Diffusion Module (DICTRA) Documentation Set

Thermo-Calc Version 2025b

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The Diffusion Module (DICTRA) User Guide

Thermo-Calc Version 2025b

Introduction to the Diffusion Module (DICTRA)

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About This Guide

This guide includes an overview of the program and describes in generic terms how you can define a system, set up and perform simulations, and then visualize the results. There is also a section to help you troubleshoot your simulation.

The guide is primarily for users already familiar with Thermo-Calc and for those who intend to use Console Mode. The Graphical Mode version is integrated into the Thermo-Calc desktop and its functionality is primarily described in the Thermo-Calc documentation.

Which Mode Should I Use?

The Diffusion Module (DICTRA) is available in both Graphical Mode and Console Mode, although Console Mode has a couple of more advanced features.

Before you start using this guide, it is recommended that you review the Thermo-Calc documentation and become familiar with using both modes. Also see Graphical Mode vs Console Mode to give you an overview of the differences. Understanding the capabilities of each mode will help you during the design of a simulation.

The two modes can be run simultaneously, but there is no communication between them. What you do in Graphical Mode does not affect the state of the Console Mode session and vice versa. This can be important to remember if you create a simulation in one mode and then decide to switch to the other mode.

What Do I Do Next?

How you proceed depends on your experience with the software as well as your level of expertise with diffusion simulations. In addition to this guide the following supplemental documentation and training resources can help you learn how to use the Diffusion Module (DICTRA).

Documentation Resources

You can search or browse all the documentation available either from within Thermo-Calc (press F1 or go to **Help → Online Help**) or browse the PDFs included with your installation by going to **Help → Manuals Folder**).

Read more about the Diffusion Module (DICTRA) on our website. There is also a Getting Started with the Diffusion Module (DICTRA) page available. If you are in Thermo-Calc, press F1 to search the help to learn about the available settings included with the Add-on Module.

The Role of Diffusion in Materials: A Tutorial is available for download on our website. It is intended for engineers interested in using the Diffusion Module (DICTRA), as well as students learning about the role of diffusion in materials. It is designed to be useful at many levels, from undergraduate studies to someone with a PhD and experience in a related field.

Training and Video Tutorials

Some of the Graphical Mode examples have video tutorials. Watching those videos may help you with your simulation in Console Mode. You may also decide to enroll in a training course or use the self-paced Learning Hub.

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

About the Diffusion Module (DICTRA)

The Diffusion Module (DICTRA) is an Add-on Module to Thermo-Calc. It is used for simulation of diffusion controlled transformations in multicomponent systems. The simulation calculations are both time- and space-dependent. The Diffusion Module (DICTRA) is available in both Graphical Mode (as the *Diffusion Calculator*) and Console Mode (as the *DICTRA module*).

The Diffusion Module (DICTRA), which is often just referred to as DICTRA, is ideally suited to solve diffusion simulations that include a moving boundary (*Stefan problems*). The multicomponent diffusion equations in the various regions of a material are solved under the assumption that thermodynamic equilibrium holds locally at all phase interfaces. Simulations are one-dimensional and three different geometries can be performed: planar, cylindrical, and spherical.

Examples of cases that have been simulated using the Diffusion Module (DICTRA) include:

- Microsegregation during solidification
- Homogenization of alloys
- Growth/dissolution of carbides, nitrides and intermetallic phases
- Coarsening of precipitate phases
- Interdiffusion in compounds, e.g. coating systems
- Austenite to ferrite transformations in steel
- Carburization, nitriding and carbonitriding of high-temperature alloys and steels
- Post weld heat treatment
- Sintering of cemented-carbides

In order to perform a simulation in the Diffusion Module, both a thermodynamic database and a kinetic database is needed. The thermodynamic database is a normal Thermo-Calc database, whereas the kinetic database contains information about the atomic mobility of individual elements in various phases.

Using the Diffusion Module (DICTRA) you can solve a variety of problems, some of which are described in Types of Diffusion Simulations.

An Important Note About Terminology

DICTRA is an acronym for *DIffusion-Controlled TRAnsformations*. The software of the same name has been included in the suite of Thermo-Calc products for many years. When you are working on Console Mode the terminology reflects this historical connection as do all the literature that cites the use of DICTRA.

With the introduction of the Graphical Mode version of DICTRA, and to better describe what the Add-on Module does, the product name is now the *Diffusion Module (DICTRA)*. However, this means some of the terminology between the modes cannot be consistent even though the theory and concept behind the software is fundamentally the same. For example, in Graphical Mode the term "DICTRA" is not used when describing the Diffusion Calculator node.

In Console Mode there is also some terminology to be aware of as there are two submodules within the program:

- The DICTRA_MONITOR: To run simulations of diffusion controlled transformations, and
- DIC_PARROT: To assess experimental data and uses this data to optimize mobilities module.

In the documentation for Console Mode, *DICTRA* and *DICTRA module* are used interchangeably to refer to the DICTRA_MONITOR module.

Graphical Mode vs Console Mode

There are two interfaces available in Thermo-Calc: *Graphical Mode* with a graphical user interface (GUI) and *Console Mode*, which uses a command line interface. Thermo-Calc and the Diffusion Module (DICTRA) are available in both modes, and all other Add-on Modules are only available in Graphical Mode.

If you are a new user, Graphical Mode is a good way to learn how to work with Thermo-Calc. Depending on what you want to simulate, in some cases Console Mode can have more functionality but until you are comfortable with the concepts, it is recommended you start in Graphical Mode, and for all new Add-on Modules, these are only available in Graphical Mode.

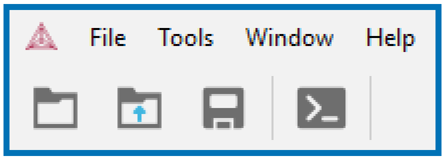
In Graphical Mode calculations are set up, carried out, and visualized as part of a *project*. The steps in the project are performed with *activities*. There are templates and a Wizard available to guide you through the process of defining the project. See Getting Started Links and Templates.

In Console Mode you work with *modules*, which are managed using commands typed at a prompt. Some modules, called *response-driven modules*, ask you a series of questions that typically take you through the process of defining your system, setting calculation conditions, performing calculations and plotting the results.

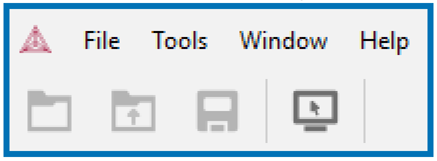
How to Switch Between Modes

The first time you open Thermo-Calc, it defaults to Graphical Mode. For any future instance it defaults to the last mode used.

Along the top of the GUI is the Graphical Mode Toolbar where you switch between modes.



In Console Mode, except for the **Switch to Graphical Mode** button, the toolbar is not used.



See Menu, Toolbar, and Keyboard Shortcuts for information about the **Tools**, **Window**, and **Help** menus, which are available in both modes.

File Extensions

The file extensions are different based on the mode you are in. In Console Mode the extensions are also based on whether you are working with Thermo-Calc or the Diffusion Module (DICTRA).

In Graphical Mode, the Thermo-Calc project files have the extension *`.tcu`. This includes the examples for the Add-on Modules.

In Console Mode, Thermo-Calc macro files have a *`.TCM` extension and the Diffusion Module (DICTRA) file extension is *`.DCM`. In addition to macro files in Console Mode the are also *Log* files and *Workspace* files, which also differ.

Modes Run Simultaneously

The two modes can be run simultaneously, but there is no communication between them. What you do in Graphical Mode does not affect the state of the Console Mode session and vice versa. One exception is the plot settings.

Global Settings: Graphical and Console Mode Plotting

Data Optimization and Thermodynamic / Kinetic Assessments

Although many calculations can be done in either mode, data optimization (i.e. PARROT) and thermodynamic or kinetic assessments (i.e. custom database development) are only available in Console Mode or using an SDK such as TC-Python.

Key Differences Between Modes in the Diffusion Module

Below are some of the main differences between the available features or simulation types in Graphical Mode (GM) and Console Mode (CM). There are also other differences not listed in the table such as slight differences between terminology and the file formats, for example.

Comparing Graphical Mode and Console Mode Features

For the Graphical Mode version of the Diffusion Module, additional functionality is scheduled for future versions of Thermo-Calc.

Feature or type of simulation	*GM*	*CM*	*Comment*
FEATURES			
Plots	x	x	
Planar, cylindrical and spherical geometries	x	x	
Homogenization	x	x	
Homogenization functions	x	x	The varieties with excluded phases are only available in Console Mode.
Tables	x	x	
Setting boundary conditions	x	x	For Graphical Mode, the Mixed activity and Zero Flux and Composition boundary conditions are available. Additional boundary conditions are planned.
Importing Scheil segregation profiles	x	x	
Importing composition profiles from file	x		
Data optimization (PARROT)		x	
SIMULATION TYPES			

Feature or type of simulation	***GM***	***CM***	***Comment***
Isothermal and Non-Isothermal simulations	x	x	
Growth of intermediate phases in compounds	x	x	
Growth or dissolution of precipitates	x	x	
Microsegregation during solidification	x	x	
Austenite to ferrite transformations	x	x	
Interdiffusion in compounds	x	x	
Coarsening		x	
Carburizing, and Nitriding and nitrocarburization	x	x	
Paraequilibrium		x	
Thermomigration		x	
Grain boundary models		x	
Pearlite models		x	
Interpolation scheme		x	
Cell calculations		x	

Diffusion Module (DICTRA) Licenses

You can start (and install) the Thermo-Calc software without a valid license but you cannot do any calculations. To show information about the available and installed licenses, from the main menu select **Help → Show License Info**.

Network License Restrictions

The Diffusion Module (DICTRA) requires a separate license. If you are using a network client installation of Thermo-Calc, then you may not be able to use the Diffusion Module (DICTRA) even if you have access to a license server with a valid network license file. This is because other clients who are part of your network installation may have checked out all instances of the network license allowed to run simultaneously.

Graphical Mode and Entering Demo Mode

In Graphical Mode only, and for users with a network license, you must exit Thermo-Calc to release the license for use. The license is checked out as soon as you add a Diffusion Calculator and remains unavailable to others until you exit the program.

With a network license, and if as per above you temporarily do not have access to a license, you are automatically put into *Demo Mode*. Then the Diffusion Calculator is available with three elements. See Available Graphical Mode Features for more information.

Console Mode

In Console Mode, a license is checked out when you enter the DICTRA module and it is checked back in when you leave the module. You do not need to exit the program.

If you are working in Console Mode and try to enter DIC_PARROT after having been in the PARROT module earlier in the session, a message displays: `DICTRA PARROT disabled after using PARROT`. To enter DIC_PARROT relaunch Thermo-Calc and enter these commands starting in the SYS module: GOTO_MODULE DIC_PAR.

Search the online help or see the *Thermo-Calc Installation Guide* for more about network licenses.

Diffusivity Theory and Diffusion Types

In this section:

Types of Diffusion Simulations

The Diffusion Module (DICTRA) is used to simulate diffusion-controlled transformations in multicomponent alloys. A short summary of the types of simulations it can handle are listed below and whether it is available in Graphical (GM) or Console (CM) Mode.

The three main simulation types that are available for both modes are briefly discussed in this section.

For Graphical Mode, see the *Quick Start Guide* for examples of single phase, moving boundary phase, and multiphase simulations.

For Console Mode, also see Models in the Diffusion Module and the *Quick Start Guide*.

Simulation type	***Examples***	***Graphical Mode***	***Console Mode***
One-phase simulations	Homogenization of alloys	x	x
	Carburizing and decarburizing of e.g. steel in austenitic state		x
Moving boundary simulations	Growth or dissolution of precipitates	x	x
	Microsegregation during solidification	x	x
	Austenite to ferrite transformations	x	x
	Growth of intermediate phases in compounds	x	x
	Coarsening of precipitates		x
Long-range diffusion in multiphase systems	Interdiffusion in compounds, e.g. coating systems	x	x
	Nitriding and nitrocarburization		x
	Carburizing of high-temperature alloys	x	x
Cooperative growth	Growth of pearlite in alloyed steels		x

Simulation type	***Examples***	***Graphical Mode***	***Console Mode***
Deviation from local equilibrium	Calculations under paraequilibrium conditions		x

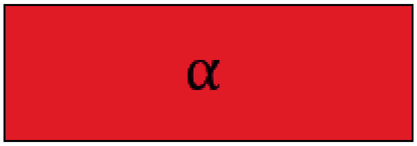
Diffusion in a Single-Phase System

The simplest simulation is one where certain elements in one phase diffuse over time in that single phase. To simulate this, you create one region and enter one phase into that region. You can set up the system under various conditions by defining profiles for how temperature and pressure change over time.

This type of simulation is available for both Graphical and Console Mode.

In Console Mode you can also simulate how the boundary conditions of the region change over time.

Simulate diffusion in a single-phase system



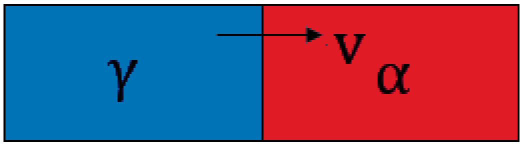
Moving Boundary Muftiphase System

With two regions in a single cell you can simulate how diffusion causes phase transformations. For example, you can simulate how an individual particle grows or dissolves as a function of time. The result is a simulation of how the boundary between the regions migrate over time. As in the case of a one-phase simulation, you can set up the system under various conditions by defining profiles for how temperature changes over time.

This type of simulation is available for both Graphical and Console Mode.

In Console Mode you can also set up the system to see how the boundary conditions of the region change over time.

Simulate a moving boundary multiphase system



Normally, simulations are performed under the assumption that thermodynamic equilibrium holds locally at all phase interfaces.

In Console Mode it is also possible to simulate a moving phase boundary problem while assuming that para-equilibrium conditions apply at the phase boundary.

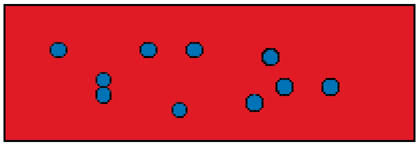
Diffusion in Disperse Systems

You can perform simulations where one or more dispersed phases are present in a matrix phase. For example, you can simulate how carburization causes precipitation of carbides in an austenitic matrix phase.

In both Graphical Mode and Console Mode, problems involving diffusion in disperse systems are handled with the homogenization model.

In Console Mode and if you are using the disperse model instead of the recommended homogenization model, the dispersed phases act as point sinks or sources of solute atoms in the simulation and the fraction and composition is calculated from the average composition in each node, assuming that equilibrium holds locally in each volume element.

Simulate diffusion in a disperse system

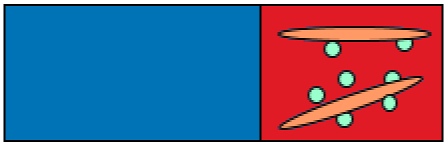


The homogenization model allows you to take into account diffusion in all phases for which you have kinetic data; the homogenization model treats all phases in the same way regardless of which phase is entered as type matrix and which phases are entered as type spheroid.

In Graphical Mode, the *Homogenization* model is automatically selected as the default solver when multiple phases are selected in a region.

In Console Mode, there are two ways in which you can simulate diffusion in a system that contains a dispersed phase, but it is strongly recommended that you use the *homogenization model*. See About the Homogenization Model.

Simulate diffusion with the homogenization model



Diffusivity Theory

In order to perform simulations using the Diffusion Module (DICTRA), both thermodynamic and kinetic descriptions are needed. Moreover, the results and the accuracy of the simulations critically depend on the quality of these descriptions. So far there is much less kinetic data which has been systematically assessed in the same way as thermodynamic data.

In the theoretical treatment of diffusive reactions one usually works with diffusion coefficients which are evaluated from experimental measurements. In a multicomponent system a large number of diffusion coefficients have to be evaluated, and moreover, they are generally functions of alloy composition and are interrelated. A database would thus be very complex. A superior alternative is to store atomic mobilities in the database, rather than diffusion coefficients. The number of parameters which need to be stored in a multicomponent system are then substantially reduced and the parameters are independent. The diffusion coefficients, which are used in the simulations, can then be obtained as a product of a thermodynamic and a kinetic factor.

The thermodynamic factor is essentially the second derivatives of the molar Gibbs energy with respect to the concentrations, and is known if the system has been assessed thermodynamically. The kinetic factor contains the atomic mobilities, which are stored in the kinetic database. The purpose of this topic is to describe how concentration, temperature and pressure dependence of the atomic mobility can be modeled, as well as to describe relations between the different diffusion coefficients and the atomic mobility.

Modeling of the Atomic Mobility

From absolute-reaction rate theory arguments the mobility coefficient for an element B, $\mathrm{M_B}$ may be divided into a frequency factor M_B^0 and an activation enthalpy, $\mathrm{Q_B}$, i.e.

[Eq. 1]

$$M_B = M_B^0 \exp\left(-\frac{Q_B}{RT}\right)\frac{1}{RT}{}^{mg}\Gamma$$

${}^{mg}\Gamma$ is a factor taking into account the effect of the ferromagnetic transition [Jönsson, 1994a]. ${}^{mg}\Gamma$ is a function of the alloy composition. It has been suggested by Jönsson, 1994b that one should expand the logarithm of the frequency factor, $\ln M_B^0$, rather than the value itself, thus the mobility, $\mathrm{M_B}$, is expressed as:

[Eq. 2]

$$M_B = \exp\left(\frac{RT\ln M_B^0}{RT}\right)\exp\left(-\frac{Q_B}{RT}\right)\frac{1}{RT}{}^{mg}\Gamma$$

Both $\mathrm{RT}\ln M_B^0$ and $\mathrm{Q_B}$ generally depend upon the composition, temperature, and pressure. In the spirit of the CALPHAD approach [Ågren, 1996], the composition dependency of these two factors, is represented with a linear combination of the values at each endpoint of the composition space, and a Redlich-Kister expansion, viz.

[*Eq. 3*]

$$\Phi_B = \sum_i x_i \Phi_B^i + \sum_i \sum_{J>i} x_i x_j \left[\sum_{r=0}^{m} {}^r\Phi_B^{i,j} (x_i - x_j)^r \right]$$

where Φ_B represents $\mathrm{RT}\ln \mathrm{M_B}$ or -$\mathrm{Q_B}$. Φ_B^i is the value of Φ_B for pure *i* and thus represents one of the endpoint values in the composition space. ${}^r\Phi_B^{i,j}$ are binary interaction parameters. The commas separate different species interacting with each other. $\mathrm{x_i}$ and $\mathrm{x_j}$ are mole fractions of elements *i* and *j* respectively. Each individual Φ parameter, i.e. Φ_B^i and ${}^r\Phi_B^{i,j}$ is stored in the database and may be expressed as a polynomial in temperature and pressure, if necessary. The Φ_B^i and ${}^r\Phi_B^{i,j}$ are referred to in the database as MF and MQ parameters, e.g.

$$\mathrm{MF(BCC\_A2\&CR,NI:VA;0) = R*T*LN(+8.50E\text{-}05)}$$

is used to represent the frequency factor to the mobility of Cr in pure Ni, i.e. $\mathrm{RT}\ln M_{Cr}^{Ni0}$, whereas:

$$\mathrm{MQ(BCC\_A2\&CR,NI:VA;0) = \text{-}2.18E{+}05}$$

represents $-Q_{Cr}^{Ni}$. The magnetic effect is represented by Jönsson's model [1994a].

[*Eq. 4*]

$${}^{mg}\Gamma = \exp(6\alpha\xi)\exp\left(\frac{-\alpha\xi Q_B}{RT}\right)$$

where ξ represents the state of the magnetic order ($0 < \xi < 1$) at the temperature under consideration and α is treated as a constant, approximately equal to 0.3 in bcc alloys. For fcc alloys the ferromagnetic effect on diffusion is usually neglectable, i.e. $\alpha \approx 0$. When there is magnetic ordering it is thus necessary to make the division into MF and MQ because ${}^{mg}\Gamma$ depends on $\mathrm{Q_B}$, i.e. MQ. The full expression then becomes:

$$RT\ln[RTM_B] = RT\ln M_B^0 - Q_B + RT\ln {}^{mg}\Gamma = \sum MF + \sum MQ + RT\ln {}^{mg}\Gamma$$

Both MF and MQ may be arbitrary polynomials in temperature and if there is no magnetic effect, i.e. $\mathrm{RT}ln^{mg}\Gamma = 0$, it is sufficient to enter either one of them. For example, the mobility of Cr in pure Ni may as well be stored as:

$$\mathrm{MF(FCC\_A1\&CR,\ NI:VA;0) = 0}$$

and

$$\mathrm{MQ(FCC\_A1\&CR,NI:VA;0)} = -Q_{Cr}^{Ni} + \mathrm{RT}\ln M_{Cr}^{Ni0}$$

In order to build a database it is necessary to find values on MF and MQ (or when no magnetic effect is considered MQ alone). In many cases such data can be found in the literature. The tracer diffusivity D_B^* is directly related to the mobility M_B by means of the Einstein relation

[*Eq. 5*] $$D_B^* = RTM_B$$

and when there is no magnetic effect on the mobility, e.g. ${}^{mg}\Gamma = 1$, then from Equation 2 and Equation 5 it is found that:

[*Eq. 6*] $$\mathrm{MQ} = RT\ln M_B^0 - Q_B = RT\ln D_B^*$$

In a more complex database the model parameters are determined from an optimization procedure, where all experimental information is taken into account, see for example Jönsson, 1995 and Engström and Ågren, 1996.

Relationship Between Diffusion Coefficients and Atomic Mobilities

Phenomenological Coefficients

For crystalline phases the vacancy-exchange mechanism of diffusion is predominant, i.e. diffusion occurs by atoms jumping into neighboring vacant lattice sites. From the absolute reaction rate theory, and by assuming that the vacancy concentration is governed by thermodynamic equilibrium, the diffusional flux of a component *k* in the lattice fixed frame of reference can be expressed as [Andersson and Ågren, 1992]:

[*Eq. 7*] $$\tilde{J}_k = -c_k y_{Va} \Omega_{kVa} \frac{\partial \mu_k}{\partial z}$$

Here $\mathrm{c_k}$ is the amount of *k* per unit volume, $\mathrm{y_{Va}}$ is the fraction of vacant lattice sites on the sublattice where *k* is dissolved, Ω_{kVa} is a kinetic parameter which gives the rate of exchange if there is a vacancy adjacent to a *k*-atom,

and μ_k is the chemical potential of component *k*. The mobility $\mathrm{M_k}$ is here defined as:

[*Eq. 8*] $\mathrm{M_k} = \mathrm{y_{Va}}\Omega_{\mathrm{kVa}}$ when *k* is substitutional

[*Eq. 9*] $\mathrm{M_k} = \Omega_{\mathrm{kVa}}$ when *k* is interstitial

From Equation 7, Equation 8 and Equation 9 it is possible to identify the so called phenomenological parameters that relate the flux of *k* to all the driving forces, i.e. $\mathrm{L_{kk}} = \mathrm{c_k M_k}$ when *k* is substitutional, $\mathrm{L_{kk}} = \mathrm{c_k y_{Va} M_k}$ when *k* is interstitial, and $\mathrm{L_{ki}} = 0$ when $\mathrm{k} \neq \mathrm{i}$. The fluxes in the lattice-fixed frame of reference may now be expressed as:

[*Eq. 10*] $$\tilde{J}_k = -\sum_{i=1}^{n} L_{ki}\frac{\partial \mu_i}{\partial z} = -L_{kk}\frac{\partial \mu_k}{\partial z}$$

Transformation to the volume-fixed frame of reference, or the number-fixed frame of reference with respect to the substitutional elements, which may be regarded as the same, if as assumed in the Diffusion Module (DICTRA), the partial molar volumes are independent of concentration, and the partial molar volumes of the interstitials are neglected, yields

[*Eq. 11*] $$J_k = -\sum_{i=1}^{n} L'_{ki} \frac{\partial \mu_i}{\partial z}$$

where

[*Eq. 12*] $$L'_{ki} = \sum_{j=1}^{n} (\delta_{jk} - c_k V_j) L_{ji}$$

where δ_{jk} is the Kronecker delta, i.e.,=1 when j=k and 0 otherwise. $\mathrm{V_j}$ is the partial molar volume of element *j*.

Interdiffusion Coefficients

Generally, it is much more convenient to express the fluxes as functions of concentration gradients, rather than gradients in chemical potential. This is accomplished by rewriting Equation 11 using the chain rule of derivation, i.e.

[*Eq. 13*] $$J_k = -\sum_{i=1}^{n} L'_{ki} \sum_{j=1}^{n} \frac{\partial \mu_i}{\partial c_j} \frac{\partial c_j}{\partial z}$$

or equally if the unreduced diffusivities, D_{kj} are introduced,

[*Eq. 14*] $$J_k = -\sum_{j=1}^{n} D_{kj} \frac{\partial c_j}{\partial z}$$

The D_{kj} matrix introduced in Equation 14 may be identified by comparing with Equation 13,

[*Eq. 15*] $$D_{kj} = \sum_{i=1}^{n} L'_{ki} \frac{\partial \mu_i}{\partial c_j}$$

The $\frac{\partial \mu_i}{\partial c_j}$ are purely thermodynamic quantities, sometimes they are referred to as thermodynamic factors. It is now evident that the diffusivities may be looked upon as consisting of two separate parts, one purely thermodynamic and one kinetic.

There is a relation between the n concentration gradients in Equation 14 and for practical calculations one usually chooses to eliminate one of them. The reduced diffusivities in a volume-fixed frame of reference, where it is assumed that all the substitutional species have the same partial molar volumes, and furthermore, only the substitutional species contribute to the volume, i.e. the Diffusion Module (DICTRA) frame of reference, is expressed as,

[*Eq. 16*] $$D^n_{kj} = D_{kj} - D_{kn} \text{ when } j \text{ is substitutional}$$

[*Eq. 17*] $D^n_{kj} = D_{kj}$ when *j* is interstitial

where *n* is taken as the dependent species. Using these diffusivities Equation 14 now becomes,

[*Eq. 18*] $$J_k = -\sum_{j=1}^{n-1} D^n_{kj} \frac{\partial c_j}{\partial z}$$

Equation 18 contains the so-called interdiffusion coefficients, sometimes referred to as chemical diffusivities. These diffusivities may be evaluated experimentally from e.g. diffusion couple experiments.

Intrinsic Diffusion Coefficients

The individual or intrinsic diffusion coefficients, that are defined in the lattice-fixed frame of reference by:

[*Eq. 19*] $$\tilde{J}_k = -\sum_{j=1}^{n-1} {}^iD^n_{kj} \frac{\partial c_j}{\partial z}$$

can also be evaluated from diffusion couple experiments, if in addition to concentration profiles the Kirkendall velocity can be estimated from the movement of inert markers. As the interdiffusion coefficients, the intrinsic diffusion coefficients can also be calculated from the mobilities. However, this time by applying the chain rule of derivation on Equation 10 and remembering that $\mathrm{L_{ki}} = 0$ when $\mathrm{k} \neq \mathrm{i}$, i.e.

[*Eq. 20*] $$\tilde{J}_k = -\sum_{j=1}^{n} L_{kk} \frac{\partial \mu_k}{\partial c_j} \frac{\partial c_j}{\partial z}$$

The intrinsic diffusion coefficients may be identified in Equation 20 as:

[*Eq. 21*] $${}^iD_{kj} = L_{kk} \frac{\partial \mu_k}{\partial c_j}$$

Also here there is a relation between the *n* concentration gradients. If one of the concentrations are chosen as dependent, and if the same approximation as previously used for the partial molar volumes of the different elements is applied, then the intrinsic diffusion coefficients defined in Equation 19 are finally found.

[*Eq. 22*] ${}^iD^n_{kj} = {}^iD_{kj} - {}^iD_{kn}$ when *j* is substitutional

[*Eq. 23*] ${}^iD^n_{kj} = {}^iD_{kj}$ When *j* is interstitial

Self-diffusion Coefficient

The self-diffusion coefficient of A is the diffusivity of A in the limit of pure A. Studies of self-diffusion usually utilize radioactive tracer atoms A* of the same element.

Impurity Diffusion Coefficient

When the diffusion of a solute B in a solvent A is studied at an extremely small concentration of B, which e.g. radio tracers permit, then the impurity diffusion coefficient of B in A is observed.

References

[1992And] Andersson, Jan-Olof, and John Ågren. 1992. “Models for Numerical Treatment of Multicomponent Diffusion in Simple Phases.” Journal of Applied Physics 72 (4): 1350–55.

[1994aJon] Jönsson, Björn. 1994a. “Ferromagnetic Ordering and Diffusion of Carbon and Nitrogen in BCC Cr-Fe-Ni Alloys.” Zeitschrift Fur Metallkunde 85 (7): 498–501.

[1994bJon] Jönsson, Björn. 1994b. “Assessment of the mobility of carbon in C-Cr-Fe-Ni FCC alloys.” Zeitschrift Fur Metallkunde 85 (7): 502–9.

[1995Jon] Jönsson, Björn. 1995. “Assessment of the Mobilities of Cr, Fe and Ni in Bcc Cr-Fe-Ni Alloys.” ISIJ International 35 (11): 1415–21.

[1996Agr]Ågren, John. 1996. “Calculation of Phase Diagrams: Calphad.” Current Opinion in Solid State and Materials Science 1 (3): 355–60.

[1996Eng]Engström, Anders, and John Ågren. 1996. “Assessment of Diffusional Mobilities in Face-Centered Cubic Ni-Cr-Al Alloys.” Zeitschrift Fur Metallkunde 87 (2): 92–97.

Working in Graphical Mode

Working with the Diffusion Module (DICTRA) in Graphical Mode is directly related to working with Thermo-Calc through the use of the Diffusion Calculator. See the Thermo-Calc documentation for more details about working in Graphical Mode.

In this section:

Available Graphical Mode Features

The Diffusion Module is an Add-on Module to the core Thermo-Calc software.

> A separate license is required to perform calculations for more than three elements. Without it you are able to use the module in *Demo Mode*. This is not available in Console Mode.

Diffusion Templates

Under **Non-Equilibrium Calculations**, the **Homogenization** and **Diffusion** templates are available to all Thermo-Calc users when in Graphical Mode.

> If you are using the Diffusion Module in Demo Mode, see Demonstration (Demo) Mode for what is available to you. Even if you have a license, you may find yourself in Demo Mode if you have a network license and all the licenses are checked out.

Using the Templates

After opening Thermo-Calc in Graphical Mode, in the templates section under **Non-Equilibrium Calculations** click:

- **Homogenization** to add a *System Definer*, *Scheil Calculator*, *Diffusion Calculator*, and two *Plot Renderer* nodes to the **Project** tree.
- **Diffusion** to add a *System Definer*, *Diffusion Calculator*, and *Plot Renderer* to the **Project** tree.

Creating a Project from a Template

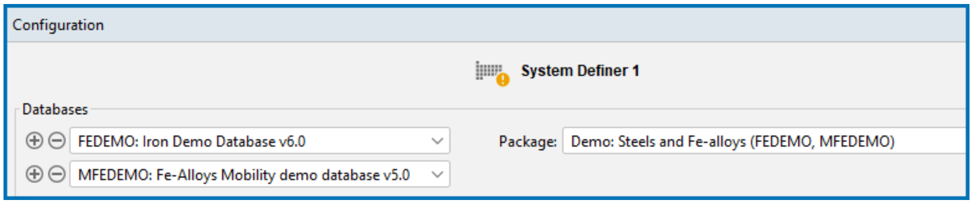
Diffusion Calculator

A Diffusion Calculator allows you to set the conditions for your calculation that define the geometry, regions, phases, grids, composition profiles, and the thermal profile, plus additional options. Many of the settings are automatically set as you define your system. Details about this activity are described in Diffusion Calculator.

Demo Database Packages for the Examples Collection

Both a thermodynamic and mobility database are required to run the Diffusion Module simulation. If you have a Diffusion Module (DICTRA) license you can run all the examples because the demonstration database packages are included with your installation.

Select the database packages from the **System Definer Configuration** window to run a simulation.



FEDEMO: Iron Demo Database v6.0

MFEDEMO: Fe-Alloys Mobility demo database v5.0

Package: Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)

Demonstration (Demo) Mode

The Diffusion Module and some examples are available to all Thermo-Calc users but only for simulations with three elements. If you do not have a license then you are in *Demo Mode* when using the Diffusion Calculator, or either of the templates.

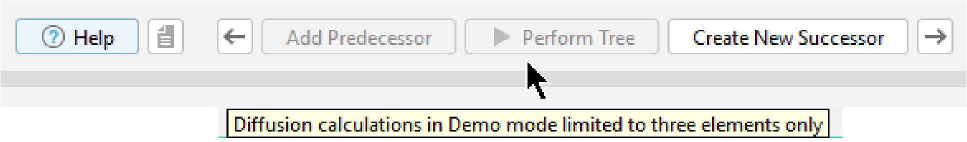
Diffusion Templates

If you are in DEMO mode then this is indicated by the addition of **DEMO** text under the button.

Diffusion Calculator

If you are experimenting with the Diffusion Calculator in Demo Mode then you may have access to a variety of databases based on your license. However, you can only define three elements for a demo simulation.

If you define more than three elements on the System Definer, when you go to the Diffusion Calculator, the **Perform** button is unavailable and the tooltip explains why.



Diffusion calculations in Demo mode limited to three elements only

Even if you have more than three elements, the Plot Renderer **Perform** button is still available. However, if you click the button and try to run the simulation the **Event Log** displays an error message.

Additive Manufacturing (AM) Module

There is connectivity between the Diffusion Module (DICTRA) or the Precipitation Module (TC-PRISMA) and the Additive Manufacturing (AM) Module when you have full licenses available for all relevant Add-on Modules and databases.

You can add a Diffusion Calculator or Precipitation Calculator as a successor to the AM Calculator and then when probes are included with the AM Calculator this data can be further used with the thermal profile.

Details are in the AM Module documentation. See AM Calculator: Working with Probe Data.

Basic Terminology in Graphical Mode

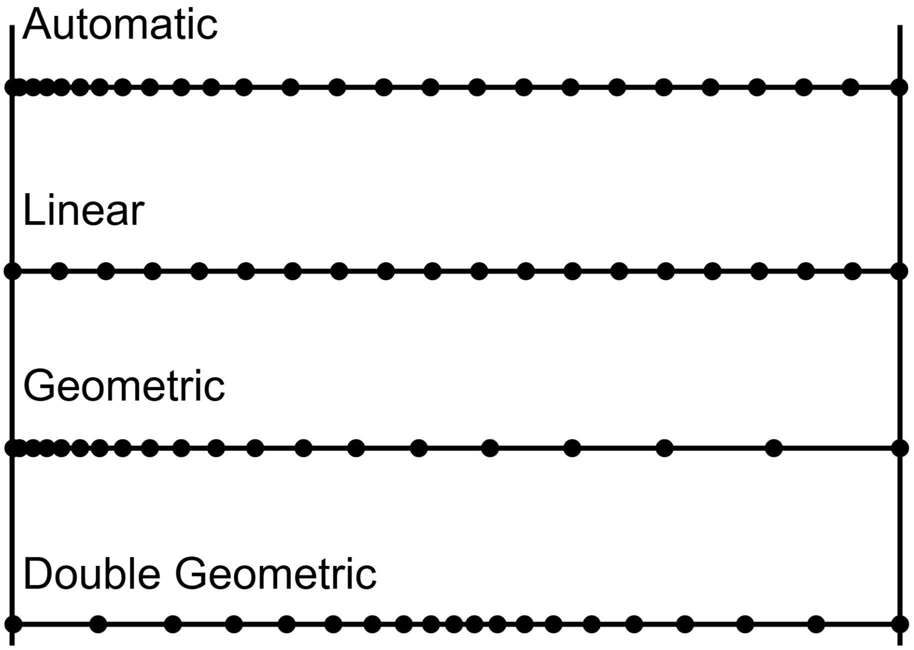
These terms are specific to working in Graphical Mode. The overall simulation in Console Mode is comparable but there are some differences in terminology and functionality.

Region

In Graphical Mode, a system consists of one *cell* with one or multiple *regions* in which the diffusion problem is to be solved.

Grid Types

These grid types are used in diffusion simulations: automatic, linear, geometric, and double geometric. When you are setting up the simulation, in either Console Mode or Graphical Mode, a region must have a grid defined.



Phases

Each region must contain at least one *phase*. The so-called *homogenization model* is used if multiple phases are added inside a region, then the average properties of the local phase mixture is used. Phase(s) can also be added to interphases of region(s) and then only participate in the simulation if the driving force for precipitation of the phase exceeds a predefined value. A new region is then created where the name of the region is set to the name of the phase but with `R_` added as a prefix.

Composition

These types of composition variables are used in the configuration of the Diffusion Calculator: *mass (weight) fraction*, *mass (weight) percent*, *mole fraction*, or *mole percent*.

The *u-fractions* are used in the diffusion equations. The u-fraction of a component *k* is defined as

$$\mu_k = \frac{x_k}{\sum\limits_{j \in S} x_j}$$

The summation is only performed over the substitutional elements. The choice of the volume fixed frame of reference in the calculations make it convenient to use a composition variable which is related to the volume. The definition of the u-fraction is based upon the assumption that a species may or may not contribute to the volume of a phase. An interstitial element is assumed to not contribute to the volume. Substitutional elements are assumed to contribute equally to volume. Weight fraction, mole fraction or u-fraction can be used when plotting the results from a simulation.

Geometry and Coordinates

The Diffusion Module (DICTRA) can only handle diffusion problems where compositions vary along one spatial coordinate. The geometry of your system can be *planar*, *cylindrical*, or *spherical*.

The *planar* geometry corresponds to an infinitely wide plate of a certain thickness. If the system has a planar geometry then the lower boundary (the zero coordinate) is at the left side of the system. The upper boundary (the coordinate with the highest value) is at the right side of the system.

Boundary Conditions

Boundary conditions are conditions that define how matter behaves at the boundaries of your system. By default, matter is not allowed to cross the system boundaries.

You can change the setting for both the lower boundary (left side/centre) and the upper boundary (right side/surface) of the system.

Next see Setting up a Diffusion Simulation in Graphical Mode then go to Working in Graphical Mode for links to the other relevant content.

Setting up a Diffusion Simulation in Graphical Mode

When you are using the Graphical Mode version of the Diffusion Module (DICTRA), the steps to set up a simulation are a combination of adding *Activity* nodes (the System Definer, Diffusion Calculator, and Plot Renderer) and then defining the applicable settings for each of these nodes in a Configuration window.

The following is a general overview of the steps to set up the simulation.

1. Use the **Diffusion** template to add the System Definer, Diffusion Calculator, and Plot Renderer activity nodes.
2. On the **System Definer**, you select the thermodynamic and kinetic databases, add elements and phases, and generally define the system.
3. On the **Diffusion Calculator**, you set the geometry (by default the geometry is planar), add region(s) and enter grid(s) and phase(s) in the region(s). You then enter composition(s) of phase(s).
4. On the **Plot Renderer** or **Table Renderer**, you choose how to visualize your diagrams, and then run the simulation, i.e. you **Perform** the sequence of nodes you have defined in the tree to produce the output simulation.

Graphical Mode Diffusion Calculator Examples

? About the Examples

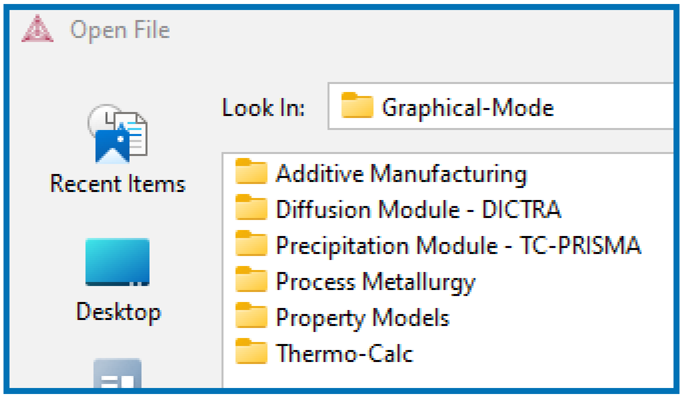
? See Diffusion Module (DICTRA) Examples Collection for links to the examples.

Opening the Diffusion Calculator Examples

Graphical Mode examples are available for Thermo-Calc and the Add-on Modules. There are also examples for the Property Models, including the material specific model libraries (i.e. Steel, Nickel, etc.). These are in the format of project files (*.tcu).

To open an example project file:

1. Open Thermo-Calc.
2. Confirm you are in Graphical Mode. If not, click the **Switch to Graphical Mode** button.
3. There are these ways to open the folders and files:
   - From the main menu select **File →** **Examples Files**
   - From the main menu select **Help →** **Examples Files**.
   - Click the **My Project** node and on the **Configuration** window, click the **Example Calculation** button.
4. The examples are divided into folders. Navigate to the folder and project file you want and double-click to open.

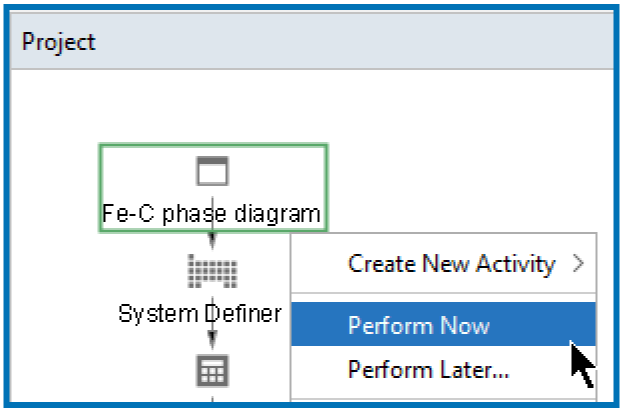


Look In: Graphical-Mode

- Additive Manufacturing
- Diffusion Module - DICTRA
- Precipitation Module - TC-PRISMA
- Process Metallurgy
- Property Models
- Thermo-Calc

5. The Graphical Mode examples are stored without calculated results so you will want to run the example calculation and generate a plot or table. To do this, click the first node in the tree at the top of the **Project** window. Then right-click and select

Perform Now. Some examples require additional licenses in order for the calculation to run.



Working in Console Mode

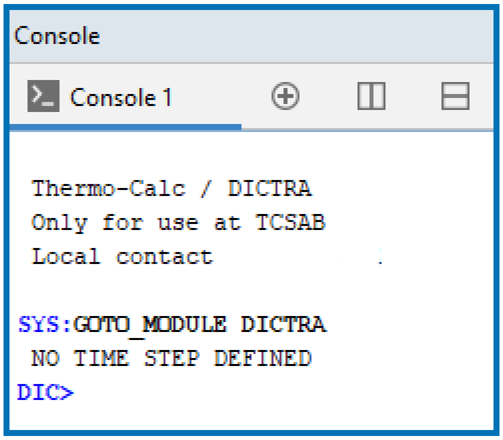
In this section:

Opening DICTRA in Console Mode

1. Open Thermo-Calc in Console Mode.

> By default, Thermo-Calc opens in the most recently used state. If it opens in Graphical Mode, on the toolbar, click **Switch to Console Mode**.

2. In the `SYS` module, type `GOTO_MODULE DICTRA`. For a list of all the available commands in the current module, at the prompt type a question mark (?) and press <Enter>. For a description of a specific command, type `Help` followed by the name of the command.



```
 Thermo-Calc / DICTRA
 Only for use at TCSAB
 Local contact

SYS:GOTO_MODULE DICTRA
 NO TIME STEP DEFINED
DIC>
```

Opening a Macro File in Console Mode

You can open the macro files (*.TCM or *.DCM files) in different ways.

- From the main menu,
- Using a command,
- By dragging and dropping the file into the Console window, or
- Navigate to the file location on your computer and double-click to open it. If you already have Thermo-Calc open, the macro opens in a new tab. Otherwise a new instance of Thermo-Calc is launched.

> If you are using the advanced pipe or redirect option (Technical Note: Pipe or Redirect Output Data from Console Mode) then a new instance of Thermo-Calc is always started.

- You can also read the commands listed in the macro file using a text editor.

> If you only open and read the macro file in a text editor, you do not see the output that Thermo-Calc gives in response to the commands stored in the macro file.

How to Open an Example Macro

To open a specific macro file from the Examples folders included with your installation:

1. Open Thermo-Calc.
2. Confirm you are in Console Mode. If not, click the **Switch to Console Mode**button.
3. From the main menu, select **File →** or **Help → Examples Files**. The Console Mode folder opens.
4. Double-click the **Diffusion Module - DICTRA** folder to view the subfolders.

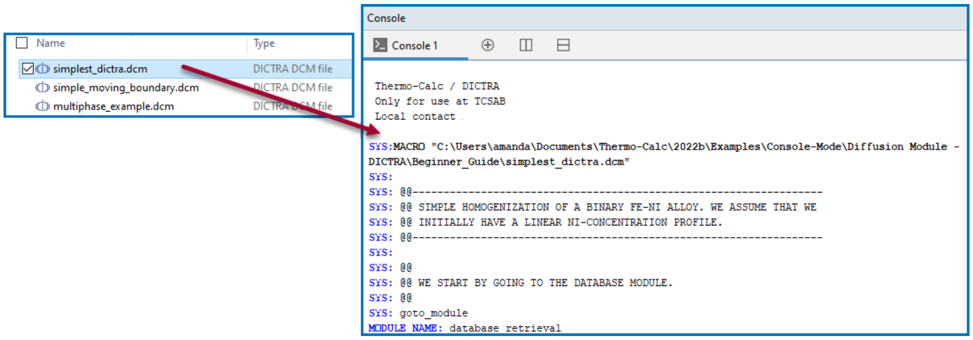
> The three Quick Start example macros and the PDF guide are in the first folder called **Beginner Guide**.

How to Open a Macro with a Command

At the `SYS` prompt, type MACRO_FILE_OPEN and press <Enter>. In the file dialogue window that opens, locate and select the macro file on your computer.

How to Open a Macro File by Dragging and Dropping it into Console Mode

For example, navigate to the **Beginner Guide** folder and then drag the file from its location into Thermo-Calc Console window. The macro automatically runs after you drop it into the Console window.



☐ Name	Type
☑ simplest_dictra.dcm	DICTRA DCM file
simple_moving_boundary.dcm	DICTRA DCM file
multiphase_example.dcm	DICTRA DCM file

```
 Thermo-Calc / DICTRA
 Only for use at TCSAB
 Local contact

SYS:MACRO "C:\Users\amanda\Documents\Thermo-Calc\2022b\Examples\Console-Mode\Diffusion Module -
DICTRA\Beginner_Guide\simplest_dictra.dcm"
SYS:
SYS: @@-----------------------------------------------------------------
SYS: @@ SIMPLE HOMOGENIZATION OF A BINARY FE-NI ALLOY. WE ASSUME THAT WE
SYS: @@ INITIALLY HAVE A LINEAR NI-CONCENTRATION PROFILE.
SYS: @@-----------------------------------------------------------------
SYS:
SYS: @@
SYS: @@ WE START BY GOING TO THE DATABASE MODULE.
SYS: @@
SYS: goto_module
MODULE NAME: database retrieval
```

Double-click to Open a File

Navigate to the macro file location, for example where each set of file examples is in its own folder. If you already have Thermo-Calc open, the macro opens in a new tab. Otherwise a new instance of Thermo-Calc is launched.

About the Console Mode File Formats

The Diffusion Module (DICTRA) in Console Mode uses different file formats: *log* files (*.TCM), *macro* files (*.DCM) and *workspace* files (*.DIC).

Also see Graphical Mode vs Console Mode. If you are working with Thermo-Calc in Console Mode, see Working with the Console Mode File Types.

Log Files

Log files (*.TCM) are plain text files and are just macro files used to save a sequence of commands. These files can be edited in a text editor.

- To start saving your input into a file, in the SYS module type `SET_LOG_FILE`, followed by the name of the file that you want to save your command sequence to.
- When creating a command sequence, and if you want to save the output in the log file, type `SET_ECHO` before SET_LOG_FILE. This is useful if you later want to use the log file as a macro file because the macro file lists the full commands instead of only the short names.

Macro Files

Macro files (*.DCM) are plain text files used to save a sequence of commands that can be loaded and executed. Macro files can be edited in a text editor. When creating a command sequence, you add comments to the file by starting a line with @@.

- To run a macro file, in the SYS or DICTRA module type `MACRO_FILE_OPEN`, followed by the name of the macro file. DICTRA runs the MACRO_FILE_OPEN sequence that the file contains.
- To remain in the console and keep working in the DICTRA module, in the SYS, DICTRA, POLY, or POST module add the command SET_INTERACTIVE at the end of the macro file. Alternatively, use `EXIT` as the final command.

Workspace Files

Workspaces files for the Diffusion Module (DICTRA) have the file extension *.DIC, which allow you to save all the data in your current workspace. A workspace contains all the data, specified settings and the result of any calculations performed. The saved data includes original and modified thermodynamic data, the last set of conditions and options, and the results of any simulations.

- At the `DIC` prompt use SAVE_WORKSPACES.
- To load the data and calculation results of a workspace file, at the `DIC` prompt use READ_WORKSPACES.

Overview of a System

In this section:

Typical Console Mode Workflow

The basic work flow in Console Mode is as follows.

1. You are in the **SYS** module when you start Thermo-Calc in Console Mode.
2. In the **DATA** module you define the system. Before performing a calculation, you must define your system and retrieve thermodynamic and kinetic data. The data is retrieved from the database files.
3. The data needed to describe a system is sent to the **GIBBS** module. When the data is in GIBBS, the software can access the retrieved data. The retrieved data is accessible to the **POLY** module, which is involved in simulations that require that equilibrium calculations are performed.
4. In the **DICTRA_MONITOR** you:
   a. Set the initial state of the system and define its geometry and boundary conditions. The simplest system has one cell that contains one region, but you may put additional regions in a cell and put additional cells in your system.
   b. Define the phases each region contains.
   c. Set various parameters for the numerical calculations.
   d. Run the simulation from within the DICTRA_MONITOR.
5. In the **POST** module you plot and visualize your data.
   a. Choose the data to plot
   b. Change the appearance of the diagram
   c. Save the diagram as an image file (available in several formats).

About Regions and Grids

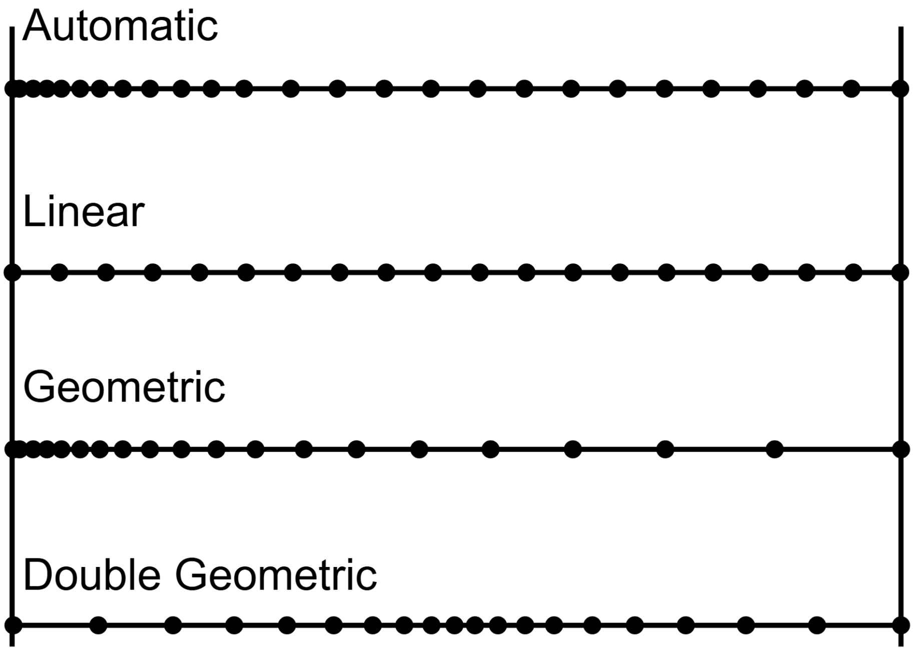
For Graphical Mode, see Diffusion Module Terminology in Graphical Mode.

Also see Creating Regions and Gridpoints.

A *region* contains one or more phases. If a region contains several phases one of those must be entered as a *matrix phase* whereas the others are entered as *spheroid*.

A region must also contain a number of *grid points*. The composition is only known at these grid points and the software assumes that the composition varies linearly between them. The amount and composition of all the phases present at a single grid point in a certain region are those given by thermodynamic equilibrium keeping the over-all composition at the grid point fixed.

These grid types are used in diffusion simulations: automatic, linear, geometric, and double geometric. When you are setting up the simulation, in either Console Mode or Graphical Mode, a region must have a grid defined.



About System, Cells and Regions

For Graphical Mode, see Diffusion Module Terminology in Graphical Mode.

A system normally consists of one *cell*. This cell contains one or several *regions* in which the diffusion problem is to be solved. A system of diffusion equations is solved for each region. The size of the system is the sum of sizes of all the regions in all the system's cells.

The interface between two regions typically moves as the result of a simulation, that is, the regions grow or shrink. Such an interface is called an *inner interface*. The boundary of a cell is called an *outer interface* and the condition of this type of interface may be affected by the choice of boundary conditions.

For some simulations it is useful to have several cells in a system. Matter can move between cells. However, it is assumed that there is diffusional equilibrium between all cells (this means that there are no differences in diffusion potentials between cells). In other words, the size of a cell is fixed during the simulation.

By default this is a *closed system*, which means that matter cannot move across its boundaries. However, you can change this setting for both the *lower boundary* (left side/centre) and the *upper boundary* (right side/surface) of the system. You can also set these boundary conditions to vary as a function of time, temperature and/or pressure.

About Phases

For Graphical Mode, see Diffusion Module Terminology in Graphical Mode.

Entering Phases in Regions and Specifying Phase Compositions in a Region.

Each region contains one or more *phases*. A phase can be of the *matrix*, *spheroid* or *lamellar* type. A phase can be introduced with the status *active* (the default) or *inactive*.

An inactive phase is a phase which does not participate in the calculations until it is stable. If a phase is inactive, then the driving force for precipitation of the phase is continuously monitored. When the driving force exceeds a predefined positive value, the phase take parts in the simulation and the phase automatically becomes active. A new region is then created and the formerly inactive phase is entered as the matrix phase of the new region. The name of the region is set to the name of the phase that just became active but with `R_` added as a prefix.

Region Phase Types

Phase type	*Description*
Matrix	The region’s primary phase. If there is only one phase in a region, then that phase is automatically a matrix.
Spheroid	Used to treat one or several dispersed phases in a matrix. Unless the homogenization model is invoked, which happens automatically when a spheroid phase is entered, then diffusion is only considered in the matrix phase; the spheroid phases then only act as sources and sinks of the diffusing elements.
Lamellar	Used to simulate the growth of a eutectic or eutectoid region. The software only treats the growth, not the dissolution, of such a region. The *pearlite calculation model* is used for a phase that is lamellar.

About Composition Variables

For Graphical Mode, see Diffusion Module Terminology in Graphical Mode.

Two types of composition variables are used within the program: site-fractions and u-fractions, although you can also use weight fraction or mole fraction, for example.

The *site-fractions* are used to set up the problem and interface with POLY-3 (in Console Mode). The site fraction of a species *k*, y_k, is the fraction of equivalent lattice sites occupied by species k. It is the only concentration variable that uniquely defines the composition and the constitution of a phase and it is necessary to use the site fraction in the storage of the data during a simulation.

The *u-fractions* are used in the diffusion equations. The u-fraction of a component *k* is defined as

$$u_k = \frac{x_k}{\sum\limits_{j \in S} x_j}$$

The summation is only performed over the substitutional elements. The choice of the volume fixed frame of reference in the calculations make it convenient to use a composition variable which is related to the volume. The definition of the u-fraction is based upon the assumption that a species may or may not contribute to the volume of a phase. An interstitial element is assumed to not contribute to the volume. Substitutional elements are assumed to contribute equally to volume.

About Global Conditions

There are several global parameters that influence the diffusion rate in simulations: temperature, pressure and heat content removal. These parameters are defined as functions of time. The temperature can also be a function of the spatial position, and heat content removal can be a function of temperature or pressure.

For heat content removal, the amount of extracted heat per time unit is normalized and the size of the system is normalized to one mole of atoms.

Setting Global Conditions

About Boundary Conditions in Console Mode

Boundary conditions are conditions that define how matter behaves at the boundaries of your system. By default, matter is not allowed to cross the system boundaries.

You can change the setting for both the lower boundary (left side/centre) and the upper boundary (right side/surface) of the system.

SET_CONDITION

Boundary Condition Descriptions

Boundary condition	***Description***
FIX_FLUX_VALUE	Enter functions that yield the flux times the molar volume for the independent components. Can be a function of time, temperature and pressure. Use this boundary condition with caution as it may cause unrealistic compositions.
STATE_VARIABLE_VALUE	A legal equilibrium condition expression in POLY-3 syntax that reduces the degrees of freedom. This type should be used with care as no checks are done in advance to determine if it is a legal expression. Do not specify the conditions for temperature and pressure here as these are taken from the global conditions.
POTENTIAL_FLUX_ FUNCTION	Use to take into account the finite rate of a surface reaction. The flux for the independent components must be given in the format: $$J_k * V_m = f_k(T,P,TIME)^* \left[POTENTIAL_k^N - g_k(T,P,TIME)\right]$$ The functions f and g may have time (TIME), temperature (T), and/or pressure (P) as arguments. N is an integer. The potentials are those with user defined reference states.
ACTIVITY_FLUX_FUNCTION	Use to take into account the finite rate of a surface reaction. The flux for the independent components must be given in the format: $$J_k * V_m = f_k(T,P,TIME)^* \left[ACTIVITY_k^N - g_k(T,P,TIME)\right]$$ The functions f and g may have time (TIME), temperature (T), and/or pressure (P) as arguments. N is an integer. The activities are those with user-defined reference states.
ITERATIVE_ACTIVITY_FLUX_ FUNCTION	Same as ACTIVITY_FLUX_FUNCTION but an iterative scheme is used to determine the flux. Use this if the other command encounters problems.
CLOSED_SYSTEM	Corresponds to a fix flux value, which is set to zero at all times. This is the default boundary condition.
MIXED_ZERO_FLUX_AND_ ACTIVITY	The flux of selected components is set to zero and the activity of others may be set to a prescribed value.
GAS	This option can cause a change in system volume. The flux of selected components is set to zero and the activity of others can be set to a prescribed value. Use this to treat an expanding system, e.g. the growth of an external oxide scale.

About Geometry and Coordinates

Specifying the Geometry

The Diffusion Module (DICTRA) can only handle diffusion problems where composition vary along one spatial coordinate. The geometry of your system can be *planar*, *cylindrical* or *spherical*.

PLANAR GEOMETRY

This geometry corresponds to an infinitely wide plate of a certain thickness. If the system has a planar geometry then the lower boundary (the zero coordinate) is at the left side of the system. The upper boundary (the coordinate with the highest value) is at the right side of the system.

CYLINDRICAL AND SPHERICAL GEOMETRIES

- Cylindrical geometry corresponds to an infinitely long cylinder of a certain radius.
- Sypherical geometry corresponds to a sphere with a certain radius.

By default for both geometries, the lower boundary (the zero coordinate) is at the centre of the cylinder/sphere. The upper boundary (the coordinate with the highest value) is at the *surface* of the cylinder/sphere. You can enter a left most coordinate that is larger than zero to allow for tube and hollow sphere geometries.

About Operators and Functions

Sometimes you need to specify functions when setting up a system. For example, to make global and boundary conditions vary as a function of time.

The following operators can be used in writing functions. Use a semi-colon (`;`) to mark the end of a function.

Available Operators for Writing Functions

Operator	*Description*
+, -, *, /	Addition, subtraction, multiplication, division
**	Exponentiation, raising one quantity to the power of another, e.g. x^2.
ABS()	Absolute value
ERF(X)	Error function

Operator	***Description***
EXP(X)	Exponential
LOG(X)	Natural logarithm
LOG10(X)	Base 10 logarithm
SIGN(X)	Sign function SIGN(X) is -1 when X<0, is 0 when X=0 and is 1 when X>0.
SIN(X), COS(X), TAN(X), ASIN(X), ACOS(X), ATAN(X)	• Trigonometric functions: sine, cosine, tangent • Inverse trigonometric functions: arcsine, arccosine, arctangent
SINH(X), COSH(X), TANH(X), ASINH(X), ACOSH(X), ATANH(X)	• Hyperbolic trigonometric functions • Inverse hyperbolic functions
SQRT(X)	Square root

Creating a DICTRA Simulation

These topics describe in general terms what options you have when setting up your diffusion simulation in Console Mode.

In this section:

Defining a System in Console Mode

Define your system with as few elements (components) and phases as possible; keep the simulation as simple as possible to avoid making the simulation unsolvable.

In order to perform a simulation in the Diffusion Module, both a thermodynamic database and a kinetic database is needed. The thermodynamic database is a normal Thermo-Calc database, whereas the kinetic database contains information about the atomic mobility of individual elements in various phases.

Database (TDB) Module Commands

1. Open Thermo-Calc in Console Mode. At the `SYS` prompt, type `GOTO_MODULE DATA`.
2. Use SWITCH_DATABASE to select databases. Unless you directly specify the name of the database as a parameter to the command, the available databases are listed. Specify the one to use.
3. Use DEFINE_ELEMENTS followed by a list of the elements that you want in your system. (To list the elements available in the current database, type `LIST_DATABASE Elements`.)
4. Use REJECT with the keyword, `Phases` to make sure that unnecessary phases are not retrieved from the database.
5. Use RESTORE with the keyword, `Phases` to restore any phases that have been excluded.
6. Use GET_DATA to read from the database and send the thermodynamic data about your system to the GIBBS and DICTRA workspace.
7. Use APPEND_DATABASE to select the database from which you want to retrieve kinetic data.
8. Define your elements and specify whether to reject and restore any phases. Do this in exactly the same way as you would for the thermodynamics data (see steps 2, 3 and 4).
9. Use GET_DATA to read from the database and add the kinetic data to the thermodynamic data that already exists in the GIBBS and DICTRA module workspace.
10. Use APPEND_DATABASE again to add thermodynamic or kinetic data from another database. When all the data needed is retrieved, you can start using the DICTRA module.

Setting Up and Running a Simulation

1. Before you can set up and start a simulation, you must have retrieved thermodynamic and kinetic data and defined your system. See Defining a System in Console Mode.
2. Set conditions that hold globally in the system using SET_CONDITION `Global`. Normally, this is the temperature condition.
3. Enter a region into the current cell using ENTER_REGION. Give the region an arbitrary name. If the region that you create is not the cell's first region, then by default it is attached to the right side of the last region created in the cell.
4. For each region, use ENTER_GRID_COORDINATES to specify the region's size (width) as well as the type of grid and the number of grid points to be used in the region. The size is specified in meters.
5. Use ENTER_PHASE_IN_REGION to enter a phase into a region. Specify whether the phase is active/inactive, which type of phase it is, and what the name of the phase is.
6. Use ENTER_COMPOSITIONS to specify the initial composition of a phase that you have entered in a region. You can specify the composition in terms of site fraction, mole fraction, mole percent, weight fraction, weight percent or u-fraction. The composition profile may be entered by a user or be read from a file.
7. Use SET_CONDITION `Boundary` to set non-default boundary conditions.
8. Use ENTER_GEOMETRICAL_EXPONENT to enter the geometrical exponent that defines the geometry of the system. If you do not specify the geometrical exponent, then it is assumed that the system has a planar geometry.
9. Use SET_SIMULATION_TIME to set the simulation time.
10. If you want to use a specific model for the simulation calculations, then set the DICTRA module to use a COARSENING_MODEL, PARA_EQUILIBRIUM_MODEL, HOMOGENIZATION_MODEL or GB_MODEL. Also see About the Pearlite Model .
11. You are now ready to run the simulation. However, it is recommended that you use SAVE_WORKSPACES to save the setup before running the simulation.
12. Use SIMULATE_REACTION to start the simulation. To ensure that the simulation is run with default settings (answer `Y`), otherwise you may be prompted to specify certain values during the running of the simulations (if phases appear or disappear in the simulation).

Setting Global Conditions

Use SET_CONDITION and choose `Global`. Global conditions include temperature (T), heat content removal (Q) and pressure (P), and these reduce the degrees of freedom for equilibrium calculations.

About Global Conditions

> If the heat content removal is specified then only the initial temperature should be entered with the SET_INITIAL_TEMPERATURE command.

- In practice, the pressure is rarely specified. By default the pressure is assumed to be constant and equal to 1 bar.
- For each condition, you can define a profile over time that consists of several intervals of time, or *ranges*, with each range having its own function to define the value of the condition.
- Temperature can be entered as a function of time (TIME) and/or spatial coordinate (X). The pressure condition can be defined as a function of time (TIME). The heat content removal can be defined as a function of temperature (T), pressure (P) and/or time (TIME).

  For example, the following function could specify a cooling rate if it is used to specify how the global condition temperature (T) changes with time (TIME) during a certain range: `1900-1*TIME;`

- Temperature can also be entered as time/temperature pair values.

Specifying Time-Dependent Profiles

In the DICTRA module you are often prompted to specify a time-dependent profile for a condition.

To define the profiles or intervals, enter information as follows:

LOW TIME LIMIT

To determine the time when the function starts to apply.

HIGH TIME LIMIT

To determine the time when the function stops applying. Use an asterisk (*) to set the high limit to the time when the simulation ends.

ANY MORE RANGES

Enter `Y` to specify an additional range with a time-dependent function, which starts to apply at the time step after the high time limit of the previous range is reached.

Creating Regions and Gridpoints

Enter a new region by specifying its name and, unless it is the first region, how it should be located with respect to one already existing region. The size of a region is determined when a grid is entered into the region.

About System, Cells and Regions and About Regions and Grids

How to Create a Region

1. Complete Defining a System in Console Mode.
2. Use ENTER_REGION to enter a region into the system.
3. Enter an arbitrary name for the region at the `Region name` prompt.
4. If this is the first region you create in your system, then you are finished. Otherwise, continue to the next step.
5. Enter the name of an already existing region to which the new region is attached.
6. Specify whether the new region should be `Attached to the right of` the existing region. Enter `Y` to attach to the existing region’s right side or `N` to attach it to its left side.
7. If the system has a cylindrical or spherical geometry, then this is a question of whether to put the new region outside the existing region, so that the new region surrounds the existing one, or to put it at the existing region’s centre, so that the existing region surrounds the new region.

How to Add Gridpoints to a Region

This topic describes how you specify the size and grid point distribution to use in a region.

1. Complete Defining a System in Console Mode and Creating a region.
2. Use ENTER_GRID_COORDINATES followed by the name of the region.
3. Specify the width of the region in meters.
4. At the `Number of points` prompt enter the number of grid points for the region.

5. Specify the type of grid point distribution to have in the region.
    - `Linear` for an equally spaced grid.
    - `Read_Point_by_Point` to read a number of specific grid points from a data file.
    - `Geometric` for a grid that yields a varying density of grid points in the region. Enter the `Value of R in the geometrical series`, which determines the distribution. A geometrical factor larger than one yields a higher density of grid points at the lower end of the region and a factor smaller than one yields a higher density of grid points at the upper end of the region.
    - `Double_Geometric` to have a high number of grid points in the middle or at both ends of a region. Specify two geometrical factors. `Value of R in the geometrical series for lower part of region` for the distribution in the lower (left) part of a region, and `Value of R in the geometrical series for upper part of subregion` for the distribution in the upper (right) part of a region.

Entering Phases in Regions

> There is no supersaturation locally within a given region.

When defining a region you need to enter one or more phases into the region. The number and type of phases depends on the simulation you want to run.

- To simulate diffusion of components within one phase, enter one matrix phase into the region.
- To simulate how an interface between regions moves, enter two regions with at least one phase in each.
- To simulate growth of one or more dispersed phases in a matrix phase, enter one matrix phase and one or more spheroid phases.

About Phases

Entering Phases in a Region

1. Complete Defining a System in Console Mode and Creating Regions and Gridpoints.
2. Use ENTER_PHASE_IN_REGION. Specify whether the phase is to be `Active` or `Inactive`.
3. For an inactive phase, specify the following:
   - Enter the name of the region and the side of that region which the phase is attached to.
   - Enter the required driving force (evaluated as DGM[1], and it is dimensionless (phase) in POLY-3) to be used for determining whether an inactive phase is stable.
   - Enter the `CONDITION TYPE` that the phase boundary condition should be set to if the inactive phase becomes stable. (Inactive phases are only considered in the simulation calculations once it is stable.)
4. For an active phase specify the following:
   - `REGION NAME` for the region in which the phase is to be entered.
   - `PHASE TYPE`: `Matrix`, `Lamellar` or `Spheroid`. `SPHEROID` is only available if a `MATRIX` phase is created first. You can only enter one matrix phase in each region.
   - Enter the `PHASE NAME`. You can append a hash sign (`#`) and a digit at the end of the phase name to designate the composition set number (e.g. `FCC#2`). If you do not append this and the phase has more than one composition set, then you are prompted to specify a composition set number.

Specifying Phase Compositions in a Region

When you specify the composition of a phase, you do this by specifying the composition of the phase within its region—a composition profile.

DICTRA Module Commands

How to Specify Phase Compositions in a Region

1. Complete Defining a System in Console Mode, Creating Regions and Gridpoints and Entering Phases in Regions.
2. Use ENTER_COMPOSITIONS to enter a composition of a phase in a certain region.

---

[1] DGM is the POLY variable for the driving force that is already divided by RT.

3. Enter the `Region name` of the region in which the phase has previously been entered.
4. Enter the `Phase name` of the phase whose composition you want to specify.
5. If the phase is spheroid, then for `Use equilibrium value` enter `Y` to automatically calculate the equilibrium fractions of the phase and its constitution at the start of the simulation. Specify the initial `Volume fraction of` the spheroid phase.
6. Enter the `Dependent component`. Sometimes the dependent component is automatically set and there is no prompt.
7. Enter a `Composition type` for the constitution of the phase. The options are: SITE_FRACTION, MOLE_FRACTION, MOLE_PERCENT, WEIGHT_FRACTION, WEIGHT_PERCENT, and U_FRACTION.
8. Enter the `Type` of composition profile (that is, the type of composition profile). The options are:

- `Linear` to have an equally spaced composition distribution. Specify the composition at the first (leftmost) grid point (`Value of first point`) and at the last (rightmost) grid point (`Value of last point`).
- `Read_point_by_point` to read the composition at each grid point. The specification of these can either be read from a DATA-file that you are prompted to select or entered directly at the terminal. If you want to enter them at the terminal, then enter `READ_POINT_BY_POINT` and press <Enter>.
- `Geometric` for a distribution that yields a higher concentration of the component at the lower end of the region if a geometrical factor larger than one is given and a higher concentration at the upper end of the region if the factor is smaller than one. You are prompted to specify the `Value of R in the geometrical series` which determines the distribution.
- `Function` for the global distance denoted ‘gd’. Useful functions include the error function (`erf(gd)`) and the heavy-side step function (`hs(gd)`). For example, the function `3+2hs(x-1e-4)` specifies a concentration of 3 at the region’s left side and 5 at the region’s right side, with a sharp step in the concentration profile at 1e-4m=100µm.

Specifying the Geometry

By default a DICTRA module system has a planar geometry. To change the geometry of the system, use ENTER_GEOMETRICAL_EXPONENT followed by a number `0` (planar), `1` (cylindrical) or `2` (spherical).

About Geometry and Coordinates

With a cylindrical or spherical geometry, the system's zero coordinate (left boundary) is at the centre of the cylinder or sphere. The highest coordinate (right boundary) is defined by the cylinder or sphere radius. If you want a geometry corresponding to a tube or a hollow sphere, then use SET_FIRST_INTERFACE to locate the system's left boundary at a coordinate that is greater than zero.

Setting Boundary Conditions

Boundary conditions are conditions that define how matter behaves at the boundaries of your system. By default, matter is not allowed to cross the system boundaries.

You can change the setting for both the lower boundary (left side/centre) and the upper boundary (right side/surface) of the system.

How to Set Boundary Conditions

1. Complete Defining a System in Console Mode and Creating Regions and Gridpoints.
2. Use SET_CONDITION and choose `Boundary`. Then specify whether you want to set the LOWER or the UPPER boundary.
3. Specify which condition type you want to set the boundary to.
4. Enter any parameter values that are necessary for the condition type you have chosen.
5. Specify the `LOW TIME LIMIT`, when the function you define starts to apply.
6. If required, enter the function that is applied during the time interval. For most condition types, the function may have time, temperature and pressure as arguments.
7. Enter the `HIGH TIME LIMIT` for the interval.
8. If you want to define a different function for another time interval, then enter `Y` when prompted with `ANY MORE RANGES`. Then enter another function for the next range.
9. When you have defined functions for all the ranges you want, enter `N` at the `ANY MORE RANGES` prompt.

Adding (Creating) Cells

If you add cells to a system, then each new cell is always placed next to the system's right outer boundary. Use the command CREATE_NEW_CELL.

Importing a Scheil Segregation Profile

You can import a previously calculated Scheil segregation profile into the Diffusion Module (DICTRA). A Scheil calculation is a conservative estimate of the segregation that occurs during solidification and is useful when estimating the necessary time/temperature for a homogenizing heat treatment.

From a practical point of view it is also a simple and fast calculation compared to a more accurate, but computationally more difficult, diffusion simulation.

In order to limit the computational effort, this feature cannot be combined with the fast diffusers option in the Scheil module.

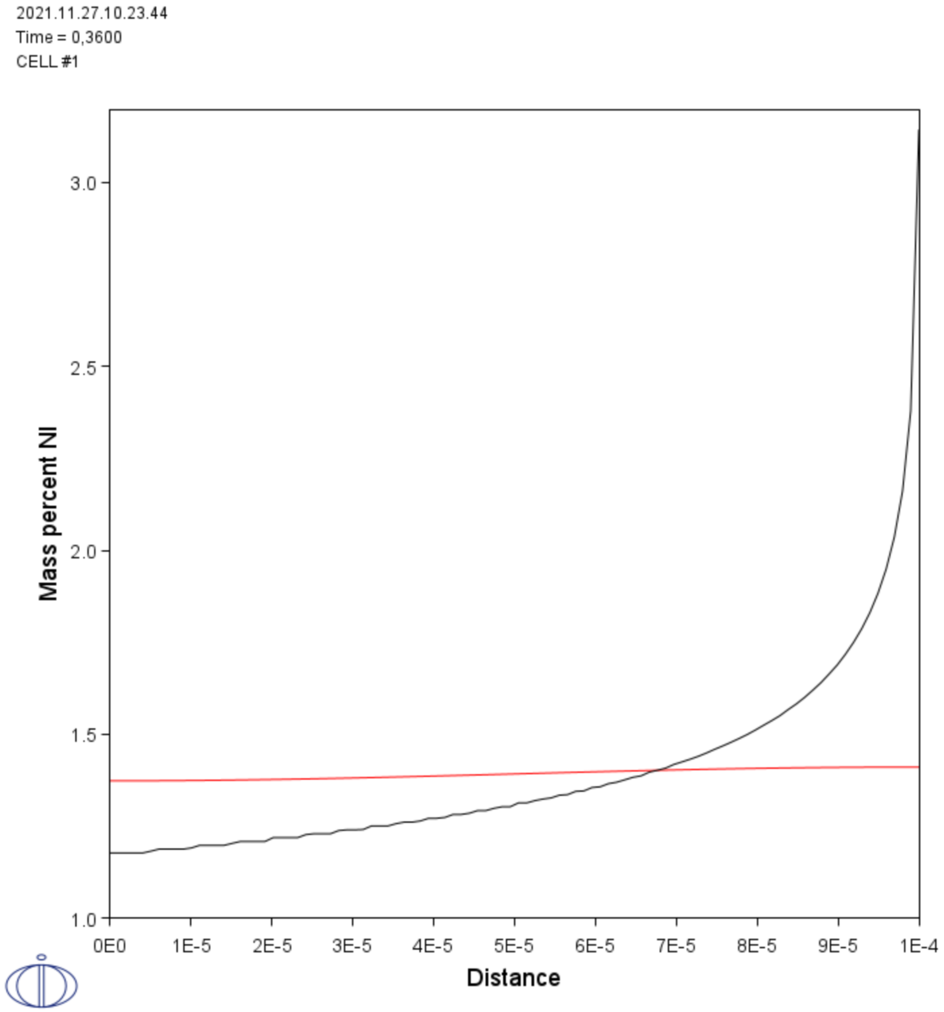
Press F1 in Thermo-Calc to search the help for more information.

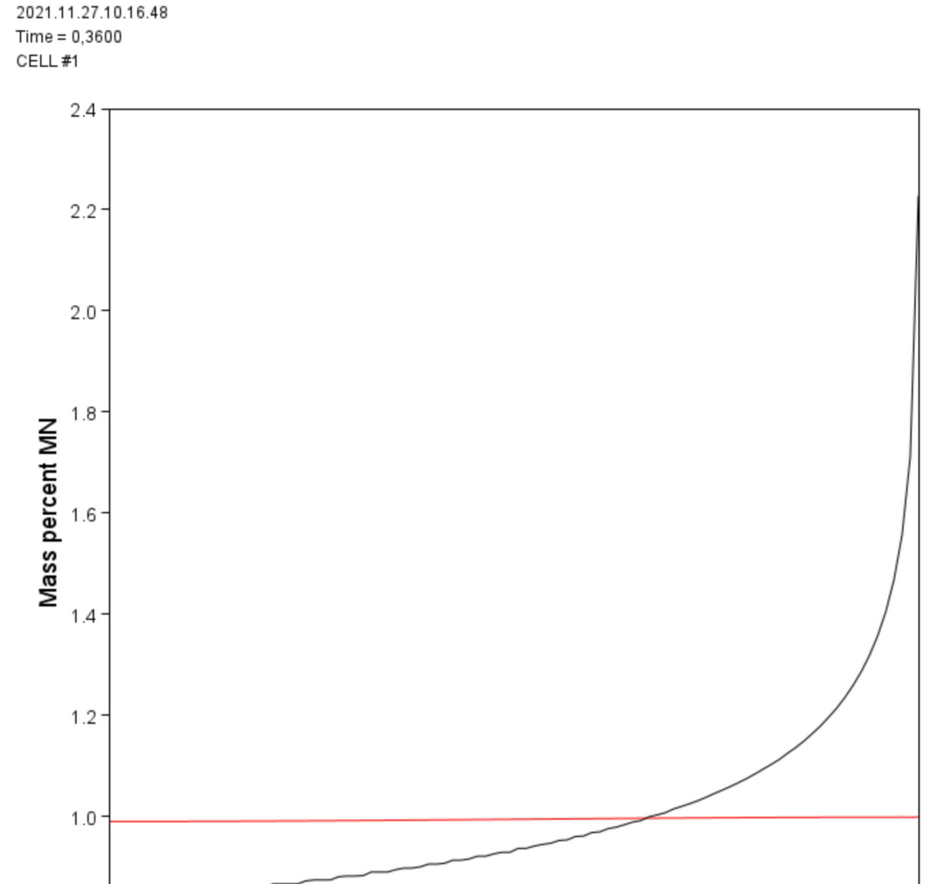
This is available in Graphical Mode using the **Homogenization** template. Also see Graphical Mode example *D_10_Fe _Homogenization_from_Scheil.tcu*.

Example exa7

In the following example, taken from the Diffusion Module example collection (see About the Examples in the Thermo-Calc documentation), the Scheil segregation profile for a ferritic stainless steel (Fe-17Cr-1.4Ni-1Mn) was calculated in the Scheil module in Thermo-Calc.

The profile was then imported into the DICTRA module and a one hour homogenizing heat treatment at 1200° C was simulated. For the simulation a domain size of 100 µm was assumed, which approximately corresponds to the secondary dendrite arm spacing.


2021.11.27.10.23.44
Time = 0,3600
CELL #1
Mass percent NI
3.0
2.5
2.0
1.5
1.0
0E0
1E-5
2E-5
3E-5
4E-5
5E-5
6E-5
7E-5
8E-5
9E-5
1E-4
Distance


2021.11.27.10.16.48
Time = 0,3600
CELL #1
Mass percent MN
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0

The plots show the initial (left) and final (right) Ni profile.

Models in the Diffusion Module

In this section:

About the Homogenization Model

This section or topic is specific to Console Mode.

If you enter a spheroid phase when you configure your calculation, then the homogenization model is automatically used. This is useful when you want to simulate long-range diffusion through a multiphase mixture, under the assumption that local equilibrium holds at each node point.

You can also explicitly set the DICTRA module to use the HOMOGENIZATION_MODEL. This way, you can use it when calculating a one phase or a moving boundary simulation.

When the homogenization model is used, simulations are run using an implicit finite volume method to increase numerical stability. Because of this, and other factors, homogenization model simulations generally run slower than other comparable simulations. You can increase or decrease the `Degree of implicity when integrating PDEs` with the command SET_SIMULATION_CONDITION.

There are several special commands for use with this model. The UTILITIES_ HOMOGENIZATION and SPECIAL_HOMOGENIZATION_OPTIONS commands are described individually in the *Diffusion Module Command Reference*. Search the help (press F1 in Thermo-Calc) for information.

If you have entered a spheroid phase in a region and want to use the older so-called dispersed system model, then you must explicitly disable the Homogenization Model after all phases have been entered.

About the Disperse Model

This section or topic is specific to Console Mode.

This model can be used to calculate diffusion of a phase that is dispersed in a matrix phase. However, it is recommended that you use the HOMOGENIZATION_MODEL for this type of calculation instead.

There is no specific command to activate this model. It is only available if a phase of type "spheroid" is entered in a region.

The disperse model has the following limitations:

- There must be a continuous matrix phase otherwise the simulation breaks down.
- There is no implicit integration of the partial differential equations (PDEs), leading to a lower accuracy.
- Only diffusion in the matrix phase can be simulated. It is assumed that no diffusion occurs in the dispersed phase.

After a spheroid phase is entered, the homogenization model must explicitly be *inactivated* in order to run the simulation with the dispersed model. To do this, enter the command HOMOGENIZATION_MODEL and then choose `N` to make it inactive.

About the Para Equilibrium Model

The model allows you to calculate a moving phase boundary simulation while assuming that para-equilibrium conditions hold at the boundary. You must explicitly set the DICTRA module to use this model with the PARA_EQUILIBRIUM_MODEL command.

When this model is used, it implies that the local equilibrium assumption is no longer valid and that substitutional components are regarded as one composite component. You can only simulate a single moving boundary in one cell.

About the Thermomigration Model

This section or topic is specific to Console Mode.

The thermomigration model allows you to simulate thermally induced diffusion in temperature gradients. To use the model, you must set the temperature to depend on the spatial coordinate (x) in your calculation. In addition, you must also enter the heat of transport quantity (Q*) using the ENTER_HEAT_TRANSFER_PARAMETER command. You must enter this parameter separately for each element in each phase.

The model is automatically used once this is done.

See Console Mode example exh3 in the *Diffusion Module Examples Guide*.

About the Grain Boundary Model (GB_Model)

This section or topic is specific to Console Mode.

You must explicitly set the DICTRA module to use this model with GB_MODEL. This model allows you to simulate grain-boundary and dislocation-assisted diffusion.

The grain boundaries and the dislocations contribute to the total amount of diffusion according to the weighted fractions. The parameters are entered separately for each region in order to allow for different expression for different phases.

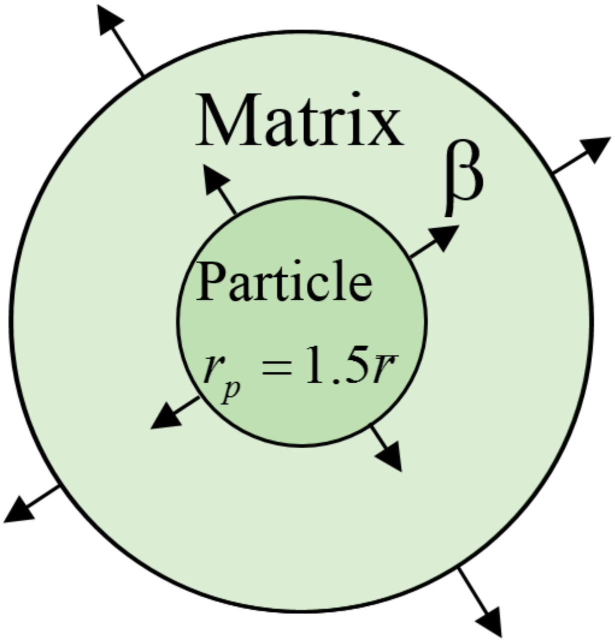
See the *TCNI Examples Collection* for an example using this model.

Coarsening Processes

This type of simulation is available for Console Mode. See About the Coarsening Model for more information.

You can run a simulation of a coarsening process. In accordance with Lifshitz-Slyozov-Wagner theory, this is done by assuming that the coarsening can be simulated by calculating the growth of a single particle of the maximum size in the particle size distribution.

Simulate a coarsening process



About the Coarsening Model

This section or topic is specific to Console Mode.

The model is based on LSW theory (after Lifshitz and Slyozov (1961)[1] and Wagner (1967)[2]. The model is also described in Gustafson, Höglund, and Ågren (1998)[3] and Björklund, Donaghey, and Hillert (1972)[4].

LSW theory is strictly only valid for low volume fractions of the particle phase. The theory predicts that the normalized particle size distribution obtains a constant shape where the largest particles have a radius equal to 1.5 times the average particle radius.

The calculations are performed in one cell on a maximum size particle which thus is assumed to be 1.5 times the size of the average particle size. The matrix phase is on one side in contact with the maximum size particle and on the other the matrix phase is in local equilibrium with an average sized particle. The effect of the surface energy is such that both the maximum size particle as well as the matrix phase grows.

The model allows you to perform coarsening simulations. You must explicitly set the DICTRA module to use this model with the command COARSENING_MODEL.

To use this mode, configure the calculation as follows:

- Have one cell only, with a single particle that is 1.5 times larger than the average particle size.
- The matrix phase should be in contact with the maximum size particle on the left/lower side, and then the model specifies a local equilibrium with an average sized particle on the right/upper side.
- The surface energy then results in growth of both the maximum size particle and the matrix phase. Use the SET_SURFACE_TENSION command to enter the surface energy to enable coarsening.

About the Pearlite Model

This section or topic is specific to Console Mode.

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[1] Lifshitz, I.M., and V.V. Slyozov. 1961. “The Kinetics of Precipitation from Supersaturated Solid Solutions.” Journal of Physics and Chemistry of Solids 19 (1–2): 35–50.

[2] Wagner, Carl. 1967. “Theorie Der Alterung von Niederschlägen Durch Umlösen (Ostwald-Reifung).” Berichte Der Bunsengesellschaft Für Physikalische Chemie 65 (7–8): 581–91.

[3] 'Simulation of carbo-nitride coarsening in multicomponent Cr-steels for high temperature applications'. In *Advanced heat resistant steels for power generation* (San Sebastian, Spain 27/04/1998

[4] Björklund, Stig, L F Donaghey, and Mats Hillert. 1972. “The Effect of Alloying Elements on the Rate of Ostwald Ripening of Cementite in Steel.” Acta Metallurgica 20 (7): 867–74.

The pearlite model is automatically used if there is lamellar phase in a region.

About Cooperative Growth

This section or topic is specific to Console Mode.

You can simulate the growth of pearlite in alloyed steels by calculating the Eutectoid reaction $\gamma \rightarrow \alpha + \beta$, where α and β grow cooperatively as a lamellar aggregate into the γ matrix.

About Using Volume in the Diffusion Module (DICTRA)

This section or topic is specific to Console Mode.

The following is applicable to the use of the classic models in the Diffusion Module (DICTRA). That is, all models *except* the homogenization model.

DICTRA uses a simplified treatment of volume, i.e. DICTRA does not use volume data from the thermodynamic databases. This implementation in the original software development was because most databases did not contain volume data at that time.

The basic rule to use when applying the classic model is that only substitutional phase constituents contribute to volume and the partial molar volume of such constituents are assumed to be constant and equal. The partial molar volume of interstitial phase constituents are assumed to be zero. The actual value used as partial molar volume of substitutional phase constituents is 10-5 [m^3/mol] and this is entered in databases as a constant `VS`.

The databases contain definitions of *zero volume species* and these species can then be interstitial phase constituents. Typically, C, N and O are entered as zero volume species.

There is, however, a rule that supersedes the basic rule, that is, for a phase that consists of a single sublattice, such as graphite, all constituents are considered to be substitutional. Another case is the liquid, which in most databases is described with a single sublattice. In such a liquid all constituents are then considered to be substitutional.

Thus, a given species can be interstitial in one phase but substitutional in another.

For the homogenization model the treatment of volume is, unfortunately, but for good reason, slightly different. The homogenization model only considers the elements of the system and regards each element as being either substitutional or interstitial. This status is the same in all phases. For many cases this treatment yields the same result as the rules for the classic model described above. However, it does not work for graphite, which has zero volume.

Plotting Simulations in the POST Module

You can plot or tabulate the results of your simulation in the POST_PROCESSOR module, also called the POST module and accessed within the DICTRA module. The resulting diagram is on a plot tab in the Console Results window. Once the simulation results are plotted, you can then change its appearance in the Plot Properties window.

In this section:

Plotting Simulation Results

? [Saving and Printing the Output in Console Mode]

Plotting a diagram is to graphically represent how a dependent variable varies with an independent variable. The independent variable is either distance or time.

1. Complete all the steps to run your simulation.
2. At the `DIC` prompt type `POST_PROCESSOR` (or just `POST`).
3. Use SET_DIAGRAM_AXIS to specify the variables to plot on the X- and Y-axes of the diagram. One of the axes must be set to either TIME or DISTANCE.

   For example, to set the X-axis to plot the distance from the lower boundary of the calculation (rather than from the lower boundary of the current region) and the Y-axis to plot the weight-percent composition of the Si element, at the `POST` prompt type:

   ```
   SET_DIAGRAM_AXIS X DISTANCE GLOBAL
   SET_DIAGRAM AXIS Y WEIGHT-PERCENT SI
   ```

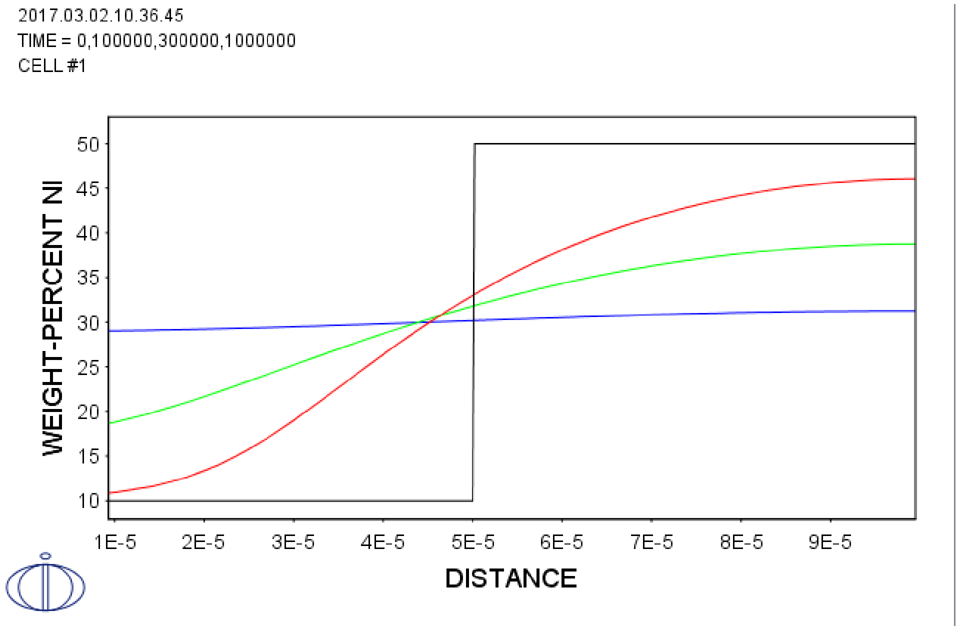
4. You can specify a Z-axis, which is represented as tick marks on the curve in the XY-plane.
5. When one of the axes is set to TIME or DISTANCE, the variable automatically becomes the independent variable. If you do not want the independent variable plotted along an axis, use SET_INDEPENDENT_VARIABLE and set it to `Time` or `Distance`.
6. Simulation calculations depend on both time and a spatial coordinate; these variables must be fixed during the plotting process. Use SET_PLOT_CONDITION to set the variable to keep fixed. These variables can be set as the fixed plot condition:
   - `Time`: The integration time. More than one value can be entered using commas or spaces to separate the values. One graph is plotted for each value.
   - `Distance`: The distance in the system (from the lower boundary).
   - `Interface`: At the location of a certain interface between two phases.
   - `Intergral`: The value of the plot condition is integrated over the phase, region or system volume.

7. Use PLOT_DIAGRAM to plot the results. The plot is added as a tab to the **Console Results** window.

   The plot example below is from example exa2a, which is part of the Diffusion Module example collection (see About the Examples in the Thermo-Calc documentation). Distance is set as the independent variable and the weight-percent of Ni is on the Y-axis. The plot condition is `TIME`: the plot shows four graphs, each with the spatial distribution of Ni in the region at the time steps 0, 1e5, 3e5, and 10e5.

8. To print the plotted graphs direct to a postscript-file, type `Plot` and a file name.
9. In the **Plot** window, right click the diagram and choose **Properties** to adjust its appearance and colors.

Editing the Plot Properties.



2017.03.02.10.36.45
TIME = 0,100000,300000,1000000
CELL #1

Editing the Plot Properties

To change the appearance of a plotted diagram, right click the diagram and select **Properties**. In the **Plot Properties** window you can change the fonts and colours, and add a title, for example.

You can also change the colour, stroke (solid/dashed/dotted/dash_dot) and line width of a particular series of lines in the plot by double-clicking one of the lines in the series. In this way, you can also toggle whether data points should be shown or not for a series of lines.

The crosshair cursor turns into a cursor resembling a pointing hand when it is placed over a line that can be clicked but if you hold down the <Ctrl> key, this does not happen (the cursor continues to be shown as a crosshair).

To configure the default settings for plotting, go to the **Options** window and on the Console Mode tab click the **Plotting** node in the tree.

Global Settings

Tabulating Simulation Results

DICTRA Module Commands

1. Complete all the steps to run your simulation.
2. At the DIC prompt type `POST_PROCESSOR` (or just `POST`).
3. Use ENTER_SYMBOL `Table` to specify the variables to be shown in the table columns. Separate the variables by commas (,).
4. Use SET_INDEPENDENT_VARIABLE to specify the variable that the rows in the table should represent.
5. Use TABULATE to generate the table.

Troubleshooting

The following topics contain some general advice to consider in order to avoid having your simulation fail to converge when you calculate different kinds of simulations in the Diffusion Module (DICTRA).

In this section:

Tips for a Successful Diffusion Simulation

The following tips are useful to help you fine-tune the design of your simulation.

Simplify Your Simulation

For example, if you have an alloy with five or six elements, first run a simulation with only the main elements. When this simulation works, you can then add more elements as necessary.

Start with a Low Accuracy and Refine It

If you start with a high accuracy setting, then computing the simulation takes much longer, and problems are more likely. Check the profiles and the overall mass balance, and if the accuracy is insufficient then you can improve the accuracy values.

To change the accuracy:

In Console Mode use SET_ACCURACY and increase or decrease `Max relative error` and `Max absolute error`.

In Graphical Mode the setting is on the Diffusion Calculator in the section *Time step control*.

Modify the Grid or Time Step

If you get large fluctuations in the composition or phase boundary profiles, then you can try modifying the grid or the time step of the simulation. You can increase the time step by lowering the accuracy if automatic time step control is used (the default).

If you increase the tolerated relative and/or absolute error then the automatic time step control increases the time step.

In Console Mode use the SET_ACCURACY command.

In Graphical Mode the setting is on the Diffusion Calculator in the section *Time step control*.

Integrate the PDEs

The composition or phase boundary profiles can often also be improved if the partial differential equations (PDEs) are integrated fully implicitly (i.e. Euler backward).

To integrate the PDEs in this way:

In Console Mode use SET_SIMULATION_CONDITION to set the parameter `Degree of Implicity when Integrating PDEs` to a value of `1`.

In Graphical Mode, the setting is on the Diffusion Calculator on the **Options** tab. Under *Simulation Conditions*, you can try a different **Time integration method**. The default method is Trapezoidal, which is equivalent to a 0.5 numerical setting in Console Mode. If you choose Euler backward, this is equivalent to a 1.0 numerical setting in Console Mode.

Debug (Console Mode)

If your Console Mode simulation fails to converge, then debugging may give you some clues about the source of the failure. To receive more detailed information about what is happening during the simulation use the command DEBUGGING.

Moving Boundary Simulations

Grid Distribution

Check the grid distribution at the interfaces. If the grid is too coarse or too fine-grained then the fluxes may not be defined well.

Use Activities Instead of Potentials

Use activities instead of potentials when the content of one or more of the elements becomes very low. If you do this, then the activity approaches zero, which is easier to handle than a potential that approaches infinity.

In Console Mode, use SET_SIMULATION_CONDITION to set the parameter `Vary potentials or activities` to `Activities`.

In Graphical Mode the setting is on the Diffusion Calculator in the section *Classic model specific*. From the list, choose **activity** [**Use the activity of a component in order to find the correct tieline at the phase interface**].

Starting Values

Use the automatic starting values when you run the simulation the first time. If the first time step does not converge try decreasing the starting values for the velocities. Alternatively, increase the duration of the first time step.

If the simulation fails during the first time step, then check how the starting values affect the residuals.

In Console Mode, use the command SET_SIMULATION_CONDITION and set the parameter `NS01A PRINT CONTROL`to `1`.

When you adjust this setting, the software then prints the tried unknown value and the residual for each flux balance equation in each iteration. The equations are organized so that the first unknown value is always the migration rate of the phase interfaces followed by the unknown potentials. All unknown values are scaled by the starting value or the calculated value in the previous time step.

Cell Calculations

This section or topic is specific to Console Mode.

In cell calculations, determine start values for each cell separately and thereafter connect the individual cells. You can even start out simulating in planar and/or cylindrical geometry in order to determine sufficient starting values if you want to use a spherical geometry.

Diffusion in Dispersed Systems

This section or topic is specific to Console Mode.

If you simulate diffusion in a dispersed system and the homogenization model is turned off, then time integration is explicit. The maximum time step allowed, or the highest time step actually taken in the calculation, affects the final result of the simulation. This effect is most evident if one or more of the diffusing species have low solubility in the matrix phase. When this is the case, a supersaturation is created in the matrix phase during a diffusion step and if too large a time step is allowed, then too much supersaturation is created. Consequently, always check your results by performing a second simulation with a maximum time step that is ten times lower than in the first run. If there is large difference in results between the first and the second run, then decrease the time step again with a factor of ten and perform a third run. Repeat this process until the results can be trusted.

If a simulation fails because the program is not able to calculate an equilibrium, then try to calculate the initial equilibrium yourself using Thermo-Calc and enter the composition and fraction of each phase separately instead of having the DICTRA module calculate it. Also enter starting values for each phase with the command SET_ALL_START_VALUES. Alternatively, you may force the software to use certain start values using SET_SIMULATION_CONDITION.

Cooperative Growth

This section or topic is specific to Console Mode.

If your simulation fails to converge, try calculating the A1e temperature with Thermo-Calc and start your simulation at a temperature slightly below that temperature. Use the equations given in the interactive help in order to estimate S0 and the growth rate.

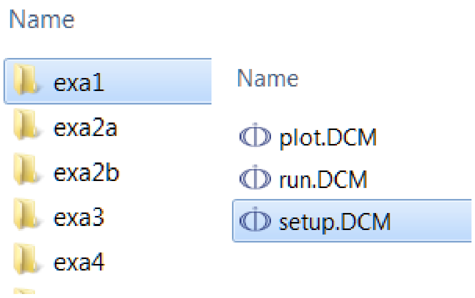
Diffusion Module (DICTRA) Console Mode Examples

To learn more about how to use the add-on software you can open and run the example files. These macro files (with the extension *.`DCM`) include comments, which you can either run in the Thermo-Calc program or open and read in a text editor.

> If you read the macro file in a text editor, you do not see the output that Thermo-Calc gives in response to the commands stored in the macro file.

Opening the Setup, Run, and Plot Macro Files

For the main set of examples (this is different for the Quick Start examples), there are three macro files: a **setup**, **run** and a **plot**. You must run these macros in order.



To begin, double-click the **setup.DCM** file to open it. It launches a new session of Thermo-Calc and opens in Console Mode.

All the macro files and the outputs are also combined into one file that you can search and read. This is included with your installation as a PDF (go to **Help → Manuals folder → Diffusion Module (DICTRA)** and open *Diffusion Module Console Mode Example Macros*.

Quick Start Guide Examples

These examples are used in the *Diffusion Module Quick Start Guide (Console Mode)*. It is recommended you review this guide before going to the additional examples.

File Name	Description
simplest_dictra.dcm	Simple homogenization of a binary Fe-Ni alloy. Initially it is assumed to have a linear Ni-concentration profile.
simple_moving_ boundary.dcm	Calculating a ferrite(bcc)/austenite(fcc) transformation in a binary Fe-C alloy
multiphase_ example.dcm	Shows the use of the homogenization model for multiphase simulations. It is taken from [2006Lar]. Experimental data is from [1995Eng].

References

[1995Eng] A. Engström, Interdiffusion in multiphase, Fe-Cr-Ni diffusion couples. Scand. J. Metall. 24, 12–20 (1995).

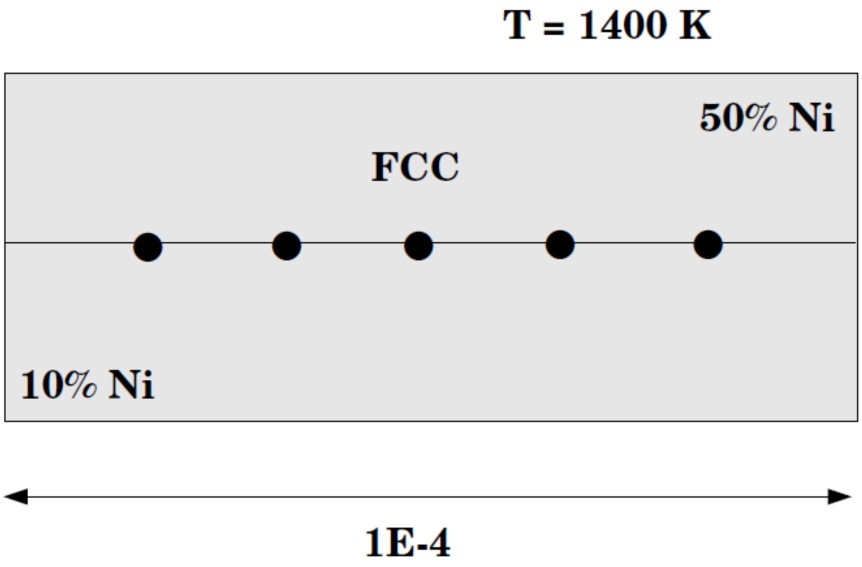
[2006Lar] H. Larsson, A. Engström, A homogenization approach to diffusion simulations applied to α+γ Fe–Cr–Ni diffusion couples. Acta Mater. 54, 2431–2439 (2006).

One Phase Examples

Example exa1

Homogenization of a binary Fe-Ni alloy: Linear concentration profile

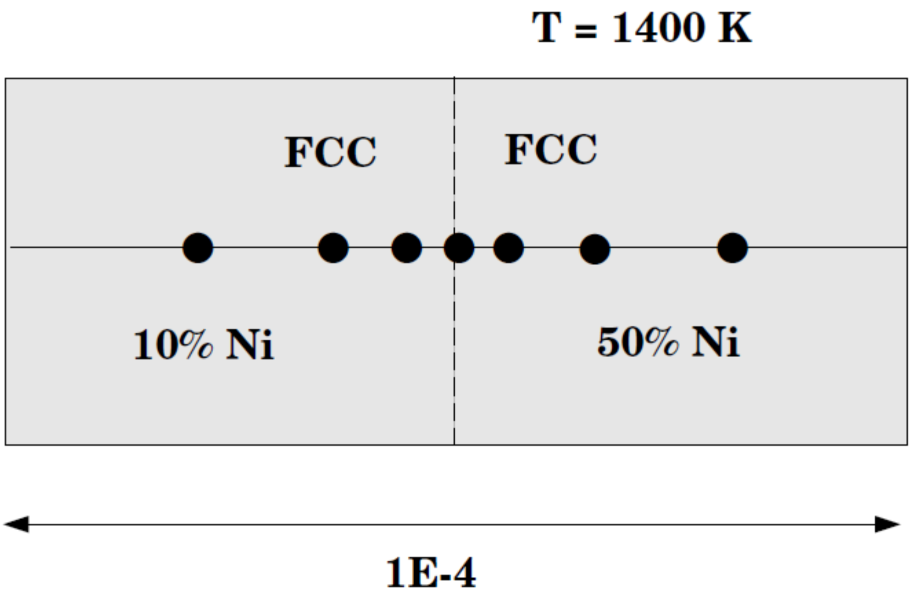
Simple homogenization of a binary Fe-Ni alloy. It is assumed there is initially a linear Ni-concentration profile.



Example exa2a and exa2b

Homogenization of a binary Fe-Ni alloy

- Example exa2a **Step Profile:** Simple homogenization of a binary Fe-Ni alloy. A Ni rich and a Ni lean alloy are put together and initially there is a step profile.
- Example exa2b **Time Integration:**This example is identical to a2a but instead it uses implicit time integration instead of the trapezoidal method for solving the PDEs.



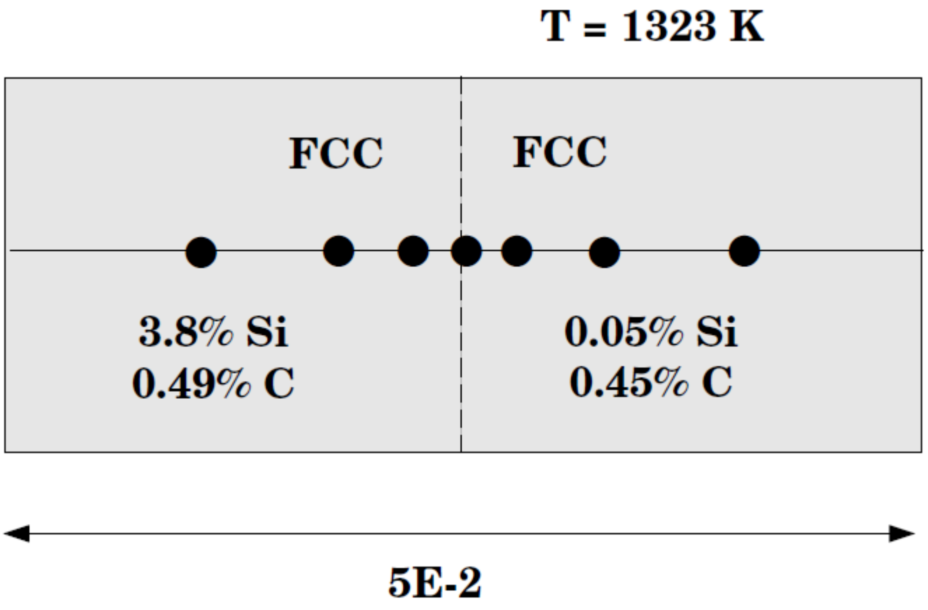
Example exa3

Uphill diffusion in an Fe-Si-C alloy

This is an example to simulate uphill diffusion in a ternary single phase austenite matrix due to the classical Darken experiment published by Darken, 1949 [1949Dar].

In this example, two pieces of austenite (3.80 wt%Si, 0.49 wt%C) and (0.05 wt%Si, 0.45 wt%C) are put together and are subsequently annealed at 1050 C for 13 days. As both pieces are austenite they must be entered into the same region. This is done by individually giving the compositions of Si and C in each grid point. These data are then stored to file.

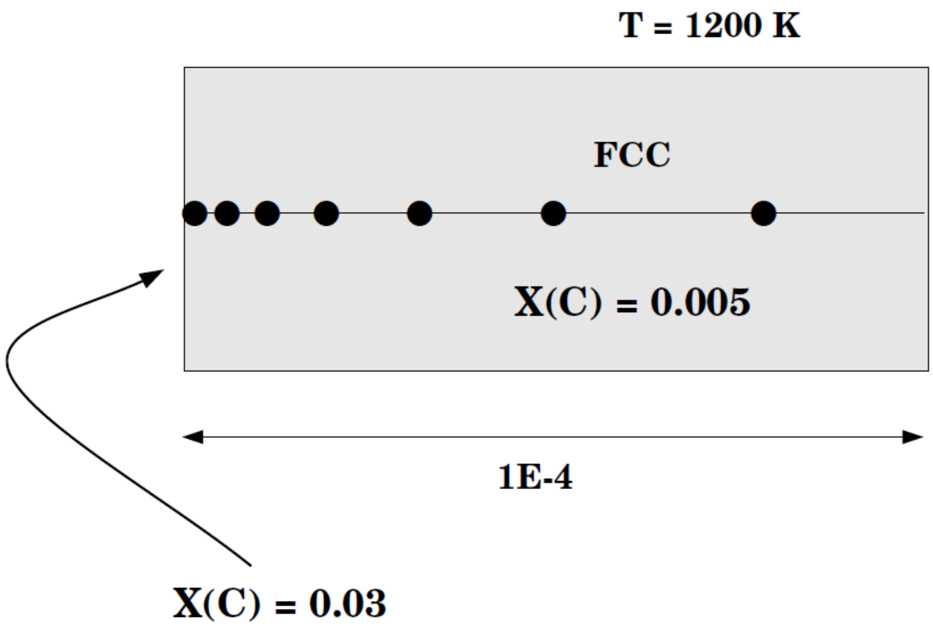
This example uses the TCFE and MOBFE databases. These licenses are required to run the example.



Example exa4

Carburization of binary Fe-C alloy: Comparison to an analytical erf solution

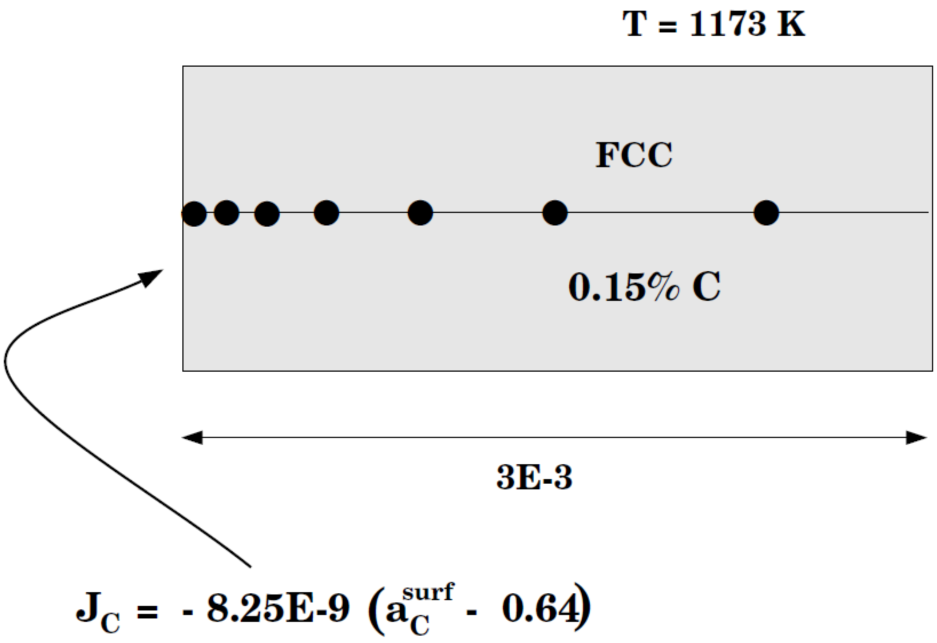
This is a simple binary simulation with one single phase region. The numerical simulation is compared with an analytical erf-solution. A special database is created (*erf.tdb*) where the diffusion coefficient is set to a concentration independent value.



Example exa5

Carburization of a binary Fe-0.15 wt% C alloy

A mixture of 40% N2 and 60% cracked methanol is used as carrier gas. The carburizing "carbon potential" in the gas is 0.85 wt% and a surface reaction controls the flux of C at the surface.

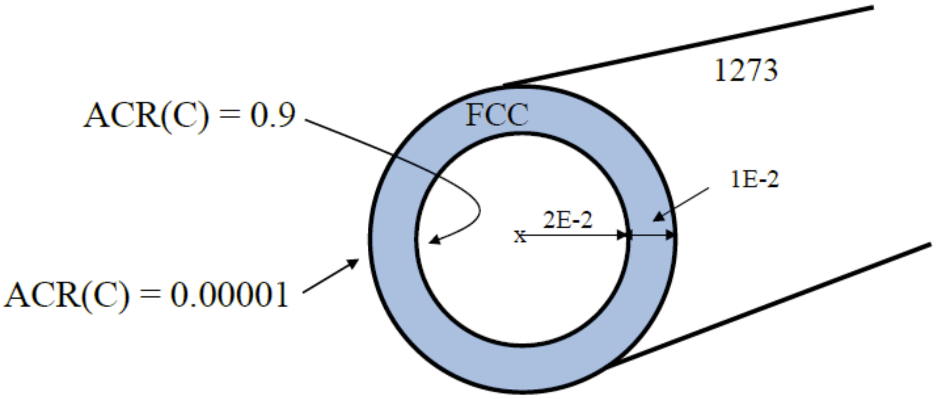


Example exa6

Diffusion through a tube wall

A simple example of diffusion through a tube wall. The tube material is an Fe-0.6%Mn-0.7%Si-0.05%C alloy. On the inside wall a carbon activity of 0.9 is maintained whereas on the outside the C-activity is very low. This example demonstrates the use of the command SET-FIRST-INTERFACE as well as the use of MIXED boundary conditions.

This example uses the TCFE and MOBFE databases. These licenses are required to run the example.

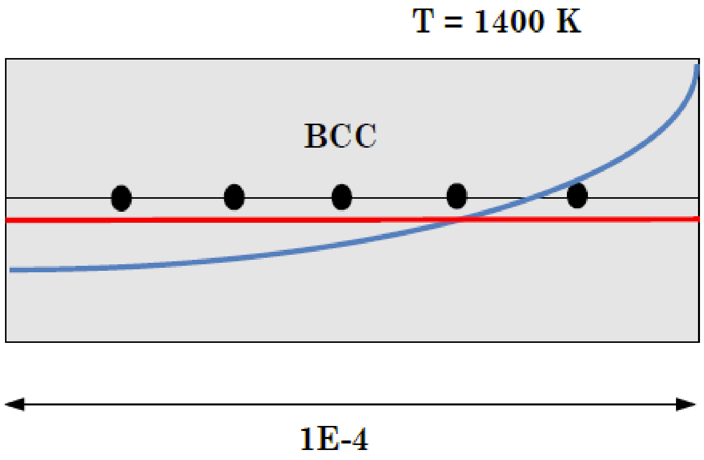


A modified version of this example is also available in Graphical Mode as example D_06. For Graphical Mode you do not need a Diffusion Module (DICTRA) license. You can open the example from Thermo-Calc when in Graphical Mode (**File → Examples Files → Diffusion Module**).

Example exa7

Homogenization heat treatment

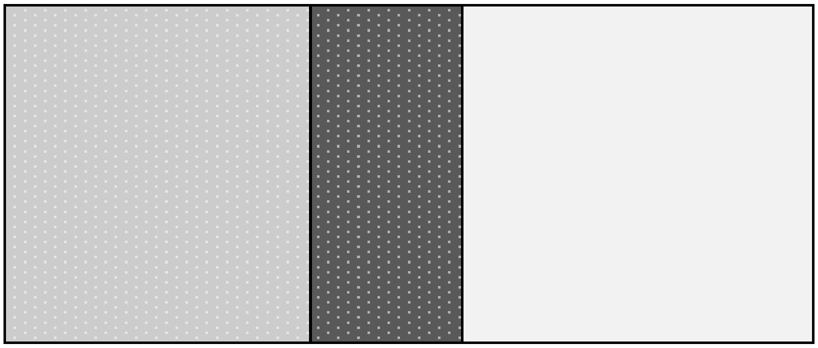
The initial segregation profile is created from a Scheil calculation (see `macro create_ initial_profile.TCM`). The command INPUT_SCHEIL_PROFILEin the DICTRA monitor performs most of the setup. Only time and temperature must be entered after the INPUT_ SCHEIL_PROFILE command is executed.



Reference

[1949Dar] L. S. Darken, Diffusion of Carbon in Austenite with a Discontinuity in Composition. Trans. Am. Soc. Met. AIME 180, 430–438 (1949).

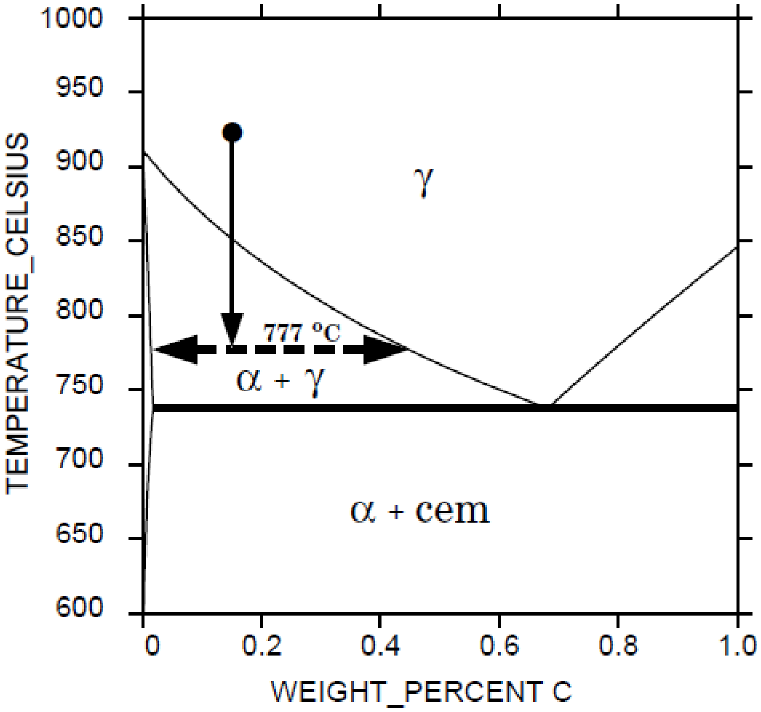
Moving Boundary Examples

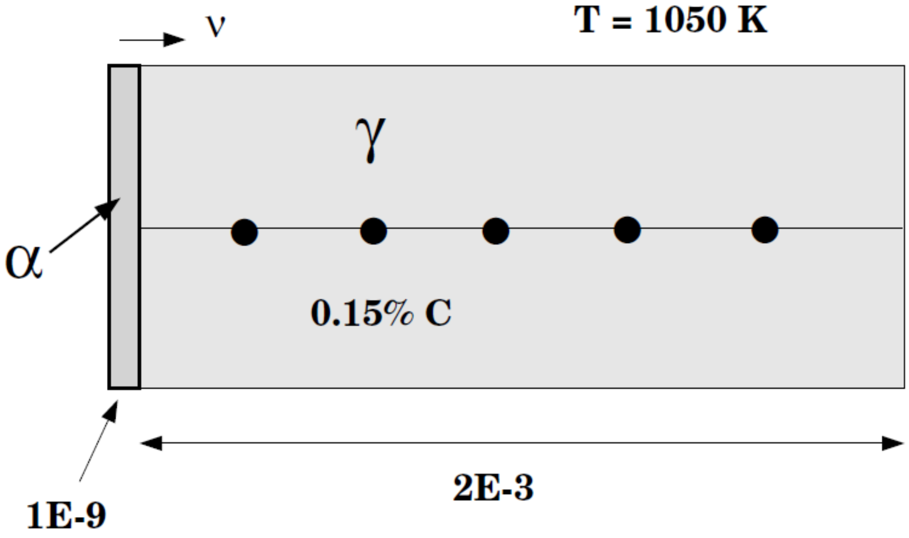


Example exb1a

Austenite (γ) to ferrite (α) transformation in a binary Fe-C alloy

This example calculates a ferrite (BCC)/austenite (FCC) transformation in a binary Fe-C alloy. The initial state is an austenite of 2 mm thickness. The composition of the austenite is Fe-0.15wt%C. After austenitization the specimen is quenched down to 1050K. The system is assumed closed, so no boundary conditions are set (a closed system is the default). Ferrite is expected to grow into the austenite. For this reason you start with a thin region with ferrite adjacent to the austenite.

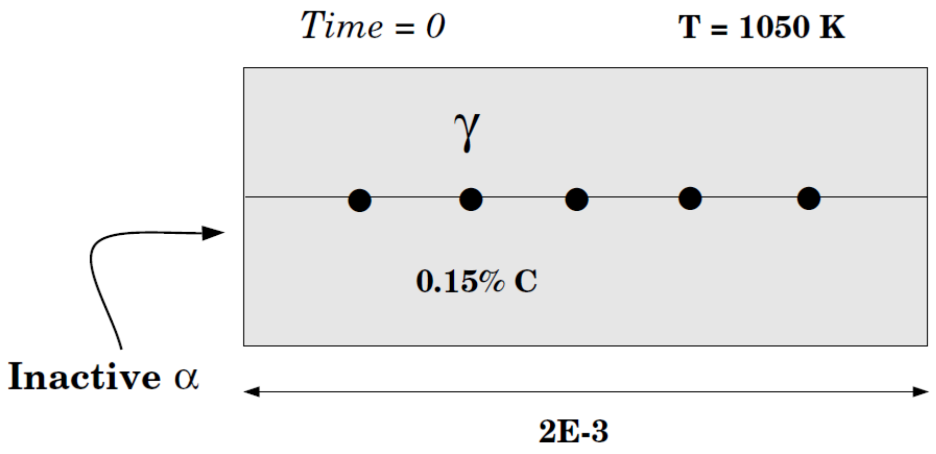


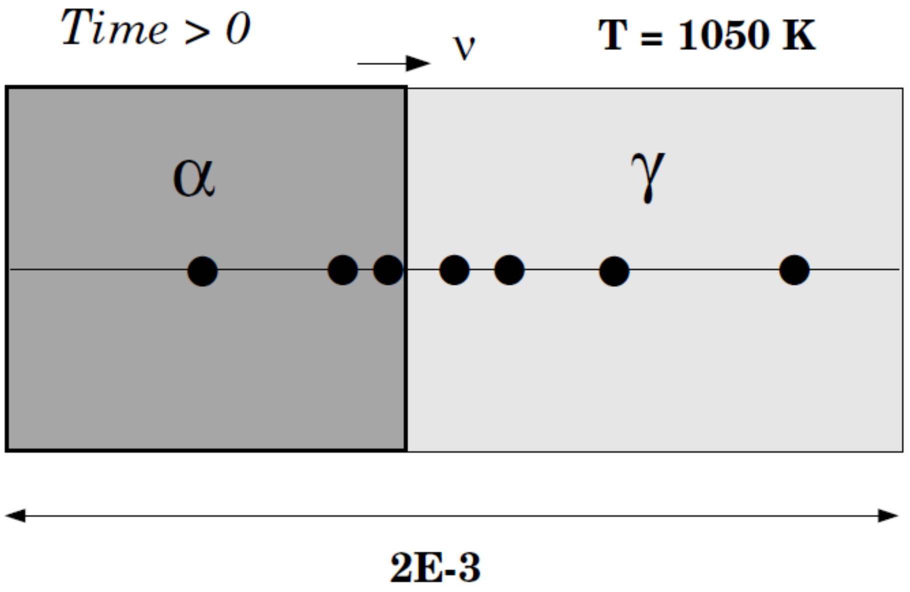


Example exb1b

Austenite (γ) to ferrite (α) transformation in a binary Fe-C alloy: Inactive α

This is the same example as in exb1a but now the problem is with ferrite as an inactive phase adjacent to the initial austenite.



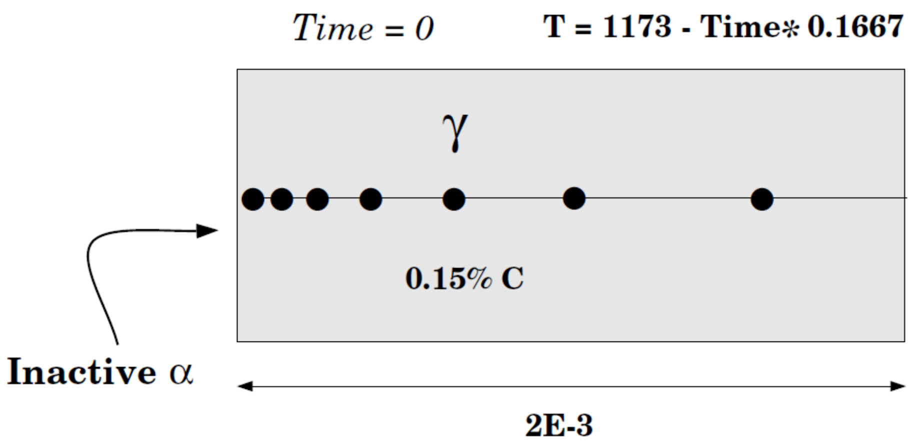


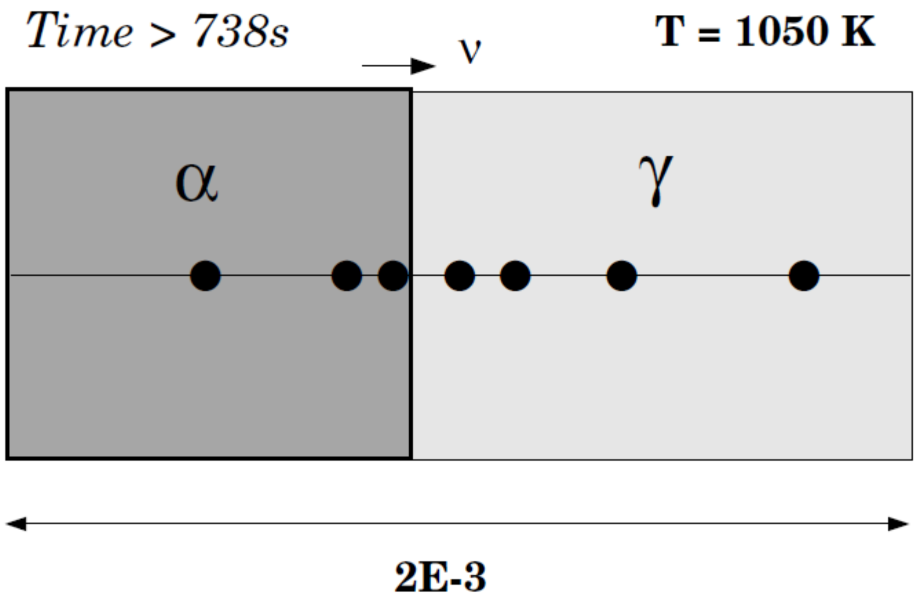
Example exb1c

Austenite (γ) to ferrite (α) transformation in a binary Fe-C alloy: Gradual cool down to 1050K

This is the same example as in exb1a and exb1b but now the simulation starts at a higher temperature and assumes a gradual cooling down to 1050 K.

When 1050 K is reached, the temperature is kept constant and thus has an isothermal transformation. As in exb1b, ferrite is in an inactive phase adjacent to the initial austenite.



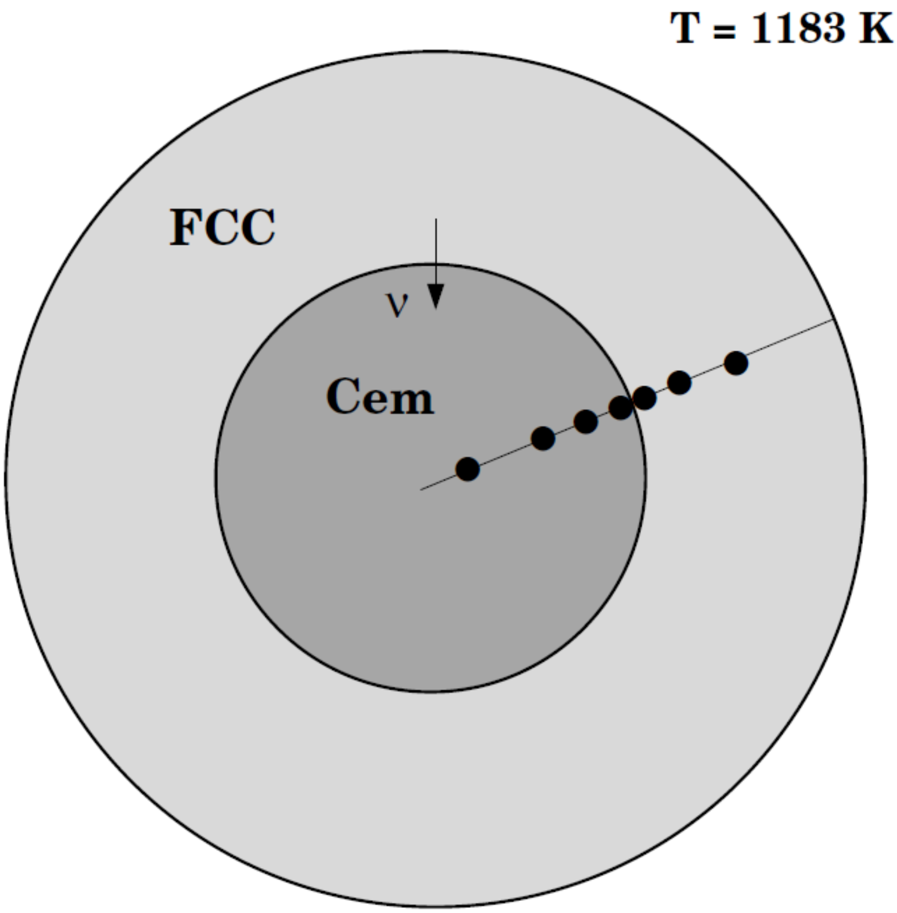


Example exb2

Cementite dissolution in an Fe-Cr-C alloy

This example calculates the dissolution of a spherical cementite particle in an austenite matrix. This case is from [1991Liu].

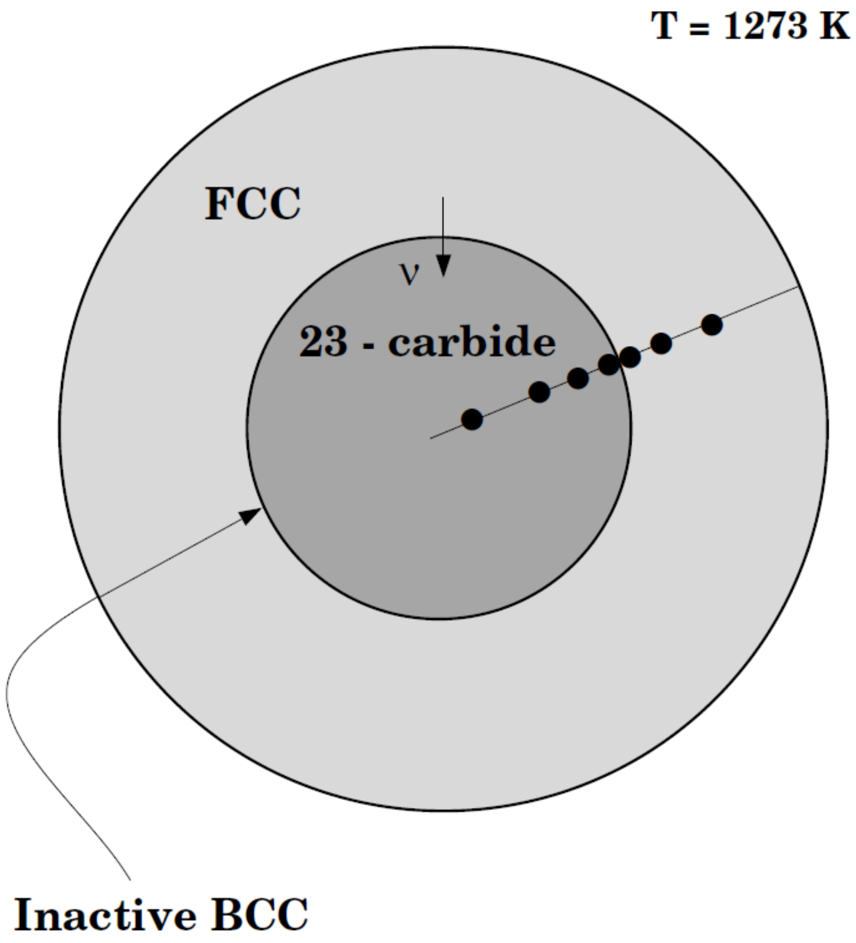
In order to achieve the correct average composition in the calculation it is necessary to take into account the fact that the calculation is set up using the volume fraction of the phases. To calculate the initial state at the heat treatment temperature we need first to determine the state at the normalizing temperature. To calculate the volume fraction of the phases we need to enter a number of functions that calculate these quantities.



Example exb3

Dissolution of 23-carbide in an austenitic matrix

This example calculates the dissolution of an M23C6 particle in an austenite matrix. A film of ferrite is allowed to nucleate around the carbide during the precipitation.

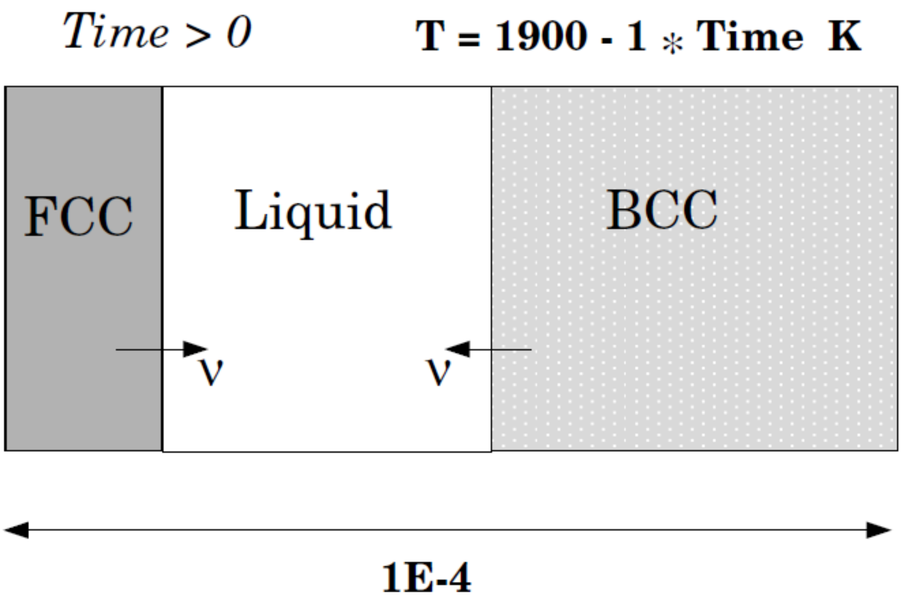


Example exb4a

Solidification path of an Fe-18%Cr-8%Ni alloy: Eutectic reaction

This example demonstrates the solidification path of an Fe-18%Cr-8%Ni alloy. A eutectic reaction is assumed, LIQUID -> BCC + FCC. Hence the BCC and FCC regions should be on separate sides of the liquid region. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both done in Thermo-Calc.

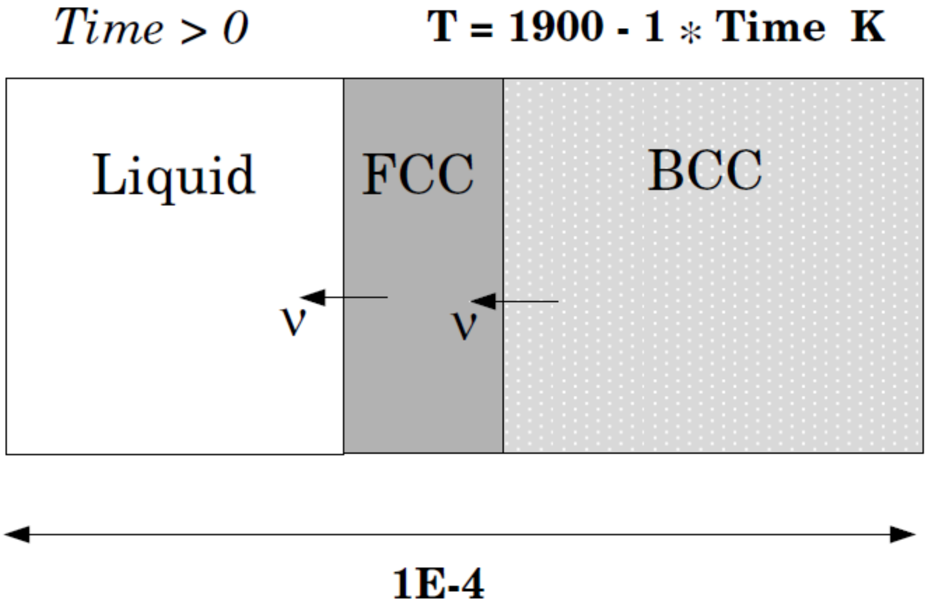
This example uses the TCFE and MOBFE databases. Licenses are required to run the example.



Example exb4b

Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction

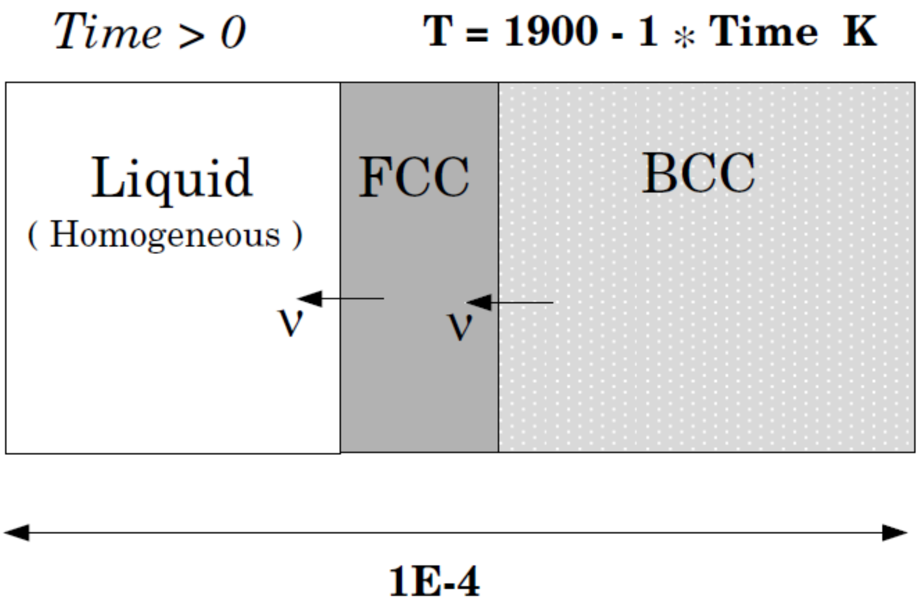
This example is the same as exb4a but now a peritectic reaction is assumed: LIQUID + BCC -> FCC. Hence the FCC region should appear in between the LIQUID and the BCC. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both done in Thermo-Calc.



Example exb4c

Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction, homogeneous liquid

This example is the same as exb4b but now the diffusivity data is amended for the LIQUID and a very high value for the diffusivity is used in order to simulate a case where we assume that the composition in the LIQUID is always homogeneous. This case should be considered less realistic than exb4b. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both done in Thermo-Calc.

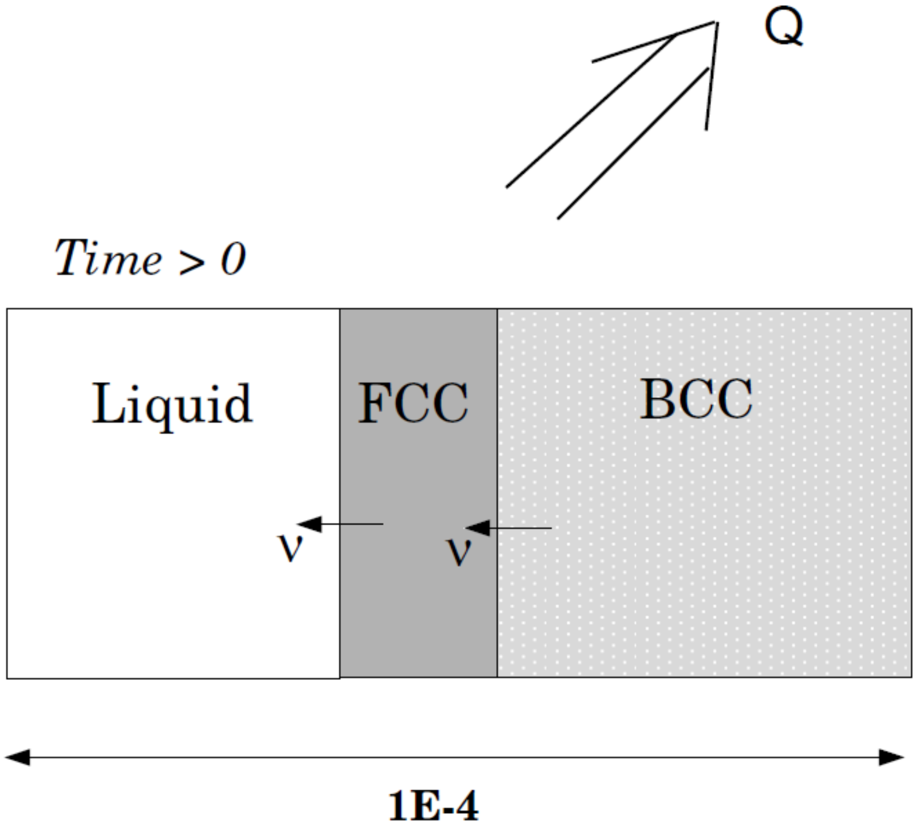


Example exb4d

Solidification path of an Fe-18%Cr-8%Ni alloy: Peritectic reaction, heat-flux controls the temperature

This example is the same as exb4b but instead of controlling the temperature the amount of heat extracted is given. Comparison is made with both a Scheil-Gulliver simulation and equilibrium solidification conditions, both done in Thermo-Calc.

> This example uses the FEDEMO and MOBFE2 database. A license is required for the MOBFE database to run the example.

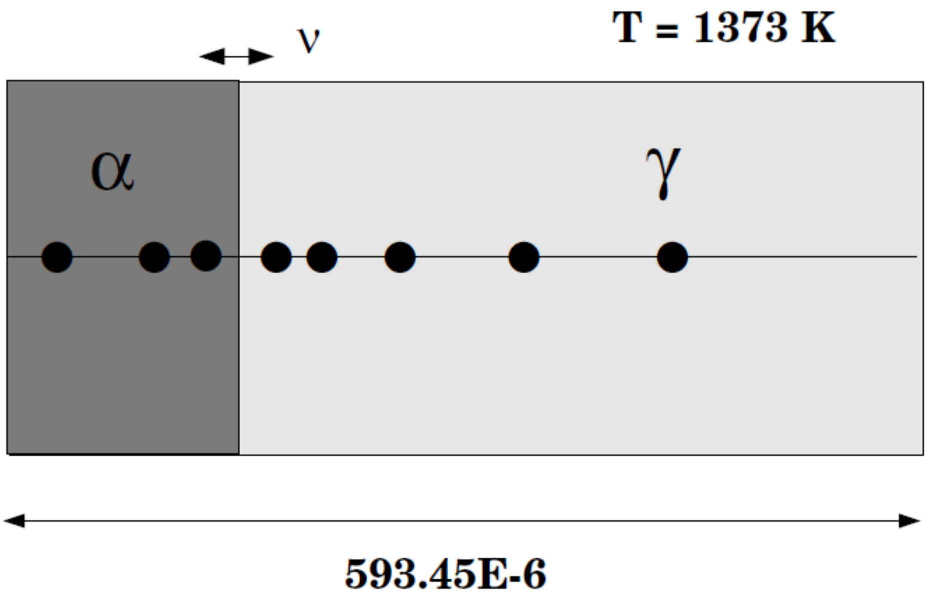


Example exb5

γ/α/γ Diffusion couple of Fe-Ni-Cr alloys

This example demonstrates the evaluation of a ternary Fe-Cr-Ni diffusion couple. A thin slice of α phase (38%Cr,0%Ni) is clamped between two thicker slices of γ phase (27%Cr, 20%Ni). The assembly is subsequently heat treated at 1373K.

This set up corresponds to diffusion couple in [1993Kaj-1]. Also see [1993Kaj-2].



Example exb6

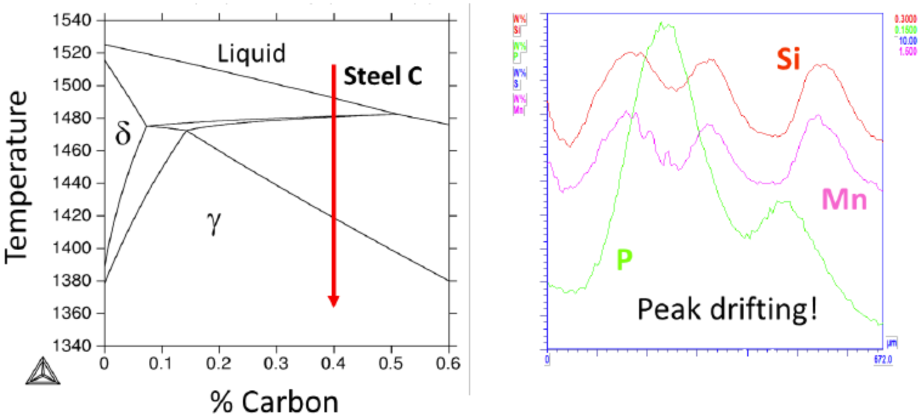
Microsegregation of phosphorus

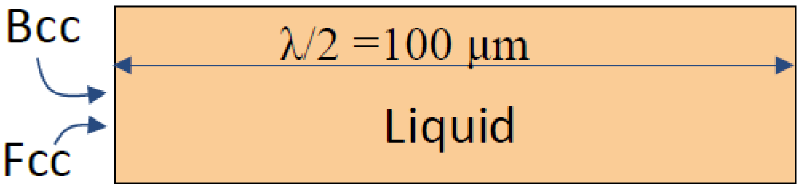
This example illustrates the effect of microsegregation of phosphorus during peritectic solidification in steel.

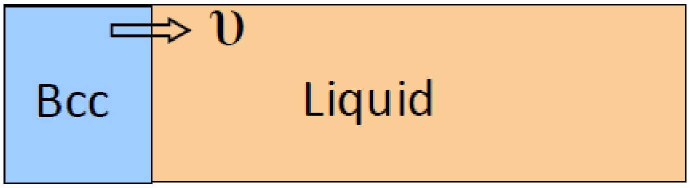
This example uses the TCFE and MOBFE databases. These licenses are required to run the example.

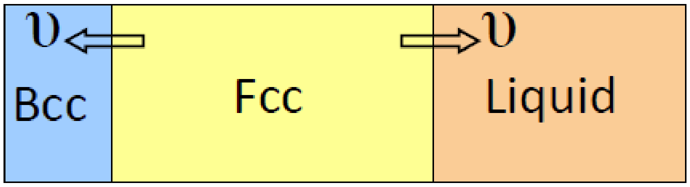
Steel C:

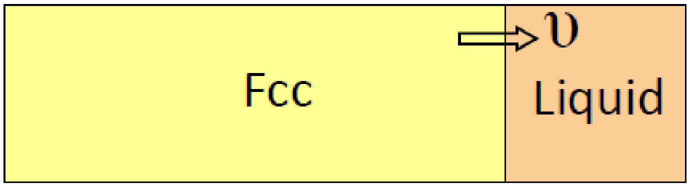
Fe - 0.8% Mn – 0.7%Si – 0.03%P – 0.4% C









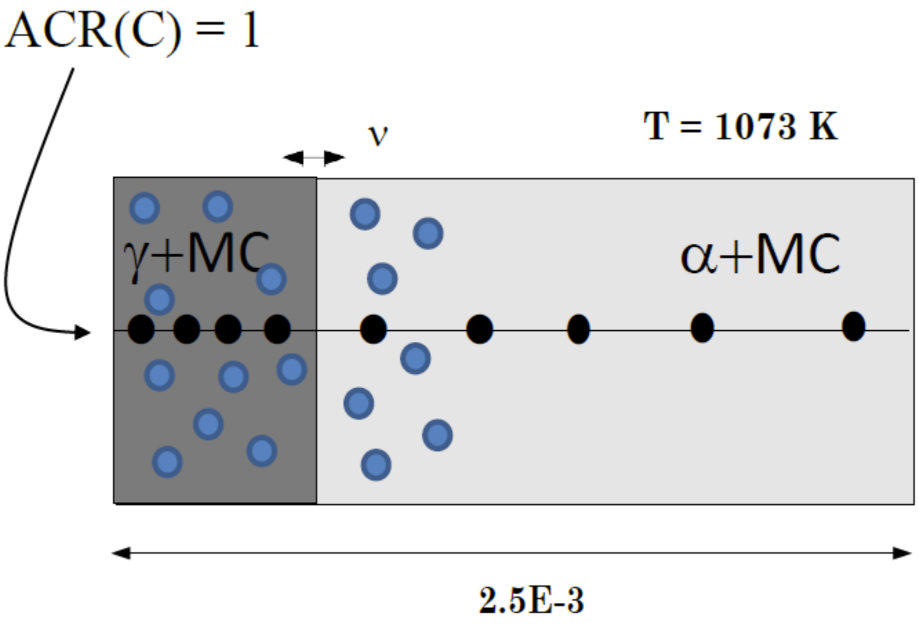


Example exb7

Moving boundary problem with multiple phases on each side of the boundary

This example shows how to enter dispersed phases on either side of a phase interface. The particular case shows how the kinetics of a ferrite to austenite transformation is affected by simultaneous precipitation of niobium carbide. The transformation is caused by carburization.

This example uses the TCFE, SSUB and MOBFE databases. These licenses are required to run the example.



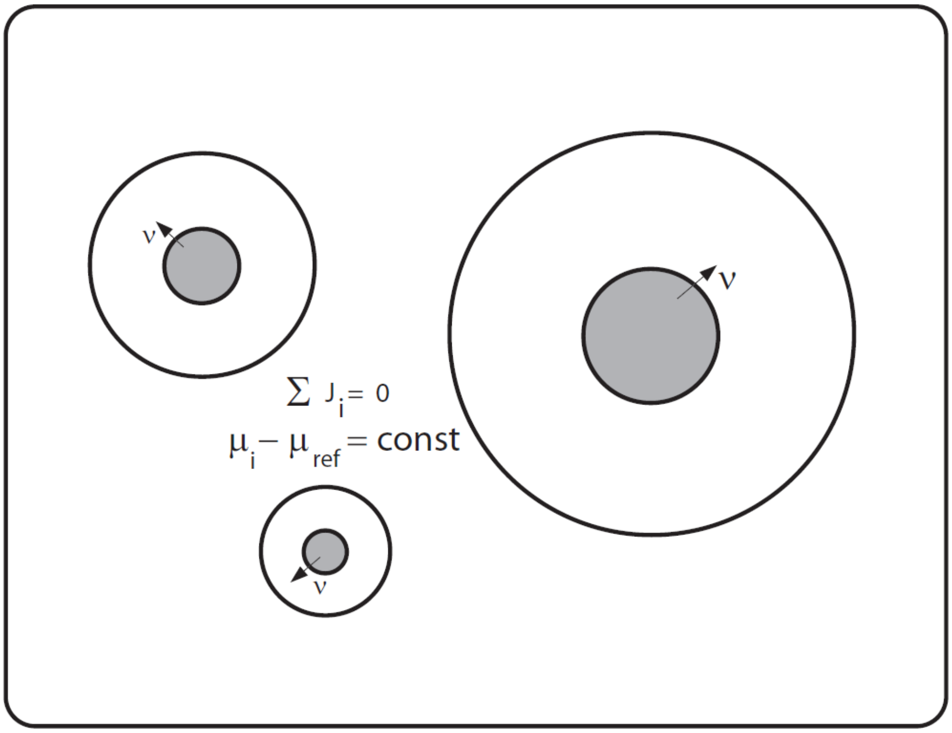
References

[1991Liu] Z.-K. Liu, L. Höglund, B. Jönsson, J. Ågren, An experimental and theoretical study of cementite dissolution in an Fe-Cr-C alloy. Metall. Trans. A 22, 1745–1752 (1991).

[1993Kaj-1] M. Kajihara, C.-B. Lim, M. Kikuchi, Experimental Study on Dissolution of ALPHA Phase in GAMMA/ALPHA/GAMMA Diffusion Couples of the Fe-Cr-Ni System. ISIJ Int. 33, 498–507 (1993).

[1993Kaj-2] M. Kajihara, M. Kikuchi, Numerical analysis of dissolution of α phase in γ/α/γ diffusion couples of the Fe-Cr-Ni system. Acta Metall. Mater. 41, 2045–2059 (1993).

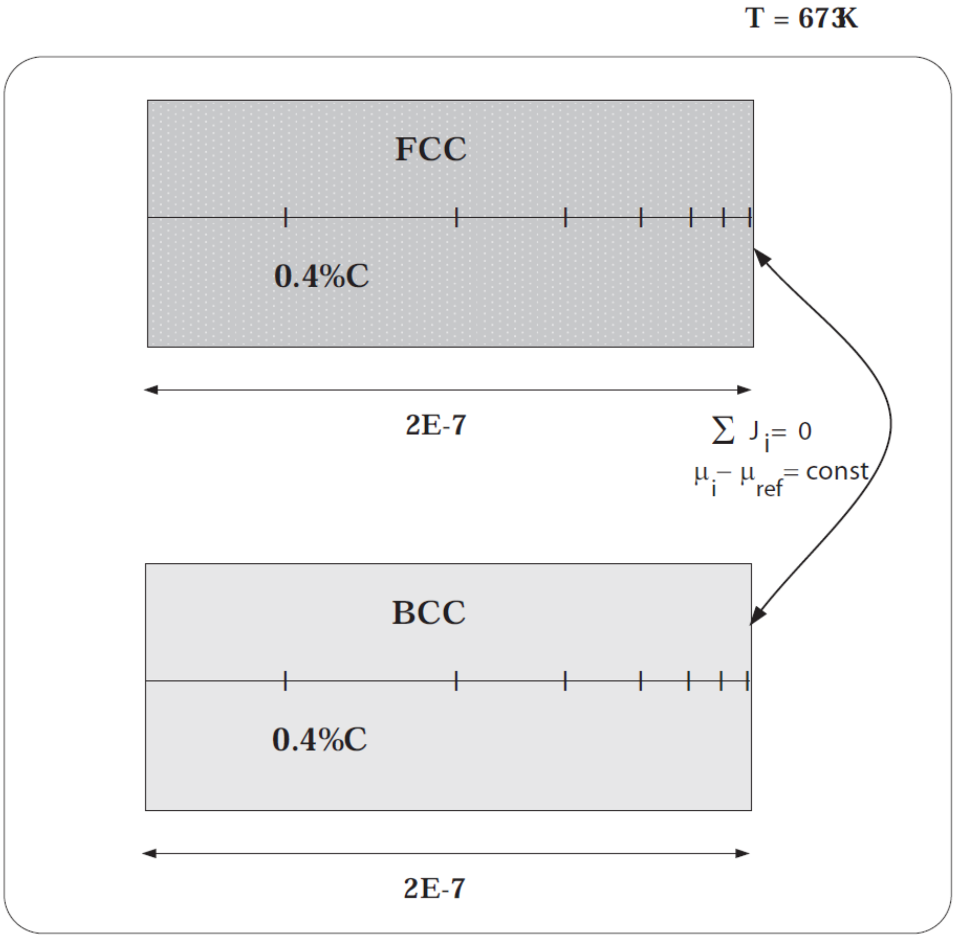
Cell Calculation Examples



Example exc1

Carbon cannon in ferrite/austenite (α/γ): Fe-C system, two-cell calculation

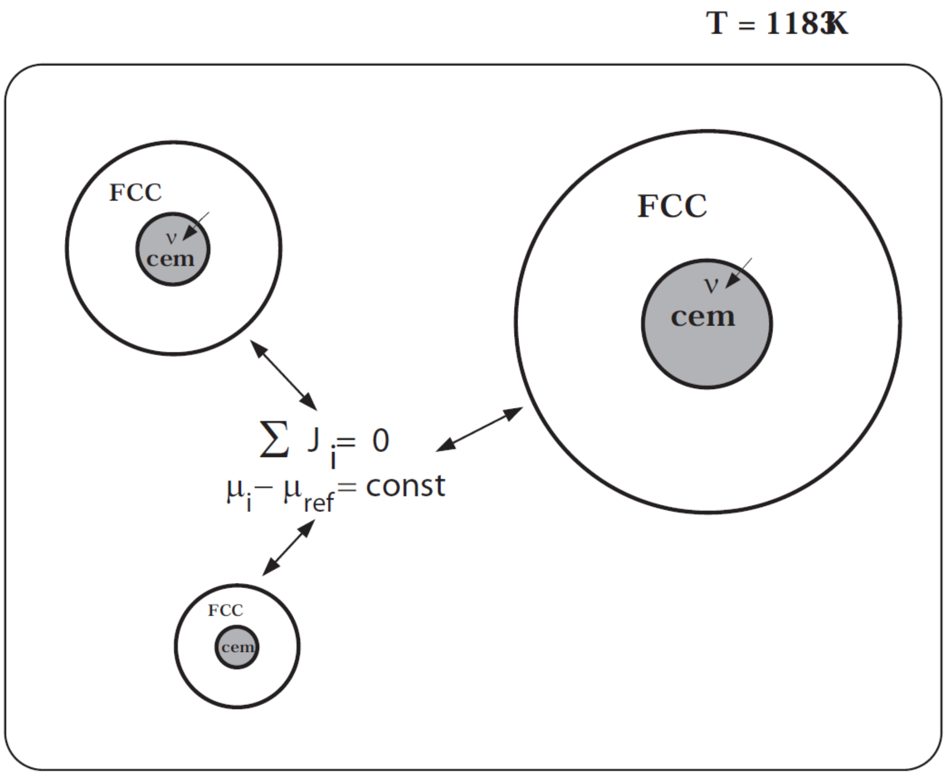
This example simulates what happens to a ferrite plate that has inherited the carbon content of its parent austenite. The ferrite plate formed is embedded in an austenite matrix. This setup corresponds to a proposed mechanism for formation of Widmannstätten ferrite or for the ferrite phase of the bainite structure. It is assumed that the phase boundary between ferrite and austenite is immobile, this is achieved in the simulation by putting the ferrite and the austenite in two different cells. Also see [1993Hil].



Example exc2

Cementite dissolution in an Fe-Cr-C alloy: Three particle sizes and three different cells

This example calculates the dissolution of cementite particles in an austenite matrix. This is the same as exc1 except that there are three particle sizes. Altogether six particles are considered using three different cells. This is to be able to represent some size distribution among the cementite particles. Also see [1991Liu].

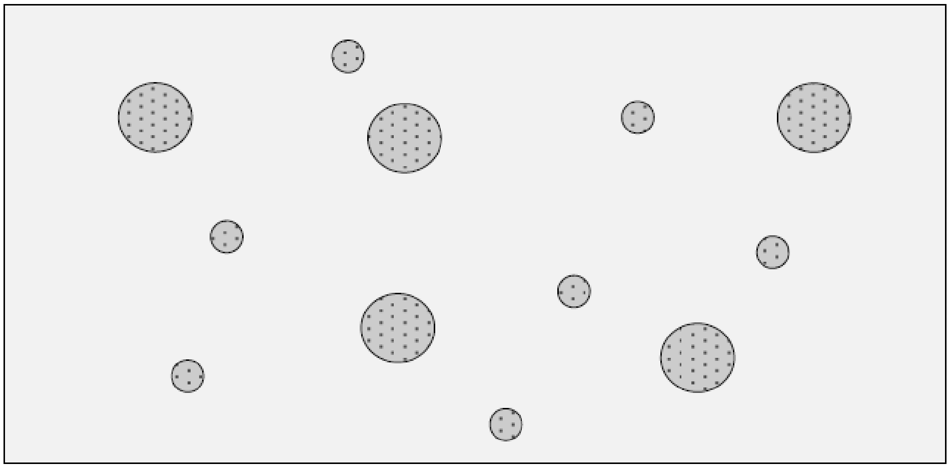


References

[1991Liu] Z.-K. Liu, L. Höglund, B. Jönsson, J. Ågren, An experimental and theoretical study of cementite dissolution in an Fe-Cr-C alloy. Metall. Trans. A 22, 1745–1752 (1991).

[1993Hil] M. Hillert, L. Höglund, J. Ågren, Escape of carbon from ferrite plates in austenite. Acta Metall. Mater. 41, 1951–1957 (1993).

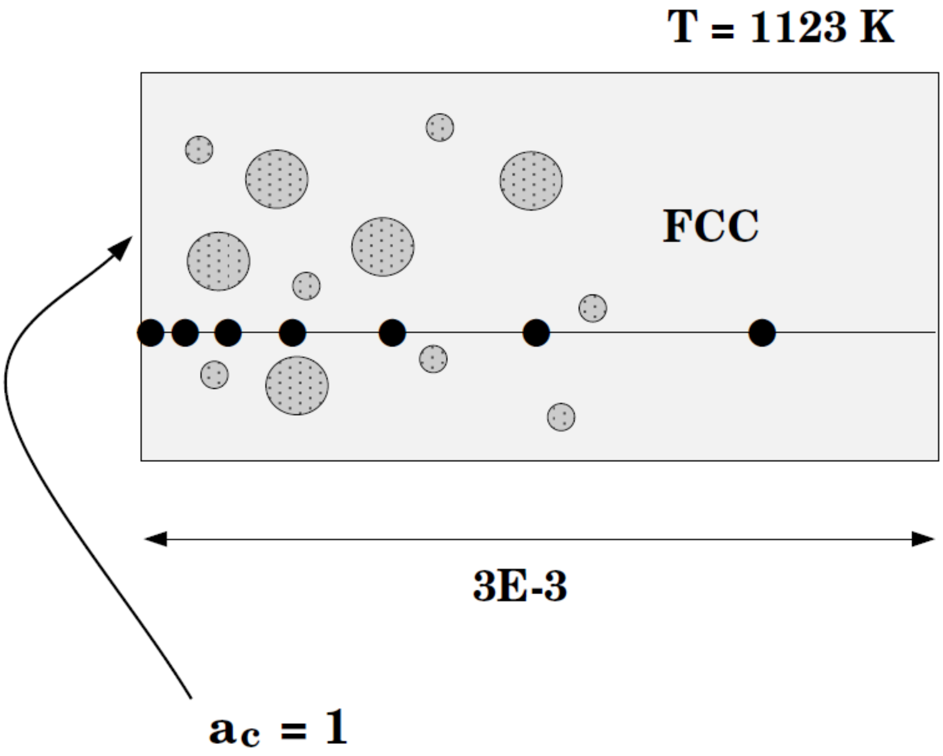
Diffusion in Dispersed Systems Examples



Example exd1a

Carburization of Ni-25%Cr alloy: Dispersed system model

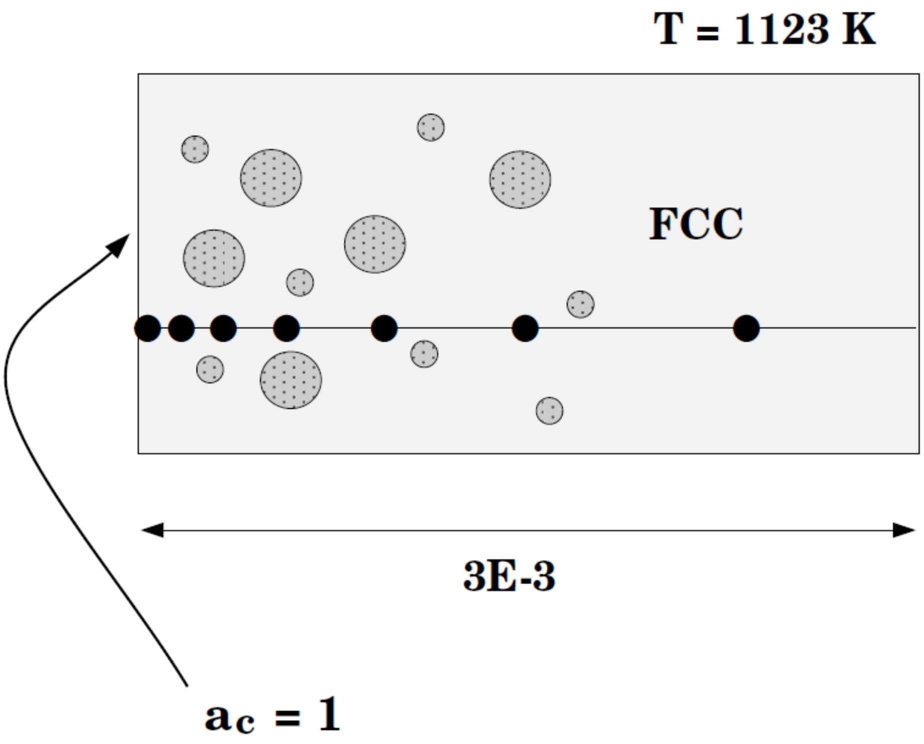
This example is about carburization of a Ni-25Cr alloy. In this case the M3C2 and M7C3 carbides are entered as spheroid phases in a FCC matrix. This simulation can be run with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL. In this example the DISPERSED SYSTEM MODEL is used. This case is from [1994Eng].



Example exd1b

Carburization of Ni-25%Cr alloy: Homogenization model

This example is about carburization of a Ni-25Cr alloy. In this case the M3C2 and M7C3 carbides are entered as spheroid phases in a FCC matrix. It is similar to exd1a except the default HOMOGENIZATION MODEL is used and then ENTER_HOMOGENIZATION_FUNCTION should be used instead of ENTER_LABYRINTH_FUNCTION. This case is from [1994Eng].

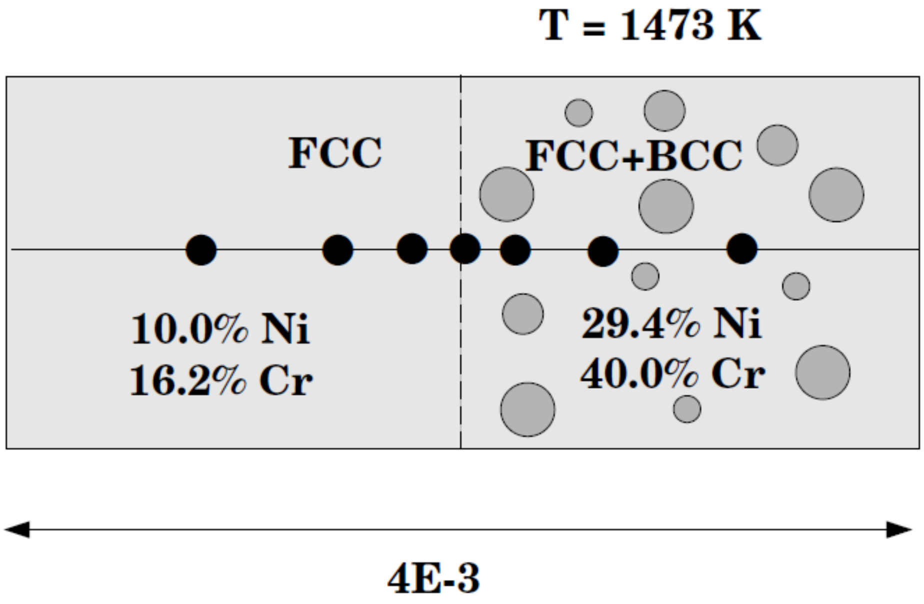


A modified version of this example is also available in Graphical Mode as example D_07. For Graphical Mode you do not need a Diffusion Module (DICTRA) license. You can open the example from Thermo-Calc when in Graphical Mode (**File →Examples Files → Diffusion Module**).

Example exd2a

Diffusion couple of Fe-Cr-Ni alloys: Dispersed system model

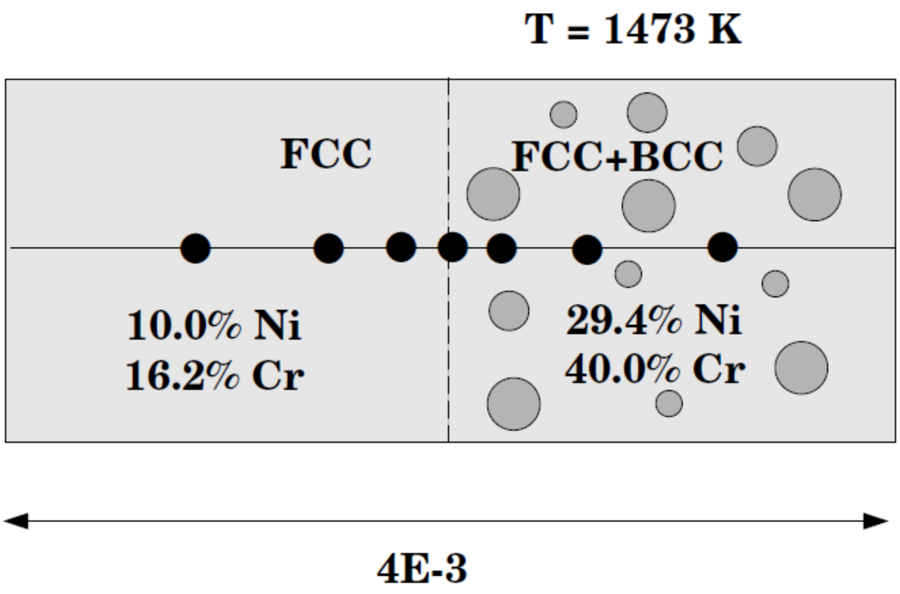
This example calculates the interdiffusion in a diffusion couple between a two-phase (FCC+BCC) and a single-phase (FCC) Fe-Ni-Cr alloy. Initially it has a step profile. This simulation can be run with either the DISPERSED SYSTEM MODEL or the HOMOGENIZATION MODEL. In this example the DISPERSED SYSTEM MODEL is used. This case is from [1995Eng].



Example exd2b

Diffusion couple of Fe-Cr-Ni alloys: Interdiffusion and the Homogenization Model

This example calculates the interdiffusion in a diffusion couple between a two-phase (FCC+BCC) and a single-phase (FCC) Fe-Ni-Cr alloy. Initially it has a step profile. It is similar to exd2a except the default HOMOGENIZATION MODEL is used and then ENTER_ HOMOGENIZATION_FUNCTION is used instead of ENTER_LABYRINTH_FUNCTION. This case is from [1995Eng].

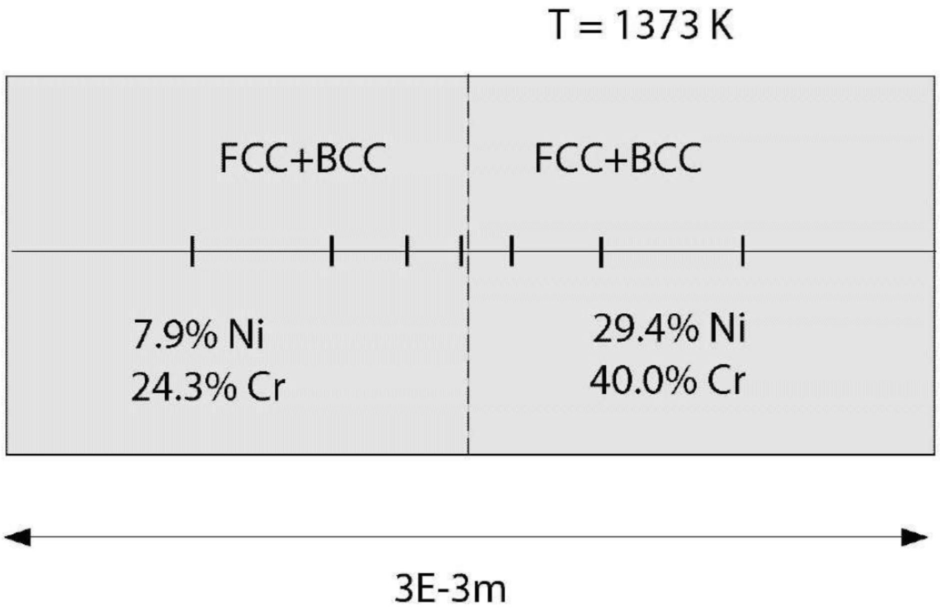


Example exd3

Diffusion couple of Fe-Cr-Ni alloys: Homogenization model

This example uses the homogenization model. It is taken from [2006Lar]. Experimental data is from[1995Eng].

The homogenization model can be used for multiphase simulations like the dispersed system model, but unlike the dispersed system model there is no need to have a single continuous matrix phase and, furthermore, there is no need to limit the size of time-steps. The set-up is performed in the same manner as for the dispersed system model, which means that a certain phase is entered as the matrix phase and the other phases are entered as spheroidal, but the choice of matrix phase does not affect the simulation.



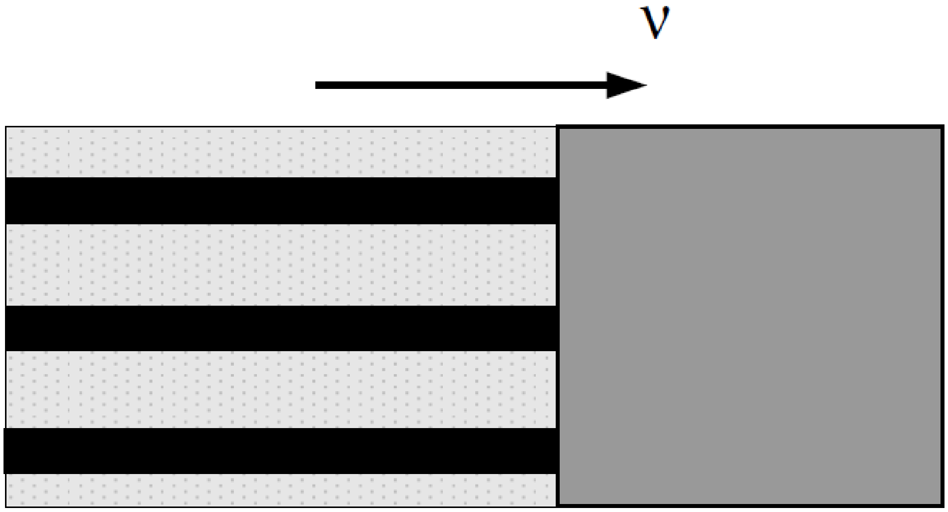
References

[1994Eng] A. Engström, L. Höglund, J. Ågren, Computer simulation of diffusion in multiphase systems. Metall. Mater. Trans. A 25, 1127–1134 (1994).

[1995Eng] A. Engström, L. Höglund, J. Ågren, Computer simulation of diffusion in multiphase systems. Metall. Mater. Trans. A 25, 1127–1134 (1994).

[2006Lar] H. Larsson, A. Engström, A homogenization approach to diffusion simulations applied to α+γ Fe–Cr–Ni diffusion couples. Acta Mater. 54, 2431–2439 (2006).

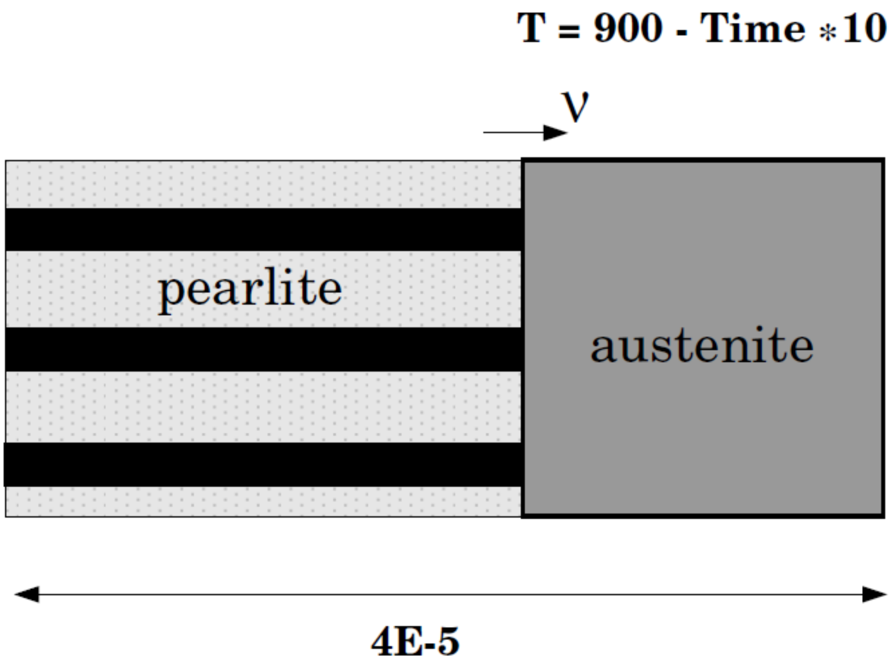
Cooperative Growth Example



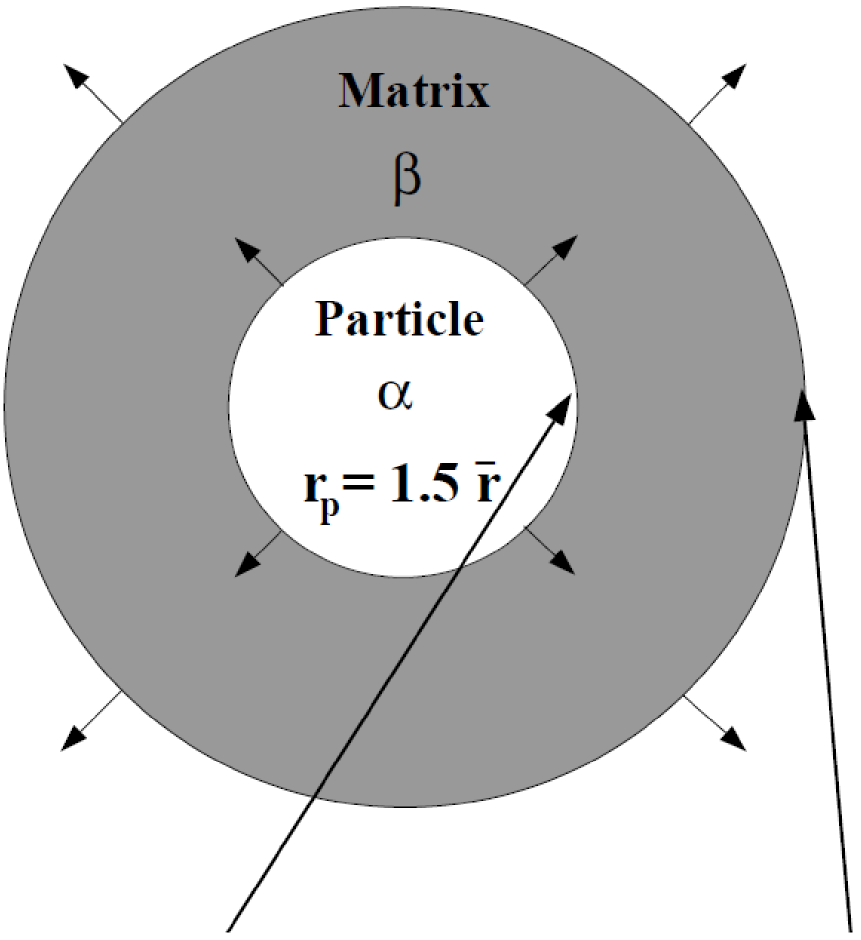
Example exe1

Growth of pearlite in an Fe-Mn-C alloy

This is an example of pearlite growth in an Fe-0.50wt%C-0.91wt%Mn steel.



Coarsening Example



Moving phase interface with α and β in local equilibrium.

$\frac{2\sigma V_m}{r}$ Interfacial energy contribution for α phase

Equilibrium as defined by the average composition in the system.

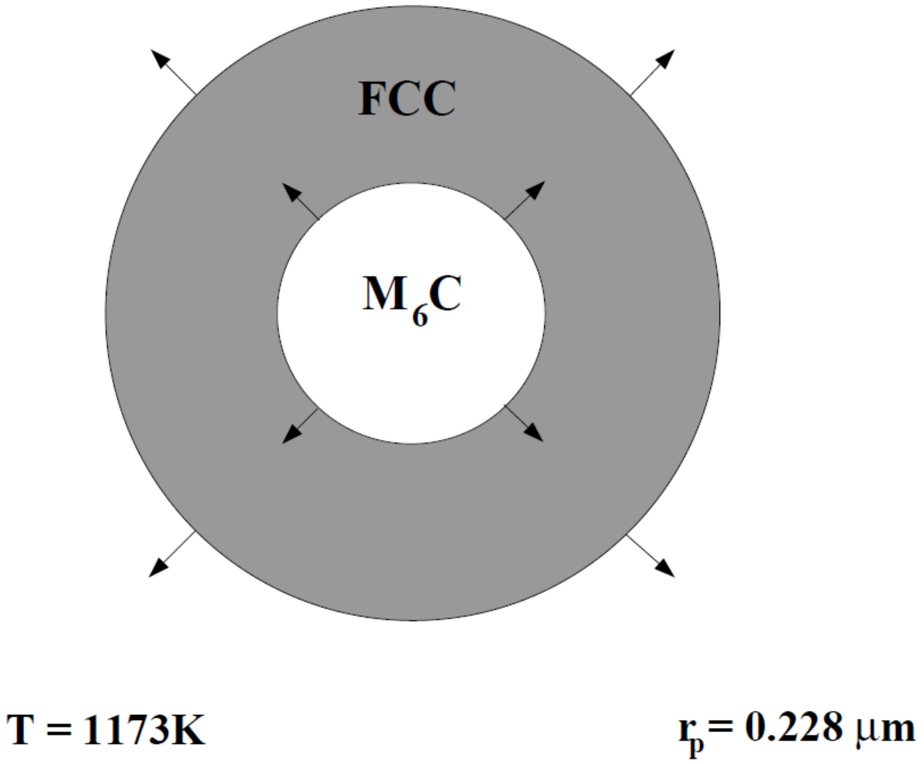
$\frac{2\sigma V_m}{r_p}$ Interfacial energy contribution for α phase

Example exf1

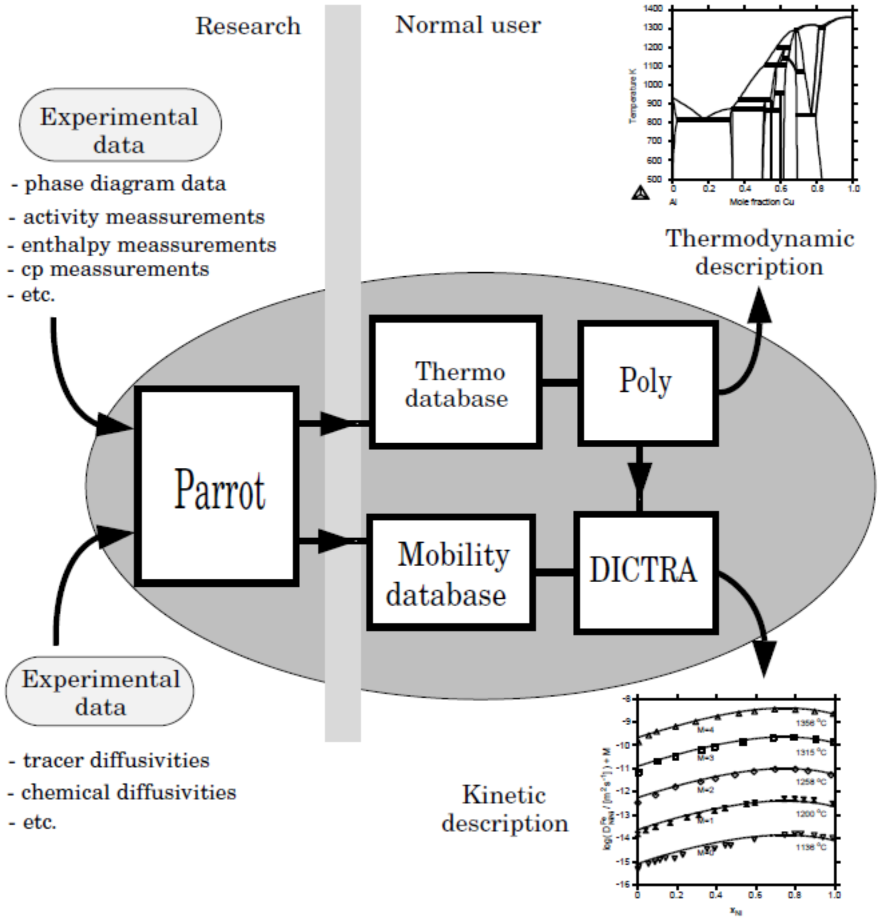
Coarsening of M6C precipitate in an Fe-Mo-C alloy

This example calculates the Ostwald-ripening of a spherical M6C carbide in an austenite matrix.

This example uses the TCFE and MOBFE databases. These licenses are required to run the example.



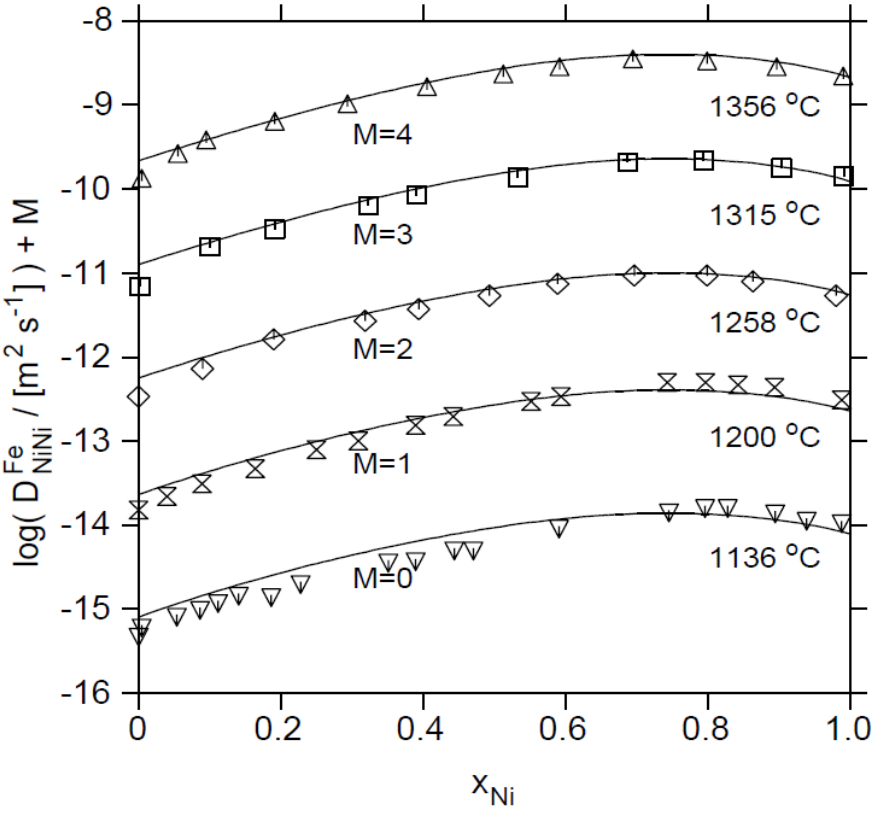
Kinetic Data Examples



Example exg1

Checking mobilities and diffusivities in an Fe-Ni alloy

This is an example file to check the mobilities and diffusivities in an Fe-Ni alloy.

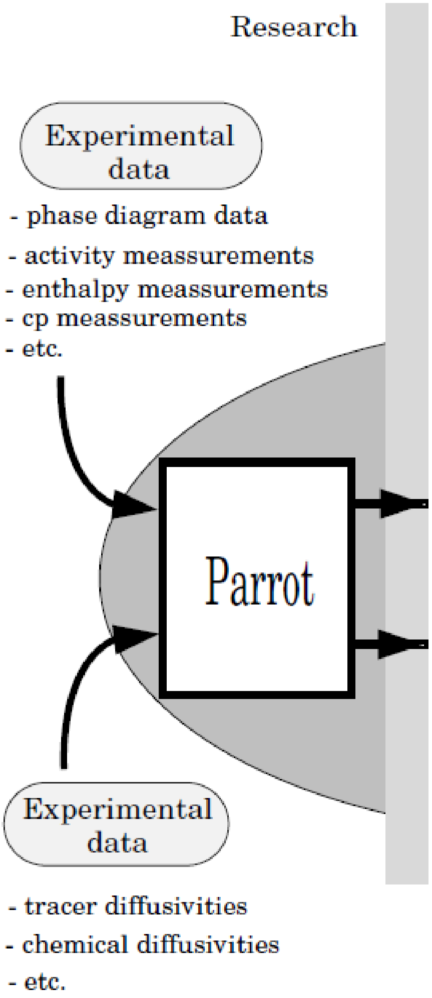


Example exg2

Optimization of mobilities in Ni-Al fcc alloys

A file for reading thermodynamic data and setting up the kinetic parameters that are needed for an optimization of the FCC phase in the binary Ni-Al system. Also see [1996Eng].

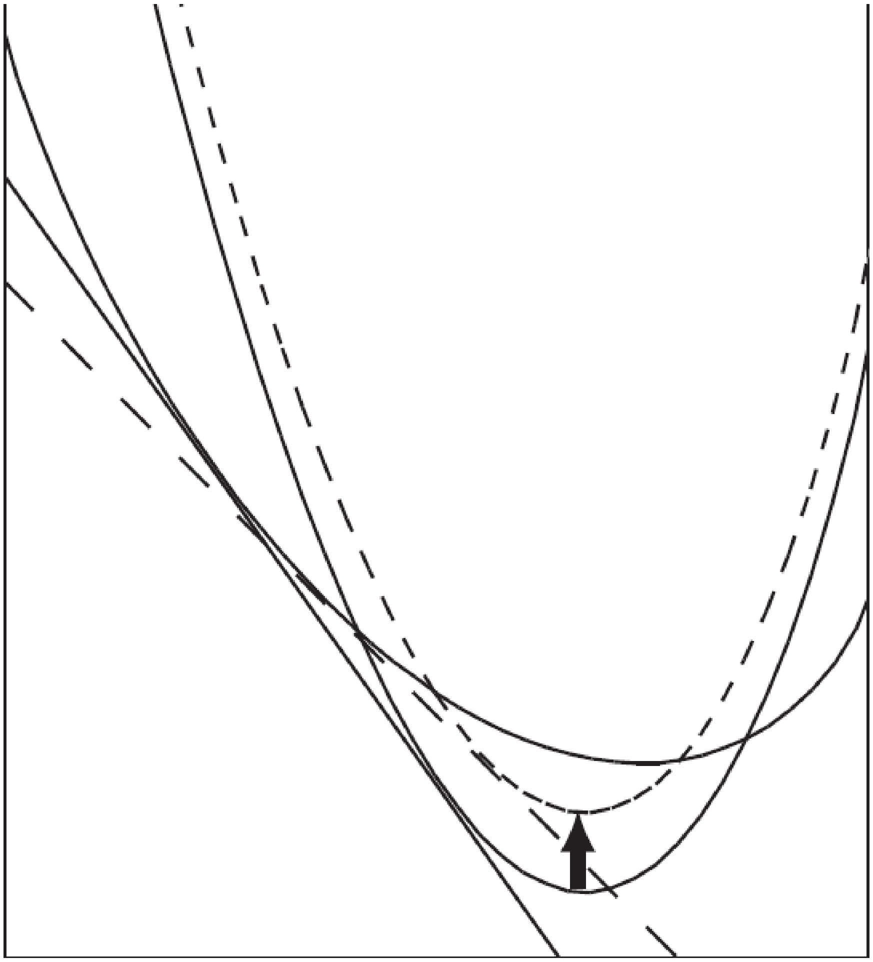
This example uses the MOB2 database. This license is required to run the example.



Reference

[1996Eng] A. Engström, J. Ä. Ägren, Assessment of Diffusional Mobilities in Face-centered Cubic Ni-Cr-Al Alloys. Int. J. Mater. Res. (Zeitschrift für Met. 87, 92–97 (1996).

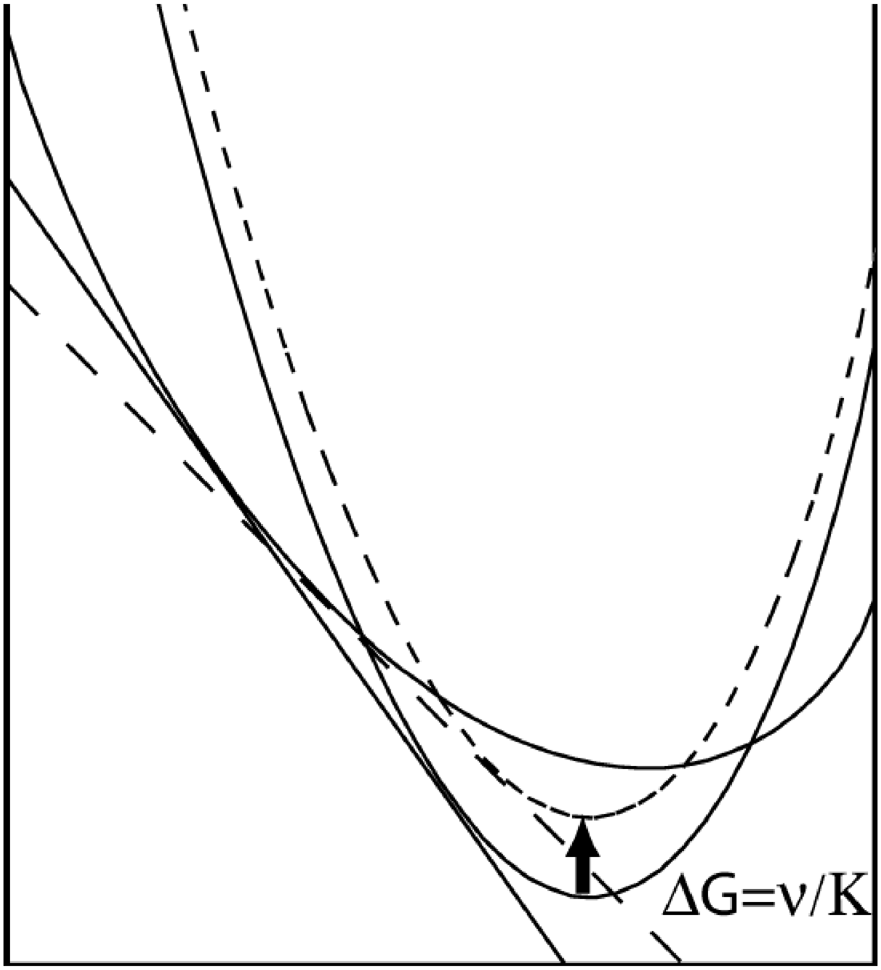
Deviation from Local Equilibrium Examples



Example exh1

Ferrite/austenite (α/γ) diffusion couple with interface mobility

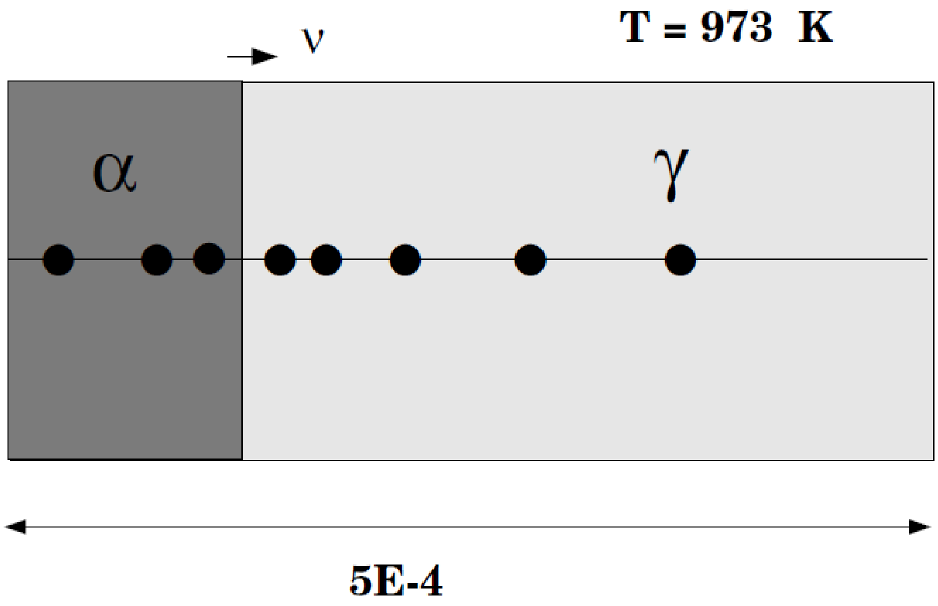
This example calculates the growth of ferrite (α) into austenite (γ) with a limited interface mobility. This is done by adding a Gibbs-energy contribution to the ferrite using the SET-SURFACE-ENERGY command.



Example exh2

Ferrite/austenite (α/γ) para-equilibrium in an Fe-Ni-C alloy

This example calculates the growth of ferrite (α) into austenite (γ) in an Fe-2.02%Ni-0.0885%C alloy using the para-equilibrium model. The results are compared with experimental information from Hutchinson, Fuchsmann, and Brechet [2004Fuc].

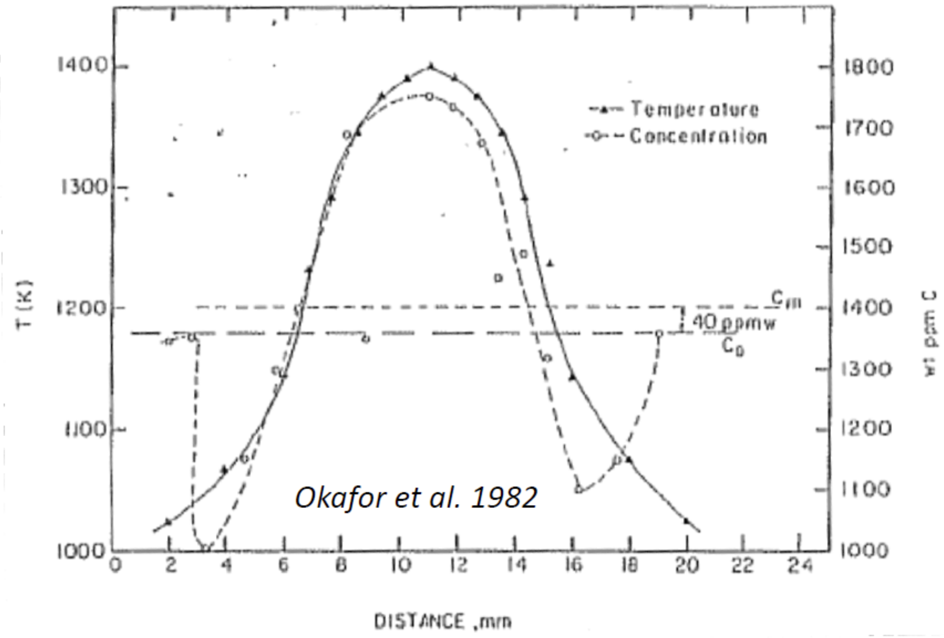


Example exh3

Diffusion induced by a temperature gradient (thermomigration)

This calculation shows how a temperature gradient induces diffusion.

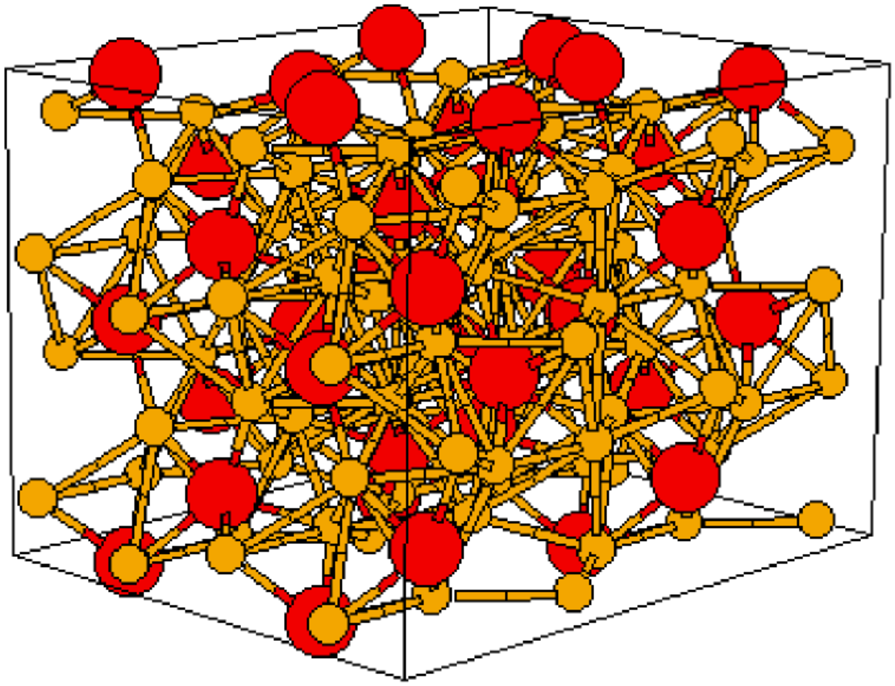
$$J_C = -\frac{u_C}{V_s} y_{Va} M_{CVa} \left(\frac{\partial \mu_C}{\partial x} + \frac{Q_C^*}{T} \frac{\partial T}{\partial x} \right)$$



Reference

[2004Fuc] C. R. Hutchinson, A. Fuchsmann, Y. Brechet, The diffusional formation of ferrite from austenite in Fe-C-Ni alloys. Metall. Mater. Trans. A 35, 1211–1221 (2004).

Diffusion in Complex Phases Examples



Example exi1

Diffusion in a system with B2 ordering

In this example folder, there is also a datafile `AlFeNi-data.TDB`, which contains both a thermodynamic and kinetic description for the ordered and disordered bcc.

Example exi2

Diffusion of carbon in cementite

This example demonstrates the use of the model for calculation of diffusion through a stoichiometric phase. The flux of a component in the stoichiometric phase is assumed to be proportional to the difference in chemical potential at each side of the stoichiometric phase multiplied with the mobility for the component in the phase. The mobility is assessed from experimental information and is basically the tracer diffusivity for the component.

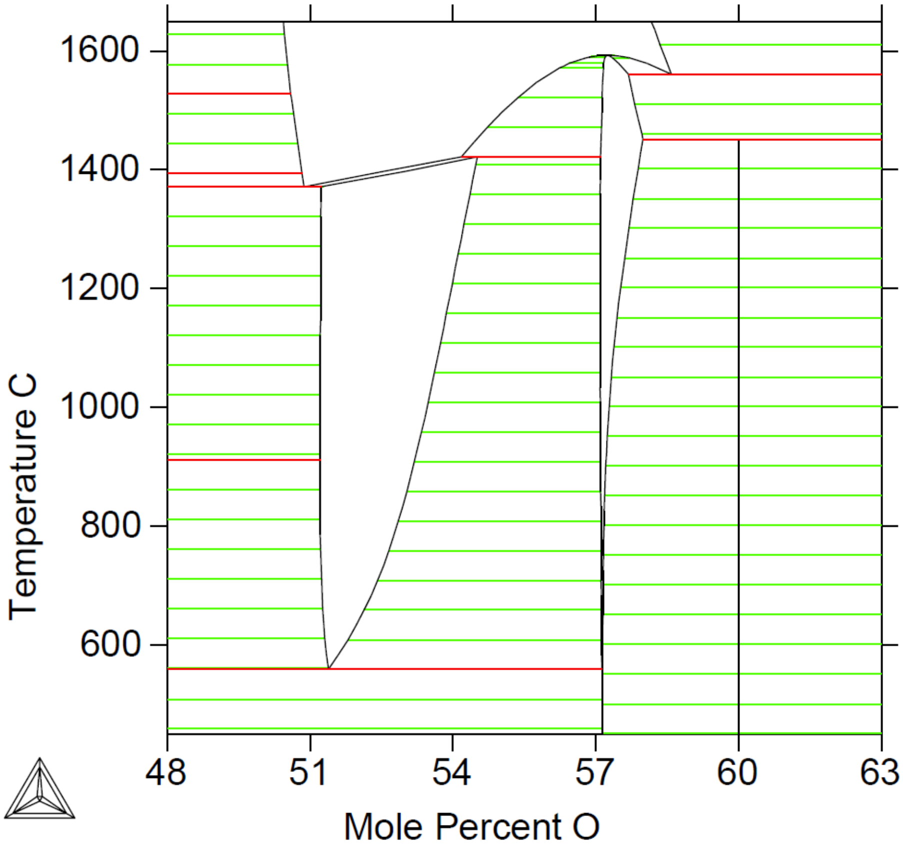
This calculation is compared with experimental data where a sample of pure iron has been exposed to a gas atmosphere with a certain carbon activity. The weight gain is then measured as a function of time. The experimental data is obtained from [1982Ozt].

$J \sim \Delta\mu$

Example exi3a

Diffusion in iron oxide (FeO)

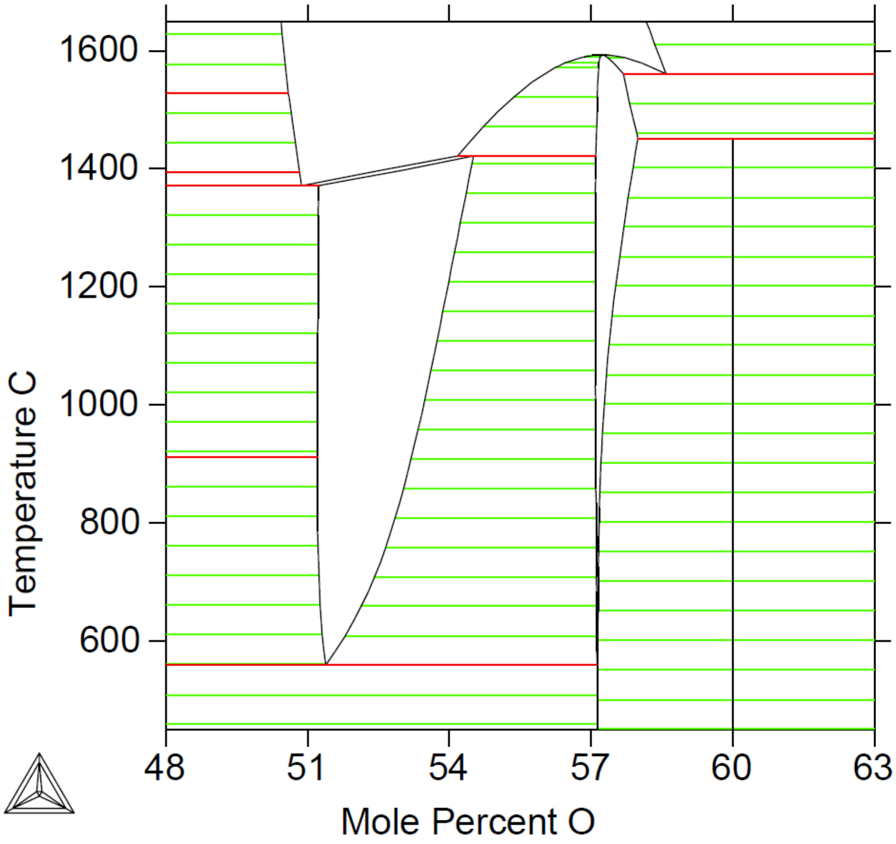
This example shows the oxidation of an iron sample and the consequent growth of an oxide layer.



Example exi3b

Diffusion in iron oxide (FeO) with a grain boundary contribution

This example shows the oxidation of an iron sample and the consequent growth of an oxide layer using the grain boundary diffusion contribution model.



Reference

[1982Ozt] B. Ozturk, V. L. Fearing, J. A. Ruth, G. Simkovich, Self-Diffusion Coefficients of Carbon in Fe3C at 723 K via the Kinetics of Formation of This Compound. Metall. Trans. A 13, 1871–1873 (1982).

Diffusion Module (DICTRA) Quick Start Guide - Graphical Mode

Thermo-Calc Version 2025b

Introduction to the Diffusion Module (DICTRA)

The Diffusion Module (DICTRA) is an Add-on Module to the Thermo-Calc software package. It is used for simulation of diffusion controlled transformations in multicomponent systems. The simulations are both time- and space-dependent.

The Diffusion Module (DICTRA) is suitable for solving diffusion problems that include a moving boundary (so-called *Stefan problems*). The multicomponent diffusion equations in the various regions of a material are solved under the assumption that thermodynamic equilibrium holds locally at all phase interfaces. The concentration fields only vary along one spatial coordinate, but the geometry may be either planar, cylindrical or spherical.

In this section:

About this Quick Start Guide

The following introduces you to the basic concepts, steps and theory to start using the Diffusion Module (DICTRA). An understanding of this information is necessary to ensure accurate calculations.

More details about the use of DICTRA can be found in [2002And] and [2000Bor].

If you are not familiar with Graphical Mode, it is recommended you review the documentation and additional resources available on our website.

The Role of Diffusion in Materials: A Tutorial is available for download on our website. It is intended for engineers interested in using the Diffusion Module (DICTRA), as well as students learning about the role of diffusion in materials. It is designed to be useful at many levels, from undergraduate studies to someone with a PhD and experience in a related field.

References

[2000Bor] A. Borgenstam, L. Höglund, J. Ågren, A. Engström, DICTRA, a tool for simulation of diffusional transformations in alloys. J. Phase Equilibria 21, 269–280 (2000).

[2002And] J.-O. Andersson, T. Helander, L. Höglund, P. Shi, B. Sundman, Thermo-Calc & DICTRA, computational tools for materials science. Calphad 26, 273–312 (2002).

Diffusion Module Terminology in Graphical Mode

The following definitions are useful to help you understand the examples in this guide. For more detailed information search or browse the online help (press F1 or from the main menu select **Help → Online Help**).

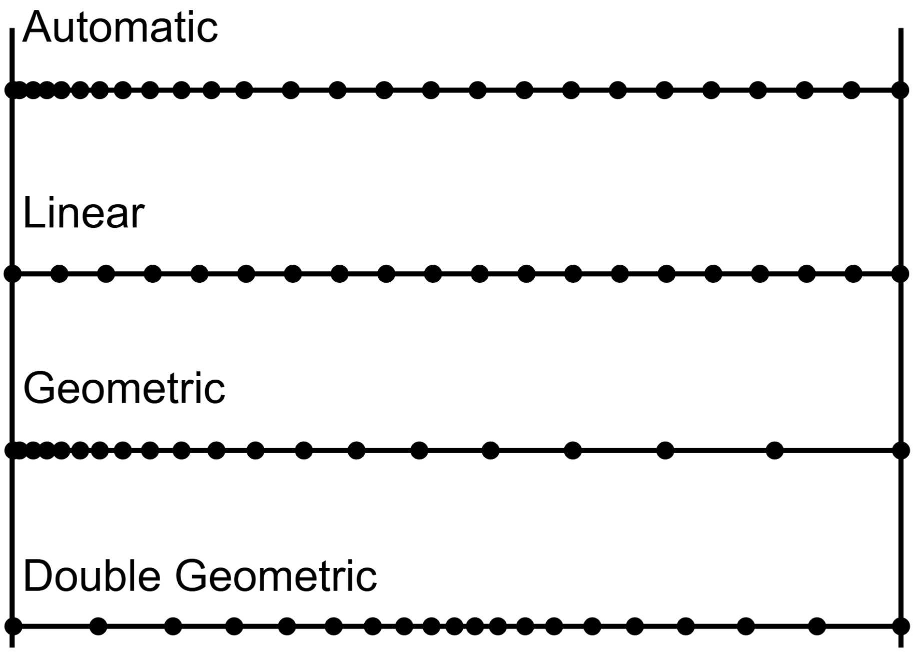
These terms are specific to working in Graphical Mode. The overall simulation in Console Mode is comparable but there are some differences in terminology and functionality.

Region

In Graphical Mode, a system consists of one *cell* with one or multiple *regions* in which the diffusion problem is to be solved.

Grid Types

These grid types are used in diffusion simulations: automatic, linear, geometric, and double geometric. When you are setting up the simulation, in either Console Mode or Graphical Mode, a region must have a grid defined.



Phases

Each region must contain at least one *phase*. The so-called *homogenization model* is used if multiple phases are added inside a region, then the average properties of the local phase mixture is used. Phase(s) can also be added to interphases of region(s) and then only participate in the simulation if the driving force for precipitation of the phase exceeds a predefined value. A new region is then created where the name of the region is set to the name of the phase but with `R_` added as a prefix.

Composition

These types of composition variables are used in the configuration of the Diffusion Calculator: *mass (weight) fraction*, *mass (weight) percent*, *mole fraction*, or *mole percent*.

The *u-fractions* are used in the diffusion equations. The u-fraction of a component *k* is defined as

$$\mu_k = \frac{x_k}{\sum\limits_{j \in S} x_j}$$

The summation is only performed over the substitutional elements. The choice of the volume fixed frame of reference in the calculations make it convenient to use a composition variable which is related to the volume. The definition of the u-fraction is based upon the assumption that a species may or may not contribute to the volume of a phase. An interstitial element is assumed to not contribute to the volume. Substitutional elements are assumed to contribute equally to volume. Weight fraction, mole fraction or u-fraction can be used when plotting the results from a simulation.

Geometry and Coordinates

The Diffusion Module (DICTRA) can only handle diffusion problems where compositions vary along one spatial coordinate. The geometry of your system can be *planar*, *cylindrical*, or *spherical*.

The *planar* geometry corresponds to an infinitely wide plate of a certain thickness. If the system has a planar geometry then the lower boundary (the zero coordinate) is at the left side of the system. The upper boundary (the coordinate with the highest value) is at the right side of the system.

Boundary Conditions

Boundary conditions are conditions that define how matter behaves at the boundaries of your system. By default, matter is not allowed to cross the system boundaries.

You can change the setting for both the lower boundary (left side/centre) and the upper boundary (right side/surface) of the system.

Setting up a Diffusion Simulation in Graphical Mode

When you are using the Graphical Mode version of the Diffusion Module (DICTRA), the steps to set up a simulation are a combination of adding *Activity* nodes (the System Definer, Diffusion Calculator, and Plot Renderer) and then defining the applicable settings for each of these nodes in a Configuration window.

The following is a general overview of the steps to set up the simulation.

1. Use the **Diffusion** template to add the System Definer, Diffusion Calculator, and Plot Renderer activity nodes.
2. On the **System Definer**, you select the thermodynamic and kinetic databases, add elements and phases, and generally define the system.
3. On the **Diffusion Calculator**, you set the geometry (by default the geometry is planar), add region(s) and enter grid(s) and phase(s) in the region(s). You then enter composition(s) of phase(s).
4. On the **Plot Renderer** or **Table Renderer**, you choose how to visualize your diagrams, and then run the simulation, i.e. you **Perform** the sequence of nodes you have defined in the tree to produce the output simulation.

Single Phase Simulations

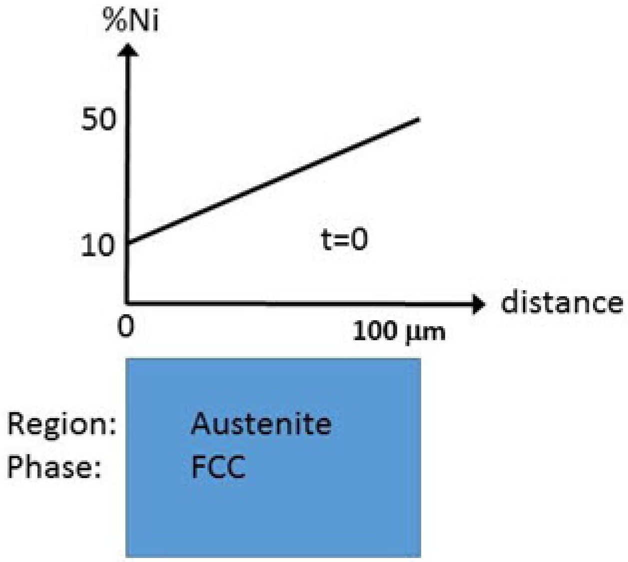
In this section:

About the Single Phase Simulation

In a 100 µm wide planar domain, the single phase example simulates the diffusion of Fe and Ni at a temperature of 1400 K. At this temperature the material is fully austenitic, i.e. the only phase present is the so-called fcc (face centered cubic) phase (in Thermo-Calc the name of this phase is FCC_A1). Initially, there is a linear variation in Ni going from 10 mass-% on the left-hand side to 50 mass-% on the right-hand side.

The simulation time is slightly different between the modes. For Console Mode it is 10^5 s and for Graphical Mode it is 30 hours.

By default the boundaries are closed. The plot generated shows the initial and final Ni profile.



Schematic view of the initial state of Single Phase Diffusion example. The width of the domain is 100 µm and there is a linear gradient in composition going from 10 to 50 mass-% Ni. There is a single region named Austenite that consists of an fcc phase.

Theory for the Single Phase Simulation

The flux of a component k in the z-direction in an isobarothermal system is in general given by

$$J_k = \sum_{i=1}^{n} L_{ki} \frac{\partial \mu_i}{\partial z}$$

where L_{ki} is a matrix of kinetic coefficients and μ_i is the chemical potential of component i. The correlation effects, i.e. the coupling of the flux of k component to the chemical potential gradients of the other elements, are normally neglected

$$(L_{ki} = 0, k \neq i)$$

and thus

$$J_k = L_{kk} \frac{\partial \mu_k}{\partial z} = M_k c_k \frac{\partial \mu_k}{\partial z}$$

where c_k is the concentration and M_k the mobility of component k.

The equation for the flux is combined with the equation of continuity, which takes the following form in a planar domain,

$$\frac{\partial c_k}{\partial t} = \frac{\partial}{\partial z}(-J_k)$$

which relates the local evolution of the concentration of k to the divergence of the flux.

The expression for the flux can be expanded in terms of concentration gradients

$$J_k = -\sum_{i=1}^{n} M_k c_k \frac{\partial \mu_k}{\partial c_j} \frac{\partial c_j}{\partial z} = -\sum_{i=1}^{n} D_{kj} \frac{\partial c_j}{\partial z}$$

where the diffusion coefficient of component k with respect to the concentration gradient of component j has been introduced.

$$D_{kj} = M_k c_k \frac{\partial \mu_k}{\partial c_j}$$

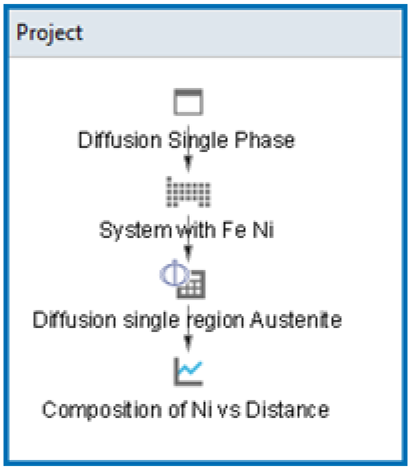
The flux expressions above are given in the so-called lattice-fixed frame of reference. In practical calculations it is more common to use a volume-fixed frame of reference. For a discussion of these concepts, see Andersson and Ågren [1992And].

References

Setting Up the Single Phase Simulation

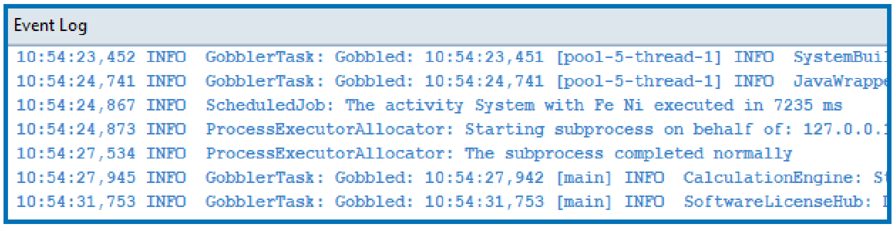
For the single phase example, you can open the example project file included with your installation to first see how it is set up:

1. Open Thermo-Calc.
2. There are different ways to access the examples.
    - From the main menu, select **File →** or **Help → Examples Files**. The Graphical Mode folder opens by default.
    - Click the **My Project** node and on the **Configuration** window under **Getting Started**, click **Example Files**.
3. Click to open the **Diffusion Module - DICTRA** folder and locate the **D_01_Diffusion_Single_Phase.tcu** file. Double-click to open it.
4. The project opens in Thermo-Calc and adds this tree structure:



5. Click the top Project node (renamed to *Diffusion Single Phase*). At the bottom of the **Configuration** window click **Perform Tree**. You can also right-click the node and select **Perform Now**.

   The **Event Log** shows the progress of the calculations:



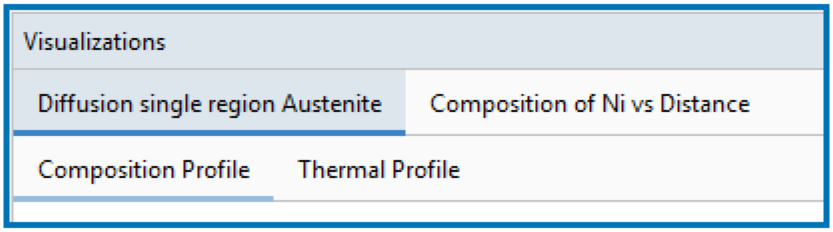
```
10:54:23,452 INFO  GobblerTask: Gobbled: 10:54:23,451 [pool-5-thread-1] INFO  SystemBui
10:54:24,741 INFO  GobblerTask: Gobbled: 10:54:24,741 [pool-5-thread-1] INFO  JavaWrapp
10:54:24,867 INFO  ScheduledJob: The activity System with Fe Ni executed in 7235 ms
10:54:24,873 INFO  ProcessExecutorAllocator: Starting subprocess on behalf of: 127.0.0.
10:54:27,534 INFO  ProcessExecutorAllocator: The subprocess completed normally
10:54:27,945 INFO  GobblerTask: Gobbled: 10:54:27,942 [main] INFO  CalculationEngine: S
10:54:31,753 INFO  GobblerTask: Gobbled: 10:54:31,753 [main] INFO  SoftwareLicenseHub:
```

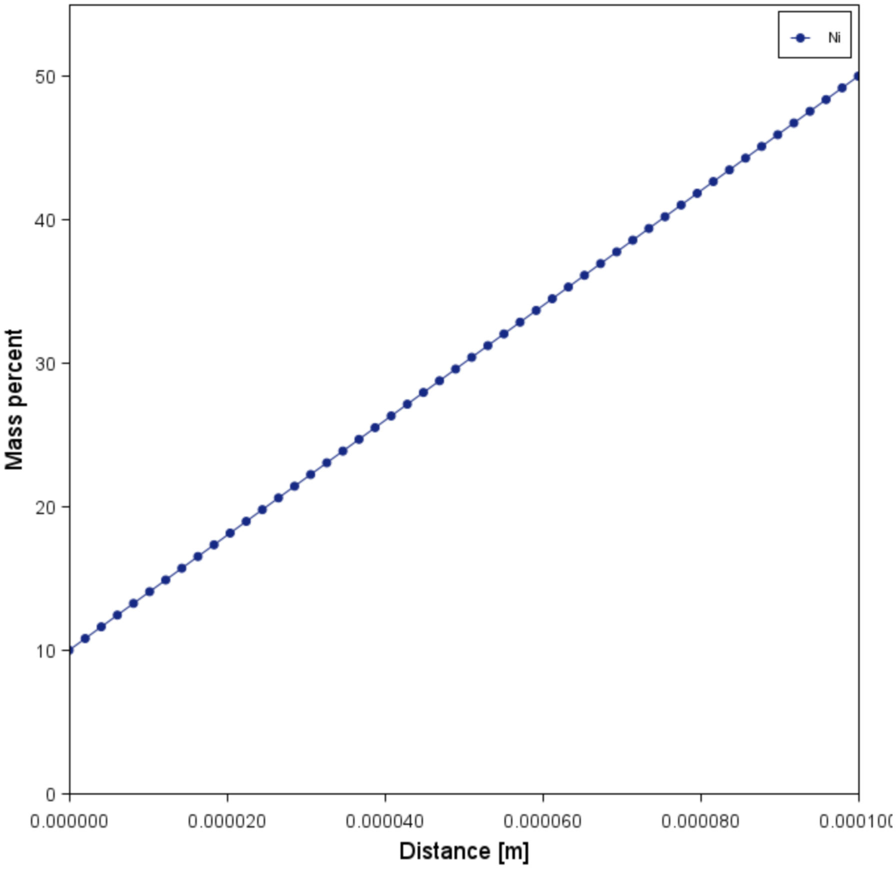
When completed, the results are plotted in the **Visualizations** window as shown below.

Visualizations

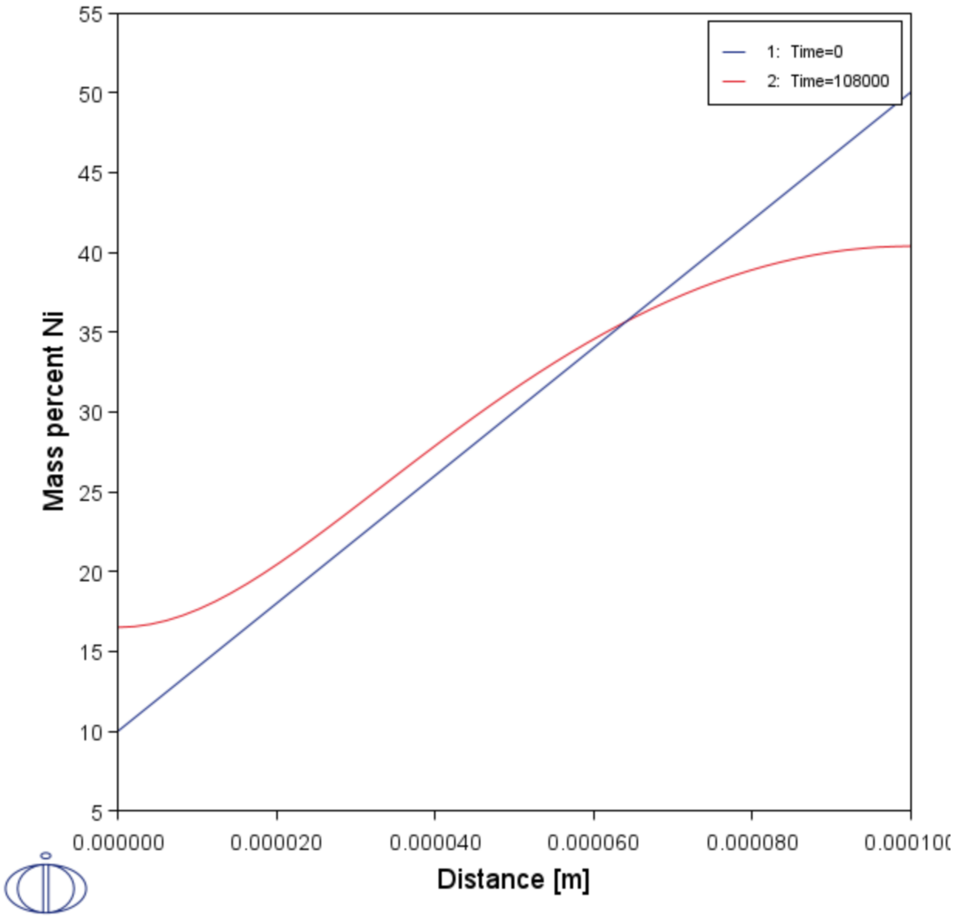
There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Composition Profiles** and **Thermal Profile**: When setting up a calculator on a **Configuration** window you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.
- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.





During set up of the calculation, you can preview the Composition Profile (shown) or Thermal Profile. Click the tab(s) in the Visualizations window to switch between these previews and adjust settings on the Diffusion Calculator Configuration window. For an Isothermal Thermal Profile this shows the constant temperature as entered.



After performing the calculation, you can view the final Plot Renderer result on the Composition of Ni vs Distance tab, which shows the initial and final Ni profile. In this example, the Plot Renderer is renamed and this matches the tab name in the Visualizations window.

For the rest of the exercise, you will learn how to build this example step-by-step.

System Definer Settings

The following describes how to set up the *D_01_Diffusion_Single_Phase.tcu* example from the beginning.

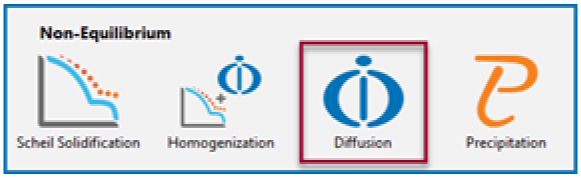
> To learn more about the activity nodes and tree structure see 'Project Activities and the Tree Structure' in the *Thermo-Calc User Guide*.

Add a System Definer Node

1. Open Thermo-Calc.
2. In the **Project** window, right-click **My Project** and select **Create New Activity → System Definer**.
3. In the **System Definer Configuration** window, you select the thermodynamic and kinetic databases to use and select the elements.

Tip: The Diffusion Template

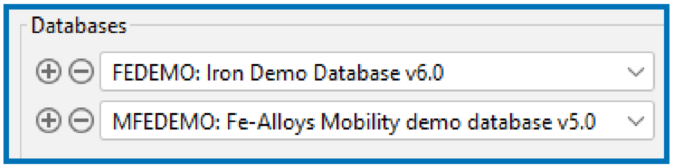
For this first example the activity nodes are added one at a time. A faster way to add all the nodes you need is to use the **Diffusion** template (click **My Project** node then under **Non-Equilibrium** click **Diffusion**).



Choose the Databases

There are databases for different purposes and material types. This example uses two demonstration databases: **FEDEMO** (the thermodynamic steels/Fe-alloys database) and **MFEDEMO** (the kinetic/mobility steels/Fe-alloys database).

1. In the System Definer **Configuration** window click the **Databases** list and select the **FEDEMO** database.
2. Click the ⊕ **Add a database** button.
3. Select the **MFEDEMO** database.

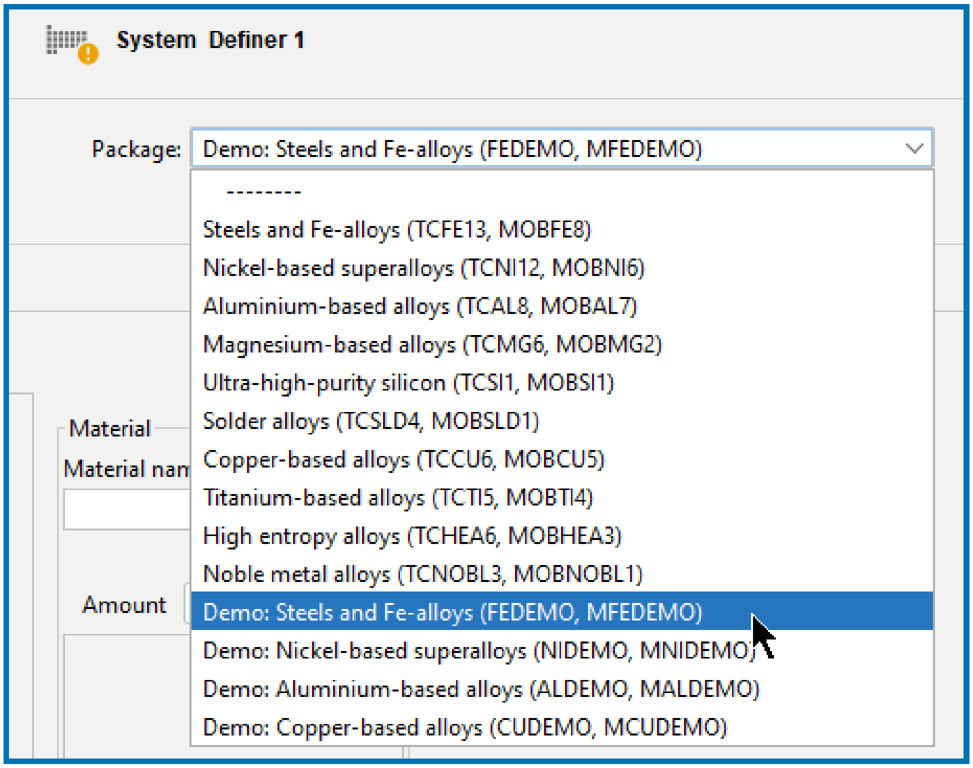


FEDEMO: Iron Demo Database v6.0

MFEDEMO: Fe-Alloys Mobility demo database v5.0

Tip: Database Packages

For this first example the databases are added one at a time. A faster way to add both the databases is to add a predefined database **Package**.



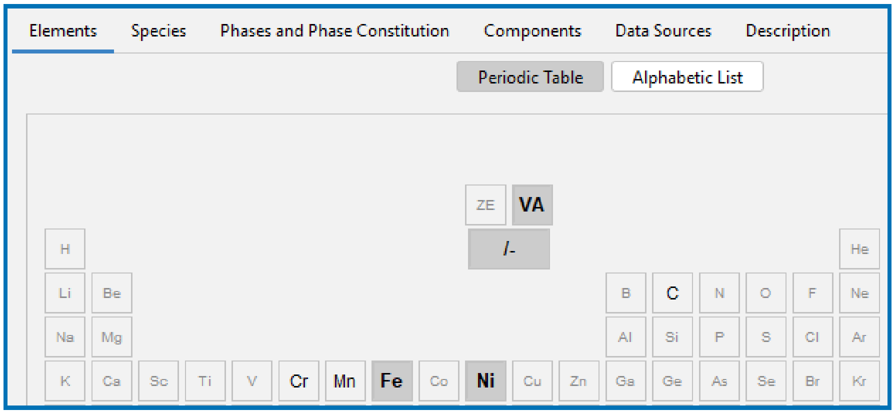
Package: Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)

- --------
- Steels and Fe-alloys (TCFE13, MOBFE8)
- Nickel-based superalloys (TCNI12, MOBNI6)
- Aluminium-based alloys (TCAL8, MOBAL7)
- Magnesium-based alloys (TCMG6, MOBMG2)
- Ultra-high-purity silicon (TCSI1, MOBSI1)
- Solder alloys (TCSLD4, MOBSLD1)
- Copper-based alloys (TCCU6, MOBCU5)
- Titanium-based alloys (TCTI5, MOBTI4)
- High entropy alloys (TCHEA6, MOBHEA3)
- Noble metal alloys (TCNOBL3, MOBNOBL1)
- Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)
- Demo: Nickel-based superalloys (NIDEMO, MNIDEMO)
- Demo: Aluminium-based alloys (ALDEMO, MALDEMO)
- Demo: Copper-based alloys (CUDEMO, MCUDEMO)

Choose the Elements

On the **Elements** tab, and based on the databases selected, you can select and review elements using a **Periodic Table** or **Alphabetic List** format. The demonstration databases have only a small number of elements to choose from.

1. In the **Periodic Table**, click **Fe**.
2. Click **Ni**.



When using the System Definer with the Diffusion Calculator, you can keep all phases selected on the **Phases and Phase Constitution** tab.

Diffusion Calculator Settings

After you have completed the settings for the System Definer you start defining the diffusion parameters on the Diffusion Calculator.

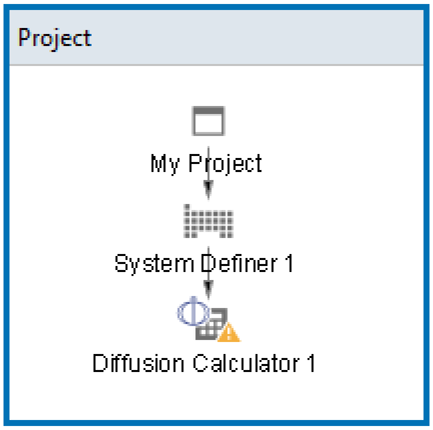
In any simulation at least one *region* must be defined. This is a named container that designates a certain part of the domain. In this case it is the whole domain. The name of a region is arbitrary and specified by you.

> The use of regions becomes clearer in the context of moving phase boundary simulations.

A region must contain a numerical *grid* specified by width and type. In this example, a 10^{-4} m (1e-4 m) wide, linear (i.e. equidistant) grid is used with 50 grid points.

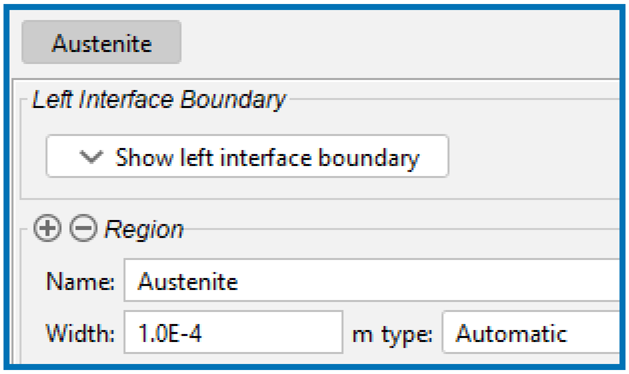
Define the Region and Composition Profiles

1. In the **Project** window, right click the **System Definer** node and select **Create New Successor → Diffusion Calculator**. A Diffusion Calculator node is added to the tree structure.



> If you used the **Diffusion** template, then this activity node is already there. Click the **Diffusion Calculator** node to access the **Configuration** window settings.

2. You are now going to add the settings to the Configuration window on the **Conditions** tab. Keep the defaults for *Composition unit* (**Mass percent**) and *Length unit* (**Meter**). A **Planar** *Geometry* is used for all the examples.
3. In the *Region* **Name** field, enter `Austenite`. This name is automatically updated on the tab.



Name: Austenite

Width: 1.0E-4

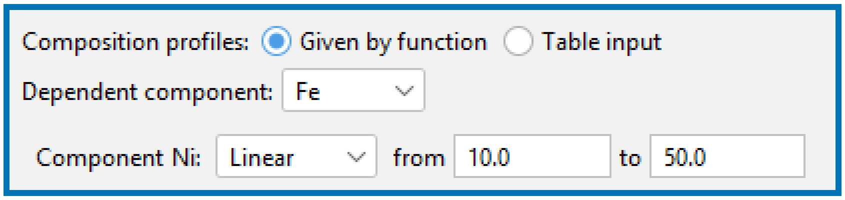
m type: Automatic

4. In the **Width** field replace the default with `1e-4`. Keep the defaults for number of points (`50`) and type of grid (`Automatic`).
5. From the **Phase** list, select **FCC_A1**.

   In the **Visualizations** window, the **Composition Profile** tab displays a preview. The initial composition profile must be specified for all regions. Since there are only two elements, Fe and Ni, the initial composition profile must only be given for one of them.

6. Next to **Composition profiles** the default selected is **Given by function**. Choose **Fe** as the **Dependent component**.

   There are many ways to specify the composition profile, e.g. an arbitrary position dependent function. In this example, the default *Linear* type is used. The initial profile for Ni is a **Linear** variation. In the **from** field enter `10` and in the **to** field enter `50`. These settings mean that the profile goes from 10 (mass-%) on the lower/left hand side of the system to 50 (mass-%) on the upper/right hand side of the system.



Composition profiles: ● Given by function ○ Table input

Dependent component: Fe

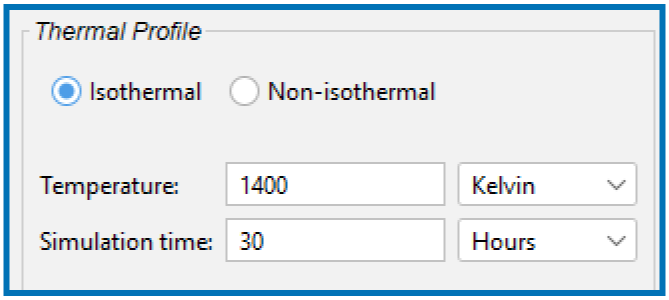
Component Ni: Linear from 10.0 to 50.0

Watch as the **Composition Profile** changes on the **Visualizations** window to match these values.

Define the Thermal Profile

The default **Isothermal** profile is used for this example. A constant temperature of 1400 K is used during the simulation, which is run for 30 hours. Enter these values in the fields:

1. In the **Temperature** field, enter `1400`. Keep **Kelvin** as the default unit.
2. In the **Simulation time** field, enter `30`. Select **Hours** from the list.



● Isothermal ○ Non-isothermal

Temperature: 1400 Kelvin

Simulation time: 30 Hours

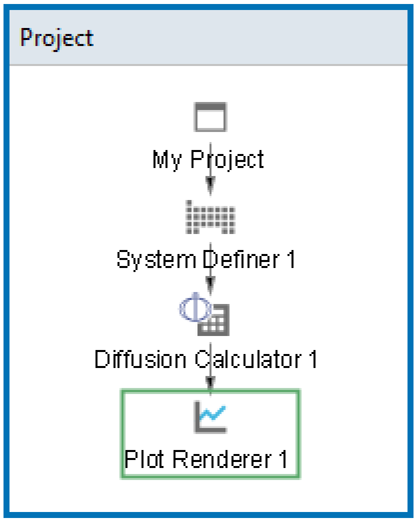
Watch as the **Thermal Profile** tab on the **Visualizations** window updates to match these values.

There are no changes to the default settings on the **Options** tab. You can click the tab to see what settings are available and then search the Online Help (press F1) for more information.

Plot Renderer Settings

After you have completed the settings for the System Definer and Diffusion Calculator you define the plot parameters and run (perform) the simulation.

1. In the **Project** window, right click the **Diffusion Calculator** node and select **Create New Successor → Plot Renderer**. A Plot Renderer node is added to the tree structure.



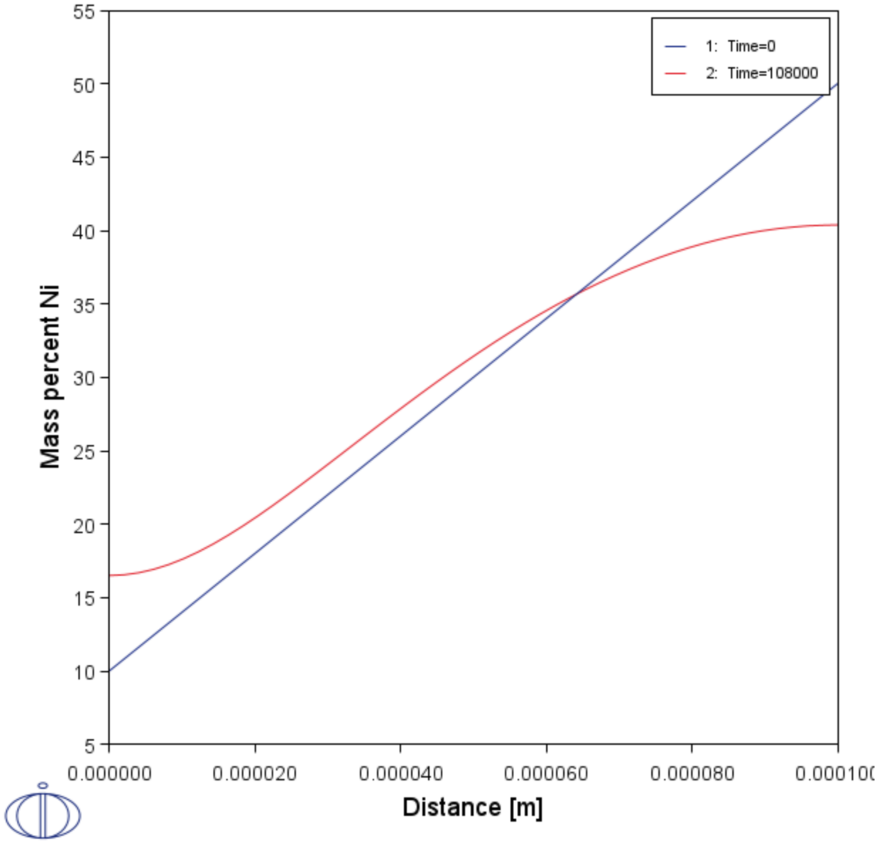
> If you used the **Diffusion** template, then this activity node is already there. Click the **Plot Renderer** node to access the **Configuration** window settings.

For this first example, some of the defaults are kept and there are only two settings to add. In most cases, either a specific position in the domain or one or more specific times must be specified depending on whether time or spatial position is chosen as independent (*X-axis*) variable.

2. In the *Axes* section for *Y* and next to **Composition**, choose **Ni**.
3. In the **Value(s)** field, enter `0.0` before the `30.0`, which is automatically taken from the Diffusion Calculator setting.

Time Hours Value(s) 0.0 30.0

4. Click **Perform**. If you have entered everything correctly, you will get this plot showing the composition profile of Ni at the initial (0 hours) and final time (30 hours or 108,000 seconds).



Renaming the Nodes and Saving the Project

You can rename the nodes in the tree at any time during the creation of a project. For this first example it was left until the end so you could become familiar with the System Definer, Diffusion Calculator and Plot Renderer settings. It is also important at this point to save the project. You can do this at any time and it is good practice to save your project often.

The following renaming can be done to match the example file included with your installation:

> When you rename a node, associated tabs are also renamed automatically. For example, when the Plot Renderer is renamed, so is the tab in the **Visualizations** window.

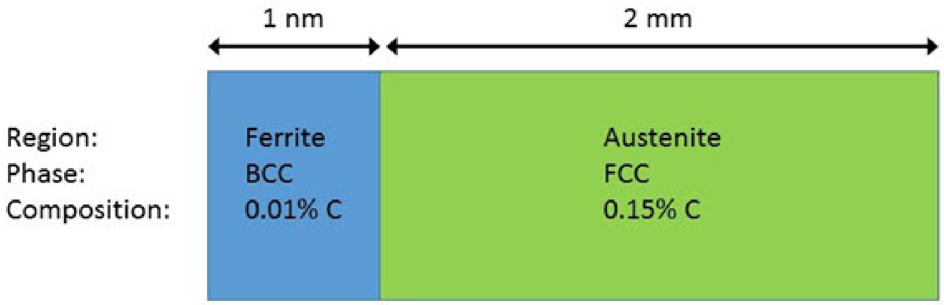
1. Right-click the **My Project** node and select **Rename**.
2. In the **New name** field enter `Diffusion Single Phase`. Click **OK**. Continue renaming the other nodes.
3. Right-click the **System Definer**, select **Rename** and enter `System with Fe Ni`.
4. Right-click the **Diffusion Calculator**, select **Rename** and enter `Diffusion single region Austenite`.
5. Right-click the **Plot Renderer**, select **Rename** and enter `Composition of Ni vs Distance`.
6. Save the project. To do this, click the **Save** button and navigate to a location on your computer where you can easily find this project file.

Moving Phase Boundary Simulations

In this section:

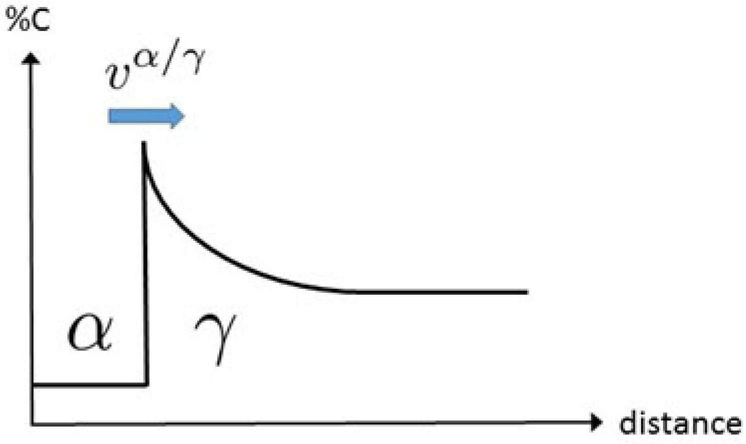
About the Moving Phase Boundary Simulation

The growth of ferrite (bcc) into austenite (fcc) is simulated in this example. The austenite is assumed to be initially homogeneous with the composition Fe - 0.15 mass-% C and the transformation temperature is 1050 K. The initial thickness of the austenite is 2 mm and an initially very thin ferrite (1 nm) is also present at the start of the simulation. The initial state is as below.



The set-up of the Moving Boundary example. There are two regions, Ferrite and Austenite, consisting of bcc and fcc, respectively.

A schematic graph of the carbon profile during the transformation is shown in the image below. Crusius et al. [1992Cru-1] is recommended as further reading.



Schematic view of the carbon profile during the transformation from austenite (γ) to ferrite (α) in the Moving Boundary example.

? References

Theory for the Moving Phase Boundary Simulation

It is assumed that local equilibrium holds at the phase interface, i.e. the chemical potentials of all elements are continuous across the boundary, but the chemical potential gradients are in general discontinuous.

In order to maintain mass balance a set of flux balance equations must be satisfied at the phase interface:

$$v^{\alpha/\gamma}(c_k^\alpha - c_k^\gamma) = J_k^\alpha - J_k^\gamma \qquad k = 1, \ldots, n-1$$

where v is the interfacial velocity. The concentrations and the fluxes c and J are those at the interface on the α and γ sides, respectively.

In the present case there are no degrees of freedom at the interface and the concentrations can be taken directly from a phase diagram. There is only one flux balance equation and the interface velocity can be evaluated once the fluxes at the interface are known. However, for ternary and higher systems the state at the interface must be found by some iterative procedure.

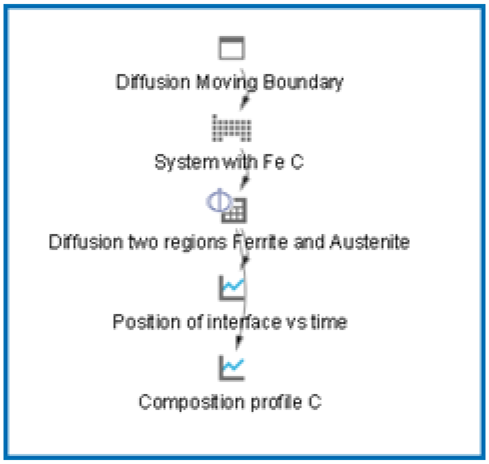
For more information on moving phase boundary problems, see, for example, [1982Ågr], [1992Cru-2], and [1997Hög].

References

Moving Phase Boundary Example Project

For the moving phase boundary simulation, you can open the example project file included with your installation to see how it is set up.

1. Open Thermo-Calc.
2. There are different ways to access the examples.
    - From the main menu, select **File →** or **Help → Examples Files**. The Graphical Mode folder opens by default.
    - Click the **My Project** node and on the **Configuration** window under **Getting Started**, click **Example Files**.
3. Click to open the **Diffusion Module - DICTRA** folder and locate the file **D_02_Diffusion_Moving_Boundary.tcu**. Double-click to open it.
4. The project opens in Thermo-Calc. Click the top Project node (renamed to *Diffusion Moving Boundary*). At the bottom of the **Configuration** window click **Perform Tree**. You can also right-click the node and select **Perform Now**.



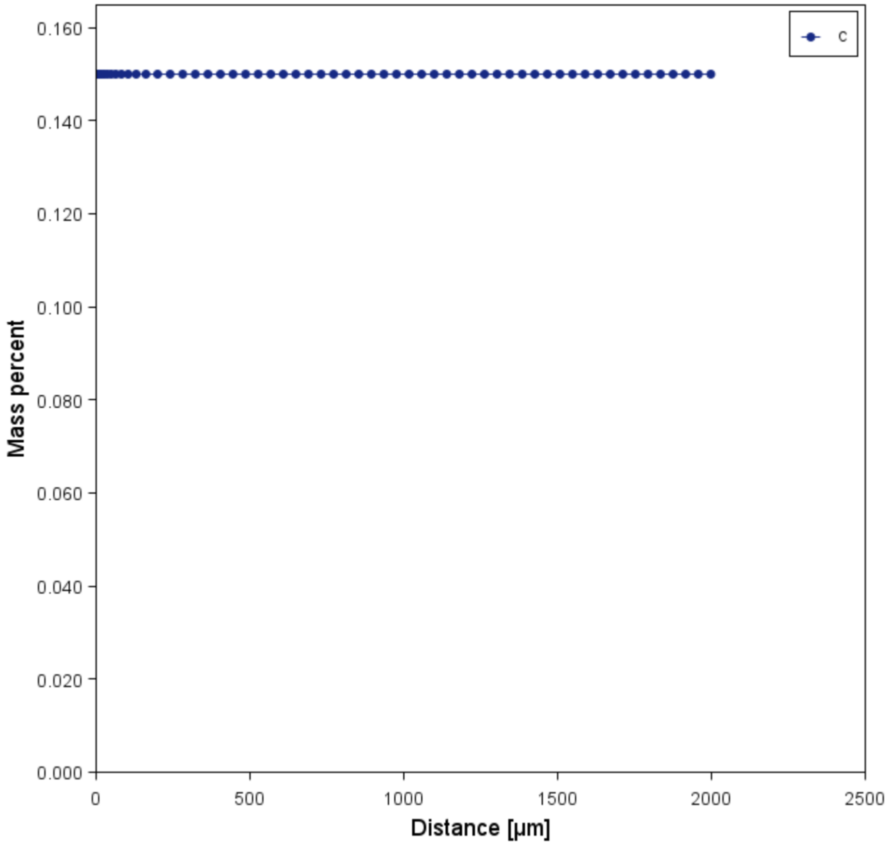
When completed, the results are plotted in the **Visualizations** window.

Visualizations

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

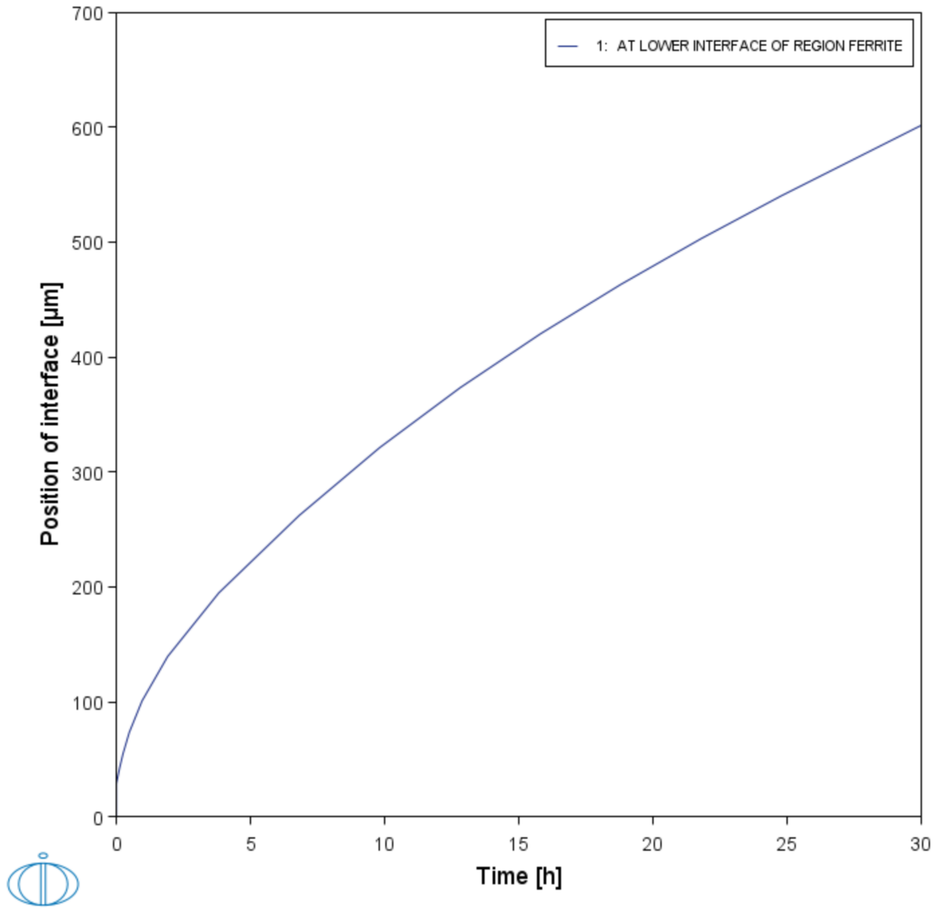
- **Composition Profiles** and **Thermal Profile**: When setting up a calculator on a **Configuration** window you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

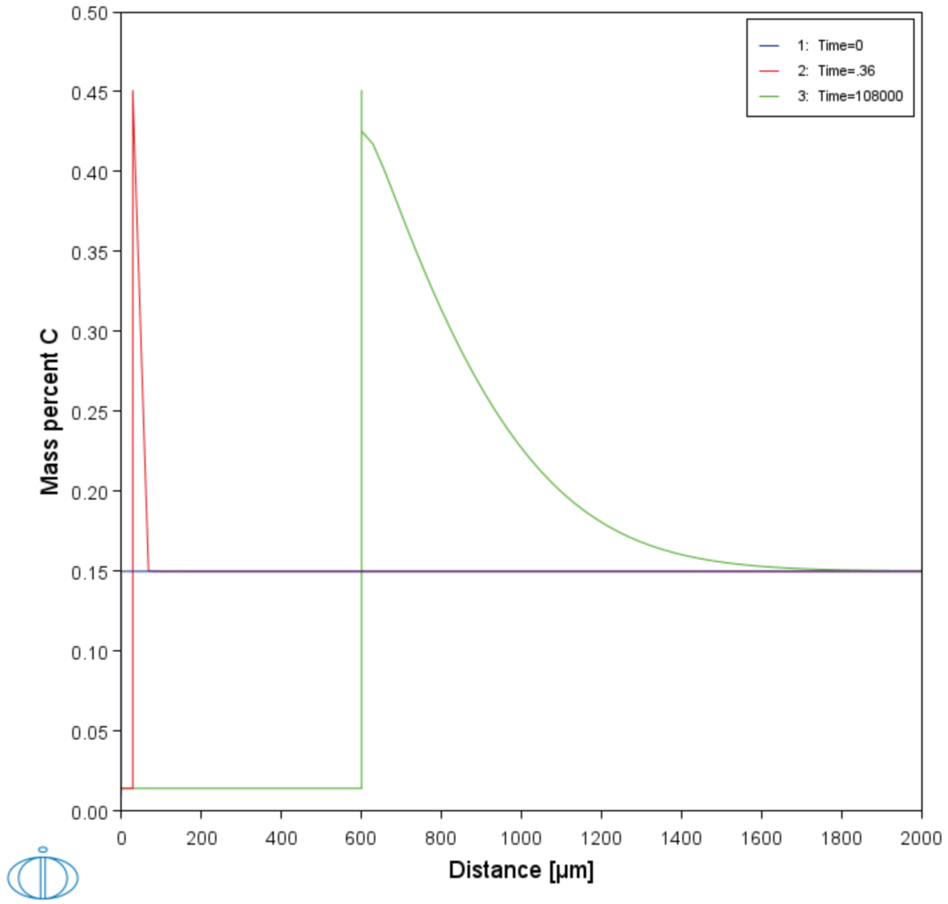


During set up of the calculation, you can preview the Composition Profile (shown) or Thermal Profile. Click the tab(s) in the Visualizations window to switch between these previews and adjust settings on the Diffusion Calculator Configuration window. For an Isothermal Thermal Profile this shows the constant temperature as entered.

There are two plot nodes, which creates two plots: The ferrite/austenite phase interface position as a function of time and the composition profile for Carbon.



After performing the calculation, you can view the final Plot Renderer result on the Position of interface vs time tab. In this example, the Plot Renderer is renamed and this matches the tab name in the Visualizations window.



After performing the calculation, you can view the final Plot Renderer result on the Composition profile C tab. In this example, the Plot Renderer is renamed and this matches the tab name in the Visualizations window.

System Definer Settings

This is a continuation from the Single Phase simulation and it describes how to set up the example file *D_02_Diffusion_Moving_Boundary.tcu*. In this example, the shortcuts explained for the Single Phase System Definerare used.

Add the Databases and the Elements

1. Open a new instance of Thermo-Calc.
2. Click the 🗀 **My Project** node and on the **Configuration** window under **Non-Equilibrium**, click the **Diffusion** template icon.
3. In the System Definer **Configuration** window click the **Package** list and choose **Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)**.
4. In the **Periodic Table**, click **Fe** then **C**.
5. Rename the nodes. Right-click **System Definer** and rename it to **System with Fe C**.
6. Right-click **My Project** and give it the same name as the project e.g. *Diffusion Moving Boundary*.
7. Save the project file with a new name, such as *Diffusion_Moving_Boundary*.

Diffusion Calculator Settings

After you have completed the settings for the System Definer you define the diffusion calculation parameters.

The phase interface between ferrite and austenite is created by introducing an austenite region that is attached to the ferrite region. Regions are always separated by phase interfaces and must therefore always contain different phases.

In this simulation both the FCC_A1 and BCC_A2 phases are included. Both phases are assumed to be initially homogeneous, the BCC phase having 0.01 mass-% C and the FCC phase 0.15 mass-% C. These settings are entered on the Diffusion Calculator.

As with the single phase example, the **Options** tab keeps all the defaults.

Add a Ferrite Region

1. In the **Project** window, click the **Diffusion Calculator** node.
2. Keep the default for **Composition unit** (**Mass percent**). Choose **Micrometer** for the **Length unit**. A **Planar** geometry is used for all the examples.
3. Under *Region* in the **Name** field enter `Ferrite` (replace the default text **Region 1**). Press <Enter>.
4. In the **Width** field enter `0.001` µm and change the default number of points to `10`. Keep the default **Automatic** grid type.

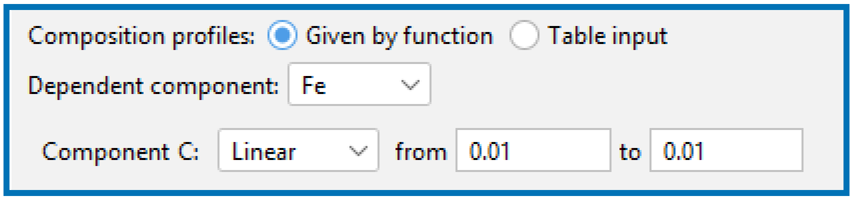
   The grid type for the ferrite region is the same as in the single-phase simulation example, i.e. equidistant.

5. From the **Phase** list select **BCC_A2**.

   In the **Visualizations** window, the **Composition Profile** tab displays a preview. The initial composition profile must be specified for all regions. Since there are only two elements, Fe and C, the initial composition profile must only be given for one of them.

6. Next to **Composition profiles** the default selected is **Given by function**. **Fe** is chosen as the **Dependent component** and the initial profile for **Component C** is a **Linear** variation.

7. Enter `0.01` in both fields to represent C going from 0.01 (mass-%) on the lower, left-hand side of the system to 0.01 (mass-%) on the upper, right-hand side of the system.



Composition profiles: ● Given by function ○ Table input

Dependent component: Fe

Component C: Linear from 0.01 to 0.01

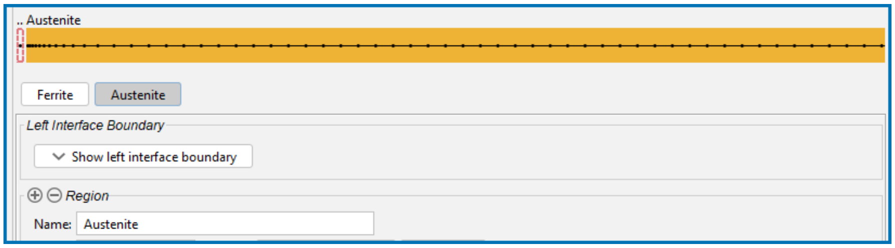
Watch as the **Composition Profile** changes on the **Visualizations** window to match these values.

Add an Austenite Region

1. Next to *Region*, click the add button ⊕. A new tab called **Region 1** is added.

> If you add a region and then need to change the order, right-click the applicable tab and choose **Move left** or **Move right**.

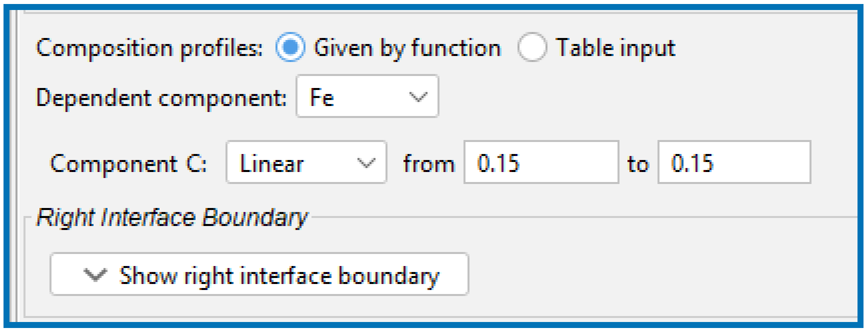
2. In the *Region* **Name** field, enter `Austenite`. This name is automatically updated on the tab and above the grid points in a new section for the second region.



Name: Austenite

3. In the **Width** field enter `2000` µm.
4. Select a **Automatic** type of grid and choose **Medium**.
5. From the **Phase** list, select **FCC_A1**.
6. Next to **Composition profiles** the default selected is **Given by function** and **Fe** is the **Dependent component**. Enter `0.15` in both the **from** and **to** fields to represent **Component C** going from 0.15 (mass-%) on the lower, left-hand side of the system to 0.15 (mass-%) on the upper, right-hand side of the system. The Austenite grid shows the points and the **Composition Profile** changes on the **Visualizations** window to

match these values.



Composition profiles: ● Given by function ○ Table input

Dependent component: Fe

Component C: Linear from 0.15 to 0.15

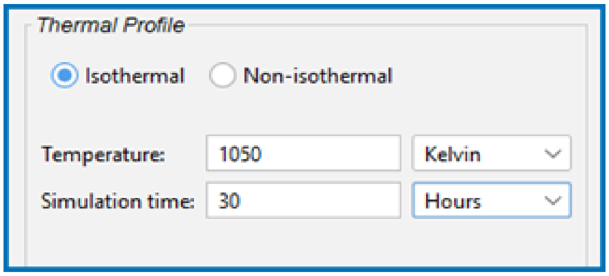
Right Interface Boundary

The domain now consists of two regions: Ferrite and Austenite.

Define the Thermal Profile

The default **Isothermal** profile is used.

1. In the **Temperature** field, enter `1050`. Keep the default unit, **Kelvin**.
2. In the **Simulation time** field, enter `30`. Choose **Hours** from the list.
3. Right-click **Diffusion Calculator** and rename it to `Diffusion two regions Ferrite and Austenite`.



Thermal Profile

● Isothermal ○ Non-isothermal

Temperature: 1050 Kelvin

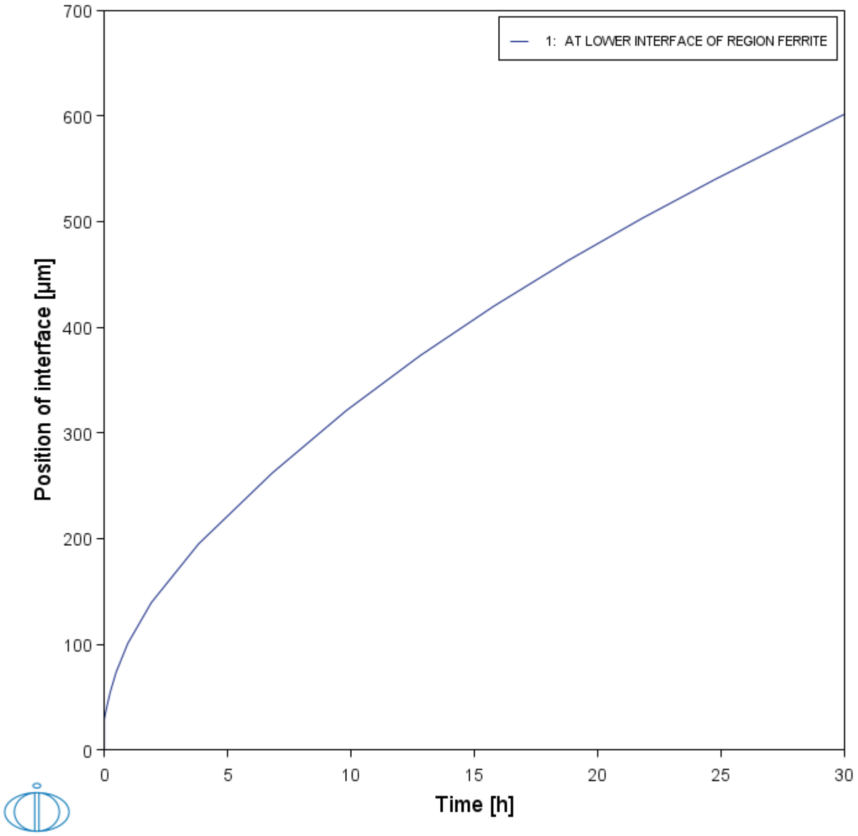
Simulation time: 30 Hours

Plot Renderer Settings

After you have completed the settings for the System Definer and Diffusion Calculator you define the plot parameters.

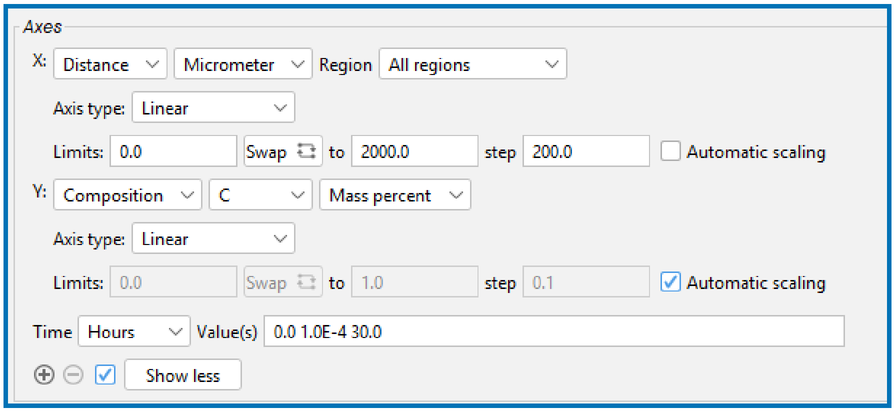
1. In the **Project** window, click the **Plot Renderer** node.
2. In the *Axes* section, choose **Time** for *X* and select **Hours**.
3. Choose **Position of interface** for *Y*. After you click **Perform**, the **Interface** list is populated.
4. Right-click the **Plot Renderer** and rename it to `Position of interface vs time`.
5. Click **Perform**. If you have entered the same settings the plot shows the ferrite/austenite phase interface position as a function of time. The plot has the parabolic appearance characteristic for many types of diffusion simulations.

Plot result from the example showing the phase interface position as a function of time.



Add a Second Plot

1. Right-click the **Diffusion Calculator** node. Remember it is renamed to *Diffusion two regions Ferrite and Austenite*.
2. From the **Create New Successor** list, click **Plot Renderer**.
3. In the new Plot Renderer node **Configuration** window *Axes* section, for *X*, change the **Distance** units to **Micrometer**.
4. Click **Show more**, then click to clear the **Automatic scaling** checkbox.
5. In the **Limits** fields, keep `0.0` as the lower limit, enter `2000` for the upper limit and `200` for **step**.
6. For *Y*, keep the default **Composition** and choose **C** from the list.
7. Choose **Hours** as the **Time** unit and enter `0.0 1.0E-4 30.0` in the field.



Axes

X: Distance, Micrometer, Region: All regions

Axis type: Linear

Limits: 0.0 Swap to 2000.0 step 200.0 ☐ Automatic scaling

Y: Composition, C, Mass percent

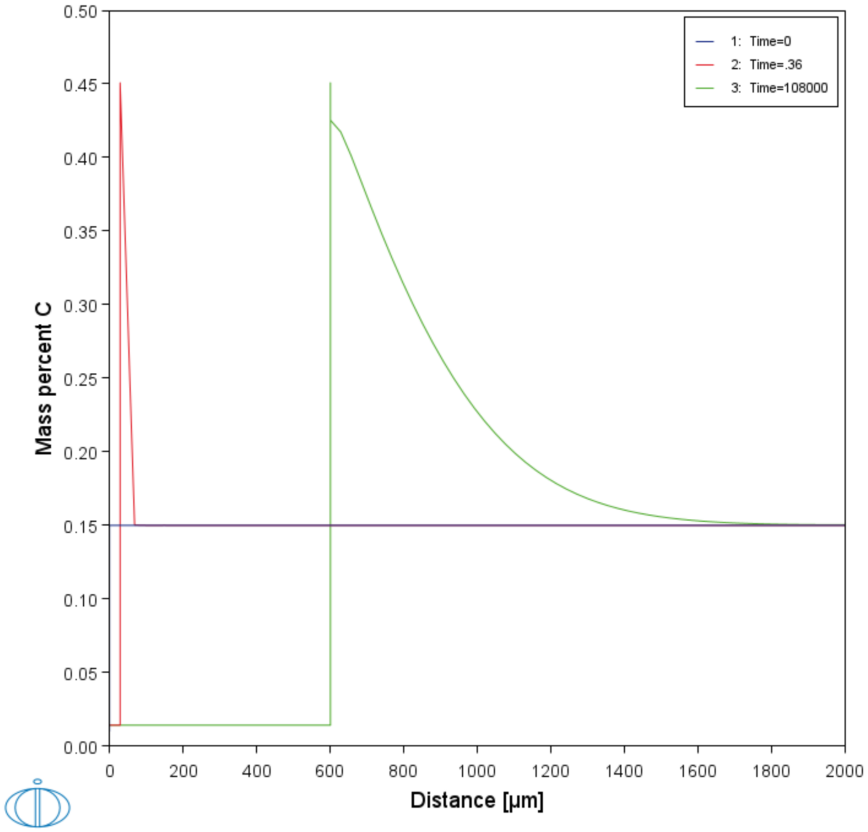
Axis type: Linear

Limits: 0.0 Swap to 1.0 step 0.1 ☑ Automatic scaling

Time: Hours Value(s): 0.0 1.0E-4 30.0

8. Right-click **Plot Renderer** and rename it to `Composition profile C`.

9. Click **Perform** If you have entered the same settings the plot shows the composition profile of C.



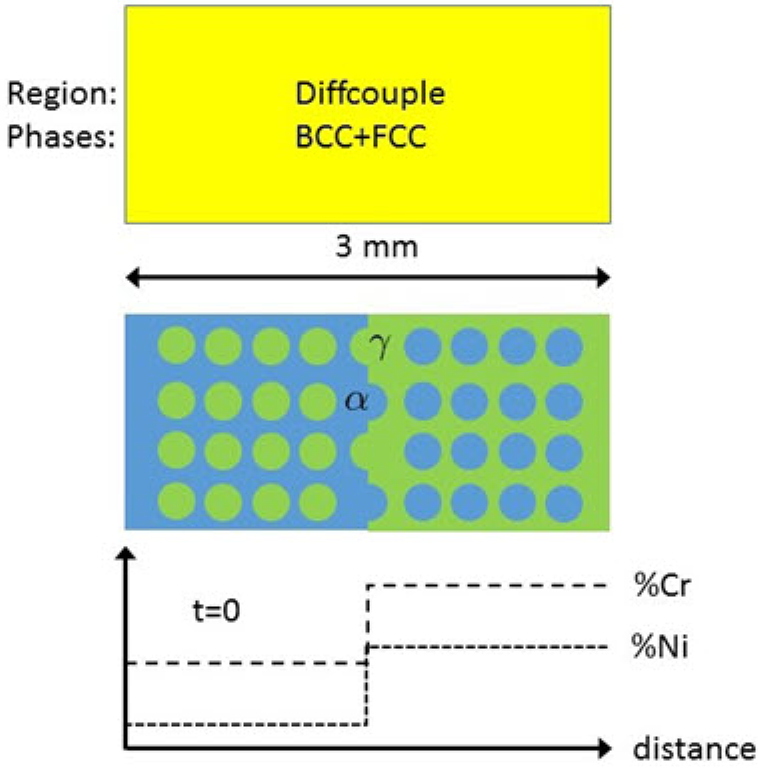
Multiphase Simulations

In this section:

About the Multiphase Simulation

This example simulates the evolution of an Fe-Cr-Ni diffusion couple during a 100 hour heat treatment at 1100° C (1373.15 K). Both end members of the diffusion couple are duplex ferrite plus austenite, but the majority phase is ferrite on the left-hand side and austenite on the right.

With this type of simulation it is assumed that the material is fully equilibrated at each grid point, i.e. the local phase fractions, phase compositions and so forth are obtained from an equilibrium calculation with the local overall composition as a condition.



Schematic view of the initial state of the Multiphase example. Two ternary Fe-Cr-Ni alloys form a diffusion couple. There is a single region (diffcouple) where both the bcc and fcc phases are entered. Both alloys are duplex bcc+fcc, but the majority phase is bcc (α) in the left-hand side alloy and fcc (γ) in the right.

Theory for the Multiphase Simulation

More details about the homogenization model for multiphase simulations can be found in Larsson and Engström [2006Lar] and Larsson and Höglund [2009Lar]. As mentioned in the description of this simulation, it is assumed that the material is locally fully equilibrated and that the local phase fractions, phase compositions and so forth are obtained from an equilibrium calculation with the local overall composition as a condition. From a numerical point of view the homogenization model treats the multiphase material as a single phase having the “average”, or “effective”, properties of the local phase mixture.

When estimating the effective kinetics of a multiphase mixture the product of solubility and mobility in each phase is considered. It is therefore convenient to define

$$\Gamma_k^\phi = M_k^\phi c_k^\phi$$

for each phase ϕ. The effective kinetics of the multiphase mixture is denoted and in this example it was evaluated using the lower Hashin-Shtrikman bound. The default method is a simple rule of mixtures

$$\Gamma^\star = \sum_\phi f^\phi \Gamma_k^\phi$$

where f^ϕ is the volume fraction of ϕ. The flux is obtained as

$$J_k = -\Gamma_k^\star \frac{\partial \mu_k}{\partial z}$$

which replaces the single-phase equation

$$J_k = L_{kk} \frac{\partial \mu_k}{\partial z} = M_k c_k \frac{\partial \mu_k}{\partial z}$$

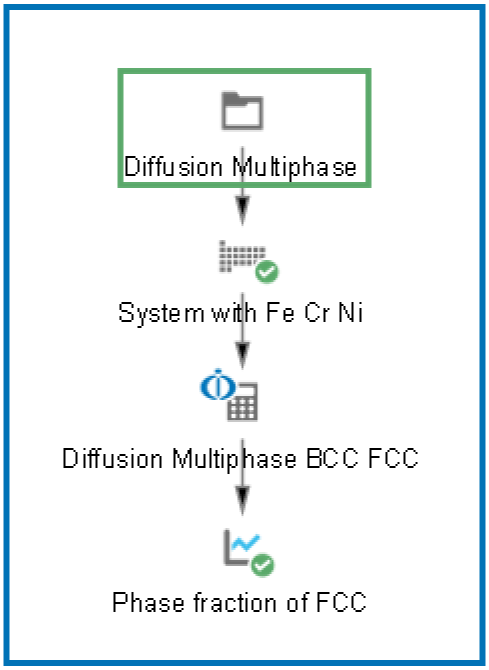
for multiphase simulations.

References

Multiphase Example Project

For the multiphase simulation, you can open the example project file included with your installation to see how it is set up.

1. Open Thermo-Calc.
2. There are different ways to access the examples.
    - From the main menu, select **File →** or **Help → Examples Files**. The Graphical Mode folder opens by default.
    - Click the **My Project** node and on the **Configuration** window under **Getting Started**, click **Example Files**
3. Click to open the **Diffusion Module - DICTRA** folder and locate the **D_03_Diffusion_Multiphase.tcu** file. Double-click to open it.
4. The project opens in Thermo-Calc. Click the top Project node (renamed to *Diffusion Multiphase*). At the bottom of the **Configuration** window click **Perform Tree**.

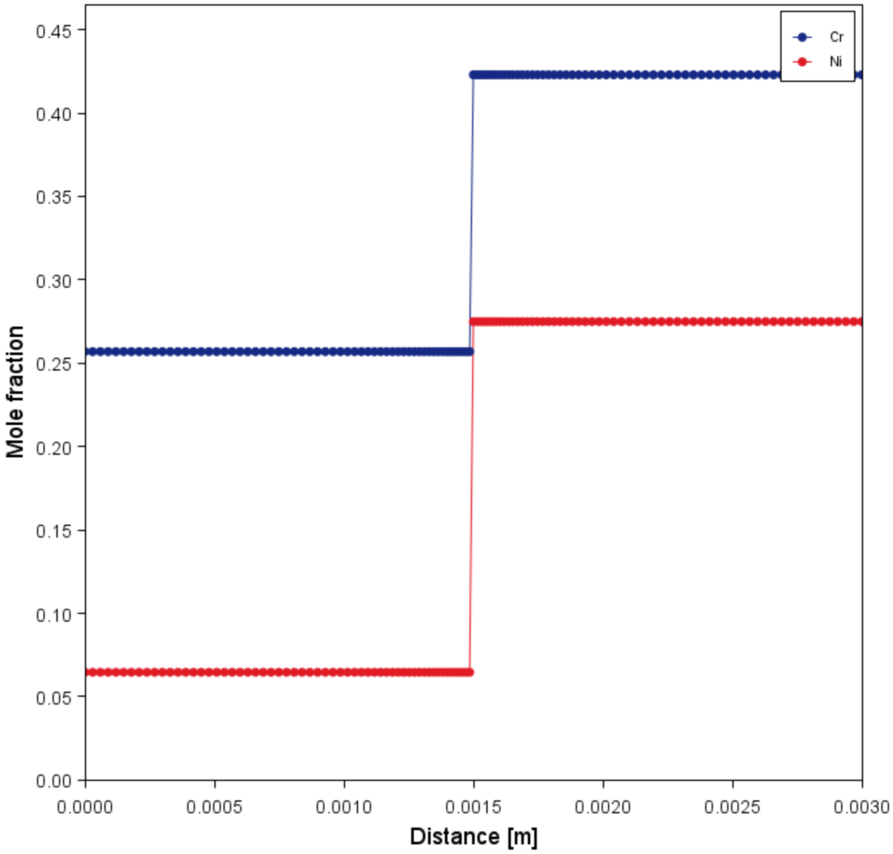


When completed, the results are plotted in the **Visualizations** window.

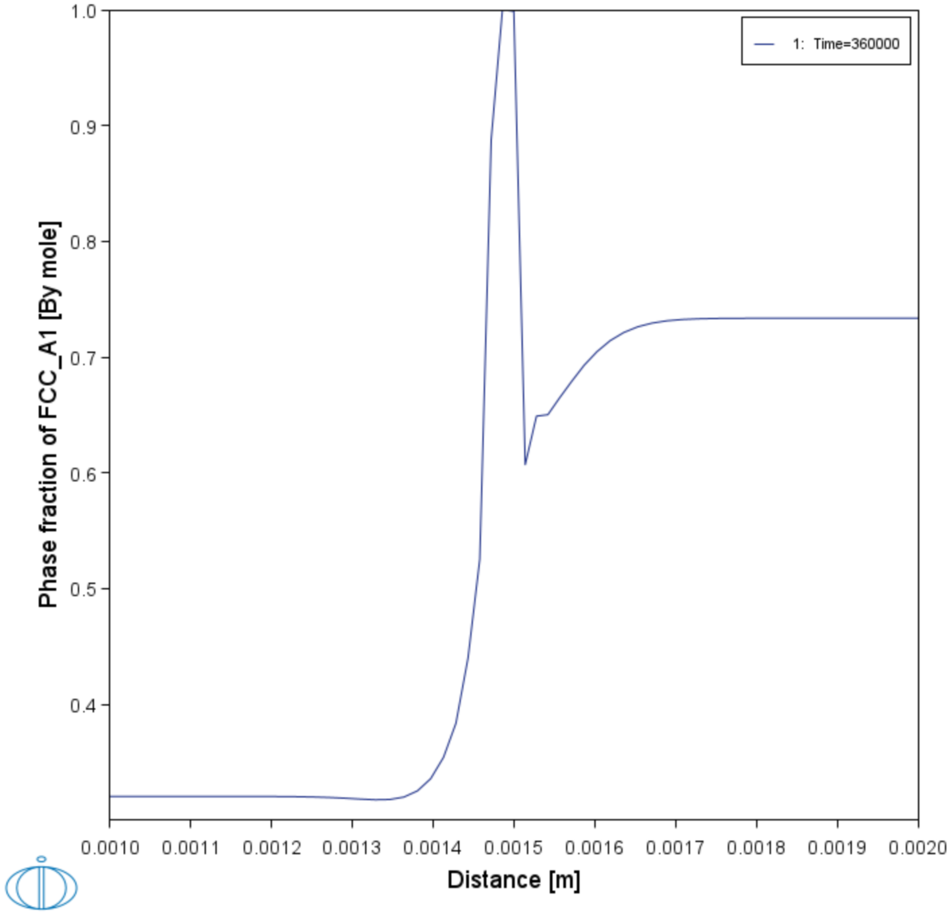
Visualizations

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Composition Profiles** and **Thermal Profile**: When setting up a calculator on a **Configuration** window you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.
- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.



During set up of the calculation, you can preview the Composition Profile (shown) or Thermal Profile. Click the tab(s) in the Visualizations window to switch between these previews and adjust settings on the Diffusion Calculator Configuration window. For an Isothermal Thermal Profile this shows the constant temperature as entered.



After performing the calculation, you can view the final Plot Renderer result on the Phase fraction of FCC tab. In this example, the Plot Renderer is renamed and this matches the tab name in the Visualizations window.

System Definer Settings

This is a continuation from the previous examples and uses the short cuts already described. You can alternatively open a saved project and edit the settings.

Add the Databases and the Elements

1. Open a new instance of Thermo-Calc.
2. In the 🗀 **My Project** window under **Non-Equilibrium**, click the **Diffusion** template icon.
3. In the System Definer **Configuration** window click the **Package** list and choose **Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)**.
4. In the **Periodic Table**, click **Fe**, then **Cr** and **Ni**.
5. Right-click **System Definer** and rename it to `System with Fe Cr Ni`.
6. Save the project file with a new name, e.g. *Diffusion_Multiphase*.

Diffusion Calculator Settings

After you have made the settings to the System Definer, you add the diffusion calculation parameters.

Define the Ferrite and Austenite Regions

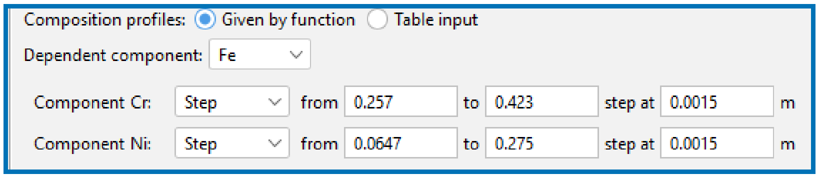
1. In the **Project** window, click the **Diffusion Calculator** node.
2. For **Composition unit** select **Mole fraction**.

   Keep the default **Length unit** as **Meter**. A **Planar** geometry is used for all the examples.

3. Under *Region* in the **Name** field enter `Diffcouple`.
4. In the **Width** field enter `0.003`.
5. Select **Automatic** as the grid type. Select **Fine**.
6. Choose **FCC_A1** from the **Phase** list.
7. Next to **Phase** click the ⊕ **Add phase** button. From the **Phase** list select **BCC_A2**.

   In the **Visualizations** window, the **Composition Profile** tab displays a preview of these changes.

8. Next to **Composition profiles** the default selected is **Given by function**. **Fe** is chosen as the **Dependent component**.
   a. Define **Component Cr** and **Component Ni**. Choose **Step** for both the Cr and Ni elements.
   b. In each of the fields for Cr (**from**, **to**, **step at**) enter `0.257`, `0.423` and `0.0015`, respectively.
   c. In each of the fields for Ni (**from**, **to**, **step at**) enter `0.0647`, `0.275` and `0.0015`, respectively.



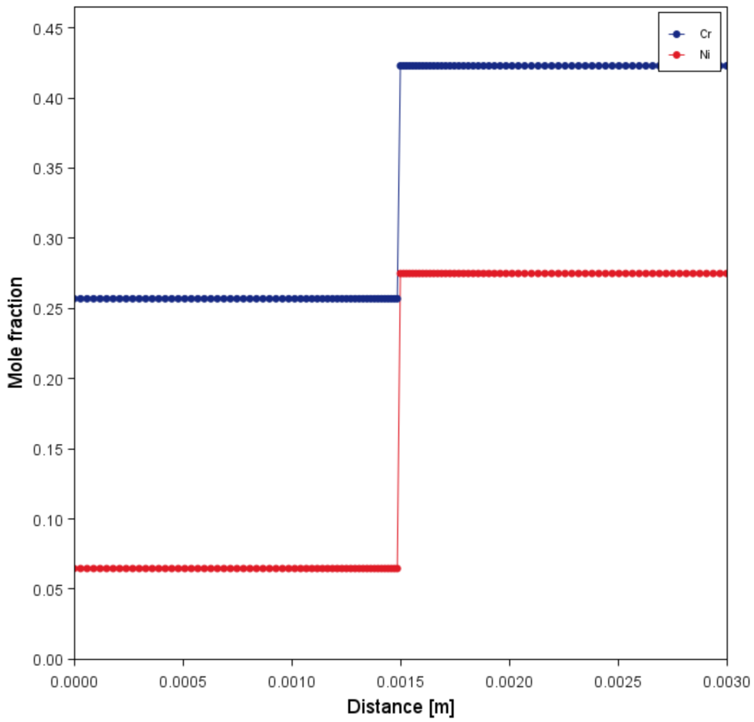
Composition profiles: ● Given by function ○ Table input

Dependent component: Fe

Component Cr: Step from 0.257 to 0.423 step at 0.0015 m

Component Ni: Step from 0.0647 to 0.275 step at 0.0015 m

In the **Visualizations** window, the **Composition Profile** tab displays a preview of these changes.



During set up of the calculation, you can preview the Composition Profile (shown) or Thermal Profile. Click the tab(s) in the Visualizations window to switch between these previews and adjust settings on the Diffusion Calculator Configuration window. For an Isothermal Thermal Profile this shows the constant temperature as entered.

The resulting Cr profile is thus 0.257 on the left half of the domain and 0.423 on the right with a sharp step at the center (as shown in About the Multiphase Simulation).

Define the Thermal Profile

The default **Isothermal** profile is used for this example.

1. In the **Temperature** field, enter `1100` and choose **Celsius** as the unit from the list.
2. In the **Simulation time** field, enter `100` and choose **Hours** from the list.
3. Right-click **Diffusion Calculator** and rename it to `Diffusion Multiphase BCC FCC`.

Choose the Homogenization Function

The local kinetics of the multiphase mixture must be estimated by means of some function that may depend on the local phase fractions, phase compositions, and the mobilities of the individual phases.

There are many such homogenization functions to choose from. In this particular example the **General lower Hashin–Shtrikman bound** is a good choice [1962Has].

1. To choose this homogenization function, click the **Diffusion Calculator** and then click the **Options** tab.
2. Under *Simulation Conditions*, select **Homogenization** as the **Default solver**.
3. Under *Homogenization Model Specific*, from the **Homogenization function** list, select **General lower Hashin–Shtrikman bound**.

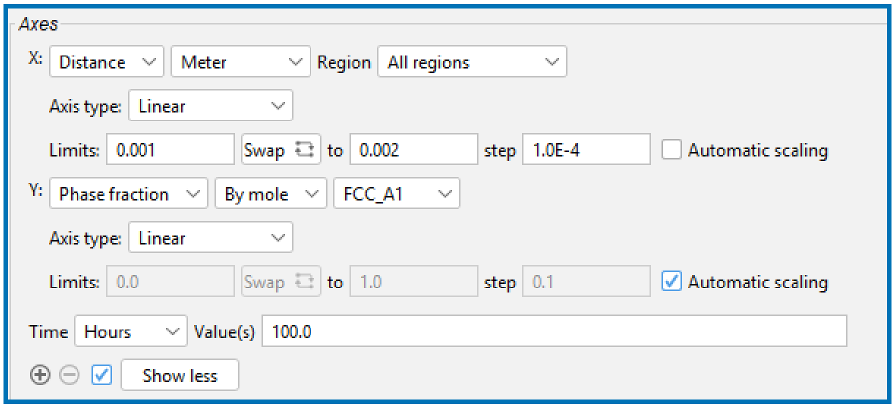
References

Plot Renderer Settings

After you enter the settings for the System Definer and Diffusion Calculator, you define the plot parameters. For this example you want to plot the mole fraction fcc phase as a function of distance at the end of the heat treatment.

The plot of phase fraction vs distance shows that a single phase fcc zone has formed and this was also observed experimentally, see [1995Eng].

1. Click the **Plot Renderer** node.
2. Click **Show more**. Then under *Axes* for *X*, click to clear the **Automatic scaling** checkbox.
3. Enter the **Limits**: `0.001` **to** `0.002` **step** `1.0E-4`.
4. For *Y*, choose **Phase fraction** and **FCC_A1**.



Axes

X: Distance, Meter, Region: All regions

Axis type: Linear

Limits: 0.001 to 0.002 step 1.0E-4 ☐ Automatic scaling

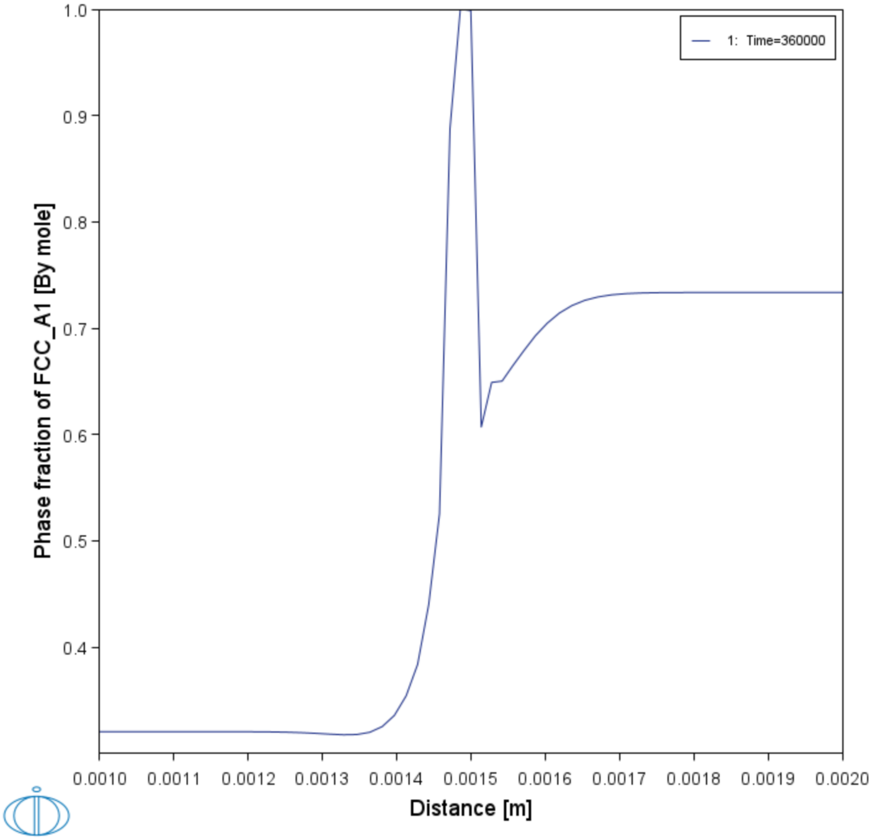
Y: Phase fraction, By mole, FCC_A1

Axis type: Linear

Limits: 0.0 to 1.0 step 0.1 ☑ Automatic scaling

Time: Hours, Value(s): 100.0

5. Click **Perform** If you have entered the same settings you will get this plot result.



6. Right-click **Plot Renderer** and rename it to `Phase fraction of FCC`.

[References](#)

References

[1962Has] Z. Hashin, S. Shtrikman, A Variational Approach to the Theory of the Effective Magnetic Permeability of Multiphase Materials. J. Appl. Phys. 33, 3125–3131 (1962).

[1982Ågr] J. Ågren, Numerical treatment of diffusional reactions in multicomponent alloys. J. Phys. Chem. Solids 43, 385–391 (1982).

[1992And] J.-O. Andersson, J. Ågren, Models for numerical treatment of multicomponent diffusion in simple phases. J. Appl. Phys. 72, 1350–1355 (1992).

[1992Cru-1] S. Crusius, L. Höglund, U. Knoop, G. Inden, J. Ägren, On the Growth of Ferrite Allotriomorphs in Fe - C Alloys / Das Wachstum von allotriomorphem Ferrit in Fe — C-Legierungen. Int. J. Mater. Res. (Zeitschrift für Met. 83, 729–738 (1992).

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[1995Eng] A. Engström, Interdiffusion in multiphase, Fe-Cr-Ni diffusion couples. Scand. J. Metall. 24, 12–20 (1995).

[1997Hög] L. Höglund, “Computer simulation of diffusion controlled transformations in multicomponent alloys,” PhD Thesis, KTH Royal Institute of Technology, Stockholm, Sweden (1997).

[2000Bor] A. Borgenstam, L. Höglund, J. Ågren, A. Engström, DICTRA, a tool for simulation of diffusional transformations in alloys. J. Phase Equilibria 21, 269–280 (2000).

[2002And] J.-O. Andersson, T. Helander, L. Höglund, P. Shi, B. Sundman, Thermo-Calc & DICTRA, computational tools for materials science. Calphad 26, 273–312 (2002).

[2006Lar] H. Larsson, A. Engström, A homogenization approach to diffusion simulations applied to α+γ Fe–Cr–Ni diffusion couples. Acta Mater. 54, 2431–2439 (2006).

[2009Lar] H. Larsson, L. Höglund, Multiphase diffusion simulations in 1D using the DICTRA homogenization model. Calphad 33, 495–501 (2009).

Next Steps

Below are suggestions for you to learn more about using the Diffusion Module (DICTRA).

- Browse the Online Help (press F1) or open one of the available PDFs included with your installation (**Help → Manuals Folder**).
- You have been working within Graphical Mode. You might also want to try the *Diffusion Module Console Mode Quick Start Guide* (**Help → Manuals Folder**). This further prepares you to work with the Console Mode examples (**Help → Examples Files**), which contain some simulation types and advanced functionality not yet available in Graphical Mode.
- You can also go to the Thermo-Calc website to see if there are other options suited to you, such as a course or video tutorials. To go to the web page, in the **Project** window, click the top **My Project** node and then click **Video Tutorials**. Or from the main menu, select **Help → Video Tutorials**.

There are several resources available on our website to help you learn how to use Thermo-Calc and other Add-on Modules. Go to the Getting Started Guides page and choose one of the guides that provides new users an introduction to setting up simple calculations in Graphical Mode. The information there is also in this help documentation.

The Role of Diffusion in Materials: A Tutorial is available for download on our website. It is intended for engineers interested in using the Diffusion Module (DICTRA), as well as students learning about the role of diffusion in materials. It is designed to be useful at many levels, from undergraduate studies to someone with a PhD and experience in a related field.

Diffusion Module (DICTRA) Quick Start Guide - Console Mode

Thermo-Calc Version 2025b

Introduction to the Diffusion Module (DICTRA)

The Diffusion Module (DICTRA) is an Add-on Module to the Thermo-Calc software package. It is used for simulation of diffusion controlled transformations in multicomponent systems. The simulations are both time- and space-dependent.

The Diffusion Module (DICTRA) is suitable for solving diffusion problems that include a moving boundary (so-called *Stefan problems*). The multicomponent diffusion equations in the various regions of a material are solved under the assumption that thermodynamic equilibrium holds locally at all phase interfaces. The concentration fields only vary along one spatial coordinate, but the geometry may be either planar, cylindrical or spherical.

In this section:

About this Quick Start Guide

The following introduces you to the basic concepts, steps and theory to start using the Diffusion Module (DICTRA). An understanding of this information is necessary to ensure accurate calculations.

More details about the use of DICTRA can be found in [2002And] and [2000Bor].

If you are not familiar with Graphical Mode, it is recommended you review the documentation and additional resources available on our website.

The Role of Diffusion in Materials: A Tutorial is available for download on our website. It is intended for engineers interested in using the Diffusion Module (DICTRA), as well as students learning about the role of diffusion in materials. It is designed to be useful at many levels, from undergraduate studies to someone with a PhD and experience in a related field.

References

[2000Bor] A. Borgenstam, L. Höglund, J. Ågren, A. Engström, DICTRA, a tool for simulation of diffusional transformations in alloys. J. Phase Equilibria 21, 269–280 (2000).

[2002And] J.-O. Andersson, T. Helander, L. Höglund, P. Shi, B. Sundman, Thermo-Calc & DICTRA, computational tools for materials science. Calphad 26, 273–312 (2002).

About the DICTRA File Formats

The Diffusion Module (DICTRA) in Console Mode uses different file formats: *log*, *macro*, and *workspace* files.

> When working with the DICTRA module in Graphical Mode, the file formats are the same as when using Thermo-Calc.

Log Files

Log files (*.TCM) are plain text files and are just macro files used to save a sequence of commands. These files can be edited in a text editor.

- To start saving your input into a file, in the SYS module type `SET_LOG_FILE`, followed by the name of the file that you want to save your command sequence to.
- When creating a command sequence, and if you want to save the output in the log file, type `SET_ECHO` before SET_LOG_FILE. This is useful if you later want to use the log file as a macro file because the macro file lists the full commands instead of only the short names.

Macro Files

Macro files (*.DCM) are plain text files used to save a sequence of commands that can be loaded and executed. Macro files can be edited in a text editor. When creating a command sequence, you add comments to the file by starting a line with @@.

- To run a macro file, in the SYS or DICTRA module type `MACRO_FILE_OPEN`, followed by the name of the macro file. DICTRA runs the MACRO_FILE_OPEN sequence that the file contains.
- To remain in the console and keep working in the DICTRA module, in the SYS, DICTRA, POLY, or POST module add the command SET_INTERACTIVE at the end of the macro file. Alternatively, use `EXIT` as the final command.

Workspace Files

Workspaces files for the Diffusion Module (DICTRA) have the file extension *.DIC, which allow you to save all the data in your current workspace. A workspace contains all the data, specified settings and the result of any calculations performed. The saved data includes original and modified thermodynamic data, the last set of conditions and options, and the results of any simulations.

- At the `DIC` prompt use SAVE_WORKSPACES.
- To load the data and calculation results of a workspace file, at the `DIC` prompt use READ_WORKSPACES.

Opening the Module and Macro Files

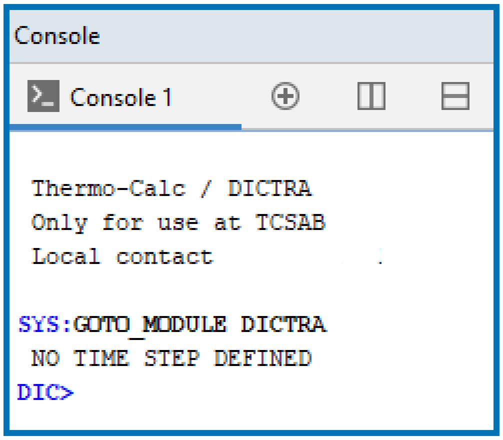
You can go to into the Console Mode to explore the command options, or continue with this quick start guide, which uses macro files to demonstrate how to use the software.

How to Open the DICTRA Module in Thermo-Calc

1. Open Thermo-Calc in Console Mode.

> By default, Thermo-Calc opens in the most recently used state. If it opens in Graphical Mode, on the toolbar, click **Switch to Console Mode**.

2. In the `SYS` module, type `GOTO_MODULE DICTRA`. For a list of all the available commands in the current module, at the prompt type a question mark (?) and press <Enter>. For a description of a specific command, type `Help` followed by the name of the command.



```
 Thermo-Calc / DICTRA
 Only for use at TCSAB
 Local contact

SYS:GOTO_MODULE DICTRA
 NO TIME STEP DEFINED
DIC>
```

How to Open the Beginner Guide Examples

For the Console Mode examples included with your installation, you can open the .DCM files from the main menu. You can also open any macro file with a command or by dragging it into the Console window.

How to Open a Macro File from the Examples Folder

To open a specific macro file from the Examples folders included with your installation:

1. Open Thermo-Calc.
2. Confirm you are in Console Mode. If not, click the **Switch to Console Mode**button.
3. From the main menu, select **File →** or **Help → Examples Files**. The Console Mode folder opens (these are the Thermo-Calc macro files).
4. Double-click the **Diffusion Module - DICTRA** folder and navigate to an example folder.

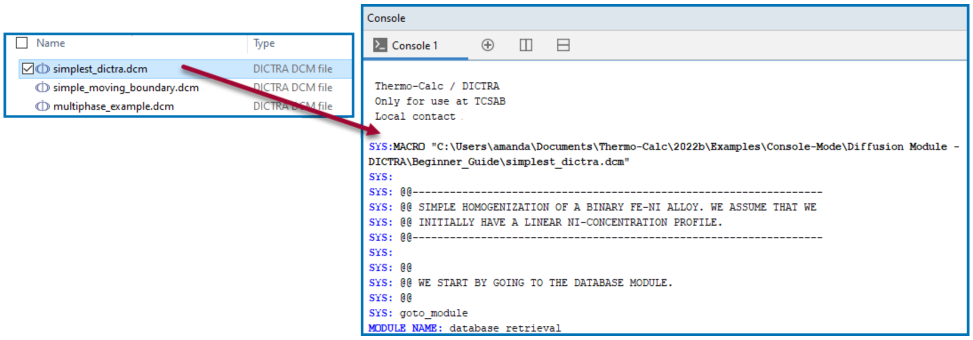
The three Quick Start example macros are in the first folder called **Beginner Guide**.

How to Use a Command in Console Mode

At the `SYS` prompt, type MACRO_FILE_OPEN and press <Enter>. In the file dialogue window that opens, locate and select the macro file on your computer.

Drag and Drop a Macro File into Console Mode

For example, navigate to the **Beginner Guide** folder and then drag the file from its location into Thermo-Calc Console window. The macro automatically runs after you drop it into the Console window.



☐ Name	Type
☑ simplest_dictra.dcm	DICTRA DCM file
simple_moving_boundary.dcm	DICTRA DCM file
multiphase_example.dcm	DICTRA DCM file

```
 Thermo-Calc / DICTRA
 Only for use at TCSAB
 Local contact

SYS:MACRO "C:\Users\amanda\Documents\Thermo-Calc\2022b\Examples\Console-Mode\Diffusion Module -
DICTRA\Beginner_Guide\simplest_dictra.dcm"
SYS:
SYS: @@------------------------------------------------------------------
SYS: @@ SIMPLE HOMOGENIZATION OF A BINARY FE-NI ALLOY. WE ASSUME THAT WE
SYS: @@ INITIALLY HAVE A LINEAR NI-CONCENTRATION PROFILE.
SYS: @@------------------------------------------------------------------
SYS:
SYS: @@
SYS: @@ WE START BY GOING TO THE DATABASE MODULE.
SYS: @@
SYS: goto_module
MODULE NAME: database retrieval
```

Double-click to Open a File

Navigate to the macro file location, for example where each set of file examples is in its own folder. If you already have Thermo-Calc open, the macro opens in a new tab. Otherwise a new instance of Thermo-Calc is launched.

Basic Terminology

The following definitions are useful to help you understand the examples and commands in this guide. For more detailed information search or browse the online help (**Help →Online Help**).

Cells and Regions in a System

A system normally consists of one *cell*. This cell contains one or several *regions* in which the diffusion problem is to be solved. A system of diffusion equations is solved for each region. The size of the system is the sum of sizes of all the regions in all the system's cells.

The interface between two regions typically moves as the result of a simulation, that is, the regions grow or shrink. Such an interface is called an *inner interface*. The boundary of a cell is called an *outer interface* and the condition of this type of interface may be affected by the choice of boundary conditions.

For some simulations it is useful to have several cells in a system. Matter can move between cells. However, it is assumed that there is diffusional equilibrium between all cells (this means that there are no differences in diffusion potentials between cells). In other words, the size of a cell is fixed during the simulation.

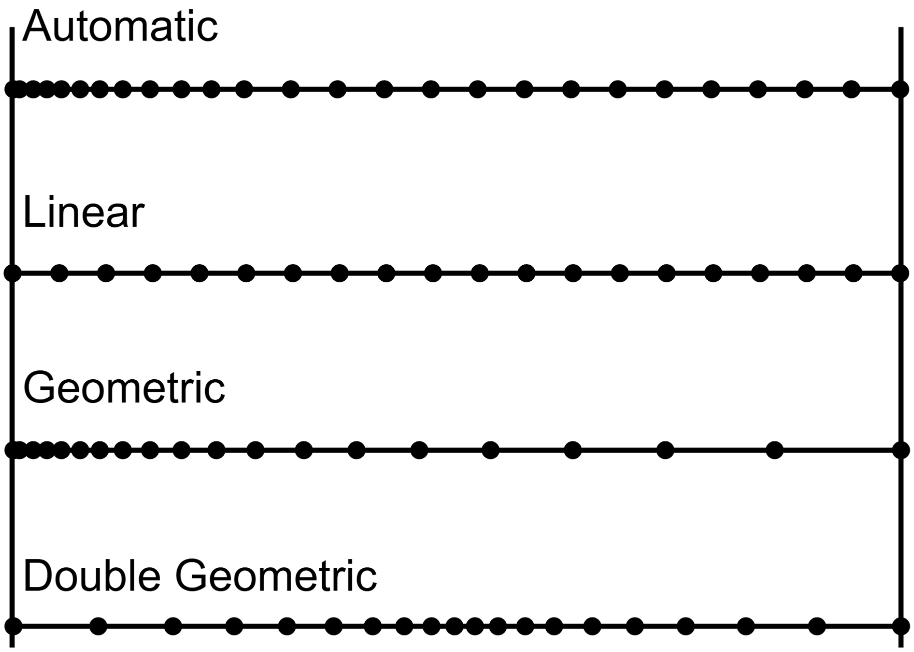
By default this is a *closed system*, which means that matter cannot move across its boundaries. However, you can change this setting for both the *lower boundary* (left side/centre) and the *upper boundary* (right side/surface) of the system. You can also set these boundary conditions to vary as a function of time, temperature and/or pressure.

Regions and Grids

A *region* contains one or more phases. If a region contains several phases one of those must be entered as a *matrix phase* whereas the others are entered as *spheroid*.

A region must also contain a number of *grid points*. The composition is only known at these grid points and the software assumes that the composition varies linearly between them. The amount and composition of all the phases present at a single grid point in a certain region are those given by thermodynamic equilibrium keeping the over-all composition at the grid point fixed.

These grid types are used in diffusion simulations: automatic, linear, geometric, and double geometric. When you are setting up the simulation, in either Console Mode or Graphical Mode, a region must have a grid defined.



Phases

Each region contains one or more *phases*. A phase can be of the *matrix*, *spheroid* or *lamellar* type. A phase can be introduced with the status *active* (the default) or *inactive*.

An inactive phase is a phase which does not participate in the calculations until it is stable. If a phase is inactive, then the driving force for precipitation of the phase is continuously monitored. When the driving force exceeds a predefined positive value, the phase take parts in the simulation and the phase automatically becomes active. A new region is then created and the formerly inactive phase is entered as the matrix phase of the new region. The name of the region is set to the name of the phase that just became active but with `R_` added as a prefix.

Composition

For Graphical Mode, see Diffusion Module Terminology in Graphical Mode.

Two types of composition variables are used within the program: site-fractions and u-fractions, although you can also use weight fraction or mole fraction, for example.

The *site-fractions* are used to set up the problem and interface with POLY-3 (in Console Mode). The site fraction of a species *k*, y_k, is the fraction of equivalent lattice sites occupied by species k. It is the only concentration variable that uniquely defines the composition and the constitution of a phase and it is necessary to use the site fraction in the storage of the data during a simulation.

The *u-fractions* are used in the diffusion equations. The u-fraction of a component *k* is defined as

$$u_k = \frac{x_k}{\sum_{j \in S} x_j}$$

The summation is only performed over the substitutional elements. The choice of the volume fixed frame of reference in the calculations make it convenient to use a composition variable which is related to the volume. The definition of the u-fraction is based upon the assumption that a species may or may not contribute to the volume of a phase. An interstitial element is assumed to not contribute to the volume. Substitutional elements are assumed to contribute equally to volume.

Geometry and Coordinates

The Diffusion Module (DICTRA) can only handle diffusion problems where composition vary along one spatial coordinate. The geometry of your system can be *planar*, *cylindrical* or *spherical*.

Planar Geometry

This geometry corresponds to an infinitely wide plate of a certain thickness. If the system has a planar geometry then the lower boundary (the zero coordinate) is at the left side of the system. The upper boundary (the coordinate with the highest value) is at the right side of the system.

Cylindrical and Spherical Geometries

- Cylindrical geometry corresponds to an infinitely long cylinder of a certain radius.
- Sypherical geometry corresponds to a sphere with a certain radius.

By default for both geometries, the lower boundary (the zero coordinate) is at the centre of the cylinder/sphere. The upper boundary (the coordinate with the highest value) is at the *surface* of the cylinder/sphere. You can enter a left most coordinate that is larger than zero to allow for tube and hollow sphere geometries.

Boundary Conditions

Boundary conditions are conditions that define how matter behaves at the boundaries of your system. By default, matter is not allowed to cross the system boundaries.

You can change the setting for both the lower boundary (left side/centre) and the upper boundary (right side/surface) of the system.

Setting up a Simulation in Console Mode

Although there are several commands to learn to correctly set up a DICTRA module simulation, the sequence in which to proceed is basically the same:

1. Define and read **thermodynamic** and **kinetic** data.
2. Set **global conditions** (i.e. temperature, *T*, and pressure, *P*).
3. Enter **region(s)**.
4. Enter **grid(s)** in region(s).
5. Enter **phase(s)** in region(s).
6. Enter **composition(s)** of phase(s).
7. Set **geometry** (optional – by default, the geometry is planar).
8. Set **boundary conditions** (optional – by default, the boundaries are closed).
9. Set the simulation **time**.
10. **Run** the simulation.

? For definitions of the above, see Basic Terminology.

The following sections describe each step in more detail for these simulation types:

- About the Single Phase Simulation
- About the Moving Phase Boundary Simulation
- About the Multiphase Simulation

Single Phase Simulations

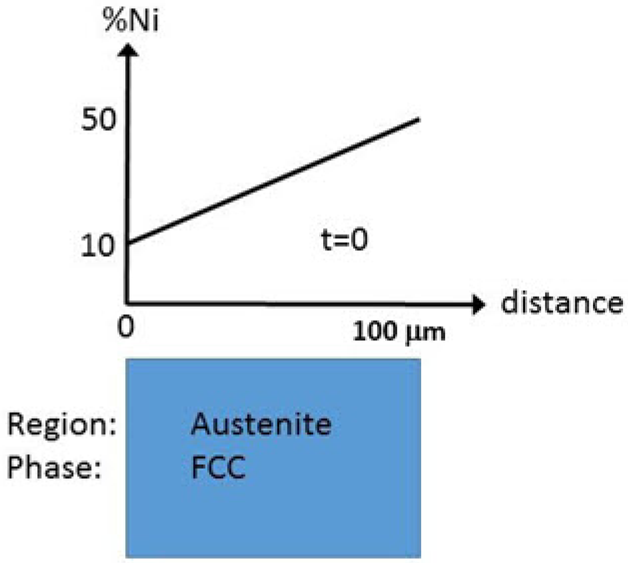
In this section:

About the Single Phase Simulation

In a 100 µm wide planar domain, the single phase example simulates the diffusion of Fe and Ni at a temperature of 1400 K. At this temperature the material is fully austenitic, i.e. the only phase present is the so-called fcc (face centered cubic) phase (in Thermo-Calc the name of this phase is FCC_A1). Initially, there is a linear variation in Ni going from 10 mass-% on the left-hand side to 50 mass-% on the right-hand side.

The simulation time is slightly different between the modes. For Console Mode it is 10^5 s and for Graphical Mode it is 30 hours.

By default the boundaries are closed. The plot generated shows the initial and final Ni profile.



Schematic view of the initial state of Single Phase Diffusion example. The width of the domain is 100 µm and there is a linear gradient in composition going from 10 to 50 mass-% Ni. There is a single region named Austenite that consists of an fcc phase.

Theory for the Single Phase Simulation

The flux of a component k in the z-direction in an isobarothermal system is in general given by

$$J_k = \sum_{i=1}^{n} L_{ki} \frac{\partial \mu_i}{\partial z}$$

where L_{ki} is a matrix of kinetic coefficients and μ_i is the chemical potential of component i. The correlation effects, i.e. the coupling of the flux of k component to the chemical potential gradients of the other elements, are normally neglected

$$(L_{ki} = 0, k \neq i)$$

and thus

$$J_k = L_{kk} \frac{\partial \mu_k}{\partial z} = M_k c_k \frac{\partial \mu_k}{\partial z}$$

where c_k is the concentration and M_k the mobility of component k.

The equation for the flux is combined with the equation of continuity, which takes the following form in a planar domain,

$$\frac{\partial c_k}{\partial t} = \frac{\partial}{\partial z}(-J_k)$$

which relates the local evolution of the concentration of k to the divergence of the flux.

The expression for the flux can be expanded in terms of concentration gradients

$$J_k = -\sum_{i=1}^{n} M_k c_k \frac{\partial \mu_k}{\partial c_j} \frac{\partial c_j}{\partial z} = -\sum_{i=1}^{n} D_{kj} \frac{\partial c_j}{\partial z}$$

where the diffusion coefficient of component k with respect to the concentration gradient of component j has been introduced.

$$D_{kj} = M_k c_k \frac{\partial \mu_k}{\partial c_j}$$

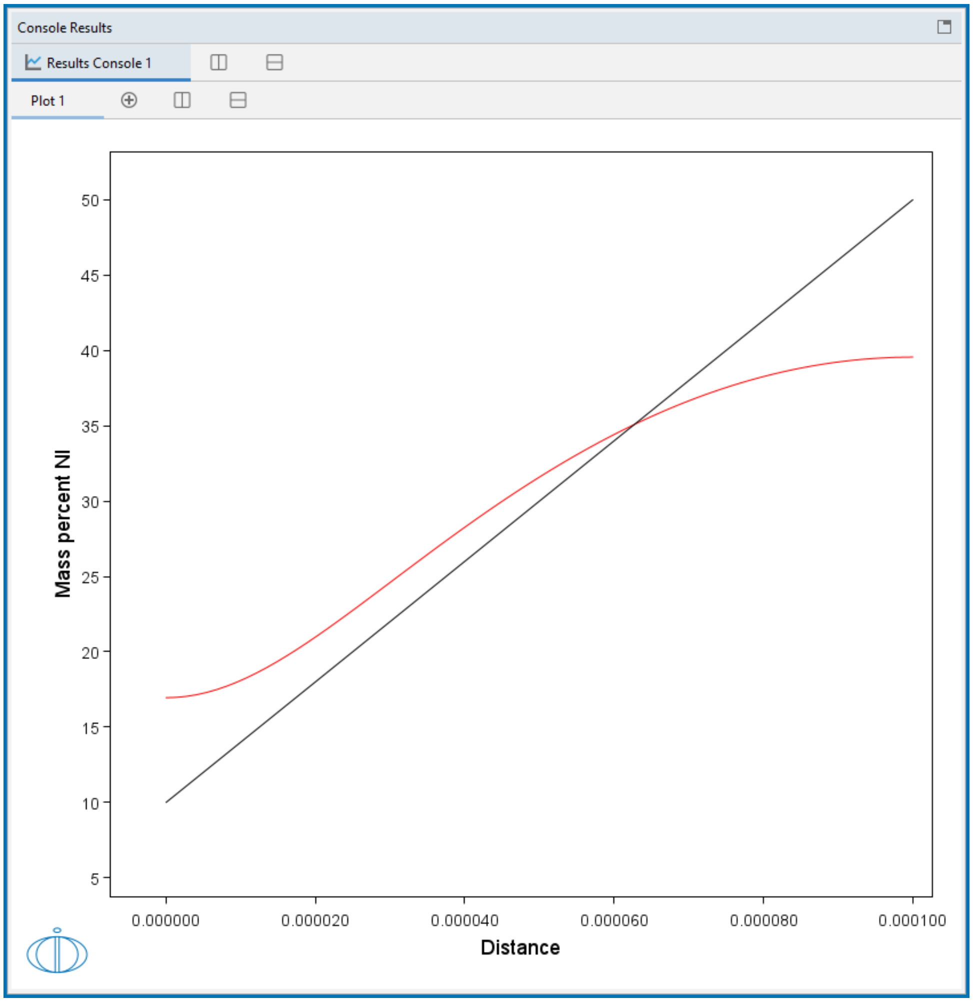
The flux expressions above are given in the so-called lattice-fixed frame of reference. In practical calculations it is more common to use a volume-fixed frame of reference. For a discussion of these concepts, see Andersson and Ågren [1992And].

References

Running the Single Phase Simulation

For the single phase simulation, you use an example macro file called `simplest_dictra.dcm`. Open this file in in Console Mode as described in Opening the Module and Macro Files.

The simulation should automatically be set up, executed and finished within a matter of seconds. Results are plotted in the **Console Results** plot window.

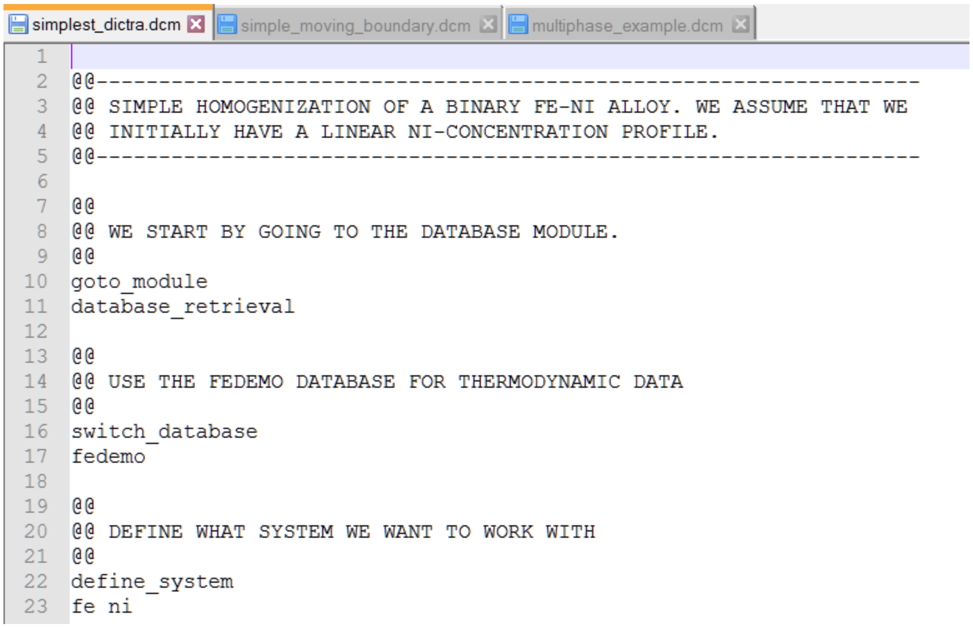


Output from the Single Phase example showing the initial and final Ni profile.

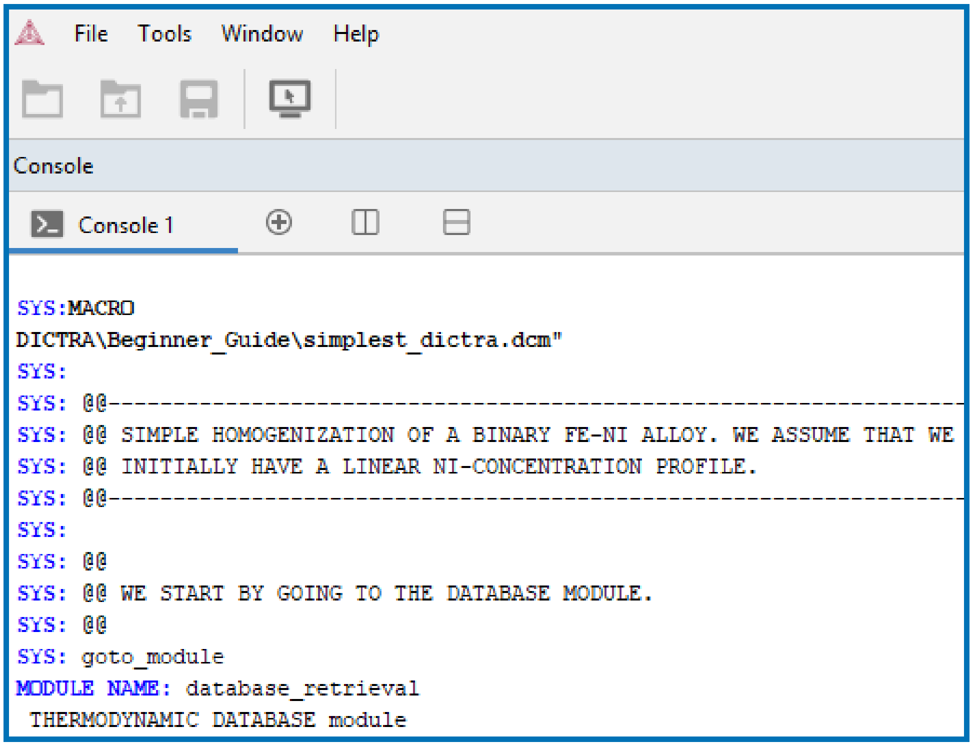
For the rest of the exercise, you will learn how to build this example step-by-step.

Single-Phase Command Details

To examine the commands in the macro file, you can either open the file `simplest_dictra.dcm` in a text editor or scroll to the top of the **Console** window.



```

@@------------------------------------------------------------------
@@ SIMPLE HOMOGENIZATION OF A BINARY FE-NI ALLOY. WE ASSUME THAT WE
@@ INITIALLY HAVE A LINEAR NI-CONCENTRATION PROFILE.
@@------------------------------------------------------------------

@@
@@ WE START BY GOING TO THE DATABASE MODULE.
@@
goto_module
database_retrieval

@@
@@ USE THE FEDEMO DATABASE FOR THERMODYNAMIC DATA
@@
switch_database
fedemo

@@
@@ DEFINE WHAT SYSTEM WE WANT TO WORK WITH
@@
define_system
fe ni
```

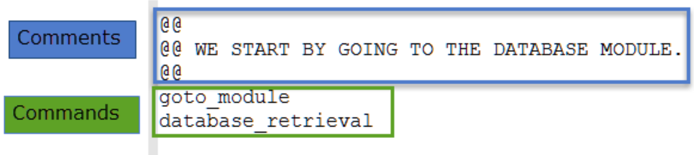


```
SYS:MACRO
DICTRA\Beginner_Guide\simplest_dictra.dcm"
SYS:
SYS: @@------------------------------------------------------------------
SYS: @@ SIMPLE HOMOGENIZATION OF A BINARY FE-NI ALLOY. WE ASSUME THAT WE
SYS: @@ INITIALLY HAVE A LINEAR NI-CONCENTRATION PROFILE.
SYS: @@------------------------------------------------------------------
SYS:
SYS: @@
SYS: @@ WE START BY GOING TO THE DATABASE MODULE.
SYS: @@
SYS: goto_module
MODULE NAME: database_retrieval
 THERMODYNAMIC DATABASE module
```

In the following sections, the commands are discussed in the order they are executed. The first time a command appears it is listed in its general form in UPPERCASE and then using `code font` to detail the specific form of the example. For subsequent examples, only the new commands are detailed. All commands may be abbreviated as long as they are unambiguous.

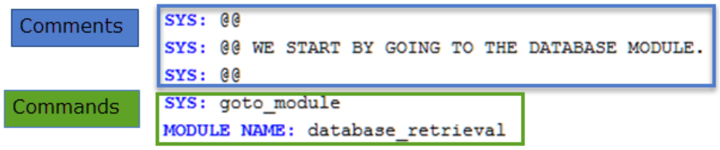
You can also review the comments included in the example files. The first command you will use is shown in the macro file as follows:

In a Text Editor



```
@@
@@ WE START BY GOING TO THE DATABASE MODULE.
@@
goto_module
database_retrieval
```

In Thermo-Calc



```
SYS: @@
SYS: @@ WE START BY GOING TO THE DATABASE MODULE.
SYS: @@
SYS: goto_module
MODULE NAME: database_retrieval
```

Single Phase - Specifying the Thermodynamic System

Thermo-Calc Console Mode has several modules used for different purposes. In order to define the thermodynamic system the DATABASE_RETRIEVAL module is used.

GOTO_MODULE <MODULE>

`goto_module database_retrieval`

There are many databases for different purposes and material types. In this example the *fedemo* database is used. This is the thermodynamic iron demonstration database.

SWITCH_DATABASE <DATABASE>

`switch_database fedemo`

Determine what elements to use in the simulation, in this case `Fe` and `Ni`.

DEFINE_SYSTEM <LIST OF ELEMENTS>

`define_system fe,ni`

Only the FCC_A1 phase takes part in this simulation and therefore all phases are initially rejected (the wildcard * means *all phases* in this context) and then, with the next command, the FCC_A1 phase is restored.

REJECT <ELEMENTS, SPECIES, PHASES, CONSTITUENT OR SYSTEM> <LIST OF THE RELEVANT TYPE>

```
reject phases *
```

RESTORE <ELEMENTS, SPECIES, PHASES OR CONSTITUENTS> <LIST OF THE RELEVANT TYPE>

```
restore phases fcc_a1
```

The thermodynamic system now consists of the elements `Fe` and `Ni` and the `fcc_a1` phase.

To actually read the data from file into computer memory the GET_DATA command must be executed.

GET_DATA

```
get_data
```

At this stage only the thermodynamic data is defined and read. The kinetic data (mobilities) are, in this case, stored in another database. This is normally the case though it is possible to have both thermodynamic and kinetic data in a single database.

To add data from a different database the APPEND_DATABASE command is used. The kinetic data in this example is stored in the *mfedemo* database. This is the kinetic iron demonstration database.

APPEND_DATABASE <DATABASE>

```
append_database mfedemo
```

The same sequence of commands used for thermodynamic data is used to read kinetic data from this database.

```
define_system fe,ni
reject phases *
restore phases fcc_a1
get_data
```

Setting up the Single-Phase Simulation

The simulation set-up is performed in the DICTRA_MONITOR module.

```
goto_module
dictra_monitor
```

In this example only one *global* condition is set, temperature. The other global condition that can be set is pressure, but that is rarely done as the default value (1 atm) is set automatically and usually accepted.

SET_CONDITION <GLOBAL OR BOUNDARY>

```
set_condition global
```

The SET_CONDITION command is immediately followed by these sub-prompts:

<T OR P>

```
T
```

The T is for temperature. Then follows a standard procedure for entering temporally piecewise functions:

<LOW TIME LIMIT> <FUNCTION> <HIGH TIME LIMIT> <Y/N> <IF Y, THEN NEXT FUNCTION> <...>

```
0 1400; * N
```

These prompts start with the *low time limit*, here zero (`0`), then the *function* (here the constant value `1400`) closed by a semicolon (`;`), then the *high time limit* (here a wildcard `*` is entered), then a `Y` or a `N` depending on whether more functions will be entered (in this case `N` because only a single function is entered).

The wildcard * used for the upper time limit means that the entered function is valid for the whole simulation. What this means is that a constant temperature equal to 1400 K is used during the whole simulation.

In any simulation at least one *region* must be defined. This is a named container that designates a certain part of, in this case the whole, domain. The name of a region is arbitrary and specified by you.

ENTER_REGION <NAME OF REGION>

```
enter_region austenite
```

The use of regions becomes clearer in the context of so-called moving phase boundary simulations (see About the Moving Phase Boundary Simulation).

A region must contain a numerical *grid* specified by width and type.

ENTER_GRID_COORDINATES

<NAME OF REGION FOR WHICH GRID IS TO BE ENTERED>

<WIDTH OF REGION>

<TYPE OF GRID>

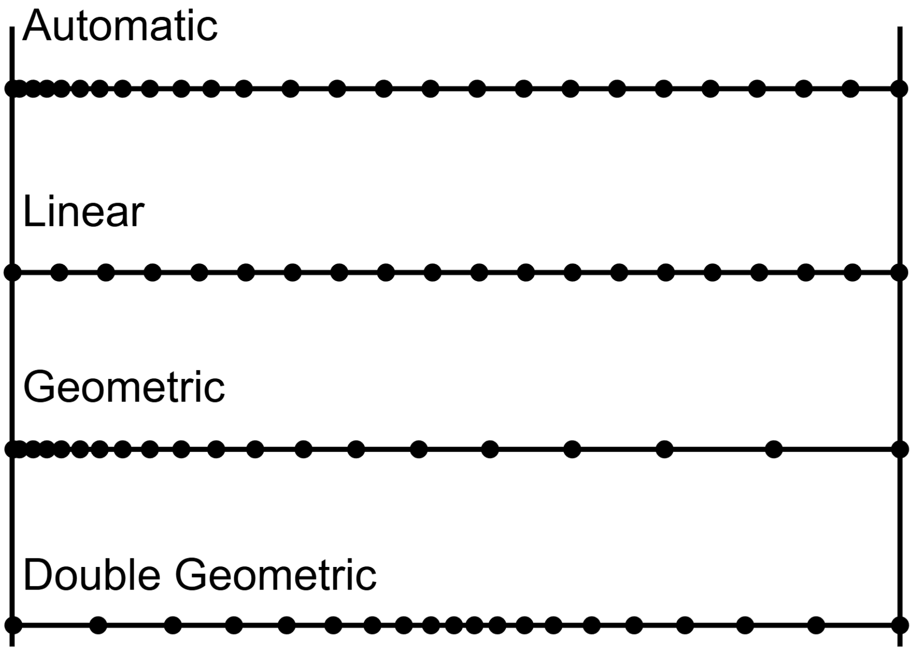
<NUMBER OF GRID POINTS>

```
enter_grid_coordinates
austenite
1e-4
```

```
auto
```

In the entries above, a 10^{-4} m wide (`1e-4`), `auto`. There are many types of grids, and a good choice is the automatic (`auto`) grid point distribution. An appropriate grid is generated at the start of the simulation where the grid points are automatically distributed according to the entered composition profile and boundary conditions.

These grid types are used in diffusion simulations: automatic, linear, geometric, and double geometric. When you are setting up the simulation, in either Console Mode or Graphical Mode, a region must have a grid defined.



A region must contain one *active* phase of type *matrix*. The meaning of active/inactive and phase type is explained in the next examples.

ENTER_PHASE_IN_REGION

<ACTIVE OR INACTIVE>

<NAME OF REGION>

<PHASE TYPE IN REGION>

<PHASE NAME>

```
enter_phase_in_region
active
austenite
matrix
```

```
fcc_a1
```

In this example only one phase participates, the `fcc_a1` phase, and it must therefore be `active` and of type `matrix`.

The initial composition profile must be specified for all phases that take part in a simulation. Since there are only two elements, Fe and Ni, in the present simulation the initial *composition profile* must only be given for one of them.

ENTER_COMPOSITIONS

<REGION NAME>

<PHASE NAME>

<DEPENDENT COMPONENT>

<COMPOSITION TYPE>

<COMPONENT NAME>

<TYPE OF COMPOSITION PROFILE>

<COMPOSITION PROFILE DEPENDENT INPUT>

```
enter_compositions
austenite
fcc_a1
fe
weight_percent
ni
linear
10
50
```

In the above entries, `Fe` is chosen as the dependent component and the initial profile for Ni is a `linear` variation going from `10` mass-% on the lower/left hand side of the system to `50` mass-% on the upper/right hand side of the system. The composition type can be chosen among a number of different types, e.g. `weight percent` or mole fraction. There are also many different ways of specifying the composition profile, e.g. an arbitrary position dependent function or reading it for each grid point from file. Here the simplest possible type is used a `linear` function.

Now you set the simulation time. If not specified the initial time is set to zero.

SET_SIMULATION_TIME

<SIMULATION END TIME>

<AUTOMATIC TIMESTEP CONTROL Y/N>

<MAXIMUM TIMESTEP>

<INITIAL SIZE OF TIMESTEP>

<SMALLEST ALLOWED TIMESTEP>

```
set_simulation_time
1E5
y
1E4
1E-7
1E-7
```

Here the simulation time is set to 10^5 [s] (`1E5`), the maximum timestep size to 10^4 (`1E4`) and the initial and smallest acceptable to 10^{-7} (both `1E-7`). The *automatic timestep control* should normally always be turned on, which it is by default (you answer `Y` above).

Now you save the workspace:

SAVE_WORKSPACES <FILENAME> <OVERWITE EXISTING FILE Y/N>

```
save_workspaces simplest_dictra y
```

> The command name SAVE_WORKSPACES can be misleading. The meaning of this command is roughly set result file. The set-up is saved immediately, but all results during the simulation are also saved to the selected file.

Running and Plotting the Simulation

The SIMULATE_REACTION command starts the simulation.

```
simulate_reaction
```

In order to plot results it is necessary to enter the POST_PROCESSOR sub-module (note that the GOTO_MODULE command is not used).

```
post_processor
```

In most cases, either a specific position in the domain or one or more specific times must be specified with the SET_PLOT_CONDITION command, depending on whether time or spatial position is chosen as independent (x-axis) variable.

SET_PLOT_CONDITION <CONDITION WITH ARGUMENTS>

```
set_plot_condition time 0,1e5
```

Here, the composition profile of Ni at the initial and final time is plotted and thus `time` is chosen as plot condition.

In other cases distance can be given relative to, for example, a phase interface, hence the global specification.

SET_DIAGRAM_AXIS <X OR Y> <AXIS QUANTITY>

```
set_diagram_axis x distance global
```

In this example the only meaningful measure of distance is relative to the domain as a whole, i.e. the leftmost position is zero and the rightmost position corresponds to the width of the region (10^{-4} m).

The dependent property to be plotted is mass-% Ni.

```
set_diagram_axis y weight_percent ni
```

Then plot the diagram:

PLOT_DIAGRAM

```
plot_diagram
```

In the **Console Results** plot window, graphs of the initial and final Ni profile display. Finally, the SET_INTERACTIVE_MODE command is executed to return control to the user. If the command is absent in a macro the program terminates when the end of the macro file is reached.

SET_INTERACTIVE_MODE

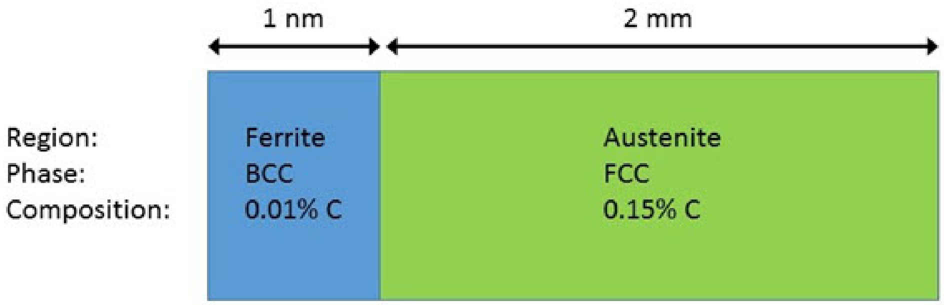
```
set_interactive_mode
```

Moving Phase Boundary Simulations

In this section:

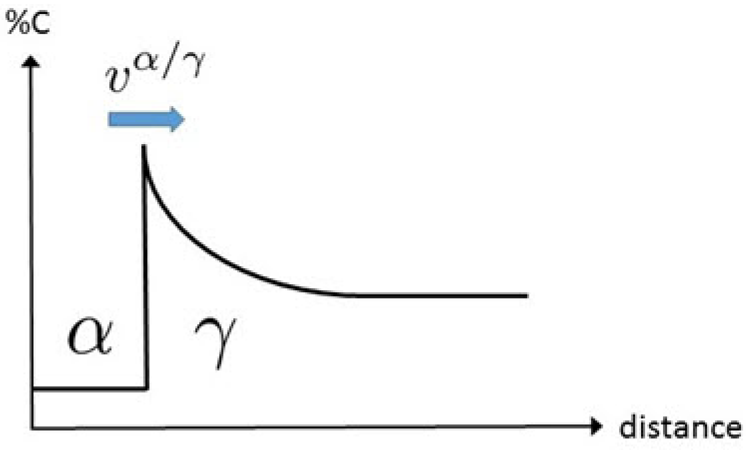
About the Moving Phase Boundary Simulation

The growth of ferrite (bcc) into austenite (fcc) is simulated in this example. The austenite is assumed to be initially homogeneous with the composition Fe - 0.15 mass-% C and the transformation temperature is 1050 K. The initial thickness of the austenite is 2 mm and an initially very thin ferrite (1 nm) is also present at the start of the simulation. The initial state is as below.



The set-up of the Moving Boundary example. There are two regions, Ferrite and Austenite, consisting of bcc and fcc, respectively.

A schematic graph of the carbon profile during the transformation is shown in the image below. Crusius et al. [1992Cru-1] is recommended as further reading.



Schematic view of the carbon profile during the transformation from austenite (γ) to ferrite (α) in the Moving Boundary example.

References

Theory for the Moving Phase Boundary Simulation

It is assumed that local equilibrium holds at the phase interface, i.e. the chemical potentials of all elements are continuous across the boundary, but the chemical potential gradients are in general discontinuous.

In order to maintain mass balance a set of flux balance equations must be satisfied at the phase interface:

$$v^{\alpha/\gamma}(c_k^\alpha - c_k^\gamma) = J_k^\alpha - J_k^\gamma \qquad k = 1, \ldots, n-1$$

where v is the interfacial velocity. The concentrations and the fluxes c and J are those at the interface on the α and γ sides, respectively.

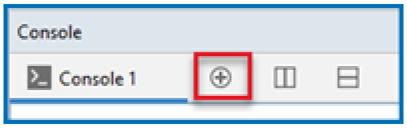
In the present case there are no degrees of freedom at the interface and the concentrations can be taken directly from a phase diagram. There is only one flux balance equation and the interface velocity can be evaluated once the fluxes at the interface are known. However, for ternary and higher systems the state at the interface must be found by some iterative procedure.

For more information on moving phase boundary problems, see, for example, [1982Ågr], [1992Cru-2], and [1997Hög].

References

Run the Macro File and Learn the Commands

If the single phase example has just been run, then either restart the software program or open another Console window by clicking the green button with the plus sign.



At the `SYS` prompt, type `macro` (short for the MACRO_FILE_OPEN command) and press <Enter>. Locate and select the macro file called `simple_moving_boundary.dcm` as described in Opening the Module and Macro Files. The commands in the macro file set up, run and plot the simulation in the Console Results window.

In the macro file some abbreviations of the commands are used. You can shorten command names in an arbitrary manner as long as the abbreviations are unambiguous.

In the macro file most commands are first given as comments with the full name and then abbreviated. Commands that were not used in the single-phase simulation, or are used differently, are explained in more detail.

> Comments in the macro file can be entered after two `@@` symbols. In most cases the arguments of a command can be entered on the same line as the command itself.

Single-Phase Command Details

Moving Phase - Specifying the Thermodynamic System

This set of commands is the same as in the single-phase simulation example. Thermodynamic and kinetic data is read for Fe and C and the bcc and fcc phases.

```
@@ goto_module database_retrieval
go da
@@ switch_database fedemo
sw fedemo
@@ define_system fe,c
def-sys fe c
@@ reject phase *
rej ph *
```

```
@@ restore phase fcc_a1,bcc_a2
rest ph fcc,bcc
@@ get_data
get
@@ append_database mfedemo
app mfedemo
@@ define_system fe,c
def-sys fe c
@@ reject phase *
rej ph *
@@ restore phase fcc_a1,bcc_a2
rest ph fcc,bcc
@@ get_data
Get
```

Setting Up the Moving Phase Boundary Simulation

The first region to be entered is entered in the same way as in the single-phase simulation.

```
@@ goto_module dictra_monitor
go d-m
@@ set_condition global T 0 1050; * N
set-cond glob T 0 1050; * N
```

A constant temperature equal to `1050` K is used in this simulation.

```
@@ enter_region ferrite
ent-reg ferrite
```

The phase interface between ferrite and austenite is created by introducing a region called austenite that is attached to the ferrite region. Regions are always separated by phase interfaces and must therefore always contain different *matrix* type phases.

ENTER_REGION

<NAME OF REGION>

<NAME OF EXISTING REGION TO ATTACH TO>

<ATTACH TO THE RIGHT OF EXISTING REGION Y/N>

```
enter_region
austenite
```

```
ferrite

y
```

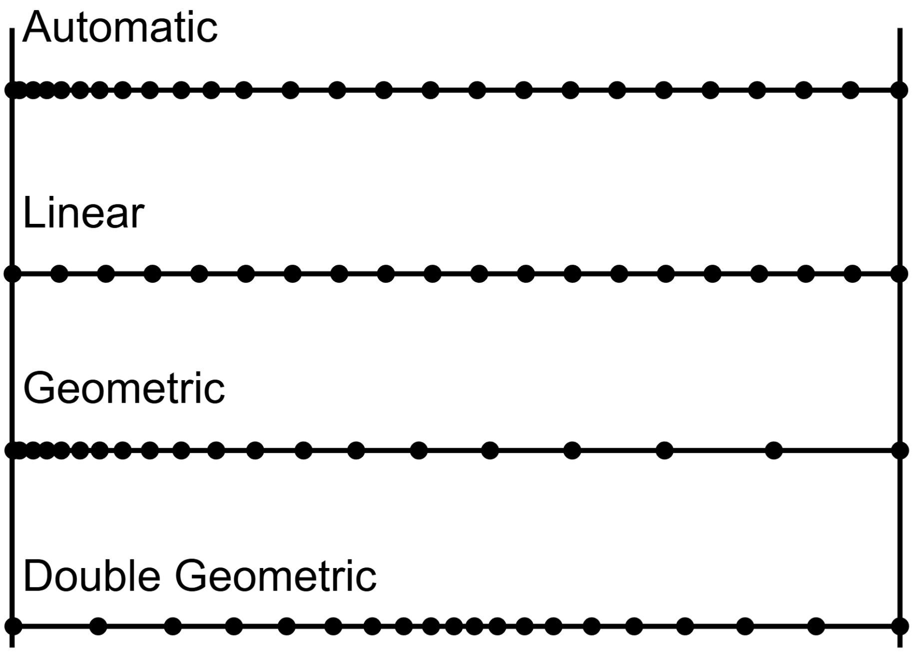
The domain now consists of two regions: `ferrite` and `austenite`.

As in the single-phase simulation example, the regions must contain both grids and one *active* phase of type *matrix*. These are entered separately for both regions.

```
enter-grid

ferrite

1e-9

auto

enter-grid

austenite

1e-9

auto
```

For both the `ferrite` and `austenite` regions, the same grid is used as in the single-phase simulation example, i.e. the automatic (`auto`) grid point distribution. An appropriate grid is generated at the start of the simulation where the grid points are automatically distributed according to the entered composition profile and boundary conditions.

These grid types are used in diffusion simulations: automatic, linear, geometric, and double geometric. When you are setting up the simulation, in either Console Mode or Graphical Mode, a region must have a grid defined.



Now the initial composition of both phases is entered. In this case Fe is automatically chosen to be the dependent component.

```
enter-phase
active
ferrite
matrix
bcc
enter-phase
active
austenite
matrix
fcc
```

Both phases are assumed to be initially homogeneous, the bcc phase having `0.01` mass-% C and the fcc phase `0.15` mass-% C, as shown in the following:

```
enter-composition
ferrite
bcc
w-p
C
linear
0.01
0.01
enter-composition
austenite
fcc
w-p
C
linear
0.15
0.15
```

Set the simulation time and other parameters related to the time-step size.

```
set-simulation-time
1e5
y
```

```
1e4
1E-7
1E-7
```

Finally, save the simulation set-up to file.

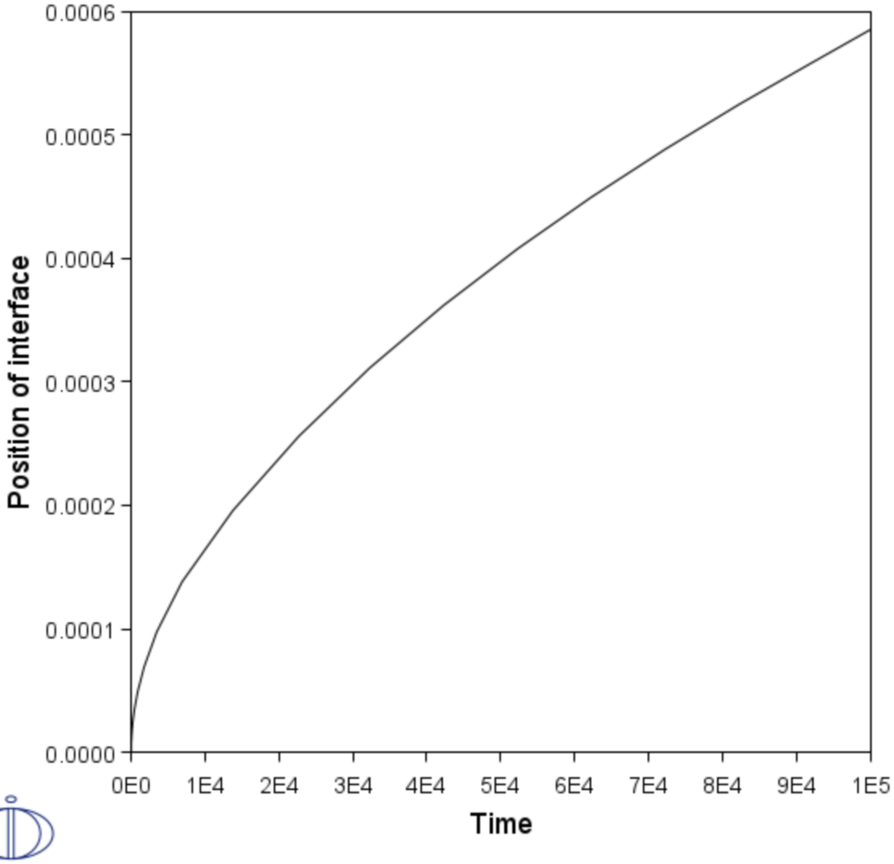
```
save simple_moving_boundary yes
```

Running and Plotting the Moving Phase Simulation

These commands are the same as in the single-phase example.

```
@@simulate_reaction
sim
@@ post_processor
post
```

The ferrite/austenite phase interface position as a function of time is plotted.



Output from the example simple_moving_boundary showing the phase interface position as a function of time.

As mentioned in the single phase example, in general either a specific spatial position or a specific time must be set as a plot condition. Here the phase `interface` is set as plot condition and it can be referenced as the lower interface of the austenite region or as the `upper` interface of the `ferrite` region.

SET_PLOT_CONDITION

<TYPE OF PLOT CONDITION>

<FOR INTERFACE CONDITION, SPECIFY REGION>

<LOWER OR UPPER INTERFACE OF REGION>

```
set-plot-condition

interface

ferrite

upper
```

Set time as x-axis variable

```
@@set-diagram-axis x time

s-d-a x time
```

Now set the interface position as y-axis variable

```
s-d-a y
```

POSITION_OF_INTERFACE

<SPECIFY REGION>

<LOWER OR UPPER INTERFACE OF REGION>

```
pos-of-int ferrite upper

@@ plot_diagram

plot
```

The plot has the parabolic appearance characteristic for many types of diffusion simulations.

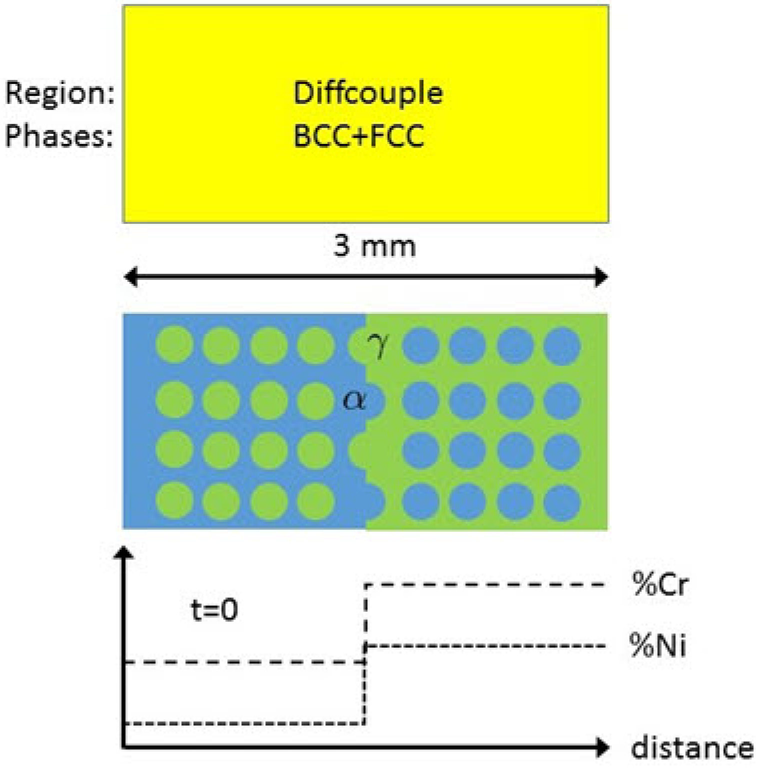
Multiphase Simulations

In this section:

About the Multiphase Simulation

This example simulates the evolution of an Fe-Cr-Ni diffusion couple during a 100 hour heat treatment at 1100° C (1373.15 K). Both end members of the diffusion couple are duplex ferrite plus austenite, but the majority phase is ferrite on the left-hand side and austenite on the right.

With this type of simulation it is assumed that the material is fully equilibrated at each grid point, i.e. the local phase fractions, phase compositions and so forth are obtained from an equilibrium calculation with the local overall composition as a condition.



Schematic view of the initial state of the Multiphase example. Two ternary Fe-Cr-Ni alloys form a diffusion couple. There is a single region (diffcouple) where both the bcc and fcc phases are entered. Both alloys are duplex bcc+fcc, but the majority phase is bcc (α) in the left-hand side alloy and fcc (γ) in the right.

Theory for the Multiphase Simulation

More details about the homogenization model for multiphase simulations can be found in Larsson and Engström [2006Lar] and Larsson and Höglund [2009Lar]. As mentioned in the description of this simulation, it is assumed that the material is locally fully equilibrated and that the local phase fractions, phase compositions and so forth are obtained from an equilibrium calculation with the local overall composition as a condition. From a numerical point of view the homogenization model treats the multiphase material as a single phase having the “average”, or “effective”, properties of the local phase mixture.

When estimating the effective kinetics of a multiphase mixture the product of solubility and mobility in each phase is considered. It is therefore convenient to define

$$\Gamma_k^\phi = M_k^\phi c_k^\phi$$

for each phase ϕ. The effective kinetics of the multiphase mixture is denoted and in this example it was evaluated using the lower Hashin-Shtrikman bound. The default method is a simple rule of mixtures

$$\Gamma^\star = \sum_\phi f^\phi \Gamma_k^\phi$$

where f^ϕ is the volume fraction of ϕ. The flux is obtained as

$$J_k = -\Gamma_k^\star \frac{\partial \mu_k}{\partial z}$$

which replaces the single-phase equation

$$J_k = L_{kk} \frac{\partial \mu_k}{\partial z} = M_k c_k \frac{\partial \mu_k}{\partial z}$$

for multiphase simulations.

? References

Run the Macro File and Learn the Commands

At the `SYS` prompt, type `macro` and pres <Enter>. Locate and select the macro file called `multiphase_example.dcm` as described in Opening the Module and Macro Files. The commands in the macro file should set up the simulation, run it and then produce a graph in the Console Results window.

Most of the set-up is the same as the single phase and moving phase boundary examples. Detailed comments are only given for the new commands for this simulation.

Single-Phase Command Details

Specifying the Multiphase Thermodynamic System

Data for Fe, Cr, and Ni and the fcc and bcc phases are read from the *fedemo* (thermodynamics) and *mfedemo* (mobility/kinetic) databases.

```
go da
sw fedemo
def-sys fe cr ni
rej ph *
rest ph bcc,fcc
get
app mfedemo
def-sys fe cr ni
rej ph *
rest ph bcc,fcc
get
```

Setting Up the Multiphase Simulation

Set the temperature `T` during the simulation to 1100° C (`1373.15` K) and enter a region `diffcouple`.

```
go dictra-monitor
set-cond glob T 0 1373.15; * N
ent-reg diffcouple
ent-grid
diffcouple
3e-3
```

```
auto
set-auto-grid-option
fine
```

The automatic (`auto`) grid point distribution is used as with the other examples. One more command SET-AUTO-GRID-OPTION is used and `fine` is chosen to set the number of equidistant points in a region (e.g. maximum distance between two adjacent grid points is the size of the region divided by this number) and the maximum factor that is allowed in the geometric series defining the initial grid.

As always, a region must contain exactly one `active` phase that is of type `matrix`. In this example it is arbitrary whether it is the bcc or the fcc phase that is entered as matrix.

```
enter-phase
active
diffcouple
matrix
fcc
```

The bcc phase is entered in the same manner as the fcc phase, except that the type is set as `spheroid`.

```
enter-phase
active
diffcouple
spheroid
bcc
```

The initial composition profile of the fcc phase is entered as a `function` of distance.

```
enter-composition
diffcouple
fcc
fe
m-f
cr
function
2.57e-1+(4.23e-1-2.57e-1)*hs(x-1.5e-3);
ni
function
6.47e-2+(2.75e-1-6.47e-2)*hs(x-1.5e-3);
```

In the above entries, the `hs` denotes the Heaviside step function that has the following properties:

$$hs(x) = \begin{cases} 0, & x < 0 \\ 1, & x \geq 0 \end{cases}$$

The resulting Cr profile is thus `0.257` on the left half of the domain and `0.423` on the right with a sharp step at the center.

As shown in About the Multiphase Simulation.

The initial composition of the fcc phase is actually the initial overall composition. This is due to the choice of initial composition of the spheroid bcc phase.

ENTER_COMPOSITIONS

<REGION NAME>

<PHASE NAME>

<USE EQUILIBRIUM VALUE Y/N>

```
enter-comp

diffcouple

bcc

y
```

When entering the composition for a type spheroid phase it is possible to either, as here, let the composition of the matrix phase be the overall composition or manually enter a start composition and volume fraction.

The local kinetics of the multiphase mixture must be estimated by means of some function that may depend on the local phase fractions, phase compositions and the mobilities of the individual phases. The command for choosing the function to use is ENTER_HOMOGENIZATION_FUNCTION. There are many such homogenization functions to choose from. In this particular example the so-called lower Hashin–Shtrikman bound [1962Has] is a good choice.

ENTER_HOMOGENIZATION_FUNCTION

<ENTER FUNCTION NUMBER>

```
enter-homo-fun

1
```

Finally, set simulation time (100 h) and select the name of the result file:

```
set-sim-time

3.6e5

yes
```

```
3.6e4
1e-7
1e-7
save multiphase_example y
```

References

Running and Plotting the Multiphase Simulation Results

Run the simulation.

```
simulate
```

Go to the post processor.

```
post
```

Plot the mole fraction fcc phase as a function of distance at the end of the heat treatment.

```
set-plot-condition time last
set-diagram-axis x distance global
set-diagram-axis y npm(fcc)
```

Instead of explicitly entering the final time it is possible to use the keyword `last`. The `np` of npm stands for *number of moles* of the phase argument and the `m` is the normalizing quantity (moles). The limits of an axis can be set with the SET_SCALING_STATUS command. You manually set the scaling of the axis and then restore automatic scaling:

SET_SCALING_STATUS

<X OR Y AXIS>

<USE AUTOMATIC SCALING Y/N>

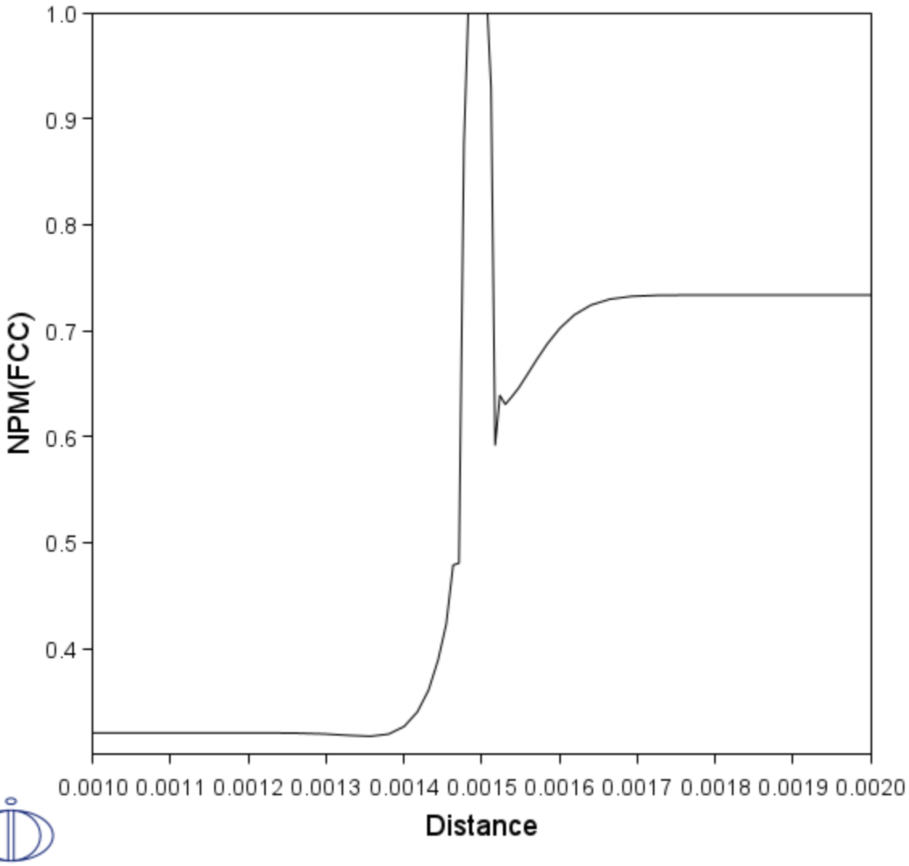
<IF MANUAL SCALING, ENTER LIMITS>

```
set-scaling-status x n 1e-3 2e-3
```

Plot the diagram.

```
plot
```

The plot below shows that a single phase fcc zone has formed and this was also observed experimentally, see [1995Eng].



Output from the multiphase_example showing the mole fraction fcc phase as a function of distance at the end of the heat treatment.

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Next Steps

Below are suggestions for you to learn more about using the Diffusion (DICTRA) Module.

- Browse the Online Help (press F1) or open one of the available PDFs included with your installation (**Help → Manuals Folder**).
- You have been working within Console Mode. You might also want to try the *Diffusion Module Graphical Mode Quick Start Guide* (**Help → Manuals Folder**). This further prepares you to work with the Console Mode examples.

There are several resources available on our website to help you learn how to use Thermo-Calc and other Add-on Modules. Go to the Getting Started Guides page and choose one of the guides that provides new users an introduction to setting up simple calculations in Graphical Mode. The information there is also in this help documentation.

- Run other Console Mode examples (**Help → Examples Files**), which contain some simulation types and advanced functionality not available in Graphical Mode. It is a good starting point when you are thinking of creating a new simulation. When you are setting up a new simulation there are two recommended ways to proceed:
  - Copy and gradually adjust an existing macro file from the examples collection.
  - Enter the set-up directly while recording a log file. The command for recording a log file is SET_LOG_FILE and this should be done immediately when starting the program in the SYS module. The log file can then be directly used as a macro file (it has the file extension *.TCM).
- You can also go to the Thermo-Calc website to see if there are other options suited to you, such as a course or video tutorials. To go to the web page, in the **Project** window, click the top **My Project** node and then click **Video Tutorials**. Or from the main menu, select **Help → Video Tutorials**.

The Role of Diffusion in Materials: A Tutorial is available for download on our website. It is intended for engineers interested in using the Diffusion Module (DICTRA), as well as students learning about the role of diffusion in materials. It is designed to be useful at many levels, from undergraduate studies to someone with a PhD and experience in a related field.

Diffusion Module (DICTRA) Command Reference

Thermo-Calc Version 2025b

About This Guide

The guide is for users already familiar with Console Mode and it includes all the commands applicable to the Diffusion Module (DICTRA). It is a supplement to the commands described for Thermo-Calc and which can be found by searching the online help.

How you proceed depends on your experience with the software as well as your level of expertise with diffusion problems. In addition to this guide, the following supplemental documentation and training resources can help you learn how to use the Diffusion Module (DICTRA) in Console Mode.

Documentation Resources

You can search or browse all the documentation available either from within Thermo-Calc (press F1 or go to **Help → Online Help**) or browse the PDFs included with your installation by going to **Help → Manuals Folder**).

Read more about the Diffusion Module (DICTRA) on our website. There is also a Getting Started with the Diffusion Module (DICTRA) page available. If you are in Thermo-Calc, press F1 to search the help to learn about the available settings included with the Add-on Module.

The Role of Diffusion in Materials: A Tutorial is available for download on our website. It is intended for engineers interested in using the Diffusion Module (DICTRA), as well as students learning about the role of diffusion in materials. It is designed to be useful at many levels, from undergraduate studies to someone with a PhD and experience in a related field.

Training and Video Tutorials

Some of the Graphical Mode examples have video tutorials. Watching those videos may help you with your simulation in Console Mode. You may also decide to enroll in a training course or use the self-paced Learning Hub.

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help →** **Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

DICTRA Module Commands

In this section:

General Commands

These commands are universal in Console Mode.

Command/Syntax	Description and Prompts
BACK	Return to the previous module. From the POST-processor you go back to the DICTRA-MONITOR module.
EXIT	Terminates the program and returns to the operating system. Unless a SAVE_WORKSPACES command has been given before all data entered is lost.
GOTO_MODULE	`Module name` Select and go to another module. The name of the module must be given. In order to obtain a list of available modules give a return.
HELP ?	Enter HELP or ? to either a list of all commands or specific help for a command by giving the command (abbreviated) `Command` The command for which a description is wanted should be given. If the abbreviation is not unique a list of all matching commands are given.

ADD_STOP_CRITERION

The ADD_STOP_CRITERION command is available to use once there is data included with a simulation. Use this command to add an alternative criteria (instead of the final time) to terminate the simulation.

SET_PLOT_CONDITION and Plot Condition and Independent Variable

Most of the "plot-conditions" in the post-processor can now be used as termination criteria for a DICTRA simulation.

Syntax	ADD_STOP_CRITERION
Prompts	`TYPE OF STOP CONDITION /INTEGRAL/:` An overall condition corresponding to the PLOT_CONDITION used in the post-processor to define where/how the criteria for termination is defined. Enter one of the following: • `DISTANCE`: Distance in the system. It defines a local or global position where the value of a state variable defines if the simulation should be terminated. • `INTERFACE`: At an interface where the value of a state variable defines if the simulation should be terminated. • `INTEGRAL`: Value is integrated over the phase/region/system volume (the default). An INTEGRAL VARIABLE value should be used to define the termination. See below for additional prompt details.

If `DISTANCE` is entered, then	`TYPE OF DISTANCE /GLOBAL/:`
	Fixed distance in the system. Enter one of the following:
	• `GLOBAL`: i.e. counted from the leftmost interface (the default).
	• `LOCAL`: i.e. counted from the interface to the left of the region. If this is entered then also enter,
	  • `NAME OF REGION`
	  • `DISTANCE`

If `INTEGRAL` is entered then	`INTEGRAL VARIABLE:` Enter the integral variable used to define the termination criteria. Integral Variables details how to construct the value.
If `INTERFACE` is entered then	Enter the interface of the system. Enter ? to list the options based on the set up. Options are:

Syntax	ADD_STOP_CRITERION
	- Region name - FIRST - LAST If a "region name" is entered, then you are further prompted: `UPPER OR LOWER INTERFACE OF REGION:` This then defines the position at as the interface at the UPPER or LOWER part of the named region.
	`STATE VARIABLE:` Enter the state variable used to define the termination criteria. See State Variables in Console Mode DICTRA for details about how to construct the value.
For either the `INTEGRAL VARIABLE` or `STATE VARIABLE`	`TERMINATION VALUE:` The criteria for the value of the variable that should trigger a termination of the simulation. Valid answers are for a numeric value.

ADVANCED_HOMOGENIZATION_OPTIONS

? UTILITIES_HOMOGENIZATION

Use this command and its subcommands with the HOMOGENIZATION_MODEL. Go to each command listed below for details.

Syntax	SPECIAL_HOMOGENIZATION_OPTIONS
Prompts	`Which option?` Enter ? to list the available commands as below. • BC_FOR_DEPENDENT_ELEMENT • SOLVE_IN_LATTICE_FIXED_FRAME • DEPENDENT_ELEM_BALANCE_FLUXES • USE_TWO_TYPES_OF_BOUNDARY_CON • CHECK_PHASE_SET

AMEND_CELL_DISTRIBUTION

Use this to amend the cell distribution factor of the currently selected cell.

Syntax	AMEND_CELL_DISTRIBUTION
Prompt	`Cell distribution factor /1/` A parameter that determines the weight of the cell, it can be used to simulate a distribution of different cell sizes. The default value is 1, i.e. a single copy of the same cell. Integer values are not required.

AMEND_MOBILITY_DATA

Use this command to change an existing parameter.

Also see ENTER_MOBILITY_DATA for information about the parameter names and prompts.

Syntax	AMEND_MOBILITY_DATA
Prompt	`Parameter name <Identifier> (<Phase>, <Component array>; <Digit>)` Enter `?` to get an overview

BC_FOR_DEPENDENT_ELEMENT

Use this command to allow an "active" boundary condition (BC) for a dependent element. It is available with the HOMOGENIZATION_MODEL as a command within the ADVANCED_ HOMOGENIZATION_OPTIONS.

The command enables you to enter a “fix flux” or an “activity-/potential-flux function” type of boundary condition for the dependent substitutional element if such a boundary condition is already entered for the independent elements.

Use of this command automatically ensures that the flux of the dependent element is not used to balance the independent fluxes, i.e. the feature “dependent element balance fluxes” is set to `No`.

Syntax	BC_FOR_DEPENDENT_ELEMENT
Prompts	`Enter BC for dependent element on lower boundary /NO/` If `YES` is entered, the subsequent prompts are the same as when the boundary condition was entered for the independent elements on the lower boundary; it is a prerequisite that such a boundary condition is already entered. This feature is only allowed with a “fix flux” or an “activity/potential flux function” type of boundary condition.
	`Enter BC for dependent element on upper boundary /NO/` If `YES` is entered, the subsequent prompts are the same as when the boundary condition was entered for the independent elements on the upper boundary; it is a prerequisite that such a boundary condition is already entered. This feature is only allowed with a “fix flux” or an “activity/potential flux function” type of boundary condition.

CHECK_DIFFUSION_MATRIX

Display the diffusion coefficient matrix for a phase at a given composition, pressure and temperature.

Syntax	CHECK_DIFFUSION_MATRIX
Prompts	`Output to screen or file /Screen/`
	`Phase name` Name of the phase for which the diffusion coefficient matrix is to be displayed.
	`Concentration of` Concentration of the component in U-fraction for which the diffusion coefficient matrix is to be displayed.
	`Pressure` Pressure for which the diffusion coefficient matrix is to be displayed.
	`Temperature` Temperature at which diffusion coefficient matrix is to be displayed. Use one or several of the options: • `D`: reduced diffusion matrix • `L:L` matrix (diagonal) • `P:L'` matrix • `B:L"` matrix • `M:MU(k)` array • `X:dMU(k)/dCj` matrix • `0`: unreduced diffusion matrix • `E`: Eigen values of matrix

CHECK_PHASE_SET

This command is available with the HOMOGENIZATION_MODEL as a command within the ADVANCED_HOMOGENIZATION_OPTIONS.

This command is only available with single region simulations.

One difficulty with single region multiphase simulations is to choose which phases should take part in the simulation, i.e. which phases should be entered in the region; what phases are stable, or become stable, is often a part of the question and the diffusion path is not known *a priori*. With this command it may be checked which, if any, phases read from the database but not entered in the region have become stable. The interval at which checks are made can be set to some extent. Whether a simulation should be terminated when a non-entered phase become stable can also be set. Finally, it can also be set whether some phases should be excluded from the check, if for example a phase has been read only to be used to define a reference state.

Syntax	CHECK_PHASE_SET

Prompt	`CHECK SET OF PHASES ENTERED INTO SIMULATION (Y/N):`
	`USE THIS FEATURE WITH DEFAULT SETTINGS? (Y/N):`
	if NO, the following settings can be made:
	`OPTIONS FOR CHECK INTERVAL:`
	`1. BEGINNING AND END OF SIMULATION`
	`2. EVERY TIME RESULTS ARE SAVED`
	`3. AS #2, BUT TERMINATE SIMULATION IF NON-ENTERED PHASE BECOME STABLE`
	`CHOOSE OPTION 1-3:`
	`PERFORM CHECK USING GLOBAL MINIMIZATION? (Y/N):`
	`SHOULD ANY PHASE BE EXCLUDED FROM THE CHECK? (Y/N):`
	if YES, then those phases are prompted for.

COARSENING_MODEL

About the Coarsening Model in the *Diffusion Module User Guide*

The model allows you to perform coarsening simulations. Use this command to explicitly set the DICTRA module to use this model.

Enable or disable the use of the simplified model for calculating Ostwald-ripening in multicomponent systems. This also must be used together with the SET_SURFACE_TENSION command.

To use this mode, configure the calculation as follows:

- Have one cell only, with a single particle that is 1.5 times larger than the average particle size.
- The matrix phase should be in contact with the maximum size particle on the left/lower side, and then the model specifies a local equilibrium with an average sized particle on the right/upper side.
- The surface energy then results in growth of both the maximum size particle and the matrix phase. Use SET_SURFACE_TENSION to enter the surface energy to enable coarsening.

Syntax	COARSENING_MODEL
Prompt	`Enable coarsening model /N/` By default the coarsening model is not used. Enter Y to enable the use of this model.

CREATE_NEW_CELL

Create a new cell and attach it to the list of current existing cells.

Syntax	CREATE_NEW_CELL
Prompt	`Cell distribution factor` A parameter that determines the weight of the cell, this parameter can be used in order to simulate a distribution of different cell sizes. This value can be viewed as the number of copies of the same cell. When modeling a particle size distribution it is useful to be able to enter different number of copies of different sized particles. However, it is not required to use integer values.

DEBUGGING

Determines the debugging level. Depending on the value given, different amounts of information are written onto the output device. This can be used to determine what causes the program to crash during a simulation.

Syntax	DEBUGGING
Prompt	`Debug level (Yes, No, 0, 1, 2, 3, 4) /N/` The level of debugging information to be displayed.

DELETE_REGION

Delete a region and all its associated data from the current cell.

Syntax	DELETE_REGION
Prompt	`Region name` The region name to delete.

DEPENDENT_ELEM_BALANCE_FLUXES

Use this command to set whether the dependent element should balance fluxes at the boundaries. This command is available with the HOMOGENIZATION_MODEL as a command within the ADVANCED_HOMOGENIZATION_OPTIONS.

For most boundary conditions (the notable exception being the “gas” type of boundary condition) the default behavior is that the boundary flux of the dependent substitutional element balances the fluxes of all other substitutional elements such that the size of the domain is preserved. This generally means that the flux of the dependent element equals minus the sum of all other substitutional elements.

This feature allow the balancing of boundary fluxes to be turned off and consequently the domain may change its size as a result of the boundary condition.

The input for this feature is `Yes` or `No`, where `No` mean that the balancing of boundary fluxes is turned off.

Syntax	DEPENDENT_ELEM_BALANCE_FLUXES
Prompt	`Dependent element balance the fluxes /Yes/:`

ENTER_COMPOSITIONS

Enter the composition into the phases in a region.

The Diffusion Module (DICTRA) in Graphical Mode uses a Diffusion Calculator instead of the Console Mode commands. Most of the Console Mode functionality is available on the Diffusion Calculator, described in the *Thermo-Calc User Guide*. However, you cannot use both Graphical Mode and Console Mode in the same simulation.

Syntax	ENTER_COMPOSITIONS
Prompts	`Region name` Name of the region into which the compositions are to be entered.
	`Phase name` Name of the phase in a region into which the compositions are to be entered.
	`Use equilibrium value` This is only for spheroid phases in simulations with dispersed phases. If this option is used the program automatically calculates the equilibrium fractions of the spheroid phase and its constitution at the start of the simulation.
	`Dependent substitutional species` A dependent substitutional species is required in order to be able to determine which species are independent. The program only queries for the compositions of the independent species. Sometimes the dependent species is chosen by the program and thus this question is never given. This may be due to stoichiometric constraints or to the fact that it has been set already in the kinetics database due to the model selected for the diffusion.
	`Dependent interstitial species` A dependent interstitial species is required in order to be able to determine which species are independent. The program only queries for the compositions of the independent species. Vacancies are always regarded as dependent and therefore if vacancies are present in the phase then this question is never given.
	`Composition type` Type of composition used for the constitution of the phase. Options are: SITE_FRACTION, MOLE_FRACTION, MOLE_PERCENT, WEIGHT_FRACTION, WEIGHT_PERCENT and U_FRACTION.
	`Type`

Syntax	ENTER_COMPOSITIONS
	Type of composition profile to be entered, options are: LINEAR, READ_POINT_BY_POINT, FUNCTION, and GEOMETRIC. • If READ_POINT_BY_POINT is chosen note the following. When compositions are read from a file it may often be the case that both grid coordinates and the composition at the grid points are given on the same line, e.g. the grid coordinates in the first column, the mole fraction of the first element at that grid point in the second column and so on. The column that contain the composition of a given element can then be specified in a macro file by, for example, having a line "read_point_by_point foo.dat 2". The "2" mean that the grid coordinates are in the 2nd column in the file foo.dat. In a corresponding manner the column that contain the grid point coordinates can be specified (see ENTER_GRID_COORDINATES). • If FUNCTION is chosen the composition profile can be given as a function of the global distance denoted X. Some useful functions are the error function denoted `erf(X)` and the Heaviside step-function denoted `hs(X)`. For example the function `3+2hs(x-1e-4)` provides a concentration of 3 at the left side and 5 at the right side with a sharp step in the concentration profile at 1e-4m=100µm.
	`Value of first point` Composition in the first gridpoint. Values in between are interpolated linearly if a LINEAR type of profile is specified.
	`Value of last point` Composition for the last gridpoint. Values in between are interpolated linearly if a LINEAR type of profile is specified.
	`Input file` The input source from which to read the points when entering values point by point, default is TERMINAL.
	`Value of point` The value of the point when entering values point by point.
	`Value of R in the geometrical serie` Use the same geometrical factor as for the geometrical grid.
	`Volume fraction of` Initial volume fraction of a spheroid phase.

ENTER_ENHANCEMENT_FACTOR

Change the mobility of a specific element in a specific phase. The mobility of the element in the phase is multiplied by a factor which is specified as an argument to the command.

Syntax	ENTER_ENHANCEMENT_FACTOR
Prompt	`Mobility enhancement factor for phase`

ENTER_GEOMETRICAL_EXPONENT

The Diffusion Module (DICTRA) in Graphical Mode uses a Diffusion Calculator instead of the Console Mode commands. Most of the Console Mode functionality is available on the Diffusion Calculator, described in the *Thermo-Calc User Guide*. However, you cannot use both Graphical Mode and Console Mode in the same simulation.

Enter the geometrical exponent which defines the geometry of the system. The program handles one-dimensional geometries defined by the geometrical exponent. These geometries are:

- **Planar**. This corresponds to an infinitely wide plate of a certain thickness.
- **Cylindrical**. This corresponds to an infinitely long cylinder of a certain radius.
- **Spherical**. Sphere with a certain radius.

Syntax	ENTER_GEOMETRICAL_EXPONENT
Prompt	`Geometrical exponent` Enter an integer value between 0 and 2.

ENTER_GRID_COORDINATES

The Diffusion Module (DICTRA) in Graphical Mode uses a Diffusion Calculator instead of the Console Mode commands. Most of the Console Mode functionality is available on the Diffusion Calculator, described in the *Thermo-Calc User Guide*. However, you cannot use both Graphical Mode and Console Mode in the same simulation.

Enter the size and gridpoint distribution of the grid in each region separately. The size of the region is specified in the units that the diffusion data is entered in. The grid in a specific region may also be subdivided into several parts, where the type of each part is chosen independently, by first entering SUB_REGION as the overall grid type.

SET_AUTO_GRID_OPTION

Syntax	ENTER_GRID_COORDINATES
Prompts	`Region name` Name of the region into which a grid is to be entered.
	`Width of region /1/` The actual size of the region is entered. The size of the region is specified in units compatible with those of the diffusion data.
Options	**Description**
`TYPE` of grid	`Type /Automatic/` Type of grid to enter, options are: • `AUTOMATIC`: Use this for automatic grid point distribution. An appropriate grid is generated at the start of the simulation where the grid points are automatically distributed according to the entered composition profile and boundary conditions. • `LINEAR`: For an equally spaced grid. • `READ_POINT_BY_POINT`: Can be done either from the keyboard or from a predefined file. When grid coordinates are read from a file it may often be the case that both grid coordinates and the composition at the grid points are given on the same line, e.g. the grid coordinates in the first column, the mole fraction of the first component at that grid point in the second column and so on. The column that contain the grid coordinates can then be specified in a macro file by, for example, having a line "read_point_by_point 30 foo.dat 1". The "1" mean that the grid coordinates are in the 1st column in the file foo.dat (and "30" is the total number of grid points). In a corresponding manner the column that contain the composition of a specific component can be specified (see ENTER_COMPOSITIONS).

Syntax	ENTER_GRID_COORDINATES
	- `GEOMETRIC`: Yields a higher number of gridpoints at the lower end of the region if a geometrical factor larger than one is given and a higher number of gridpoints at the upper end of the region if the factor is smaller than one. - `DOUBLE_GEOMETRIC`: Divides the region in two halves and generates a separate geometrical grid in each half. It gives a high number of gridpoints in the middle or at both ends of a region, two geometrical factors should be entered.
`Sub_region`	If `SUB_REGION` is entered when you are prompted to enter the grid type, then the next prompt is `End coordinate in Sub-Region /1/` Enter a value equal to or less than the total width of the region. You are then prompted for the number of grid points and the grid type to be used between the left-hand side of the region and the end coordinate. As long as the end coordinate is less than the total width of the region you are prompted for an end coordinate and the grid to be used in the sub region starting at the end of the former sub region. Thus, progressively higher end coordinates must be entered and the final end coordinate must be equal to the total width of the region.
	`Number of points /50/` The number of points present in the region. Please consider the interspacing of the grid when determining the number of points.
	`Input file` The input source from which to read the points when entering values point by point, default is TERMINAL.
	`Value of point` The value of the point when entering values point by point.
	`Value of R in the geometrical series` Value in the geometrical factor in the series determining the distribution of the grid points. A geometrical factor larger than one yields a higher density of gridpoints at the lower end of the region and a factor is smaller than one yields a higher density of gridpoints at the upper end of the region.
	`Value of R in the geometrical serie for lower part of region` The geometrical factor in the series for the lower (left) part of a region in a double geometrical grid
	`Value of R in the geometrical serie for upper part of region` The geometrical factor in the series for the upper (right) part of a region in a double geometrical grid.

ENTER_HEAT_TRANSFER_PARAMETER

A model for thermos-migration simulates the thermal induced diffusion in temperature gradients. This model requires that the temperature depends on the length coordinate in the system and that the quantity `heat of transport` (`Q*`), is entered.

Syntax	ENTER_HEAT_TRANSFER_PARAMETER
Prompt	`Heat transfer parameter for phase` The phase for which the parameter is to be entered. This parameter is entered separately for each component in each phase.
	The implementation and functionality of this model is described in Höglund and Ågren (2010)[1].

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[1] Höglund, Lars and John Ågren(2010)."Simulation of Carbon Diffusion in Steel Driven by a Temperature Gradient", *J. Phase Equilibria Diffus.* 31, 212–215.

ENTER_HOMOGENIZATION_FUN

Use this with the homogenization model for multiphase simulations. The homogenization model is based on the assumption of local equilibrium at each node point, which yields the local chemical potentials at each node point from which the local chemical potential gradients may be estimated. The chemical potential gradients are the driving forces for diffusion. The local kinetics must also be evaluated by some averaging procedure, the choice of which is determined by this command. The local kinetics is evaluated by considering the product of mobility times u-fraction for each component in each phase and the volume fraction of each phase.

The Diffusion Module (DICTRA) in Graphical Mode uses a Diffusion Calculator instead of the Console Mode commands. Most of the Console Mode functionality is available on the Diffusion Calculator, described in the *Thermo-Calc User Guide*. However, you cannot use both Graphical Mode and Console Mode in the same simulation.

Syntax	ENTER_HOMOGENIZATION_FUN
Prompt	`Enter homogenization function # /5/` Enter a digit between 1 and 14 (default is 5). The options corresponding to the numbers are listed below.

Homogenization Functions

Enter a digit between 1 and 14 (default is #5) to assign the homogenization function then follow the prompts. The homogenization functions are:

No.	**Function name**
1	General lower Hashin-Shtrikman bound*
2	General upper Hashin-Shtrikman bound*
3	Hashin-Shtrikman bound with prescribed matrix phase*
4	Hashin-Shtrikman bound with majority phase as matrix phase*
5	Rule of mixtures (upper Wiener bound)
6	Inverse rule of mixtures (lower Wiener bound)
7	Labyrinth factor f with prescribed matrix phase
8	Labyrinth factor f**2 with prescribed matrix phase

No.	Function name
9	General lower Hashin-Shtrikman bound with excluded phase(s) *
10	General upper Hashin-Shtrikman bound with excluded phase(s) *
11	Hashin-Shtrikman bound with prescribed matrix phase with excluded phase(s) *
12	Hashin-Shtrikman bound with majority phase as matrix phase with excluded phase(s) *
13	Rule of mixtures (upper Wiener bound) with excluded phase(s)
14	Inverse rule of mixtures (lower Wiener bound) with excluded phase(s)
	* For the Hashin-Shtrikman bounds, see Hashin, Z. & Shtrikman, S. “A Variational Approach to the Theory of the Effective Magnetic Permeability of Multiphase Materials”. *J. Appl. Phys.* 33, 3125–3131 (1962).

About the Homogenization Functions

The geometrical interpretation of the Hashin-Shtrikman bounds are concentric spherical shells of each phase. For the general lower Hashin-Shtrikman bound the outermost shell consists of the phase with the most sluggish kinetics and vice versa for the general upper bound. The geometrical interpretation of the Hashin-Shtrikman bounds suggest further varieties of the bounds, viz. *Hashin-Shtrikman bound with prescribed matrix phase* and *Hashin-Shtrikman bound with majority phase as matrix phase*, where the outermost shell consist of a prescribed phase or the phase with highest local volume fraction, respectively.

The geometrical interpretation of the Wiener bounds are continuous layers of each phase either parallel with (upper bound) or orthogonal to (lower bound) the direction of diffusion.

The labyrinth factor functions (described below) are available in Console Mode and when using TC-Python.

The labyrinth factor functions implies that all diffusion takes place in a single continuous matrix phase. The impeding effect on diffusion by phases dispersed in the matrix phase is taken into account by multiplying the flux with either the volume fraction (*Labyrinth factor f with prescribed matrix phase*), or the volume fraction squared (*Labyrinth factor f**2 with prescribed matrix phase*), of the matrix phase.

The varieties with excluded phases (described below) are available in Console Mode and when using TC-Python.

The varieties with excluded phases are useful in several respects. First, if a phase is modeled as having zero solubility for a component, the mobility of that component in that phase is undefined, which causes a (non-terminal) error. Setting a phase as excluded causes the mobility of all components in that phase to be set to zero. Second, often there are some major matrix solid solution phases and some minor precipitate phases. If the mobilities in the minor precipitate phases are zero the lower Hashin-Shtrikman bound is useless as it produces a kinetic coefficient of zero. However, using *General lower Hashin-Shtrikman bound with excluded phase(s)*the excluded phases are not considered when evaluating what phase has the most sluggish kinetics.

ENTER_LABYRINTH_FUNCTION

Enters a constant value or a function of temperature, pressure, or the volume fraction of the phase where diffusion occurs. This function increase or reduces the diffusion coefficient matrix. This function is primarily used when spheroid phases have been entered into a region. It may also be used for increasing or decreasing all diffusion coefficients in a certain matrix phase by a constant factor.

Syntax	ENTER_LABYRINTH_FUNCTION
Prompt	`Region` `f(T,P,VOLFR,X)=`

ENTER_MOBILITY_DATA

Use this command to enter previously non-existing mobility parameters. If there is already a function is defined for the same parameter, it is deleted.

You can also use:

- ENTER_ENHANCEMENT_FACTOR to enter a factor by which element mobilities are multiplied with.
- ENTER_MOBILITY_ESTIMATE to enter a rough mobility estimate for elements in specific phases. This can be useful for phases where there is no data in the database.

A valid parameter should have the general form of:

```
<Identifier> ( <Phase name> , <Component array> ; <Digit> )
```

The `identifier` must be followed by an opening parenthesis, a phase name, a comma and a component array. Optionally, the component array can be followed by a semicolon and a digit. The parameter name is terminated by a closing parenthesis.

These identifiers are legal:

- `MQ` (activation energy for mobility)
- `MF` (frequency factor for mobility)
- `DQ` (activation energy for diffusivity)
- `DF` (frequency factor for diffusivity)
- `OQ` (activation energy for mobility, ordered part)
- `OF` (frequency factor for mobility, ordered part).

The `phase name` must be followed by an & and directly following that the name of the diffusing species.

The `component array` consists of a list of constituent names. Interaction parameters have two or more constituents separated by a comma. If the phase has sublattices at least one constituent in each sublattice must be specified. The constituents in different sublattices must be given in sublattice order and are separated by a colon.

After the component array a subindex `digit` can be specified after a semicolon. This digit must be in the range 0 to 9. The interpretation of the subindex depends on the excess model used for the phase. If no semicolon and digit is given the subindex value is assumed to be zero.

Syntax	ENTER_MOBILITY_DATA

Prompt	`Parameter: <Parameter name>`
	As explained above, specify a correct and complete parameter name, which should contain all the necessary parts of the general form:
	`<Identifier>(<Phase>,<Component array>;<Digit>)`
	If a parameter name is not acceptable or <Enter>, is pressed, the error message displays:
	`*** Error, please re-enter each part separately`
	Examples
	• `MQ(FCC&C,Fe:Va)` Mobility of C in fcc Fe with interstitials.
	• `MQ(FCC&C,Fe,Cr;0)` The regular parameter for Fe and Cr in fcc.
	• `MQ(FCC&C,Fe,Cr;1)` The subregular interaction parameter (Redlish-Kister model).

`Identifier`	`Identifier /MQ/ <MQ, MF, DQ, Df, OQ, OF>` If this command is used one or more times, the previous value on this prompt is set as default. Press <Enter> for the same type identifier or specify a new type.
`Phase Name`	`Phase name /FCC&C/` Each parameter is valid for a specific phase. The name of that phase must be supplied. The name must not be abbreviated. The phase name must be followed by an '&' and directly following that, the name of the diffusion species.

ENTER_MOBILITY_ESTIMATE

Use this command to enter a function yielding a mobility estimate for a specific element in a specific phase.

LIST_MOBILITY_ESTIMATES

Syntax	ENTER_MOBILITY_ESTIMATE
Prompt	`Mobility estimate for phase` Interactively enter a function yielding a mobility estimate for a specific element in a specific phase. This can be used to enter mobility estimates in phases for which there is no assessed data. Estimates entered here override database values.

ENTER_PHASE_IN_REGION

Enter a phase into a previously defined region.

Syntax	ENTER_PHASE_IN_REGION
Prompts	`Active or Inactive phase` Type of phase entered. An inactive phase is a phase which does not participate in the calculations until it is stable. This is done by regarding the driving force for precipitation of the phase in an equilibrium calculation. The program then automatically retransforms the inactive phase into an active one.
	`Region name` Name of the region into which the phase is to be entered.
	`Phase type` Type of phase entered. Legal types are: • MATRIX • LAMELLAR (see ENTER_PHASE_IN_REGION - Lamellar Prompts). • SPHEROID: requires that a MATRIX phase has been previously entered.
	`Phase name` Name of the phase that is to be entered. A #-sign and a digit may append the phase name in order to specify the composition set number, e.g. FCC#2.
	`Composition set` Number of the composition set. This is needed if the phase has been amended to have more than one composition set and the number was not given directly on the phase name, see above.
	`Attach to region named` Enter the name of the region onto which the inactive phase is to be attached.
	`Attached to the right of` Enter Y to attach the inactive phase on the right side of the region. Enter N to attach on the left side.
	`Required driving force for precipitation` The required driving force (evaluated as DGM (phase) in POLY-3) to be used for determining whether an inactive phase is stable.
	`Condition type` Boundary condition used if the inactive phase becomes stable.

ENTER_PHASE_IN_REGION - Lamellar Prompts

The following are the ENTER_PHASE_IN_REGION subprompts for Lamellar.

For a LAMELLAR type of phase, the pearlite calculation model is invoked. The following is displayed:

```
eutectoid reaction is "gamma" ==> "alpha" + "beta"
```

This is to clarify what is meant with GAMMA, ALPHA and BETA in the specific sub-prompts that display as follows.

Subprompts	LAMELLAR
	`Enter name of "alpha" phase` Enter the GES phase name for the ALPHA phase of the eutectic/eutectoid decomposition product.
	`Enter name of "beta" phase` Enter the GES phase name for the BETA phase of the eutectic/eutectoid decomposition product.
	`Enter name of "gamma" phase` Enter the GES phase name for the GAMMA matrix phase.
	`Enter "alpha"/"beta" surface tension:` Enter function for the surface tension between the ALPHA and BETA phases, $\sigma^{\alpha/\beta}$
	`Enter "alpha"/"gamma" surface tension:` Enter function for the surface tension between the ALPHA and GAMMA phases,$\sigma^{\alpha/\gamma}$
	`Enter "beta"/"gamma" surface tension:` Enter function for the surface tension between the BETA and GAMMA phases,$\sigma^{\beta/\gamma}$
	`Optimum growth condition factor /2/:` Enter the Optimum-growth-rate-factor. Due to Zener's maximum growth rate criteria this factor has a value of 2 for volume controlled growth and 3/2 for boundary controlled growth. Due to Kirkaldy's extreme in entropy production criteria the values are 3 and 2, respectively.
	`Name of dependent element` Enter the name of the substitutional element to consider as the dependent one.
	`Growth model (Volume/Boundary/Kirkaldy) for element x` Select growth model to be used for element X. Choose between: • `Volume` diffusion model • `Boundary` diffusion model • `Kirkaldy`'s mixed mode diffusion model. Implies MIXED, see below.

Subprompts	LAMELLAR

	`df(x) = /Value/Automatic/Mixed/TDB/`
	Either input a numerical value on the pre-exponential factor DF or select one of the keywords:
	• AUTOMATIC
	• MIXED
	• TDB
	AUTOMATIC is only available for element Carbon. It implies a mixed type of calculation where the volume diffusion part is calculated due to J. Ågren “A revised expression for the diffusivity of carbon in binary Fe-C austenite”. *Scr. Metall.* 20, 1507–1510 (1986) (volume diffusion of C in Austenite) and the boundary diffusion part due to J. Ågren “Computer simulations of the austenite/ferrite diffusional transformations in low alloyed steels” *Acta Metall.* 30, 841–851 (1982) (boundary diffusion of C is assumed to be the same as C diffusion in Ferrite).
	The k' or k'', as appropriate, are given by B. Jönsson (1992)[1]. MIXED means a mixed mode calculation using an effective diffusion coefficient. Coefficient k' or k'' is asked for, see below. TDB means calculate the diffusion coefficient for volume diffusion for element X from the parameters stored in the database.
	`DQ(X)=`
	Input a numerical value on the activation energy DQ for element X.
	`k'=`
	`k''=`
	Input a numerical value on the k coefficient used to calculate the effective diffusion coefficient, use in MIXED mixed mode calculations, see B. Jönsson, 1992“On the Lamellar Growth of Eutectics and Eutectoids in Multicomponent Systems.” Trita-Mac 478 (January): 27.

	`DF_boundary(x)=` Input a numerical value on DF for boundary diffusion of element X in a mixed mode calculation.
	`DQ_boundary(x)=` Input a numerical value on DQ for boundary diffusion of element X in a mixed mode calculation.
	`DF_volume(x)=` Input a numerical value on DF for volume diffusion of element X in a mixed mode calculation. N.B. key word TDB may also be used, see TDB above.
	`DQ_volume(x)=` Input a numerical value on DQ for volume diffusion of element X in a mixed mode calculation.
	`Automatic start values for the s0 determination /Y/:` Enter `Y` if you want automatic start values for the unknown parameters in the S0 determination else enter `N`. S0 is the critical lamellar spacing for which the growth rate is zero.
	`Critical thickness of "alpha" lamella:` If you answered `N` this prompt displays. The critical thickness of ALPHA is about 0.9 of S0, which

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[1] "On the Lamellar Growth of Eutectics and Eutectoids in Multicomponent Systems” *Trita-Mac* 478.

Subprompts	LAMELLAR
	in turn is about 1/3 to 1/2 of the observed lamellar spacing S. For binary Fe-C alloys the observed pearlite lamellar spacing is approximately given by $S = 1.75 \cdot 10^{-5} (A_{1e} - T)^{-1}$ The equation may be used as a start value approx. for alloyed steels. However, use the $\mathrm{A}_{1\mathrm{e}}$ temperature of the steel.
	`Critical thickness of "beta" lamella:` The critical thickness of BETA is about 0.1 of S0, see above.
	`Automatic start values on potentials /Y/:` By default, automatic start values for the unknown potentials are used. Choose N to enter your own start values.
	`Give potentials for "alpha"/"gamma" equil.` Enter start values for the unknown potentials, MU, at the ALPHA/GAMMA phase boundary.
	`Give potentials for "beta"/"gamma" equil.` Enter start values for the unknown potentials, MU, at the BETA/GAMMA phase boundary.
	`Growth rate v:` Enter a start guess on the growth rate. As a hint on what value to choose we recognize that for binary Fe-C alloys the pearlite growth rate is approximately given by: $v = 8 \cdot 10^{-9} (A_{1e} - T)^2$ The equation may be used as a start value approx. for alloyed steels. However, use the $\mathrm{A}_{1\mathrm{e}}$ of the steel.
	`Automatic start values on other variables /Y/:` By default there are automatic start values for the unknowns in the determination of the growth rate.
	`Fraction of "alpha" phase:` Enter a guess on the fraction of the ALPHA phase. For pearlite it is about 0.9.
	`Give potentials for "alpha"/"gamma" equil.` Enter start values for the unknown potentials, MU, at the ALPHA/GAMMA phase boundary.
	`Give potentials for "beta"/"gamma" equil.` Enter start values for the unknown potentials, MU, at the BETA/GAMMA phase boundary.

ENTER_REGION

Enter a region into the system. Enter this before entering a grid or any phases.

Syntax	ENTER_REGION
Prompts	`Region name` Name of a region to be entered. The name of the region can be arbitrarily chosen.
	`Attach to region named` Name of a region to which the new region should be attached.
	`Attached to the right of` Relative position of the new region. Enter Y to attach the inactive phase on the right side of the region. Enter N to attach on the left side.

GB_MODEL

Grain-boundary and dislocation assisted diffusion is implemented by assuming that these contributed to the diffusion by using the same frequency factor and a modified bulk activation energy. The grain-boundaries and the dislocations contribute to the total amount of diffusion according to the weighted fractions.

Syntax	GB_MODEL
	The parameters are entered separately for each region in order to different expression for different phases.
	The used expressions for the grain-boundary and dislocation contributions are: $M^{gb} = M_0^{bulk} \cdot \exp(F_{redGB} \cdot Q^{bulk}/R/T)$ $M^{disl} = M_0^{bulk} \cdot \exp(F_{redDisl} \cdot Q^{bulk} R/T)$ where • M_0^{bulk}: frequency-factor in the bulk • Q^{bulk}: activation energy in the bulk • F_{redGB}: bulk diffusion activation energy multiplier (typical value 0.5) • $F_{redDisl}$: bulk diffusion activation energy multiplier (typical value 0.8) The weighted calculated value for the mobility M^{new} is then evaluated from: $M^{new} = \delta/d \cdot M^{gb} + \rho \cdot b^2 \cdot M^{disl} + (1 - \delta/d - \rho \cdot b^2) \cdot M^{bulk}$ where • δ: grain boundary thickness (typical value $0.5 \cdot 10^{-9}$ or $0.5 \cdot 10^{-10}$) • d: grain size as a function of time and temperature (typical value $25 \cdot 10^{-6}$) • ρ: dislocation density as a function of time and temperature • b: burgers vector (typical value $1 \cdot 10^{-10}$) • M^{bulk}: mobility in the bulk (δ/d being the fraction of grain boundaries in the bulk and $\rho \cdot b^2$ being the fraction of dislocations in the bulk)

HOMOGENIZATION_MODEL

UTILITIES_HOMOGENIZATION

ADVANCED_HOMOGENIZATION_OPTIONS

This command enables or disables the use of the homogenization model and its default settings. The homogenization model is used for multiphase simulations assuming that local equilibrium holds at each node point. When entering phases into a region one of them is entered as MATRIX phase and all other phases as SPHEROID, but it does not matter which one is entered as matrix phase and it does not affect simulations. Homogenization model simulations differs from all other DICTRA module simulations in that it is implemented using an implicit finite volume method in order to increase numerical stability (degree of implicity can be chosen using the SET_SIMULATION_CONDITION command). Because of this, and other factors, homogenization model simulations generally run slower than other comparable simulations.

The Diffusion Module (DICTRA) in Graphical Mode uses a Diffusion Calculator instead of the Console Mode commands. Most of the Console Mode functionality is available on the Diffusion Calculator, described in the *Thermo-Calc User Guide*. However, you cannot use both Graphical Mode and Console Mode in the same simulation.

Syntax	HOMOGENIZATION_MODEL
Prompts	`Enable homogenization model:` Enter `Y` to enable the homogenization model. If it is already enabled, you can enter `N` to disable it.
	`Use default settings /Y/:` Press <Enter> to keep the default settings for the homogenization model. Otherwise enter N and follow the prompts.

	`Add ideal flux contribution /N/:`
	If you enter `Y` you are prompted as follows:
	`Fractional ideal contribution(0->1) /.01/:`
	Enter a number between zero and one. In multiphase regions the system loses degrees of freedom which may cause fluctuations in the composition profiles. This can be amended by adding a small ideal contribution to the fluxes. The ideal flux contribution should normally not be used.

	`Use interpolation scheme /Y/:`
	By default the interpolation scheme is used and it normally speeds up simulations. You are then prompted with the following:
	`Enter number of steps between XMin and XMax /10000/:`
	Enter the number of steps in composition space. In the limit where an infinite number of steps are used, exactly the same solution is obtained as without the interpolation scheme. However,

Syntax	HOMOGENIZATION_MODEL

	excellent results can be obtained with a reasonable discretization.
	`Linear or logarithmic discretization /Log/:`
	The discretization can be either linear or logarithmic (the default). For the linear discretization the scheme is not used at node points where the content of one or more solutes fall below a certain critical value. For such cases, where a good discretization is required for very low solute contents, the logarithmic discretization can be tried.
	`Fraction of free physical memory to be used /.1/:`
	Enter the fraction of free physical memory to be used by the interpolation scheme. If a value larger than one (1) is entered it is interpreted as the number of MB to be used for the interpolation scheme.

	`Use global minimization /N/:` By default global minimization is not used in equilibrium calculations. In general, using global minimization significantly increases the simulation time, but there is also a significantly reduced risk for non-converged equilibrium calculations.
	`Refresh Jacobian every iteration /N/:` If there are convergence problems, enter Y to see if this solves the issue. This does increase computational demand for each iteration.
	`Default grid parameter values /Y/:` These settings only affect simulations where the grid changes during the simulation. If you enter N, you are prompted with the following.
	`Geometrical coefficient (0+ -> 1) /.98/:` The geometrical coefficient used in each region.
	`Fixed interface width (<0 DISABLES) /-1/:` A value larger than zero makes interface widths fixed to that value.
	`Grid fineness away from interface /1/:` A value other than one causes the grid away from the interface to be coarser (>1) or finer (<1) than what would be obtained just by the geometrical coefficient.
	`Interface width fraction (0+ -> 0.1) /.005/:` If the interface width is not fixed the program aims for a width equal to this factor times the cell width.
	`Consecutive critical time-steps (DT) to delete region /20/:` If the width of a region falls below a certain critical value and shrinks monotonically for this number of time-steps it is deleted.

INPUT_SCHEIL_PROFILE

As per normal procedure, and before entering the DICTRA monitor, you need to read thermodynamic and kinetic data to use this command.

This command takes a previously calculated Scheil segregation profile and performs most of the setup needed to use that profile in a simulation, for example a homogenizing heat treatment.

The command creates a region called SCHEIL_REGION. You then create a linear grid and enter the composition read from the file containing the segregation profile.

After issuing this command, you specify simulation time (SET_SIMULATION_TIME) and simulation temperature (SET_CONDITION, enter `GLOBAL` and variable `T`) to finalize setup.

In order to limit the computational effort, this feature cannot be combined with the fast diffusers option in the Scheil module.

Press F1 in Thermo-Calc to search the online help for detailed information about Scheil simulations.

Syntax	INPUT_SCHEIL_PROFILE
Prompts	`Enter file location of Scheil segregation profile` In interactive mode (the command line), a file dialogue window opens. Navigate to the file containing the Scheil profile. Alternately, if you are working from a macro file, the line should contain the name of the file. An XF.txt file can be created with the EVAL_SEGR command in the Thermo-Calc SCHEIL module. The file is available after the Scheil simulation is finished and contains one line per grid point. See EVALUATE_SEGREGATION_PROFILE for more information and to make sure to use the same number of grid points in the DICTRA region for both commands.
	`Enter width of region` Enter the width of the region [m] that contains the Scheil profile. This typically corresponds to the secondary dendrite arm spacing.

Syntax	INPUT_SCHEIL_PROFILE
	`Enter main solid solution phase` Enter the name of one of the main solid solution phases. In the next prompt you can enter other phases that enter the simulation.
	`Should more phases be entered in the region` Enter Y to enter more phases then enter the phase name as prompted next.
	`Enter phase name` Enter the name of another phase that should be entered into the region.

INTERFACE_SURFACE_TENSION

This command enters a distance- and velocity-dependent function that is added to the Gibbs energy of the phase at left side of a specified interface. This can then be used to emulate the effect of surface tension on the equilibrium between at the phase interface or limited phase mobility. This command is similar to the SET_SURFACE_TENSIONcommand but more flexible because if there is more than one interface in a cell, the user can add different Gibbs energy expressions to different interfaces, each specified by the two neighboring phases.

Syntax	INTERFACE_SURFACE_TENSION

Prompt	`PHASE ON LEFT SIDE OF INTERFACE`
	The name of the phase on the left side of the specified interface.
	`PHASE ON RIGHT SIDE OF INTERFACE`
	The name of the phase on the right side of the specified interface.
	`Function F(X,V,TIME,T):`
	Enter a function which adds to the Gibbs energy expression for the phase located at the lower (left) side of the interface. The expression is multiplied with the volume per mole substitutional atoms (10-5m^3/mole). This command is also used to simulate a limited interfacial mobility control where the energy function is a function of the interface velocity.
	It is used to enter the surface energy to enable coarsening. However, it can also be used to simulate a case with a limited interfacial mobility.
	For detailed syntax for the function, see the SET_SURFACE_TENSION command.

LIST_CONDITIONS

Use the LIST_CONDITIONS command to lists the conditions defined with the SET_CONDITION command.

Syntax	LIST_CONDITIONS
Prompt	`Output file` File where the information is to be written.

LIST_MOBILITY_DATA

This command does not work for encrypted databases.

Lists the mobility data from the database or entered interactively by the ENTER_MOBILITY_DATA command.

Syntax	LIST_MOBILITY_DATA
Prompt	`Output file` File where the information is to be written.

LIST_MOBILITY_ESTIMATES

Use the LIST_MOBILITY_ESTIMATES command to list on screen the mobility estimate entered interactively using the ENTER_MOBILITY_ESTIMATE command.

LIST_PROFILES

Lists the concentration profiles and grid coordinates in the cell.

Syntax	LIST_PROFILES
Prompts	`Name of region` Name of region(s) in which the profiles are to be listed.
	`Output file` File where the information is to be written.
	`Composition type` Composition type in which the profiles are to be written. Legal composition types are: • SITE_FRACTION • MOLE_FRACTION • WEIGHT_FRACTION • U_FRACTION
	`Components` The output information may be limited to the specified components.
	`Constituents` The output information may be limited to the specified constituents.

LIST_REGION

List the names of the defined regions, active and inactive phases and the global coordinates of the interfaces.

Syntax	LIST_REGION
Prompt	`Output file` File where the information is to be written.

LIST_TIMESTEPS

This for the DICTRA module. Also see LIST_TIME_STEPS for the POST module.

Use the LIST_TIMESTEPS command to list the time steps in the workspace and those stored on file during a simulation.

MACRO_FILE_OPEN

Use this to predefine sequences of commands on a file and then execute them with the MACRO command. This is useful when the same calculation is made often with just small changes. One good case for applying this is when calculating diagrams from an assessment. With a macro file all commands can be stored on a file and you just type MACRO <filename>.

Syntax	MACRO_FILE_OPEN
Prompt	`Macro filename` Give the name of the file with the macro commands. Default extension is DCM.
	The macro file can contain any legal DICTRA module commands. The macro must be terminated with EXIT or in the SYS, DICTRA, POLY-3 or POST module with the command SET_INTERACTIVE_MODE.

PARA_EQUILIBRIUM_MODEL

Turns on the para-equilibrium model in the simulation. Using this model implies that the local equilibrium assumption is no longer valid and that substitutional components are regarded as one composite component.

The model is limited to treating only one single moving interface in one cell.

See the Diffusion Module (DICTRA) example EXH2, which is briefly described in Deviation from Local Equilibrium Examples

Syntax	PARA_EQUILIBRIUM_MODEL
Prompts	`Enable paraeq` Enables or disables the use of this model by using one of the key words YES or NO.
	`Auto` Choose this to set it to the value at the region’s lower or upper boundary.
	`Value %` Enter a value followed by a percentage sign (%) to set it to a certain percentage from the moving boundary inside the region.
	`-Value` Enter a hyphen (-) followed by a value to set it to a fixed distance from the moving boundary.
	`Value` Enter a value to set the composition to that specific value,

POLY_COMMAND

This command sends a string to the POLY-3 module interpreter where it is then executed.

An example of the use of this command is as follows. There are some differences in the default settings for equilibrium calculations based on whether the equilibrium calculation is performed from the DICTRA module or POLY. The changes in the defaults are performed automatically every time the DICTRA module is entered. By using this command it is possible to override those changes.

Syntax	POLY_COMMAND
Prompt	`To POLY` Command line sent to the POLY-3 module.

POST_PROCESSOR

Use the POST_PROCESSOR command to "give control" to the post processor. Then you can start using the commands.

? POST PROCESSOR Commands

READ_WORKSPACES

Both GES6 and GES5 data are saved to/read from a dic-file. For information about GES versions, see About the Gibbs Energy System (GES) Module.

The DICTRA, POLY-3 and GES workspaces can be read from a file where they must be already saved with a SAVE command. This file is not printable.

Syntax	READ_WORKSPACES
Prompt	`File name` Name of the file where the workspaces shall be read from. The default file extension is `dic`.

REINITIATE_MODULE

Use the `REINITIATE_MODULE` command to reset the state of the DICTRA module to what it was when you first entered the workspace.

REMOVE_STOP_CRITERION

The REMOVE_STOP_CRITERION command can be used as long as you have already set up the simulation and included a stop criterion using the ADD_STOP_CRITERION command.

? ADD_STOP_CRITERION

Syntax	REMOVE_STOP_CRITERION
Prompts	There are no prompts. You enter arguments, either a number referring to a specific criterion (as shown inLIST_CONDITIONS) or a wildcard `*` referring to all criteria.

SAVE_WORKSPACES

Both GES6 and GES5 data are saved to/read from a dic-file. For information about GES versions, see About the Gibbs Energy System (GES) Module.

The workspaces in DICTRA, POLY-3 and GES are saved in a file. Return to the state before the SAVE command by entering a READ command. The SAVE command should normally be given before starting a simulation with SIMULATE_REACTION.

Syntax	SAVE_WORKSPACES
Prompts	`File name` Name of the file where the workspaces shall be saved on. The default file extension is DIC.
	`Overwrite current file content`
	`Proceed with save` If there is already a file with this name and if you answer Y the previous content is overwritten. If you have results from SIMULATE_REACTION these are lost when SAVE is used. You may append several results by the SIMULATE_REACTION command without destroying the previous results but SAVE erases them all.

SELECT_CELL

Selects the current cell from the list of existing cells and enables you to enter and display data into that cell. This command is for the DICTRA.

? See also POST PROCESSOR prompt of the same name SELECT_CELL.

Syntax	SELECT_CELL
Prompt	`Number` Specify the cell number by giving an integer or one of the key words NEXT or PREVIOUS.

SELECT_TIMESTEP

Select a time step from those stored on file during a simulation. The profiles can be listed and simulation can be continued from this time step.

Syntax	SELECT_TIMESTEP
Prompt	`Timestep` The time step to be selected, legal syntax is: • `FIRST` • `LAST` • `time` • `#nnn` • `#?` When selecting a time no interpolation is performed but the time step closest to the time entered is selected. #nnn can be obtained from the number given by LIST_TIMESTEPS or by typing `#?`.
	`Delete all other timesteps` Clears the current workspace from all other time steps except the one selected. This is necessary if the simulation is to be continued from this time step.

SET_ACCURACY

Enter the accuracy requirements to use in the determination of the time step when using the automatic time step procedure. It may also be necessary to modify the parameters to control the removal of grid points and set manual starting values for velocities and potentials at the phase interfaces.

The Diffusion Module (DICTRA) in Graphical Mode uses a Diffusion Calculator instead of the Console Mode commands. Most of the Console Mode functionality is available on the Diffusion Calculator, described in the *Thermo-Calc User Guide*. However, you cannot use both Graphical Mode and Console Mode in the same simulation.

Syntax	SET_ACCURACY
Prompts	`Max relative error` The maximum allowed relative error of the profile during one time step integration.
	`Max absolute error` Maximum allowed absolute error of the profile during one time step integration. This parameter must be chosen with some relation to the smallest concentration in the profiles.

SET_ALL_START_VALUES

Enter starting values for various quantities, such as velocities and potentials.

Syntax	SET_ALL_START_VALUES
Prompts	`Start value for velocity of interface` A starting value for velocity at the named interface is required.
	`Start value for potential` A starting value for a potential at the named interface is required. If an AUTOMATIC value is specified the program attempts to determine a starting value and also selects a suitable component for which the potential is varied.
	`Varying species in interface` The species which potential is treated as unknown.
	`Automatic starting values for phase compositions` Compositions used as starting values in the equilibrium calculations using POLY-3. When using automatic starting values the compositions are taken from the entered profiles.

SET_AUTO_GRID_OPTION

Use the SET-AUTO-GRID-OPTION command to set the number of equidistant points in a region (e.g. maximum distance between two adjacent grid points is the size of the region divided by this number) and the maximum factor that is allowed in the geometric series defining the initial grid.

HOMOGENIZATION_MODEL

Syntax	SET_AUTO_GRID_OPTION
Prompt	`GRID ACCURACY/MEDIUM/:` Press enter to accept the default (MEDIUM), or enter FINE, COARSE, or CUSTOM. The values for the Grid Accuracy settings for each option differ when calculated by Thermo-Calc based on whether it is the Classic or Homogenization model. • If you are using a Classic model: Fine 75/1.25, Medium 50/1.2, Coarse 25/1.15 (Number of points/Max geometric factor) • If you are using the Homogenization model: Fine 100/1.03, Medium 80/1.02, Coarse 60/1.01 (Number of points/Max geometric factor)
Custom	If CUSTOM is entered then further define these settings. MAX NUMBER OF EQUIDISTANT POINTS IN A REGION: /50/: This value must be more than 2. VALUE OF R IN THE GEOMETRICAL SERIE : /1.2/: Value in the geometrical factor in the series determining the distribution of the grid points. A geometrical factor larger than one yields a higher density of gridpoints at the lower end of the region and a factor is smaller than one yields a higher density of gridpoints at the upper end of the region.

SET_CONDITION

Define conditions to reduce the degrees of freedom at equilibrium or defines the boundary conditions at the outer rims of the system. Use it to set the temperature, pressure or heat extracted from the system.

Conditions can be a function of time and different time-dependent functions can be specified at different time intervals. The syntax for this is approximately the same as used in the GES to specify temperature ranges for thermodynamic parameters.

DICTRA uses a constant molar volume, which is included in the flux, i.e. the unit of flux as entered in boundary conditions is:

$$\texttt{flux*molar volume} = \texttt{mol*m}^{-2}\texttt{*s}^{-1}\texttt{*m}^{3}\texttt{*mol}^{-1} = \texttt{m*s}^{-1}$$

Syntax	SET_CONDITION
Prompts	`Global or Boundary Condition /Global/` Type of condition to be specified. A global condition is either pressure (P), temperature (T) or heat content removal (P) and may be specified as a function of time. Boundary conditions determine how the cell interacts with the world outside the cell.

	`Variable`
	Legal variables are pressure (P), temperature (T) or heat extracted (Q) as a function of time (TIME), TIME_TEMPERATURE_PAIRS (T-T-P) that specifies temperature at a specific time and lets the program calculate the cooling or heating rate, or LOOKUP_TABLE_TEMPERATU that reads a file with time-temperature pairs. For Q the amount of extracted heat per time unit is normalized and the size of the system is normalized to 1 mole of atoms.
	For example, if you enter T-T-P at the Variable prompt then at the next prompt:
	`TIME,TEMPERATURE`
	Specify temperature and time pairwise such as e.g.:
	`0 1400`
	`60 1200`
	`* 1200`
	Where entering an asterisk(`*`)" is required in order to indicate the end time of a simulation.
	For LOOKUP_TABLE_TEMPERATU the file should look similar except for the end time:
	`0 1473`
	`60 1273`
	`1000 1173`
	For the lookup table some optimization is done. Redundant pairs are removed when reading the data.

Syntax	SET_CONDITION
	Tips to Determine the Temperature as a Function of Time The two methods to determine the temperature as a function of time, TIME_TEMPERATURE_PAIRS and LOOKUP_TABLE_TEMPERATU, are used in different ways based on the type of simulation. • TIME_TEMPERATURE is a shortcut to the ordinary temperature condition and is translated into a series of different temperature conditions. For example, they appear as a series of conditions if the conditions are listed. This sets some limits on the time-step that is used, occasionally overriding the limit set in the SET_SIMULATION_TIME command. The time-step is also adjusted to always coincide with the time giving in the time-temperature pair. Therefore it is recommended that this option is only used for a limited number of pairs, e.g. a linear approximation of a heat-treatment cycle. For the input to be valid, the last time in the set of pairs must be given as a wildcard *. • LOOKUP_TABLE stores the time and temperature pairs and interpolates within the table in order to obtain the correct temperature for a certain time. The time-step is limited by how much the temperature is allowed to change over the time-step besides the maximum limit provided by the SET_SIMULATION_TIME command. This allows for the use of a very large dataset containing several hundred values, e.g. a measured temperature from a solidification. Should the simulation exceed the last time given in the table, an error message is shown but the simulation will continue using the last temperature in the list.
	`Boundary` Defines on which side of the system the boundary conditions are to be specified. Options are UPPER (the rightmost side of the system) and LOWER (the leftmost side of the system).
	`Condition type` Defines the type of boundary condition to be specified. The options may in most cases be functions of both TIME, T (temperature) and P (pressure). The default is CLOSED_SYSTEM which is equivalent to setting the fluxes of all components to zero at the boundary. Options are: • `FIX_FLUX_VALUE`: Enter functions that yield the flux times the molar volume for the independent components. May be a function of time, temperature and pressure. • `STATE_VARIABLE_VALUE`: A legal expression in POLY-3 syntax that reduces the degrees of freedom. This type of boundary condition should be used with the uttermost care as no checks are done if it is a legal expression in advance. • `ACTIVITY_FLUX_FUNCTION` or `POTENTIAL_FLUX_FUNCTION`: These types of boundary conditions are used to take into account the finite rate of a surface reaction. The flux for the independent components must be given in the format: $J_k * V_m = f_k(T,P,TIME)^* \left[ACTIVITY_k^N - g_k(T,P,TIME)\right]$ or $J_k * V_m = f_k(T,P,TIME)^* \left[POTENTIAL_k^N - g_k(T,P,TIME)\right]$ where *f* and *g* may be functions of time (TIME), temperature (T), and pressure (P), and N is an integer.

Syntax	SET_CONDITION
	The activities are those with user defined reference states. The function f_k is the mass transfer coefficient, g_k is the activity of the corresponding species in the gas and *N* is a stoichiometric coefficient. For more details see L. Sproge and J. Ågren, “Experimental and theoretical studies of gas consumption in the gas carburizing process” *J. Heat Treat*. 6, 9–19 (1988). - `ITERATIVE_ACTIVITY_FLUX_FUNCTION`: Same as activity flux function above. However, an iterative scheme is used to determine the flux. This method may be used instead of activity flux function when the latter has problems. - `CLOSED_SYSTEM`: Corresponds to a fix flux value, which is set to zero at all times. - `MIXED_ZERO_FLUX_AND_ACTIVITY`: The flux of selected components is set to zero and the activity of others may be set to a prescribed value. - `GAS`: The flux of selected components is set to zero and the activity of others may be set to a prescribed value. This option is used for treating an expanding system, e.g. the growth of an external oxide scale.
	`Low time limit` The lower time limit to be used when entering a time dependent function.
	`High time limit` The upper time limit to be used when entering a time dependent function. An asterisk * indicates the high limit as infinity.
	`Any more ranges` To specify whether any additional time dependent functions exists or not.
	`Type of condition for component` The type of condition when setting a boundary condition of the type MIXED. Options are ZERO_ FLUX and ACTIVITY.

SET_FIRST_INTERFACE

Set the coordinate of the first interface in the cell, when a value other than zero is required, for instance when simulating diffusion through a tube wall or a hollow sphere. The default value is zero.

Syntax	SET_FIRST_INTERFACE
Prompt	`Coordinate for first interface` The coordinate to which the first interface is to be set.

SET_INITIAL_TEMPERATURE

This command is only used when the heat removal rate from the system is specified. It yields the initial temperature of the system. How the temperature then varies during the simulation is a result of the heat removed from the system.

Syntax	SET_INITIAL_TEMPERATURE
Prompt	`Initial temperature /2000/`

SET_LOG_LEVEL

Use the SET_LOG_LEVEL command to choose the amount of output to the logs during a homogenization model simulation. The default (`2`) keeps the log output to a minimum and thus limits the possibility of slowing down a calculation.

Syntax	SET_LOG_LEVEL
Prompt	`HOMOGENIZATION MODEL LOG LEVEL(1=NORMAL, 2=MINIMAL): /2/:`
	Choose `1` to set the amount of logging to normal and `2` to set it to a minimal amount (the default).

SET_NUMERICAL_LIMITS

Set parameters to control the integration, the solution of the flux balance equations, diffusion equations and the equilibrium calculation during the simulation.

The Diffusion Module (DICTRA) in Graphical Mode uses a Diffusion Calculator instead of the Console Mode commands. Most of the Console Mode functionality is available on the Diffusion Calculator, described in the *Thermo-Calc User Guide*. However, you cannot use both Graphical Mode and Console Mode in the same simulation.

Syntax	SET_NUMERICAL_LIMITS
Prompts	`Required sum of squares in NS01A` Required accuracy during the solution of the flux-balance equations.
	`Max number of calls to Calfun of NS01A` The maximum number of iterations when solving the flux-balance equations. This number acts as a *safety valve*, a moderate choice is 10*(number_of_interfaces *(number_of_components - 1)) but use a larger value if necessary.
	`Step used by NS01A` A user supplied parameter which is used to calculate the estimates of the partial derivatives numerically when solving the flux-balance equations.
	`Max step used by NS01A` A parameter which must be set to a generous estimate of the 'distance' between the initial approximation and the required solution of the flux-balance equations.
	`Max number of equidistant points in a region` The number of equidistant parts in which a region is divided into that is required to describe the profile. This parameter is used by the procedure that removes unnecessary gridpoints from the profile during the simulation; the number of gridpoints is normally not allowed to be less than this number if a linear grid is used.
	`Fraction of region assigned to the interface` Fraction of a region at the region border that is to be regarded as part of the interface. This parameter is used by the procedure that removes unnecessary gridpoints from the profile during the simulation.
	`Smallest number used in scaling flux equations` The flux-balance equations are scaled by the velocities calculated in the previous time step. This number may however decrease to such a small value so that convergence may be affected. The scaling factor is therefore not allowed to decrease below this value.
	`Default driving force for inactive phases` Sets the necessary driving force needed before an inactive phase is allowed to start to precipitate.

SET_REFERENCE_STATE

The reference state for a component is important when using activities, chemical potentials and enthalpies and it is determined by the data. For each component the data must be referred to a selected phase, temperature and pressure the *reference state*. All data in all phases where this component dissolves must use the same reference state. However, different datasets may use different reference states for the same element. Thus one must mix data from different databases with caution.

By default activities etc. are computed relative to the reference state used by the database and this may thus differ depending on the database. You can select the reference state of a component if the reference state in the database is not suitable.

Syntax	SET_REFERENCE_STATE
Prompts	`Component` The name of the component must be given.
	`Reference state` The name of a phase that must be either entered or dormant must be given. The component must be a constituent of this phase of course. A subtle problem is if the component exists in several species in the phase, for example oxygen as O, O2 and O3 in a gas. Normally one would like to have the most stable species as reference state of oxygen, i.e. O2 in this case. Therefore the program calculates the Gibbs energy of all possible states with the phase with the pure component at the current temperature and selects the most stable one.
	`Temperature` Select the temperature for the reference state. The value * means the temperature used for the calculation.
	`Pressure` Select the pressure for the reference state.

SET_SIMULATION_CONDITION

Set parameters used to control output and certain parameters during the simulation.

The Diffusion Module (DICTRA) in Graphical Mode uses a Diffusion Calculator instead of the Console Mode commands. Most of the Console Mode functionality is available on the Diffusion Calculator, described in the *Thermo-Calc User Guide*. However, you cannot use both Graphical Mode and Console Mode in the same simulation.

Syntax	SET_SIMULATION_CONDITION
Prompts	`NS01A print control` Determines whether data should be printed about the iterative procedure to solve flux-balance equations. This parameter is normally set to 0 but can be set to 1 when difficulties with convergence occur. NS01A prints out the values used in the iterations and the residuals.
	`Flux correction factor` This parameter controls if the flux correction scheme should be used in the calculations. The value should normally always be 1.
	`Number of delta timesteps in calling MULDIF` This parameter specifies the number of equally large time steps that one time step should be subdivided into.
	`Check interface position` This parameter determines whether the time step is to be controlled by the phase interface displacement during the simulation. The default is `Auto`.
	`Vary potentials or activities or LNAC` Determines whether the program should use the potential or the activity of a component in order to find the correct tie-line at the phase interface. The potential or the activity is varied by the program and is set in order to reduce the degrees of freedom at the local equilibrium. The default is `Activities`.
	`Allow automatic switching of varying element` Determines whether the program is allowed to itself switch the component that is used to reduce the degrees of freedom at the local equilibrium. The scheme used is that of choosing the components which activities or potentials varied most during the previous time step. The default is `Yes`.
	`Save workspace on file` This parameter determines whether the workspaces are to be saved to file during the course of the simulation. Options are `Yes` (the default) to always save to file, `No` to never save to file, or `##` to save every *n*th time to file where ## is a integer value ranging from 0 to 99.
	`Degree of implicity when integrating PDEs` The default is `Auto` where the default degree of implicity corresponds to trapezoidal (0.5) for classic and Euler Backward (1.0) for the homogenization model. If large fluctuations occur in the profiles it may be necessary to use the value 1.0 (Euler backwards).

Syntax	SET_SIMULATION_CONDITION
	• `Auto` • `0.0` Euler forwards • `0.5` Trapezoidal rule • `1.0` Euler backwards
	`Max timestep change per timestep` Factor specifying the maximum increase in the time step taken from one time step to another. For example, if the default, `2` is used the maximum time step is twice as long as the previous time step taken.
	`Use forced starting values in equilibrium calculation` This concerns the calculation of the equilibrium when using the disperse model where the equilibrium calculations sometimes fail due the abrupt changes in the composition over the region. The default `Auto` means it always sets forced starting values for composition and phase amounts before preforming the equilibrium calculation.
	`Always calculate stiffness matrix in MULDIF` This determines how often the diffusion coefficient matrix is calculated when solving the partial differential equations (PDE) of diffusion problem. The default setting `Yes` calculates the diffusion coefficient matrix, yielding the stiffness matrix, at each iteration. However, when setting this parameter to `No`, it is only calculated at the first iteration and a constant stiffness matrix is used to obtain the solution to the PDEs. This then leads to an implicit solution and therefore the degree of implicitly is automatically set to 1.
	`Calculate residual for dependent component /No/` Keep the default.

SET_SIMULATION_TIME

Enter the time specific conditions for a simulation.

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Syntax	SET_SIMULATION_TIME
Prompts	`Eend time for integration` The time up to which the simulation is to be carried out.
	`Automatic timestep control` Determines whether the time step should be controlled by an automatic procedure or not. If you answer `N` you are prompted for the fixed time step to use during the simulation. The time step determined by the automatic time step control procedure is controlled by the parameters set by the command SET_ACCURACY.
	`Max timestep during integration` The maximum time step allowed during the simulation. This is required when using the automatic procedure to determine the time step.
	`Timtestep during integration` Fixed time step used when the automatic time step procedure is disabled.
	`Initial timestep` Time step used as the initial time step.
	`Smallest acceptable timestep` The smallest time step allowed during the simulation. This is required when using the automatic procedure to determine the time step.

SET_SURFACE_TENSION

This command enters a distance- and velocity-dependent function which is added to the Gibbs energy of the phase at left side of each phase interface. This can then be used to emulate the effect of surface tension on the equilibrium between at the phase interface or limited phase mobility.

Syntax	SET_SURFACE_TENSION
Prompt	`Function` Enter a surface energy function which adds to the Gibbs Energy expression for the phase located at the lower (left) side of the interface. The expression is multiplied with the volume per mole substitional atoms. This command is also used to simulate a limited interfacial mobility control where the energy function is a function of the interface velocity. It is used to enter the surface energy to enable coarsening. However, it can also be used to simulate a case with a limited interfacial mobility.

> This function should only be used in spherical geometries if the function is solely dependent of the interface position.

Function describing how the (surface) energy function varies with the particle radius and/or the interface velocity.

The classical expression for the surface energy contribution has the form of $\frac{2\sigma V_m}{r}$.

The molar volume should be given relative to the molar volume used by default in DICTRA, 1 x 10^{-5} (m^3/mole). The volume should also be given per mole of substitutional atoms. For a precipitate of type M_xC_y this means multiplying with a factor (y+x)/x. If we use M_6C as an example with surface tension 0.5 (J/m^2) and molar volume of 0.71 x 10^{-5} (m^3/mole), the entered function should be 2*0.5*0.71*(7/6)/X;

Commonly the surface tension function is defined as:

```
delta-G = 2 * SIGMA * Vm / R
```

The function to be entered will then be:

```
2*SIGMA/X;
```

A limited interface mobility can be expressed as:

```
delta-G = v * Vm /const
```

The function to be entered is then:

```
v/"const";
```

> The expression is multiplied by the partial molar volume of the substitutional components.

SIMULATE_REACTION

This command starts the simulation. If given without any argument, you are prompted for certain values during simulations where phases appear or disappear.

Syntax	SIMULATE_REACTION
Prompt	The command can also be given with the argument YES typed on the same line: `Simulate_Reaction Yes` With the YES argument, default values are used during simulation and no user input can be given. This is especially useful when using batch mode.

SOLVE_IN_LATTICE_FIXED_FRAME

Use this command to solve a diffusion problem in the lattice-fixed frame of reference. This command is available with the HOMOGENIZATION_MODEL as a command within the ADVANCED_HOMOGENIZATION_OPTIONS.

Syntax	SOLVE_IN_LATTICE_FIXED_FRAME
Prompts	`Solve in the lattice-fixed frame of reference /NO/` Enter `Yes` to enable this feature.

By default, DICTRA solves diffusion problems in a volume-fixed frame of reference under the assumption that the partial molar volume of all substitutional elements is constant and equal and that the partial molar volume of interstitial elements is zero. When you enable this command, the diffusion problem will instead be solved in a lattice fixed frame of reference. In addition, this option forces the use of the assessed molar volumes read from the current thermodynamic database.

Simulations with moving boundaries as well as cell simulations are currently not available with this feature.

For all geometries the leftmost/lower coordinate is fixed during a simulation (by default it is zero). This command also enforces some constraints for planar and cylindrical geometry. For a planar geometry the size of the domain in the plane orthogonal to the direction of diffusion is fixed. For a cylindrical geometry the length of the cylinder is fixed. For all geometries there may be changes in the size of the domain as a result of the diffusion process, even with closed boundaries, since the assessed molar volumes of the thermodynamic database is used.

All elements are set as substitutional. Though the notion of substitutional/interstitial elements has no meaning when running a simulation with this feature turned on, it does have implications in the POST processor.

The DICTRA POST processor does not use assessed molar volumes, which means that certain plots will be erroneous. There may for example be changes in the total domain size even for a single phase simulation with a closed system due to changes in the molar volume. A plot of the total number of moles in the domain would then, erroneously, show a change over time. Other axis quantities that in general will be incorrect are, for example, IV(*) and VP(*).

Further, when solving in the lattice-fixed frame of reference the unit of the flux is mol*$m^{-2}s^{-1}$, which differs from the default unit wherein the assumed constant substitutional molar volume (10^{-5} m^3*mol^{-1}) is included in the flux. This must be taken into account for certain types of boundary conditions, that is, the conditions of type

- FIX_FLUX_VALUE
- POTENTIAL_FLUX_FUNCTION
- ACTIVITY_FLUX_FUNCTION
- ITERATIVE_ACTIVITY_FLUX_FUNCTION

? See SET_CONDITION for details about the above commands.

In order to roughly get the same result for these boundary conditions the evaluated flux must be a factor 10^5 higher when solving in the lattice-fixed frame of reference compared to simulations with the default setting.

STORE_HOMOGENIZATION_DATA

Read/write the interpolation scheme data to file. The interpolation scheme is an option of the homogenization model that is used to speed up simulations. Use if this option can speed up simulations further.

Syntax	STORE_HOMOGENIZATION_DATA
Prompt	`Store/Read homogenization model interpolation data <Y/N>` Answering `Y` or `N` enables/disables read/write of interpolation scheme data to file.

SWITCH_MODEL

Use the SWITCH_MODEL command to use the HOMOGENIZATION_MODELto solve a problem if the classic model fails.

There are two solvers for moving phase boundary problems. The classic computationally efficient model and the more robust, but computationally more demanding, homogenization model. By default, the classic solver is tried first. If this fails, then the new solver is tried for a few time-steps before switching back to the classic solver, and so on.

The Diffusion Module (DICTRA) in Graphical Mode uses a Diffusion Calculator instead of the Console Mode commands. Most of the Console Mode functionality is available on the Diffusion Calculator, described in the *Thermo-Calc User Guide*. However, you cannot use both Graphical Mode and Console Mode in the same simulation.

Syntax	SWITCH_MODEL
Prompts	`Enable automatic switch of model (Y/N)` Determine if automatic switching from the classic solver to the homogenization model is allowed.

USE_INTERPOLATION_FOR_D

In Graphical Mode, `Complex` is the default and cannot be changed.

An interpolation scheme can be used to calculate the chemical diffusivities of complex phases. If this is enabled, the performance gain from this ranges in orders of magnitude. This is ON by default for complex phases and can be set to OFF with this command.

Syntax	USE_INTERPOLATION_FOR_D

Prompts	`The following phases will be affected if complex is selected:`
	When there are phases in the system that will be affected, these are listed. The phases are based on the thermodynamic model.
	`Interpolate diffusivities in /None/Complex/All phases /Complex/`
	The default is `Complex`. A complex phase means that an equilibrium calculation is needed in order to determine the site-fractions in a phase with converting from *u*-fraction (or any other type of composition variable).

	`Enter number of steps between Xmin and Xmax /10000/:` Enter what is essentially the number of steps in each dimension in composition-P-T space for each equilibrium condition (Nk, P, T). In the limit where an infinite number of steps are used, exactly the same solution is obtained as without the interpolation scheme. However, excellent results can be obtained with a reasonable discretization.
	`Linear or Logarithmic discretisation /Log/:` The discretization can be either linear or logarithmic. For the linear discretization the scheme will not be used at node points where the content of one or more solutes fall below a certain critical value. For such cases, where composition span many orders of magnitude, the logarithmic discretisation can be tried.

	The system confirms the discretization setting and displays the amount of free memory available for the calculation. You are prompted to enter how much of this memory to use for the simulation.
	`Discretisation set as Logarithmic (or Linear)`
	`Free physical memory (mb): 8535`
	`Fraction of free physical memory to be used /.1/:`
	The fraction of free physical memory to be allocated for the interpolation scheme.

USE_TWO_TYPES_OF_BOUNDARY_CON

This command enables you to use two types of boundary conditions (BC). This command is available with the HOMOGENIZATION_MODEL as a command within the ADVANCED_HOMOGENIZATION_OPTIONS. During the simulation one arbitrary boundary will be closed, but for the other open boundary and for each element, you can select which of the two entered boundary conditions should apply.

Syntax	USE_TWO_TYPES_OF_BOUNDARY_CON
Prompts	`Use two types of boundary conditions /NO/` Enter `Yes` to define the boundary conditions further.
	`Close the upper boundary /YES/` Select whether the upper or lower boundary should be closed during the simulation.
	`For <element>, use lower boundary BC: /YES/` You are prompted for each element whether the boundary condition entered for the lower or the upper boundary should apply.

UTILITIES_HOMOGENIZATION

ADVANCED_HOMOGENIZATION_OPTIONS

Use this with the HOMOGENIZATION_MODEL for the available utilities.

Syntax	UTILITIES_HOMOGENIZATION
Prompts	`Set temperature according to solidus temperature /N/:` Set the global temperature such that it goes to a certain value T_{target}=T_{sol}-X, where X is an entered value. Also enter the rate by which the temperature approaches T_{target}. The solidus temperature is determined with a +/- 1 K accuracy. Input guesses of the minimum and maximum temperature to occur during the simulation. This utility can be useful to optimize homogenization heat treatments. The liquid phase must be entered into the system.
	`Dump results to text files /N/:` Enter `Y` to save simulation results to various text files. The names of these files are fixed and are saved to the current working directory.
	`Read initial composition from text file /N/:` Enter `Y`to read initial composition from a text file `XF.TXT` that must be present in the working directory. The file should contain the mole fractions of all elements, in alphabetical order, starting from the first grid point, in the first region, in the first cell.
	`Enter ghost phase /N/:` Enter `Y`to force the so-called ghost phase to be created. This phase has full solubility of all components and zero diffusivity. The Gibbs energy surface of the ghost phase is set above all other phases. The name of this phase is ZZDICTRA_GHOST. It can be used for numerical reasons. It is created automatically if there is a phase that lack solubility range of one or more components and then used internally by the program.
	`Enter inactive phases into one region /N/:` Enter `Y`to make all inactive phases at a given interface to be entered into a single multiphase region when any one of the phases becomes stable.
	`Explicitly set substitutional/interstitial /N/:` Enter `Y` to explicitly select for each element whether it should be substitutional or interstitial. There must be at least one substitutional element in each region. These settings only have effect for the homogenization model and results viewed in the post processor must be interpreted with care; use `DUMP RESULTS TO TEXT FILES` to get results corresponding to the settings entered here.
	`Save average finite volume composition /N/:` Save the average finite volume composition instead of a converted piece-wise linear composition.
	`Set constant phase addition /N/:` Add constant Gibbs energy contributions to phases (in J/mol formula unit).

Syntax	UTILITIES_HOMOGENIZATION
	`Use element mobility prefactor /N/:` Enter constant factors which the mobilities of elements are multiplied with in all phases.
	`Enter element mobility constant value /N/:` Interactively enter a constant mobility estimate for specific elements in specific phases. This can be used to enter mobility estimates in phases for which there is no assessed data. Estimates entered here override database values.
	`Enter minimum save interval /Y/:` Enter a minimum time interval (in seconds) that must pass between subsequent saved time-steps. This is useful in cases where a large number of small time-steps may occur in order to keep down the size of the result file.
	`Simplified evaluation of activity boundary condition /N/:` Enter `Y` to evaluate the fluxes on boundaries directly from the activity gradient, i.e. without taking into account the change of state on the boundary caused by the prescribed boundary activities.
	`Enter explicit limits on composition /N/:` Use this setting with caution to explicitly enter upper and lower limits on composition for all components (in mole fraction).
	`Enter chemical potential contribution /N/:` Enter a function (in valid POLY-3 syntax) that is evaluated separately at all grid points and added to the chemical potential of all elements. The contribution affects the flux between grid points.
	`Do not balance external boundary fluxes /N/:` For all boundary conditions except type GAS, the flux of substitutional elements into the domain is balanced with the flux of the dependent substitutional elements such that the size of the domain is preserved. Enabling this setting disables the balancing of the substitutional fluxes. This feature is now available under the ADVANCED_HOMOGENIZATION_OPTIONS command. The use of this feature under the command UTILITIES HOMOGENIZATION is deprecated.
	`Fix external boundary flux of dependent component /N/:` This feature is disabled. A more general version is available under the ADVANCED_HOMOGENIZATION_OPTIONS command. It is still visible for backwards compatibility reasons.
	`Modified kinetics on boundary /N/:` Use this to modify the kinetics on the boundary and enter a factor. If the factor is greater/smaller than one, the mobilities of all elements on the boundary is set equal to the maximum/minimum mobility of all elements times the factor. This can be useful in order to quickly saturate an outermost finite volume.

POST PROCESSOR Commands

In this section:

Purpose and Methodology

The purpose of the POST PROCESSOR is to read and process data from the internal data structure of the DICTRA module in order to present the result of a simulation in either* GRAPHICAL (command PLOT_DIAGRAM) or* TABULAR FORM (command MAKE_EXPERIMENTAL_DATAFILE).

Before plotting/printing, you have to specify what variables should be plotted on the diagram axis or printed in the table columns. For this purpose there is a command SET_DIAGRAM_AXIS. After having SET both X- and Y-axis variables, you have to SET also plot condition and independent variable. It is also possible to specify a Z-axis. Its values appear as tick marks on the XY-curve.

Plot Condition and Independent Variable

There are two free variables after a simulation is done by the DICTRA module. One is the simulation TIME and the other is a DISTANCE in the system.

In general, when plotting a diagram you MUST set either type as fixed, i.e. the *plot condition*, use command SET_PLOT_CONDITION. The plot condition chosen is printed on a separate line above the diagram.

The other variable is then the independent variable, use command SET_INDEPENDENT_VARIABLE. The independent variable is used as stepping variable. It varies along the calculated curve.

Legal Plot Conditions

- `TIME`: Integration time
- `DISTANCE`: Distance in the system. It can be a GLOBAL distance counted from the rightmost interface of the system. A LOCAL distance is counted from the LOWER interface of the specific region prompted for.
- `INTERFACE`: At a certain interface. An interface is identified by the NAME of the adjacent region, with the addition that you will be prompted to specify if the interface is at the upper or lower end of the region.
- `INTEGRAL`: Is automatically SET when using an INTEGRAL VARIABLE as axis variable.
- `TIE_LINE`: At a certain interface. Allows you to plot a certain quantity from both sides of an interface. The typical application is for plotting tie-lines.

Legal Independent Variables

- `TIME`: Integration time. Is automatically SET when using an INTEGRAL VARIABLE' or TIME as axis variable.
- `DISTANCE`: Space coordinate. It may be GLOBAL. It is then counted from the rightmost interface of the system. Alternatively, it may be LOCAL. The distance is then counted from the LOWER interface of the specific region prompted for.

APPEND_EXPERIMENTAL_DATA

Add experimental data and text on a calculated diagram. The experimental data and text are added to a file prepared according to the syntax of the DATAPLOT graphical language. The picture generated from the data is superimposed on the ordinary graphical output from the POST PROCESSOR. The experimental data file can be created with an ordinary text editor. Another use of the APPEND_EXPERIMENTAL_DATA command is to superimpose plots from several independent calculations. For this purpose, there is a command MAKE_EXPERIMENTAL_DATAFILE which dumps a calculated diagram on a file according to the DATAPLOT syntax. With the aid of a basic text editor many such files may be merged. Remember to have only one prologue section on the file (see below).

? About DATAPLOT Files

Syntax	APPEND_EXPERIMENTAL_DATA
Prompts	`Use experimental data (Y or N) /N/:` By default, no experimental data is plotted.
	`Experimental datafile` Specify the name of the file with the experimental data. Default file extension is exp.
	`Prologue number` Select which prologue to use. In a prologue one may e.g. give the scaling of an axis, the axis texts, and so on. -1 gives a list of all prologues on the file. Read more about prologues below.
	`Dataset number(s)` Select from which dataset(s) data should be read. Several datasets may be given separated with commas or spaces. -1 gives a list of all datasets on the file.

DETERMINE_KIRK_PLANE

To use this command a certain time must be set as plot condition. You are prompted for the position of a plane at time zero. The position of the plane at the plot condition time is then calculated. The difference in position is equal to the Kirkendall shift, i.e. how much an inert marker would drift in the material due to a net flux of vacancies.

Syntax	DETERMINE_KIRK_PLANE
Prompt	`Initial zero plane /-1/`

DIFFERENTIATE_VALUES

Use the DIFFERENTIATE_VALUES command to determine differences between values in a plotted curve.

DUMP_DIAGRAM

An alternative way to create plots. Supported graphical formats are PNG, BMP, PDF, JPEG and TIFF. The plot is saved to a file.

Syntax	DUMP_DIAGRAM
Prompt	`Output format (PNG,BMP,PDF,JPEG,TIFF)` Specifies which graphical format to use.
	`Resolution (Low, Medium, High)` Specifies the resolution of the plot.

ENTER_SYMBOL

The information about this command is specific to the Diffusion Module (DICTRA) Console Mode. The ENTER_SYMBOL command is also available in the GIBBS, POLY3 and POST modules in Thermo-Calc.

Define a symbolic name to represent either a table or an 'arbitrary' function. Legal variables in functions and columns in tables are described in the sections state variables, auxiliary variables, integral variables or can be previously defined functions. Functions are a useful feature of the POST PROCESSOR to define quantities.

Syntax	ENTER_SYMBOL
Prompts	`Function or table /Function/` Select what kind of symbol to enter.
	`Name` Each symbol has a unique name that must start with a letter and can have maximum 8 characters. If one wishes to enter the name and the value on the same line they must be separated with an equal sign =.

	`Function`
	Functions are evaluated from an expression of state variables, auxiliary variables, integral variables or previously defined functions. The expression is a Fortran-like expression and operators +, -, *, / and ** can be used (** only with integer powers). Unary functions like LOG, LOG10, EXP, SIN, COS, ABS and ERF can also be used. An expression can be continued on more than one line. An expression should be terminated by a semicolon or an empty line.
	Examples
	`POI(CEM,U)-POI(CEM,L);`
	The thickness of the region named CEMENTITE
	`AC(CR)/X(FCC,CR);`
	The activity coefficient for Cr in phase FCC
	`SQRT(TIME);`
	The square root of the simulation time
	`&`
	The ampersand & sub-prompt displays if the function was not terminated by a semicolon. It allows a user to continue to write the function on the new line if one line is not enough for the function. If one has finished the function just press return again.

	`Variable(s)` When entering a table, specify what variables are to be in the various columns. Separate the variables with commas or space characters. At present a maximum of 15 columns are allowed.

Syntax	ENTER_SYMBOL
	The independent variable is always printed in the first column. Auxiliary Variables, Integral Variables, and State Variables in Console Mode DICTRA for details and examples of the short names (mnemonics).

INFORMATION

Some general information about the POST PROCESSOR module is given.

Syntax	INFORMATION
Prompt	`Which subject` Select which subject you want additional information about. Type ? to get a list of topics. • PURPOSE • STATE VARIABLES • INTEGRAL VARIABLES • AUXILIARY VARIABLES • PLOT CONDITION AND INDEPENDENT VARIABLE • BASIC METHODOLOGY

INTEGRATE_VALUES

Use the INTEGRATE_VALUES command to mathematically integrate the plotted curve.

LABEL_CURVES

Create labels. Each label is explained with to the right of the diagram.

Syntax	LABEL_CURVES
Prompt	`Label curves` Enter Y or N. For example: *1. X: X(CR); Y: TIME; PC:3* is read as *1 is a curve with X(CR) on the x-axis, TIME on the y-axis and plot condition PC according to value 3 specified on the plot condition line printed above the diagram*.

LIST_PLOT_SETTINGS

Use the LIST_PLOT_SETTINGS command to list on screen the present values of most parameters specifying the type of diagram to be plotted.

LIST_REGION_NAMES

All region names have a #-sign and the cell number appended.

Use the LIST_REGION_NAMES command to list all region names that are defined.

LIST_SYMBOLS

Use the LIST_SYMBOLS command to list a specific symbol or enter an asterisk (*) to list all defined symbols.

Syntax	LIST_SYMBOLS
Prompt	`Name` Give the name of a symbol or an asterisk * to list all defined symbols.

MAKE_EXPERIMENTAL_DATAFILE

Save graphical information in a file with the DATAPLOT format. To merge two or more diagrams from separate calculations, use the MAKE_EXPERIMENTAL_DATAFILE command to export it and add them together with a normal text editor.

APPEND_EXPERIMENTAL_DATA and About DATAPLOT Files

Syntax	MAKE_EXPERIMENTAL_DATAFILE
Prompt	`Output file` File where the graphical information is written. Default file extension is `exp`

PLOT_DIAGRAM

Plot graphical information on the specified device using the plot format set by SET_PLOT_FORMAT.

Syntax	PLOT_DIAGRAM
Prompt	`Plot file` The name of the file or graphical device.

PRINT_DIAGRAM

This command is only available for Windows operating systems.

Use the PRINT_DIAGRAM command to print a plot or diagram using the printers defined in Windows.

QUICK_EXPERIMENTAL_PLOT

Use the QUICK_EXPERIMENTAL_PLOT command to define a pair of axes, sets the axis labels to X and Y, and scale both x- and y-axis between 0.0 and 1.0 unless a prologue is read from the data file. It is similar to the APPEND_EXPERIMENTAL_DATA command but can be used when there is no graphical information to be plotted in the DICTRA module workspace.

See APPEND_EXPERIMENTAL_DATA about the format of the data file.

REINITIATE_PLOT_SETTINGS

Use the REINITIATE_PLOT_SETTINGS command to give all parameters describing the diagram as default values.

SET_AXIS_LENGTH

Change the relative length of an axis, i.e. the number of tic-marks on the axis. The default number of tic-marks on an axis is 10 when the relative length is 1. The number of units per tic-mark must be a multiple of 1, 2, or 5 to obtain a reasonable scaling of an axis.

Syntax	SET_AXIS_LENGTH
Prompts	`Axis` Specify the axis to set the axis length.
	`Axis length` Specify the relative axis length. The relative length 1 corresponds to 10 tic-marks on the axis.

SET_AXIS_PLOT_STATUS

Specify to plot a diagram axis. Use it to merge different diagrams on a pen-plotter or to obtain the diagram faster. The default to plot the axes.

Syntax	SET_AXIS_PLOT_STATUS
Prompt	`Axis plot` `Y` or `N` to plot axis.

SET_AXIS_TEXT_STATUS

Change the axis text from the automatic text given by the axis specification to another text.

Syntax	SET_AXIS_TEXT_STATUS
Prompts	`Axis (X, Y or Z)` Specify which axis text status to change (if the axis type is INVERSE, X2 or Y2 may be used to set the corresponding opposite linear axis text).
	`Automatic axis text (Y or N)` Specify if automatic axis text is to be used or not.
	`Axis text` Enter axis text.

SET_AXIS_TYPE

Select a linear, logarithmic or inverse axis.

Syntax	SET_AXIS_TYPE
Prompts	`Axis (X, Y or Z)` Specify which axis to change the axis type.
	`Axis type` Specify which axis type to set. Select `LIN`ear (default), `LOG`arithmic or `INV`erse. Only the three first characters are needed.

SET_COLOR

On devices that support colors/(line types), select different colors/(line types).

Syntax	SET_COLOR
Prompt	• Text and axis Color • Diagram Color • DATAPLOT Color

SET_DIAGRAM_AXIS

Specify the axis variables of a plot. At least two axis variables (x and y) must be specified.

Also see Auxiliary Variables, Integral Variables, and State Variables in Console Mode DICTRA for lists of variables including its abbreviated name (i.e. the mnemonic) as well of the names of these variables.

Syntax	SET_DIAGRAM_AXIS
Prompts	`Axis (X,Y or Z)` Specifies the axis to set a variable.
	`Variable` Specifies the variable to plot along this axis. A variable is specified by its mnemonic (i.e. its abbreviated name) or by name. The variable types are None, Integral Variables, Functions, Auxiliary Variables or State Variables. - `NONE`: Use this variable to clear an axis setting. - `INTEGRAL VARIABLES`: A quantity obtained by integration in space over the whole system or over a specific region. In a planar geometry values are given per unit area, in a cylindrical geometry they are given per unit length, and in a spherical geometry they are absolute values. See Integral Variables for examples. - `FUNCTIONS`: These are identified by a name which is entered with the ENTER_FUNCTION command. Use the LIST_SYMBOLS command to get a list of valid function names. - `AUXILIARY VARIABLES`: As a complement to state variables and integral variables the auxiliary variables are defined. The variables can be called by their mnemonic names, which are shown in the rightmost column. These are useful in user-defined functions. See Auxiliary Variables for examples. - `STATE VARIABLES`: State variables in the DICTRA POST module are similar to those defined in POLY-3. Examples of state variables are temperature, mole fraction, enthalpy, etc. In POLY-3 a general notation method based on character mnemonics is designed for a predefined set of state variables. See State Variables in Console Mode DICTRA for examples. Depending on the axis variable some sub-prompts may be available.
	`For component` When an activity, flux, mole-, weight- or U-fraction or percent is plotted the name of the component must be supplied.
	`In region` When the lamellar spacing, e.g. for pearlite, is plotted the name of the region must be supplied.
	`For phase` When the lamellar thickness, e.g. for ferrite in pearlite, is plotted the name of the phase must be supplied.
	`Interface`

Syntax	SET_DIAGRAM_AXIS
	When the velocity or the position of an interface is plotted the name of the interface must be given. An interface is identified by the name of the region on its upper side.
	`Type` When choosing distance as variable one has additionally to specify what type of distance. A distance may be GLOBAL, i.e. counted from the leftmost interface, or LOCAL, i.e. counted from the interface to the left of the region whose name you are prompted for.
	`Region name` Name of the region wherein the local distance is measured.

SET_DIAGRAM_TYPE

Set the diagram to a square (the default) or triangular plot (Gibbs triangle).

Syntax	SET_DIAGRAM_TYPE
Prompts	`Triangular diagram` Select `Y` for a triangular plot.
	`Plot 3rd Axis` For triangular plots is selected specify if a 3:rd axis, connecting the end points of the x- and y-axis is plotted.
	`Clip along the 3rd axis` Remove all lines outside the region limited by a line joining the end points of the X- and Y-axis.

SET_FONT

Select the font to use for labels and numbers when plotting the diagram. For some devices (e.g. PostScript) there may be other fonts available and these are selected by the SET_PLOT_FORMAT command.

Syntax	SET_FONT
Prompts	`Select Font number` Give the number for the font to select. Type ? to get an online list of the available fonts.
	`Font size` A value of 0.3 is recommended.

SET_INDEPENDENT_VARIABLE

There are two free variables after a simulation is done in theDiffusion Module (DICTRA). One is the simulation TIME, the other is a DISTANCE in the system. When plotting a diagram you must choose either one to vary along the curve, i.e. the independent variable, the other one is then the plot condition.

> ❗ When plotting integral quantities TIME should be the independent variable.

Syntax	SET_INDEPENDENT_VARIABLE
Prompts	`Variable` Select which variable TIME (integration time) or DISTANCE (space coordinate) to treat as the independent variable.
	`Type` When choosing distance as independent variable specify the type of distance. A distance may be GLOBAL, i.e. counted from the leftmost interface, or LOCAL, i.e. counted from the interface to the left of the region whose name you are prompted for.
	`Name of region` For a LOCAL distance supply the name of the region within which the distance is measured. Type a ?, to get a list of valid region names.

SET_PLOT_CONDITION

There are two free variables after a simulation is done in theDICTRA module. One is the simulation TIME, the other one is a DISTANCE in the system. In general, when plotting a diagram you must choose either type as fixed (i.e. the plot condition), the other one is then the independent variable. However, when plotting integral quantities, plot condition is automatically set to INTEGRAL and TIME is chosen as independent variable.

> You cannot mix different kinds of plot conditions. However, for TIME and DISTANCE you can give up to 15 different condition values, see sub-prompt VALUE(S) below. The plot condition chosen is printed on a separate line above the diagram.

Plot Condition and Independent Variable

Syntax	SET_PLOT_CONDITION
Prompts	`Condition` Specify the type of condition to set. Valid conditions are: • `NONE`: Condition not set. • `TIME`: Integration time. • `DISTANCE`: Distance in system. • `INTERFACE`: At a certain interface. • `INTEGRAL`: Value is integrated over the phase/region/system volume • `TIE_LINE`: Pair of values from both sides of certain interface. Depending on the condition some or none of these sub-prompts may display.
	`Interface` Specify at which interface the condition should be set. FIRST and LAST refer to the leftmost and the rightmost interface of the system, respectively. Type ? to get a full list of relevant region names.
	`Type` When distance is chosen as plot condition specify the type of distance. A distance may be GLOBAL, i.e. counted from the leftmost interface, or LOCAL, i.e. counted from the interface to the left of the region whose name you are prompted for.
	`Name of region` Give the name of the region within which the distance is measured.
	`At upper interface of region` Give the name of the region which upper interface is specified for the TIE_LINE plotting. This plot-condition allows you to plot a certain quantity from both sides of an interface. The typical

Syntax	SET_PLOT_CONDITION
	application is for plotting tie-lines.
	`Upper or lower interface of region` Specify if the condition is at the LOWER or UPPER interface of a region. The LOWER interface is placed on the left side of a region and the UPPER interface on its right side.
	`Value(s)` Supply up to 15 numerical values separated by commas or spaces for the condition set. If plot condition TIME was chosen FIRST, LAST or #n (where n is an integer number) may be specified. #? provides a list of time steps.

SET_PLOT_FORMAT

Adjust the format of the graphical output to another graphical device. This default can be changed with the SET_PLOT_ENVIRONMENT command in the SYSTEM MONITOR.

Syntax	SET_PLOT_FORMAT
Prompt	`Graphic device number /#/: <Number of the device>` Specify a graphic device number. Depending on the hardware, different plot formats (graphic devices) may be available. These are listed online by giving a question mark `?`. For some formats there can be additional sub-prompts (Y or N) about the available fonts being used for the chosen format. Also enter Y for further specifications, e.g. font type and size.

SET_PLOT_OPTIONS

Toggle on/off the plotting options on the diagram.

Syntax	SET_PLOT_OPTIONS
Prompts	`Plot header` Toggle the plot of the text above the diagram.
	`Plot logo` Toggle the plot of the logo at lower-left corner of the diagram.
	`Plot footer` Toggle the plot of the footer identifier text (only on postscript devices).
	`White contoured PS CHARS` Toggle the option of having a thin white contour around postscript characters (only on postscript devices).
	`Plot remote exponents` Toggle the plot of the remote exponents on the axis.
	`Plot cell #` Toggle the plot of the cell number text at the upper-right corner of the diagram.
	`Plot condition status` Toggle the plot of the plot-condition status line above the diagram.

SET_PLOT_SIZE

Specify a relative scale factor to change the size of the diagram. The default value of the scaling factor depends on what output device is chosen by the SET_PLOT_FORMAT command. The default plot size is adjusted to the chosen device.

Syntax	SET_PLOT_SIZE
Prompt	`Relative plot size` Enter the relative scaling factor.

SET_PREFIX_SCALING

When prefix scaling is enabled the remote exponent for an axis is automatically chosen to have a value which is a multiple of three, i.e. ..., -6, -3, 0, 3, 6,...

Syntax	SET_PREFIX_SCALING
Prompts	`Axis (X or Y)` Specify `X`- or `Y`- axis.
	`Use prefix scaling` Enables or disables prefix scaling, `Y` or `N`. Give an integer value to select a prefix power of your own.

SET_RASTER_STATUS

Set to have a raster plotted in the diagram. Default is no raster plotted.

Syntax	SET_RASTER_STATUS
Prompt	`Raster plot (Y or N) /Y/` Enables (`Y`) or disables (`N`) the raster plot.

SET_SCALING_STATUS

Choose between manual or automatic scaling on a specified axis. If manual scaling is chosen specify a minimum and a maximum value. Manual scaling can be used to magnify interesting parts of a diagram. When an axis variable is selected by the SET_DIAGRAM_AXIS command the scaling status for the axis is always set to automatic scaling.

Syntax	SET_SCALING_STATUS
Prompts	`Axis (X, Y or Z)` Specify what axis to set the scaling status.
	`Automatic scaling (Y or N)` Automatic (`Y`) and manual (`N`) scaling.
	`Min value` For manual scaling specify the value of the starting point of the specified axis.
	`Max value` For manual scaling specify the value of the end point of the specified axis.

SET_TIC_TYPE

Change the size of the tic marks and the placement either inside or outside of the axis.

Syntax	SET_TIC_TYPE
Prompt	`TIC type` Place on either the inside or the outside of the diagram axis. The absolute value of TIC TYPE determines the length. • `TIC TYPE > 0` (outside the axis) • `TIC TYPE < 0` (inside the axis)

SET_TITLE

Specify a title that displays on all listings and diagrams from the POST PROCESSOR.

Syntax	SET_TITLE
Prompt	`Title` Enter the title to include on all output. There is a maximum length of about 60 characters.

SET_TRUE_MANUAL_SCALING

Use the SET_TRUE_MANUAL_SCALING command to turn manual scaling on and off. The default is where the tic marks on the axis are placed in even intervals using the whole axis length. The scaling routine adjusts the given minimum and maximum values slightly to accomplish this.

Syntax	SET_TRUE_MANUAL_SCALING
Prompt	`Axis (X or Y)` Specify the axis you want to toggle between automatic adjustment or avoiding the adjustment of the given maximum and minimum values.

DATPLOT Files

In this section:

About DATAPLOT Files

A DATAPLOT file can be divided into two sections. The prologue, which contains directives for manipulating the default settings on the diagram layout, and the dataset, which contains the actual data and any text to be plotted in the diagram. The sections may contain multiple PROLOGUE and DATASET statements, respectively.

DATAPLOT User Guide included with this documentation set.

- All prologues must be placed before the first DATASET statement. See Keywords for Prologues and Keywords for Datasets.
- The syntax must be used for the DATAPLOT file.
- In general, each line in a DATAPLOT file must consist of a legal keyword plus its parameters or an XY coordinate pair.
- An XY coordinate pair is two real numbers and an optional graphical operation code (GOC). See Available Graphical Operation Codes (GOCs).

Example

```
700 2.54

50 1.91 WRDS

1.1 0.9 NS3

100 20'This is a text

BLOCK GOC=C3,MWAS; X=C1+273.15; Y=C2*4.184;

600 -1400 S1'text

700 -1500

BLOCKEND
```

Keywords for Prologues

Keyword	Parameters
PROLOGUE	inumb text
XSCALE	min max
YSCALE	min max
XTEXT	text
YTEXT	text
XTYPE	LIN, LOG or INV
YTYPE	LIN, LOG or INV
XLENGTH	rnumb
YLENGTH	rnumb
DIAGRAM_TYPE	TRIANGULAR or SQUARE
TIC_TYPE	rnumb
TITLE	text

Keywords for Datasets

Keyword	Parameters
DATASET	inumb text
FONT	inumb
CHARSIZE	rnumb
COLOR	inumb
GLOBALSIZE	rnumb
LFSIZE	rnumb
LINETYPE	inumb
BLOCK GOC=C3,DEFGOC; X=C1+273.15; Y=LOG10(C2);	Select one X and one Y variable
BLOCK GOC=C3,DWR; X1=C1+273.15; X2=C1; Y=C1+C2*4.184;	or multiple X and one Y variable
BLOCK GOC=C4,MWAS; X=C1+273.15; Y1=C2*4.184; Y2=C3;	or one X and multiple Y variables
BLOCK GOC=C5,DWA; X1=C1; X2=C4; Y1=C2*4.184; Y2=C3;	or multiple XY pairs
BLOCKEND	
DRAWLINE	x,y x,y
TEXT	text or ~name (of a string, see below)
ATTRIBUTE	TOP, CENTER or BOTTOM
STRING	name text The text string may contain text formatting codes namely: ^S# to set font size, ^G for Greek font, ^F# to set font type, ^U# for positioning the text upwards, ^D# for positioning the text downwards, ^R#for positioning the text to the right, ^L# for positioning the text to the left, and finally ^N for printing without updating current position to the end of the character. These text formatting codes only work for soft fonts not hardcopy postscript fonts.
INCLUDE	filename
CLIP	ON or OFF

Keyword	Parameters
`SYMBOLSIZE`	rnumb
`FUNCTION Y=203 (X); or X=203 (Y);`	<start end steps GOC> The < > denotes an optional parameter.
`PAINT`	<code> <video> <mode> The <> denotes optional parameters. Paint the area enclosed by the current path in the current pattern. The current path starts at the last 'moveto' given and includes all subsequent 'draws'. Also see PCFUNCTION below. Default is <code>=0, <video>=NORMAL and <mode>=TRANSPARENT. To set a new current pattern supply any or all of the optional parameters. <code> is a single letter 0-9, A-Z or a-t (if <code>=t supply also a number in the range 0.00 - 1.00, e.g. PAINT t 0.25.) <video> is a string reading NORMAL or INVERSE. <mode> is a string reading TRANSPARENT or OPAQUE.
`PCFUNCTION Y=203 (X); or X=203 (Y);`	<start end steps GOC> The <> denotes an optional parameter. May be used to add a function to the current path.

Available Graphical Operation Codes (GOCs)

These are the available GOCs:

- `W`: World coordinates (* DEFAULT)
- `V`: Virtual coordinates
- `N`: Normalized plot box coordinates (NPC)
- `M`: Move to this XY (*)
- `D`: Draw to this XY
- `A`: XY is absolute values (*)
- `R`: XY are relative values
- `S`: Plot current symbol at XY
- `B`: Apply soft spines on the drawn curve (use only on BLOCK data)
- `S2`: Change current symbol to 2 and plot at XY
- `'`: Plot the following text at XY

State, Integral and Auxiliary Variables

In this section:

State Variables in Console Mode DICTRA

State variables in the DICTRA POST module are similar to those defined in Thermo-Calc POLY-3 module. Examples of state variables are temperature, mole fraction, enthalpy, etc. In POLY-3 a general notation method based on character mnemonics is designed for a predefined set of state variables.

The numerical values of some state variables, e.g. activity, chemical potential, and the energetic extensive properties, are given relative to some reference state which has been defined in the thermodynamic database file. Sometimes you may have specified a reference state using SET_REFERENCE_STATE. To get numerical values relative to the user-defined reference state, append an R to the mnemonic names as defined.

Intensive Properties

Mnemonic	Description
T	temperature
P	pressure
AC(component)	activity
MU(component)	chemical potential

Extensive Properties

NORMALIZATION of extensive properties: For all extensive properties a suffix can be added to the mnemonic name to indicate a normalized extensive property. The following tables describe each mnemonic .

Extensive Property `Z at Each Grid Point

Mnemonic	Description
Z	Extensive property `Z at each grid point.
ZM	Extensive property `Z per moles of atoms.
ZW	Extensive property `Z per mass (gram).

Mnemonic	Description
ZV	Extensive property `Z per volume (m^3).

Extensive Property `Z for a Phase at Each Grid Point

Mnemonic	Description
Z	Extensive property `Z for the current amount of the phase.
ZM	Extensive property `Z per mole of atoms of the phase.
ZW	Extensive property `Z per mass (gram) of the phase.
ZV	Extensive property `Z per volume (m^3) of the phase.
ZF	Extensive property `Z per mole formula unit of the phase.

Energetic Extensive Properties

Suffixes M, W, V and F can be applied.

Mnemonic	Description
S	entropy
S(phase)	entropy of a phase
V	volume
V(phase)	volume of a phase
G	Gibbs energy
G(phase)	Gibbs energy of a phase

Mnemonic	Description
H	enthalpy
H(phase)	enthalpy of a phase
A	Helmholtz energy
A(phase)	Helmholtz energy of a phase

Amount of Components

Suffixes M, W and V can be applied.

Mnemonic	Description
N(component)	Number of moles of a component.
N(phase,component)	Number of moles of a component in a phase.
B(component)	Mass of a component.
B(phase,component)	Mass of a component in a phase.

Total Amount

Suffixes M, W and V can be applied.

Mnemonic	Description
N	Number of moles
B	Mass

Mnemonic	Description
	The legal combination BW is not very interesting as it will always be unity. BV is the density

Amount of a Phase

Suffixes M, W and V can be applied.

The normalizing properties are calculated at each grid point.

Mnemonic	Description
NP(phase)	Number of moles of a phase.
BP(phase)	Mass of a phase.
VP(phase)	Volume of a phase.
Y(phase,species#sublattice)	site fraction This quantity is dependent upon the model chosen for the phase.

Constitution

This quantity is dependent upon the model chosen for the phase.

Mnemonic	Description
Y(phase,species#sublattice)	site fraction

Integral Variables

An integral variable is a quantity that has been obtained by integration in space over the whole system or over a specific region. In a planar geometry values are given per unit area, in a cylindrical geometry they are given per unit length, and in a spherical geometry they are absolute values.

SET_DIAGRAM_AXIS and ENTER_SYMBOL commands in the DICTRA POST module.

The variable mnemonics are constructed in the following way.

- The first letter is always I for INTEGRAL VARIABLE.
- The second letter specifies quantity.
- The third letter is OPTIONAL and specifies the normalizing quantity.

First and Second Letter

Class	Quantity	Description
I	N	for number of moles
I	W	for mass
I	V	for volume
I	U	for number of moles of volume-contributing elements
II	S	for entropy
II	H	for enthalpy
II	G	for Gibbs energy
II	A	for Helmholtz energy

Class I

Integral quantities of CLASS=I may take 0-3 arguments.

The arguments MUST be given in 'falling' order of significance.

1. Region name
2. Phase name
3. Component name

Class II

Integral quantities of CLASS=II may take 0-2 arguments.

The arguments MUST be given in 'falling' order of significance.

1. Region name
2. Phase name

Third Letter - Normalizing Quantity

Quantity	Description
N	for total number of moles in system
W	for total mass of system
V	for total volume of system
U	for total number of moles of volume-contributing elements in system

Examples

Variable	Definition
`IW(PEARLITE,BCC,CR)`	The mass of CR in the BCC phase in region PEARLITE.
`IW(PEARLITE,BCC)`	The mass of BCC phase in region PEARLITE. IW is the total mass in the system.
`IVV(Austenite)`	The volume fraction of Austenite in a single cell calculation.
`IVV(2, Austenite)`	The volume fraction of Austenite in Cell 2 for a multi cell calculation.

Auxiliary Variables

The following table lists auxiliary variables that are associated with both names and mnemonics.

SET_DIAGRAM_AXIS and ENTER_SYMBOL in the DICTRA POST module.

Interface names are the same as the region names with the addition that you also have to specify if the interface is at the U(pper) or L(ower) end of the regions.

Name and Mnemonic Auxiliary Variables

Name	***Mnemonic***	***Argument***
ACTIVITY	AC(component)	component
DISTANCE		
FLUX	JV(component)	component
LAMELLAR-SPACING	LS(name)	region name
LAMELLAR-THICKNESS	LT(name)	phase name
MOLE-FRACTION	X(component)	component
MOLE-PERCENT		component
POSITION-OF-INTERFACE	POI(name,U/L)up*)	interface name
TEMPERATURE-KELVIN	T	
TEMPERATURE-CELSIUS	-	
U-FRACTION	UF(component)	component
VELOCITY-OF-INTERFACE	VOI(name,U/L)up*)	interface name
WEIGHT-FRACTION	W(component)	component
WEIGHT-PERCENT		component

Mnemonic Auxiliary Variables

There are also auxiliary variables that are only associated with a mnemonic.

Mnemonic	Description
GD	global distance
LD	local distance
M(phase,J)	mobility coefficient where J=diffusing species
LOGM(phase,J)	^{10}log of the mobility coefficient
DT(phase,J)	tracer diffusion coefficient where J=diffusing species
LOGDT(phase,J)	10log of the tracer diffusion coefficient
DC(phase,J,K,N)	chemical diffusion coefficient where K=gradient species, and N=reference species
LOGDC(phase,J,K,N)	^{10}log of chemical diffusion coefficient
DI(phase,J,K,N)	intrinsic diffusion coefficient
LOGDI(phase,J,K,N)	^{10}log of intrinsic diffusion coefficient
JV(phase and/or species)	flux in volume fixed frame of reference
JL(phase and/or species)	flux in lattice fixed frame of reference
QC(phase,J,K,N)	Q=R(ln (DC{T1}) - ln (DC{ T1+e}))/(1/(T1+e) - 1/ T1)
QT(phase,J)	Q=R(ln (DT{T1}) - ln (DT{T1+e}))/(1/(T1+e) - 1/ T1)
QI(phase,J,K,N)	Q=R(ln (DI{T1}) - ln (DI{T1+e}))/(1/(T1+e) - 1/T1)
FC(phase,J,K,N)	D0=exp(ln (DC{T1})+Q/R/ T1)
FT(phase,J)	D0=exp(ln (DT{T1})+Q/R/T1)
FI(phase,J,K,N)	D0=exp(ln (DI{T1})+Q/R/T1)

The Thermo-Calc Documentation Set

Thermo-Calc Version 2025b

About the Thermo-Calc Software

In this section:

Thermo-Calc Software

Thermo-Calc Software develops computational tools used to predict and understand materials properties, allowing you to generate computational materials data without costly, time-consuming experiments or estimations based on the limited data available.

Thermo-Calc can be used to fill the gaps in material property data and make predictions of material behavior throughout the materials life cycle. With Thermo-Calc, you can make better decisions about your products and improve your material processing conditions with accurate, reliable materials data.

The Thermo-Calc software (also referred to as the *Thermo-Calc program* or *the software* to distinguish it from the company name) is used to perform thermodynamic calculations. It can calculate complex homogeneous and heterogeneous phase equilibria, and then plot the results as property diagrams and phase diagrams.

The software fully supports stoichiometric and non-ideal solution models and databases. These models and databases can be used to make calculations on a large variety of materials such as steels, nickel, aluminum, magnesium, titanium and titanium aluminide-based alloys, high entropy alloys, copper, slags, salts, ceramics, solders, polymers, subcritical aqueous solutions, supercritical electrolyte solutions, non-ideal gases, and hydrothermal fluids or organic substances. The calculations take into account a wide range of temperature, pressure, and compositions conditions.

There are several resources available on our website to help you learn how to use Thermo-Calc and other Add-on Modules. Go to the Getting Started Guides page and choose one of the guides that provides new users an introduction to setting up simple calculations in Graphical Mode. The information there is also in this help documentation.

Databases

There are over 40 high quality kinetic, properties and thermodynamic databases for use in our software. Each database is developed for a specific materials system or application, and all databases are developed using the proven CALPHAD methodology.

The quality of the predictions in Thermo-Calc is strongly dependent on the quality of the databases because they provide the data for the calculations. This makes the databases as important, if not more so, than the software itself.

Thermo-Calc Software has long experience in the field of database generation using the proven CALPHAD methodology. We employ a highly qualified team of people working on database development internally and through international collaboration projects. With our kinetic, properties, and thermodynamics databases, you can rest assured that you are working with the most advanced CALPHAD databases available.

Go to our website to review the databases available. The online help contains all the content including technical information and examples.

About the Thermo-Calc Add-on Modules

Thermo-Calc Software offers several Add-on Modules that allow users to extend the functionality of the software in your area of specialization. All Add-on Modules are built into the Thermo-Calc platform, so there is no need for additional installation. This also creates a unified workflow and allows data to move seamlessly between the modules.

Go to the Add-On Modules page on our website for more information about license requirements, which is also mentioned throughout the documentation.

Additive Manufacturing (AM) Module

The Additive Manufacturing (AM) Module (also referred to as the AM Module) is an Add-on Module to Thermo-Calc and it is available in Graphical Mode as the AM Calculator. The aim of the Additive Manufacturing Module is to better understand the laser powder bed fusion (LPBF) process by predicting the temperature distribution and melt pool geometry as a function of process parameters and using material properties from the Thermo-Calc thermodynamic and properties databases. Special focus is to have a unified treatment of alloy-dependent material properties and process parameters when solving the multiphysics problem of a moving heat source that melts and solidifies metal powder. The multiphysics simulation involves thermal conduction, fluid flow, evaporation-, radiation-, and convective-heat loss.

The Module can simulate the transition from conduction- to keyhole-mode. With experimental melt pool data you can calibrate the heat source. The calibrated heat source can be used to predict additional process conditions and/or to construct printability (aka process) maps.

Furthermore, once you have the temperature distribution, for instance as a function of time and space, you can also use this information for other Thermo-Calc Add-on-Module simulations such as with the Diffusion Module (DICTRA) or the Precipitation Module (TC-PRISMA), or for input to other external finite element programs.

Diffusion Module (DICTRA)

The Diffusion Module (DICTRA) is an Add-on Module to Thermo-Calc. It is used for simulation of diffusion controlled transformations in multicomponent systems. The simulation calculations are both time- and space-dependent. The Diffusion Module (DICTRA) is available in both Graphical Mode (as the *Diffusion Calculator*) and Console Mode (as the *DICTRA module*).

The Diffusion Module (DICTRA), which is often just referred to as DICTRA, is ideally suited to solve diffusion simulations that include a moving boundary (*Stefan problems*). The multicomponent diffusion equations in the various regions of a material are solved under the assumption that thermodynamic equilibrium holds locally at all phase interfaces. Simulations are one-dimensional and three different geometries can be performed: planar, cylindrical, and spherical.

Examples of cases that have been simulated using the Diffusion Module (DICTRA) include:

- Microsegregation during solidification
- Homogenization of alloys
- Growth/dissolution of carbides, nitrides and intermetallic phases
- Coarsening of precipitate phases
- Interdiffusion in compounds, e.g. coating systems
- Austenite to ferrite transformations in steel
- Carburization, nitriding and carbonitriding of high-temperature alloys and steels
- Post weld heat treatment
- Sintering of cemented-carbides

Precipitation Module (TC-PRISMA)

The Precipitation Module, or TC-PRISMA, is an Add-on Module to Thermo-Calc and it is available in Graphical Mode as the *Precipitation Calculator*.

The Module treats concurrent nucleation, growth/dissolution and coarsening under arbitrary heat treatment conditions in multi-component and multi-phase systems using Langer-Schwartz theory and the Kampmann-Wagner numerical approach. It is a general computational tool for simulating kinetics of diffusion controlled multi-particle precipitation processes in multicomponent and multiphase alloy systems.

You can use the Precipitation Module for:

- Concurrent nucleation, growth/dissolution and coarsening of precipitates
- Normal grain growth and Zener pinning
- Temporal evolution of particle size distribution
- Average particle radius and number density
- Volume fraction and composition of precipitate
- Nucleation rate and coarsening rate
- Time-Temperature-Precipitation (TTP) diagrams

- Continuous-Cooling-Transformation (CCT) diagrams
- Estimation of multi-component interfacial energy
- Estimation of yield stress using the Yield Strength Property Model

Process Metallurgy Module

The Process Metallurgy Module is an Add-on Module to Thermo-Calc and it is available in Graphical Mode as the *Process Metallurgy Calculator*. The Add-on Module is designed to model reactions that occur in metallurgical processes. Although primarily used in steelmaking and steel refining processes—such as basic oxygen furnaces, electric arc furnaces, ladle furnace metallurgy, and so forth—applications are not limited to steelmaking.

There are two main branches of calculations possible: **Equilibrium** and **Process simulation**. Equilibrium calculations do not consider any kinetics, the process simulation includes reaction kinetics.

In general, for both types, the main difference compared to using a standard Equilibrium Calculator is that it is easy to handle the different materials present in a metallurgical process. The materials used in the process can be pre-defined, saved and used for the equilibrium calculations. Metallic materials can be defined in element weight percent, oxide materials in weight percent of oxide components, the gas phase in volume percent of gas components and its amount can be defined in normal cubic meters, and so forth. In principle this can be done in a standard Equilibrium Calculator. However, it is much easier when using the Process Metallurgy Calculator as this is designed for this specific purpose.

When using the **Equilibrium** branch of calculations, both isothermal and adiabatic calculations are possible. Adiabatic calculations assume no heat and mass exchange with the environment during the equilibrium reaction, meaning that the temperature changes as a result of exothermal or endothermal reactions taking place.

For a **Process simulation** branch of calculation, the reaction kinetics of the process are considered. This is done by dividing the system into zones. Typically one would have one steel zone containing liquid metal and a slag zone containing liquid oxide (slag). The kinetic model assumes that only a fraction of the steel zone reacts with a fraction of the slag zone per time step. This reacting fraction of the whole system is termed the reaction zone (in literature it has become known as Effective Equilibrium Reaction Zone or EERZ).

You can use the Process Metallurgy Module to calculate the following:

- The equilibrium between custom-defined steels, slags, and gasses.
- The equilibrium between other metallic and non-metallic phases.
- Desulfurization, dephosphorization, and decarburization.

- Any partition coefficient, for example the partitioning of sulfur between the liquid steel and slag phase.
- Slag characteristics, such as slag basicity or sulfur capacity.
- The fraction of liquid and solid in the slag.
- The temperature change in an adiabatic process.
- Kinetics of the reaction between phases. Typically this is the reaction between a liquid metal and slag phase, but it could also be the reaction between a solid oxide and slag (simulation of refractory wear) or between a solid metal and liquid metal (simulation of dissolution of alloy), etc.

Material Specific Property Model Libraries

There are specialized Property Models available for those working with specific materials such as steel, nickel, and titanium. The libraries, also sometimes referred to Add-on Modules, are available with the Property Model Calculator and the applicable database licenses.

- The *Nickel Model Library* includes the following models specially designed for those working with nickel alloys: Antiphase Boundary Energy, Coarsening, Equilibrium with Freeze-in Temperature, Solvus for Ordered Phase, and Strain-Age Cracking.
- The *Noble Metal Alloys Model Library* includes the Optical Properties Property Model.
- The *Steel Model Library*includes the following models for those working in the steel industry: Bainite, CCT Diagram, Critical Transformation Temperatures, Ferrite, Martensite Fractions, Martensite Temperatures, Martensitic Steel Strength, Pearlite, and TTT Diagram.
- The *Titanium Model Library* includes the following models specially designed for those working with titanium alloys: Alloy Strength and Martensite Temperatures.

Graphical Mode vs Console Mode

There are two interfaces available in Thermo-Calc: *Graphical Mode* with a graphical user interface (GUI) and *Console Mode*, which uses a command line interface. Thermo-Calc and the Diffusion Module (DICTRA) are available in both modes, and all other Add-on Modules are only available in Graphical Mode.

If you are a new user, Graphical Mode is a good way to learn how to work with Thermo-Calc. Depending on what you want to simulate, in some cases Console Mode can have more functionality but until you are comfortable with the concepts, it is recommended you start in Graphical Mode, and for all new Add-on Modules, these are only available in Graphical Mode.

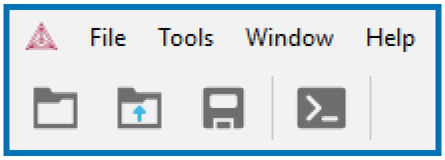
In Graphical Mode calculations are set up, carried out, and visualized as part of a *project*. The steps in the project are performed with *activities*. There are templates and a Wizard available to guide you through the process of defining the project. See Getting Started Links and Templates.

In Console Mode you work with *modules*, which are managed using commands typed at a prompt. Some modules, called *response-driven modules*, ask you a series of questions that typically take you through the process of defining your system, setting calculation conditions, performing calculations and plotting the results.

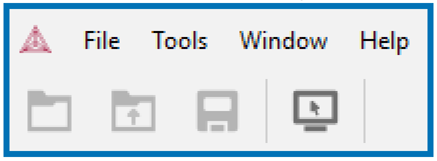
How to Switch Between Modes

The first time you open Thermo-Calc, it defaults to Graphical Mode. For any future instance it defaults to the last mode used.

Along the top of the GUI is the Graphical Mode Toolbar where you switch between modes.



In Console Mode, except for the **Switch to Graphical Mode** button, the toolbar is not used.



See Menu, Toolbar, and Keyboard Shortcuts for information about the **Tools**, **Window**, and **Help** menus, which are available in both modes.

File Extensions

The file extensions are different based on the mode you are in. In Console Mode the extensions are also based on whether you are working with Thermo-Calc or the Diffusion Module (DICTRA).

In Graphical Mode, the Thermo-Calc project files have the extension *.`tcu`. This includes the examples for the Add-on Modules.

In Console Mode, Thermo-Calc macro files have a *.`TCM` extension and the Diffusion Module (DICTRA) file extension is *.`DCM`. In addition to macro files in Console Mode the are also *Log* files and *Workspace* files, which also differ.

Modes Run Simultaneously

The two modes can be run simultaneously, but there is no communication between them. What you do in Graphical Mode does not affect the state of the Console Mode session and vice versa. One exception is the plot settings.

Global Settings: Graphical and Console Mode Plotting

Data Optimization and Thermodynamic / Kinetic Assessments

Although many calculations can be done in either mode, data optimization (i.e. PARROT) and thermodynamic or kinetic assessments (i.e. custom database development) are only available in Console Mode or using an SDK such as TC-Python.

Graphical Mode Activities vs Console Mode Modules

Although many calculations can be done in either Graphical Mode (GM) or Console Mode (CM), only data optimization and thermodynamic or kinetic assessments are available in Console Mode. Conversely, Calculators are only available in Graphical Mode as indicated in the table.

About the Activity Nodes (Graphical Mode) and Console Mode Modules

Graphical Mode (GM) versus Console Mode (CM)

GM Activity	***CM module (Short Name)***	***Primary Functions***
AM Calculator	–	Run additive manufacturing (AM) simulations using the Add-on Additive Manufacturing (AM) Module. In addition, probe data generated from an AM calculation can be used with the Diffusion Calculator and/or Precipitation Calculator. Additional licenses are required for full access to this Add-on Module and/or the extended use of the probe data.
Binary Calculator	BIN	Calculate binary phase diagrams. Access to specific databases designed for BIN, such as TCBIN, is required.
System Definer	DATA	Select appropriate databases, define chemical systems and retrieve the data required for calculations.
Diffusion Calculator	DICTRA	Run simulations of diffusion controlled transformations in Thermo-Calc using the Diffusion Module (DICTRA). An additional license is required for full access to this Add-on Module.
–	DIC_PARROT	This is to do data optimization for the Diffusion Module (DICTRA) and Precipitation Module (TC-PRISMA). It allows you to assess experimental data and use such data to optimize calculations. An additional license is required for full access to this Add-on Module.
–	ED_EXP	Part of the PARROT submodule, use it to edit experimental data points to make reliable optimizations.
This is the calculation engine	GIBBS or GES	Handles thermodynamic models and quantities. Generally you do not need to use this, but you can get information about models, and list, add or amend the thermodynamic parameters in use.
–	PARROT	Used for data optimization to assess experimental data and use the data to optimize calculations.
Precipitation	–	Set the conditions for, and perform, a precipitation calculation using the

GM Activity	*CM module (Short Name)*	*Primary Functions*
Calculator		Precipitation Module (TC-PRISMA). An additional license is required for full access to this Add-on Module.
Property Model Calculator	–	Predict and optimize material properties based on their chemical composition and temperature. There are preconfigured **General Models** available for all users and specialized material specific models such as **Nickel Models**, **Noble Metal Alloys Models**, **Steel Models**, and **Titanium Models** available with additional licenses.
Equilibrium Calculator	POLY	Equilibrium calculation command module. Specify conditions and make calculations.
Material to Material Calculator	–	To calculate materials transitioning from one into the other.
Plot Renderer	POST	This is a submodule to POLY and is for post-processing and plotting of calculation results. Modify property and phase diagrams, add labels, change the diagram colors and so forth.
Ternary Calculator	POTENTIAL	Calculate and plot gas potential diagrams in a ternary system. The potential of two gas species are used as the diagram axes.
–	POURBAIX	Calculate and plot pH-Eh diagrams (Pourbaix diagrams) and property diagrams for heterogeneous interaction systems involving aqueous solutions.
Process Metallurgy Calculator	–	Use this to model with the Process Metallurgy Module and for reactions that occur in metallurgical processes. Although primarily used in steelmaking and steel refining processes (such as basic oxygen furnaces, electric arc furnaces, ladle furnace metallurgy and so forth), applications are not limited to steelmaking. An additional license is required for full access to this Add-on Module.
–	REACTOR	Simulate chemical reaction processes in several feed-forward steady-state stages or in several dynamic stages.
Scheil Calculator	SCHEIL	Simulate and plot Scheil-Gulliver solidification processes with no diffusion in the solid phases and with/without consideration of back diffusion of interstitial components (such as C, N, O, S).
–	SYS	Interact with the operating system and change environmental settings. Create and execute macro files.
–	TAB	Tabulate properties of chemical reactions and substances (stoichiometric or solution phases).

GM Activity	*CM module (Short Name)*	*Primary Functions*
Ternary Calculator	TERN	Calculate ternary phase diagrams.

Graphical Mode vs Console Mode: Calculation Types

When you are using Thermo-Calc and the Add-on Modules, you generally first set up a system, select the databases to use, and then define various parameters related to the simulation you want to conduct. Once this is set up you decide what *Calculation Type* to perform, choose a *Plot type* (or a table for single equilibrium, for example) to use and then eventually get a result.

How Thermo-Calc handles the calculation behind the scenes is the same whether you use Graphical Mode (GM) or Console Mode (CM). However, there are differences with the workflow and for historical reasons some calculation types are named differently based on whether you are in one mode or another.

? Calculation Types in Graphical Mode and Graphical Mode vs Console Mode: Calculation Types

In addition, the plot types (diagrams) you choose to output the information are also different based on whether you are in Graphical or Console Mode. These plot types are often based on the type of calculation being done, where in some cases you can only do it in one mode and not the other. For example, precipitation calculations are only available with the Precipitation Calculator, GM only, but you can do diffusion calculations in both modes.

Comparison of Calculation Types in Graphical Mode vs Console Mode

The table lists most of the calculation types that you will want to perform. The first column is primarily based on the calculation types you can select when working in GM and when using the various calculators as indicated in the second column. The third column is the module or command in CM that you would use to perform the same, or similar, type of calculation.

Calculation Type	*Graphical (GM)*	*Console (CM)*	*Definition*
Equilibrium calculations	Equilibrium Calculator	POLY3 module	An equilibrium defines the amount(s) and composition(s) of one or several phases that have the minimum Gibbs energy at a given temperature and pressure. A prerequisite for a successful equilibrium calculation is that the number of degrees of freedom according to Gibb's phase rule

Calculation Type	*Graphical (GM)*	*Console (CM)*	*Definition*
			must be zero. This means that the right number of independent conditions must be set in order to successfully be able to calculate an equilibrium.
Single equilibrium	Property Model Calculator (Equilibrium model), Equilibrium Calculator, and Material to Material Calculator	POLY3 module	To calculate a single equilibrium. The results from this calculation are displayed as follows: - Graphical Mode: In the Visualizations window for a Table Renderer or in the Event Log window (for the Property Model Calculator) - Console Mode: With the LIST_EQUILIBRIUM command.
Single (no axes)	Property Model Calculator and Process Metallurgy Calculator	POLY3 module	To calculate a single point. The results from this calculation are displayed as follows: - Graphical Mode: In the Visualizations window for a Table Renderer or in the Event Log window. - Console Mode: With the LIST_EQUILIBRIUM command.
One Axis	Property Model Calculator, Equilibrium Calculator, Material to Material Calculator, and Process Metallurgy Calculator	POLY3 module	To vary a quantity on the X-axis.
Property diagrams	One Axis: available with Equilibrium Calculator, Material to Material Calculator, and Property Model Calculator	POLY3 module, *STEP* command	A property diagram is calculated by stepping one of the conditions that were defined for the equilibrium calculation and plotting some other property against this variable. For example stepping through temperature and plotting equilibrium composition of a certain phase, or stepping through composition and plotting equilibrium phase fractions, and so forth.
Phase diagrams	Equilibrium Calculator, Binary Calculator, Material to Material Calculator, and Ternary Calculator	POLY3 module, *MAP* command, BINARY module, and TERNARY module The Material to	A phase diagram is mapped within a specific space constructed by two (or more) independent mapping variables. These are mostly temperature and composition, but can be many other, such as temperature and pressure, activity of oxygen and activity of sulfur, and so forth.

Calculation Type	*Graphical (GM)*	*Console (CM)*	*Definition*
		Material Calculator is not available in Console Mode	
Scheil calculations	Scheil Calculator	Scheil module	Simulate a non-equilibrium transformation or partial-equilibrium transformation, also called a Scheil-Gulliver solidification.
Gibbs energy curves	Binary Calculator	BINARY module	To calculate at a constant temperature over the whole composition range.
Activity curves	Binary Calculator	BINARY module	To calculate at a constant temperature over the whole composition range.
Phase fractions	Binary Calculator	BINARY module	To calculate as a function of temperature at a constant composition.
Isothermal section	Ternary Calculator	TERNARY module	To calculate the ternary system for the whole composition range at a constant temperature.
Monovariant lines	Ternary Calculator	TERNARY module	To calculate the variation of the liquid compositions with temperature.
Liquidus projection	Ternary Calculator	TERNARY module	The projection liquid surface and the monovariant lines are calculated over the given temperature range.
Potential diagrams	not available	Potential Diagram module and POLY3 module	A potential diagram uses the activities of two major species in the gaseous mixture phase as mapping variables. For example, use this for a metal-oxide/sulphide-gas interaction system to calculate a diagram based on a specific temperature and pressure .
T0 temperature simulations	This is available as the T-Zero Temperature Property Model using the Property Model Calculator	POLY3 module	The T0-temperature is the temperature at which two phases have the same Gibbs energy for a certain composition for a certain alloy composition.
Paraequilibrium	not available	POLY3 module	A paraequilibrium is a partial equilibrium where one interstitial component, such as carbon (C) and nitrogen (N), in a multicomponent alloy can diffuse much faster than the other components (the

Calculation Type	*Graphical (GM)*	*Console (CM)*	*Definition*
			substitutional elements, including the matrix element and alloying elements).
Grid	Property Model Calculator, Equilibrium Calculator, Process Metallurgy Calculator, and AM Calculator	not available	With the Equilibrium Calculator, it computes the equilibrium of each grid point in a two-dimensional grid. With the Property Model Calculator and Process Metallurgy Calculator, it evaluates two axis variables of the selected quantities in the specified range and number of steps. For the AM Calculator it is available with the Additive Manufacturing (AM) Module and a Steady-state simulation. It evaluates two axis variables of power and scanning speeds in the specified range and number of steps.
Batch	Property Model Calculator and AM Calculator	not available	With the Property Model Calculator, it allows for high throughput calculations and reads data from a file, such as a spreadsheet, rather than, for example, having a fixed grid or random values. Results from these batch calculations can then be compared to experimental values (as long as this data is included). For the AM Calculator it is available with the Additive Manufacturing (AM) Module and a Steady-state simulation.It is to include power and scan speed data, which is read from a file such as a spreadsheet. You can optionally include experimental melt pool width and depth (if there is data), and compare this to the calculated results.
Min/Max	Property Model Calculator	not available	Evaluates the Property Model(s) for all variations of the selected quantities at the given limits.
Uncertainty	Property Model Calculator and Process Metallurgy Calculator	not available	Evaluates the Property Model(s) where the values of the quantities are sampled from Gaussian distributions.
Aqueous solutions, Pourbaix diagram	Equilibrium Calculator	Pourbaix Diagram module, POLY module	A Pourbaix diagram is a kind of phase diagram that shows the stability boundaries for a metal-aqueous interaction system. The phase boundaries are shown as a function of pH (acidity) and Eh (standard hydrogen electronic potential).
Tabulation reaction	not available	TAB module	To tabulate thermodynamic functions of any type of substance, stoichiometric phase or solution phase, or reaction.

Calculation Type	***Graphical (GM)***	***Console (CM)***	***Definition***
Diffusion simulation	Diffusion Calculator	DICTRA monitor	Detailed simulation of diffusion controlled reactions in multicomponent systems.
Isothermal	See below	POLY3, DICTRA monitor	Isothermal calculations in general can be done in all Console Mode modules, for example an Isothermal diffusion in DICTRA monitor and an isothermal calculation in POLY3 using the STEP command.
Isothermal and non-isothermal	Precipitation Calculator	See above	You can calculate nucleation, growth/dissolution and coarsening of particles size classes under these conditions: isothermic (precipitation simulation at constant temperature) or non-isothermic (precipitation simulation with user-defined temperature profile).
TTT and CCT	Precipitation Calculator	not available	The TTT (Time-Temperature-Transformation) and CCT (Continuous Cooling Transformation) diagram can be simulated for one or more particles.
Heat source calibration	AM Calculator	not available	This is available for the Additive Manufacturing (AM) Module for Steady-state simulations, import parameters for a range of experimental melt pool data then store the calibrated heat source for further use.

About the File Types and Formats

The file formats (and the file extensions / suffixes) are based on whether you are working in Graphical or Console Mode, and in Console Mode, whether you are working with Thermo-Calc and/or the Diffusion Module (DICTRA).

Graphical Mode

In Graphical Mode you work with one file type, a *project* file, which has a `*.tcu` file extension. This is applicable to Thermo-Calc and all the Add-on Modules and Property Model Libraries.

Console Mode

In Thermo-Calc Console Mode there are file *types*—**macro** (including log files) and **workspace**—and *extensions* —`*.TCM`, `*.POLY3`, `*.GES5`, `*.PAR`, `*.POP`, and `*.EXP`.

A reminder that Linux and macOS are case sensitive; when applicable ensure you enter file extensions with capital letters.

Workspace files are not currently available with GES6.

Working with the Console Mode File Types

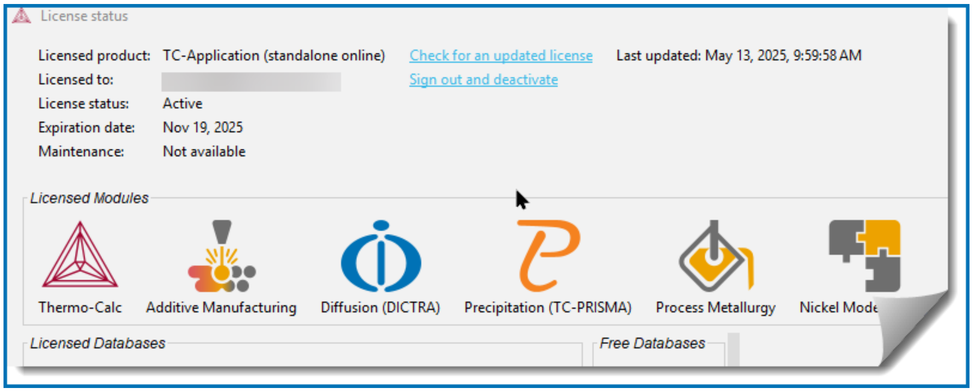
Displaying Thermo-Calc License Information

You can start (and install) the software without a valid Thermo-Calc license but you cannot do any calculations. To show information about the available and installed licenses, from the main menu select **Help →** **Show License Info**.

> There are two **license activation types** available with Thermo-Calc 2025b: One using a *license file* that is installed on your computer (this also includes the different network installation types using Sentinel License Management Software), and the new type where *user credentials* (user name and password) are entered after installation and when you first open (launch) Thermo-Calc.

User Credentials Activations

Below is an example of part of a **License Information** window for a Standalone installation using the **User credentials** activation type. The details are unique for each installation.



License status

Licensed product: TC-Application (standalone online)

Licensed to: [redacted]

License status: Active

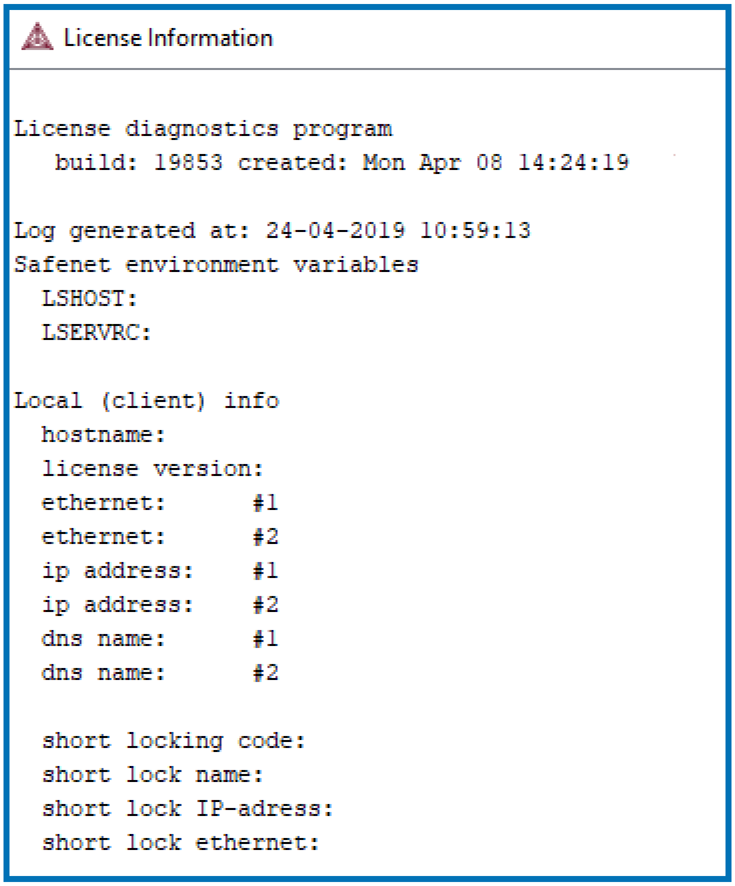
Expiration date: Nov 19, 2025

Maintenance: Not available

Last updated: May 13, 2025, 9:59:58 AM

License File Activations

Below is an example of part of a **License Information** window for a network installation using the **license file** activation type. It only shows the fields you would expect to see as the details are unique for each installation.



```
License diagnostics program
   build: 19853 created: Mon Apr 08 14:24:19

Log generated at: 24-04-2019 10:59:13
Safenet environment variables
  LSHOST:
  LSERVRC:

Local (client) info
  hostname:
  license version:
  ethernet:       #1
  ethernet:       #2
  ip address:     #1
  ip address:     #2
  dns name:       #1
  dns name:       #2

  short locking code:
  short lock name:
  short lock IP-adress:
  short lock ethernet:
```

Network Licenses

For a *network* license, under each license type with instances checked out, there is a list of who checked out each license.

In Graphical Mode, an instance is checked out when an Equilibrium Calculator activity is created, and checked back in when that Equilibrium Calculator is removed. For the Add-on Diffusion (DICTRA), Precipitation (TC-PRISMA), and/or Additive Manufacturing Modules this also applies to the Diffusion Calculator, Precipitation Calculator, AM Calculator, and Process Metallurgy Calculator, respectively.

In Console Mode, an instance is checked out when you enter the POLY module and is checked back in when you exit the POLY module.

- The **Features** column is a list of the specific software, databases and API licenses purchases.
- The **Version** is an internal version number for the feature.
- The **number of licenses** column is how many instances of each license type available to be checked out simultaneously.
- The **in use** column shows how many license instances are checked out.

Console Mode License Restrictions

- If you start Thermo-Calc without a valid Thermo-Calc license you cannot leave the SYS module.
- If all the licenses are checked out for a network client installation of Thermo-Calc, you may not be able to enter the POLY or DICTRA modules until a license is available.
- To enter the DICTRA and the DIC_PARROT modules, you need a valid Diffusion Module (DICTRA) license key.
- If you enter and use either the DIC_PARROT module or the PARROT module, then you cannot enter the other module in the same session. You must close down Thermo-Calc and launch the program again to enter the other data optimization module.

Network Computer License Restriction

If you have a network computer installation of Thermo-Calc, then you may not be able to do any calculations even if you have access to a valid network license file. This is because others who are part of your network installation may have checked out all allowed instances of the software.

If you are running a network installation of Thermo-Calc, you can see how many instances of the client licenses are currently checked out and how many of them are left. You can also see which client computers have checked out the licenses.

About the Documentation and Examples

In this section:

Installed Examples, Manuals, and Materials Folders

There are several ways to access the examples, manuals (containing PDF documentation), and materials data folders included with your installation.

Item	*Main Menu*	*My Project Configuration window*	*System Definer or Material to Material Calculator*	*From the Windows Start Menu*	*On your Computer*	*Website*
Manuals (PDF documentation, DATAPLOT EXP files, TC-Python and TC-Toolbox for MATLAB® HTML help)	x	-	-	x	x	x
Software Development Kits (SDKs) (TC-Python, TC-Toolbox for MATLAB®, TQ-Interface)*	x	-	-	-	x	x
Examples (project and macro files)*	x	x	-	x	x	x
Materials**	-	-	x	x	x	x
Property Models	-	-	-	-	x	-
Process Metallurgy Materials***	-	-	-	-	x	-

* The SDK folder is installed during installation and available when you have a license for the applicable SDK. There are also differences based on the API as to where examples are installed.

** The Material Properties libraries for the Additive Manufacturing (AM) Module are handled by the software.

*** The Process Metallurgy Module user-defined material compositions are saved from the Process Metallurgy Calculator and managed from the **Options** tab.

From the Main Menu

Once your Thermo-Calc software is installed you can open the Examples and PDF documentation (*Manuals*) from the main menu:

- To open the Manuals folder select **Help → Manuals Folder**. Note for Linux openSUSE users: This link is not functional. To access the folder, navigate to the default location based on your installation type
- To open the Examples based on whether you are in Console Mode or Graphical Mode, select **File → Examples Files** or **Help → Examples Files**.

My Project Configuration Window

When in Graphical Mode, click the **My Project** node. In the **Configuration** window under **Getting Started**, click **Example Files**.

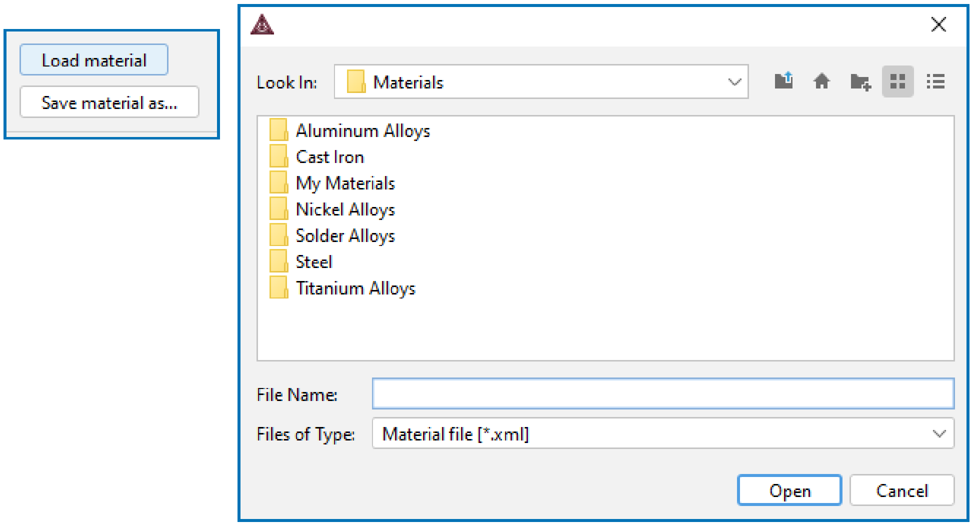
Installed Materials Folder

When you are working with the System Definer or Material to Material Calculator you can open the default **Materials** folder included with your installation.

At the bottom of the window under **Material**, click **Load material** to navigate to a material file.

There is a separate folder for materials saved using the Process Metallurgy Calculator. See Installation Default Directory: Process Metallurgy Materials.

For the Additive Manufacturing (AM) Module, the Material Properties library is managed by the software.



The default directory where these material files are stored is based on operating system:

Operating System	*Materials Installation Directory*
Windows	`C:\Users\<user>\Documents\Thermo-Calc\2025b\Materials`
Linux	On Linux all user files are installed where the program is installed. If installed as root the default is: `/opt/Thermo-Calc/2025b/Materials`
macOS	`/Users/Shared/Thermo-Calc/2025b/Materials`

Start Menu (Windows Only)

On Windows, once Thermo-Calc is installed, you can locate the Examples and Materials folders, plus all the Manuals. Go to the Start menu and in the search field enter **Thermo-Calc**. A list of the installed versions is provided or click the **Apps** or other tabs to browse search results.

On Your Computer (All Operating Systems)

The PDFs, example files and materials xml files are included with your installation in a folder location based on the operating system.

In the table, *<user>* stands for the username and *<version>* for the version of Thermo-Calc, for example 2025b.

WINDOWS FILE PATHS

User Type	*Default Directory*
Administrator	**Software** Program Files\Thermo-Calc\<*version*> **Examples, Manuals, Materials, Property Models, Process Metallurgy Materials and SDK folders:** Users\Documents\Thermo- Calc\<*version*>

MACOS FILE PATHS

User Type	*Default Directory*
Administrator (user name and password required)	**Examples, Manuals, Materials, Property Models, Process Metallurgy Materials and SDK folders:** /Users/Shared/Thermo-Calc/<*version*> To go to this folder, in Finder, from the **Go** main menu select **Go to folder**. Enter the above file path and click **Go**.

LINUX FILE PATHS

User Type	*Default Directory*
Non root user	home/<*user*>/Thermo-Calc/<*version*>
Root user	usr/local/Thermo-Calc/<*version*>

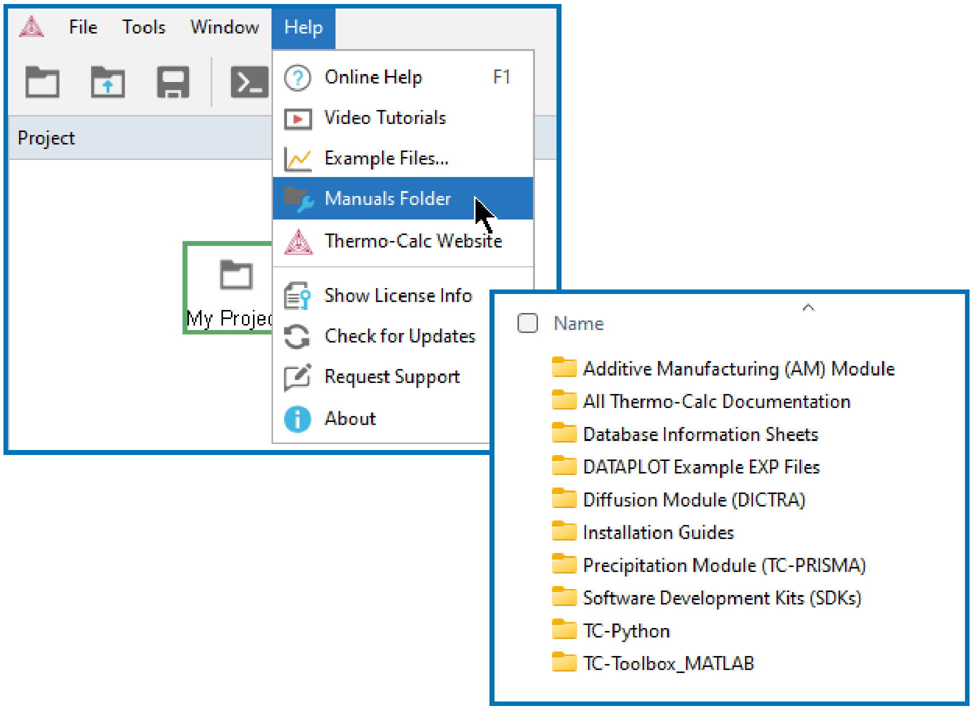
Website

Many resources are available from our website. On the Support → Documentation page you can download the current and archived PDF documentation and examples, or navigate to the TC-Python and TC-Toolbox for MATLAB® help and diagnostics tools. For current technical information and examples collections for the databases, you can access these by database starting on the Products → Databases page.

About the Manuals (Documentation) Folder

There is documentation available in PDF format from the **Help** → **Manuals** folder as part of your installation. Except for two of the SDKs, this is the same information as is contained in the Thermo-Calc online help, just in a different format. The contents of each folder are described below.

It is recommended you search the help (press F1 in Thermo-Calc) if you cannot find what you are looking for in a particular folder or PDF.



Additive Manufacturing (AM) Module
All Thermo-Calc Documentation
Database Information Sheets
DATAPLOT Example EXP Files
Diffusion Module (DICTRA)
Installation Guides
Precipitation Module (TC-PRISMA)
Software Development Kits (SDKs)
TC-Python
TC-Toolbox_MATLAB

A *Documentation Set* contains a variety of user guides packaged together in one PDF. For the Process Metallurgy Module and specialized material specific Property Models (i.e. Steel or Nickel), all the content is contained in the *Thermo-Calc Documentation Set* or online help.

Additive Manufacturing (AM) Module

The *Additive Manufacturing Module User Guide* is a summary PDF for the functionality of the Additive Manufacturing (AM) Module and its AM Calculator. This is a highly specialized product and it is interconnected to Thermo-Calc features such as the Scheil Calculator, Diffusion Calculator, and Precipitation Calculator. It requires additional licenses for some functionality. The user guide is not comprehensive. Use the *Thermo-Calc Documentation Set* or online help for all other content.

All Thermo-Calc Documentation

The *Thermo-Calc Documentation Set* is one large PDF that includes the information needed to work with the Thermo-Calc software. By having all content in one PDF it enables you to search the content just like you would when in the online help (with some exceptions). For example, this PDF does not include specific database or other specialized content that can require additional licenses.

The Thermo-Calc Documentation Set includes the following.

Thermo-Calc Installation Guides

Includes all installation instructions for all platforms and license types.

Graphical Mode User Guide

Includes details about all features and calculators included with Graphical Mode. For example, it includes details about calculators available with add-on products such as the AM Calculator, Diffusion Calculator, Precipitation Calculator, Process Metallurgy Calculator, and all the Add-on Material Specific Property Model Libraries (i.e. Steel, Nickel, etc.). For the Add-on Diffusion Module (DICTRA) and Precipitation Module (TC-PRISMA), additional information is included in the separate documentation.

Console Mode User Guide

Includes details about the functionality and features available with the Console Mode version of Thermo-Calc.

For example, the following is only in Console Mode and the associated documentation is included in the respective documentation.

- The PARROT module optimization content is described in the *Data Optimization User Guide*.
- If you develop your own custom databases, this is described in the *Database Manager User Guide*. There is some other generally related documentation that is found under General Reference.
- If you use the old DATAPLOT functionality for plotting, this is included in the *DATAPLOT User Guide*.
- The POURBAIX module is only in Console Mode and there is the *Pourbaix Diagrams Educational Material* guide included.
- A separate *Thermo-Calc Console Mode Example Macros* PDF is available in the folder but NOT included in the Documentation Set due to its file size and page length.

Thermo-Calc General Reference

This is content that spans some of the general topics applicable to multiple applications within Thermo-Calc, i.e. it might be for both Console Mode and Graphical Mode, or needed for a specific database calculation in Thermo-Calc (i.e. model information, variables, and functions for thermophysical and elastic properties).

- **Parameters, Functions, and Variables**: Information applicable to both Console Mode and Graphical Mode with respect to understanding the format these are to be written in for Thermo-Calc to use the parameter, function, or variable. However, many of the sections are specific to Console Mode where the explicit use of these terms is more often used.
- **Thermophysical Properties Data**: This includes the model descriptions and data parameters you would need in combination with a database that has the relevant thermophysical property.
- **Elastic Properties Variables**: This includes the model descriptions and data parameters you would need in combination with a database that has the relevant elastic properties.
- **Database Files and Database Checker**: Information about the database initialization file, differences between Thermo-Calc encrypted and user-defined unencrypted databases, about cached database files, and more. Some content is more specific to those developing their own databases, other information is intended for advanced users, for example, the Database Checker information is a supplement to the *Database Manager User Guide*.
- **Global Settings**: In the **Options** window you can globally set general settings for Graphical Mode as well as default settings for any new activities for both Graphical Mode and Console Mode.

Database Information Sheets (Technical Information)

The *Technical Information* content available as a PDF is also included in the online help system and contains details such as the elements, systems, phases, and properties available with a specific database. It includes the revision history for the database.

> Starting with Thermo-Calc 2020b, databases are transitioning from the *Extended Info* PDF, which can include examples, to individual *Validation and Calculation Examples Collection*. The examples are only available on the website or in the help.

All *Technical Information* and *Validation and Calculation Examples Collection* PDFs for the **current version** of the database are available for download from the Thermo-Calc website.

DATAPLOT Example EXP Files

The examples are available as supplementary information as described in the *DATAPLOT User Guide*, which you can find in either the online help, *Thermo-Calc Documentation Set* or *Diffusion Module (DICTRA) Documentation Set*.

Diffusion Module (DICTRA)

The *Diffusion Module Documentation Set* is one large PDF that includes the information needed to work with the Add-on Diffusion Module (DICTRA) and Thermo-Calc software in Graphical Mode and Console Mode. By having all content in one PDF it enables you to search the content just like you would when in the online help (with some exceptions). For example, this PDF does not include specific database or other specialized content that can require additional licenses.

The Documentation Set includes:

- All the content available in the *Thermo-Calc Documentation Set* and described above.
- Diffusion Module (DICTRA) *Quick Start Guide—Graphical Mode* and *Quick Start Guide—Console Mode*.
- *Diffusion Module (DICTRA) Command Reference* (for Console Mode only)

Also available separately in this folder:

- *Diffusion Module Quick Guide - Console Mode*
- *Diffusion Module Quick Guide - Graphical Mode*
- The *Diffusion Module (DICTRA) Console Mode Example Macros* PDF is available in the folder but NOT included in the Documentation Set due to its file size and page length.

Installation Guides

Includes the *Quick Install* guides for Standalone (SUNLL) Windows and macOS systems, instructions for TC-Python and TC-Toolbox for MATLAB®, with the full installation instructions for all platforms and license types.

For convenience, the *TC-Python Installation Guide* is also included as a separate PDF in this folder.

Precipitation Module (TC-PRISMA)

There is a user guide in this folder, which includes examples, Precipitation Calculator settings, references, and details about the theoretical models and numerical methods. Use the *Thermo-Calc Documentation Set* or online help for all other content.

Software Development Kits (SDKs)

Separate TC-Python and TC-Toolbox for MATLAB® documentation is stored in its own folder and each is available from our website. This folder has the PDF version of this content.

- **TC-Python API Programmer Guide**: This guide is the PDF format of the HTML help described below.
- **TQ-Interface Programmer Guide**
- **TC Toolbox for MATLAB® Programmer Guide**: This guide is the PDF format of the HTML help described below.

TC-Python

This folder contains the TC-Python HTML files. Double-click `Index.html` file to open it. This help is also available on our website. TC-Python includes details about working with custom property models.

TC Toolbox_MATLAB

This folder contains the TC Toolbox for MATLAB® HTML files. Double-click `Index.html` file to open it. This help is also available via our website.

About the Examples

To learn more about how to use the software you can open and run the example projects (Graphical Mode) and macro files (Console Mode).

Graphical Mode Examples

Graphical Mode examples are available for Thermo-Calc and the Add-on Modules. There are also examples for the Property Models, including the material specific model libraries (i.e. Steel, Nickel, etc.). These are in the format of project files (*.tcu).

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Console Mode Examples

Console Mode examples are available for Thermo-Calc and the Diffusion Module (DICTRA). The *macro* files are in the format of *.TCM and *.DCM, respectively.

There are other file types when you are working in Console Mode. Search the Help for *About the File Formats* or *About the DICTRA File Formats*.

Examples by Product

Thermo-Calc Examples

A description of the Thermo-Calc examples, and how to access them, is based on whether you are using Graphical Mode or Console Mode.

- Thermo-Calc Examples Collection
- Console Mode Examples

Additive Manufacturing (AM) Module Examples

A description of examples using the AM Calculator, which is only available in Graphical Mode, is included in the Thermo-Calc documentation.

Additive Manufacturing (AM) Module Examples Collection

Diffusion Module (DICTRA) Examples

A description of Diffusion Module (DICTRA) examples, which are available for both Graphical Mode and Console Mode, is included in both the Thermo-Calc and Diffusion Module (DICTRA) documentation.

For Graphical Mode, see Diffusion Module (DICTRA) Examples Collection

For Console Mode, search the help or go to the Diffusion Module (DICTRA) documentation set.

All the macro files and the outputs are also combined into one file that you can search and read. This is included with your installation as a PDF (go to **Help → Manuals folder → Diffusion Module (DICTRA)** and open *Diffusion Module Console Mode Example Macros*.

Precipitation Module (TC-PRISMA)

A description of examples using the Precipitation Calculator, which is only available in Graphical Mode, is included in both the Thermo-Calc and Precipitation Module (TC-PRISMA) documentation.

Precipitation Module (TC-PRISMA) Examples Collection

Process Metallurgy Module Examples

A description of examples using the Process Metallurgy Calculator, which is only available in Graphical Mode, is included in the Thermo-Calc documentation.

Process Metallurgy Module Examples Collection

Property Models including Material Specific Model Library Examples

A description of examples using the Property Model Calculator, which is only available in Graphical Mode, is included in the Thermo-Calc documentation.

- Thermo-Calc General Property Models Examples Collection
- Nickel Model Library Examples Collection
- Noble Metal Alloys Model Library Examples Collection
- Steel Model Library Examples Collection
- Titanium Model Library Examples Collection

TC-Python Examples

There are examples for TC-Python available after installing the SDK. A brief description of the TC-Python SDK examples, and how to access these, is available in the Help.

TQ-Interface Examples

There are examples for the TQ-Interface available. See the *TQ-Interface Guide* for brief descriptions.

TC-Toolbox for MATLAB® Examples

There are included examples with all TC-Toolbox installations. These are generally the same as the examples included with TC-Python although with a different suffix (`matex`) and prefix (*`.m` or *`.mlx`) in the file name. Not all examples included with TC-Python are available for this SDK. You can read summaries about the examples as described in the online help.

See Installation Default Directory: TC-Toolbox and the Examples to learn where these are located.

Database Examples

Most of the databases have a *Validation and Calculation Examples Collection* available as a PDF you can download from the website. The information there is included in the help content.

Help Resources: Installed and Web Versions

The technical content is available in HTML format as an Online Help system that you can access from two locations. Both versions are viewed in your browser.

- A local version that is available with each Thermo-Calc installation and does not require an Internet connection.
- A web version available online. The web help also matches the most recently released version of Thermo-Calc.

> Between releases there may be minor updates to the web version compared to the installed version. All updates made to the web version are included in the next installed release version.

> There are several resources available on our website to help you learn how to use Thermo-Calc and other Add-on Modules. Go to the Getting Started Guides page and choose one of the guides that provides new users an introduction to setting up simple calculations in Graphical Mode. The information there is also in this help documentation.

Opening the Web Version of the Help

- A web version **specific to each release version** is available at https://help.thermocalc.com/2025b/content/intro/help-home.htm
- The help at the link also matches the most recently released version of Thermo-Calc.

Opening the Installed Help: No Internet Required

There are several ways to access online help in a browser. The content opens in a browser but uses local content so you do not need an Internet connection except for links to external websites.

First open Thermo-Calc, then choose one of these options to go to the local browser version of the help:

- Press <F1> on the keyboard.
- Select **Help** → **Online Help**.
- On the **My Project Configuration** window, click **Online Help**.
- At the bottom of any **Configuration** window, click **Help**.

Opening the Console Mode Help

Console Mode is for Thermo-Calc and the Diffusion Module (DICTRA).

In Console Mode at the command line prompt, you can access help in these ways:

- For a list of all the available commands in the current module, at the prompt type a question mark (`?`) and press <Enter>.
- For a description of a specific command, type `Help` followed by the name of the command. You can only get online help about a command related to the current module you are in.
- For general system information type `Information`. Specify the subject or type `?` and the available subjects are listed. This subject list is specific to the current module.

Typographical Conventions

The following typographical conventions are used throughout the documentation, both online and in the PDF documents.

Text

Convention	***Definition***
Forward arrow symbol →	The forward arrow symbol → instructs you to select a series of menu items in a specific order. For example, **Tools → Options** is equivalent to: From the **Tools** menu, select **Options**.
Boldface font	A **boldface** font indicates that the given word(s) are shown that way on a toolbar button or as a menu selection. For example, if you are told to select a menu item in a particular order, such as **File → Save Project**, or to click **Save**.
Italic font	An *italic* font in the body of the text indicates the introduction of important terminology. Expect to find an explanation in the same paragraph or elsewhere in the guide.
COMMAND	For features in Thermo-Calc that use Console Mode (i.e. the command line), this font and all capital letters indicates that this is a Console Mode COMMAND. Examples of how you can use a command are written with code font. For example: Use DEFINE_ELEMENTS followed by a list of the elements that you want in your system. (To list the elements that are available in your current database, use LIST_DATABASE and choose `Elements`).
HELP	Text in blue and underline and a page number is a link to another topic in the current or referenced guide. Command names are often also topics. Clicking the link takes you to more detail about a particular command or subject in the PDF or documentation set.
<Enter>	Text with <angle brackets> indicates a keyboard entry. Usually to press <Enter> (or Return) or to use a series of keys such as <Ctrl + S>.
`code` and **`code bold`**	A `code` font shows a programming code or code example. The **`code bold`** font highlights the entry. It is also used for file names or paths to help distinguish it from other text. e.g. • For Windows users, the documents, materials, examples and other folders that sometimes require additional licenses are installed in C:\Users\Public\Public Documents\Thermo-Calc\<*version*>."
click vs press	In general, you *click* with the mouse to perform an action on the screen (e.g. click **Save**) and you *press* keys on a keyboard to enter a set of commands (e.g. press Ctrl+S).

Convention	*Definition*
	>_ When working in Console Mode, you can use keyboard shortcuts. Sometimes a window opens where you have the option to **Save**, **Cancel** or **Open** a file, for example. In these cases the instructions might say *click* Save, whereas you would need to *press* the applicable keys to perform the action.

Icons

Convention	*Definition*
Important	❗ Provides important information. It is recommended that you read the text or follow the link.
License Required	🔑 This indicates that additional licenses are required for the feature, database, or example.
Note	📄 The information can be of use to you. It is recommended that you read the text or follow the link to more information.
Time	⏳ Indicates that something you are going to do will take some time, usually related to running an example.
Tip	💡 This is general information that can be of use but is not required knowledge.
Read More	📖 Read more at the link, which may be to our website or another source of general information.

Convention	***Definition***
See More	Go to the link or guide to see more general information about the topic being discussed.
Training	Indicates there may be training opportunities available, usually related to a specific feature.
Link to more information	Click the link to more information in the content.
Examples	Go to the example collection to learn more.
Console Mode	This note relates specifically to something in Console Mode.
Video	Indicates there is a video tutorial on our website, usually in relation to an example.
Graphical Mode	This note relates specifically to something in Graphical Mode.
Diffusion Module (DICTRA)	This indicates that the information relates to the Add-on Diffusion Module (DICTRA).
Precipitation Module (TC-PRISMA)	This indicates that the information relates to the Add-on Precipitation Module (TC-PRISMA).
Process Metallurgy Module	This indicates that the information relates to the Add-on Process Metallurgy Module.
Property Models	This indicates that the information relates to the Property Models. This includes all material specific libraries, i.e. Steel Model Library, Nickel Model Library, etc. as well as the general Models included with all installations.

Convention	Definition
Additive Manufacturing (AM) Module	This indicates that the information relates to the Add-on Additive Manufacturing (AM) Module.

Installation Guide

Windows®, macOS®, and Linux Operating Systems

Thermo-Calc Version 2025b

Including the TC-Python and TC-Toolbox for
MATLAB® Installation Guides

Thermo-Calc
Software

Introduction to Installing Thermo-Calc

This guide is NOT applicable to installations of the Free Educational Package, which does not require a license file and is not currently available with the new license system. Installation instructions are available separately after you request the free version from this page on our website.

In this section:

Key to Using this Guide

Starting with the 2025a release, Thermo-Calc Software began to migrate to a new License Entitlement System. The new license system greatly simplifies the licensing process and has many advantages. Licenses are now handled through a login (where *user credentials* are entered), rather than downloading and storing license files on a computer. The majority of users are already migrated to this new system. However, for the short term, a few users continue to use the old license file system. For more information about the changes and migration plan, contact us by email at info@thermocalc.com.

In this guide learn how to:

- Download and install the software on Windows, macOS, and Linux operating systems. This is applicable to new users and existing users who are installing a new or updated version of Thermo-Calc, where the new version is installed next to the old version.
- Activate your license using user credentials or a license file/license server.
- Locate various items in the default installation directories (i.e. databases, Database Checker, TDB Editor, materials, custom Property Models).
- Install selected components using the custom installation option.
- Install the *TC-Python* and *TC-Toolbox for MATLAB®* SDKs.
- Work with existing installations, i.e. add new components, update or uninstall the software.
- Deactivate online or offline user credentials licenses.
- Install silently over a network (unattended installations)
- Troubleshoot to solve common installation problems related to the license file/license server activation type.

This guide is NOT applicable to installations of the Free Educational Package, which does not require a license file and is not currently available with the new license system. Installation instructions are available separately after you request the free version from this page on our website.

Installation instructions are generally organized based on the *license activation type*:

- **User credentials**: The new License Entitlement System, where a user name and password are entered after the installation is complete. This new system is available for standalone (SUNLL) and floating network licenses (NWL) (i.e. on a Cloud Hosted License Server), but not currently for On Premise License Servers.
- **License file**: The soon-to-be phased out license system where the license file is installed on either a standalone computer or a network server. This includes On Premise License Server installations involving the Sentinel license management software.

Visit our website to watch the installation video showing how to install with user credentials (in both online and offline mode), which will replace the license files. The video library also includes the installation videos using the old method (license files) and other installations such as for TC-Python.

This guide is available in PDF format: (1) On the website or (2) when in Thermo-Calc go to **Help → Manuals Folder → Installation**.

Typographical Conventions and Terminology

Typographical Conventions

Convention/Name	*Definition*
User credentials	This indicates that the information is applicable to the new license entitlement system. **User credentials** are a type of *license activation type* where a user name and password are entered after installation and when Thermo-Calc is first launched. The information is managed via an online portal system as well as from within Thermo-Calc.
License file	This indicates details related to the Thermo-Calc **license file**, which contains the license keys and is installed on either a standalone computer or a network server. This is a *license activation type* that is being replaced by *user credentials*.
Important	Provides important information and indicates that more detail is located in the linked or named topic.
Note	The information can be of use to you. It is recommended that you read the text or follow the link.
Forward arrow →	The forward arrow symbol → instructs you to select a series of menu items in a specific order. For example, **File → Save Project** is equivalent to: From the **File** menu, select **Save Project**.
Boldface font	A **boldface** font indicates that the given word(s) are shown that way in on a toolbar button or as a menu selection. For example, if you are told to select a menu item in a particular order, such as **File → Save Project**, or to click **Save**.
Italic font	An *italic* font indicates the introduction of important terminology. Expect to find an explanation in the same paragraph or elsewhere in the guide.
`code` and **`code bold`**	A `code` font indicates you are to make a keyboard entry. It also shows a programming code or code examples. The **`code bold`** font highlights the entry.

Installation Terminology

Term	*Definition*
client*	A computer without a license file of its own but connected through the network to a computer with the license information. The client receives a license token from the computer where the license management software is installed.
consolidated network*	A type of network installation where the Thermo-Calc software and a Thermo-Calc licensing software are installed on a single server computer. This allows all computers in the network to access both the software and a license on the server via a client installation.
distributed network*	A type of network installation where the Thermo-Calc software is installed on one server computer in a network and the Thermo-Calc licensing software is installed on a different computer. After a thin client installation, all computers in the network can access both the software and the network license key via the server.
host ID*	The MAC address on the computer that a license is locked to.
license file*	The file (called *lservrc*) that contains all the purchased license keys. It is issued by Thermo-Calc Software, usually by email. This is a *license activation type* that is being replaced by user credentials.
license key*	The information contained in the license file that represents the products purchased and which is then authorized for installation.
license management software (see Sentinel RMS License Software)*	The Thermo-Calc license management software. When working in Windows it is called *License Manager* (full name is Sentinel RMS License Manager by SafeNet) and on Linux it is called *License Server* (full name is Sentinel License Sever by Safenet).
license server*	The use of the term *license server* (lower case letters) is reserved for use for scripts and option files (for example, in an Unattended or Silent Network Client Installations (License File)). For the purposes of the step-by-step instructions it is not used to refer to the type of network installation that runs the license management program. See *Sentinel RMS Software* below.
Network Floating License (NWL)	A license type available and activated using user credentials. A NWL can only be used on one specific computer that hosts the licensing software. It is still referred to as an NWL license but is different than the one used with license file activations. The software may be used on the number of sites you have paid for and by the number of persons you have paid for on any number of network connected computers.
Network License (NWL)*	The license type used with the Sentinel RMS licensing software. The NWL can only be used on one specific computer that hosts the licensing software. This restricts license usage to a certain subnet or subnets. The software may be used on the number of sites you have paid for and by the number of persons you have paid for on any number of network connected computers.

Term	***Definition***
Operating system	The operating system is named when the information is specific to a *Windows*, *macOS*, or *Linux* machine.
Sentinel RMS License Software*	The Thermo-Calc license management software that supplies the client computers in your network with license tokens when it runs the Thermo-Calc software. This is available for both Windows (called the License Manager) and Linux (called the License Server, but not to be confused with *license server* in lower case letters reserved for scripts).
Single User Node Locked License (SUNLL)	A unique license that can be used for one designated computer at one designated site. It cannot be copied or moved outside the site. If the software is installed on a portable computer, it can be temporarily used off-site. For *license file* activation types, a file is automatically installed on the computer, upon activation, and the license can be used without network access (to the License Server).
standalone computer	A computer which uses a SUNLL license type.
TC-Toolbox	The short name for the TC-Toolbox for MATLAB® SDK.
thin client*	An installation where the software is installed on a file server but is run from a client computer. The licensing software may be installed on the file server (consolidated network installation) or on a different computer (distributed network installation).
user credentials	A type of *license activation type* where user credentials (a user name and password) are entered after installation and when Thermo-Calc is first launched. The information is managed via an online portal system as well as from within Thermo-Calc.
XQuartz	An open-source X Windows System, which is required to run Thermo-Calc on a Mac.

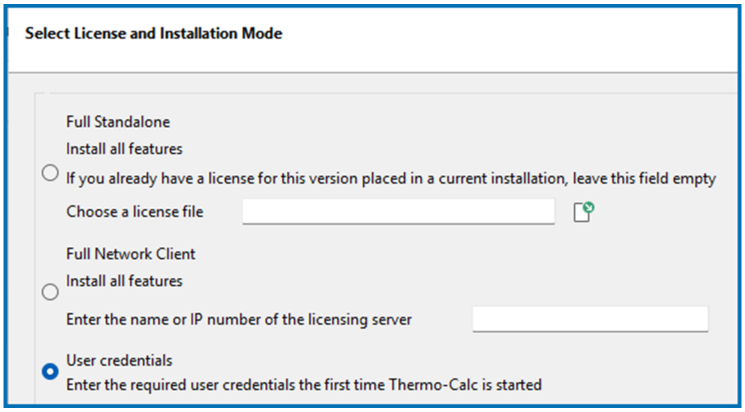
* A term only applicable to license files or license server systems, which are being replaced by the user credentials licensing.

About the Thermo-Calc Installed Components

What is Installed?

At the start of the installation process, you choose the *license activation type* (license file, licensing server, or user credentials) and whether to install all features.

The following components are installed when you choose any of the options, **Full Standalone**, **Full Network Client**, or **User credentials**. If you want to exclude a component (perhaps one of the SDKs), then click the **Custom** button instead (see below).



Select License and Installation Mode

○ Full Standalone
Install all features
If you already have a license for this version placed in a current installation, leave this field empty
Choose a license file

○ Full Network Client
Install all features
Enter the name or IP number of the licensing server

● User credentials
Enter the required user credentials the first time Thermo-Calc is started

A full installation (*Install all features*) means that all listed feature components are installed but the availability of the individual components is based on the license you have. This is also applicable to the user credentials option, as well as databases and software development kits (SDKs).

Thermo-Calc

The Thermo-Calc software "component" includes several add-on features and capabilities that are packaged with the software and included with a full standalone, network client, or user credentials type installation. For example, there are the specialized add-on products, such as the Diffusion Module (DICTRA), Precipitation Module (TC-PRISMA), Process Metallurgy Module, and Additive Manufacturing (AM) Module. There are also material specific Property Model libraries included such as the Steel Model Library, Nickel Model Library, etc. For some of these specialized features, demonstration (*demo*) versions and examples are available for all users but advanced features are only available with a license.

Databases

All the latest databases are installed. As with the software features, availability of a specific database in the software itself is based on license. However, several demonstration (*demo*) databases are included and available to all users.

Software Development Kits (SDKs)

When the **Full Standalone**, **Full Network Client**, or **User credentials** option is chosen, it also installs the software development kits (SDKs).

- **TC-Python**: The TC-Python program is installed when the **Full Standalone**, **Full Network Client**, or **User credentials** option is chosen, but there are additional steps required to complete the installation as described in the *TC-Python Installation Guide*, which is available in this guide or as a standalone guide.
- **TC-Toolbox for MATLAB®**: If a MATLAB® installation on your computer is found during this installation process, the TC-Toolbox for MATLAB® (available only for Windows) is automatically installed, otherwise you may need to do a manual installation. For details, see the section related to *TC-Toolbox for MATLAB Installation Guide®*.
- **TQ-Interface**: The TQ-Interface program is installed when the **Full Standalone**, **Full Network Client**, or **User credentials** option is chosen. However, it is currently only available with the license file activation type. For more information about the changes and migration plan, read the latest Release News on our website.

What is the Custom Option?

During the installation process, there is some flexibility to choose what to include or exclude with the installation by choosing the **Custom** option. This is primarily to the level of being able to choose the SDKs or to exclude all databases or Thermo-Calc itself. That is, you cannot choose specific Thermo-Calc features or databases as these are controlled by the license and not the installation procedure.

System Requirements

General

About the Thermo-Calc Installed Components

A full list of system requirements and program availability is found on the Thermo-Calc website. You can also see the roadmap for platform support to use for planning purposes.

Network Client Installations: Sentinel RMS License Software

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

Network client installations using the Sentinel RMS license management software require the use of the most recent version, 9.7.

For details of the system requirements to install Sentinel RMS, see Windows: About Installing the License Manager and Linux: About Installing the License Server.

For macOS, the Sentinel RMS License software is installed on a Windows or Linux computer server where the Thermo-Calc license file must also be located.

Platforms Tested and SDK Availability

A full list of system requirements and program availability is found on the Thermo-Calc website. You can also see the roadmap for platform support to use for planning purposes.

Platforms Tested

Thermo-Calc and its components are tested on these platforms for Thermo-Calc 2025b:

Windows	***macOS[1]***	***Linux[2]***
• Windows 10 • Windows 11	• Sequoia (15.1) • Sonoma 14.x	• Red Hat RHEL 9 • OpenSUSE 15.6 (Leap) • Ubuntu 24.04 (Noble Numbat) • Ubuntu 22.04 (Jammy Jellyfish)

[1] Works with Rosetta 2 emulation on all M1, M2 and M3 Macs (2020, 2022, 2023).

[2] Thermo-Calc Software cannot guarantee full functionality if the software is installed on other Linux distributions.

SDK Availability by Platform

The software development kits (SDKs) are available as follows for the indicated platforms:

SDK	***Windows***	***macOS***	***Linux***
TC-Python	x	x	x
TQ-Interface	x	not available	x
TC-Toolbox for MATLAB®	x	not available	not available

License Activation and Installation Types

There are two **license activation types** available with Thermo-Calc 2025b: One using a *license file* that is installed on your computer (this also includes the different network installation types using Sentinel License Management Software), and the new type where *user credentials* (user name and password) are entered after installation and when you first open (launch) Thermo-Calc.

This guide is NOT applicable to installations of the Free Educational Package, which does not require a license file and is not currently available with the new license system. Installation instructions are available separately after you request the free version from this page on our website.

Installation procedures are based on the license types, license activation types, installation type, and the operating system.

User Credentials Activations

About User Credentials License Activations

Troubleshoot User Credential License Activations

License type	*Installation Type*	*Windows*	*macOS*	*Linux*
Single User Node Locked License (SUNLL)	Standalone (aka Single User)	Yes	Yes	Yes
Floating Network License (NWL)	Cloud Hosted License Server	Yes	Yes	Yes
	On Premise License Server*	No	No	No

* A few users will continue to use the License Management Software system for the short term until the change over is complete and implemented in a future release. Until then, users who require an On Premise License Server need to use License File and License Server Activations, see the next section. For more information about the changes and migration plan, contact us at info@thermocalc.com.

License File and License Server Activations

For macOS, the Sentinel RMS License software is installed on a Windows or Linux computer server where the Thermo-Calc license file must also be located.

License type	*Installation Type*	*Windows*	*macOS*	*Linux*
Single User Node Locked License (SUNLL)	Standalone	Yes	Yes	Yes
Network License (NWL)	Consolidated network	Yes	No	Yes
	Distributed network	Yes	No	Yes
	License installations on a server network	Yes	Yes	Yes

Sentinel RMS License Management Software: Use Current Version

The most recent version (9.7) of the Sentinel RMS License Manager (Windows) and License Server (Linux) is included with the network license Thermo-Calc software download.

However, due to security issues reported by the vendor, it is important that previous network license installations of the Sentinel RMS are upgraded to this version number.

For more information for your operating system, see Windows: About Installing the License Manager and Linux: About Installing the License Server

User Credential License Activation Installations

Starting with the 2025a release, Thermo-Calc Software began to migrate to a new License Entitlement System. The new license system greatly simplifies the licensing process and has many advantages. Licenses are now handled through a login (where *user credentials* are entered), rather than downloading and storing license files on a computer. The majority of users are already migrated to this new system. However, for the short term, a few users continue to use the old license file system. For more information about the changes and migration plan, contact us by email at info@thermocalc.com.

In this section:

About User Credentials License Activations

All users are being migrated to this new *user credentials* license activation type. For this type of activation, the information is managed via an online portal system as well as accessible from within Thermo-Calc. Customers are being contacted directly by email to provide the necessary information to install and use your purchased products. During the transition from using the old license file activations, some users may need to contact support for assistance.

Visit our website to watch the installation video showing how to install with user credentials (in both online and offline mode), which will replace the license files. The video library also includes the installation videos using the old method (license files) and other installations such as for TC-Python.

What is Not Available in the New License System as of Thermo-Calc 2025b

- TQ-Interface
- Floating licenses for TC-Python and TC-Toolbox for MATLAB®
- Free Educational Package installations
- On Premise License Server installations

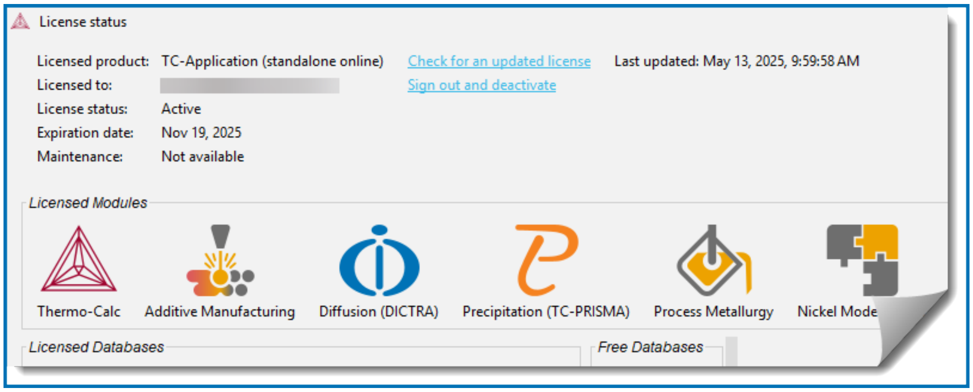
With respect to downloading and installing the software, there are subtle differences based on operating system (Windows, macOS, or Linux). One benefit of the new user credentials license activation type is that its use is independent of OS and the activation steps are the same across platforms.

Although many steps are the same, separate instructions are available for all the OS and for custom single user installations: Windows® User Credentials Installations, macOS® User Credentials Installations, or Linux User Credentials Installations. There are also instructions for Custom User Credentials Installations.

Viewing Product License Information

After you have installed Thermo-Calc and activated your license by entering your user credentials, you can view the license information by selecting **Help** → **Show License Info**.

In the **License status** window, it is an overview of your license as well as where you can check for updates, sign out or deactivate the license, and review its status and when it expires. If you have a Maintenance & Support Subscription (M&SS) the date of expiration is also displayed.



License status

Licensed product: TC-Application (standalone online)
Licensed to: [redacted]
License status: Active
Expiration date: Nov 19, 2025
Maintenance: Not available

Last updated: May 13, 2025, 9:59:58 AM

Checking for License Updates

After you have installed Thermo-Calc and activated your license by entering your user credentials, you can remotely check to see if your product license is up-to-date.

> Internet access is required. If you have chosen to use an offline license activation, this option is not available. Access to this update service is one reason the online activation type is recommended.

1. Open Thermo-Calc.
2. Select **Help** → **Show License Info**.
3. In the **License status** window, click **Check for an updated license**.
4. The program synchronizes with the license software management database and updates the licenses accordingly.

When you update to a new version of Thermo-Calc, you may also need to update your license if you have added additional modules or databases.

TC-Python Additional License Activation Steps

When you also have a license for TC-Python, there are additional steps required to complete the activation. This is covered in the sections:

- TC-Python: Configuring a License
- TC-Python: Setting Environment Variables

TC-Toolbox Additional License Activation Steps

When you also have a license for TC-Toolbox for MATLAB®, there are additional steps required to complete the activation. This is covered in the section:

- TC-Toolbox: Configuring a License

Reminder that TC-Toolbox is not available with macOS or Linux installations.

Windows® User Credentials Installations

There are two *license activation types* available as of 2025b: (1) **User credentials**, which are entered after installation and managed via an online portal or (2) where a **license file** is installed directly on the computer or a licensing server. Many users have already started using the *user credentials* activation type and all users will eventually be migrated to the new system.

Visit our website to watch the installation video showing how to install with user credentials (in both online and offline mode), which will replace the license files. The video library also includes the installation videos using the old method (license files) and other installations such as for TC-Python.

This section is applicable to:

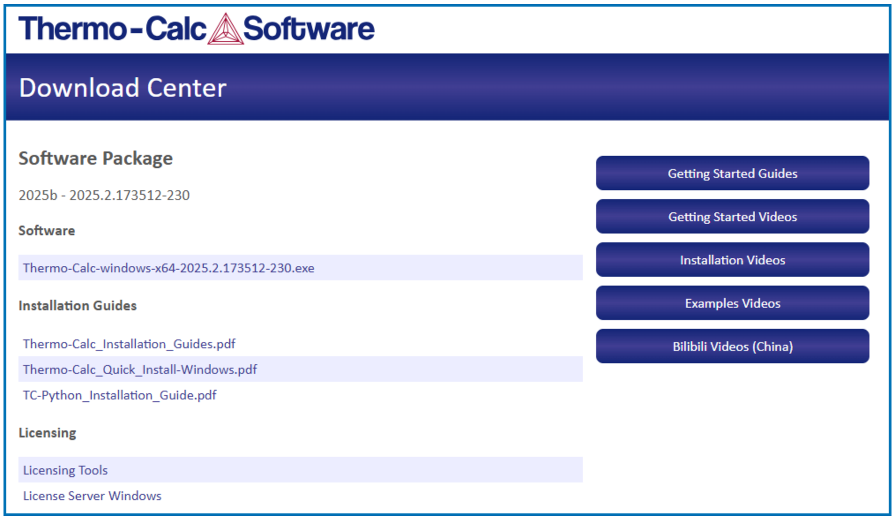
- Operating system: Windows
- Installation type: Single User (SUNLL) or Floating Network Licenses (NWL)
- License activation type: User credentials (online and offline)
- Upgrading to a new version of Thermo-Calc (M&SS maintenance plan only)

For instructions about other operating systems, network installations, or installing an SDK (e.g. TC-Python or TC-Toolbox for MATLAB®) search the *Thermo-Calc Installation Guide*, which is also available on our website. You can also review the Licensing Options included on our website.

Step 1: Download Thermo-Calc Software

Administrative rights are required to complete this installation. An email from Thermo-Calc Software (or from someone in your organization) includes the links and information you need to access and activate the current version of the software you want to download.

1. Click the link from the email and the first page of the **Download Center** opens. Under the **Windows** section, select the OS version. Click **Go to download page**.
2. In the **Sign in to access this site** window, enter the **Username** and **Password** (found in the email) and click **Sign in**.
3. On the **Download Center** page under **Software**, click the **.exe** link to download the file for the current software version for your operating system (2025b).



Thermo-Calc Software

Download Center

Software Package

2025b - 2025.2.173512-230

Software

Thermo-Calc-windows-x64-2025.2.173512-230.exe

Installation Guides

Thermo-Calc_Installation_Guides.pdf

Thermo-Calc_Quick_Install-Windows.pdf

TC-Python_Installation_Guide.pdf

Licensing

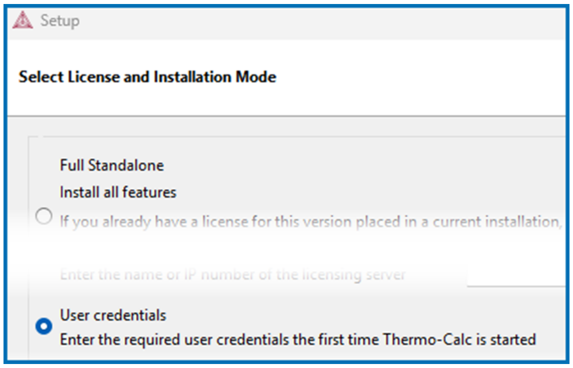
Licensing Tools

License Server Windows

Step 2: Install Thermo-Calc Software

1. Once the download is complete, navigate to the folder where you downloaded the software. Double-click the downloaded program file (the suffix is based on the operating system). Remember that administrative rights are needed, so when you are prompted for that user name and password, enter those credentials here, not the ones sent to you from Thermo-Calc.
2. Click **Yes** to continue.
3. On the **Setup - Thermo-Calc 2025b** window click **Next**.
4. On the **License Agreement** window click to accept the license agreement. Click **Next**.

5. In the **Select License and Installation Mode** window click **User credentials** and then click **Next**.



Select License and Installation Mode

○ Full Standalone
Install all features
If you already have a license for this version placed in a current installation,

Enter the name or IP number of the licensing server

● User credentials
Enter the required user credentials the first time Thermo-Calc is started

6. TC-Python is automatically installed when the **User credentials** option is chosen. The **Install TC-Python** page is a reminder for users of TC-Python that additional installation and license credential procedures are needed after Thermo-Calc is installed. Read the separate installation instructions (also included in the full installation guide) for more information if applicable. Click **Next**.
7. In the **Ready to Install** window click **Next**. The software continues installing.
8. At the end of installation, click **Finish**. Once this is done, open Thermo-Calc either from the shortcut on your desktop or from the menu.

Step 3: Activate the License

If your work environment does not allow an Internet connection to activate the license, as a last resort you can use the option **Create offline activation file**. Overall it is best to use the **Activate online** option as this provides more flexibility and future benefits including being able to easily update your license. See the last section for details.

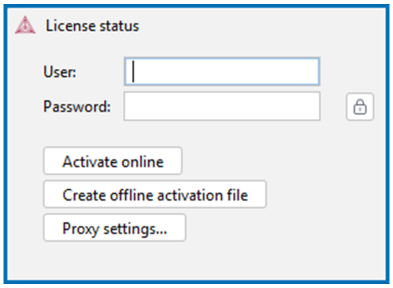
1. Open Thermo-Calc. The first window includes highlights from the current release. Click **Close**.
2. In the **License status** window, enter the **User** and **Password** provided to you.

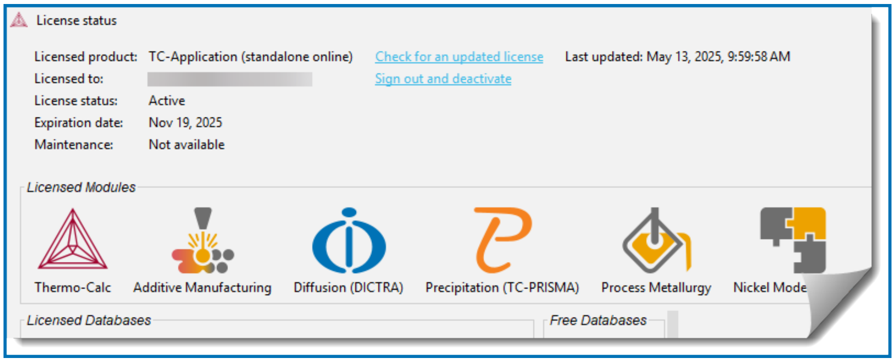
> Your license user credentials are sent to you in an email from Thermo-Calc or a representative. This is different from the Download Center login details. If you have not received the information, first ask the main Thermo-Calc contact in your organization. Otherwise, contact Support for clarification.

3. If you use a proxy server, click **Proxy settings**. Click **Use proxy** and enter your information. Click **OK**.
4. Click **Activate online**.

> If the fields become empty when you click **Activate online**, this means the activation did NOT work. See the troubleshooting section for details about next steps When Activate Online Does Not Work.

5. Once it is activated you will see the **License status** window with a list of the products you have access to. Click **Close** and start using Thermo-Calc.





License status

Licensed product: TC-Application (standalone online)
Licensed to: [redacted]
License status: Active
Expiration date: Nov 19, 2025
Maintenance: Not available

Last updated: May 13, 2025, 9:59:58 AM

At any time you can view the product license information by selecting **Help → Show License Info** from the menu in Thermo-Calc.

Step 4: Optional Offline License Activations

Offline activations are only available for single user (SUNLL) licenses and should only be used as a last resort, i.e. if there is no option provided by your organization to achieve online activation. The computer only needs to be connected to a network during the license activation, not when working with the software.

Offline activations can be an alternative for users who are in a highly secure environment that does not allow Internet connections.

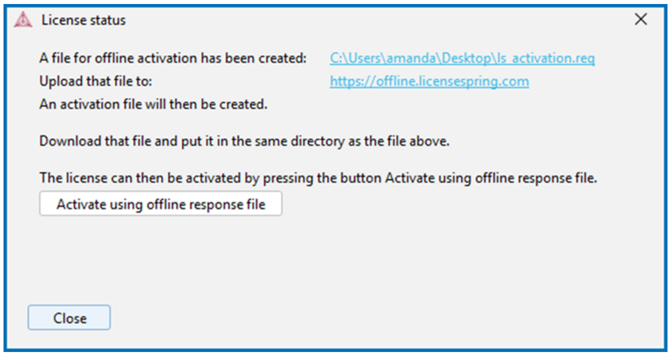
In general it is highly recommended to use the **Online activation** option as this provides more flexibility including faster and easier license updates, i.e. for offline activations license updates require repeating the full offline activation procedure.

You will need access to the Internet to complete the activation. You can do this either by:

- Accessing the Internet temporarily from the computer you will use Thermo-Calc on, or
- Activating the license on another computer then transferring the license to the computer you will use Thermo-Calc on.

These instructions are a continuation from previous steps and assume you have already installed Thermo-Calc and entered your user credentials.

1. Click **Create offline activation file**. The **License status** window opens with instructions you can refer to.



A file for offline activation has been created: C:\Users\amanda\Desktop\ls_activation.req
Upload that file to: https://offline.licensespring.com
An activation file will then be created.

Download that file and put it in the same directory as the file above.

The license can then be activated by pressing the button Activate using offline response file.

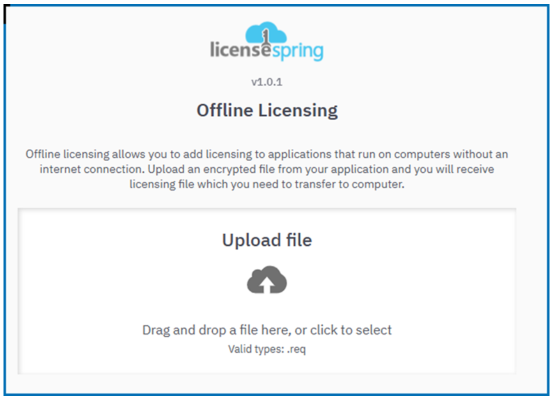
2. A local file to use for the offline activation is created and the link to where it is downloaded to your computer is provided. The file is named `ls_activation.req`. Click the link to go to this location on your computer.

If you have downloaded the file to a computer that does not have Internet access, then copy this file to one that does and continue the process. Later you will copy the generated offline license back to the computer where Thermo-Calc is installed.

3. On the computer that has Internet access, go to the URL shown on the **License status** window: https://offline.licensespring.com.

4. Navigate to the `ls_activation.req` file on your computer and drag and drop it into the center of the window. The program generates another file and downloads it to your computer. This file is named `ls_activation.lic`.

As soon as the `ls_activation.req` file is uploaded the license is considered by the software to be activated.



licensespring

v1.0.1

Offline Licensing

Offline licensing allows you to add licensing to applications that run on computers without an internet connection. Upload an encrypted file from your application and you will receive licensing file which you need to transfer to computer.

Upload file

Drag and drop a file here, or click to select

Valid types: .req

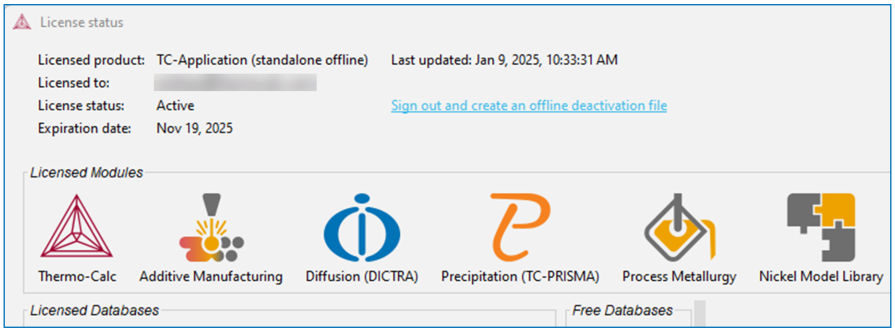
> If at this point you want to switch to an online activation instead (recommended), you can delete the `ls_activation.req` file from the computer location to end the offline activation process.

5. Navigate to the downloaded `ls_activation.lic` file. If needed, this is when you copy this file back to the computer where Thermo-Calc is installed. In both cases the new file should be copied back to the same folder where the original file `ls_activation.req` is located.

6. Once the two files are in the same folder, you are ready to generate an offline license.

7. Go to the **License status** window and click **Activate using offline response file**.

   Once activated you will see the **License status** window with a list of the products you have access to. Click **Close** and start using Thermo-Calc.



License status

Licensed product: TC-Application (standalone offline)
Last updated: Jan 9, 2025, 10:33:31 AM
Licensed to: [redacted]
License status: Active
Sign out and create an offline deactivation file
Expiration date: Nov 19, 2025

8. You do not need to keep the files you downloaded. Return to where these files are downloaded and delete them.

At any time you can view the product license information by selecting **Help → Show License Info** from the menu in Thermo-Calc.

macOS® User Credentials Installations

There are two *license activation types* available as of 2025b: (1) **User credentials**, which are entered after installation and managed via an online portal or (2) where a **license file** is installed directly on the computer or a licensing server. Many users have already started using the *user credentials* activation type and all users will eventually be migrated to the new system.

Visit our website to watch the installation video showing how to install with user credentials (in both online and offline mode), which will replace the license files. The video library also includes the installation videos using the old method (license files) and other installations such as for TC-Python.

This section is applicable to:

- Operating system: macOS
- Installation type: Single User (SUNLL) or Floating Network Licenses (NWL)
- License activation type: User credentials (online and offline)
- Upgrading to a new version of Thermo-Calc (maintenance plan only)

For instructions about other operating systems, network installations, or installing an SDK (e.g. TC-Python or TC-Toolbox for MATLAB®) search the *Thermo-Calc Installation Guide*, which is also available on our website. You can also review the Licensing Options included on our website.

Step 1: Install Required macOS Software

To install and run Thermo-Calc on a Mac computer with an ARM processor, Rosetta first needs to be installed.

The XQuartz open-source X.Org X Window system is required to run Thermo-Calc on macOS.

1. In a web browser go to https://www.macupdate.com or to download it directly from XQuartz, https://www.xquartz.org/.
2. In the **Search Mac Apps** field, enter *XQuartz*.
3. Click the **XQuartz** search result. For example, based on the recent version, the name is XQuartz-2.8.5.dmg.
4. Click **Download**.
5. Double-click the **XQuartz-***<version>***.pkg** file. Follow the instructions.
6. Click **OK** when the message about logging out displays and click **Close** when the installation is successful.

Step 2: Download Thermo-Calc Software

Administrative rights are required to complete this installation. An email from Thermo-Calc Software (or from someone in your organization) includes the links and information you need to access and activate the current version of the software you want to download.

1. Click the link from the email and the first page of the **Download Center** opens. Under the **macOS** section, select the OS version. Click **Go to download page**.
2. In the **Sign in to access this site** window, enter the **Username** and **Password** (found in the email) and click **Sign in**.
3. On the **Download Center** page under **Software**, click the **.zip** link to download the file for the current software version for your operating system (2025b).


Thermo-Calc Software

Download Center

Software Package

2025b - 2025.2.173512-230

Software

Thermo-Calc-osx-2025.2.173512-230.zip

Installation Guides

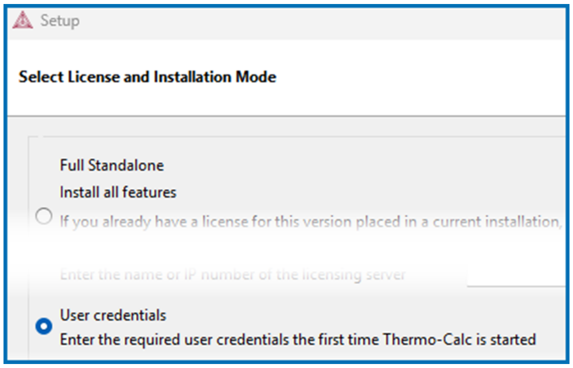
Thermo-Calc_Installation_Guides.pdf
Thermo-Calc_Quick_Install-Mac.pdf
TC-Python_Installation_Guide.pdf

Licensing

Licensing Tools

Step 3: Install Thermo-Calc Software

1. Once the download is complete, navigate to the folder where you downloaded the software. Double-click the downloaded program file (the suffix is based on the operating system). Remember that administrative rights are needed, so when you are prompted for that user name and password, enter those credentials here, not the ones sent to you from Thermo-Calc.
2. Click **Yes** to continue.
3. On the **Setup - Thermo-Calc 2025b** window click **Next**.
4. On the **License Agreement** window click to accept the license agreement. Click **Next**.
5. In the **Select License and Installation Mode** window click **User credentials** and then click **Next**.



Setup

Select License and Installation Mode

○ Full Standalone
Install all features
If you already have a license for this version placed in a current installation,

Enter the name or IP number of the licensing server

● User credentials
Enter the required user credentials the first time Thermo-Calc is started

6. TC-Python is automatically installed when the **User credentials** option is chosen. The **Install TC-Python** page is a reminder for users of TC-Python that additional installation and license credential procedures are needed after Thermo-Calc is installed. Read the separate installation instructions (also included in the full installation guide) for more information if applicable. Click **Next**.
7. In the **Ready to Install** window click **Next**. The software continues installing.
8. At the end of installation, click **Finish**. Once this is done, open Thermo-Calc either from the shortcut on your desktop or from the menu.

Step 4: Activate the License

If your work environment does not allow an Internet connection to activate the license, as a last resort you can use the option **Create offline activation file**. Overall it is best to use the **Activate online** option as this provides more flexibility and future benefits including being able to easily update your license. See the last section for details.

1. Open Thermo-Calc. The first window includes highlights from the current release. Click **Close**.
2. In the **License status** window, enter the **User** and **Password** provided to you.

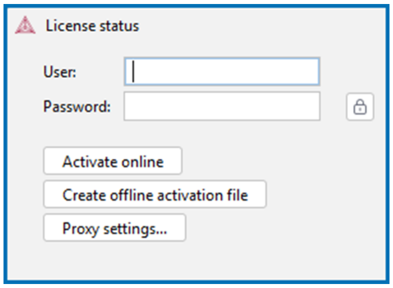
   Your license user credentials are sent to you in an email from Thermo-Calc or a representative. This is different from the Download Center login details. If you have not received the information, first ask the main Thermo-Calc contact in your organization. Otherwise, contact Support for clarification.

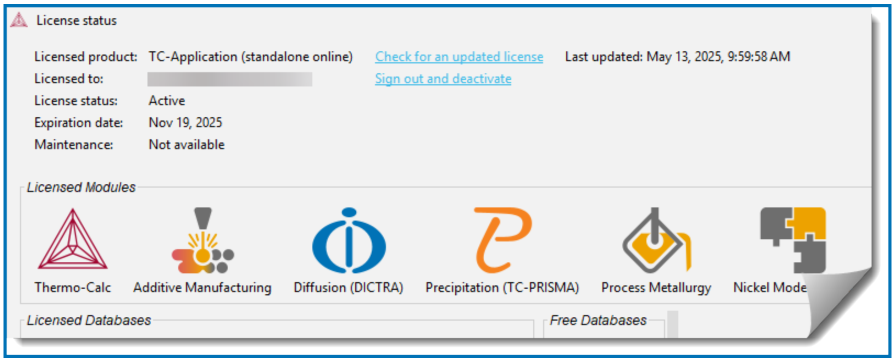
3. If you use a proxy server, click **Proxy settings**. Click **Use proxy** and enter your information. Click **OK**.
4. Click **Activate online**.

   If the fields become empty when you click **Activate online**, this means the activation did NOT work. See the troubleshooting section for details about next steps When Activate Online Does Not Work.

5. Once it is activated you will see the **License status** window with a list of the products

you have access to. Click **Close** and start using Thermo-Calc.




License status

Licensed product: TC-Application (standalone online)

Licensed to: [redacted]

License status: Active

Expiration date: Nov 19, 2025

Maintenance: Not available

Last updated: May 13, 2025, 9:59:58 AM

At any time you can view the product license information by selecting **Help → Show License Info** from the menu in Thermo-Calc.

Step 5: Optional Offline License Activations

Offline activations are only available for single user (SUNLL) licenses and should only be used as a last resort, i.e. if there is no option provided by your organization to achieve online activation. The computer only needs to be connected to a network during the license activation, not when working with the software.

Offline activations can be an alternative for users who are in a highly secure environment that does not allow Internet connections.

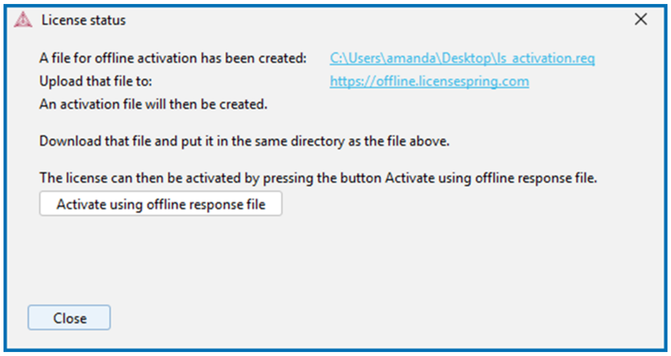
In general it is highly recommended to use the **Online activation** option as this provides more flexibility including faster and easier license updates, i.e. for offline activations license updates require repeating the full offline activation procedure.

You will need access to the Internet to complete the activation. You can do this either by:

- Accessing the Internet temporarily from the computer you will use Thermo-Calc on, or
- Activating the license on another computer then transferring the license to the computer you will use Thermo-Calc on.

These instructions are a continuation from previous steps and assume you have already installed Thermo-Calc and entered your user credentials.

1. Click **Create offline activation file**. The **License status** window opens with instructions you can refer to.



A file for offline activation has been created: C:\Users\amanda\Desktop\ls_activation.req

Upload that file to: https://offline.licensespring.com

An activation file will then be created.

Download that file and put it in the same directory as the file above.

The license can then be activated by pressing the button Activate using offline response file.

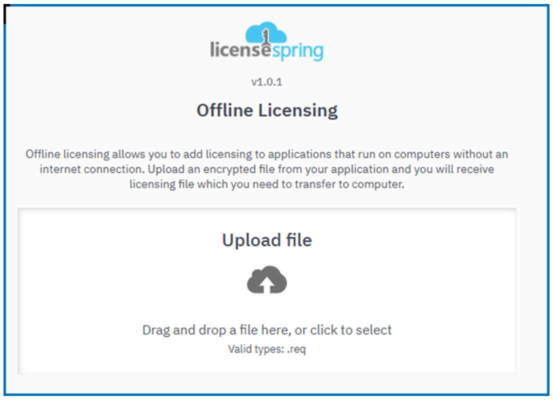
2. A local file to use for the offline activation is created and the link to where it is downloaded to your computer is provided. The file is named `ls_activation.req`. Click the link to go to this location on your computer.

If you have downloaded the file to a computer that does not have Internet access, then copy this file to one that does and continue the process. Later you will copy the generated offline license back to the computer where Thermo-Calc is installed.

3. On the computer that has Internet access, go to the URL shown on the **License status** window: https://offline.licensespring.com.

4. Navigate to the `ls_activation.req` file on your computer and drag and drop it into the center of the window. The program generates another file and downloads it to your computer. This file is named `ls_activation.lic`.

As soon as the `ls_activation.req` file is uploaded the license is considered by the software to be activated.



Offline Licensing

Offline licensing allows you to add licensing to applications that run on computers without an internet connection. Upload an encrypted file from your application and you will receive licensing file which you need to transfer to computer.

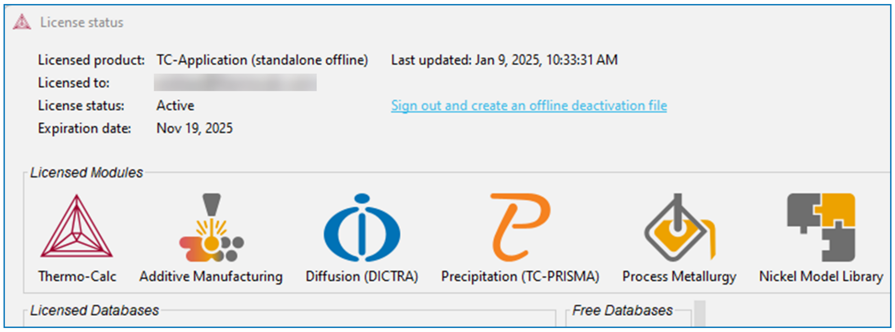
If at this point you want to switch to an online activation instead (recommended), you can delete the `ls_activation.req` file from the computer location to end the offline activation process.

5. Navigate to the downloaded `ls_activation.lic` file. If needed, this is when you copy this file back to the computer where Thermo-Calc is installed. In both cases the new file should be copied back to the same folder where the original file `ls_`

`activation.req` is located.

6. Once the two files are in the same folder, you are ready to generate an offline license.
7. Go to the **License status** window and click **Activate using offline response file**.

   Once activated you will see the **License status** window with a list of the products you have access to. Click **Close** and start using Thermo-Calc.



License status

Licensed product: TC-Application (standalone offline)

Last updated: Jan 9, 2025, 10:33:31 AM

Licensed to: [redacted]

License status: Active

Sign out and create an offline deactivation file

Expiration date: Nov 19, 2025

Licensed Modules

Thermo-Calc

Additive Manufacturing

Diffusion (DICTRA)

Precipitation (TC-PRISMA)

Process Metallurgy

Nickel Model Library

Licensed Databases

Free Databases

8. You do not need to keep the files you downloaded. Return to where these files are downloaded and delete them.

At any time you can view the product license information by selecting **Help → Show License Info** from the menu in Thermo-Calc.

Linux User Credentials Installations

There are two *license activation types* available as of 2025b: (1) **User credentials**, which are entered after installation and managed via an online portal or (2) where a **license file** is installed directly on the computer or a licensing server. Many users have already started using the *user credentials* activation type and all users will eventually be migrated to the new system.

Visit our website to watch the installation video showing how to install with user credentials (in both online and offline mode), which will replace the license files. The video library also includes the installation videos using the old method (license files) and other installations such as for TC-Python.

This section is applicable to:

- Operating system: Linux
- Installation type: Single User (SUNLL) or Floating Network Licenses (NWL)
- License activation type: User credentials (online and offline)
- Upgrading to a new version of Thermo-Calc (maintenance plan only)

For instructions about other operating systems, network installations, or installing an SDK (e.g. TC-Python or TC-Toolbox for MATLAB®) search the *Thermo-Calc Installation Guide*, which is also available on our website. You can also review the Licensing Options included on our website.

Step 1: Download Thermo-Calc Software

Administrative rights are required to complete this installation. An email from Thermo-Calc Software (or from someone in your organization) includes the links and information you need to access and activate the current version of the software you want to download.

1. Click the link from the email and the first page of the **Download Center** opens. Under the **Linux** section, select the OS version. Click **Go to download page**.
2. In the **Sign in to access this site** window, enter the **Username** and **Password** (found in the email) and click **Sign in**.
3. On the **Download Center** page under **Software**, click the **.run** link to download the file for the current software version for your operating system (2025b).


Thermo-Calc Software

Download Center

Software Package

2025b - 2025.2.173512-230

Software

Thermo-Calc-linux-2025.2.173512-230.run

Installation Guides

Thermo-Calc_Installation_Guides.pdf

TC-Python_Installation_Guide.pdf

Licensing

Licensing Tools

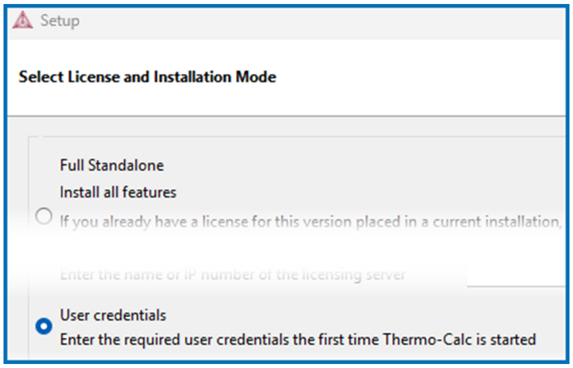
License Server Linux 32

License Server Linux 64

Step 2: Install Thermo-Calc Software

1. Once the download is complete, navigate to the folder where you downloaded the software. Double-click the downloaded program file (the suffix is based on the operating system). Remember that administrative rights are needed, so when you are prompted for that user name and password, enter those credentials here, not the ones sent to you from Thermo-Calc.
2. Click **Yes** to continue.
3. On the **Setup - Thermo-Calc 2025b** window click **Next**.
4. On the **License Agreement** window click to accept the license agreement. Click **Next**.

5. In the **Select License and Installation Mode** window click **User credentials** and then click **Next**.



Setup

Select License and Installation Mode

○ Full Standalone
Install all features
If you already have a license for this version placed in a current installation,

Enter the name or IP number of the licensing server

● User credentials
Enter the required user credentials the first time Thermo-Calc is started

6. TC-Python is automatically installed when the **User credentials** option is chosen. The **Install TC-Python** page is a reminder for users of TC-Python that additional installation and license credential procedures are needed after Thermo-Calc is installed. Read the separate installation instructions (also included in the full installation guide) for more information if applicable. Click **Next**.
7. In the **Ready to Install** window click **Next**. The software continues installing.
8. At the end of installation, click **Finish**. Once this is done, open Thermo-Calc either from the shortcut on your desktop or from the menu.

Step 3: Activate the License

If your work environment does not allow an Internet connection to activate the license, as a last resort you can use the option **Create offline activation file**. Overall it is best to use the **Activate online** option as this provides more flexibility and future benefits including being able to easily update your license. See the last section for details.

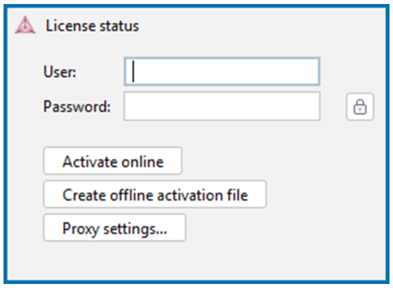
1. Open Thermo-Calc. The first window includes highlights from the current release. Click **Close**.
2. In the **License status** window, enter the **User** and **Password** provided to you.

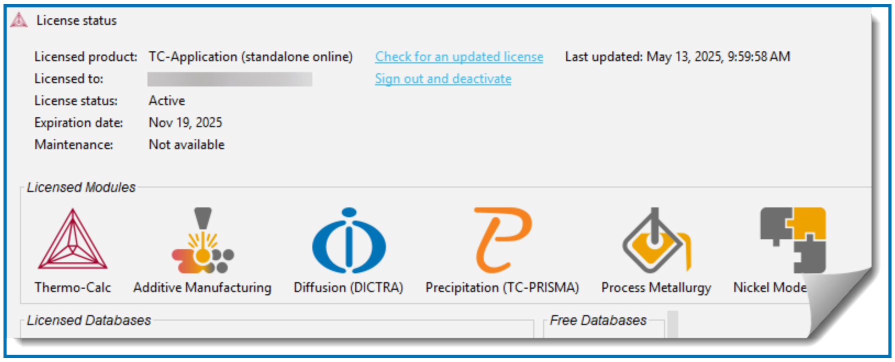
Your license user credentials are sent to you in an email from Thermo-Calc or a representative. This is different from the Download Center login details. If you have not received the information, first ask the main Thermo-Calc contact in your organization. Otherwise, contact Support for clarification.

3. If you use a proxy server, click **Proxy settings**. Click **Use proxy** and enter your information. Click **OK**.
4. Click **Activate online**.

If the fields become empty when you click **Activate online**, this means the activation did NOT work. See the troubleshooting section for details about next steps When Activate Online Does Not Work.

5. Once it is activated you will see the **License status** window with a list of the products you have access to. Click **Close** and start using Thermo-Calc.




License status

Licensed product: TC-Application (standalone online)

Licensed to: [redacted]

License status: Active

Expiration date: Nov 19, 2025

Maintenance: Not available

Last updated: May 13, 2025, 9:59:58 AM

At any time you can view the product license information by selecting **Help → Show License Info** from the menu in Thermo-Calc.

Step 4: Optional Offline License Activations

Offline activations are only available for single user (SUNLL) licenses and should only be used as a last resort, i.e. if there is no option provided by your organization to achieve online activation. The computer only needs to be connected to a network during the license activation, not when working with the software.

Offline activations can be an alternative for users who are in a highly secure environment that does not allow Internet connections.

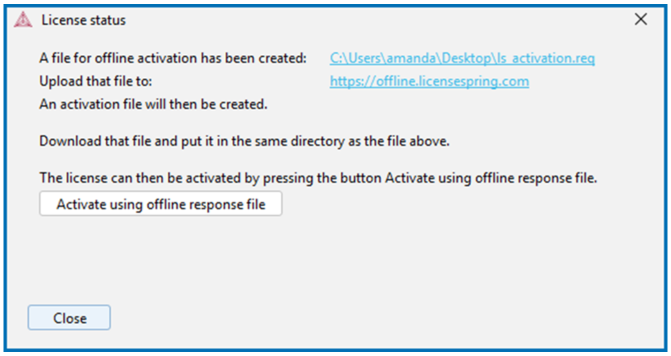
In general it is highly recommended to use the **Online activation** option as this provides more flexibility including faster and easier license updates, i.e. for offline activations license updates require repeating the full offline activation procedure.

You will need access to the Internet to complete the activation. You can do this either by:

- Accessing the Internet temporarily from the computer you will use Thermo-Calc on, or
- Activating the license on another computer then transferring the license to the computer you will use Thermo-Calc on.

These instructions are a continuation from previous steps and assume you have already installed Thermo-Calc and entered your user credentials.

1. Click **Create offline activation file**. The **License status** window opens with instructions you can refer to.



A file for offline activation has been created: C:\Users\amanda\Desktop\ls_activation.req
Upload that file to: https://offline.licensespring.com
An activation file will then be created.

Download that file and put it in the same directory as the file above.

The license can then be activated by pressing the button Activate using offline response file.

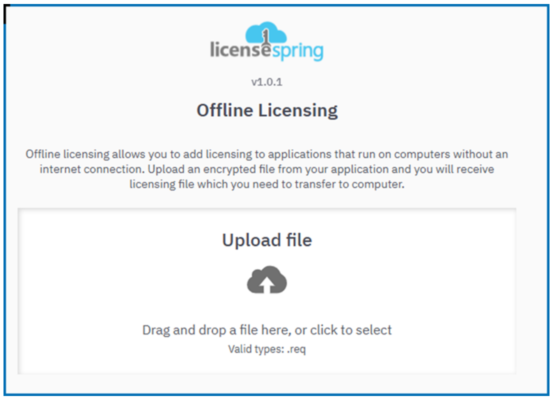
2. A local file to use for the offline activation is created and the link to where it is downloaded to your computer is provided. The file is named `ls_activation.req`. Click the link to go to this location on your computer.

If you have downloaded the file to a computer that does not have Internet access, then copy this file to one that does and continue the process. Later you will copy the generated offline license back to the computer where Thermo-Calc is installed.

3. On the computer that has Internet access, go to the URL shown on the **License status** window: https://offline.licensespring.com.

4. Navigate to the `ls_activation.req` file on your computer and drag and drop it into the center of the window. The program generates another file and downloads it to your computer. This file is named `ls_activation.lic`.

As soon as the `ls_activation.req` file is uploaded the license is considered by the software to be activated.



v1.0.1

Offline Licensing

Offline licensing allows you to add licensing to applications that run on computers without an internet connection. Upload an encrypted file from your application and you will receive licensing file which you need to transfer to computer.

Upload file

Drag and drop a file here, or click to select

Valid types: .req

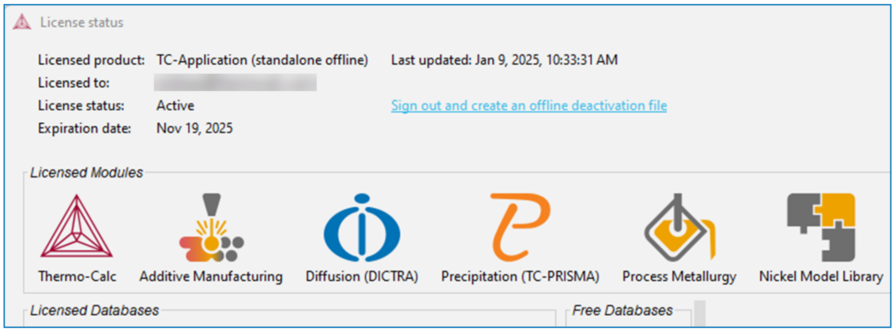
If at this point you want to switch to an online activation instead (recommended), you can delete the `ls_activation.req` file from the computer location to end the offline activation process.

5. Navigate to the downloaded `ls_activation.lic` file. If needed, this is when you copy this file back to the computer where Thermo-Calc is installed. In both cases the new file should be copied back to the same folder where the original file `ls_activation.req` is located.

6. Once the two files are in the same folder, you are ready to generate an offline license.

7. Go to the **License status** window and click **Activate using offline response file**.

   Once activated you will see the **License status** window with a list of the products you have access to. Click **Close** and start using Thermo-Calc.



License status

Licensed product: TC-Application (standalone offline)

Last updated: Jan 9, 2025, 10:33:31 AM

Licensed to: [redacted]

License status: Active

Sign out and create an offline deactivation file

Expiration date: Nov 19, 2025

8. You do not need to keep the files you downloaded. Return to where these files are downloaded and delete them.

At any time you can view the product license information by selecting **Help → Show License Info** from the menu in Thermo-Calc.

Custom User Credentials Installations

This section is applicable to:

- Operating systems: Windows, macOS, or Linux
- Installation type: Single User (SUNLL) or Floating Network Licenses (NWL)
- License activation type: User credentials (online and offline)
- Upgrading to a new version of Thermo-Calc (maintenance plan only)

Use the **Custom** option to have more control over what component features to include or exclude, for example, to exclude an SDK.

? About the Thermo-Calc Installed Components

? Add New Components to an Existing Installation

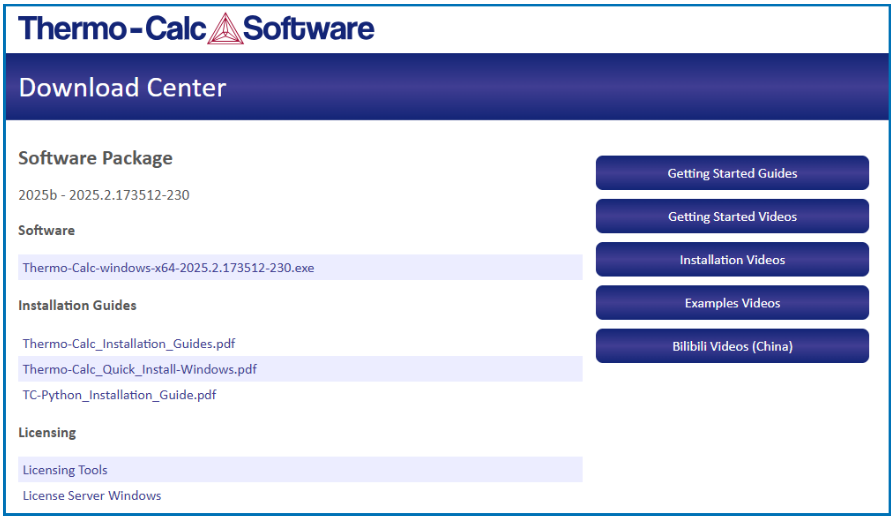
Step 1: Download Thermo-Calc Software

This section uses Windows as an example, but download the applicable OS for use.

> Administrative rights are required to complete this installation. An email from Thermo-Calc Software (or from someone in your organization) includes the links and information you need to access and activate the current version of the software you want to download.

1. Click the link from the email and the first page of the **Download Center** opens. Under the **Windows** section, select the OS version. Click **Go to download page**.
2. In the **Sign in to access this site** window, enter the **Username** and **Password** (found in the email) and click **Sign in**.

3. On the **Download Center** page under **Software**, click the **.exe** link to download the file for the current software version for your operating system (2025b).



Download Center

Software Package

2025b - 2025.2.173512-230

Software

Thermo-Calc-windows-x64-2025.2.173512-230.exe

Installation Guides

Thermo-Calc_Installation_Guides.pdf

Thermo-Calc_Quick_Install-Windows.pdf

TC-Python_Installation_Guide.pdf

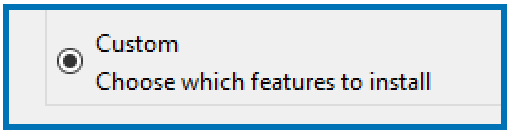
Licensing

Licensing Tools

License Server Windows

Step 2: Select the Components to Install

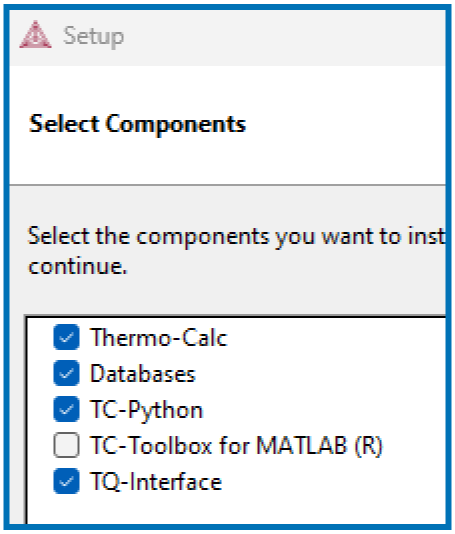
1. Once the download is complete, navigate to the folder where you downloaded the software. Double-click the downloaded program file (the suffix is based on the operating system). Remember that administrative rights are needed for Windows and macOS, so when you are prompted for that user name and password, enter those credentials here, not the ones sent to you from Thermo-Calc.
2. Click **Yes** to continue.
3. On the **Setup - Thermo-Calc 2025b** window click **Next**.
4. On the **License Agreement** window click to accept the license agreement. Click **Next**.
5. In the **Select License and Installation Mode** window click **Custom**. Click **Next**.



● Custom
Choose which features to install

6. On the **Specify Configuration** window the **Create Shortcut on Desktop** checkbox is selected by default. Click **Next**.

7. In the **Select Components** window, click to select or deselect the checkboxes as needed. Click **Next**.



Select Components

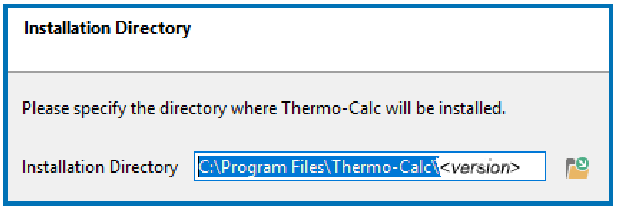
Select the components you want to inst
continue.

- ☑ Thermo-Calc
- ☑ Databases
- ☑ TC-Python
- ☐ TC-Toolbox for MATLAB (R)
- ☑ TQ-Interface

TQ-Interface is not yet available with the user credentials system.

Step 3: Finish Installing Thermo-Calc

1. In the **Installation Directory** window, either accept the default path or enter a path to where you want to install the software. Click the file button 📂 to **Browse for Folder** and navigate to another directory.

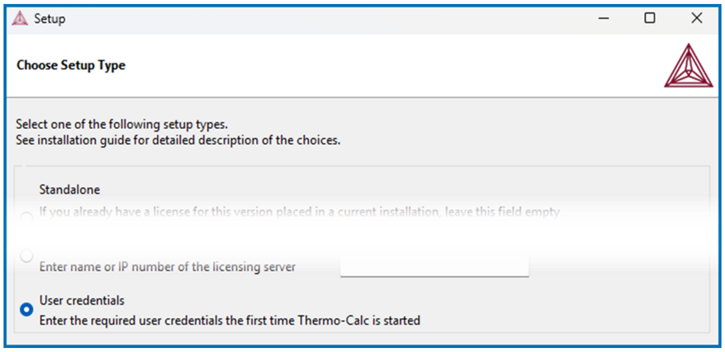


Installation Directory

Please specify the directory where Thermo-Calc will be installed.

Installation Directory C:\Program Files\Thermo-Calc*<version>*

2. In the **Choose Setup Type** window, click **User credentials**.



Setup

Choose Setup Type

Select one of the following setup types.
See installation guide for detailed description of the choices.

Standalone
○ If you already have a license for this version placed in a current installation, leave this field empty

○ Enter name or IP number of the licensing server

● User credentials
Enter the required user credentials the first time Thermo-Calc is started

3. TC-Python is automatically installed when the **User credentials** option is chosen. The **Install TC-Python** page is a reminder for users of TC-Python that additional installation and license credential procedures are needed after Thermo-Calc is installed. Read the separate installation instructions (also included in the full installation guide) for more information if applicable. Click **Next**.
4. In the **Ready to Install** window click **Next**.
5. Click **Finish** and start using Thermo-Calc. For Linux users, log out and log back in to finish the installation.

For macOS installations and if you have previous Thermo-Calc installations: When you launch Thermo-Calc with the new or updated version, the splash screen hides the **Import User Settings** dialog box. In order to proceed you need to click the splash screen and then click **Yes** or **No** in the dialog box.

Step 4: Activate the License

If your work environment does not allow an Internet connection to activate the license, as a last resort you can use the option **Create offline activation file**. Overall it is best to use the **Activate online** option as this provides more flexibility and future benefits including being able to easily update your license. See the last section for details.

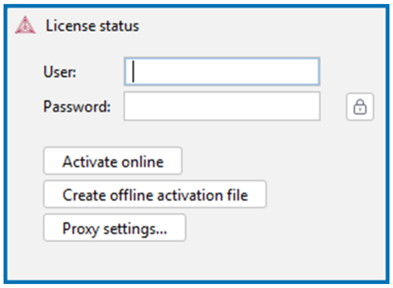
1. Open Thermo-Calc. The first window includes highlights from the current release. Click **Close**.
2. In the **License status** window, enter the **User** and **Password** provided to you.

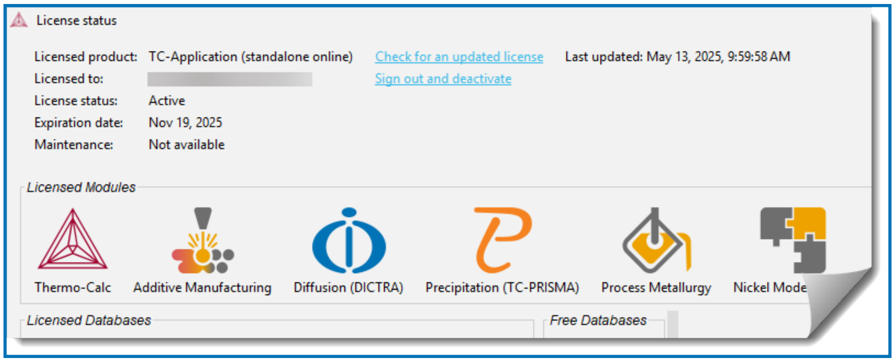
Your license user credentials are sent to you in an email from Thermo-Calc or a representative. This is different from the Download Center login details. If you have not received the information, first ask the main Thermo-Calc contact in your organization. Otherwise, contact Support for clarification.

3. If you use a proxy server, click **Proxy settings**. Click **Use proxy** and enter your information. Click **OK**.
4. Click **Activate online**.

If the fields become empty when you click **Activate online**, this means the activation did NOT work. See the troubleshooting section for details about next steps When Activate Online Does Not Work.

5. Once it is activated you will see the **License status** window with a list of the products you have access to. Click **Close** and start using Thermo-Calc.





License status

Licensed product: TC-Application (standalone online) Check for an updated license Last updated: May 13, 2025, 9:59:58 AM
Licensed to: [redacted] Sign out and deactivate
License status: Active
Expiration date: Nov 19, 2025
Maintenance: Not available

At any time you can view the product license information by selecting **Help → Show License Info** from the menu in Thermo-Calc.

Step 5: Optional Offline License Activations

Offline activations are only available for single user (SUNLL) licenses and should only be used as a last resort, i.e. if there is no option provided by your organization to achieve online activation. The computer only needs to be connected to a network during the license activation, not when working with the software.

Offline activations can be an alternative for users who are in a highly secure environment that does not allow Internet connections.

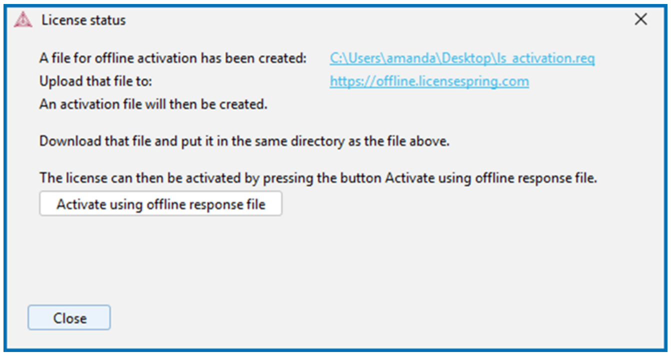
In general it is highly recommended to use the **Online activation** option as this provides more flexibility including faster and easier license updates, i.e. for offline activations license updates require repeating the full offline activation procedure.

You will need access to the Internet to complete the activation. You can do this either by:

- Accessing the Internet temporarily from the computer you will use Thermo-Calc on, or
- Activating the license on another computer then transferring the license to the computer you will use Thermo-Calc on.

These instructions are a continuation from previous steps and assume you have already installed Thermo-Calc and entered your user credentials.

1. Click **Create offline activation file**. The **License status** window opens with instructions you can refer to.



License status

A file for offline activation has been created: C:\Users\amanda\Desktop\ls_activation.req
Upload that file to: https://offline.licensespring.com
An activation file will then be created.

Download that file and put it in the same directory as the file above.

The license can then be activated by pressing the button Activate using offline response file.

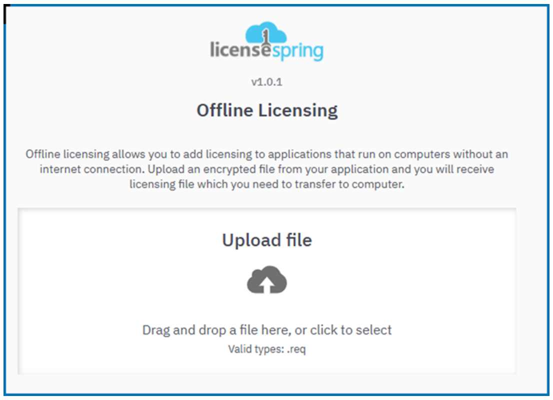
2. A local file to use for the offline activation is created and the link to where it is downloaded to your computer is provided. The file is named `ls_activation.req`. Click the link to go to this location on your computer.

If you have downloaded the file to a computer that does not have Internet access, then copy this file to one that does and continue the process. Later you will copy the generated offline license back to the computer where Thermo-Calc is installed.

3. On the computer that has Internet access, go to the URL shown on the **License status** window: https://offline.licensespring.com.

4. Navigate to the `ls_activation.req` file on your computer and drag and drop it into the center of the window. The program generates another file and downloads it to your computer. This file is named `ls_activation.lic`.

As soon as the `ls_activation.req` file is uploaded the license is considered by the software to be activated.



v1.0.1

Offline Licensing

Offline licensing allows you to add licensing to applications that run on computers without an internet connection. Upload an encrypted file from your application and you will receive licensing file which you need to transfer to computer.

Upload file

Drag and drop a file here, or click to select

Valid types: .req

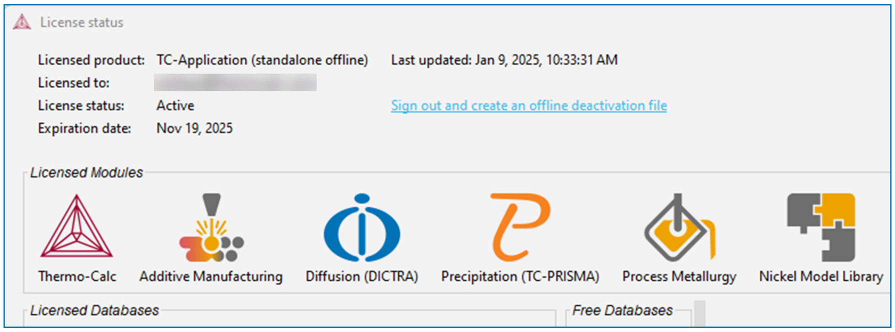
> If at this point you want to switch to an online activation instead (recommended), you can delete the `ls_activation.req` file from the computer location to end the offline activation process.

5. Navigate to the downloaded `ls_activation.lic` file. If needed, this is when you copy this file back to the computer where Thermo-Calc is installed. In both cases the new file should be copied back to the same folder where the original file `ls_activation.req` is located.

6. Once the two files are in the same folder, you are ready to generate an offline license.

7. Go to the **License status** window and click **Activate using offline response file**.

   Once activated you will see the **License status** window with a list of the products you have access to. Click **Close** and start using Thermo-Calc.


License status

Licensed product: TC-Application (standalone offline)

Last updated: Jan 9, 2025, 10:33:31 AM

Licensed to: [redacted]

License status: Active

Sign out and create an offline deactivation file

Expiration date: Nov 19, 2025

8. You do not need to keep the files you downloaded. Return to where these files are downloaded and delete them.

At any time you can view the product license information by selecting **Help → Show License Info** from the menu in Thermo-Calc.

Unattended or Silent Network Installations (User Credentials)

Sometimes it is convenient to install Thermo-Calc network clients without providing user input after the installation is initiated (an unattended network installation), i.e. a *silent installation*. This is available for Windows and Linux operating systems.

Create an Option File in a Text Editor to Enter the Options

Below is a example for installation when you have a license activation type **user credentials**:

```
installation_mode=custom

setup_type=licenseSpring
```

Go to the Directory Where the Installation File is Saved

> Thermo-Calc can only be installed in unattended mode from the command line prompt.

Start the installation in unattended mode using the option file created with this command:

- Windows: `<installationfile>.exe --mode unattended --optionfile <path\optionfile>`
- Linux: `<installationfile>.run --mode unattended --optionfile <path/optionfile>`

To see other options when you start the Thermo-Calc installation program from the command line prompt, run this command:

- Windows: `<installationfile>.exe --help`
- Linux: `<installationfile>.run --help`

Activate the User Credentials Type of License

1. In the installation folder these files are found based on OS:
    - Windows: `License-manager.bat`
    - Linux: `License-manager.sh`

2. From the command line prompt, run the command once for every product you want to activate:
    - Windows: `License-manager.bat <product> activate <user> <password>`
    - Linux: `License-manager.sh <product> activate <user> <password>`

<product> can be TC-Application, TC-Python, or TC-Toolbox. *<user>* and *<password>* are the user credentials provided by email from Thermo-Calc or a representative.

The license manager can be used for activation, updating, and so forth. Run the command `License-manager.bat --help` and it shows the available options.

Deactivating Online or Offline Licenses

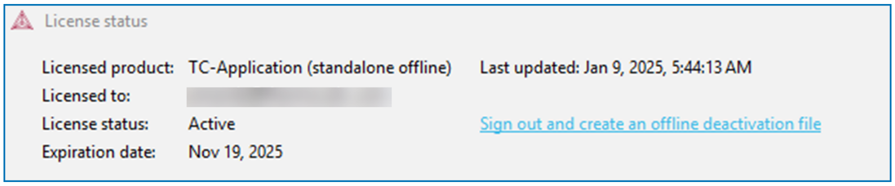
In this section is information about deactivating online and offline licenses.

Deactivating an Online License

1. Open Thermo-Calc.
2. Select **Help →** **Show License Info**.
3. In the **License status** window, click **Sign out and deactivate**.
4. The login window opens where you enter the user credentials and the license is deactivated.

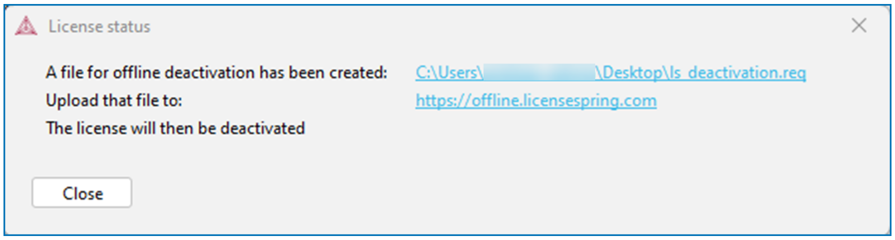
Deactivating an Offline License

1. Open Thermo-Calc.
2. Select **Help →** **Show License Info**.
3. In the **License status** window, click **Sign out and use an offline deactivation file**.



Licensed product: TC-Application (standalone offline)
Last updated: Jan 9, 2025, 5:44:13 AM
Licensed to: [redacted]
License status: Active
Expiration date: Nov 19, 2025

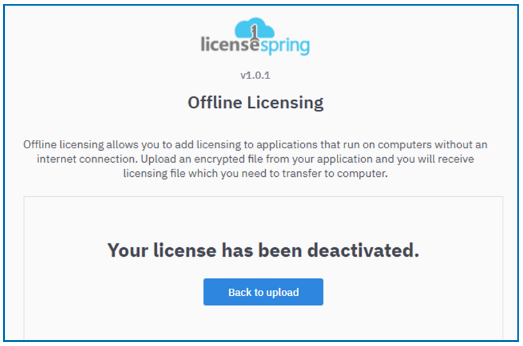
4. A local file to use for the offline deactivation is created and the link to where it is downloaded to your computer is provided. The file is named `ls_deactivation.req`. Click the link to go to this location on your computer.



A file for offline deactivation has been created: C:\Users\[redacted]\Desktop\ls_deactivation.req
Upload that file to: https://offline.licensespring.com
The license will then be deactivated

> Since you have downloaded the file to a computer that does not have Internet access, then either temporarily access the Internet, or copy the file to one where you can continue the process.

5. On the computer that has Internet access, go to the URL shown on the **License status** window: https://offline.licensespring.com.
6. Navigate to the `ls_deactivation.req` file on your computer and drag and drop it into the center of the window. The Offline Licensing window confirms that the license is deactivated.



licensespring

v1.0.1

Offline Licensing

Offline licensing allows you to add licensing to applications that run on computers without an internet connection. Upload an encrypted file from your application and you will receive licensing file which you need to transfer to computer.

Your license has been deactivated.

7. You do not need to keep the file you downloaded. Return to where the deactivation file was downloaded or saved and delete it.

Default Installation Directories

The default directories where the software and its components are installed, including where the license file is stored, vary by platform and user type.

If you want to select specific components to install or if you want to install the software in a non-default installation directory, then do a **custom** installation (Windows and Linux only). In the table, *<user>* stands for the user name and *<version>* for the version of Thermo-Calc, for example 2025b.

In this section:

Installation Default Directory: Windows

Administrative rights are required to install and uninstall Thermo-Calc.

Windows User Type	*Default Directory*

Administrator	The Thermo-Calc program is installed here:
	`Program Files\Thermo-Calc\<version>`
	The default folders where documents, materials files, examples, and other folders that sometimes require additional licenses are installed under **Public Documents** for ALL USERS.
	For a local user these files are copied to the user’s **Documents** folder where this local copy is associated to the user login. The **Public Documents** folder always contains the original set of contents as per the installation.
	`C:\Users\Public\Public Documents\Thermo-Calc\<version>`
	After installing Thermo-Calc, and when you first open the program, the set of folders is copied from the source Public Documents location into a user Documents folder:
	`C:\Users\<user>\Documents\Thermo-Calc\<version>`
	It is recommended that you work with the files that are copied to the *user* folder.
	In some cases when an interim software update is installed there is also a backup folder created in this folder. For details, see Updating the Software for Interim Releases.

Server network	This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a. License software installations on a server network (the License Manager software) `C:\Program Files (x86)\Common Files\SafeNet Sentinel\Sentinel RMS License Manager\WinNT\`

Installation Default Directory: macOS

macOS User Type	*Default Directory*

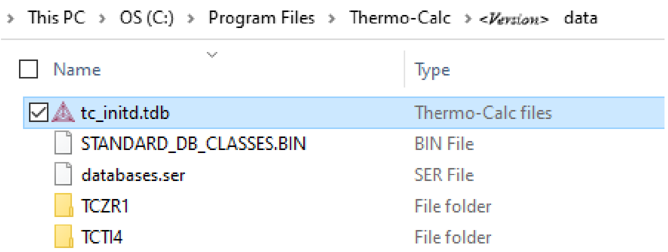
Administrator (user name and password required)	The Thermo-Calc program is installed in the **Applications** folder:
	`Thermo-Calc-<version>.app and uninstall-Thermo-Calc-<version>.app`
	The documents, materials, examples, and other folders that sometimes require additional licenses are installed here:
	`/Users/Shared/Thermo-Calc/<version>`
	In some cases when an interim software update is installed there is also a backup folder created in this folder. For details, see Updating the Software for Interim Releases.
	To go to this folder, in Finder, from the **Go** main menu select **Go to folder**. Enter the above file path and click **Go**.

Installation Default Directory: Linux

Linux User Type	*Default Directory*
Non root user	The Thermo-Calc program including the documents, materials, examples, and other folders that sometimes require additional licenses are installed here: `/home/<user>/Thermo-Calc/<version>`
Root user	The Thermo-Calc program including the documents, materials, examples, and other folders that sometimes require additional licenses are installed here: `/opt/Thermo-Calc/<version>` In some cases when an interim software update is installed there is also a backup folder created in this folder. For details, see Updating the Software for Interim Releases.
License software installations on a server network (the License Server software)	This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a. If you are doing a network installation then these files are available as a tar-file from the Thermo-Calc website. Contact Support for more information. In the downloaded tar-file, there is a **restart_lserv** script file, which can be used as a template for creating a script that starts up the License Server.

Installation Default Directory: Databases, Database Checker, and TDB Editor

The standard Thermo-Calc databases and the database initialization file `tc_initd.tdb` are located in a subfolder to the Thermo-Calc installation. For example, in a Windows Standalone installation, you can find these in a folder called **data** where the file path is *C:\Program Files\Thermo-Calc\<version>\data*.



› This PC › OS (C:) › Program Files › Thermo-Calc › <Version> data

☐ Name	Type
☑ tc_initd.tdb	Thermo-Calc files
STANDARD_DB_CLASSES.BIN	BIN File
databases.ser	SER File
TCZR1	File folder
TCTI4	File folder

Database Checker

The Thermo-Calc software package includes a program to check that the syntax of unencrypted database files is correct. The program applies the syntax rules set out in the *Database Manager User Guide* and reports errors and issues warnings. This program is intended for advanced users who develop and manage databases.

Thermo-Calc accepts some deviations from these syntax rules. Although warnings can be ignored, errors must be corrected. Reported errors must be corrected in the TDB file before the database can be loaded by the application. Sometimes the warnings can also reveal the need for additional corrections as shown in the example below.

For example, a warning is generated if a phase name is detected that is also an abbreviation of another phase name in the database. Although allowed, it is not recommended as this can (in some cases) lead to unexpected results because abbreviations are also used when entering commands in the Console and included in macro files. The following shows why in this case an abbreviation is not recommended.

Imagine that a macro file uses the abbreviation `ABC` to refer to a phase in a database that is named `ABCDE`. As long as there is no other phase in the database with the same exact name or initial abbreviation, it works. But if a new phase is added to the database and is actually named `ABC` then the macro can in error refer to the wrong phase. The macro still runs but now refers to the phase `ABC` instead of `ABCDE` because `ABC` is an exact match, *which takes precedence over abbreviations*. The Database Checker displays a warning because this situation can only occur when one phase name is an abbreviation of another.

With respect to using this tool, the executable `DatabaseChecker` file is found in the Thermo-Calc home directory.

The program can also be launched by selecting **Tools →** **Database Checker**from the main menu in Thermo-Calc.

TDB Editor

The TDB Editor is an editing tool for those who develop their own custom databases for use with Thermo-Calc or other applications. The tool speeds up the database editing process by providing immediate feedback through syntax coloring, syntax checking, and by allowing formatting and easy navigation to items of interest in the TDB file.

During installation, the `tdb-language-support.vsix` file is installed in the Thermo-Calc home directory.

In order to access the most-up-to-date version of the TDB editing functionality, it must be reinstalled every time a *new* version of Thermo-Calc is installed.

For information about installing the TDB Editor, which is separate from the main installation and can be done later, see the *Database Manager's User Guide* contained in the *Thermo-Calc Documentation Set* or press F1 in Thermo-Calc and search the help.

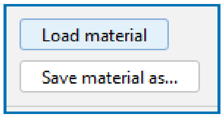
Installation Default Directory: Materials

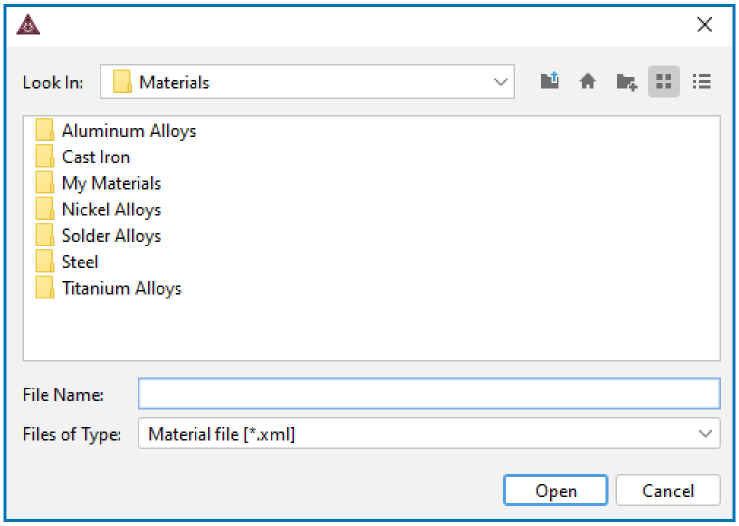
When you are working with the System Definer or Material to Material Calculator you can open the default **Materials** folder included with your installation.

At the bottom of the window under **Material**, click **Load material** to navigate to a material file.

There is a separate folder for materials saved using the Process Metallurgy Calculator. See Installation Default Directory: Process Metallurgy Materials.

For the Additive Manufacturing (AM) Module, the Material Properties library is managed by the software.





The default directory where these material files are stored is based on operating system:

Operating System	*Materials Installation Directory*
Windows	`C:\Users\<user>\Documents\Thermo-Calc\2025b\Materials`
Linux	On Linux all user files are installed where the program is installed. If installed as root the default is: `/opt/Thermo-Calc/2025b/Materials`

Operating System	***Materials Installation Directory***
macOS	`/Users/Shared/Thermo-Calc/2025b/Materials`

Installation Default Directory: Process Metallurgy Materials

With the Process Metallurgy Calculator you can save materials to work with again. This is the default folder where these are stored based on your operating system:

Operating System	*Process Metallurgy Materials Installation Directory*
Windows	`C:\Users\<user>\Documents\Thermo-Calc\2025b\ProcessMetallurgyMaterials`
Linux	On Linux all user files are installed where the program is installed. If installed as root the default is: `/opt/Thermo-Calc/2025b/ProcessMetallurgyMaterials`
macOS	`/Users/Shared/Thermo-Calc/2025b/ProcessMetallurgyMaterials`

Installation Default Directory: Custom Property Models

All Property Models (whether these are predefined or custom models) must be located in a subdirectory of the Property Model directory. You can go to the **Options** window then on the **General** tab the **Model directory** field displays the default directory.

To open the **Options** window:

- Windows: Select **Tools** → **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

Predefined models included with the Property Model Calculator are installed in the locations below based on your operating system. If you create your own models using TC-Python, this is the default directory where these are saved.

Operating System	*Property Model Installation Directory*
Windows	`C:\Program Files/Thermo-Calc/2025b\PropertyModels`

Linux	On Linux all user files are installed where the program is installed. If installed as root the default is:
	`/opt/Thermo-Calc/2025b/PropertyModels`
	or:
	`/home/<username>/Thermo-Calc/2025b/PropertyModels`

macOS	`/Applications/Thermo-Calc-2025b.app/Contents/Resources/PropertyModels`

License File and License Server Installations

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

In this section:

About License Keys and Files

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

To run Thermo-Calc and its components you need a valid license key for each product. The license keys are included in the license file emailed to you by Thermo-Calc Software.

You can copy the license file to the applicable computer(s) before or after installing the software—the license file itself is not required during the installation process. However, it is required to make calculations in Thermo-Calc.

? Request a License File from Thermo-Calc Software

First Steps of Installation

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

This section reviews some of the things you need to do before installing the Thermo-Calc software.

- Learn about the different default directories where the software and license files are installed.
- For network installations, collect subnet information.
- Make sure the person installing the software has administrator rights for Windows and macOS.
- For macOS, install XQuartz and make sure the security preferences are set correctly.
- For a Linux Cent OS 7 installation, also install gtk2 before you run the installation script.

```
yum install gtk2
```

Should I get my license file before or after software installation? The Thermo-Calc license file itself is not required during the installation process. However, it is required to make calculations in Thermo-Calc. The license file has details about your computer(s) that in some cases cannot be determined accurately until *after* installation (especially for a network installation). For most users it is recommended you request the file before you start installing.

You do not need a license file if you are provided with user credentials to activate your license. See About User Credentials License Activations and proceed to the relevant installation instructions.

Installation Default Directories and the License File

You do not need a license file if you are provided with user credentials to activate your license. See About User Credentials License Activations and proceed to the relevant installation instructions.

The default directories where the software and its components are installed, including where the license file is stored, vary by platform and user type.

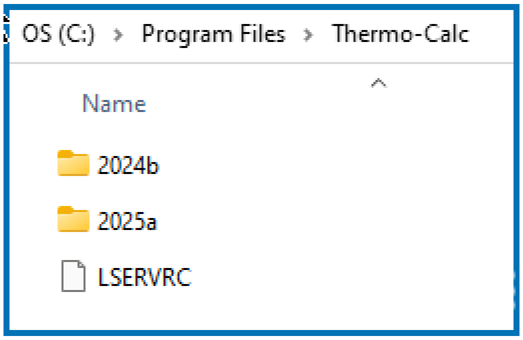
If you want to select specific components to install or if you want to install the software in a non-default installation directory, then do a **custom** installation (Windows and Linux only). In the table, *<user>* stands for the user name and *<version>* for the version of Thermo-Calc, for example 2025b.

License File Installation Location for All Operating Systems

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

The Thermo-Calc license file is installed outside of the installation program folder. If you have more than one version of Thermo-Calc installed then there are additional folders by version number with only one license file.

For macOS the license file is put in `/Users/Shared/Thermo-Calc`. The example below is for a Standalone Windows installation.


OS (C:) › Program Files › Thermo-Calc

Name

2024b

2025a

LSERVRC

More Information

See the following for more information:

- Installation Default Directory: Windows
- Installation Default Directory: macOS
- Installation Default Directory: Linux
- Installation Default Directory: Databases, Database Checker, and TDB Editor
- Installation Default Directory: Materials
- Installation Default Directory: Process Metallurgy Materials
- Installation Default Directory: Custom Property Models
- Installation Default Directory: TC-Python
- Installation Default Directory: TC-Toolbox and the Examples

Standalone Installations (License File)

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

You can either do a full or a custom standalone installation. The license type is called a Single-User Node-Locked License (SUNLL).

In this section:

Standalone Installations (SUNLL)

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

The standalone installation is used with the Single-User Node-Locked License (SUNLL). The Thermo-Calc software and a Thermo-Calc license file are installed on a standalone computer. You can do a full (all operating systems) or a custom installation (Windows and Linux only).

To get started, go to (1) First Steps of Installation and then (2) Standalone Installations (License File).

Full Standalone Installations

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

The following describes a full standalone installation. These steps assume you have completed the section First Steps of Installation.

Request your License File from Thermo-Calc Software

Upgrading to a new version of Thermo-Calc: Skip this section if you are upgrading to a new version of Thermo-Calc (and you have a maintenance plan), or you have already been provided with the license file.

For license file activations, follow the instructions for your operating system in the section Request a License File from Thermo-Calc Software. Also note that the license file name must be the same as the existing file name to ensure there are no errors during the update.

You do not need a license file if you are provided with user credentials to activate your license. See About User Credentials License Activations and proceed to the relevant installation instructions.

Download your Thermo-Calc Installation Software

Administrative rights are required for Windows and macOS to complete this installation. The email from Thermo-Calc Software (or from someone in your organization) includes the links and information you need to access the current version of the software you want to download.

1. Click the link from the email and the first page of the **Download Center** opens. Under the applicable operating system section (Windows, macOS, or Linux), select the OS version. Click **Go to download page**.
2. In the **Sign in to access this site** window, enter the **Username** and **Password** (found in the email) and click **Sign in**.
3. On the **Download Center** page under **Software**, click the relevant link for your operating system to download the file for the current software version (2025b).

Run the Applicable Installation File for your Operating System

1. Navigate to the folder for your operating system and click the link to download the software package, then go to the folder where you downloaded it.

Windows

Double-click the **.exe** file to launch the **Setup** program.

macOS

Double-click the downloaded file then follow the instructions.

> For macOS and when you first run the installer, you may see a message that *Thermo-Calc-osx-<version> can't be opened because Apple cannot check it for malicious software*. If this happens, select **Show in Finder**. Then, in the opened **Finder** window right-click the downloaded file `Thermo-Calc-osx-<version>` and select **Open**.

Linux

To start the Setup Wizard in a Terminal window, enter these commands in the directory where the installation file is saved:

```
> chmod +x linux-installation-x64-2025b.run
> ./linux-installation-x64-2025b.run
```

If you are an openSUSE root user, see Linux Installation Notes for some information about your installation.

2. On the **Setup** window click **Next**.
3. On the **License Agreement** window click the button to accept the license agreement then click **Next**.

Select the License and Installation Mode and Install the Software

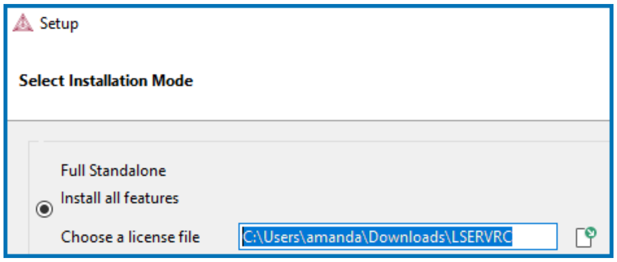
About the Thermo-Calc Installed Components

1. In the **Select License and Installation Mode** window click **Full Standalone: Install all features**.

   If you want to exclude a component (e.g. an SDK), then use the **Custom** option. See Custom Standalone Installations (License File). For TC-Toolbox for MATLAB®, also see Installing TC-Toolbox with the Custom Option.

   If you also have a license for TC-Python, it is installed when the **Full Standalone** or **Full Network Client** option is chosen, but there are additional steps required as described separately for this SDK.

2. For a **Full Standalone** installation, in the **Choose a license file** field either enter the file path or click the file button to navigate to where you saved the license file emailed to you from Thermo-Calc Software.



Select Installation Mode

● Full Standalone
Install all features

Choose a license file: C:\Users\amanda\Downloads\LSERVRC

The license file is called **lservrc**. Click **Next**. To prevent errors, leave this field blank if you did not get a license file yet. If you did not get your license file see Request a License File from Thermo-Calc Software.

TC-Python is installed for all users even if you do not have a license. The **Install TC-Python** window is a reminder that additional installation procedures are required after Thermo-Calc is installed. See the *TC-Python Installation Guide*.

3. In the **Ready to Install** window click **Next**. Click **Finish** and start using Thermo-Calc.

Additional Notes

For Linux users, log out and log back in to finish the installation.

For macOS installations and if you have previous Thermo-Calc installations: When you launch Thermo-Calc with the new or updated version, the splash screen hides the **Import User Settings** dialog box. In order to proceed you need to click the splash screen and then click **Yes** or **No** in the dialog box.

Windows® Standalone (License File) Installations

There are two *license activation types* available as of 2025b: (1) **User credentials**, which are entered after installation and managed via an online portal or (2) where a **license file** is installed directly on the computer or a licensing server. Many users have already started using the *user credentials* activation type and all users will eventually be migrated to the new system.

This section is applicable to:

- Operating system: Windows
- Installation type: Full Standalone (SUNLL)
- License activation type: License file where the software and the license file are installed together on one computer.
- Upgrading to a new standalone version of Thermo-Calc (maintenance plan only)

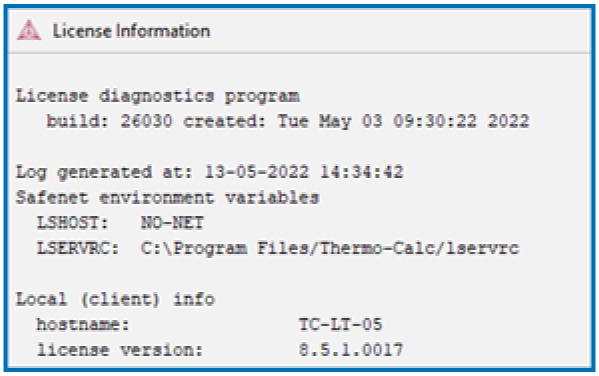
For instructions about other operating systems, network installations, or installing an SDK (e.g. TC-Python or TC-Toolbox for MATLAB®) search the *Thermo-Calc Installation Guide*, which is also available on our website. You can also review the Licensing Options included on our website.

Step 1: Request a License File

Upgrading to a new version of Thermo-Calc: Skip this section if you are upgrading to a new version of Thermo-Calc (and you have a maintenance plan), or you have already been provided with the license file.

1. Your license information is sent to you in an email from Thermo-Calc or a representative. When you are sent a *license file*, save it to your computer to use during software installation. You may also need to provide some information that is accessed from Thermo-Calc.

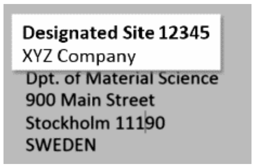
   Select **Help → Show License Info**.



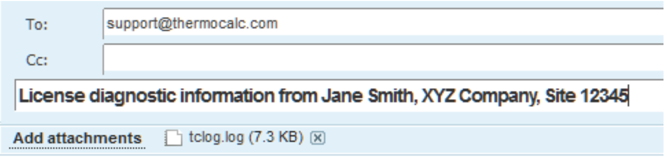
```
License diagnostics program
   build: 26030 created: Tue May 03 09:30:22 2022

Log generated at: 13-05-2022 14:34:42
Safenet environment variables
  LSHOST:    NO-NET
  LSERVRC:  C:\Program Files/Thermo-Calc/lservrc

Local (client) info
  hostname:                TC-LT-05
  license version:         8.5.1.0017
```

2. Copy the information from the **License Information** window. A lot of information may be shown below the initial screen, so make sure you scroll down to the end when you select and copy the window's contents. (Alternatively, you can copy the same information from the console by using the SYS module command DISPLAY_LICENSE_INFO.)
3. Send an email to support@thermocalc.com. Make sure to include the following in the subject line:

   License diagnostic information from <Name> where Name is replaced with your **name**, the **organization name** and the **Site Number**. *You can find the five-digit site number on an invoice or any correspondence from Thermo-Calc Software.*

   Designated Site 12345
   XYZ Company
   Dpt. of Material Science
   900 Main Street
   Stockholm 11190
   SWEDEN

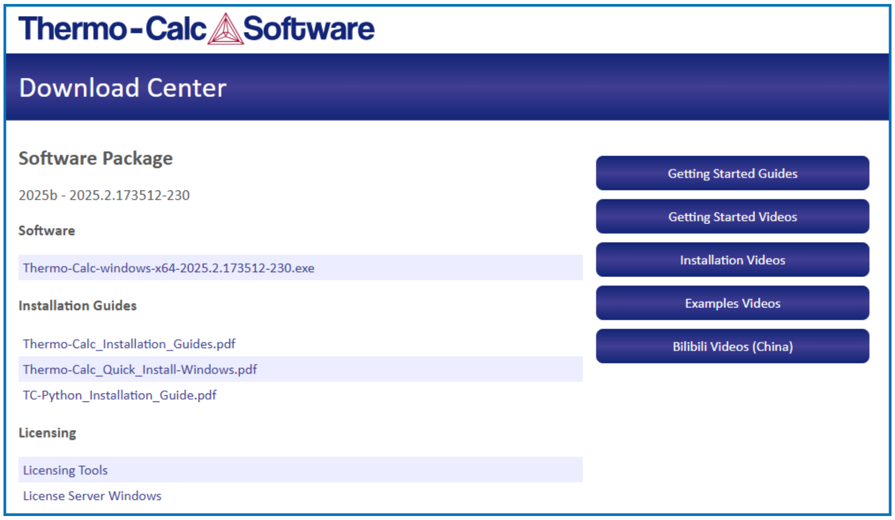
   To: support@thermocalc.com
   Cc:
   License diagnostic information from Jane Smith, XYZ Company, Site 12345

4. A representative from Thermo-Calc Software replies to the email and attaches your license file(s).
5. Save the license file(s) to your computer or network.

Step 2: Download Thermo-Calc Software

Administrative rights are required to complete this installation. An email from Thermo-Calc Software (or from someone in your organization) includes the links and information you need to access and activate the current version of the software you want to download.

1. Click the link from the email and the first page of the **Download Center** opens. Under the **Windows** section, select the OS version. Click **Go to download page**.
2. In the **Sign in to access this site** window, enter the **Username** and **Password** (found in the email) and click **Sign in**.
3. On the **Download Center** page under **Software**, click the **.exe** link to download the file for the current software version for your operating system (2025b).



Download Center

Software Package

2025b - 2025.2.173512-230

Software

Thermo-Calc-windows-x64-2025.2.173512-230.exe

Installation Guides

Thermo-Calc_Installation_Guides.pdf

Thermo-Calc_Quick_Install-Windows.pdf

TC-Python_Installation_Guide.pdf

Licensing

Licensing Tools

License Server Windows

Step 3: Install Thermo-Calc Software

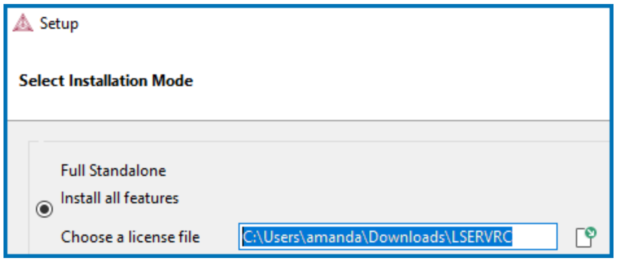
1. Navigate to the folder where you downloaded the software. Double-click the **.exe** program. Remember that administrative rights are needed, so when you are prompted for that user name and password, enter these credentials here. Click **Yes** to continue.
2. On the **Setup - Thermo-Calc 2025b** window click **Next**.
3. On the **License Agreement** window click to accept the license agreement. Click **Next**.

Step 4: Select License and Installation Mode

1. In the **Select License and Installation Mode** window click **Full Standalone: Install all features**.

> If you also have a license for TC-Python, it is installed when the **Full Standalone** or **Full Network Client** option is chosen, but there are additional steps required as described separately for this SDK.

2. For a **Full Standalone** installation, in the **Choose a license file** field either enter the file path or click the file button to navigate to where you saved the license file emailed to you from Thermo-Calc Software.



Setup

Select Installation Mode

● Full Standalone
Install all features

Choose a license file C:\Users\amanda\Downloads\LSERVRC

> The license file is called **lservrc**. Click **Next**. To prevent errors, leave this field blank if you did not get a license file yet.

> TC-Python is installed for all users even if you do not have a license. The **Install TC-Python** window is a reminder that additional installation procedures are required after Thermo-Calc is installed. See the *TC-Python Installation Guide*.

3. In the **Ready to Install** window click **Next**. Click **Finish** and start using Thermo-Calc.

macOS® Standalone (License File) Installations

There are two *license activation types* available as of 2025b: (1) **User credentials**, which are entered after installation and managed via an online portal or (2) where a **license file** is installed directly on the computer or a licensing server. Many users have already started using the *user credentials* activation type and all users will eventually be migrated to the new system.

This section is applicable to:

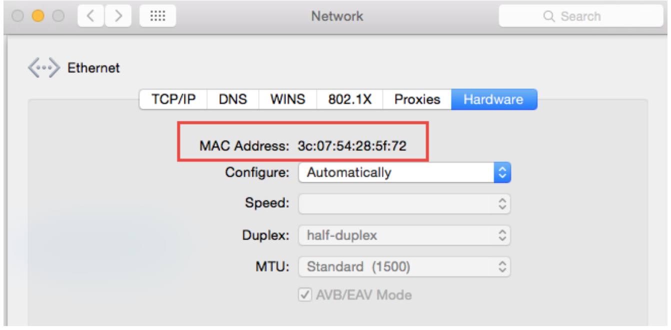
- Operating system: macOS
- Installation type: Full Standalone (SUNLL)
- License activation type: License file where the software and the license file are installed together on one computer.
- Upgrading to a new standalone version of Thermo-Calc (maintenance plan only)

For instructions about other operating systems, network installations, or installing an SDK (e.g. TC-Python or TC-Toolbox for MATLAB®) search the *Thermo-Calc Installation Guide*, which is also available on our website. You can also review the Licensing Options included on our website.

Step 1: Request a License File

Upgrading to a new version of Thermo-Calc: Skip this section if you are upgrading to a new version of Thermo-Calc (and you have a maintenance plan), or you have already been provided with the license file.

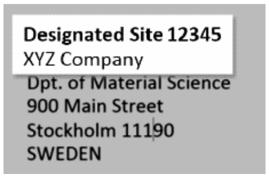
1. From the Apple main menu, select **System Preferences**.
2. Click **Network**.
3. In the left column select **Ethernet** or **Built-in Ethernet** (do not select a WiFi connection as a local static MAC address is required).
4. Click **Advanced → Hardware**. The **Network** window shows you the **MAC Address**. For example, the MAC address (the host ID) might be **3c:07:54:28:5f:72**.



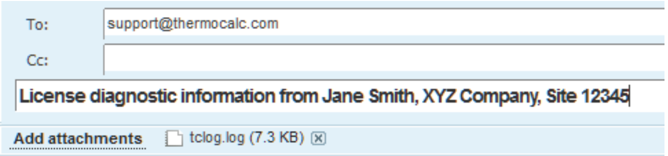
MAC Address: 3c:07:54:28:5f:72
Configure: Automatically
Speed:
Duplex: half-duplex
MTU: Standard (1500)
☑ AVB/EAV Mode

5. Send an email to support@thermocalc.com and copy and paste the MAC address into the body of the email. Make sure to include the following in the subject line:

   License diagnostic information from <Name> where Name is replaced with your **name**, the **organisation name** and the **Site Number**. *You can find the five-digit site number on an invoice or any correspondence from Thermo-Calc Software.*



Designated Site 12345
XYZ Company
Dpt. of Material Science
900 Main Street
Stockholm 11190
SWEDEN



To: support@thermocalc.com
Cc:
License diagnostic information from Jane Smith, XYZ Company, Site 12345

6. A representative from Thermo-Calc Software replies to the email address provided and attaches your license file or files.
7. Save your license file to your computer or network.

Step 2: Install Required macOS Software

To install and run Thermo-Calc on a Mac computer with an ARM processor, Rosetta first needs to be installed.

The XQuartz open-source X.Org X Window system is required to run Thermo-Calc on macOS.

1. In a web browser go to https://www.macupdate.com or to download it directly from XQuartz, https://www.xquartz.org/.
2. In the **Search Mac Apps** field, enter *XQuartz*.

3. Click the **XQuartz** search result. For example, based on the recent version, the name is XQuartz-2.8.5.dmg.
4. Click **Download**.
5. Double-click the **XQuartz-**<*version*>**.pkg** file. Follow the instructions.
6. Click **OK** when the message about logging out displays and click **Close** when the installation is successful.

Step 3: Download Thermo-Calc Software

Administrative rights are required to complete this installation. An email from Thermo-Calc Software (or from someone in your organization) includes the links and information you need to access and activate the current version of the software you want to download.

1. Click the link from the email and the first page of the **Download Center** opens. Under the **macOS** section, select the OS version. Click **Go to download page**.
2. In the **Sign in to access this site** window, enter the **Username** and **Password** (found in the email) and click **Sign in**.
3. On the **Download Center** page under **Software**, click the **.zip** link to download the file for the current software version for your operating system (2025b).

Thermo-Calc Software

Download Center

Software Package

2025b - 2025.2.173512-230

Software

Thermo-Calc-osx-2025.2.173512-230.zip

Installation Guides

Thermo-Calc_Installation_Guides.pdf

Thermo-Calc_Quick_Install-Mac.pdf

TC-Python_Installation_Guide.pdf

Licensing

Licensing Tools

Step 4: Install Thermo-Calc Software

For macOS and when you first run the installer, you may see a message that *Thermo-Calc-osx-<version> can't be opened because Apple cannot check it for malicious software*. If this happens, select **Show in Finder**. Then, in the opened **Finder** window right-click the downloaded file `Thermo-Calc-osx-<version>` and select **Open**.

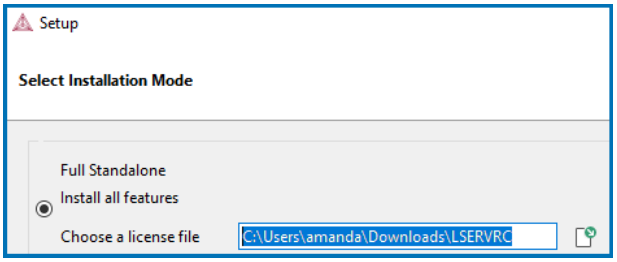
1. Navigate to the folder where you downloaded the software. Double-click the **.zip** program. Remember that administrative rights are needed, so when you are prompted for that user name and password, enter these credentials here. Click **Yes** to continue.
2. On the **Setup - Thermo-Calc 2025b** window click **Next**.
3. On the **License Agreement** window click to accept the license agreement. Click **Next**.

Step 5: Select License and Installation Mode

1. In the **Select License and Installation Mode** window click **Full Standalone: Install all features**.

   If you also have a license for TC-Python, it is installed when the **Full Standalone** or **Full Network Client** option is chosen, but there are additional steps required as described separately for this SDK.

2. For a **Full Standalone** installation, in the **Choose a license file** field either enter the file path or click the file button to navigate to where you saved the license file emailed to you from Thermo-Calc Software.



● Full Standalone
Install all features

Choose a license file C:\Users\amanda\Downloads\LSERVRC

The license file is called **lservrc**. Click **Next**. To prevent errors, leave this field blank if you did not get a license file yet.

TC-Python is installed for all users even if you do not have a license. The **Install TC-Python** window is a reminder that additional installation procedures are required after Thermo-Calc is installed. See the *TC-Python Installation Guide*.

3. In the **Ready to Install** window click **Next**. Click **Finish** and start using Thermo-Calc.

Import User Settings

For macOS installations and if you have previous Thermo-Calc installations: When you launch Thermo-Calc with the new or updated version, the splash screen hides the **Import User Settings** dialog box. In order to proceed you need to click the splash screen and then click **Yes** or **No** in the dialog box.

Custom Standalone Installations (License File)

Use the **Custom** option to have more control over what component features to include or exclude, for example, to exclude an SDK.

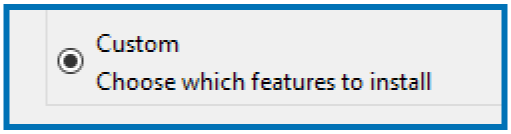
This topic describes how to do a custom installation on a standalone computer for either a Windows or Linux operating system. These steps assume you have completed these sections:

- First Steps of Installation
- Steps 1 to 3 of a Full Standalone Installations where you request your license file, download the software and then have started to set up the program up to the **Select Installation Mode** window.

Choose the Components to Install

About the Thermo-Calc Installed Components

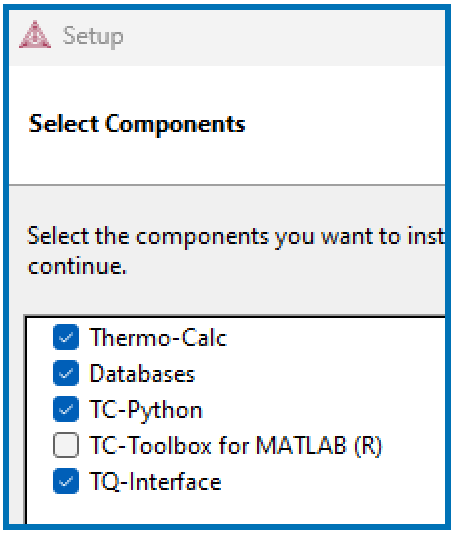
1. In the **Select License and Installation Mode** window click **Custom**. Click **Next**.



● Custom
Choose which features to install

2. On the **Specify Configuration** window the **Create Shortcut on Desktop** checkbox is selected by default. Click **Next**.

3. In the **Select Components** window, click to select or deselect the checkboxes as needed. Click **Next**.



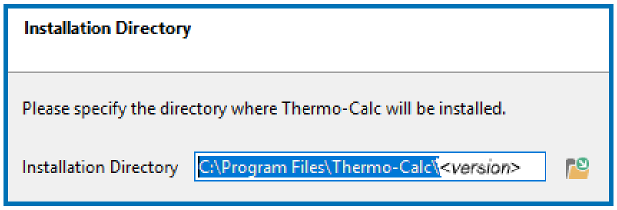
Select Components

Select the components you want to inst
continue.

☑ Thermo-Calc
☑ Databases
☑ TC-Python
☐ TC-Toolbox for MATLAB (R)
☑ TQ-Interface

Set the Installation Directory and Choose the License File

1. In the **Installation Directory** window, either accept the default path or enter a path to where you want to install the software (see Installation Default Directories and the License File). Click the file button to **Browse for Folder** and navigate to another directory.



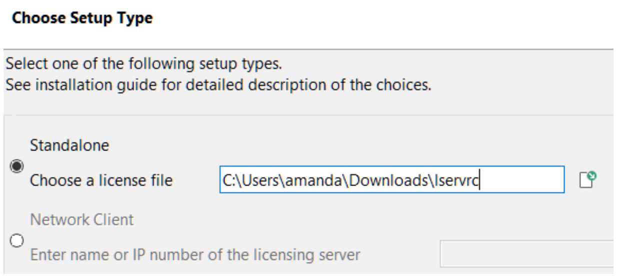
Installation Directory

Please specify the directory where Thermo-Calc will be installed.

Installation Directory: C:\Program Files\Thermo-Calc\<version>

> To prevent errors, leave this field blank if you do not have a license file yet.

2. In the **Choose Setup Type** window, click **Standalone**.



Choose Setup Type

Select one of the following setup types.
See installation guide for detailed description of the choices.

● Standalone
Choose a license file C:\Users\amanda\Downloads\lservrc

○ Network Client
Enter name or IP number of the licensing server

3. In the **Choose a license file** field enter the path to your license file (called **lservrc**) or click the file button to navigate to a location on the computer and open the file.
4. TC-Python is automatically installed when the **User credentials** option is chosen. The **Install TC-Python** page is a reminder for users of TC-Python that additional installation and license credential procedures are needed after Thermo-Calc is installed. Read the separate installation instructions (also included in the full installation guide) for more information if applicable. Click **Next**.

Install the Software and Start Using Thermo-Calc

1. In the **Ready to Install** window click **Next**.

   See the separate instructions for TC-Toolbox for MATLAB®.

2. Click **Finish** and start using Thermo-Calc. For Linux users, log out and log back in to finish the installation.

For macOS installations and if you have previous Thermo-Calc installations: When you launch Thermo-Calc with the new or updated version, the splash screen hides the **Import User Settings** dialog box. In order to proceed you need to click the splash screen and then click **Yes** or **No** in the dialog box.

If you did not get your license file see Request a License File from Thermo-Calc Software.

Network Client Installations (License Files)

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

This installation type is available for all operating systems, however for macOS the License Server must be run on a Windows or Linux computer. It is applicable to the consolidated and distributed network types of installations as well as for the licensing installation on a server network.

[About the Thermo-Calc Installed Components](#)

In this section:

Subnet Information for Network Licenses

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

This is related to Full Network Client Installations.

For network licenses, the subnet information is also required. Ask your network administrator for the *network address for the subnet*. Additional requirements are included elsewhere for network installations.

- Subnets should be in the format aaa.bbb.ccc*** (for example: 192.168.29.0/24 or 192.168.29.*
- When installing on Sentinel RMS License Server version 9.7, a maximum of seven (7) subnets are permitted.

An alternative way to get this information is to run the command:

- *Windows:* `ipconfig /all`
- *macOS/Linux*: `ip a`

Multi-User Network Installations (NWL)

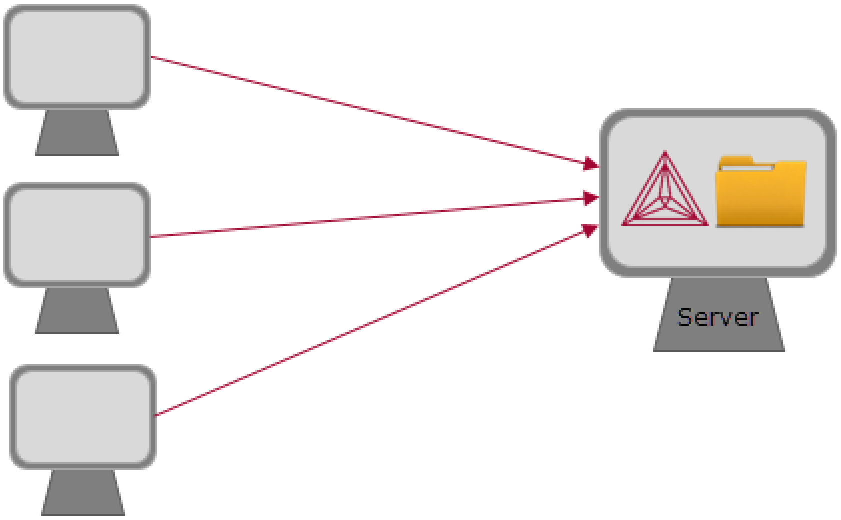
This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

There are different types of multi-user network installations: consolidated, distributed, and where the licensing software is installed on a computer network. There is also a subtype of installation called thin client, which is a step done with the consolidated and distributed network installations.

Thin client installations: A thin client installation is where the Thermo-Calc software is installed on a computer server but is run from a client computer. The licensing software can be installed on the computer server (a consolidated network) or on a different computer (a distributed network). This type of installation is available for Windows and Linux operating systems. The client computer must have the Thermo-Calc software installed. This type of installation mainly sets environmental variables and paths on the client computer.

Consolidated Network Installations

The consolidated network installation is used with a Network License (NWL) and it is available for Windows and Linux operating systems.

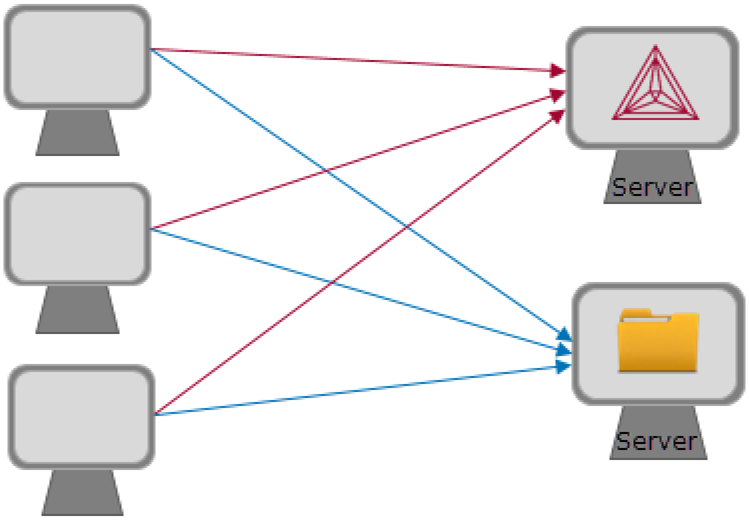


The Thermo-Calc software and the license management program are installed on the same server where the license file is also copied. A thin client installation allows all computers (the clients) in the server network to access both the software and the licensing on the same computer server.

To get started, go to (1) First Steps of Installation and then (2) Network Client Installations (License Files).

Distributed Network Installations

The distributed network installation is used with a Network License (NWL) and is available for Windows and Linux operating systems.

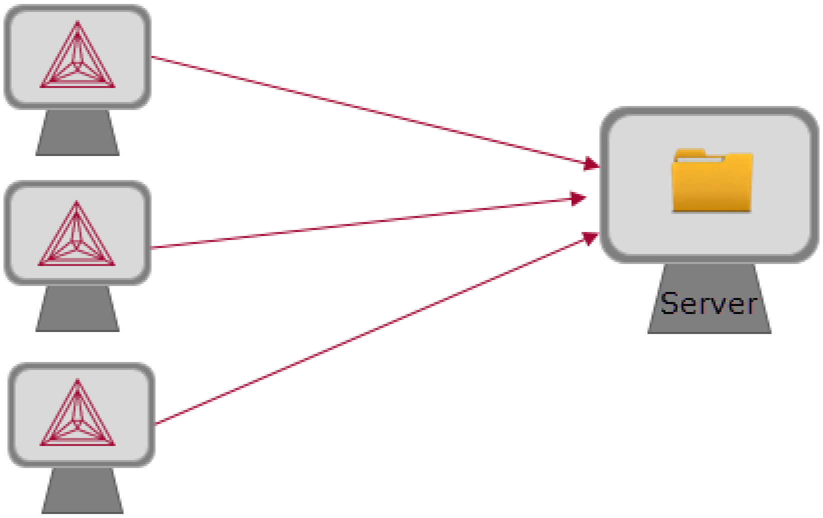


The Thermo-Calc software is installed on one computer server in a network and the licensing software is installed on a different computer server where the license file is also copied. A thin client installation allows all computers (the clients) in the server network to access both the software and the licensing on the two computer servers.

To get started, go to (1) First Steps of Installation and then (2) Network Client Installations (License Files).

License Installations on a Server Network

When a license file is installed on a server network, it is used with a Network License (NWL). It is available for all platforms. However, for macOS the server containing the licensing software must be set up on Windows or Linux.



The licensing software is installed on a computer server where the license file 📁 is also copied. The Thermo-Calc software is installed on every computer in the network that needs it.

To get started, go to (1) First Steps of Installation and then (2) Network Client Installations (License Files).

Full Network Client Installations

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

The following outlines how to do a full network client installation.

Install the Sentinel RMS Management License Software

Follow the instructions for your operating system:

Windows

- Windows: About Installing the License Manager
- Windows: Installing the Sentinel RMS License Manager

Linux

- Linux: About Installing the License Server
- Linux: Installing the Sentinel RMS License Server

Complete Steps 1 to 3 of a Full Standalone Installation

These steps assume you have completed the instructions for Full Standalone Installations to download and run the software up to the **Select Installation Mode** window. It is up to you whether you get the computer information for the license files before or after installing the software.

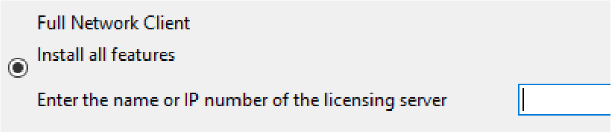
Choose the Installation Type and Enter the Computer Server Details

About the Thermo-Calc Installed Components

1. In the **Select Installation Mode** window click **Full Network Client** to **Install all features**.

> If you want to exclude a component (perhaps one of the SDKs), then use the **Custom** option and see Custom Network Client Installations.

2. In the field, enter the name or IP number of the computer where the licensing software is installed. Click **Next**.



Full Network Client

● Install all features

Enter the name or IP number of the licensing server

3. TC-Python is installed for all users even if you do not have a license. The **Install TC-Python** window is a reminder that additional installation procedures are required after Thermo-Calc is installed. See the *TC-Python Installation Guide* for details.
4. In the **Ready to Install** window click **Next**.
5. When the **Completing the Thermo-Calc Setup Wizard** window opens, click **Finish**. For *Linux* users, log out and log back in to start using Thermo-Calc.

> For macOS installations and if you have previous Thermo-Calc installations: When you launch Thermo-Calc with the new or updated version, the splash screen hides the **Import User Settings** dialog box. In order to proceed you need to click the splash screen and then click **Yes** or **No** in the dialog box.

If you did not get your Thermo-Calc license file see Request a License File from Thermo-Calc Software.

Windows: About Installing the License Manager

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

If you have previously installed an older version of Sentinel RMS License Manager, you must first uninstall the old version then **reboot** the server before starting with a new installation.

The Sentinel RMS License Manager service supplies the client computers in your network with license tokens when it runs Thermo-Calc software. The Sentinel RMS License Manager software is installed on a computer that acts as a license server in your network. This is related to Full Network Client Installations and administrative rights are required for all steps.

Remember to collect subnet information before beginning. See Subnet Information for Network Licenses.

A network license can only be used on one specific computer that hosts the License Manager. The network license determines which client computers receive license tokens using the IP addresses and IP ranges.

Supported Windows Versions

These Windows operating systems are supported for the installation of Sentinel RMS License Manager. When ready, go to Windows: Installing the Sentinel RMS License Manager.

For macOS, the Sentinel RMS License software is installed on a Windows or Linux computer server where the Thermo-Calc license file must also be located.

Windows 32-bit Operating Systems

- Windows 7
- Windows 8.1
- Windows 10 v1909
- Windows Server 2008

Windows 64-bit Operating Systems

- Windows 7
- Windows 8.1
- Windows 10 v1909
- Windows Server 2008
- Windows Server 2008 R2
- Windows Server 2012
- Windows Server 2012 R2
- Windows Server 2016
- Windows Server 2019

Windows: Installing the Sentinel RMS License Manager

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

First review Windows: About Installing the License Manager. Then if this is a new installation of the Sentinel RMS License Manager, start with Step 2.

Uninstall Any Older Versions of Sentinel RMS License Manager

1. With Administrator rights, log onto the server that hosts the Sentinel RMS License Manager.
2. Save a copy of the license file LSERVRC found in the default directory—the license file can be saved as a text file: `C:\Program Files (x86)\Common Files\SafeNetSentinel\Sentinel RMS License Manager\WinNT\`.

   After saving the existing license file and uninstalling the old version of Sentinel RMS, ensure you delete the old license file (LSERVRC) in the above folder. This license is not required anymore.

3. Reboot the computer hosting the Sentinel RMS License Manager.
4. Continue with the installation and use the preselected default settings.

Download and Install Thermo-Calc

This step is not required to complete the server installation, however some administrators may want to do it at this point.

1. Download Thermo-Calc.

- *Web downloads*: For web links sent in an email from Thermo-Calc Software, go to the URL and log in with the information provided to download the software.
- *DVD installations*: Insert the DVD and follow the instructions.

2. Install Thermo-Calc. For testing purposes, and in order to confirm the installation is working correctly, install the Thermo-Calc software on the same computer as the Sentinel RMS License Manager. If required after testing, Thermo-Calc can always be uninstalled.

Install the Sentinel RMS License Manager Software

1. From the download, extract the files `license_server_win_9.7.zip` and `LS_tools_win.zip`.
2. Right-click `setup.exe` and select **Run as Administrator** from the menu.

Choose the Installation Directory

1. Click to accept the license agreement.
2. Enter your **User Name** and **Organization** and select to install the License Manager for **All users**.
3. In the **Destination Folder** window click **Next** to accept the suggested destination directory or **Change** to select another directory.

Choose the Setup Type and Install the Software

1. In the **Setup Type** window, select **Complete**. Click **Next**.
2. Select the **Unblock the system firewall for the Sentinel RMS License Manager** checkbox.

> Selecting the checkbox is required to run Thermo-Calc.

3. Click **Next** and then **Install**.
4. Click **Finish** to exit the InstallShield Wizard.

Install the Thermo-Calc Network License Using WlAdmin

Only the WlAdmin tool can be used to update the network license used by the License Manager.

1. Save the source file containing the license code. The source file can be kept as a .txt file
2. Go to the previously saved file `LS_tools_win.zip`.
3. Right-click the file `WlmAdmin.exe` and select **Run as Administrator** from the menu.
4. If the license server is not found under subnet servers, go to **Edit → Defined Server List**.
5. Enter the host name or IP address of the license server.
6. Click **Add** and then **OK**.
7. Click **View → Refresh All** to update the list.
8. In the left main window right-click the name of a License Manager.
9. From the menu select **Add Feature → From a File → To Server and its File**.
10. To add the license from a file, select **From a File**. This permanently adds the license code to the License Manager license file as well as to the License Manager memory.
11. In the windows that open, browse to the source file that contains the license code and click **Open**.

Install Additional Tool Options

Sentinel RMS License 9.7 Tools

Linux: About Installing the License Server

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

The Sentinel RMS License Server service supplies the client computers in your network with license tokens when it runs Thermo-Calc software. The Sentinel RMS License Server software is installed on a computer that acts as a license server in your network. This is related to Full Network Client Installations.

Preparing for Installation

Read and be aware of the following before you begin the section Linux: Installing the Sentinel RMS License Server.

Remember to collect subnet information before beginning. See Subnet Information for Network Licenses.

Uninstall Older Versions of the License Server

- Older versions of the License Server must be stopped by with `lsrvdown` before running the new installation. This is Step 1 in Linux: Installing the Sentinel RMS License Server.
- If you have a license server: Upgrade your license server if the new one is a higher version than the present one. Clients work with newer license servers (managers) but not necessarily with ones older than the client.

Requires Root Access or sudoers List

Root access to your computer is required or you need to be on the `sudoers` list.

Linux 32-bit Installations on a 64-bit OS

To run a license server 32-bit on a Linux 64-bit OS, 32-bit library support is needed.

Thermo-Calc License File

The name of the **license file** must be in lower case letters (**lservrc**) because Linux commands and operations are case-sensitive.

- You need a valid **lservrc** network license file supplied by Thermo-Calc Software (Requesting the License File for Windows or Linux) as well as the actual License Server—a file (program) called **lserv**.
- The Thermo-Calc license file needs to be readable and writable by the license server (license manager).

Differences Between 32- and 64-bit Scripts

Sentinel RMS License Server version 9.7 supports both 32- and 64-bit. However, when writing scripts be aware of script naming and do not mix the scripts.

- All 32-bit scripts are named *<script_name>*, for example `restart_lserv`
- All 64-bit scripts are named *<script_name>64*, for example, `restart_lserv64`

It is not possible to use Linux 32-bit scripts/tools to manage license server 64-bit and vice versa, you cannot use Linux 64-bit scripts/tools to manage license server 32-bit

openSUSE Administration (sudo) Users

Note the following if you are a sudo user (administrator) in openSUSE installing Thermo-Calc using this command:

```
sudo ./Thermo-Calc-linux-<full-version-number>.run
```

When this command is used, you will do a text-based installation instead of having a graphical interface to guide you. The information is the same, just without the user interface.

For example, the *<full-version-number>* is not just 2025b, it is what is found in the **Help → About** window in Thermo-Calc and it changes every release. You can find the current full version number listed on our website.

Supported Linux Operating Systems and Versions

For macOS, the Sentinel RMS License software is installed on a Windows or Linux computer server where the Thermo-Calc license file must also be located.

Both Linux 32-bit and 64-bit operating systems are supported for the installation of Sentinel RMS License Server.

- Red Hat Enterprise Linux (RHEL) 7.x
- Red Hat Enterprise Linux (RHEL) 8.x
- SUSE Linux Enterprise Server (SLES)12.x
- SUSE Linux Enterprise Server (SLES) 15.x
- Debian Linux 9.x
- Debian Linux 10.x
- Ubuntu Linux 16.x (LTS)
- Ubuntu Linux 18.x (LTS)
- Ubuntu Linux 20.x (LTS)
- OpenSUSE Leap 42.x
- OpenSUSE Leap 15.x

Linux: Installing the Sentinel RMS License Server

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

First review Linux: About Installing the License Server. Then if this is a new installation of the Sentinel RMS License Server, start with Step 2.

Sentinel RMS License Server version 9.7 supports both 32- and 64-bit. However, when writing scripts be aware of script naming and do not mix the scripts.

- All 32-bit scripts are named <*script_name*>, for example `restart_lserv`
- All 64-bit scripts are named <*script_name*>*64*, for example, `restart_lserv64`

It is not possible to use Linux 32-bit scripts/tools to manage license server 64-bit and vice versa, you cannot use Linux 64-bit scripts/tools to manage license server 32-bit

Stop Older Versions of the Sentinel RMS License Server

1. To stop an old version of the License Server already running, go to the directory where the old file is found, and enter the commands:
   - 32-bit license server

     ```
     >chmod +x <lsrvdown>
     >./lsrvdown <host_name>
     ```

   - 64-bit license server

     ```
     >chmod +x <lsrvdown64>
     >./lsrvdown64 <host_name>
     ```

2. Edit existing scripts that start the older version of the License Server so that they start the newer version instead.

   For more information about the **lservdown utility**, go to https://docs.sentinel.thalesgroup.com/softwareandservices/rms/

Write a Script to Start the License Server

The following is an excerpt from the template script for starting the License Server found in the restart_lserv file.

Replace the paths for LICENSE_SERVER_DIR, LICENSE_FILE_DIR and LOG_DIR to match your system. Save it as a script:

```
# set the directory where the executables are located

LICENSE_SERVER_DIR=/usr/local/Thermo-Calc/2025b/Licensing-files

# set the directory of the license file lservrc

LICENSE_FILE_DIR=/usr/local/Thermo-Calc/2025b/Licensing-files

# set the directory where you wish to save the log-files

LOG_DIR=/tmp

# stop the running server

# (omit this line if calling this script at startup)

$LICENSE_SERVER_DIR/lsrvdown $HOSTNAME

# start the license server

$LICENSE_SERVER_DIR/lserv -s $LICENSE_FILE_DIR/lservrc -l $LOG_DIR/lserv_use.log
-f $LOG_DIR/lserv_err.log
```

Confirm the HOSTNAME variable and open the UDP port

The hostname should always correspond to the DNS record verify this by doing the following.

1. Before starting the License Server make sure that the value of the $HOSTNAME variable is correct. This value can be shown by typing the `> nslookup $HOSTNAME` command in the terminal window:

   The value should be the same IP address that is shown when you use the ifconfig command.

2. Open the UDP port 5093 in your firewall. In case you have installed SELinux you might also need to disable it by setting `SELINUX=permissive` in the `/etc/selinux/config` file.

Start the License Server

1. To start the License Server, run the script created as root. Enter these commands in the console:

```
> chmod +x <name_of_script_file>
> ./<name_of_script_file>
```

2. If you want the License Server to start when you boot the system, put a copy of the start script under `/etc/rc.d/init.d` and start the script from the file `/etc/rc.d/rc.local`.

Install Additional Tool Options

Sentinel RMS License 9.7 Tools

Thin Client Installations

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

This topic describes how you install a thin Thermo-Calc client to run Thermo-Calc from a file server. It is applicable to consolidated and distributed network installations for either a Windows or Linux operating system.

Installation Requirements

- You need access to the directory where Thermo-Calc is installed on the file server.
- You need the IP number or name of the computer where the license file is installed.
- For *Linux* you may have to disable your firewall. If SELinux is installed, try disabling it by setting `SELINUX=permissive` in `/etc/selinux/config`.

Windows Installations

The following details may also be of use to those installing in a Windows environment.

- Requests license server name or address and sets LSHOST as a user environment variable accordingly.
- Sets TC*<version>*_HOME (where *<version>* is the software version, e.g. TC22A_HOME) as a user environment variable to point to the location from which the thin client installer is running.

The default folders where documents, materials files, examples, and other folders that sometimes require additional licenses are installed under **Public Documents** for ALL USERS. See Installation Default Directory: Windows.

How to Install a Thin Client on Windows

1. Map the file server share as a network drive so that it gets an assigned drive letter (e.g. **E:**).
2. Open the **\Thermo-Calc**<*version*>\ directory on the file server, where *version* is the current version of the software.
3. Open the directory **Thin-client**. Double-click the `Thermo-Calc-client-windows-<version>.exe` file.
4. Click to accept the terms of the license agreement. Click **Next**.
5. Enter the name or IP number of where the license file and the License Manager software is installed. Click **Next**.
6. By default the **Create Shortcuts on Desktop** checkbox is selected. Click **Next**.

> The shortcuts to the program are added to the user's Windows roaming profile as well as placed on the user's Desktop (not the system's).

7. In the **Ready to Install** window, click **Next**.
8. Click **Finish**. To start Thermo-Calc find the program on the server and start it from there.

How to Install a Thin Client on Linux

1. Add the following to the `smb.conf` file, where *<user>* is your user name:

```
[public]
path=/home/<user>/Thermo_Calc/2025b
public=yes
writable=yes
comment=smb share
guest OK=yes
force user=<user>
```

2. From the client, mount the directory on the server computer that contains the Thermo-Calc server installation (by default, this directory is called **/Thermo-Calc/2025b**). How the directory is mounted depends on the Linux distribution being used as well as how the Thermo-Calc directory on the server computer is shared. Use the Linux command `mount`. For example:

   ```
   > mkdir public
   ```

   ```
   > sudo mount -t cifs //ip_number_server_computer/public ./public -o
   user=<user>
   ```

3. Open the mounted directory on your computer, and run `client-install-linux-x64.run` or `client-install-linux-x86.run` in the **/Thin-client** directory.
4. If you do this from the terminal window, use the following to start the installation (assuming that the file server is a 64-bit computer):

   > ./client-install-linux-x64.run

5. Click **Forward** and click to select the license agreement. Click **Forward**.
6. Enter the name or IP number of the License Server. Click **Forward**.
7. If you are installing as a non-root user, by default, the **Create Shortcuts on Desktop** checkbox is selected. Click **Forward**.
8. In the **Ready to Install** window click Forward.
9. Click **Finish**. Log out and log back in to start using Thermo-Calc.

Custom Network Client Installations

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

This installation type is available for all operating systems, however for macOS the License Server must be run on a Windows or Linux computer.The requirements are the same as for a full client installation.

Install the Licensing Software

Follow the instructions for your operating system:

- Windows: About Installing the License Manager, or
- Linux: About Installing the License Server

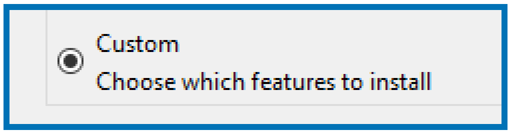
Complete Steps 1 to 4 of a Full Standalone Installation

Follow the instructions for Full Standalone Installations to download and run the software. It is up to you whether you get the computer information for the license files before or after installing the software.

Select the Installation Mode and the Components to Include or Exclude

About the Thermo-Calc Installed Components

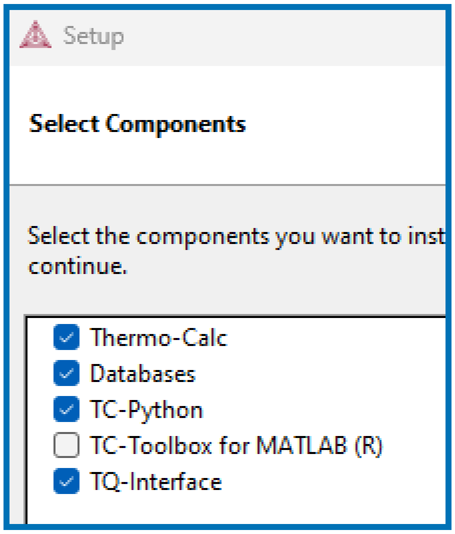
1. In the **Select License and Installation Mode** window click **Custom**. Click **Next**.



● Custom
Choose which features to install

2. On the **Specify Configuration** window the **Create Shortcut on Desktop** checkbox is selected by default. Click **Next**.

3. In the **Select Components** window, click to select or deselect the checkboxes as needed. Click **Next**.



Setup

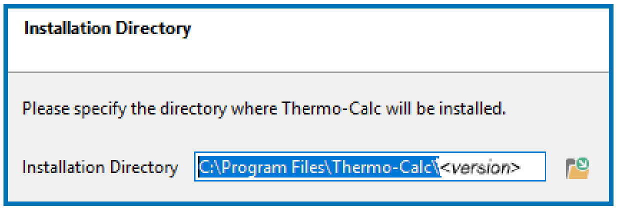
Select Components

Select the components you want to inst
continue.

- ☑ Thermo-Calc
- ☑ Databases
- ☑ TC-Python
- ☐ TC-Toolbox for MATLAB (R)
- ☑ TQ-Interface

Set the Installation Directory and the File Path to the License

1. In the **Installation Directory** window, either accept the default path or enter a path to where you want to install the software (see Installation Default Directories and the License File). Click the file button to **Browse for Folder** and navigate to another directory. Click **Next**.



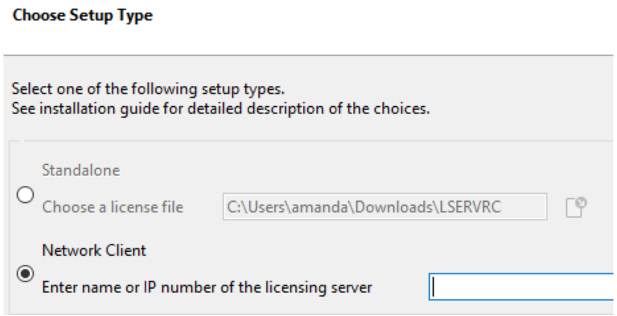
Installation Directory

Please specify the directory where Thermo-Calc will be installed.

Installation Directory: C:\Program Files\Thermo-Calc\<version>

To prevent errors, leave this field blank if you do not have a license file yet.

2. In the **Choose Setup Type** window, click **Network Client** and enter the name or IP number of the computer where the licensing software is installed. Click **Next**.



Choose Setup Type

Select one of the following setup types.
See installation guide for detailed description of the choices.

○ Standalone
Choose a license file: C:\Users\amanda\Downloads\LSERVRC

● Network Client
Enter name or IP number of the licensing server

> If you have selected to install **TC-Python** there is a reminder window that additional installation procedures are required after Thermo-Calc is installed. See the *TC-Python Installation Guide*.

Install the Software and Start Using Thermo-Calc

1. In the **Ready to Install** window click **Next**.

   See the separate instructions for TC-Toolbox for MATLAB®.

2. Click **Finish** and start using Thermo-Calc. For Linux users, log out and log back in to finish the installation.

> For macOS installations and if you have previous Thermo-Calc installations: When you launch Thermo-Calc with the new or updated version, the splash screen hides the **Import User Settings** dialog box. In order to proceed you need to click the splash screen and then click **Yes** or **No** in the dialog box.

If you did not get your license file see Request a License File from Thermo-Calc Software.

Unattended or Silent Network Client Installations (License File)

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

Terminology note: The use of the term *license server* (lower case letters) is applicable to the option files as described in this section. For the purposes of the step-by-step instructions it is not used to refer to the type of network installation that runs the licensing software.

Sometimes it is convenient to install Thermo-Calc network clients without providing user input after the installation is initiated (an unattended network client installation), i.e. a *silent installation*. This is available for Windows and Linux operating systems.

Make sure you know the name or IP number of the computer where the licensing software and the license file are to be installed.

Create an Option File in a Text Editor to Enter the Options

The following is an example of an option file for a custom network client installation, where *<name/IP number>* is the name or IP number of the computer where the license file is installed:

```
installation_mode=custom

setup_type=client

enable-components=thermo,databases,tq,toolbox,tcpython

icons=1

license_server=<name/IP number>
```

Below is a shorter example, specifying that a full Thermo-Calc network client should be installed:

```
installation_mode=full_client

license_server=<name/IP number>
```

Go to the Directory Where the Installation File is Saved

Thermo-Calc can only be installed in unattended mode from the command line prompt.

Start the installation in unattended mode using the option file created with this command:

- Windows: `<installationfile>.exe --mode unattended --optionfile <path\optionfile>`
- Linux: `<installationfile>.run --mode unattended --optionfile <path/optionfile>`

To see other options when you start the Thermo-Calc installation program from the command line prompt, run this command:

- Windows: `<installationfile>.exe --help`
- Linux: `<installationfile>.run --help`

TC-Python Installation Guide

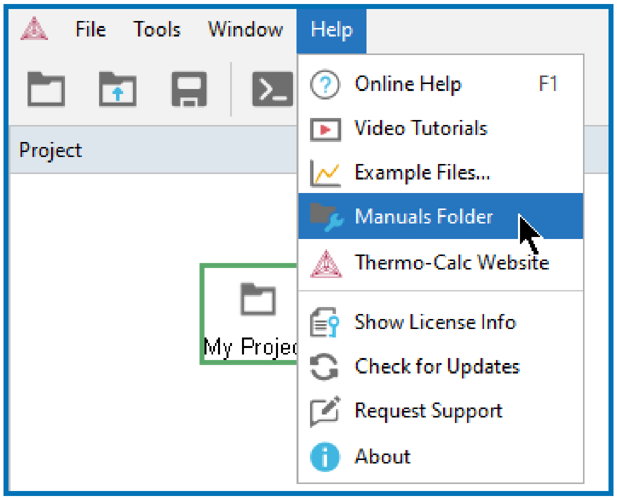
In this section:

About the TC-Python Documentation

The TC-Python help is available on the Thermo-Calc website where you can also access additional resources. You can alternatively access the locally installed documentation from the **Help** menu in Thermo-Calc.

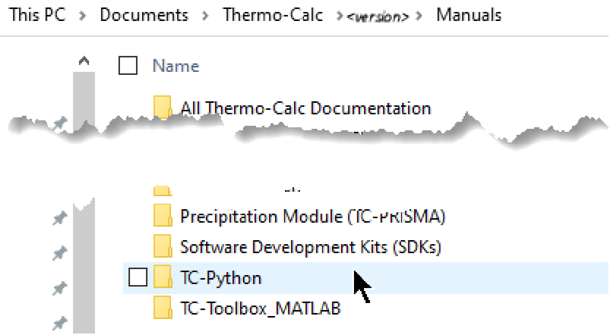
Opening the Locally Installed Documentation

1. In Thermo-Calc from the menu, select **Help → Manuals Folder**.

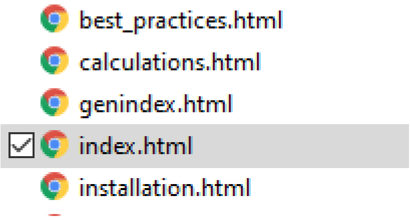


You can also navigate to the **Manuals** folder outside of Thermo-Calc and based on your operating system installation location.

2. In the window that opens, double-click to open the **TC-Python** folder.



3. Double-click the **Index** HTML file (or any of the HTML files).



4. The API reference documentation opens as a searchable HTML file in your local browser.

Which TC-Python Installation Should I Choose?

A license is required to run TC-Python. Also remember to review the System Requirements page on our website.

There are these options to install TC-Python.

See the Videos about TC-Python page for additional learning resources.

Install with the Bundled Python-interpreter

This is a straightforward installation where TC-Python is preinstalled together with some popular Python packages.

This is the recommended option for new users to TC-Python who may only want to run the examples. The available preinstalled packages (e.g. numpy, scipy, scikit-learn, pyvista, and matplotlib) can also be sufficient for many advanced users.

Installing TC-Python with a Bundled Python-interpreter.

Optional Packages

Install with a Python-interpreter of Your Choice

This installation requires additional steps and is the recommended option for more advanced use and has full flexibility.

Installing TC-Python Into a Python-interpreter of Your Choice.

Installing TC-Python with a Bundled Python-interpreter

TC-Python can be installed using a Python-interpreter that is bundled to Thermo-Calc. This interpreter has TC-Python preinstalled together with some popular Python packages. This is the recommended option for new users to TC-Python who may only want to run the examples.

The bundled interpreter package is also used to run the Property Models in Thermo-Calc. Do not make changes to interpreter packages or this can stop Thermo-Calc from working correctly. To fix issues caused by changes to an interpreter, completely uninstall Thermo-Calc and start over, either with the bundled interpreter package or using interpreters of your choice.

If you are planning to do more advanced calculations that require other external packages then you may want to follow these instructions instead: Installing TC-Python Into a Python-interpreter of Your Choice

Limitations

The following examples cannot be run with the bundled Python-interpreter as additional packages are required: `pyex_M_01_Input_from_file.py` (pandas) and `pyex_M_02_Output_to_file.py` (pandas, lxml, h5py).

The bundled Python 3 interpreter contains the following major packages:

- colour-science
- matplotlib
- numpy
- scikit-learn
- scipy
- pandas

- pyvista
- TC-Python
- tmm

If you have recommendations for additional packages to include (see below), send an email to Thermo-Calc Support.

These TC-Python examples require additional packages that are not available in the bundled Python-interpreter, and thus cannot be run: `pyex_M_01_Input_from_file.py` and `pyex_M_02_Output_to_file.py`.

Install an IDE (Integrated Development Environment)

Any editor can be used to write the Python code, but an IDE is recommended, e.g. PyCharm. These instructions are based on the use of PyCharm.

Use of an IDE gives you access to code completion, which helps when you use the API as it gives you the available methods on the objects you are working with.

1. Navigate to the PyCharm website: https://www.jetbrains.com/pycharm/download.
2. Click to choose your OS and then click **Download**. You can use the **Community** version of Pycharm.
3. Follow the instructions. It is recommended you keep all the defaults.

For Mac installations, you also need to set some environment variables as described below in macOS: Setting Environment Variables.

Configure PyCharm to Use the Bundled Python-interpreter

Open PyCharm and configure the interpreter:

1. Go the menu **File → Settings**.
2. Navigate in the tree to **Project: YourProjectName** and choose **Project Interpreter**.
3. Click on the settings symbol close to the **Project Interpreter** dropdown menu and choose **Add**.
4. Select **System Interpreter** and add the bundled Thermo-Calc Python 3 interpreter, which is located in a folder based on the operating system:

Operating system	*Path to the bundled Python-interpreter*
Windows	`C:\Program Files\Thermo-Calc\2025b\python\python.exe`
Linux	`/home/UserName/Thermo-Calc/2025b/python/bin/python3`
macOS	`/Applications/Thermo-Calc-2025b.app/Contents/Resources/python/bin/python3`

5. Select the interpreter and confirm.

Run a TC-Python Example

It is recommended that you open one or more of the included examples to both check that the installation has worked and to start familiarizing yourself with the code.

If you have a license activation type based on **user credentials** you first need to activate your license. See License Activation with User Credentials.

Open the TC-Python Project in PyCharm

When you first open the TC-Python project and examples, it can take a few moments for the Pycharm IDE to index before some of the options are available.

1. Open PyCharm and then choose **File** → **Open**. The first time you open the project you will need to navigate to the path of the TC-Python installation based on your operating system.

Operating system	*Path to the TC-Python folder*
Windows	`C:\Users\UserName\Documents\Thermo-Calc\2025b\SDK\TC-Python`
Linux	`/home/UserName/Thermo-Calc/2025b/SDK/TC-Python`
macOS	`/Users/Shared/Thermo-Calc/2025b/SDK/TC-Python`

2. Click the **Examples** folder and then click **OK**.
3. From any subfolder:
    - Double-click to open an example file to examine the code.
    - Right-click an example and choose **Run**.

If you are not following the recommended approach and create a *new* project (**File → New Project…**), you need to consider that by default the options to choose the interpreter are hidden within the **Create Project** window. For this, click **Project Interpreter: New Virtual Environment** and in most cases choose your *System Interpreter* containing the Python bundled to Thermo-Calc instead of the default *New Virtual Environment*.

Installing TC-Python Into a Python-interpreter of Your Choice

TC-Python can be installed using a Python-interpreter of your choice. This is the recommended option for any more advanced usage and provides full flexibility.

> If you are new to TC-Python and want to mainly run the examples, then it is recommended you install the bundled Python-interpreter. The available preinstalled packages (e.g. numpy, scipy, scikit-learn, pyvista, and matplotlib) can also be sufficient for many advanced users. See Installing TC-Python with a Bundled Python-interpreter.

Install a Python Distribution

> If you already have a Python distribution installation, version 3.8 or newer, skip this step.

These instructions are based on using the Anaconda platform for the Python distribution. Install version 3.8 or newer to be able to work with TC-Python, although it is recommended that you use the most recent version.

INSTALL ANACONDA

1. Navigate to the Anaconda website: https://www.anaconda.com/download/.
2. Click to choose your OS (operating system) and then click **Download**. Follow the instructions. It is recommended you keep all the defaults.

Install Thermo-Calc and the TC-Python SDK

1. Install Thermo-Calc.
2. When the installation is complete, open the TC-Python folder that includes the *.whl file needed for the next step. There is also an **Examples** folder with Python files you can use in the IDE to understand and work with TC-Python.

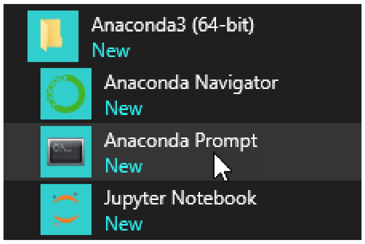
Install TC-Python

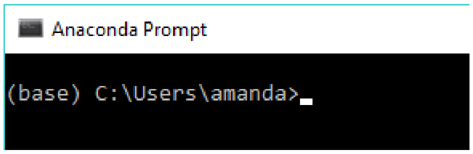
Updating to a Newer Version

On Windows, it is recommended you use the Anaconda distribution prompt (i.e. Anaconda), especially if you have other Python installations.

> Do not use Virtual Environments unless you have a good reason to do so. Also see Fixing Potential Issues with the Environment.

1. Open the command line. For example, in Anaconda on a Windows OS, go to **Start → Anaconda → Anaconda Prompt**.





```
(base) C:\Users\amanda>_
```

2. At the command line, enter the following. Make sure there are no spaces at the end of the string or in the folder name or it will not run:

```
pip install <path to the TC-Python folder>/TC_Python-<version>-
py3-none-any.whl
```

> On Linux, and depending on the interpreter, *pip3* is typically used.

Operating system	***Path to the TC-Python folder***
Windows	`C:\Users\UserName\Documents\Thermo-Calc\2025b\SDK\TC-Python`

Operating system	*Path to the TC-Python folder*
Linux	`/home/UserName/Thermo-Calc/2025b/SDK/TC-Python`
macOS	`/Users/Shared/Thermo-Calc/2025b/SDK/TC-Python`

3. Press <Enter>. When the process is completed, there is a confirmation that TC-Python is installed.

> If your computer is located behind a proxy-server, the default pip-command will fail with a network connection error. In that case you need to install the dependency py4j in a special configuration:

```
pip install -proxy user:password@proxy_ip:port py4j jproperties
```

Go to the TC-Python Help **Troubleshooting** section for detailed information. This can be found on our website or from the installed documentation where you can search for "pip install fails" with “Failed to establish a new network connection” or similar.

Install an IDE (Integrated Development Environment)

Any editor can be used to write the Python code, but an IDE is recommended, e.g. PyCharm. These instructions are based on the use of PyCharm.

Use of an IDE gives you access to code completion, which helps when you use the API as it gives you the available methods on the objects you are working with.

1. Navigate to the PyCharm website: https://www.jetbrains.com/pycharm/download.
2. Click to choose your OS and then click **Download**. You can use the **Community** version of Pycharm.
3. Follow the instructions. It is recommended you keep all the defaults.

> For Mac installations, you also need to set some environment variables as described below in macOS: Setting Environment Variables.

Open the IDE and Run a TC-Python Example

After you complete all the software installations and set up the pip install path, you are ready to open the IDE to start working with TC-Python.

It is recommended that you open one or more of the included examples to both check that the installation has worked and to start familiarizing yourself with the code.

> If you have a license activation type based on **user credentials** you first need to activate your license. See License Activation with User Credentials.

Open the TC-Python Project in PyCharm

> When you first open the TC-Python project and examples, it can take a few moments for the Pycharm IDE to index before some of the options are available.

1. Open PyCharm and then choose **File** → **Open**. The first time you open the project you will need to navigate to the path of the TC-Python installation based on your operating system.

Operating system	*Path to the TC-Python folder*
Windows	`C:\Users\UserName\Documents\Thermo-Calc\2025b\SDK\TC-Python`
Linux	`/home/UserName/Thermo-Calc/2025b/SDK/TC-Python`
macOS	`/Users/Shared/Thermo-Calc/2025b/SDK/TC-Python`

2. Click the **Examples** folder and then click **OK**.
3. From any subfolder:
   - Double-click to open an example file to examine the code.
   - Right-click an example and choose **Run**.

Also see Optional Packages if you are using the Additive Manufacturing Module for simulations.

Installation Default Directory: TC-Python

These are the default paths to the TC-Python folder based on your operating system.

Operating system	*Path to the TC-Python folder*
Windows	`C:\Users\UserName\Documents\Thermo-Calc\2025b\SDK\TC-Python`
Linux	`/home/UserName/Thermo-Calc/2025b/SDK/TC-Python`
macOS	`/Users/Shared/Thermo-Calc/2025b/SDK/TC-Python`

For a bundled Python-interpreter installation, these are the paths to this location based on your operating system.

Operating system	*Path to the bundled Python-interpreter*
Windows	`C:\Program Files\Thermo-Calc\2025b\python\python.exe`
Linux	`/home/UserName/Thermo-Calc/2025b/python/bin/python3`
macOS	`/Applications/Thermo-Calc-2025b.app/Contents/Resources/python/bin/python3`

macOS: Setting Environment Variables

In order to use TC-Python on macOS you need to set some environment variables.

```
TC25B_HOME=/Applications/Thermo-Calc-2025b.app/Contents/Resources
```

User Credentials License Activations

```
TC_LICENSE_SPRING=y
```

License File Type Activations

If you use a license server:

```
LSHOST=<name-of-the-license-server>
```

If you have a node-locked license:

```
LSHOST= NO-NET
LSERVRC=/Users/Shared/Thermo-Calc/lservrc
```

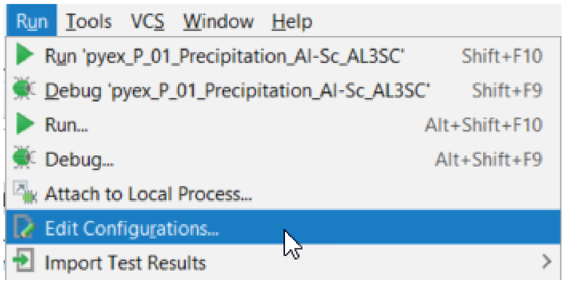
PyCharm IDEs

In PyCharm, you can add environment variables in the configurations.

Select **Run** → **Edit Configurations** to open the **Run/Debug Configurations** window. Enter the environment variable(s) by clicking the button to the right of the **Environment Variables** text field. Now the environment variables(s) will be set for each new configuration by default.

Existing configurations need to be removed and recreated to obtain the environment variables in them.

The same way for configuring the environment variables can be used on other operating systems as if necessary.



Fixing Potential Issues with the Environment

In most cases you should run TC-Python within your **global** Python 3 interpreter and not use Virtual Environments unless you have a good reason to do so.

If there are problems with the interpreter settings, for example, a common problem when you first use TC-Python is the message *No module named tc_python*, which you can resolve in the Settings window as follows:

1. Go the menu **File → Settings**.
2. Navigate in the tree to *<Project.YourProjectName>* and choose **Project Interpreter**.
3. Click on the settings symbol close to the **Project Interpreter** drop-down menu and choose **Add**.
4. Now choose **System Interpreter** and add your existing Python 3 interpreter.
5. Select your added interpreter and confirm.

If you are not following the recommended approach and create a *new* project (**File → New Project…**), you need to consider that by default the options to choose the interpreter are hidden within the **Create Project** window. For this, click **Project Interpreter: New Virtual Environment** and in most cases choose your *System Interpreter* containing the Python bundled to Thermo-Calc instead of the default *New Virtual Environment*.

If you really need to use a Virtual Environment, it is recommended you review the hints provided in the **Best Practices** section in the full TC-Python HTML help or PDF.

Optional Packages

Plotting results of Additive Manufacturing simulations requires the package *pyvista*. It is automatically installed if using the option *[am-plotting]* during the installation:

```
pip install <path to the TC-Python folder>/TC_Python-<version>-py3-none-any.
whl[am-plotting]
```

The bundled interpreter contains *pyvista* by default.

TC-Python: Configuring a License

TC-Python requires a license to run. If you do not yet have the information about your license, contact Thermo-Calc Support at support@thermocalc.com.

> ⓘ If you have no valid license, an exception is thrown that states: `NO LICENSE: No activated license for TC-Python.`

Depending on the type of license, different steps are required to configure TC-Python to use it.

Environment Variables

Some environment variables need to be set. On Windows this is normally done during the installation of Thermo-Calc, but on Linux and macOS this needs to be performed for each used IDE or terminal.

? TC-Python: Setting Environment Variables

License Activation with User Credentials

This section is applicable to licenses that are activated after entering user credentials (i.e. user name and password).

> ⓘ The TC-Python license is a separate license from the Thermo-Calc software license. You need to activate the TC-Python license once on your computer after, or in addition to, activating the Thermo-Calc license.

It is recommended to run the included example to perform the activation and deactivation. By default an online activation is performed, but you can choose other methods, which are both included in the example and described in the API documentation.

- Open and run the example `pyex_M_04_license.py`, which is located in the **Miscellaneous** folder.
- The license activation is completed with the methods in the class `tc_python.license.LicenseManager`.
- Depending on the type of license other methods are available, for example for online and offline activation plus the use of proxy settings are described.

Once the license is activated, either by using online or offline activation methods, you can view the license status and information in Thermo-Calc. Select **Help → Show License Info** from the menu.

To use the license on a different computer, the license must first be deactivated on the original computer. This is for both online and offline activations.

TC-Python: Setting Environment Variables

macOS and Linux

In order to use TC-Python on macOS and Linux you need to set some environment variables.

```
TC25B_HOME=/Applications/Thermo-Calc-2025b.app/Contents/Resources
```

User Credential License Types

If you have a license based on user credentials:

```
TC_LICENSE_SPRING=y
```

License File Type Activations

If you use a license server:

```
LSHOST=<name-of-the-license-server>
```

If you have a node-locked license:

```
LSHOST=NO-NET
LSERVRC=/Users/Shared/Thermo-Calc/lservrc
```

If running in the terminal these can be set using export `LSHOST=NO-NET`, etc.

PyCharm IDEs

In PyCharm, you can add environment variables in the configurations.

> For other operating systems, the configuration can be done in the same way as described below.

1. Select **Run → Edit Configurations** to open the **Run/Debug Configurations** window.
2. Choose **Templates** and then **Python**.
3. Enter the environment variable(s) by clicking the button to the right of the **Environment Variables** text field. Now the environment variables(s) are set for each new configuration by default.

Existing configurations need to be removed and recreated to obtain the environment variables in them.

Updating to a Newer Version

If you are using the bundled Python-interpreter automatically installed with Thermo-Calc, these steps are not required.

These steps are required if you have previously followed the instructions in Installing TC-Python Into a Python-interpreter of Your Choice.

When updating to a newer version of Thermo-Calc, you always need to also install the latest version of TC-Python. It is not sufficient to run the installer of Thermo-Calc (except for bundled versions of the Python interpreter).

```
pip install <path to the TC-Python folder>/TC_Python-<version>-py3-none-any.whl
```

In case of problems you may wish to uninstall the previous version of TC-Python in advance:

```
pip uninstall TC-Python
```

```
pip install <path to the TC-Python folder>/TC_Python-<version>-py3-none-any.whl
```

However, this should not normally be required.

On Linux typically *pip3* is used.

You can check the currently installed version of TC-Python by running:

```
pip show TC-Python
```

TC-Python Diagnostic Script

A diagnostic script is available to help you if you have problems running TC-Python.

It is important to run the diagnostic script EXACTLY the same way as you run your TC-Python script (in the same IDE, same project, same Python environment, same Jupyter notebook, etc).

The script automatically prints useful suggestions that, in many cases, will help you to fix the problem yourself. If you are unable to solve the problem, contact us for support. You can find the script in these locations:

- Miscellaneous example (diagnostics.py)
- In the **Troubleshooting** section of the *TC-Python API Reference Documentation*. Also refer to the **Best Practices** in the same guide to see if there are any other solutions or tips.
- On our website.

TC-Toolbox for MATLAB® Installation Guide

In this section:

About TC-Toolbox for MATLAB®

TC-Toolbox for MATLAB® (TC-Toolbox) provides an interface to the commonly used MATLAB® software for scientific and engineering computing. This software development kit (SDK) is ideal for fast realization of ideas and visualization of results during research and development activities. The TC-Toolbox API includes calculation types available in Thermo-Calc such as single point equilibrium, property (step) and phase (map) diagrams, Scheil solidification simulations, as well as all the general Thermo-Calc Property Models (e.g. yield strength, spinodal, driving force, etc.).

With the addition of licenses for the applicable software and databases, you can further maximize your integration with MATLAB® to include the capabilities of the Steel Model Library Property Models (e.g. bainite, pearlite, etc.), as well as access the range of functionality included with the Diffusion Module (DICTRA) and the Precipitation Module (TC-PRISMA). Generally, all the functionality available in Graphical Mode or via the TC-Python SDK is available.

TC-Toolbox for MATLAB® is available on Windows platforms.

A license is required to run TC-Toolbox for MATLAB® and MATLAB® must also be installed on your computer prior to the TC-Toolbox installation. Also remember to review the System Requirements page on our website.

TC-Toolbox Documentation

There are various locations and formats of the documentation you need related to this SDK.

> The *TC-Toolbox for MATLAB® API Reference Documentation* is available from these general locations (1) within the MATLAB® environment—both as help and as part of the tab completion (2) directly on the Thermo-Calc website, and (3) locally in the Thermo-Calc installation (**Help>Manuals Folder**).

API Reference Documentation

The *TC-Toolbox for MATLAB® API Reference Documentation* is available either as interactive help (in HTML format or when in MATLAB® using tab completion or accessed via different menus or key combinations) or as a standalone PDF.

There are these ways to access the content:

- Directly in MATLAB® via the Help menu then under **Supplemental Software** click **TC-Toolbox**. Help is also available when writing code and using the tab completion feature and/or pressing different key combinations as described in the *Best Practices* section of the help.
- From the website: HTML Help or PDF
- Locally in a Thermo-Calc installation:
  - HTML: **Help > Manuals Folder > TC-Toolbox_MATLAB**, then click any HTML file.
  - PDF: **Help > Manuals Folder > Software Development Kits (SDKs)**, then double-click to open the *TC-Toolbox for MATLAB® API Programmer Guide*. This is a copy of the HTML API reference documentation.

Installation Instructions

The installation instructions are only included in the Thermo-Calc help (press F1), and in the PDF version of the main installation guide found, for example:

- On our website as part of the full Thermo-Calc Installation Guide.
- Once Thermo-Calc is installed:
  - Locally in a Thermo-Calc installation: **Help > Manuals Folder >Installation Guides**.
  - Press F1 in Thermo-Calc to search the help.

Thermo-Calc Help (Limited)

For TC-Toolbox, there is limited content included in the Thermo-Calc help (press F1 when in Thermo-Calc) because it is replaced by the *TC-Toolbox for MATLAB® API Reference Documentation*. The exception is installation instructions to describe how to install the SDK.

Installation Default Directory: TC-Toolbox and the Examples

The software component and the examples are installed as described below.

This is the default path to the installation folder for the TC-Toolbox component on Windows operating systems. Be aware that the initial *installation files and examples* are placed in **Public\Documents**, then after opening Thermo-Calc for the first time, these are copied to the **Documents** folder for each user. The *documentation* is installed elsewhere and as described in TC-Toolbox Documentation.

There are included examples with all TC-Toolbox installations. These are generally the same as the examples included with TC-Python although with a different suffix (`matex`) and prefix (*`.m` or *`.mlx`) in the file name. Not all examples included with TC-Python are available for this SDK. You can read summaries about the examples as described in the online help.

Path to the TC-Toolbox folder

Both the installation files AND the examples are installed in the following folders.

The default Windows folders where the TC-Toolbox examples are installed starts with the original installation placing these under **Public Documents** for ALL USERS.

For a local user, and after Thermo-Calc is opened for the first time, these files are copied to the user's **Documents** folder where this local copy is associated to the user login. The **Public Documents** folder always contains the original set of contents as per the installation.

```
C:\Users\Public\Public Documents\Thermo-Calc\<version>\SDK\TC-Toolbox-MATLAB
```

After installing Thermo-Calc, and when you first open the program, the set of folders containing the examples is copied from the source Public\Documents location into a user Documents folder:

```
C:\Users\<user>\Documents\Thermo-Calc\<version>\SDK\TC-Toolbox-MATLAB\Examples
```

It is recommended that you work with the files that are copied to the *user* folder.

Installing TC-Toolbox

There are automatic or manual installation instructions for TC-Toolbox for MATLAB®.

Automatic Installation of TC-Toolbox

When the following conditions are met, Thermo-Calc automatically installs the TC-Toolbox for MATLAB® component on your computer.

1. MATLAB® is already installed.
2. There is only one Windows user on the computer where TC-Toolbox is being installed.

> Administrator privileges are needed when you start the Thermo-Calc installer.

Then follow the regular installation instructions for Thermo-Calc, choosing whether you use a Standalone or Network installation. If required also see Testing a TC-Toolbox Installation.

> A reminder regarding the license. Although you do not need to have a license file during the installation process (it can be added after the fact), you do need to have purchased a license for TC-Toolbox for MATLAB® to run the program within MATLAB®.

Manual Installation of TC-Toolbox

The installation is not automatic if:

- There are multiple Windows users on the same machine, or
- The installer cannot find the directory path to the MATLAB installation.

Multiple Windows Users on Same Machine

If there are multiple windows users on the same machine, then the following manual steps are done at the end of the automatic installation.

1. A message at the end of the Thermo-Calc installation process displays with instructions.
2. An Explorer window automatically opens to the `C:\Users\Public\Documents\Thermo-Calc\2025b\SDK\TC-Toolbox-MATLAB` folder.
3. Double-click the `InstallTCToolboxMATLAB.cmd` file to finalize the process. This briefly launches MATLAB® and installs TC-Toolbox. If required see Testing a TC-Toolbox Installation.

Installer Cannot Find the MATLAB® Installation Directory

If the Thermo-Calc installer cannot find the MATLAB® installation directory,

1. Start the version of MATLAB® that you want to install TC-Toolbox in.
2. Open and run the MATLAB® script included with your installation of Thermo-Calc.

   For example on Windows, `C:\Users\<username>\Documents\Thermo-Calc\2025b\SDK\TC-Toolbox-MATLAB\setupTCToolbox.m`

> You can also follow the instructions for Installing TC-Toolbox with the Custom Option.

TC-Toolbox: Configuring a License

TC-Toolbox requires a license to run. If you do not yet have the information about your license, contact Thermo-Calc Support at support@thermocalc.com.

Depending on the type of license, an additional step is required to configure TC-Toolbox for MATLAB® to use it.

License Activation

This section is applicable to licenses that are activated after entering user credentials (i.e. user name and password).

The TC-Toolbox for MATLAB® license is a separate license from the Thermo-Calc software license. You need to activate the TC-Toolbox license once on your computer after, or in addition to, activating the Thermo-Calc license.

It is recommended to run the included example to perform the activation and deactivation. By default an online activation is performed, but you can choose other methods, which are both included in the example and described in the API documentation.

- Open and run the example `matex_M_04_license.m`, which is located in the **Miscellaneous** folder.
- The license activation is completed with the methods in the class `tc_toolbox.LicenseManager`.
- Depending on the type of license other methods are available, for example for online and offline activation plus the use of proxy settings are described.

Once the license is activated, either by using online or offline activation methods, you can view the license status and information in Thermo-Calc. Select **Help → Show License Info** from the menu.

To use the license on a different computer, the license must first be deactivated on the original computer. This is for both online and offline activations.

Installing TC-Toolbox with the Custom Option

MATLAB® must be installed before you install TC-Toolbox.

As described in Installing TC-Toolbox, if MATLAB® is already installed, then Thermo-Calc automatically installs the files you need either using the *Full Standalone* or *Full Network Client* installation where you **install all features**. Otherwise you need to use the **Custom** installation.

The following generally describes the **Custom** option for either a Standalone or Network installation. Use the **Custom** option if MATLAB® is installed but the Thermo-Calc installer is not finding the directory path so you need to enter the path manually.

Some steps are described in more detail in other parts of this guide.

Request your License File from Thermo-Calc Software

A reminder regarding the license. Although you do not need to have a license file during the installation process (it can be added after the fact), you do need to have purchased a license for TC-Toolbox for MATLAB® to run the program within MATLAB®.

Download your Thermo-Calc Installation Software

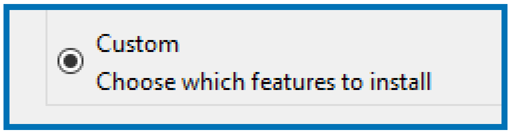
Install MATLAB®

Run the Thermo-Calc Installation File as an Administrator

1. Locate the Thermo-Calc installation file on your computer. Right-click the **.exe** file and choose **Run as administrator** to launch the **Setup** program.
2. Accept the **License Agreement** and click **Next**.

Select the Custom Installation Type

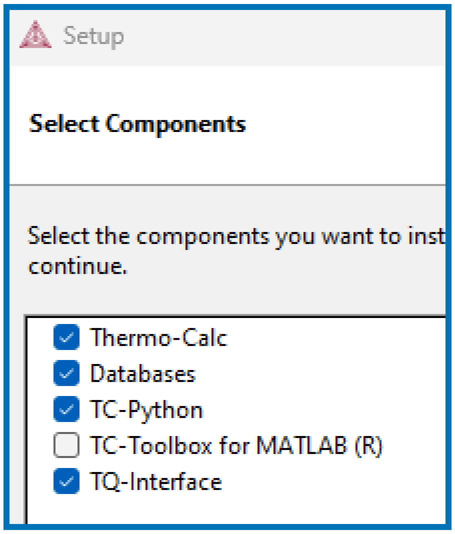
1. In the **Select Installation Mode** window click **Custom**. Click **Next**.



● Custom
Choose which features to install

2. On the **Specify Configuration** window the **Create Shortcut on Desktop** checkbox is selected by default. Click **Next**.

3. In the **Select Components** window, click to select the **TC-Toolbox for MATLAB** checkbox.



Setup

Select Components

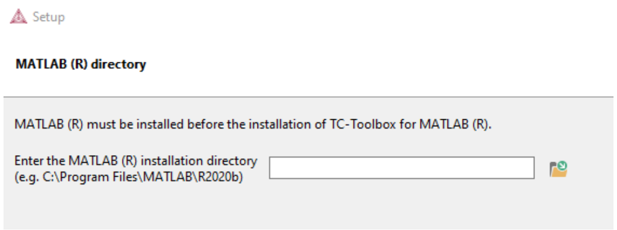
Select the components you want to inst
continue.

☑ Thermo-Calc
☑ Databases
☑ TC-Python
☐ TC-Toolbox for MATLAB (R)
☑ TQ-Interface

Remember, you must have MATLAB® already installed and may need to know the file path to the MATLAB® folder. If the **TC-Toolbox for MATLAB** checkbox is NOT selected, this confirms that the Thermo-Calc installer did NOT locate the MATLAB® installation (or it is not installed yet).

4. Click **Next**.

5. If you selected the **TC-Toolbox for MATLAB** checkbox, the **MATLAB directory** window opens.



MATLAB (R) directory

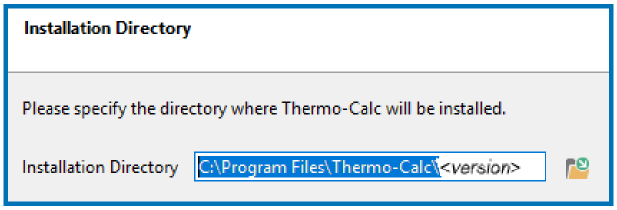
MATLAB (R) must be installed before the installation of TC-Toolbox for MATLAB (R).

Enter the MATLAB (R) installation directory
(e.g. C:\Program Files\MATLAB\R2020b)

- If MATLAB® is already installed but the Thermo-Calc installer could not find the path, then enter the file path to the MATLAB® installation directory or click the file button to **Browse for Folder** and navigate to the directory. Click **Next**.
- If MATLAB® is NOT installed, click **Cancel** to exit the Thermo-Calc installer program. Once MATLAB® is installed you can return to this process.

Set the Thermo-Calc Installation Directory and Choose the Setup Type

1. In the **Installation Directory** window, either accept the default path or enter a path to where you want to install the Thermo-Calc software. Click the file button to **Browse for Folder** and navigate to another directory.

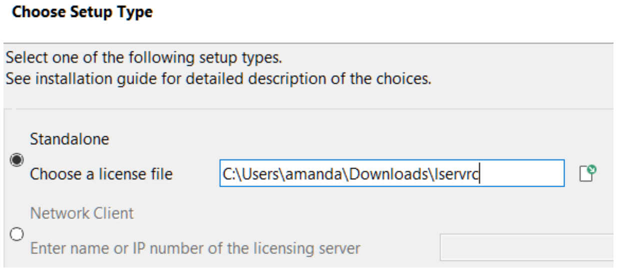


Installation Directory

Please specify the directory where Thermo-Calc will be installed.

Installation Directory C:\Program Files\Thermo-Calc\<version>

2. In the **Choose Setup Type** window, click **Standalone** or **Network Client**.



Choose Setup Type

Select one of the following setup types.
See installation guide for detailed description of the choices.

● Standalone
Choose a license file C:\Users\amanda\Downloads\lservrc

○ Network Client
Enter name or IP number of the licensing server

- For a Standalone installation: In the **Choose a license file** field enter the path to your license file (called **lservrc**).
- For a Network installation: Enter the details as required into the **Enter the name or IP number of the licensing server** field. Click **Next**.

> If the **TC-Python** checkbox is also selected to be installed (which it is by default), the **Install TC-Python** window is a reminder that additional installation procedures are required after Thermo-Calc is installed.

Install and Start Using Thermo-Calc as an Add-on in MATLAB®

1. In the **Ready to Install** window click **Next**.

> If MATLAB® is not installed (and you selected the TC-Toolbox checkbox) a message displays to confirm that TC-Toolbox will not be installed until you complete the MATLAB® installation. If MATLAB is installed, click **Back** to confirm that the installation path is correct, otherwise **Cancel** this Thermo-Calc installation, install MATLAB and start again.

2. Click **Finish**.

Test the Installation

Testing a TC-Toolbox Installation

Testing a TC-Toolbox Installation

Generally you can check the installation by first looking in the **Home** tab to see if the program is in the menu. Then proceed to running the diagnostic script or another example.

To check the installation, in MATLAB®:

1. From the **Add-Ons** menu, select **Manage Add-Ons**.

   If TC-Toolbox is in the list it is likely it installed correctly but it is recommended you run the diagnostic script or another example to confirm.

2. Run the diagnostics script from the folder `C:\Users\<user>\Documents\Thermo-Calc\2025b\SDK\TC-Toolbox-MATLAB\Examples\Miscellaneous` or open and run any other example to test.

   > The TC-Toolbox diagnostic script is also available from our website.

TC-Toolbox Installation Troubleshooting

Below are some suggestions to help troubleshoot a TC-Toolbox for MATLAB® installation.

Diagnostic Script

A diagnostic script is available to help you if you have problems running TC-Toolbox.

> ❗ It is important to run this script EXACTLY the same way as you run your MATLAB® script.

The script automatically prints useful suggestions that, in many cases, will help you to fix the problem yourself. If you are unable to solve the problem, contact us for support.

The script is based on the version of Thermo-Calc installed and named `tc-toolbox-diagnostic-script-2025b.m`. You can find the script in these locations:

- As an example (`diagnostics.m`) located in this folder `C:\Users\<user>\Documents\Thermo-Calc\2025b\SDK\TC-Toolbox-MATLAB\Examples\Miscellaneous`
- In the **Troubleshooting** section of the *TC-Toolbox for MATLAB® API Reference Documentation*. Also refer to the **Best Practices** in the same guide to see if there are any other solutions or tips.
- On our website.

MATLAB® Installation Directory Not Found

For Windows installations of the TC-Toolbox for MATLAB® component, you may get an error message or window asking for the MATLAB® installation directory path.

> The most common reason for this is that MATLAB® is not installed. If this is the case, exit the Thermo-Calc installation, install MATLAB® and then run the Thermo-Calc installation program again.

If MATLAB® is installed and Thermo-Calc just did not find the file path during the installation setup process, then enter the path in the field when prompted.

Determining the Licensing Software Version (Network Installs)

Sometimes you may need to know the version of License Manager (Windows) or License Server (Linux) software being used. This can be useful while troubleshooting network installations.

- On *Windows* open a command prompt and go to the directory where `lservnt.exe` is found. For example:

  ```
  >C:\Program Files (x86)\Common Files\SafeNet Sentinel\Sentinel RMS License Manager\WinNT
  ```

  Type the command `>lservnt.exe -help` and the version is displayed.

- On *Linux* open a Terminal window and go to the directory where the `lserv script` is saved. For example:

  ```
  >cd opt/Thermo-Calc/<version>/Licensing-files
  ```

  Type the command `>./lserv -help` and the version is displayed.

Silent Installations

Administrative rights are required to install the Thermo-Calc software package. If you or your IT department are having problems silently installing TC-Toolbox over a network, perhaps to multiple computers, you need to run a file that is available after Thermo-Calc is installed.

1. Install Thermo-Calc as usual (requires administrative rights).

2. After Thermo-Calc is installed, navigate to this folder:

   `C:\Users\Public\Documents\Thermo-Calc\<2025b>\SDK\TC-Toolbox-MATLAB\.`

3. Double-click the `InstallTCToolboxMATLAB.cmd` file to run it

> The `InstallTCToolboxMATLAB.cmd` file must be run by the user who is going to use TC-Toolbox for MATLAB®, i.e. anyone with admin rights can install Thermo-Calc, but for TC-Toolbox, the user must be logged in to run this file.

Uninstalling TC-Toolbox for MATLAB®

Uninstallation requires that the user is logged in with administrator rights and Thermo-Calc is installed for this same user. Then the uninstallation is automatically completed as part of the uninstallation of Thermo-Calc. Otherwise a manual step is required.

To uninstall TC-Toolbox (when not automatically uninstalled):

1. Start MATLAB®.
2. In the **Home** tab from the **Add-Ons** menu, select **Manage Add-Ons**.
3. Right-click **TC-Toolbox** and choose **Uninstall**.

Working with Existing Installations

Also see Uninstalling TC-Toolbox for MATLAB®

In this section:

Add New Components to an Existing Installation

If you want to add new components to an existing Thermo-Calc installation (for example, you purchased a license for TC-Toolbox for MATLAB®), run the installation again.

Custom User Credentials Installations and Custom Standalone Installations (License File)

1. For Windows and macOS you need to have administrative level rights. For example in Windows, when you double-click the executable Thermo-Calc installation **.exe** file to launch the **Setup** program.

   Linux OS: If Thermo-Calc was not installed by root the first time, then administrative rights are not required.

2. Click **Next**. Click to accept the license agreement.
3. Select the additional component(s) to install.
4. Click **Next** to start the installation, which adds the new component(s).

Use the **Uninstall** program to *remove* components. See Uninstalling Thermo-Calc or Uninstalling TC-Toolbox for MATLAB®.

Updating the Software for Interim Releases

The full version of Thermo-Calc software is released twice a year. The software releases are named after the year of the release followed by an “a” for the first release of the year or a “b” for the second release of the year. For example, this release is 2025b.

Occasionally after a full release, an interim release version, an update, is required to fix a serious bug or to address an external issue that occurred after the full release. Software licenses come with a free 12 month Maintenance & Support Subscription, starting from the time of purchase, and this includes these software updates.

> Go to our website to confirm the current distributed software version and determine if there are updates, or to learn more about Maintenance and Support options.

Check for a Software Update

You can set your software to automatically check for updates upon start up.

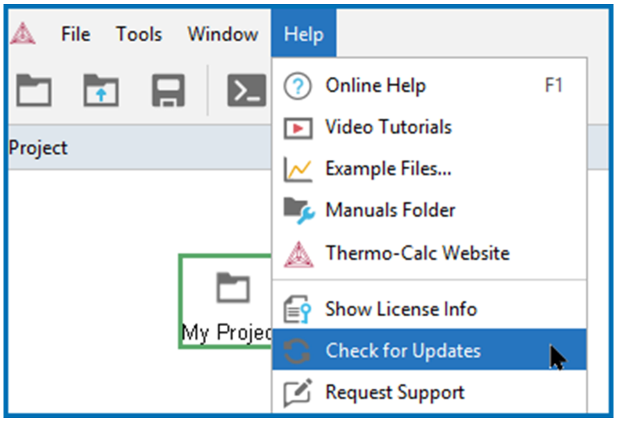
- From within the software on the **Options** window, **General** tab, set **Check update interval** to **On start up**.

  To open the **Options** window:

  - Windows: Select **Tools** → **Options**.
  - Mac: Select **Thermo-Calc** <*version*> → **Preferences** or **Settings** or press <⌘> on the keyboard.

- If you do not have Automatic Updates on you can go to **Help** → **Check for**

Updates.



Follow the Installation Instructions for the Applicable OS

After the software has checked for updates and determined there is one, the applicable installation file for your operating system is downloaded. Then follow the instructions provided in the Installation Guide for the specific operating system and license type.

For an update to the software, no additional license files or user credentials are required.

Option to Save Backup User Created Files

There are significant operating system differences regarding what backup files are saved if you are installing an update on Windows versus macOS or Linux.

During the installation process, several default folders are added to your system that include documentation, materials, and example files. This is the same for all operating systems. During an update, Thermo-Calc runs a check of these default folders to determine if there are changed or new user files that are saved in these folders. For example, you might have saved a completely new project `*.tcu` file into the Examples folder, or after running one of the included examples such as *T_06_Serial_Equilibrium_Calculators.tcu*, the default file is changed and now includes results.

On Windows operating systems, Thermo-Calc gives you the opportunity after the installation to specifically save a backup of these user created or modified files to your Documents folder when you open Thermo-Calc for the first time after the update.

However, for macOS and Linux operating systems, the behavior is different due to limitations enabling the identification of changes to some files.

Operating System	*When does backup occur?*	*What files are copied?*
Windows	After installation, when you open the software for the first time	Documents, Materials, and/or Examples files are copied when you choose **Yes** at the prompt (see the Windows section for details).
macOS	During installation	There is an option during the installation process to save a backup copy of the Examples folder even if no changes are made to files (see the macOS or Linux sections for details). Materials and Documents folders are not automatically copied even if there are file changes or additions. However, you can always manually back up these folders (see the macOS or Linux sections for details).
Linux		

Windows

First complete the installation update. Then when you open Thermo-Calc for the first time, and if Thermo-Calc identifies that there are changed files, you are prompted with a **Software Update - Action Required** window that identifies the folders where the applicable files are changed or added.

> These file types are not kept, i.e. these are excluded: dll, exe, lib, mltbx, pdf, whl, html, and htm.

Click **Yes** to save a backup of these changed files or **No** to continue opening Thermo-Calc as normal where the default set of folders are copied from the source `Public Documents` location into a user `Documents` folder.

If you choose to save a backup of the files, the new backup folder is added to this same location, for example:

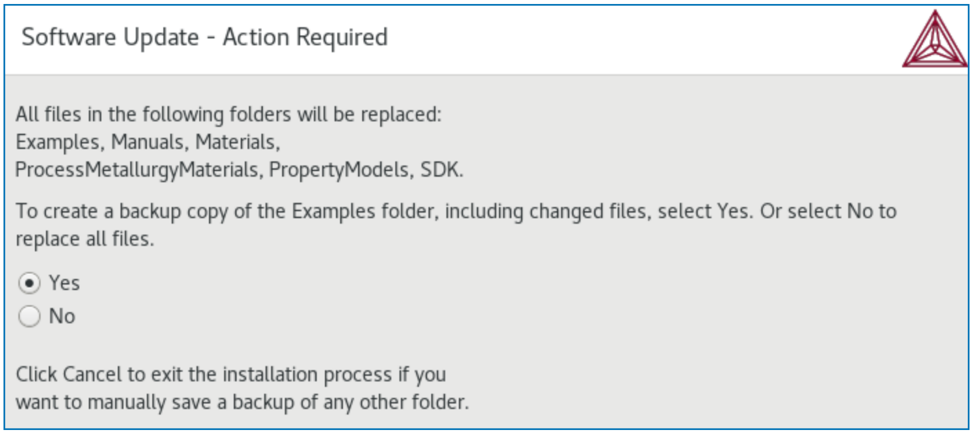
```
C:\Users\<user>\Documents\Thermo-Calc\2025b_backup
```

Installation Default Directory: Windows

macOS

During the installation process you are prompted with a **Software Update - Action Required** window.

This window always displays whether there are changes or additions to the folders or not.



Software Update - Action Required

All files in the following folders will be replaced:
Examples, Manuals, Materials,
ProcessMetallurgyMaterials, PropertyModels, SDK.

To create a backup copy of the Examples folder, including changed files, select Yes. Or select No to replace all files.

● Yes
○ No

Click Cancel to exit the installation process if you want to manually save a backup of any other folder.

The Materials and Documentation folders do not automatically have a backup saved. If you think there are user files you want to keep it is recommended that you click **Cancel** at this prompt to exit the installer, then manually copy the folders to another location. Then start the installation update process again.

To create a backup copy of the `Examples` folder, including changed files (i.e. all files are copied, not just the changed or new ones). Options at this prompt are to click:

- **Yes** to create the backup.
- **No** to replace all files.
- **Cancel** to exit the installation process, i.e. to manually save a backup of any other folder.

The default backup folder containing a full copy of all the contents of the `Examples` folder is saved to this location, for example:

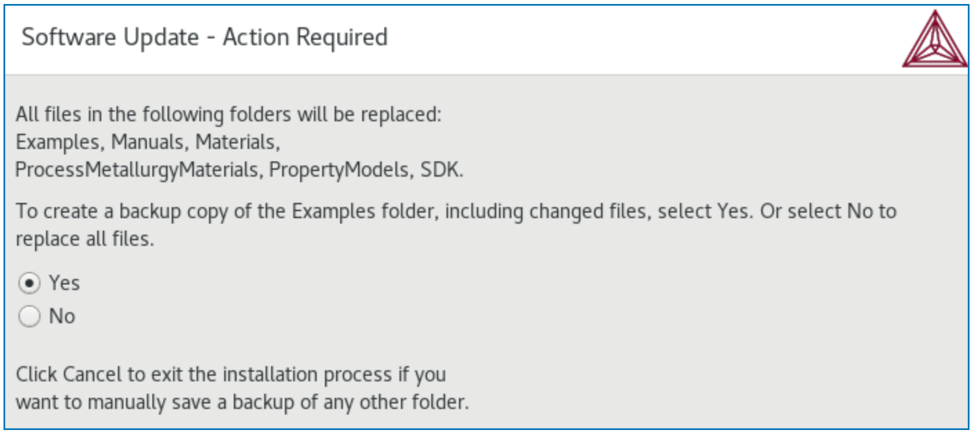
```
/Users/Shared/Thermo-Calc/2025b/Examples_backup
```

[Installation Default Directory: macOS](#)

Linux

During the installation process you are prompted with a **Software Update - Action Required** window.

This window always displays whether there are changes or additions to the folders or not.



Software Update - Action Required

All files in the following folders will be replaced:
Examples, Manuals, Materials,
ProcessMetallurgyMaterials, PropertyModels, SDK.

To create a backup copy of the Examples folder, including changed files, select Yes. Or select No to replace all files.

● Yes
○ No

Click Cancel to exit the installation process if you want to manually save a backup of any other folder.

The Materials and Documentation folders do not automatically have a backup saved. If you think there are user files you want to keep it is recommended that you click **Cancel** at this prompt to exit the installer, then manually copy the folders to another location. Then start the installation update process again.

To create a backup copy of the `Examples` folder, including changed files (i.e. all files are copied, not just the changed or new ones). Options at this prompt are to click:

- **Yes** to create the backup.
- **No** to replace all files.
- **Cancel** to exit the installation process, i.e. to manually save a backup of any other folder.

The default backup folder containing a full copy of all the contents of the `Examples` folder for Linux depends if you are a root super user requiring administrative privileges or a common user.

For example, for a common user:

```
/home/<user>/Thermo-Calc/2025b/Examples_backup
```

For example, for a root user:

```
/opt/Thermo-Calc/2025b/Examples_backup
```

Installation Default Directory: Linux

Uninstalling Thermo-Calc

Uninstalling TC-Toolbox for MATLAB®

Windows 11

1. From **Start**, go to **Settings → Apps → Installed Apps**.
2. In the list of programs, locate the version of Thermo-Calc you want to uninstall. Click the three dots to the right of the row.
3. Select **Uninstall**. Select **Uninstall** a second time.
4. Enter your admin level user credentials.
5. In the **Setup** window, **Uninstallation Mode** dialog box, choose to uninstall the **Entire application** or **Individual components**. Follow the instructions to finish.

You can also directly launch the Thermo-Calc uninstaller program:

1. Navigate to where the Thermo-Calc program is installed, i.e in the **Program Files** folder.
2. Locate the uninstaller program, named `Thermo-Calc-<version>-uninstaller.exe`.
3. Double-click and enter your admin level user credentials.
4. In the **Setup** window, **Uninstallation Mode** dialog box, choose to uninstall the **Entire application** or **Individual components**. Follow the instructions to finish.

Windows 10

1. From the **Control Panel** Desktop app, go to **Programs → Programs and Features → Uninstall or change a program**.
2. In the list of programs, locate the version of Thermo-Calc you want to uninstall. Click to highlight that row.
3. Click **Uninstall/Change**.
4. In the **Setup** window, **Uninstallation Mode** dialog box, choose to uninstall the **Entire application** or **Individual components**. Follow the instructions to finish.

macOS

Deleting the program from the Applications folder does not remove the program from your operating system. Run the **Thermo-Calc-***<version>***-uninstaller** program located in the Applications folder.

1. Go to the **Applications** folder and double click the file that starts with **Thermo-Calc-***<version>***-uninstaller**. Enter the administrator's user name and password.
2. Click **Yes** to choose **Entire application** or select individual components. Otherwise click **No** to quit.
3. The **Uninstalling Thermo-Calc** window shows the progress. Click **OK** when prompted.

Linux

1. To start the uninstallation procedure, in the Thermo-Calc installation directory use the command
   ```
   ./Thermo-Calc-2025b-uninstaller.run
   ```
   For *Thin Client* installations, use the command
   ```
   ./Thermo-Calc-client-2025b-uninstaller.run
   ```
2. To remove the whole application, including all its components, select **Entire application** and click **Forward**, or to remove specific components, select **Individual components** and click **Forward**.

> ❗ If you intend to reinstall Thermo-Calc 2025b it is important to (1) Restart the computer before you reinstall the software and (2) remove the environmental variable TC25B_HOME.

Request License Files

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

In this section:

Request a License File from Thermo-Calc Software

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

The following explains how to retrieve the necessary diagnostic and network adaptor information about your computer and then send an email to Thermo-Calc Software to get your license file(s) containing the license key(s).

To set up the correct licensing:

1. Make a note of your company or organization’s *site number*. You can find the site number on an invoice or any correspondence from Thermo-Calc Software.
2. Retrieve your computer diagnostic and network adapter information.
3. Email Thermo-Calc Software with this information.
4. A Thermo-Calc Software representative emails you the license file. Save the license file **lservrc** (there is no file suffix) to a location where you can easily access it later.

Thermo-Calc Support Center on our website

Getting License Information for License File Activations Using Thermo-Calc

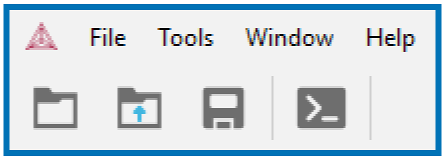
This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

Viewing and using the license information is based on the license activation type. When you have a license file activation type, you may need to copy information to provide to Thermo-Calc.

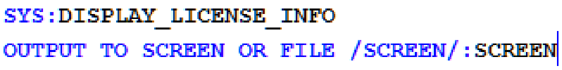
In Graphical Mode, and if you have already installed Thermo-Calc, you can view the license information by selecting **Help →** **Show License Info**.

In Console Mode you can run the SYS module command DISPLAY_LICENSE_INFO.

1. Open Thermo-Calc.
2. Click the **Switch to Console Mode** button .



3. At the `SYS:` prompt, enter `DISPLAY_LICENSE_INFO`.You can output the information to a `FILE` or to the `SCREEN`.



```
SYS:DISPLAY_LICENSE_INFO
OUTPUT TO SCREEN OR FILE /SCREEN/:SCREEN
```

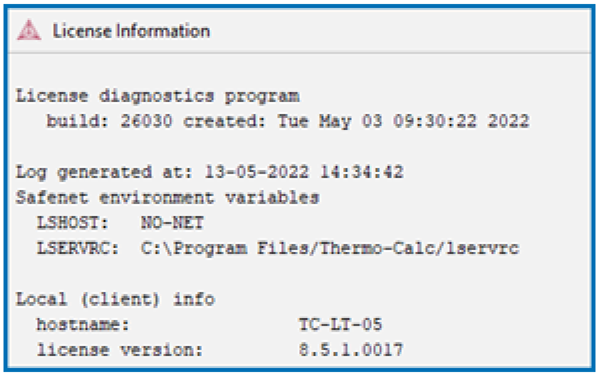
4. For both options, the information is displayed on screen. Copy the section containing the **Ethernet** and **IP address**. You can save it to a text file or paste it directly into an email. If you choose `FILE` as the output, then you can attach the file to an email.

Requesting the License File for Windows or Linux

Upgrading to a new version of Thermo-Calc: Skip this section if you are upgrading to a new version of Thermo-Calc (and you have a maintenance plan), or you have already been provided with the license file.

1. Your license information is sent to you in an email from Thermo-Calc or a representative. When you are sent a *license file*, save it to your computer to use during software installation. You may also need to provide some information that is accessed from Thermo-Calc.

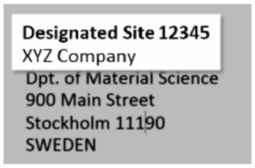
   Select **Help → Show License Info**.

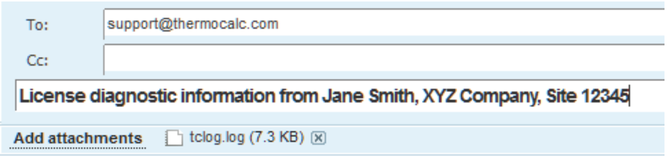
   ```
   License diagnostics program
      build: 26030 created: Tue May 03 09:30:22 2022

   Log generated at: 13-05-2022 14:34:42
   Safenet environment variables
     LSHOST:    NO-NET
     LSERVRC:   C:\Program Files/Thermo-Calc/lservrc

   Local (client) info
     hostname:               TC-LT-05
     license version:        8.5.1.0017
   ```

2. Copy the information from the **License Information** window. A lot of information may be shown below the initial screen, so make sure you scroll down to the end when you select and copy the window's contents. (Alternatively, you can copy the same information from the console by using the SYS module command DISPLAY_LICENSE_INFO.)
3. Send an email to support@thermocalc.com. Make sure to include the following in the subject line:

   License diagnostic information from <Name> where Name is replaced with your **name**, the **organization name** and the **Site Number**. *You can find the five-digit site number on an invoice or any correspondence from Thermo-Calc Software.*

   Designated Site 12345
   XYZ Company
   Dpt. of Material Science
   900 Main Street
   Stockholm 11190
   SWEDEN



support@thermocalc.com

License diagnostic information from Jane Smith, XYZ Company, Site 12345

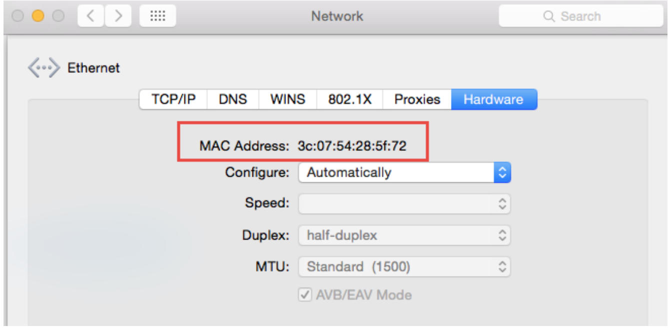
tclog.log (7.3 KB)

4. A representative from Thermo-Calc Software replies to the email and attaches your license file(s).
5. Save the license file(s) to your computer or network.

Requesting the License File for macOS

Upgrading to a new version of Thermo-Calc: Skip this section if you are upgrading to a new version of Thermo-Calc (and you have a maintenance plan), or you have already been provided with the license file.

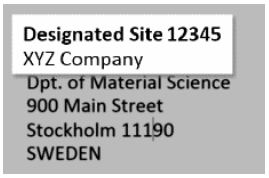
1. From the Apple main menu, select **System Preferences**.
2. Click **Network**.
3. In the left column select **Ethernet** or **Built-in Ethernet** (do not select a WiFi connection as a local static MAC address is required).
4. Click **Advanced → Hardware**. The **Network** window shows you the **MAC Address**. For example, the MAC address (the host ID) might be **3c:07:54:28:5f:72**.



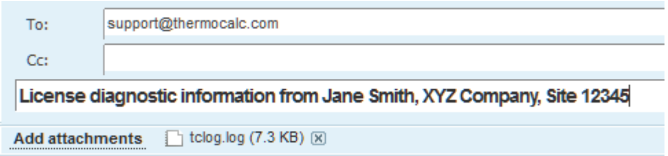
MAC Address: 3c:07:54:28:5f:72
Configure: Automatically
Speed:
Duplex: half-duplex
MTU: Standard (1500)
☑ AVB/EAV Mode

5. Send an email to support@thermocalc.com and copy and paste the MAC address into the body of the email. Make sure to include the following in the subject line:

License diagnostic information from <Name> where Name is replaced with your **name**, the **organisation name** and the **Site Number**. *You can find the five-digit site number on an invoice or any correspondence from Thermo-Calc Software.*



Designated Site 12345
XYZ Company
Dpt. of Material Science
900 Main Street
Stockholm 11190
SWEDEN



To: support@thermocalc.com
Cc:
License diagnostic information from Jane Smith, XYZ Company, Site 12345

6. A representative from Thermo-Calc Software replies to the email address provided and attaches your license file or files.
7. Save your license file to your computer or network.

Troubleshooting and Miscellaneous

There are diagnostic scripts available for TC-Python and TC-Toolbox for MATLAB® (these are included as examples in the Miscellaneous folder). These scripts are also available on our website.

Troubleshoot User Credential License Activations

In this section:

macOS Installation Notes

How to Restart After an Installation

In some types of installations (e.g. a network installation), you may have to restart your Mac to use Thermo-Calc for the first time.

Rosetta is Required when there is an ARM Processor

To install and run Thermo-Calc on a Mac computer with an ARM processor, Rosetta first needs to be installed.

How to Install XQuartz

The XQuartz open-source X Windows system is required to run Thermo-Calc on macOS but it is not required to install Thermo-Calc. Before installing Thermo-Calc, you may also need to ensure that the computer security permissions are set.

The XQuartz open-source X.Org X Window system is required to run Thermo-Calc on macOS.

1. In a web browser go to https://www.macupdate.com or to download it directly from XQuartz, https://www.xquartz.org/.
2. In the **Search Mac Apps** field, enter *XQuartz*.
3. Click the **XQuartz** search result. For example, based on the recent version, the name is XQuartz-2.8.5.dmg.
4. Click **Download**.
5. Double-click the **XQuartz-**<*version*>**.pkg** file. Follow the instructions.
6. Click **OK** when the message about logging out displays and click **Close** when the installation is successful.

How to Enable the Security Settings

1. From the Apple main menu, select **System Preferences**.
2. Click **Security and Privacy**.
3. Click **General**. At the bottom of the **Security & Privacy** window, click the lock icon to make changes. Enter the administrator password as required.
4. If you have already tried to launch the Thermo-Calc installer, you can click **Open Anyway** to proceed. Otherwise, under **Allow apps downloaded from:** click **Anywhere** and then **Allow from Anywhere**.
5. Continue with the applicable installation type (standalone or network).

Remember to reset your security after installing Thermo-Calc.

Linux Installation Notes

The following are details you need to know regarding your Linux installation as well as how to open Thermo-Calc.

openSUSE Administration (sudo) Users

Note the following if you are a sudo user (administrator) in openSUSE installing Thermo-Calc using this command:

```
sudo ./Thermo-Calc-linux-<full-version-number>.run
```

When this command is used, you will do a text-based installation instead of having a graphical interface to guide you. The information is the same, just without the user interface.

For example, the *<full-version-number>* is not just 2025b, it is what is found in the **Help → About** window in Thermo-Calc and it changes every release. You can find the current full version number listed on our website.

Opening Thermo-Calc in Linux

To open Thermo-Calc double-click the **Thermo-Calc-2025b** application or from the Thermo-Calc installation directory enter `$ ./Thermo-Calc-2025b.sh` in the terminal.

Troubleshoot User Credential License Activations

All users are being migrated to this new *user credentials* license activation type. For this type of activation, the information is managed via an online portal system as well as accessible from within Thermo-Calc. Customers are being contacted directly by email to provide the necessary information to install and use your purchased products. During the transition from using the old license file activations, some users may need to contact support for assistance.

This section is specific to troubleshoot some common problems with the *user credentials* license activation option.

When Activate Online Does Not Work

If the fields become empty (i.e. go blank) when you click **Activate Online**, this means that the final step of the license activation has failed. You need to contact support to troubleshoot further.

1. Close the license activation window.
2. Go to the bottom left corner of Thermo-Calc and click to open the **Event Log** window.
3. Copy all the red error messages and send these to your local support contact should you have one. Otherwise copy and paste these into an email and send to support@thermocalc.com.

Firewall or Anti-virus Issues

If you have trouble with a local or non-local firewall or anti-virus software blocking Thermo-Calc from accessing LicenseSpring API, then try this solution.

Make an exception allowing Thermo-Calc to connect to the following IP addresses through TCP ports 443 and 80:

- 34.250.134.210
- 34.251.49.36
- 52.18.228.254
- 54.78.102.217

Proxy Service or SSL Certification Issues

If you see this error

```
ERROR LicenseManager: . Thrown at:
com.licensespring.internal.services.LicenseSpringApiRetryer:tryCauseMessage:LineN
o:96 PKIX path
```

then it is either because you are behind a proxy server OR the SSL certification has failed.

For both of these types of issues you typically need to contact your organization's IT department for assistance.

- A proxy service is used for an Internet connection, which blocks the connection. Use the **Proxy Settings** option available on the license activation window, or contact your proxy service provider to make an exception.
- For SSL certification: The Let's Encrypt root public CA should be installed (ISRG Root X1). This is included in all supported OS, but can be missing in the organization's security service.

Other Common Errors

Some general troubleshooting suggestions are included in this section.

Problem	***Suggested Solution***
The incorrect password is entered	There can be issues when you copy and paste passwords from other sources. Check that no extra spaces were accidentally copied at the beginning or end of a password, and that all of the string is included in the selection.
Offline activation procedure was initiated but not completed, thus blocking the final activation.	It is recommended that where possible an online activation is used instead. First try to fix this issue by deleting the `ls_activation.req` file on your computer as described in the step for Offline Activation described for your specific OS. In other cases, once an offline activation is attempted, and if it does not work, the license can still be registered by the license software as being activated, thus blocking the final activation. Contact support@thermocalc.com to reset the license.

License File Activation Type Errors

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

Issue	*Platform*	*Installation type*	*Action or link to more information*
How do I add or update a standalone (SUNLL) license on a Windows computer where Thermo-Calc is already installed?	Windows	Standalone	Determining the Current License File Directory Path
How do I add or update a standalone (SUNLL) license on a Linux computer where Thermo-Calc is already installed?	Linux	Standalone	Determining the Current License File Directory Path
How do I add or update a network license on Windows?	Windows	Network	Determining the Current License File Directory Path
How do I add or update a network license on Linux?	Linux	Network	Determining the Current License File Directory Path
No license file found. Copy a valid license file to the installation directory after completing the installation.	All	All	You get this message if the wrong path or no license file is found at a path entered during the installation process. See Installation Default Directories and the License File and Determining the Current License File Directory Path
TC-Toolbox for MATLAB®	Windows	All	TC-Toolbox Installation Troubleshooting
Warning Environment variable “LSHOST” is not set. Software will not function properly.	All	Network	Specifying a New Server Name or IP Number
Problem running post-install step. Installation may not complete correctly.	Linux and Mac	Standalone	macOS Installations: Running the License Initialization Script or Linux Installations: Running the License Initialization Script

Issue	***Platform***	***Installation type***	***Action or link to more information***
Unable to run post-installation script, run the license initialization script as root after the installation.			
Firewall warnings related to license management software (License Manager and License Server)	Windows and Linux	Network	Firewalls
Client / Server naming mismatches	Windows and Linux	Network	Client/Server Mismatch
InstallScript engine missing	Windows	Network	You are not notified if the InstallScript scripting engine is not installed. Install the ISScript.msi file and then run the downloaded file from Thermo-Calc again as described in Windows: About Installing the License Manager
License initialization warning on a Mac with ARM processor	Mac	Standalone	To install and run Thermo-Calc on a Mac with ARM processor, Rosetta needs to be installed. Cancel any installation in progress, install Rosetta, then start the installation again.

Determining the Current License File Directory Path

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

This topic explains how to find out where your license file is installed, either by default or if a different directory was chosen for previously installed versions. For new installations, where you may not have had a license file when you installed Thermo-Calc, you can also use these instructions to determine the correct file path.

From Thermo-Calc

If you have already installed Thermo-Calc, you can view the path to the license file in the GUI. Select **Help → Show License Info**.

In Console Mode you can run the SYS module command DISPLAY_LICENSE_INFO.

Windows Standalone Installations

How do I add or update a standalone (SUNLL) license on a Windows computer where Thermo-Calc is already installed?

1. Unpack the .zip file that contains your standalone license and save the LSERVRC file on your computer. Find out where to place the new license file by opening a Command Prompt Window (cmd.exe) and type in the command line:

   ```
   >set LSERVRC
   ```

2. Press `Enter`. The output from the command is the path to the license file (including the name of the license file). For example: if the output is

   ```
   LSERVRC=C:\Users\<user>\Documents\Thermo-Calc\lservrc
   ```

   then the new license file should be placed in `C:\Program Files\Thermo-Calc\2025b\`

Linux Standalone Installations

How do I add or update a standalone (SUNLL) license on a Linux computer where Thermo-Calc is already installed?

Find out where to place the new license file by opening a Terminal window and type in the command line:

```
echo $LSERVRC
```

Windows Network Installations

How do I add or update a network license on Windows?

Only the WlAdmin tool can be used to update the network license used by the License Manager. See Install the Thermo-Calc Network License Using WIAdmin.

Linux Network Installations

How do I add or update a network license on Linux?

Replace your current license file with the new license file. The license file is located in the same directory as the license server.

Specifying a New Server Name or IP Number

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

The Thermo-Calc Setup wizard does not warn you if the name or IP number entered to the server (with the license management software) is incorrect.

If the name or IP number is not set at all, or if it is set to an empty string, then when you start Thermo-Calc the following message displays: *Warning Environment variable “LSHOST” is not set. Software will not function properly*.

Windows

This section explains how to specify or change the name or IP number of the server where the License Manager is installed and for a consolidated network client installation.

To install a license for an existing Thermo-Calc program, follow these steps:

1. Close all running Thermo-Calc programs.
2. Open a command line window.
3. Specify the name or IP number of the licensing software server. Type:

   ```
   set LSHOST=<name/IP number>
   ```

   To display the current name or IP number, type:

   ```
   set LSHOST
   ```

macOS

Permanently set the environmental variable LSHOST to specify a new licensing server name or IP number. Refer to the file `/Applications/Thermo-Calc-2025b.app/Contents/Info.plist`.

In this file, you can manually set the TC25B_HOME variable, which specifies the home directory of the Thermo-Calc program. See the `Info.plist` file for an example.

Linux

You can set or change the name or IP number of the license server at a later time by setting the environmental variable “LSHOST” to this name or number.

Firewalls

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

Windows

For a Windows License Manager installation you may have to change the system firewall settings to allow the License Manager to communicate with the computers running the client applications. Go to the Windows Firewall settings window to see if there are any problems. If prompted, select Unblock the system firewall for the Sentinel RMS License Manager and click Next.

Linux

For a Linux License Server installation you need to open the UDP port 5093 in your firewall. In case you have installed SELinux you might also need to disable it by setting SELINUX=permissive in the /etc/selinux/config file.

Client/Server Mismatch

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

For some network installations there can be a naming mismatch that causes errors. The server (where the license management software is installed) gets information from its DNS servers that an IP address (aaa.bbb.ccc) belongs to a computer (Computer A). But the client computer identifies itself as having a different IP address (aaa.bbb.ccc.eee) for the same computer (Computer A).

Even if the IP address of the client computer belongs to a subnet range listed in the license file, there is a problem with accessing the license file because the computer name does not match the information.

You may need your organisation’s network administrator to assist with this issue.

How to Check

Compare computer names on the client computer and server

1. On the client computer, start a command prompt **cmd.exe** and type `ipconfig /all`. Press `Enter`. A variety of data is displayed on screen. Write down the following information for later comparison:
   - Hostname
   - DNS Suffix
   - Current IPv 4 Address
2. In the command window, type `nslookup` *<client_computer_name>,* where *client_computer_name* is the actual name of the client. Press `Enter`.

   This shows what information is saved on the DNS Servers used by the client computer. This information should match what is shown in the output from the first step.

3. On the server that holds the license management software, open a command prompt and run the command line: `nslookup client_computer_name`. The output

lists the information for this server.

> Does it match the information given by the command ipconfig /all on the client computer? If not try the following.

Try these options to correct the issue

1. If the client computer has a dynamic (DHCP) IP address, either change it to a static one or make a reservation on the DHCP Server so that the computer always get the same IP address.
2. Update the records on the DNS Servers used by both the client computer and the server computer.

You can also configure the computer names and IP addresses in the local Hostfile of the client and server:

1. On the client computer, make a backup copy of the file C:\Windows\System32\drivers\etc\hosts.
2. Open the original in a simple text editor.
3. Add a new line which contains the IP and name of the server, for example: 192.168.29.27 license_server.thermocalc.se.
4. Save the changes.
5. On the server, make a backup copy of the file /etc/hosts.
6. Open the original in a simple text editor.
7. Add a new line which contains the IP and name of the client, for example: 192.168.29.47 Computer_A.thermocalc.se.
8. Save the changes.
9. In the host file, there is an example of how the operating system (Windows or Linux) wants the line in the hosts file to look like.

macOS Installations: Running the License Initialization Script

As part of the Standalone installation of Thermo-Calc, the Setup runs a license initialization script. If this part of the installation process did not complete properly for a standalone installation, you must manually run the license initialization script. You need the administrator username and password for these steps.

How to Run the Script

For this script to successfully initialize the license, the license file must be called **lservrc** and be located in the folder:

```
/Users/Shared/Thermo-Calc
```

Installation Default Directory: macOS

1. Open a terminal window. The **Terminal** application is in the */Applications/Utilities* folder.
2. At the prompt, enter this command:

   ```
   $ sudo /Applications/Thermo-Calc-
   2025b.app/Contents/Resources/license-initialization-macOS-x86_
   64.sh
   ```

   If you are not already logged in as an administrator, you probably cannot run the `sudo` command. If this is the case, then you can use the `su` command in the terminal window to login as an administrator. Contact your local system administrator for help.

3. Enter the administrator password and press `Enter`.
4. When you restart your computer and run the license initialization script, you are ready to start using Thermo-Calc.

> If you did not install a license file during this procedure, you can still start Thermo-Calc although you will get the **No license file found** message.

Linux Installations: Running the License Initialization Script

As part of a Standalone installation of Thermo-Calc, the Setup runs a license initialization script. If you get a warning message during the standalone installation `Unable to run post-installation script`, run the license initialization script as root after the installation, then you need to manually run the script as root.

openSUSE Administration (sudo) Users

Note the following if you are a sudo user (administrator) in openSUSE installing Thermo-Calc using this command:

```
sudo ./Thermo-Calc-linux-<full-version-number>.run
```

When this command is used, you will do a text-based installation instead of having a graphical interface to guide you. The information is the same, just without the user interface.

> For example, the *<full-version-number>* is not just 2025b, it is what is found in the **Help → About** window in Thermo-Calc and it changes every release. You can find the current full version number listed on our website.

How to Run the Script

> For this script to successfully initialize the license, the license file must be called **lservrc** and be located in the directory where you have installed Thermo-Calc.

Installation Default Directory: Linux

1. In the console, go to the Thermo-Calc installation directory.
    - The license file is put in `/home/<user>/Thermo-Calc`if you are installing as a non-root user, where `<user>` is your user name.
    - If you are installing as root, then this directory is `opt/Thermo-Calc/`.
2. Enter this command:

```
$ sudo sh license-initialization-linux.sh
```

If you are not able to execute the `sudo` command because you are not on the sudoers list, you must log in as a root user with the command `su`, and then use `sh` to run the license initialization script. For example, on a 64-bit computer, enter the following:

```
$ sh license-initialization-linux.sh
```

3. Log out of Thermo-Calc and then log back in to save these changes.

Sentinel RMS License 9.7 Tools

This section is applicable to installations involving a **license file** activation type. This licensing method is gradually being replaced by the **user credentials** activation type starting with Thermo-Calc 2025a.

These tools relate to Network Client installations of the Sentinel RMS License software.

Windows: Installing the Sentinel RMS License Manager or Linux: Installing the Sentinel RMS License Server

In this section:

GetHostID: Get HostID/Mac Address

GetHostID is a tool that retrieves the HostID/Mac address from the computer hosting the license server and saves it to a text file.

> For Linux the output file is called `gethostid.log`. For Windows it is called `TC_Hostid.txt`.

- This is related to the Full Network Client Installations using the Sentinel RMS License Manager (Windows) or Server (Linux), version 9.7.

- The tool is applicable to Windows and Linux (32-bit and 64-bit) operating systems. See Windows: Installing the Sentinel RMS License Manager or Linux: Installing the Sentinel RMS License Server.

Windows

1. Extract `getHostID_win.zip`.
2. Right-click `getHostID_win.bat` and select **Run as Administrator** from the menu.

   The output is saved in a file: `TC_Hostid.txt` located in the same folder as `getHostID_win.bat`.

Linux 32-bit

1. Extract `gethostid.tar`.
2. Run the command: `>./gethostid`.

   The output is saved in a file: `gethostid.log` located in the same directory as `gethostid`.

Linux 64-bit

1. Extract `gethostid64.tar`.
2. Run the command: `>./gethostid64`.

   The output is saved in a file: `gethostid.log` located in the same directory as `gethostid64`.

lsmon: Monitor License Manager Transactions

- This is related to the Full Network Client Installations using the Sentinel RMS License Manager (Windows) or Server (Linux), version 9.7.

- The tool is applicable to Windows and Linux (32-bit and 64-bit) operating systems. See Windows: Installing the Sentinel RMS License Manager or Linux: Installing the Sentinel RMS License Server.

Platforms

Windows, Linux 32-bit, Linux 64-bit

The tool retrieves information about all features currently licensed by the Sentinel RMS License Manager, licenses, and clients.

On UNIX computers, you can use "Poll-interval-in-seconds" to specify that lsmon should keep monitoring and reporting usage activity instead of displaying information once and stopping. If specified, lsmon waits for that many seconds between re-polls of the License Manager.

lsmon monitors all licensed applications supported by a License Manager. If the License Manager supports licensed applications from multiple vendors, then all licenses for all vendors are displayed.

- On Windows, use `lsmon` *[Server-host]*
- On Linux 32-bit, use `lsmon` *[Poll-interval_in_seconds] [Server-host]*
- On Linux 64-bit, use `lsmon64` *[Poll-interval_in_seconds] [Server-host]*

OPTIONS

- *Poll-interval_in_seconds*: Enable periodic update at indicated rate. This option is supported on UNIX only).
- *Server-host*: The name of the computer on which the License Manager is running. If Server-host is omitted, lsmon will attempt to talk to the Sentinel RMS License Manager on the computer indicated in the LSHOST environment variable or in the LSHOST (or lshost) file. If the variable or the file does not exist, then it will attempt to contact a License Manager using the broadcast mechanism. If lsmon fails to find a Sentinel RMS License Manager, it will display an error message and exit.

lspool: Maintain Redundant License Manager Pool

- This is related to the Full Network Client Installations using the Sentinel RMS License Manager (Windows) or Server (Linux), version 9.7.

- The tool is applicable to Windows and Linux (32-bit and 64-bit) operating systems. See Windows: Installing the Sentinel RMS License Manager or Linux: Installing the Sentinel RMS License Server.

lspool is a redundant License Manager administration utility (command-line) for Windows and UNIX.

OPTIONS

- `h` Displays a list of lspool usage options.
- `a` *<license manager>* Adds the License Manager to the redundant License Manager pool. Specify the hostname or IP address of the License Manager system. Modifies the redundant license file.. On Windows, dynamic addition of License Manager in an existing redundant pool is not supported.
- `d` *<license manager>* Deletes the License Manager from the redundant License Manager pool. Specify the hostname or IP address of the License Manager system. Modifies the redundant license file. On Windows, dynamic deletion of License Manager in an existing redundant pool is not supported.
- `l` Displays the host name of the leader redundant License Manager.
- `p` Displays the list of License Managers in the redundant License Manager pool.
- `g` *< feature> <version>* Displays the license token distribution criteria for the specified feature/version. If the version is not specified, it must be replaced with empty quotation marks: " ".
- `L` *<event> <OFF|ON>* Disables/enables logging for an event. The events you select will be logged into the License Manager trace log file (only if error logging is enabled).

LSPOOL - L OPTIONS

Events that can be logged using the -L option are given below. The following events are temporarily logged (except 1) and need to be set each time the License Manager is restarted.

- `0` Logs all events.
- `1` Logs when the License Manager is up. On by default. 2 Logs election of the leader License Manager.
- `3` Logs the two-way redundant License Manager heartbeat:> Leader License Manager periodically logs the update status received from all its followers

  > Follower License Manager periodically logs the update about the contact established with the current leader License Manager

- `5` Logs the usage information event, shared by the leader, regarding the number of tokens issued. 7 Logs the license token distribution information synchronization event.
- `9` Logs when the License Manager is down.
- `11` Logs addition of a license into the file or memory. Also logs deletion of a license from the memory.

lsrvdown: Shut Down the License Manager

- This is related to the Full Network Client Installations using the Sentinel RMS License Manager (Windows) or Server (Linux), version 9.7.

- The tool is applicable to Windows and Linux (32-bit and 64-bit) operating systems. See Windows: Installing the Sentinel RMS License Manager or Linux: Installing the Sentinel RMS License Server.

lsrvdown utility is used to shut down the named License Manager.

Platforms

Windows, Linux 32-bit, Linux 64-bit

- On Windows and Linux 32-bit use `lsrvdown host-name`
- On Linux 64-bit use `lsrvdown64 host-name`

lsrvdown can be run from the operating system command prompt by an administrative user on a client or License Manager computer.

- On UNIX, only the user logged in as “root” can use lsrvdown.
- On Windows, any user with administrative privileges may use lsrvdown unless the License Manager was started by a user logged in as Administrator, in which case only Administrator can shut the License Manager down. The computer on which you are running lsrvdown must be in the same network domain as the License Manager computer.

> The same user must install the Sentinel RMS License Manager and also run this utility.

lswhere: Display a List of License Managers

- This is related to the Full Network Client Installations using the Sentinel RMS License Manager (Windows) or Server (Linux), version 9.7.

- The tool is applicable to Windows and Linux (32-bit and 64-bit) operating systems. See Windows: Installing the Sentinel RMS License Manager or Linux: Installing the Sentinel RMS License Server.

Platforms

Windows, Linux 32-bit, Linux 64-bit

lswhere command displays the network names of the computers running the License Manager. By default, lswhere displays for each License Manager the address of the computer on which that License Manager is running as well as its host name.

lswhere can be run on Windows and UNIX. lswhere should be run from the operating system command prompt by an administrator or application user on a standalone, client, or License Manager computer.

lswhere should be run in the following format:

- Windows and Linux 32-bit: `lswhere` *[option]*
- Linux 64-bit: `lswhere64` *[option]*

OPTIONS

- `d` Displays details on the License Managers found on the network.
- `r` Displays only the IP addresses of the License Managers found on the network (resolves the host names). lswhere can also be run without specifying any command line options.

WlmAdmin Administrative Tool

- This is related to the Full Network Client Installations using the Sentinel RMS License Manager for Windows, version 9.7.

- The tool is applicable to Windows operating systems. See Windows: Installing the Sentinel RMS License Manager.

WlmAdmin performs a variety of administrative functions for the license management activities. It displays elaborate information that includes the License Manager information, feature information, and license and client information.

Platform

Windows

WlmAdmin can administer a remote Linux license server.

WlmAdmin Functions

- Provides information on the License Managers.
- Details on licenses and clients using them in the network. For example, the administrator can see which users have acquired that license and who are in a queue waiting for the license.

If you are using redundant License Managers, you can use WlmAdmin as an informational tool to:

- Add or delete a redundant License Manager from the redundant License Manager file.
- Display a list of all License Managers in the redundant License Manager pool and display the name of the License Manager leader.
- Display the distribution criteria for specific licenses (only high assurance model is allowed, where the reigning leader server keeps all the license tokens).

View License Manager Information

- Click the name of a License Manager in the left-hand pane of the main window. In the right-hand pane of the display, you see the IP address of the computer containing the License Manager and its host name.

Add or Remove a License Manager from the Defined Server List

- To add a License Manager: Right-click the name of a License Manager in the list of Subnet Servers. From the menu select **Add to Defined List**.
- To remove a License Manager: Right-click the name of a License Manager in the list of Defined Servers. From the menu select **Remove from Defined List**.

Add a License Code to the License Manager from a File

1. Right-click the name of a License Manager in the left-hand pane of the main window.
2. From the menu select **Add Feature > From a File > To Server and its File**.
3. To add the license from a file, select **From a File**. This permanently adds the license code to the License Manager license file as well as to the License Manager memory.
4. In the new windows, browse to the source file that contains the license code and click **Open**.
5. Select the license code file.

Delete Old License Features from the License Manager

1. Right-click the file `WlmAdmin.exe` and select **Run as Administrator**.

   If the license server is not found under subnet servers, go to **Edit > Defined Server List**.

2. Enter the host name or IP address of the license server.
3. Click **Add** and **OK**.
4. Click **View > Refresh All** to update the list.
5. Right-click the name of a License Manager in the left-hand pane of the main window.
6. From the menu select **Remove all Features**

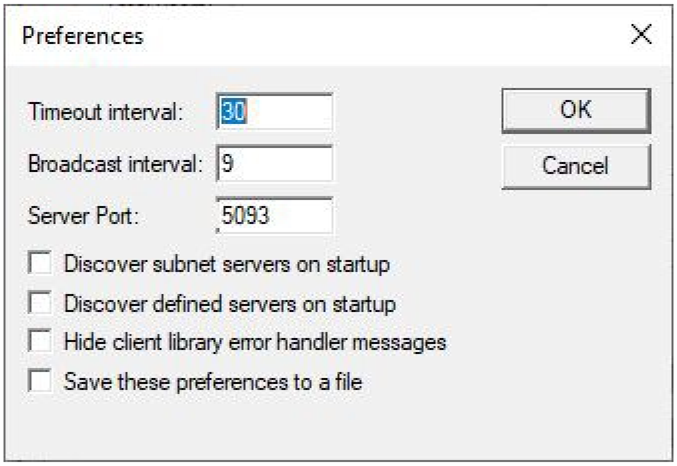
Shut Down a License Manager

- Right-click the name of a License Manager in the left-hand pane of the main window. From the menu select **Shutdown Server**.

Setting WlmAdmin Preferences

WlmAdmin allows you to choose what to display when it starts.

From the **Edit** menu, select the **Preferences** command to view WlmAdmin Preferences:



Timeout interval: 30

Broadcast interval: 9

Server Port: 5093

☐ Discover subnet servers on startup

☐ Discover defined servers on startup

☐ Hide client library error handler messages

☐ Save these preferences to a file

- **Timeout Interval**: The number of seconds after which WlmAdmin will stop trying to contact a License Manager. If you have a large network or a slow one, you might want to increase this number if you find WlmAdmin has difficulty retrieving information from License Managers.
- **Broadcast Interva**l: Specify the number of seconds between broadcasts to the network to discover License Managers.
- **Server Port**: To set any custom port (other than the default port 5093) on which the RMS License Manager is running.

> Set this port number before you add that License Manager in the list of defined servers.

- **Discover subnet servers on startup**: To automatically discover and display the License Managers on your subnet.

- **Discover defined servers on startup**: To always show the License Managers you have defined.
- **Show client library error handler messages**: To pass license management error messages from Sentinel RMS to WlmAdmin.
- **Save these preferences to a file**: To save your choices.

Sldemo: Show Basic API Functions

- This is related to the Full Network Client Installations using the Sentinel RMS License Manager for Windows, version 9.7.

- The tool is applicable to Windows operating systems. See Windows: Installing the Sentinel RMS License Manager.

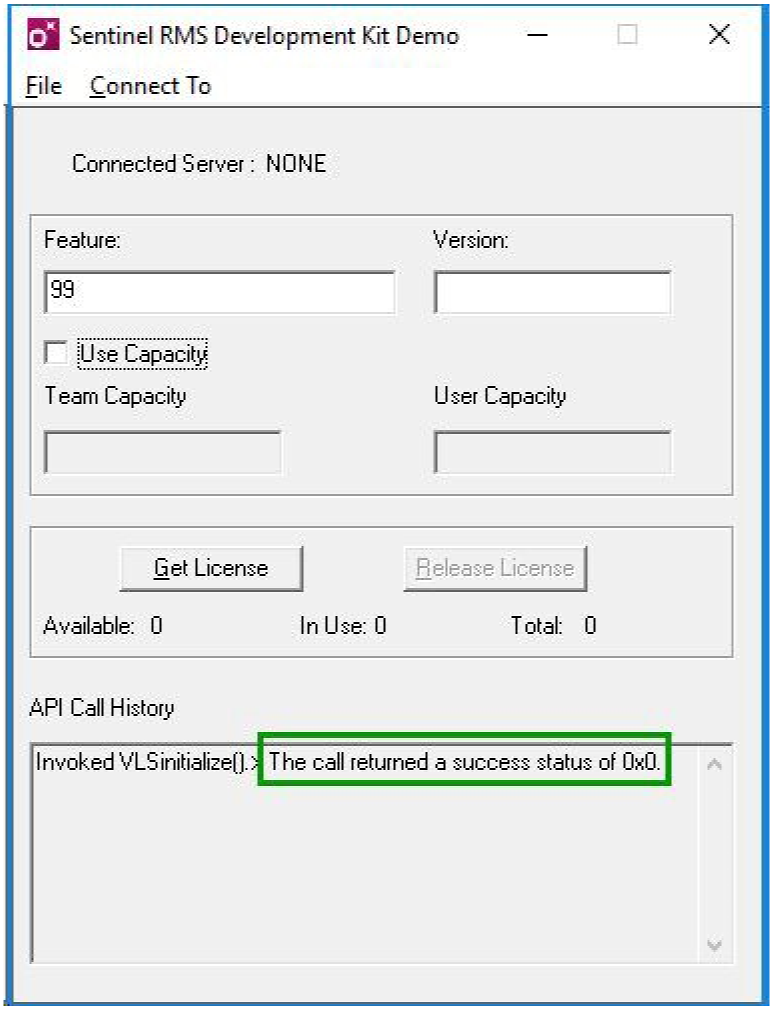
slmdemo is a Windows-based graphical sample program to show basic API functions. Evaluate it using the steps described here to understand the basic API calls and test the connectivity between client and license server

slmdemo can be used to test the connectivity to a remote Linux license server

Platform

Windows

Right-click on the executable and select **Run as administrator**. slmdemo calls the VLSinitialize API when the application is invoked successfully.



Connected Server : NONE

Feature: 99

Version:

☐ Use Capacity

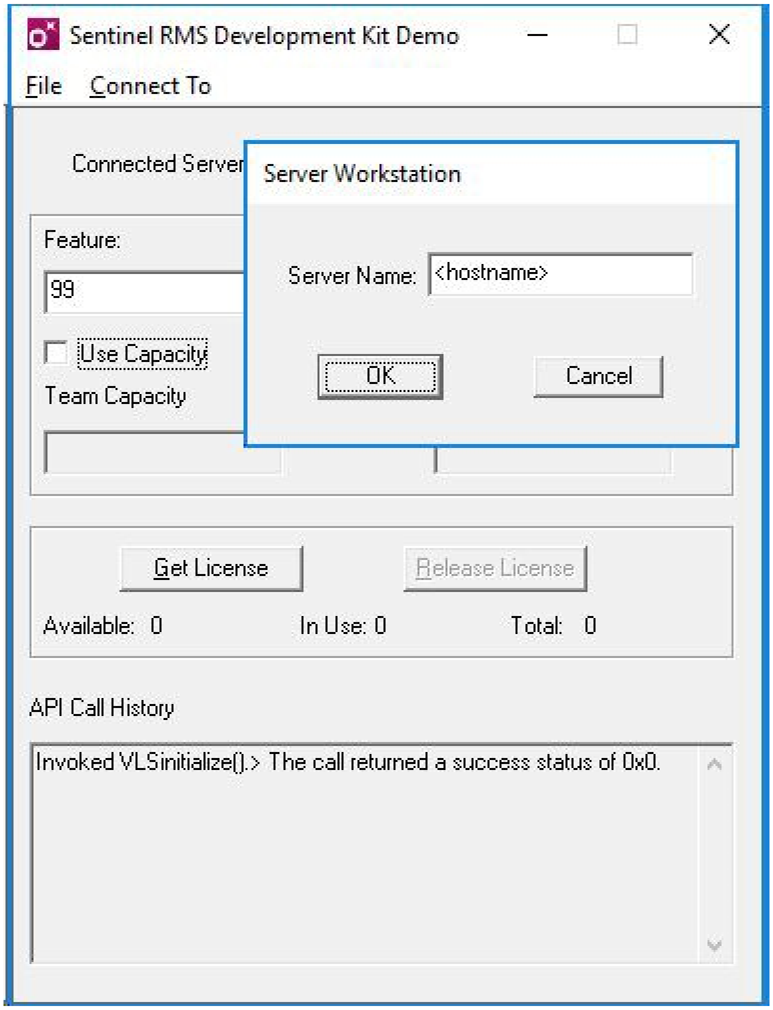
Team Capacity

User Capacity

Available: 0 In Use: 0 Total: 0

Invoked VLSinitialize().> The call returned a success status of 0x0.

Set the contact server (License Manager) under the **Connect To > Server** menu option. Enter a `hostname` , which is the hostname or IP address of the License Server.



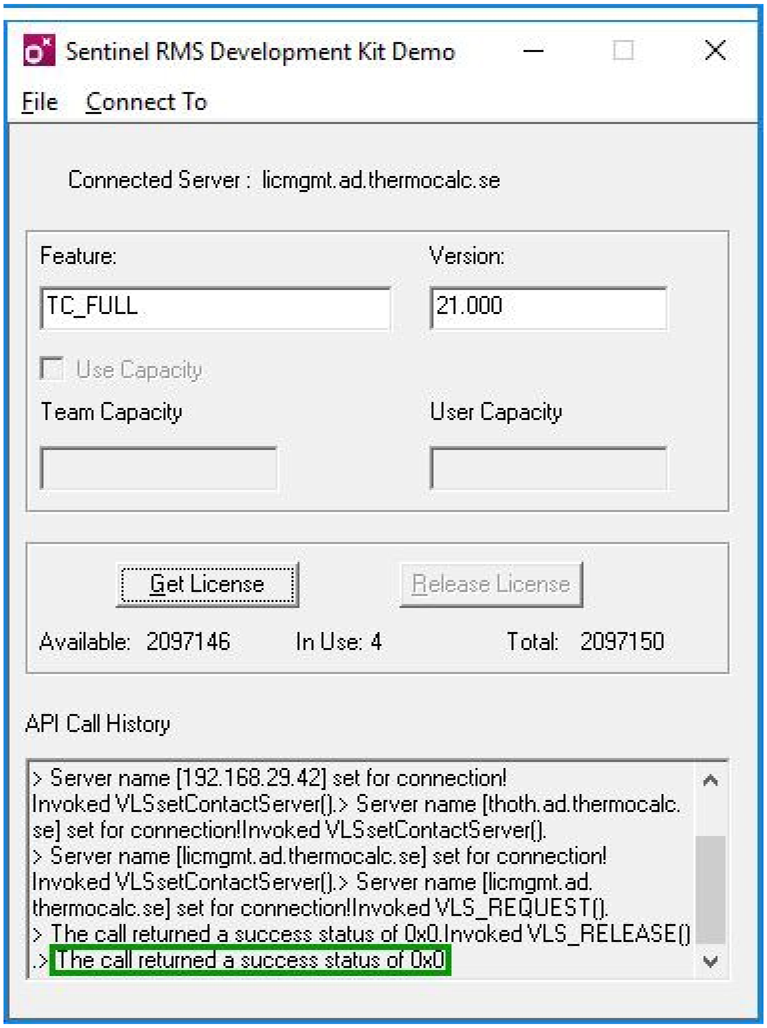
Feature: 99

Server Name: <hostname>

Available: 0 In Use: 0 Total: 0

Invoked VLSinitialize().> The call returned a success status of 0x0.

Click **OK** and enter in the field one of the license features available in the network license file. Where *Feature* is the name of the feature ex. **TC_FULL** and *Version* is the license version in the NWL (Network) license. Click **Get License**. The message `The call returned a success status of 0x0` means that the connection client <> license server works.



Connected Server : licmgmt.ad.thermocalc.se

Feature: TC_FULL

Version: 21.000

☐ Use Capacity

Team Capacity

User Capacity

Available: 2097146

In Use: 4

Total: 2097150

```
> Server name [192.168.29.42] set for connection!
Invoked VLSsetContactServer().> Server name [thoth.ad.thermocalc.
se] set for connection!Invoked VLSsetContactServer().
> Server name [licmgmt.ad.thermocalc.se] set for connection!
Invoked VLSsetContactServer().> Server name [licmgmt.ad.
thermocalc.se] set for connection!Invoked VLS_REQUEST().
> The call returned a success status of 0x0.Invoked VLS_RELEASE()
.> The call returned a success status of 0x0
```

To save the log, click **File > Save log**.

Wechoid: Get a Computer Locking Code

- This is related to the Full Network Client Installations using the Sentinel RMS License Manager for Windows, version 9.7.

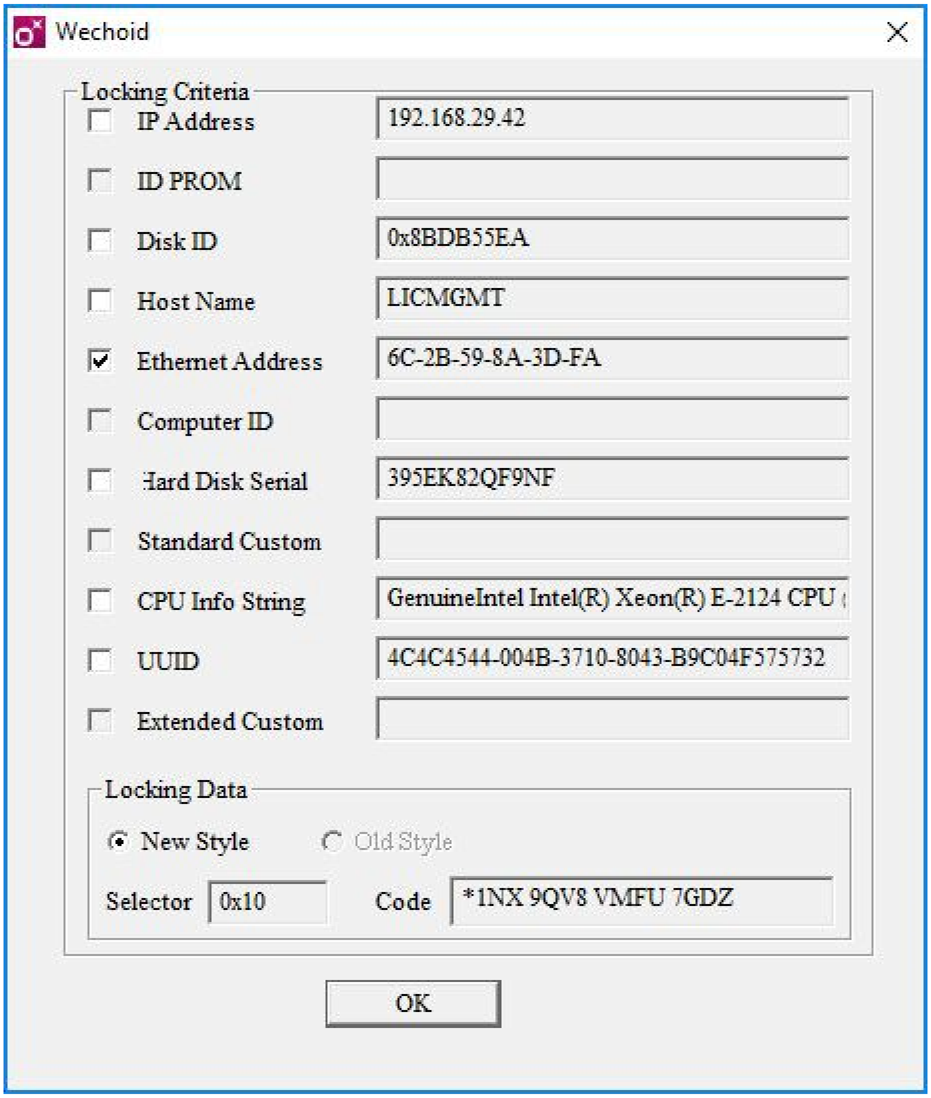
- The tool is applicable to Windows operating systems. See Windows: Installing the Sentinel RMS License Manager.

Before your software vendor creates a license code with any computer restrictions, you must get the locking code for your computer with the Wechoid program. Your software vendor will tell you which computers you must run Wechoid on. The Wechoid utility outputs either one or two hexadecimal locking codes depending upon how your software vendor has configured it. You will send all locking information to your software vendor. Your software vendor will use this information, which is specific to your computers, to generate new license codes.

Platform

Windows

When launched, the utility shows the available lock criteria (a checkmark is added next to each) and the values. Click to clear (uncheck) all checkboxes except for **Ethernet Address**.



Wechoid

Locking Criteria

☐ IP Address 192.168.29.42

☐ ID PROM

☐ Disk ID 0x8BDB55EA

☐ Host Name LICMGMT

☑ Ethernet Address 6C-2B-59-8A-3D-FA

☐ Computer ID

☐ Hard Disk Serial 395EK82QF9NF

☐ Standard Custom

☐ CPU Info String GenuineIntel Intel(R) Xeon(R) E-2124 CPU

☐ UUID 4C4C4544-004B-3710-8043-B9C04F575732

☐ Extended Custom

Locking Data

● New Style ○ Old Style

Selector 0x10

Code *1NX 9QV8 VMFU 7GDZ

Thermo-Calc User Guide: Graphical Mode

Thermo-Calc Version 2025b

Thermo-Calc Software

Working in Graphical Mode

In this section:

The Graphical Mode Desktop Layout

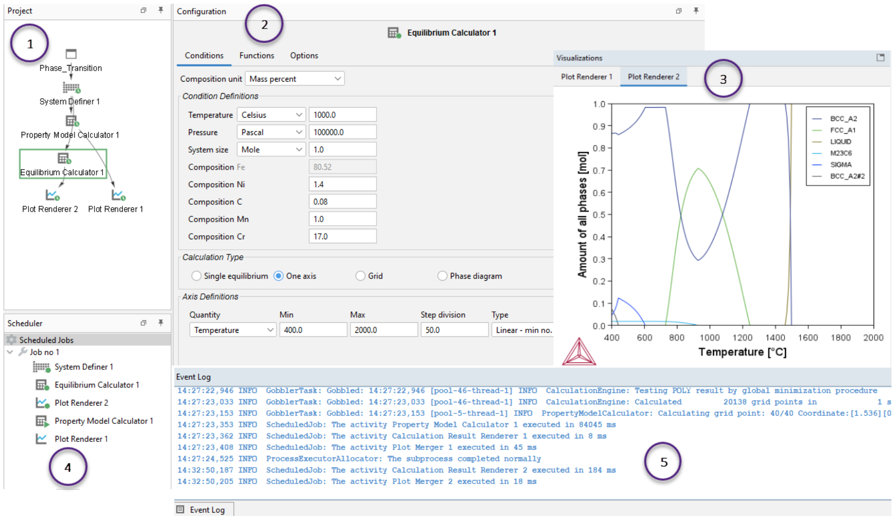
Open Thermo-Calc to view the default graphical user interface (GUI) layout for Graphical Mode. The windows are:

1. **Project**: Create, make changes, and navigate between the activities that make up a project. Click the **My Project** node to access the Quick Start wizard, a variety of templates to create projects for all the calculator types, and several other resources.
2. **Configuration**: Shows the settings that can be configured for the currently selected activity node, i.e. when you click the **Equilibrium Calculator**, the **Configuration** window has the settings for this node.
3. **Visualizations**: Shows the results of a calculation, either plotted as a diagram or displayed in table format. For some types of calculations, there are also previews of settings shown in this window. In this example, there is only a Plot Renderer *tab* in the Visualizations window.

   Previews in the **Visualizations** window are applicable to some of the Add-on Modules, i.e. for the Diffusion Calculator, Precipitation Calculator, and AM Calculator. The information is detailed in the relevant sections of the documentation.

4. **Scheduler**: Displays information about jobs, such as calculations, that are being performed or are scheduled to be performed. You can cancel scheduled jobs and if a job has failed, then you can view information about the error.
5. **Event Log**: By default this window is closed but it displays during calculation processes. You can always open it to view progress of calculations and to troubleshoot.

   In this example, the **Visualizations** window also has a **Plot Renderer** tab. You can also have a **Table Renderer** tab and when working with calculations that have specialized settings, these tabs are also included and match the names of the nodes in the **Project** window.



Composition unit: Mass percent

Condition Definitions

Temperature: Celsius, 1000.0
Pressure: Pascal, 100000.0
System size: Mole, 1.0
Composition Fe: 80.52
Composition Ni: 1.4
Composition C: 0.08
Composition Mn: 1.0
Composition Cr: 17.0

Calculation Type

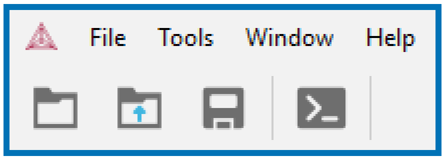
○ Single equilibrium ● One axis ○ Grid ○ Phase diagram

Axis Definitions

Quantity	Min	Max	Step division	Type
Temperature	400.0	2000.0	50.0	Linear - min no.

```
14:27:22,946 INFO  GobblerTask: Gobbled: 14:27:22,946 [pool-46-thread-1] INFO  CalculationEngine: Testing POLY result by global minimization procedure
14:27:23,033 INFO  GobblerTask: Gobbled: 14:27:23,033 [pool-46-thread-1] INFO  CalculationEngine: Calculated         20138 grid points in            1 s
14:27:23,153 INFO  GobblerTask: Gobbled: 14:27:23,153 [pool-5-thread-1] INFO  PropertyModelCalculator: Calculating grid point: 40/40 Coordinate:[1.536][0
14:27:23,353 INFO  ScheduledJob: The activity Property Model Calculator 1 executed in 84045 ms
14:27:23,362 INFO  ScheduledJob: The activity Calculation Result Renderer 1 executed in 8 ms
14:27:23,408 INFO  ScheduledJob: The activity Plot Merger 1 executed in 45 ms
14:27:24,525 INFO  ProcessExecutorAllocator: The subprocess completed normally
14:32:50,187 INFO  ScheduledJob: The activity Calculation Result Renderer 2 executed in 184 ms
14:32:50,205 INFO  ScheduledJob: The activity Plot Merger 2 executed in 18 ms
```

Menu, Toolbar, and Keyboard Shortcuts



The **File** menu and toolbar are reserved for Graphical Mode but in Console Mode the **Tools**, **Window**, and **Help** menus have the same options.

> For Mac users, the **Tools** menu has only one item. The global **Options** window is opened by selecting **Thermo-Calc** *<version>* **→ Preferences** or press <⌘> on the keyboard.

In Console Mode you use commands to access the other options, for example see Main Menu Commands.

Graphical Mode Menu and Toolbar Options

Button or Icon	*Action*	*Description*	*Action (s)*
	New Project	Create a new project. Also see Creating a Project from a Template.	• Click the **New** button on the toolbar • Select **File → New Project** • Windows: Press <Ctrl+N> • Mac: Press < ⌘ + N>
	Open Project	Open an existing project. See Opening Project Files.	• Click the **Open** button on the toolbar • Select **File → Open Project** • Windows: Press <Ctrl+O>. • Mac: Press < ⌘ + O>
--	Open Recent Project	Open a recent project. See Opening Project Files.	Select **File → Open Recent Project** and choose from the list of projects or click **Clear Recent Projects** to reset the list. Up to the last 10 projects are listed

Button or Icon	***Action***	***Description***	***Action (s)***
			and numbered in the order at which last opened.
	Save	Save a project. See Saving Project Files.	• Click the **Save** button on the toolbar • Select **File → Save Project** • Windows: Press <Ctrl+S>. • Mac: Press < ⌘ + S>
	Save Project As	Save an existing project with a new name. See Saving Project Files.	• Select **File → Save Project As** • Windows: Press <Ctrl+Shift+S> • Mac: Press < ⇧⌘ + S>
	Switch to Console Mode	This button is available when working in Graphical Mode. Click to switch to Console Mode and the command prompt.	Click the button to exit Graphical Mode and open Console Mode.
	Switch to Graphical Mode	This button is available when working in Console Mode. Click to switch to Graphical Mode and work with the GUI version.	Click the button to exit Console Mode and open Graphical Mode.
	Append Project	Combine two projects into one project file. See Appending Project Files.	• Select **File → Append Project** • Windows: Press <Ctrl+Shift+O> • Mac: < ⇧⌘+O>
	Exit	Exit the program.	• In the upper right-corner of the program, click the X. • Windows: Select **File → Exit** or press <Ctrl+Q> on the keyboard. • Mac: **Thermo-Calc** *<version>* **→ Quit** or press <⌘+Q> on the keyboard.
	Options	Change the global defaults for a variety of settings.	To open the **Options** window:

Button or Icon	***Action***	***Description***	***Action (s)***
		See Global Settings.	• Windows: Select **Tools** → **Options**. • Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.
⛁	Database Checker	Open the **Database Checker**, a program to check that the syntax of Thermo-Calc database files is correct. This is for advanced users who develop and manage databases. See About the Database Checker.	Select **Tools** → **Database Checker**
--	Window menu	Highlight a specific window on the GUI	From the **Window** menu, select an option to refocus on that specific window.
?	Help	Open the help system where you can browse or search all the Thermo-Calc documentation. This does not require an Internet connection. The content is stored locally.	First open Thermo-Calc, then choose one of these options to go to the local browser version of the help: • Press <F1> on the keyboard. • Select **Help** → **Online Help**. • On the **My Project Configuration** window, click **Online Help**. • At the bottom of any **Configuration** window, click **Help**.
▶	Video Tutorials	Open a link to the Thermo-Calc website where a variety of video tutorials are available.	• Select **Help** → **Video Tutorials** • On the **My Project Configuration** window, click **Video Tutorials**.
📈	Examples Files	Open the examples folder based on whether you are in Console Mode or Graphical Mode. Also see Opening Example Project Files in Thermo-Calc.	• Select **File** → **Examples Files**. • Select **Help** → **Examples Files**. • On the **My Project Configuration** window, click

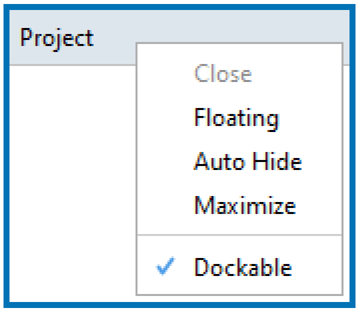
Button or Icon	***Action***	***Description***	***Action (s)***
			📈 **Example Calculation**.
📁	Manuals Folder	Open the folder on your computer that has the PDF documentation and guides. Also see About the Manuals (Documentation) Folder.	Select **Help → Manuals Folder**
🗎	Show License Info	Open the License Information window. Also see Displaying Thermo-Calc License Information and the *Thermo-Calc Installation Guide*	Select **Help → Show License Info**
⟳	Check for update	Check for updates to the software. Also see Updating the Software for Interim Releases.	Select **Help → Check for Updates**
✎	Request Support	Open a link to the Support on the Thermo-Calc website. There are instructions about how to submit your question.	Select **Help → Request Support**
	New in Thermo-Calc 2025b	Each release this pop up window includes details about the new and improved features and databases, with links to content on the website.	Select **Help → New in Thermo-Calc <version>**
ⓘ	About	Includes the version number of the installed software and information about third party software licenses.	Select **Help → About**
🗎	Notes	Open a **Notes - My Project** window to add notes to your project file.	At the bottom center of the **Configuration** window, click the Notes (🗎) button. Once a note is added, hover your mouse over the button and it is then called **Read and edit notes**.

Organizing the Windows on the Desktop

The windows on the Thermo-Calc desktop can be fixed or free floating. By default, most windows are fixed and open.

Using a combination of menu (right-click the window bar) and buttons (top right corner of a window), you can organize the windows as needed for your workflow.

For example, right-click the top of a window to select from the options to float, auto hide, maximize, or dock it. You can also left-click on the top bar of a window to float (i.e. detach) and move a window or to dock it again using the guides on the screen.



Reset the Desktop Layout

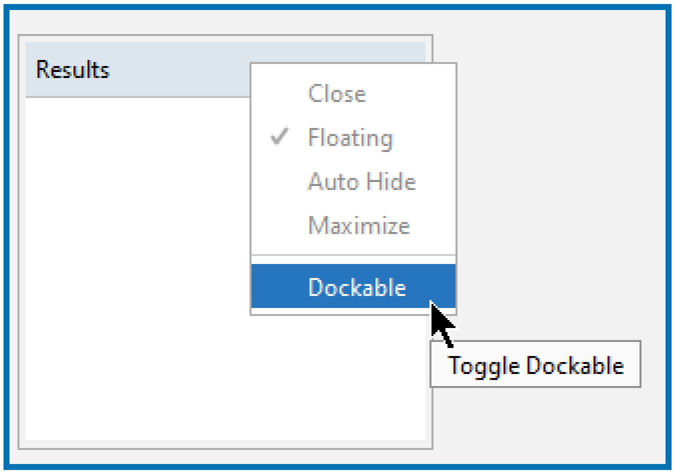
At any time to return to the standard desktop layout, from the main menu, select **Window → Reset Windows**.

Make a Window Dockable or "Permanently" Floating

By default windows are dockable, i.e. you can move the windows around using the outline guides and adjust the layout location for each window on one monitor. When a window is NOT dockable the window can be moved around it is just does not become part of the layout, it stays floating all the time (i.e. it is "permanently" floating).

> When **Dockable** is turned off (i.e. not selected) the other options are not available and there are no buttons at the top right corner of the window. However, you can reset the desktop layout to return it to the default location.

Right-click the top of a window to select **Dockable** to turn this option on and off.



Auto Hide (Minimize) a Window

When a window is fixed it can also be set to auto hide. Auto-hiding means that the window is minimized and placed as a tab either along the top or bottom or side of Thermo-Calc. A free-floating window is shown on top of the other windows and can be moved outside the frame of Thermo-Calc. when you select another window.

- Right-click the top of a window to select **Auto Hide** to turn this on and off.
- Click the pin and unpin buttons to **Toggle auto-hide** on and off. The buttons are on the top-right of a window.
- Click the minimize – button to **Hide active auto-hide window**. The window automatically minimizes if another window is selected. This button is available on the top right of a window that is already set to auto-hide.

The **Event Log** window is set by default to auto-hide.

Maximize or Restore a Window

- Double-click the top bar of a window (i.e. Project, Configuration, Visualizations, etc.) to maximize the window pane across the whole monitor. This hides the other windows. To restore the configuration (and the hidden windows) double-click the top bar of the window a second time.

> This can be useful for small screens, or if you are working on a large screen and want to compare two configurations side-by-side.

- Right-click the top of a window to select **Maximize**. To restore the window to its previous state and location, right-click the bar of the window again and select **Restore**.

Float or Fix a Window

There are several ways to float and fix a window back to its most recent location in the layout.

- Right-click the top of a window to select **Floating** and turn this on and off.
- Left-click on the top bar of a window to float (i.e. detach) and move a window or to dock it again using the guides on the screen.
- Click the **Toggle floating** ▫ button to float the window.
- Click the **Toggle floating** ☐ button to turn off floating and dock the window automatically to its last location.

Projects and Activities

In this section:

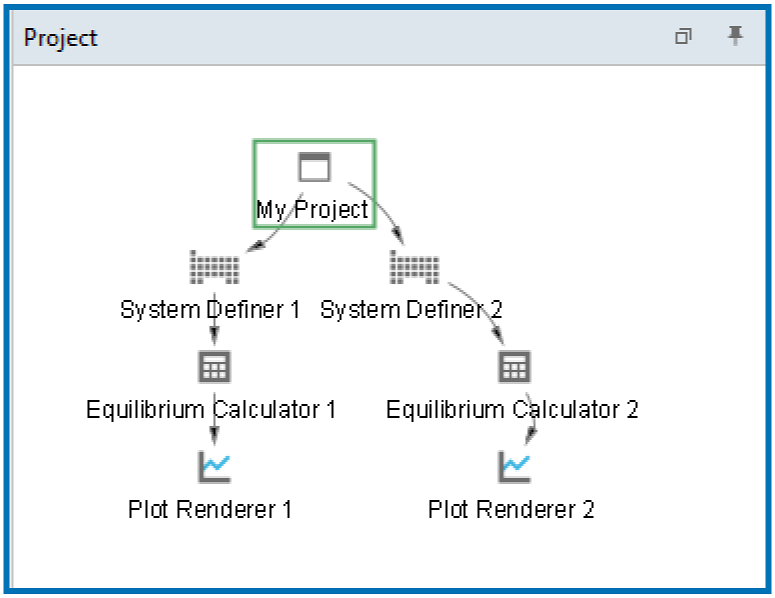
About the Activity Nodes

Graphical Mode Activities vs Console Mode Modules

In a *project*, a set of linked activities is called a *tree*. A result calculated within a tree is fed as input into the next *activity* in the tree. Consequently, if you have an Equilibrium Calculator with another Equilibrium Calculator as its *successor*, the successor takes the calculation results of the *predecessor* as the starting values for its calculation. When working with activities in the Project window these are also referred to as *nodes* (or *activity nodes*) in the tree structure.

The example below shows a *My Project* node with two trees. In each tree, settings and calculation results are propagated downward until the calculation and the visualization of the results are completed in the *Plot Renderer* nodes.

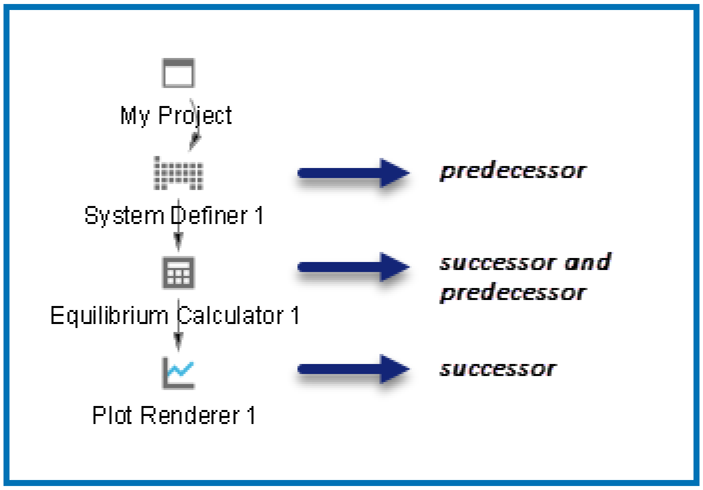
The system definitions, settings, and calculation results of the two trees are independent of each other in this example.



There are several resources available on our website to help you learn how to use Thermo-Calc and other Add-on Modules. Go to the Getting Started Guides page and choose one of the guides that provides new users an introduction to setting up simple calculations in Graphical Mode. The information there is also in this help documentation.

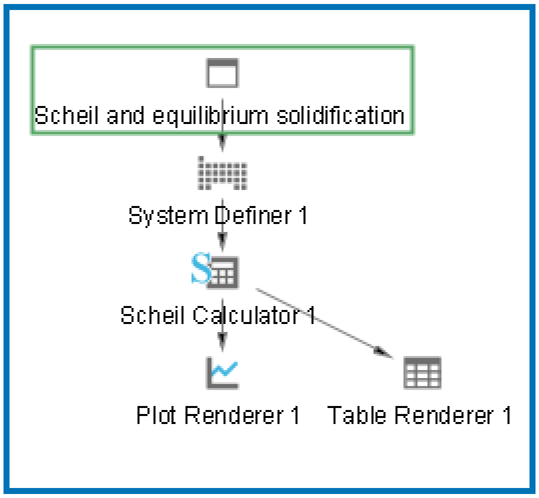
Activity Successor and Predecessor Nodes

An activity node located below another activity node in a tree is referred to as that activity's *successor*. An activity located above another activity is called that activity's *predecessor*. A predecessor is performed before the predecessor's successors and its result is fed forward to any successor activities.



For example, to calculate and display a phase diagram, create a branch with three linked activities: A **System Definer** activity linked to an **Equilibrium Calculator** activity, which in turn is connected to a **Plot Renderer** activity.

You can determine the available successors by right-clicking a node in the **Project** window to browse what is available from the menu and follow the arrows connecting the nodes. The example below shows that **Scheil Calculator 1** is a predecessor to the successors, **Plot Renderer 1** and **Table Render 1**.



Creating Activities and Successors and Cloning Activities and Trees

Activity Node Descriptions

The table below is a brief description of the activity types you work with in the **Project** window. When working with activities these are referred to as *nodes* in this documentation.

These are the project activity nodes available in Graphical Mode. Some of these require additional licenses for full feature availability. Listed in alphabetical order.

Activity Type	***Description***
AM Calculator	Using the Additive Manufacturing (AM) Module this activity is used in conjunction with either the Scheil Calculator or a Material Library to define the necessary settings to better understand the laser powder bed fusion (LPBF) process by predicting the temperature distribution and melt pool geometry as a function of process parameters. There is also connectivity with the Diffusion Calculator and Precipitation Calculator to include probe data with a Thermal Profile calculation. In DEMO mode you can view the settings and experiment with some things, but no calculations can be run.
Binary Calculator	Use it for some calculations involving two components only. It is like a combination of System Definer and Equilibrium Calculator activities with adaptations to simplify the configuration of calculations on binary systems. To perform this activity, you need a database designed for the Binary Calculator, such as the TCBIN database.
Diffusion Calculator	Using the Diffusion Module (DICTRA), this activity is where you set the geometry, add one or more regions, enter grids and phases in the regions, and then enter compositions of phases. You can also use this in DEMO mode with up to three components. There is also connectivity to the Scheil Calculator and to other Add-on Modules such as the Additive Manufacturing (AM) Module.
Equilibrium Calculator	Set thermodynamic conditions and define axis variables when a series of equilibrium calculations are to be performed in one or more dimensions.
Experimental File Reader	Read experimental data files (*.EXP). This type of file contains information specifying a plotted diagram, written in the DATAPLOT graphical language.
Material to Material Calculator	This activity calculates materials transitioning from one into the other.
Plot Renderer	Determine the layout of non-text based output.
Precipitation Calculator	Set the conditions for, and perform, a precipitation calculation using the Precipitation Module (TC-PRISMA). You can also use this in DEMO mode with up to three components. There is also

Activity Type	***Description***
	specialized connectivity to the Yield Strength Property Model and to other Add-on Modules such as the Additive Manufacturing (AM) Module.
Process Metallurgy Calculator	This calculator allows for efficient setup of advanced calculations involving slag, metal and gas. Define the composition of a steel and slag system using material groups: one each for steel, slag and gas.
Property Model Calculator	Choose one or more **General Models** to predict and optimize material properties. You can evaluate models simultaneously over a range of compositions and cross plot the results. You can then conduct an uncertainty analysis and plot the results as either a histogram or as a probability plot. With additional licenses, there are material specific libraries, i.e. **Steel Models**, **Nickel Models**, and others available.
Scheil Calculator	Perform Scheil-Gulliver calculations (also known as Scheil calculations). A default Scheil calculation is used to estimate the solidification range of an alloy assuming that i) the liquid phase is homogeneous at all times and ii) the diffusivity is zero in the solid. However, it is possible to disregard the second assumption for selected components. The Scheil Calculator is also used with other specialized Add-on Modules such as the Diffusion Module (DICTRA) and Additive Manufacturing (AM) Module.
System Definer	Define a certain thermodynamic system and read it from file into memory.
Table Renderer	Use this activity for text-based output.
Ternary Calculator	Use it for some calculations involving three components. It is like a combination of System Definer and Equilibrium Calculator activities with adaptations to simplify the configuration of calculations on ternary systems. To get a reliable result you need a database that fully assesses binary and ternary systems.

Activity Node Workflow

You can set up a tree in the **Project** window (starting with the **My Project** node) and then perform all the activities at once, or create and perform one activity at a time.

Additional licenses are required for some of the listed features.

You can also use the templates to add all the necessary activity nodes based on your simulation needs. See Creating a Project from a Template.

The typical workflow is to:

1. *Define a System*: Add a System Definer activity (in the **Project** window) where you select a database and the elements to have as system components (in the **Configuration** window).

   To the **My Project** node, you can alternatively add and define one of these activity nodes: AM Calculator, Binary Calculator, Ternary Calculator, Process Metallurgy Calculator, or Experimental File Reader.

2. *Set up and run a calculation*: Add an Equilibrium Calculator activity (a successor to the **System Definer**), where calculation conditions are set (temperature, pressure, etc.). This is where axis variables are set to create a property or phase diagram. These settings are also made in the **Configuration** window. You can also add a Property Model Calculator, Material to Material Calculator, Precipitation Calculator, Diffusion Calculator, or Scheil Calculator to the System Definer. The AM Calculator is also available and can either be added directly to the **My Project** node or as a successor to the Scheil Calculator. It depends how you work with this Add-on Module.
3. *Preview some settings*: For some specialized calculations (i.e. with the Add-on Modules), you can preview the settings in the **Visualizations** window. For example, for the Diffusion Calculator (Composition Profiles and Thermal Profiles), for the Precipitation Calculator (Thermal Profiles), and with the AM Calculator a variety of settings are previewed during the set up.
4. *Visualize the results*: Add either a Plot Renderer or a Table Renderer activity in the **Project** window. When calculated, this creates a plot or table in the **Visualizations** window. The results are shown in a **Plot Renderer** or a **Table Renderer** tab.

You need to **Perform** a Plot Renderer or a Table Renderer activity to visualize the calculation results from an Equilibrium Calculator.

Getting Started Links and Templates and About the Activity Nodes

Creating Activities and Successors

You can create a new activity in these ways:

- In the **Project** window, right-click an activity and choose **Create New Activity** (**My Project** node only) or **Create New Successor** (all other nodes).
- Select the activity you want to create from the submenu.
- At the bottom of the **Configuration** window, click **Create New Activity** or **Create New Successor** and select the activity to create.
- Use the available templates or the **Quick Start** wizard: Click the **My Project** node and select templates from the **Configuration** window to quickly add a set of activity nodes to the tree.

> The activity nodes listed in the table are in alphabetical order not in order of selection from the various menus. Additional licenses are also required to access full functionality for any Add-on Modules.

Activity	*Possible Predecessors*	*Possible Successors*
My Project	None; this is the first node of the tree structure. You can add activities using the Quick Start wizard or templates. Getting Started Links and Templates	AM Calculator, System Definer, Binary Calculator, Ternary Calculator, Process Metallurgy Calculator, or Experimental File Reader. Also choose templates from this level.
AM Calculator	My Project, Scheil Calculator	Plot Renderer, Diffusion Calculator, Precipitation Calculator When a Diffusion Calculator or Precipitation Calculator is added, a full set of nodes, including a System Definer and Plot Renderer, are added as a template to the top My Project node. The Diffusion Calculator or Precipitation Calculator is linked to the AM Calculator.

Activity	***Possible Predecessors***	***Possible Successors***
Binary Calculator	My Project	Plot Renderer
Diffusion Calculator	System Definer, AM Calculator	Plot Renderer, Table Renderer
Equilibrium Calculator	System Definer, Equilibrium Calculator	Equilibrium Calculator, Plot Renderer, Table Renderer
Experimental File Reader	My Project	Plot Renderer
Material to Material Calculator	System Definer	Plot Renderer, Table Renderer
Plot Renderer	Equilibrium Calculator, Material to Material Calculator, Property Model Calculator, Binary Calculator, Ternary Calculator, Scheil Calculator, Process Metallurgy Calculator, Diffusion Calculator, Precipitation Calculator, AM Calculator, Experimental File Reader	None
Precipitation Calculator	System Definer, AM Calculator	Plot Renderer, Table Renderer
Process Metallurgy Calculator	My Project	Plot Renderer, Table Renderer
Property Model Calculator	System Definer	Plot Renderer, Table Renderer
Scheil Calculator	System Definer	Plot Renderer, Table Renderer, AM Calculator, Diffusion Calculator
System Definer	My Project, System Definer	Property Model Calculator, Equilibrium Calculator, Precipitation Calculator, Scheil Calculator
Table Renderer	Equilibrium Calculator, Material to Material Calculator, Property Model Calculator, Binary Calculator, Scheil Calculator, Process Metallurgy Calculator, Diffusion Calculator, Precipitation Calculator	None
Ternary Calculator	My Project	Plot Renderer

Cloning Activities and Trees

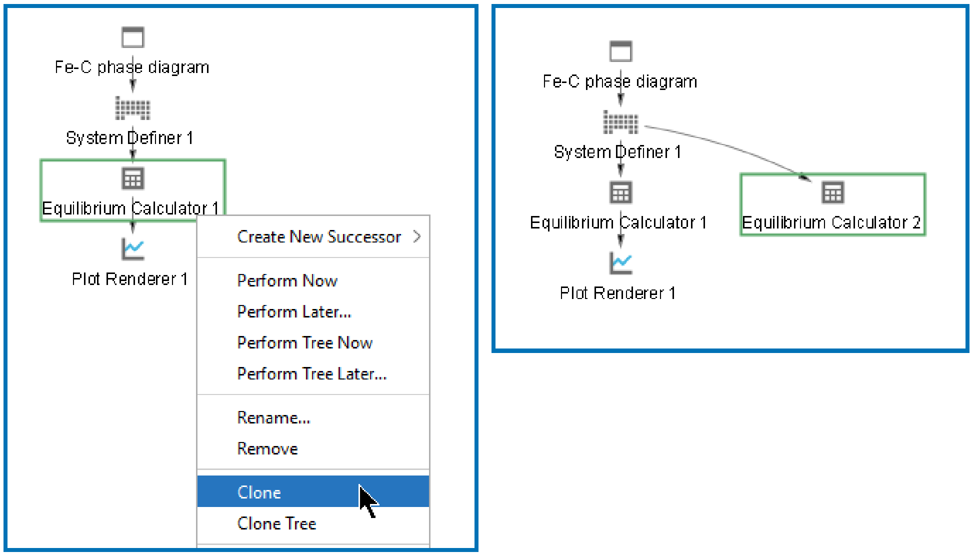
As described in Creating Activities and Successors, you can clone a single activity or the selected activity and all the activities that come after it (successors). The predecessor of the selected activity also is the predecessor of the clone.

Cloned activities are configured exactly like the activities that they were cloned from, and any results of calculations or plots are also cloned. To clone a selected activity, right-click the activity and select **Clone**.

For example, if you clone the Equilibrium Calculator in this project the result is an **Equilibrium Calculator 2** created as a successor to **System Definer 1**.

The following applies to clones.

- The new Equilibrium Calculator has the same settings for conditions, functions and options as its Equilibrium Calculator 1 clone.
- If the Equilibrium Calculator is already performed, then the calculation results are cloned.
- If the activity is a Plot Renderer or a Table Renderer, then the plot or table is cloned.
- If you want to clone all the successor activities that follow a selected activity, then right-click and select **Clone Tree** instead.



Cloning an Equilibrium Calculator activity node.

About Equilibrium Calculator Clones and Successors

If you create an Equilibrium Calculator as a successor to another Equilibrium Calculator, then the successor inherits all the settings for conditions, functions and options from its predecessor. In this respect, it is similar to a clone.

> ❗ The Equilibrium Calculator successor is different from a clone in that it does not inherit any calculated results and it is a successor to the Equilibrium Calculator instead of a successor to its predecessor.

The calculated result from an Equilibrium Calculator that is the predecessor to another Equilibrium Calculator is the starting value for the latter's calculation. On the other hand, the clone of an Equilibrium Calculator does not receive any data as input from the Equilibrium Calculator that it is cloned from.

Moving or Grouping Nodes and Using the Grid

In the **Project** window, you can work with the activity nodes in these ways.

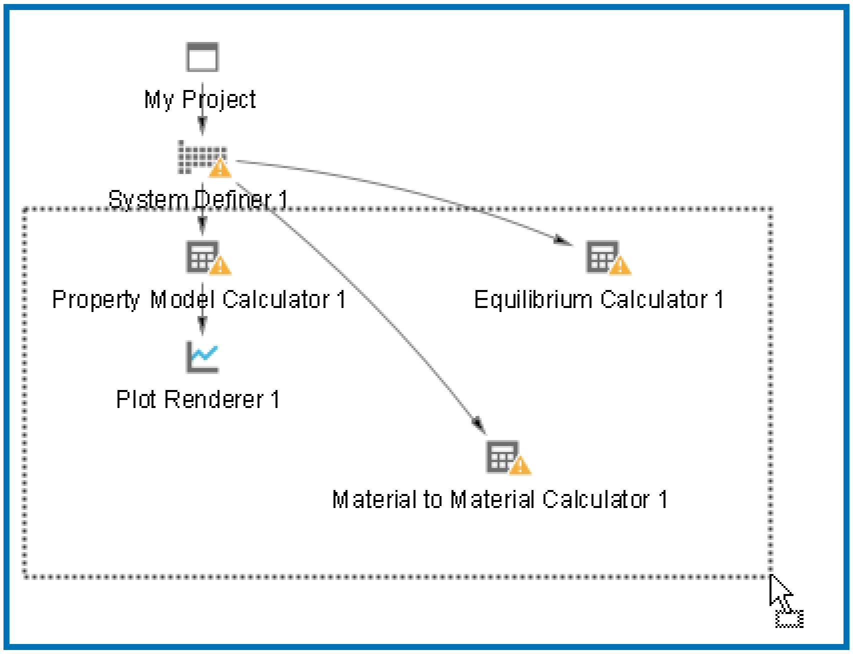
- Select and move individual nodes
- Select several nodes at a time
- Select and then group activity nodes
- Show the grid and "snap" to it
- Apply Auto Layout

Select and Move Individual Nodes

- Click an activity node to select it.
- To move activities, click and hold the activity node and move the cursor.

Select Several Nodes at a Time

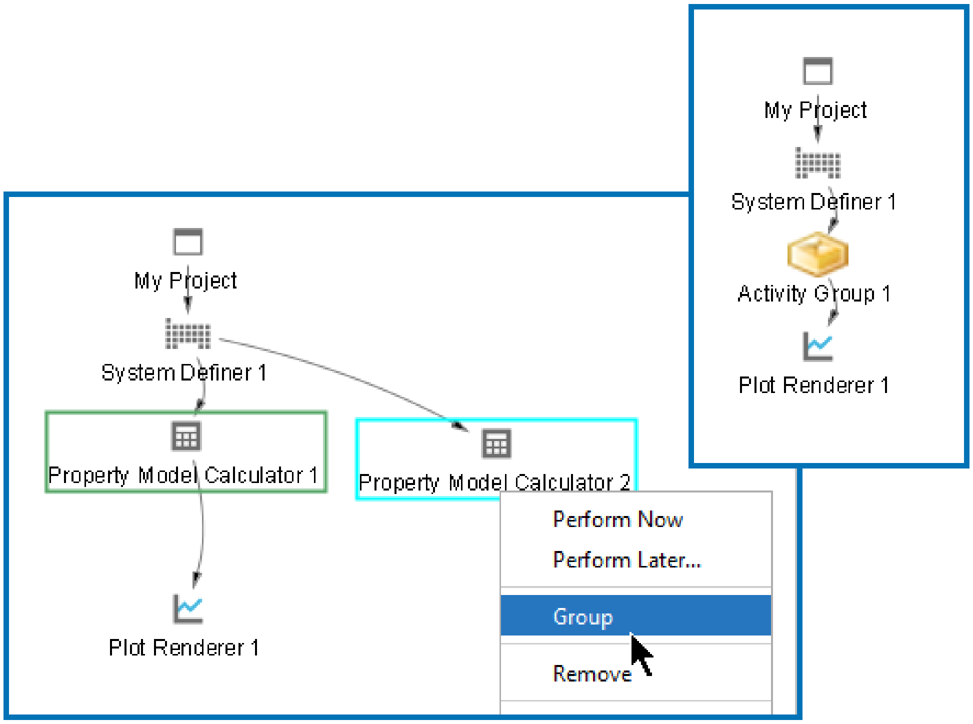
- To select several activity nodes, hold down <Ctrl> while clicking on each node you want to select.
- Click and hold the mouse button and draw a square around the activity nodes to select. Both the name and the icon that represents an activity must be within the square.



Group Activity Nodes

You can group activity nodes together on the **Project** window. This also creates separate tabs on the **Configuration** window so you can more easily edit the settings for each one. It is important to have logical groupings of nodes because the calculation relies on this connectivity.

In the **Project** window, control + click to select each node, then right-click and select **Group**. An **Activity Group** node is created (you can rename it) and on the **Configuration** window there are two tabs created, named for each of the group nodes. For example, Property Model Calculator 1 and Property Model Calculator 2. The order of the tabs is based on the order of when you select each node.



Apply Auto Layout

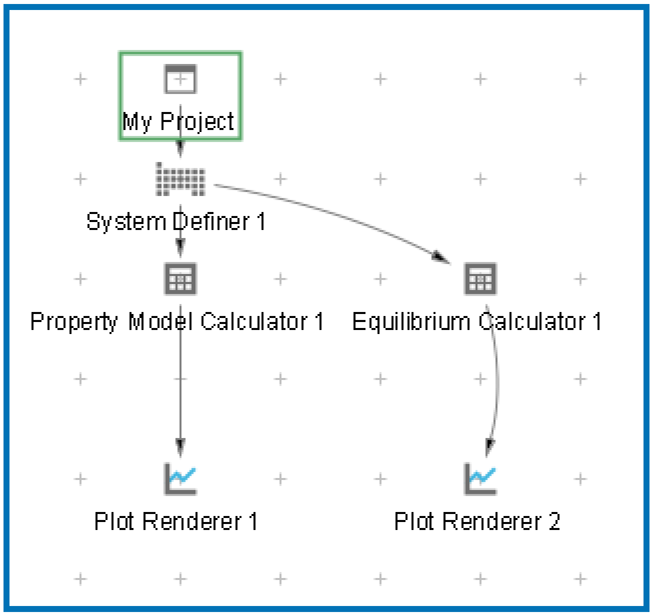
In the **Project** window, right-click anywhere and choose **Apply Auto Layout** from the menu. The nodes and the tree default to the center of the Project window.

Show Grid and Snap to Grid

To show a grid of light grey cross-hairs overlaid on a project, click **Show Grid** in the toolbar. Click the button again to turn the grid off. Or right-click in the **Project** window and select **Show Grid**.

Click **Snap to Grid** in the toolbar or right-click in the **Project** window and select **Snap to Grid** to automatically position each activity in the Project window at a cross-hairs point in the grid.

The Project window with the grid turned on and activity nodes moved from the default location. These nodes are snapped to the grid.


My Project
System Definer 1
Property Model Calculator 1
Equilibrium Calculator 1
Plot Renderer 1
Plot Renderer 2

Node or Window Status Markers

Status markers indicate whether an activity is ready to be performed, is being performed, or has been performed. The markers are overlaid on the activity nodes in the **Project** window. The status markers are displayed on a **System Definer** node.

? About the Activity Nodes

Project Window Status Markers

Status	Description
▦	No status marker means the activity is ready to be performed (i.e. it has not been performed).
▦ !	A yellow circle with an exclamation mark means there is an error or the activity needs to be run again. For example, the necessary configurations for the activity may not be set or other prerequisites are not met.
▦ ▶	A green circle with a right-facing arrow means the activity is being performed.
▦ 🕒	A pink circle with a clock face means the activity is currently scheduled to be performed or in the process of being performed.
▦ ⏸	For the Diffusion Calculator and Precipitation Calculator, you can pause a calculation. A blue circle with a the pause symbol indicates this state.
▦ ✓	A green circle with a check mark means the activity has finished its calculation, i.e. it is performed.

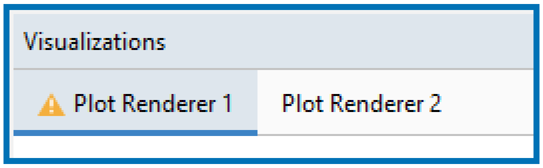
Scheduler Window Status Markers

Status	Description
▦	No status marker means the activity (the job) is scheduled to be performed (the job has not started).

Status	**Description**
!	A yellow circle with an exclamation mark means there an error happened during the activity job.
▶	A green circle with a right-facing arrow means the activity (the job) is being performed.
✓	A green circle with a check mark means the activity (the job) performed successfully.

Visualizations Window Status Marker

If you have plotted a diagram and then modify something in the tree that the Plot Renderer is associated with, then a notification —an exclamation mark enclosed in a yellow triangle— is shown in the **Visualizations** window for the applicable tab. The tab names match the node names in the **Project** window (i.e. if a node is renamed, the tab is renamed to match).

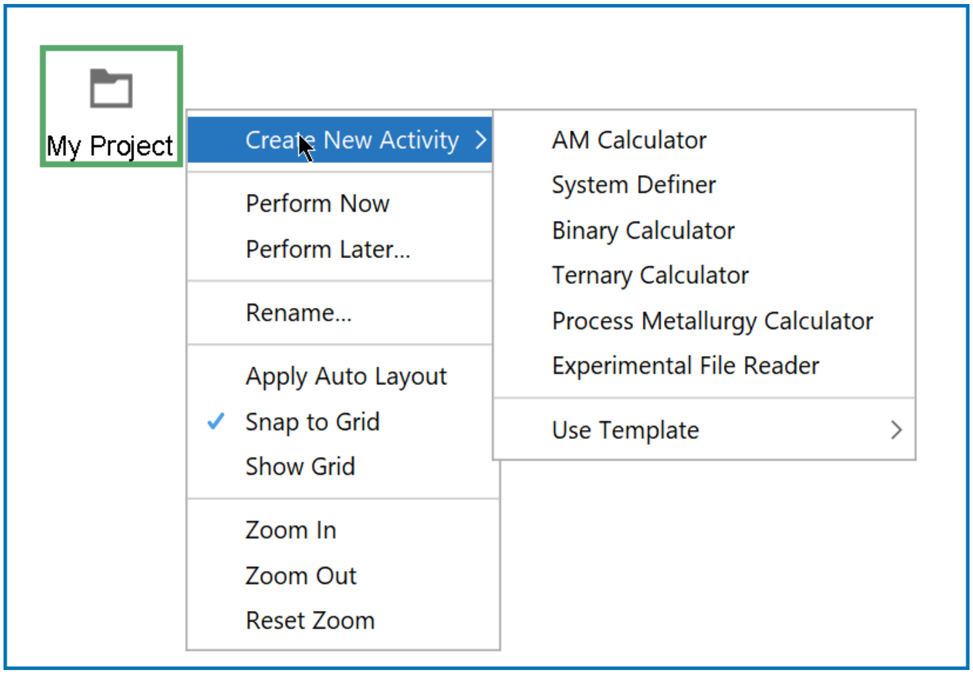


My Project and Activity Menus

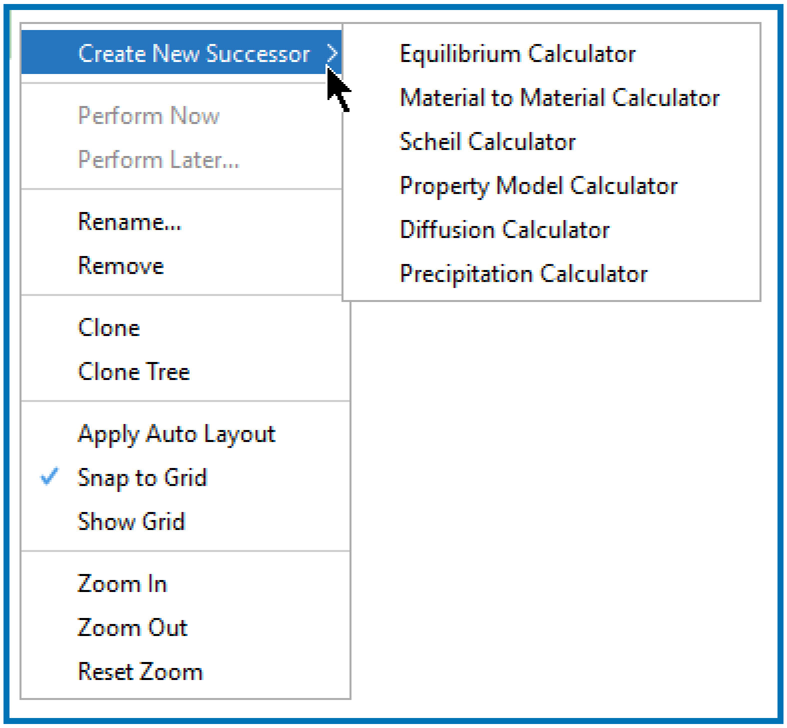
When working in the Project window you can right-click nodes to open menus with the available actions. For example, click the **My Project** node to open the menus. Most nodes in the tree have a common menu with differences due to placement in the tree and the activity type.

About the Activity Nodes

Menus



My Project Node



Activity Node General

Menu Options for Activity Nodes

Option	*Description*	*Action (s)*
Create New Activity	Add AM Calculator, System Definer, Binary Calculator, Ternary Calculator, Process Metallurgy Calculator, and Experimental File Reader nodes.	Right-click **My Project** and from the **Create New Activity** menu choose an option. ? [Creating Activities and Successors]
Create New Activity → Use Template	Choose from the available templates to use the Wizard or add predefined nodes.	Right-click **My Project** and from the **Create New Activity → Use Templates** menu choose an option. The templates are also available on the **Configuration** window, which you can access by clicking the **My Project** node, or from the **Window** menu.

Option	***Description***	***Action (s)***
		Creating a Project with the Quick Start Wizard or Creating a Project from a Template
Create New Successor	Add a successor to the selected node.	Right-click the **System Definer**, any **Calculator** node or the **Experimental File Reader**. Then from the **Create New Successor** menu choose an option. Creating Activities and Successors
Add a Predecessor	Add a predecessor to the selected node.	Right-click a node to add a predecessor to it (when available).
Perform Now or Perform Later	Perform a calculation or create a plot or table immediately, or schedule it for a time in the future.	Right-click any node. Using the Scheduler
Perform Tree Now or Perform Tree Later	Perform a calculation for the whole project immediately, or schedule it for a time in the future.	Right-click the System Definer or any Calculator node. Using the Scheduler
Rename	Change the name of the node.	Right-click any node.
Remove	Delete the selected node from the tree.	Right-click any node except My Project.
Clone	Duplicate the selected node and add it to the same tree.	Right-click any node except My Project. Cloning Activities and Trees

Option	***Description***	***Action (s)***
Clone Tree	Duplicate a tree and add it to My Project.	Right-click any node except My Project.
Apply Auto Layout	Apply an automatic layout to the nodes in the tree.	Right-click any node.
Snap to Grid	Snap a node to align it with the grid.	Right-click any node. ? Moving or Grouping Nodes and Using the Grid
Show Grid	Turn the grid on or off in the Project window.	Right-click any node.
Zoom In, Zoom Out, Reset Zoom	Zoom in and out of the Project window or reset the zoom to the default.	Right-click any node.

Saving Project Files

In Graphical Mode, Thermo-Calc uses a *project file* format with a `.tcu` suffix.

If you are working in Console Mode there are other file formats used for both Thermo-Calc and the Diffusion Module (DICTRA). See Working with the Console Mode File Types.

A project file always includes project activities and the configurations. You can also include calculated results, although there are factors and limitations that need to be considered as described below and also detailed in Opening Project Files and Converting Project Files to a Newer Version of Thermo-Calc.

In general, to save your project file, you can choose between the following methods:

- On the toolbar click the **Save** button.
- Press CTRL + S (Windows) or ⌘ + S (macOS).
- From the menu, select **File** → **Save Project**.
- When you want to give an existing project a new name, OR when saving with results, select **File** → **Save Project As** . See Including Calculated Results with Project Files and Saving a Project File with Results.

If you are working in a file that includes results, any method to save the project file continues to include the calculated results. However, if this is the first time results are being included, there are additional important factors to consider as described next.

Including Calculated Results with Project Files

Starting with Thermo-Calc version 2022b, saved calculated results are only accessible in the same version of Thermo-Calc in which it is originally created. For example, if you have a project file with saved results from version 2020a, the results are only immediately available in 2020a. You can regenerate results in a different version of the software but that can require adjustments to the configuration if new functionality or changes impact the particular project set up, especially if there is a wide gap between release versions.

When including calculated results in the project file there are these factors to consider: Future compatibility, file size, and plot design and themes.

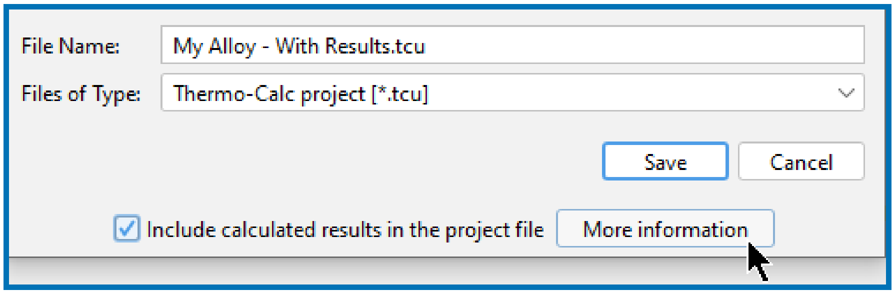
- **Future compatibility**: If you want to use this project file over time, in future versions of Thermo-Calc, it will require recalculation after opening. It also depends on the difference in versions; the project can require reconfiguration of the settings and other fine tuning. However, if you are going to work in the same version of the software for a short term project, for example, saving the file with results eliminates the need for re-calculating results when the file is re-opened. This is particularly advantageous when a simulation takes several hours to complete such as when working with the Add-on Diffusion (DICTRA), Precipitation (TC-PRISMA), and/or Additive Manufacturing Modules.
- **File size**: When results are included, the size of the file increases. This is especially true when working with the Add-on Diffusion (DICTRA), Precipitation (TC-PRISMA), and/or Additive Manufacturing Modules.
- **Plot design and themes**: When you save your results, the plot design may have local or global designs or themes applied, which are also saved as part of the calculated results. There are considerations related to this when you open the project file again, especially in future versions of the software. See Opening Project Files for more information.

Saving a Project File with Results

1. First, determine if saving results is efficient for your particular project based on future compatibility, file size, and plot design and theme factors. To save calculated results with the project file, choose an option:
   - From the menu, chose **File** → **Save Project As**or,
   - Press CTRL + Shift + S (Windows) or ⇧+⌘ + S (macOS).
2. On the **Save** window, select the **Include calculated results in the project file** checkbox.

> The checkbox is not available (it is greyed out) if no results have yet been calculated. In this case, go back to your project, click **Perform Tree** (or any other action to generate results) and then save the project file as above.

3. Click **More information** to learn about the activity nodes with calculated results that are included / saved in the project file.



File Name: My Alloy - With Results.tcu

Files of Type: Thermo-Calc project [*.tcu]

☑ Include calculated results in the project file

4. Enter a meaningful **File Name**. It can be useful to include the version of the software in the file name, especially if the file is converted in a future version of the software.
5. Navigate to the location where you want to save your project file and then click **Save**.

Converting Project Files to a Newer Version of Thermo-Calc

Opening Project Files

Opening a project file in the same software version in which it was saved, with or without results, is straight forward and there are several methods to open a file.

See the Saving Project Files topic for useful details about saving a project file to include calculated results.

- For standard instructions to open a project file with or without results, see Opening Project Files in the Same Version of Thermo-Calc. There are checkbox controls for plot themes and opening with or without results that are also described.
- To open a recent project file, see Opening Recent Project Files.

Starting with Thermo-Calc version 2022b, all older project files including results generated and saved in Thermo-Calc versions 2015a to 2022a, can only be opened with results in the original software version. You can still open a project file without results and then re-perform the calculation. However, this can require a review and update to the settings and configurations, especially if there is a wide gap between versions.

For old project files being opened in a different software version, see the topic Converting Project Files to a Newer Version of Thermo-Calc, where you can also learn about regenerating the results and the automatic creation of backup files in these instances.

Opening Project Files in the Same Version of Thermo-Calc

To Open a Project File from Thermo-Calc

1. To open a project file with or without results in the same version of the software in which it was created, choose a method below:
    - On the toolbar, click the **Open** button.
    - From the main menu, select **File** → **Open Project**.
    - Press <Ctrl+O> (Windows) or < ⌘ + O> (macOS).
2. On the **Open File** window review the checkboxes that control global plot themes and results:
    - By default the **Apply plot theme from Tools/Options** checkbox is selected and depends on whether the global setting checkbox is also selected on the **Options** window, which applies a predefined or custom theme globally to the project file. Click to deselect the checkbox to keep the original plot design in your project file. For more information about the settings, see About Project Files and Plot Themes for additional details.
    - For macOS users, **Tools/Options** refers to the **Options** window, which is accessed differently. Select **Thermo-Calc** *<version>* → **Preferences** or press <⌘> on the keyboard.
    - By default the **Open project with results if present** checkbox is selected. Click to deselect the checkbox if you want to exclude results for a file saved in the same version of the software.
3. If you are opening an older project file with results (in which case the file is converted), you are prompted by a secondary window that includes related version information and options to continue or not. **Even if the checkbox is selected, old project files still cannot be opened with results**. See Converting Project Files to a Newer Version of Thermo-Calc.
4. When you are ready, navigate to the file on your computer and click **Open**.

To Open a Project File from a File Location on the Computer

Navigate to the project file on your computer then choose between these methods:

- In an open instance of Thermo-Calc, drag and drop it into the **Project** window. This replaces any other project already open.
- Double-click to open it. This launches a new instance of Thermo-Calc.

The checkbox controls **Open project with results if present** and **Apply plot theme from Tools/Options** are not available when dragging and dropping or double-clicking to open.

For macOS users, **Tools/Options** is the same as the **Preferences** menu that accesses the **Options** window.

For old projects with results, and if you are dragging and dropping or double-clicking to open, you are also prompted to decide what to do next. See Converting Project Files to a Newer Version of Thermo-Calc.

Opening Recent Project Files

Select **File → Open Recent Project** and choose from the list of projects. Up to the last 10 projects are listed and numbered in the order in which they were last opened. You can click **Clear Recent Projects** to reset the list.

About Project Files and Plot Themes

When opening project files, a predefined or custom plot theme can be automatically applied to all plots. There are two checkboxes that control this, one is a global setting and one is a local setting applied to a specific file as it is opened.

If you double-click or drag and drop to open a project file it automatically uses the global settings in Thermo-Calc (which may or may not be to apply a theme). This means you may inadvertently apply a theme to your plots without realizing it.

On the **Open File** window, the **Apply plot theme from Tools/Options** checkbox is selected by default and applies a theme locally to the specific project file being opened. Click to clear the checkbox to allow the specific file to keep existing plot settings.

If this checkbox is selected or cleared it only applies to the specific project file being opened, i.e. the global settings **Apply the selected theme to opened file [.tcu]** checkbox on the **Tools → Options** window does not change.

For macOS users, **Tools/Options** is the same as the **Preferences** menu that accesses the **Options** window.

See Working with Plot Themes for the details about how the checkbox interacts with its counterpart.

If you have a project file with calculated results and local settings applied to plots i.e. applied from the **Visualizations** window to a specific plot via the **Plot Properties** settings window, then click to clear the local setting as you open the file using **Apply plot theme from Tools/Options** checkbox. Otherwise the default global settings are applied to all plots and you would need to individually change these settings back to your original design. Alternatively, experiment with applying a predefined theme, e.g. **Publication**, as this could be sufficient for your final output.

Opening Project Files Including Results and with Different GES Versions

When projects with calculated results created with a different Gibbs Energy System (GES) version than selected from the **Options** window, the results are discarded as these are not 100% compatible.

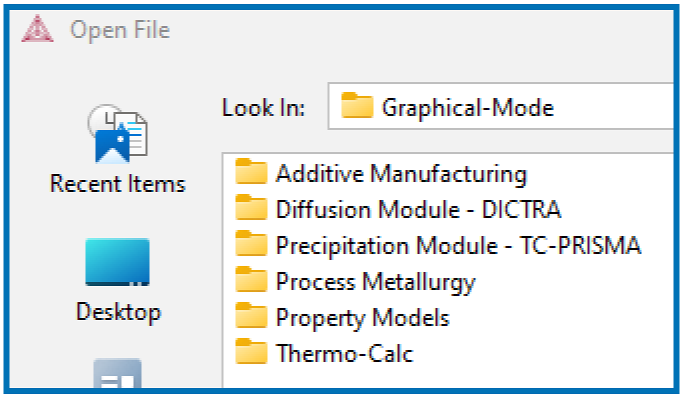
GES6 (**Version 6** is the default, but some may be using GES5 (**Version 5**). See Global General Settings for more information.

Opening Example Project Files in Thermo-Calc

Additional licenses may be required to run calculations with the examples. The individual example descriptions detail this information.

To open an example project file:

1. Open Thermo-Calc.
2. Confirm you are in Graphical Mode. If not, click the **Switch to Graphical Mode** button.
3. There are these ways to open the folders and files:
    - From the main menu select **File** → **Examples Files**
    - From the main menu select **Help** → **Examples Files**.
    - Click the **My Project** node and on the **Configuration** window, click the **Example Calculation** button.
4. The examples are divided into folders. Navigate to the folder and project file you want and double-click to open.

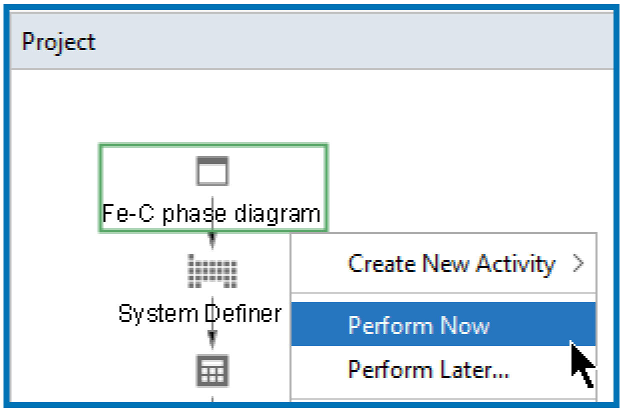


Look In: Graphical-Mode

Additive Manufacturing
Diffusion Module - DICTRA
Precipitation Module - TC-PRISMA
Process Metallurgy
Property Models
Thermo-Calc

5. The Graphical Mode examples are stored without calculated results so you will want to run the example calculation and generate a plot or table. To do this, click the first node in the tree at the top of the **Project** window. Then right-click and select **Perform Now**. Some examples require additional licenses in order for the calculation

to run.

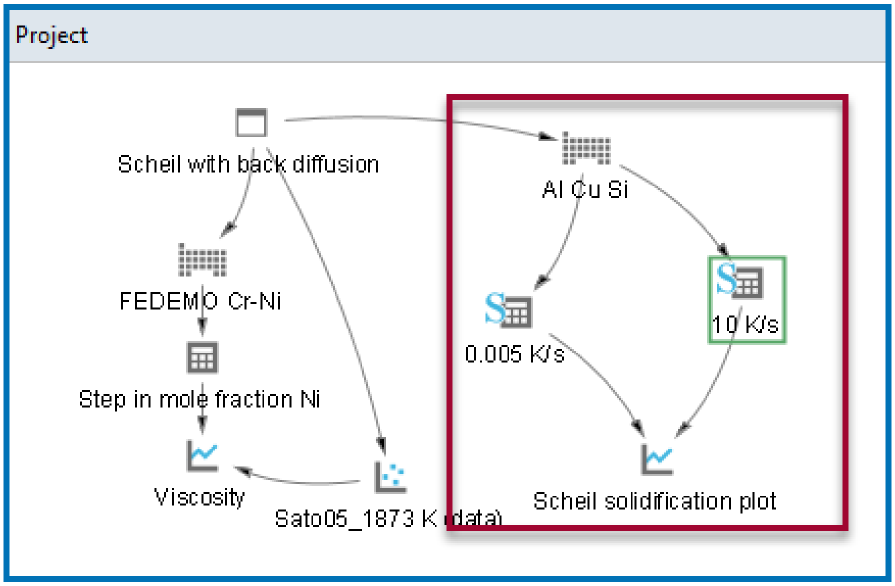

Project
Fe-C phase diagram
System Definer
Create New Activity
Perform Now
Perform Later...

Appending Project Files

You can only have one project file open at a time in any one instance of Thermo-Calc. However, you can *append* the nodes from additional project files to the topmost **My Project** node in the **Project** window.

To append a project file into the Project tree:

1. Chose an option:
   - From the main menu, select **File** → **Append Project** .
   - Press <Ctrl+Shift+O> (Windows) or < ⇧⌘O> (macOS).
2. Then in the **Append file** window, navigate to the project file and click **Open**.
3. The nodes are appended to the top node. Drag the nodes to separate and arrange within the Project window.



[Saving and Printing the Output in Graphical Mode](#) and *Saving Tabulated Data* for the [Table Renderer](#)

Converting Project Files to a Newer Version of Thermo-Calc

This topic discusses the various considerations related to opening old project files, with or without results, in a different version of Thermo-Calc, i.e. converting a project file. In both types of conversion (with or without results), a backup file is automatically created and can be useful during the review or regeneration of results for a converted file.

? Saving Project Files and Opening Project Files

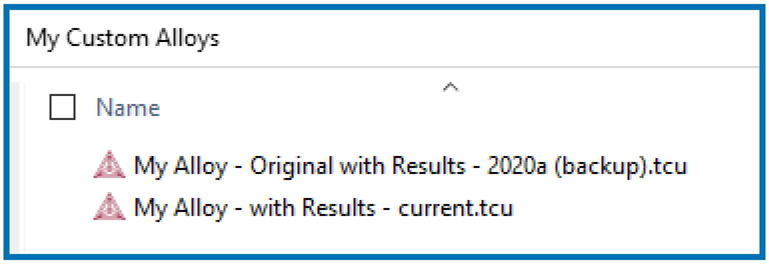
About Backup Files

When you first open a project file in a newer version of Thermo-Calc, a backup file is automatically created. The backup file has (backup) added to the end of the file name, e.g. *My Alloy (backup).tcu*. This is applicable whether the file has included results or not.

> If a file including the name (backup) is also converted, then another (backup) is added to the file name, e.g. *My Alloy (backup)(backup).tcu*.

As soon as the original project file containing results is converted, it overwrites any previously saved results. This is where the backup file can be useful.

> Since the version of the software used for the original project file is not always known, you can use the information provided in the **Old project file with results** window to rename the backup file with key information once the file is converted. See Converting Old Project Files - Original with Saved Results for information about this window.



My Custom Alloys

☐ Name

My Alloy - Original with Results - 2020a (backup).tcu
My Alloy - with Results - current.tcu

An example of the backup file created (in the same folder) when an old project file is opened in a newer version of Thermo-Calc, i.e. converted. It is recommended that users rename the file in a meaningful way in order to include a software version number and to indicate if it contains saved results.

Converting Old Project Files - No Results Saved

When opening an old project file without results, the procedure is the same as described in Opening Project Files. The main difference is that a backup file is automatically created. There can also be potential differences in setup configuration that need to be addressed.

After opening the file in the new version of Thermo-Calc, also open the **Event Log** to see if there are any messages. Try also to perform the simulation and check the results against the original or expected output, then continue as normal.

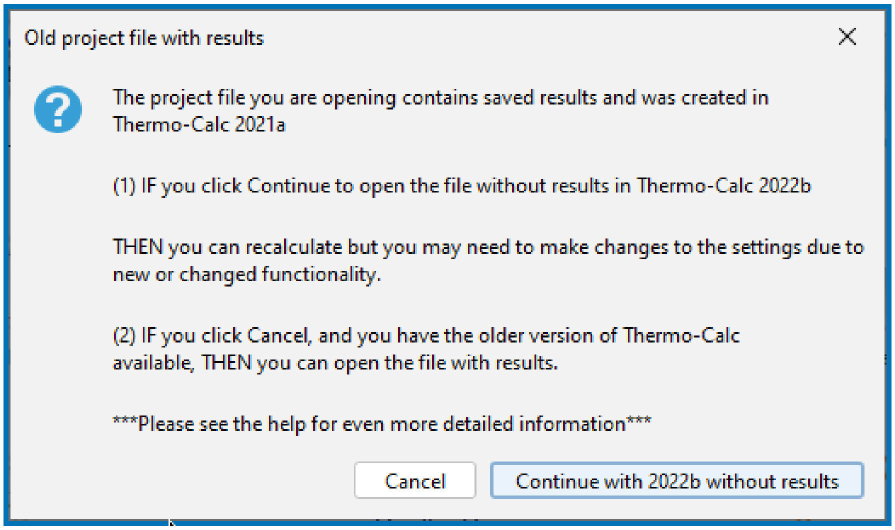
Converting Old Project Files - Original with Saved Results

> Starting with Thermo-Calc version 2022b, all older project files including results generated and saved in Thermo-Calc versions 2015a to 2022a, can only be opened with results in the original software version. You can still open a project file without results and then re-perform the calculation. However, this can require a review and update to the settings and configurations, especially if there is a wide gap between versions.

To Open and Convert a Project File with Results

1. Follow the instructions as described in Opening Project Files.
2. At the point of opening the old project file including results, the **Old project file with results** window displays. This also occurs when the **Open project with results if present** checkbox is selected because no results can be included.

The window provides information about the original Thermo-Calc version in which the results were calculated as well as the version of the software in which you are opening the project file.



The project file you are opening contains saved results and was created in Thermo-Calc 2021a

(1) IF you click Continue to open the file without results in Thermo-Calc 2022b

THEN you can recalculate but you may need to make changes to the settings due to new or changed functionality.

(2) IF you click Cancel, and you have the older version of Thermo-Calc available, THEN you can open the file with results.

Please see the help for even more detailed information

3. Click **Continue** to open and convert the file to the version of the software indicated. A backup file is automatically created, which includes the old results. Click **Cancel** to exit without converting the file.
    a. If you click **Continue**, then it is recommended that you first review the setup and then regenerate the results. Review the **Event Log** to see if there are any messages.
    b. If you click **Cancel**, or want to use the backup file to compare results between versions, then open the old or backup file in the original version of the software.

Regenerating the Results for a Converted File

As part of the project file conversion, all previous results are overwritten and the file is opened without results. However, the project structure and settings are maintained.

When the versions of the software are not far apart, then re-performing a simulation is likely to have no or few errors recorded in the Event Log.

However, to regenerate and compare results in a newer version of Thermo-Calc also depends on the original project set up and whether new or improved functionality in Thermo-Calc impacts the recalculation. Another consideration includes the availability of a newer version of a database than was used in the original calculation. In other words, there are various factors that can change the new or regenerated results compared to the original.

Opening Old Project Files in the Original Version of Thermo-Calc

There are various reasons for wanting to open an old project file in its original version of the software. For example, if you are:

- Regenerating the results in a newer version of the software and there are errors in the **Event Log** or unexplained differences.
- Reviewing or comparing the original configuration settings to update the settings.
- Comparing results from the older version of the software to the converted version of the results.

Different versions of Thermo-Calc can be installed at the same time on your computer and have project files opened alongside each other to facilitate such comparisons.

If you are having problems with opening an old project file, or are unable to access an installed version of the software that you know your organization has a license for, complete this Request Support form on our website to get help. Be sure to include all relevant details such as your organization number.

Calculation Types in Graphical Mode

A variety of Plot Types are available based on the Calculator and, in most cases, *Calculation Type* selected. Also see Graphical Mode vs Console Mode: Calculation Types.

AM Calculator

The **AM Calculator** is available with the Additive Manufacturing (AM) Module. It is used to predict the temperature distribution and melt pool geometry as a function of process parameters. There are these simulation types: **Steady-state**, **Transient**, and **Transient with heat source from Steady-state**.

For **Steady-state** simulations, you can also choose to run different *Calculation Types*:

- **Single point**: The standard steady-state calculation for a single set of processing parameters. This is available with all heat sources.
- **Heat Source Calibration**: To calibrate a heat source based on the imported or entered experimental data instead of performing a single point calculation. This is available with **Gaussian**, **Double ellipsoidal**, or **Conical** heat sources.
- **Batch**: To include power and scan speed data, which is read from a file such as a spreadsheet. You can optionally include experimental melt pool width and depth (if there is data), and compare this to the calculated results using a **Parity plot** on the Plot Renderer. Other plots are also available. This is available with all heat sources.
- **Grid**: To evaluate two axis variables of power and scanning speeds in the specified range and number of steps. This is available with all heat sources.

Binary Calculator

The following calculation types are available for a **Binary Calculator** activity node:

- **Phase diagram**: To calculate in a defined multicomponent heterogeneous system, from one or more initial equilibria. A phase diagram is usually mapped within a specific space that is constructed by two (or more) defined independent mapping axis-variables.
- **Gibbs energy curves**: To calculate at a constant temperature over the whole composition range.

- **Activity curves**: To calculate at a constant temperature over the whole composition range.
- **Phase fractions**: To calculate as a function of temperature at a constant composition.

Diffusion Calculator

Diffusion calculations are done with the **Diffusion Calculator** to have detailed simulation of diffusion controlled reactions in multicomponent systems. There are no calculation types you need to choose when setting up your simulation.

Equilibrium Calculator

The following calculation types are available for an **Equilibrium Calculator** activity node:

- **Single equilibrium** (no axes): To calculate a single point. The results from this calculation are displayed in the **Event Log**.
- **One Axis**: To vary a quantity on the X-axis.
- **Grid**: Computes the equilibrium of each grid point in a two-dimensional grid.
- **Phase diagram**: To calculate in a defined multicomponent heterogeneous system, from one or more initial equilibria. A phase diagram is usually mapped within a specific space that is constructed by two (or more) defined independent mapping axis-variables.

Material to Material Calculator

The following calculation types are available for a **Material to Material Calculator** activity node:

- **Single equilibrium** (no axes): To calculate a single point. The results from this calculation are displayed in the **Visualizations** window if a Table Renderer is used.
- **One Axis**: To vary a quantity on the *X*-axis; the fraction of one of the materials or temperature.
- **Phase diagram**: To calculate a section in a multicomponent system between two materials, transitioning from one into the other. The phase diagram is mapped within a specific space that is constructed by the two mapping axis-variables; the fraction of one of the materials and temperature.

See Plot Types for Plot Renderer choices related to the **One Axis***Calculation Type*.

Precipitation Calculator

The following calculation types are available for a **Precipitation Calculator** activity node:

- **Isothermal**: Precipitation simulation at constant temperature.
- **Non-isothermal**: Precipitation simulation with user-defined temperature profile.
- **TTT Diagram**: Time-Temperature-Transformation diagram calculation.
- **CCT Diagram**: Continuous Cooling Transformation diagram calculation.

Process Metallurgy Calculator

The following calculation types are available for a **Process Metallurgy Calculator** activity node when doing an **Equilibrium** simulation.

- **Single**: To calculate a single point. The results from this calculation can be displayed in the **Visualizations** window using a **Table Renderer**.
- **One Axis**: To vary a quantity on the *X*-axis.
- **Grid**: Evaluates two axis variables of the selected quantities in the specified range and number of steps.
- **Uncertainty**: Evaluates calculations where the values of the quantities are sampled from Gaussian distributions. The **Mean** field is as defined under *Condition Definitions* for the respective quantity. The result is visualized as a histogram or normal probability plot by adding a Plot Render activity.

Property Model Calculator

The following calculation types are available for a **Property Model Calculator** activity node:

- **Single** to calculate a single point. Any model can use this calculation type and no additional settings are required. The results from this calculation are displayed in the **Event Log** or if a **Table Renderer** is used, in the **Visualizations** window.
- **One Axis**: To vary a quantity on the *X*-axis.

- **Grid**: Evaluates two axis variables of the selected quantities in the specified range and number of steps.
- **Min/Max**: Evaluates the Property Model(s) for all variations of the selected quantities at the given limits. The **Mean** field is as defined under *Condition Definitions* for the respective quantity. The total minimum and maximum of the model(s) results are shown in the **Event** log.
- **Uncertainty**: Evaluates the Property Model(s) where the values of the quantities are sampled from Gaussian distributions. The **Mean** field is as defined under *Condition Definitions* for the respective quantity. The result is visualized as a histogram or normal probability plot by adding a Plot Renderer activity.
- **Batch**: Use this to allow for high throughput calculations and read data from a file, such as a spreadsheet, rather than, for example, having a fixed grid or random values. Results from these batch calculations can then be compared to experimental values (as long as this data is included), using a **Cross plot** on the Plot Renderer.

Scheil Calculator

When using a **Scheil Calculator** activity node there are no calculation types you need to choose when setting up your simulation.

Ternary Calculator

The following calculation types are available for a **Ternary Calculator** activity node:

- **Isothermal section**: To calculate the ternary system for the whole composition range.
- **Monovariant lines**: To calculate the variation of the liquid compositions with temperature.
- **Liquidus projection**: The projection liquid surface and the monovariant lines are calculated over the given temperature range.

About the Uncertainty Calculations

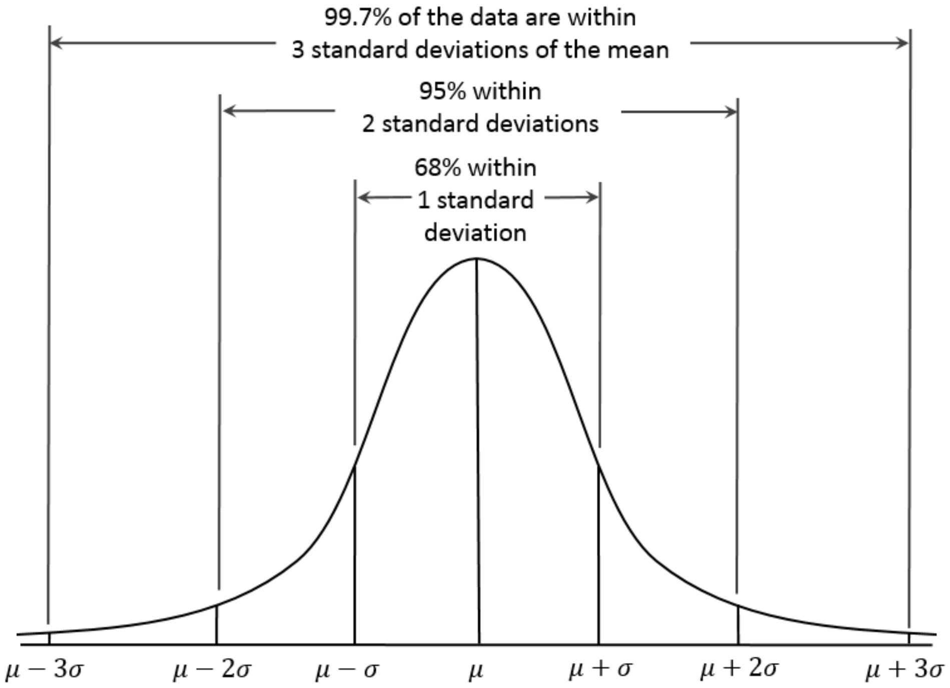
The **Uncertainty** calculation in Thermo-Calc uses the values (the mean) entered for quantities under the *Condition Definitions* section as the starting point to estimate, within a certain probability, the true variation of the quantity. Uncertainty calculations are available with the **Property Model Calculator** and the **Process Metallurgy Calculator**.

An example of a Gaussian distribution is shown next. The example uses the Phase Transition Property Model Settings and an **Uncertainty** *Calculation Type* to describe how the sampling of data is performed. The example PM_G_01: Phase Transition predicts the transition temperature to the unwanted brittle Sigma phase and shows how the temperature is influenced by changes to a steel alloy's composition.

Gaussian Distribution, the 3-Sigma Rule

- The *mean* is at the peak of the curve (labeled μ).
- The *standard deviation* (σ) is a plus and minus range, ±1σ, ±2σ or ±3σ, of the variance from the mean.

Image by Dan Kernler: https://en.wikipedia.org/wiki/Normal_distribution#/media/File:Empirical_Rule.PNG.

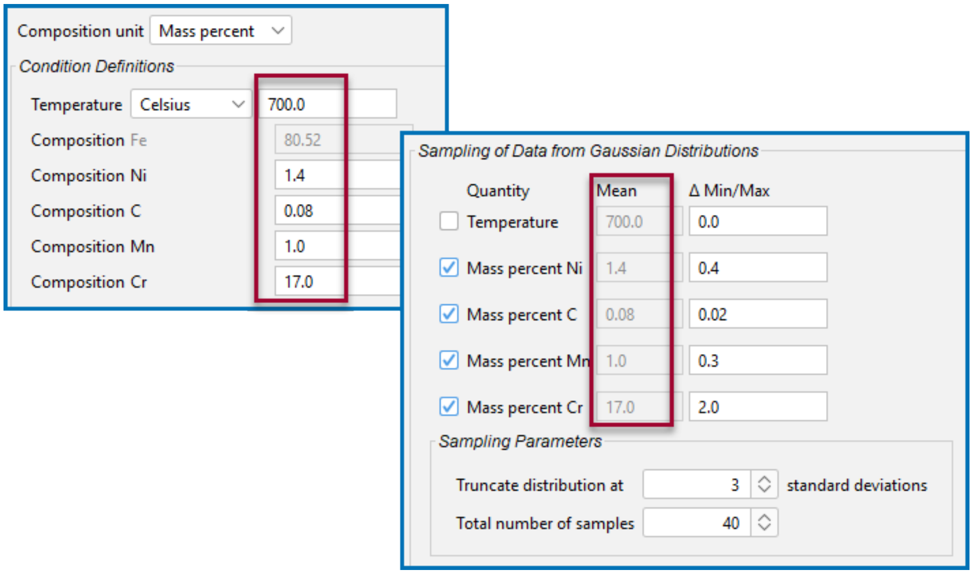


As long as the number of events (the sample size) is very large, then the Gaussian distribution function can be used to describe physical events. A Gaussian distribution is assumed to describe how each quantity varies in an uncertainty calculation, as shown next.

Condition Definitions and Sampling Settings

In Thermo-Calc, the mean of the quantity's distribution is defined in the *Condition Definitions* section. The **Mean** is then used in the *Sampling of Data from Gaussian Distributions* section as the starting point for how much you want to deviate from this value.

The mean defined under *Condition Definitions* is used during the sampling.



Composition unit: Mass percent

Condition Definitions

Temperature	Celsius	700.0
Composition Fe		80.52
Composition Ni		1.4
Composition C		0.08
Composition Mn		1.0
Composition Cr		17.0

Sampling of Data from Gaussian Distributions

	Quantity	Mean	Δ Min/Max
☐	Temperature	700.0	0.0
☑	Mass percent Ni	1.4	0.4
☑	Mass percent C	0.08	0.02
☑	Mass percent Mn	1.0	0.3
☑	Mass percent Cr	17.0	2.0

Sampling Parameters

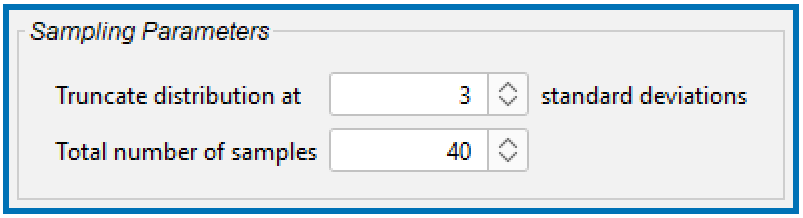
Truncate distribution at 3 standard deviations

Total number of samples 40

The values entered in the Δ **Min/Max** fields are the resulting width of the distribution corresponding to the 95% confidence interval (approximately μ ± 2σ) shown in *Gaussian distribution, the 3-sigma rule*.This confidence interval means that approximately 95% of the sampled values fall within these limits, as shown next.

Sampling Parameter Settings

The default value for truncating the distribution is set at **3 standard deviations** in the *Sampling Parameters* section. This is also where you set the **Total number of samples**. The default is 200. In order to maintain a Gaussian distribution for the varied quantities, this number should not be too low.



Truncate distribution at 3 standard deviations

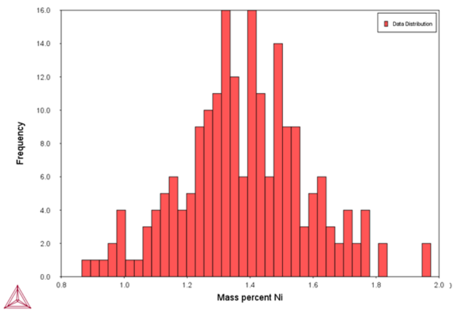
Total number of samples 40

You can experiment by varying the conditions and the number of samples to see the distribution results smooth out as is to be expected based on the Central Limit Theorem, as shown in the histogram plot. You can also plot the results as a normal probability.

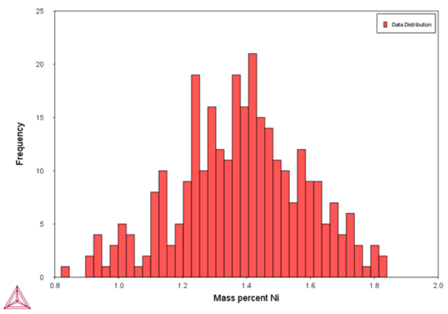
Histogram Plot

This series of histogram plots shows the uncertainty calculations sampling data from Gaussian distributions. On the **Plot Renderer** the variable is set to measure the **Composition** of **Ni**. It compares the Ni composition where the total sample size is increased. In the example, the initial sample size uses the default, 200, and then the sample size is increased to 300, 400, 600, 800, and 1000, showing how the plot follows the Gauss distribution.

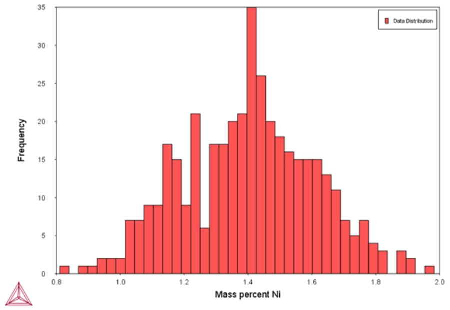
Total samples = 200



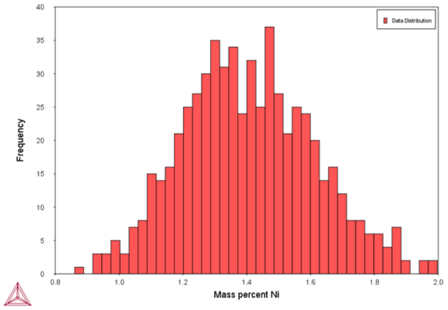
Total samples = 300



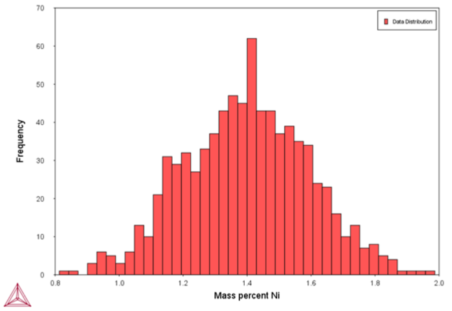
Total samples = 400



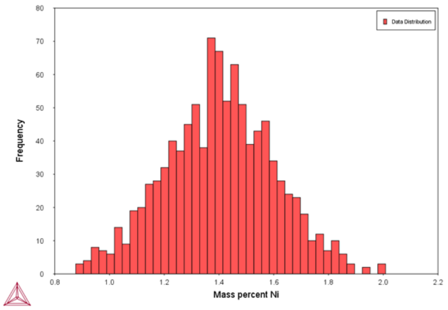
Total samples = 600



Total samples = 800

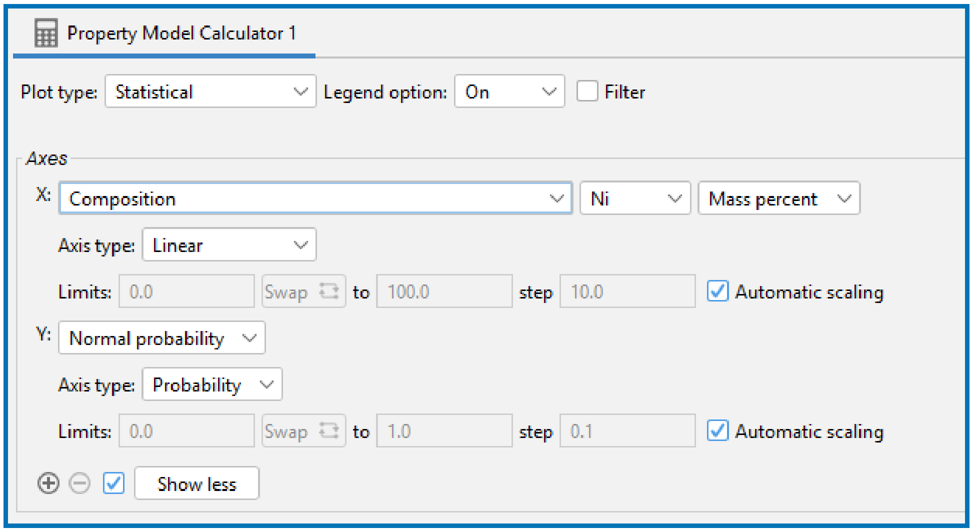


Total samples = 1000



Normal Probability Plot

You can also plot the results as a **Normal probability**. Continuing with this example, for the Property Model Calculator the *X* variable is plotted as **Composition** and the *Y* variable is plotted as the **Normal probability**.



Plot type: Statistical

Legend option: On

☐ Filter

X: Composition

Ni

Mass percent

Axis type: Linear

Limits: 0.0 Swap to 100.0 step 10.0

☑ Automatic scaling

Y: Normal probability

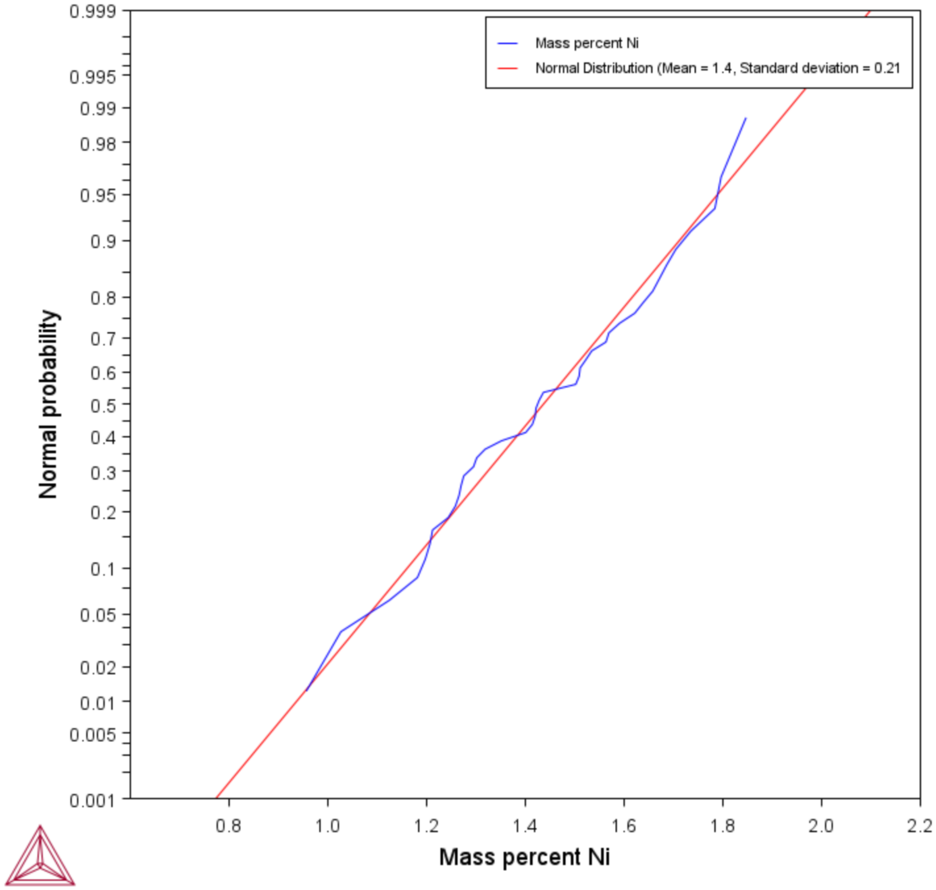
Axis type: Probability

Limits: 0.0 Swap to 1.0 step 0.1

☑ Automatic scaling

☑

This is a normal probability plot example of the uncertainty calculations sampling data from Gaussian distributions. It compares the relaxed condition where the total sample size is 200. The sampled data (blue line) closely follows the ideal normal distribution (red line). Deviations are naturally larger at the tails (≈1%Ni and ≈2%Ni) since the number of samples are fewer there compared to the center of the distribution.


Mass percent Ni
Normal Distribution (Mean = 1.4, Standard deviation = 0.21
Normal probability
0.999
0.995
0.99
0.98
0.95
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.05
0.02
0.01
0.005
0.001
0.8
1.0
1.2
1.4
1.6
1.8
2.0
2.2
Mass percent Ni

Working with Batch Calculations

When defining a **Batch** calculation for a Property Model Calculator, you choose to load (import) a configuration data file that contains predefined data. The columns that can be included in the data file are:

- Element compositions and the associated unit
- Temperature and the temperature unit
- Experimental data and a key word
- Parameters (as long as these are both available and selected for a Property Model)
- An identifier (ID) for each row of data

Only these types of data are read / used in calculations. It is important that the data file contents are correctly entered in order for the calculation to perform smoothly. The software runs a validation of the data file prior to allowing you to perform a calculation. Warnings related to this validation display on the Property Model Calculator. You can also skip this data file validation for composition or parameter inconsistencies. See below for details.

The *Batch Control* settings, which are further described in this section, are found on the Property Model Calculator **Configuration** window. See Configuration Window Settings.

Batch calculations are also available with the Additive Manufacturing (AM) Module and described separately.

Batch Controls

For the settings in this section, it is recommended you read the Data File Rules, Data File Requirements, and Skip Validation of Data File sections prior to importing the data file.

In the **Data file** field, either enter a file path or click the load data file button (📁) to navigate to a data file such as an Excel spreadsheet (with `*.xls` or `*.xlsx` extensions) or a `*.csv` file. You can also use other programs (e.g. Google Sheets) to enter data and export to a CSV format that can be read by the software.

Click **Open** to import the data. In the **Data file** field you can see the file path to the selected file. The next time you click the load data file button (📁) the program remembers the last location from where the file is opened.

Choose the delimiter—**Comma** (`,`), **Colon** (`:`), **Equals sign** (`=`), **Semicolon** (`;`), or **Tab**—that matches the delimiter in the data file and click the **Reload** (⟳) button.

The data is imported and displays on the Property Model Calculator:

- The data are used for the applicable fields that must match what already exists as a Property Model parameter (e.g. critical radius, grain size, etc.) as well as the composition, temperature, and units that you want to run the calculation for. Also, if the dependent element composition is not included in the data file, the batch calculation then sets the dependent element to be the same as defined in the user interface.
- The calculation runs once for every row of data included in the file.

> When the data file is imported into Thermo-Calc, there is also a **Row** column autogenerated by Thermo-Calc.

Select the **Set zero amount to value (in mole-/mass-fraction)** to enter a small value for the mole/mass-fraction in cases where a Property Model has problems calculating zero amounts of elements.

Select the **Skip validation of data file** checkbox to allow a calculation to perform using the data file even when certain criteria are not met.

When selected, the validation of the data file is skipped:

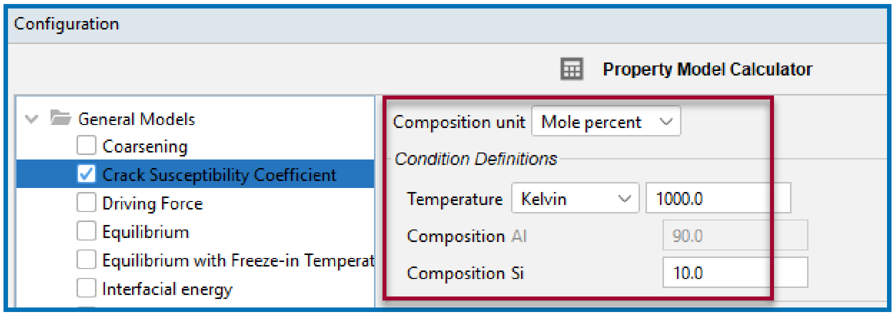
- If the **Composition** (elements) do not match the system composition entered on the GUI in the System Definer or Property Model Calculator.
- If one or more **Parameters** are not correctly entered, not selected for the specific Property Model, or are unavailable with the selected Property Model, then these are ignored in the calculation.

If there are any data file validation error(s), a tooltip on the **Perform** button lists and describes these.

Data File Rules

GENERAL RULES

- No abbreviations are allowed.
- All header text must be in English, i.e. no translations into other languages will be read correctly by the data file.
- For the settings on the Property Model Calculator (**Composition unit**, **Composition**, **Temperature**, and **Temperature unit**) when there is nothing specified in the data file, the default is taken from the GUI and used in the calculation. Also, if the dependent element composition is not included in the data file, the batch calculation then sets the dependent element to be the same as defined in the user interface.



☐ Coarsening
☑ Crack Susceptibility Coefficient
☐ Driving Force
☐ Equilibrium
☐ Equilibrium with Freeze-in Temperat
☐ Interfacial energy

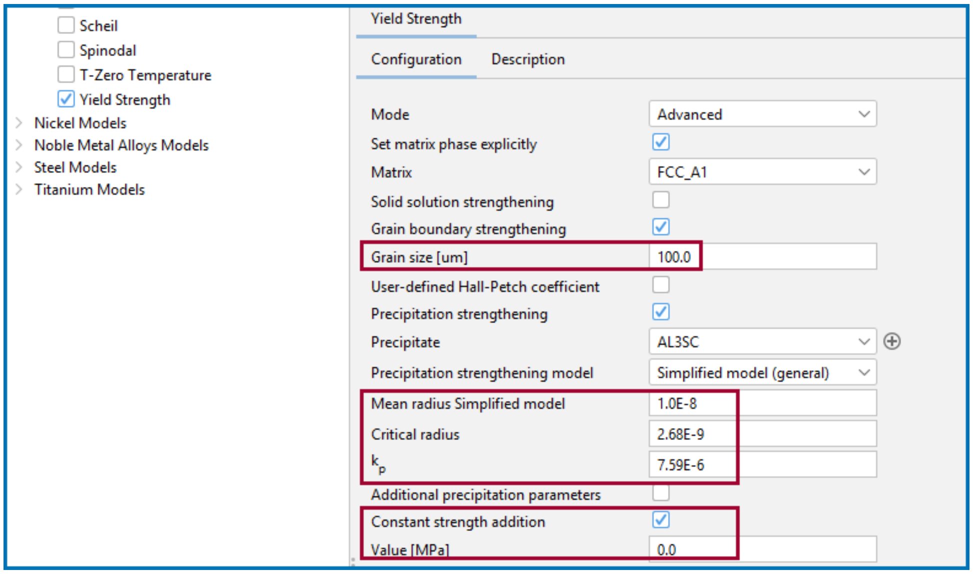
Composition unit: Mole percent
Temperature: Kelvin 1000.0
Composition Al: 90.0
Composition Si: 10.0

PARAMETER, PARAMETER NAME, AND PARAMETER VALUE RULES

Only numeric parameters available on the **Configuration** tab for the selected Property Model can be included in the calculation.

The column entries for the Parameter + <*parameter name*> plus the row entries for the <*parameter value*> must adhere to these rules. The validation checks for inconsistencies, which could be the result of any of the following criteria not being met.

- When including **Parameters** in the data file, these must be existing Property Model parameters and the applicable Property Model must be selected on the GUI.
- The *<parameter name>* is case sensitive and must be entered exactly as you see on the GUI, no abbreviations are allowed.
- The *<parameter value>* must be numeric or it is not included in the calculation.



Mode: Advanced
Set matrix phase explicitly: ☑
Matrix: FCC_A1
Solid solution strengthening: ☐
Grain boundary strengthening: ☑
Grain size [um]: 100.0
User-defined Hall-Petch coefficient: ☐
Precipitation strengthening: ☑
Precipitate: AL3SC
Precipitation strengthening model: Simplified model (general)
Mean radius Simplified model: 1.0E-8
Critical radius: 2.68E-9
k_p: 7.59E-6
Additional precipitation parameters: ☐
Constant strength addition: ☑
Value [MPa]: 0.0

An example of the Yield Strength Property Model numeric parameters available for the Batch calculations. These are available on the Property Model Calculator Configuration tab after selecting Yield Strength under General Models. The parameter name must be entered in the data file exactly as you see on the GUI. No parameters from other calculators are accepted.

Data File Requirements

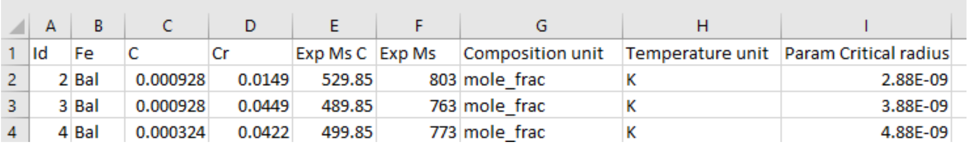
Only the columns described here are read / used in the calculation. It is important to enter the information exactly as described. It is recommended that the data file is cleaned up before importing / loading it and performing calculations. All header text must also be written in English, i.e. no translations into other languages will be read correctly by the data file.

In the table below, `code font` indicates something entered into the data file (or it is an example) and any *<text in italic with angle brackets>* is a generic name for an entry.

Column Heading Description	*Column Heading Requirements and Options*	*Row Cell Requirements and Options*
Composition Each element of the composition is in a separate heading column using the *<element short name>* e.g. Fe, C, Mn, Si, etc.	Enter an *<element short name>*. It is not case sensitive. For example: `Fe`. It is not case sensitive, so alternatives in this example are `fe` or `FE`.	Valid format and entries of the *<composition value>*: • A number for the composition e.g. `0.1`, `8.7`, `1.00E-05`, etc. • Text entry `Bal` to define the balanced element. • Empty cells are read as zero (`0`) amounts.
Composition unit	Enter the text `Composition unit`. No abbreviations allowed but it is not case sensitive. For example, it is acceptable to enter `composition unit` or `Composition Unit`, or `COMPOSITION UNIT`, etc.	Valid format and entries of the *<composition unit>*: • `mass_pct` • `mass_frac` • `mole_pct` • `mole_frac`
Temperature	Enter the text `Temperature`. No abbreviations allowed but it is not case sensitive. For example, it is acceptable to enter `temperature` or `Temperature`, or `TEMPERATURE`.	Valid format and entries – • Any number e.g. `273.15`
Temperature unit	Enter the text `Temperature unit`. No abbreviations allowed but it is not case sensitive. For example, it is acceptable to enter `temperature unit` or `Temperature Unit`, or `TEMPERATURE UNIT`, etc.	Valid format and entries – • `C` • `F` • `K`
Parameters with numerical values only. The heading column is defined with `Param` in front of a Property Model *<parameter name>*	`Param` + *<parameter name>* For example: `Param Critical radius` The *<parameter name>* has requirements–	Valid format and entries – The *<parameter value>* must be numeric or it is not included in the calculation. An example of an accepted Property

Column Heading Description	***Column Heading Requirements and Options***	***Row Cell Requirements and Options***
	• It is case sensitive based on the available and selected Property Model parameter • It must be an existing Property Model parameter and be included with any selected Property Model • No abbreviations	Model parameter is for the **Yield Strength** model where *Grain size* and *Critical radius* are accepted (these have fields for numerical entries) but you cannot use *Matrix* or *Precipitate* as these are text choices from a drop down list.
Experimental value. The heading column is defined with `Exp` followed by any *<keyword>*.	`Exp` + *<keyword>* where the *<keyword>* is defined by the user. For example: `Exp Ms`.The keyword is not case sensitive so alternatives are `MS` or `ms`.	Valid format and entries – • Each *<experimental value>* must be numeric
Identifier (i.e. an alloy name). The heading column is defined as `Id`	Enter the text `Id`. It is not case sensitive so alternatives are `id` or `ID`.	Valid format and entries – • An *<identifier>* can be any text or number defined by the user.

DATA FILE EXAMPLE AND COLUMN DEFINITIONS



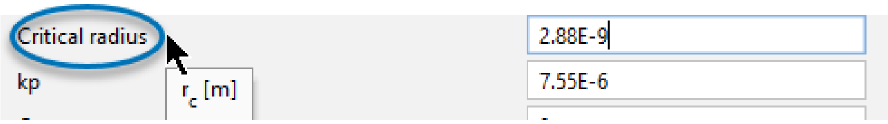
	A	B	C	D	E	F	G	H	I
1	Id	Fe	C	Cr	Exp Ms C	Exp Ms	Composition unit	Temperature unit	Param Critical radius
2	2	Bal	0.000928	0.0149	529.85	803	mole_frac	K	2.88E-09
3	3	Bal	0.000928	0.0449	489.85	763	mole_frac	K	3.88E-09
4	4	Bal	0.000324	0.0422	499.85	773	mole_frac	K	4.88E-09

This is an example of data entered into an Excel spreadsheet. When this is imported into Thermo-Calc, an additional "Row" column is automatically added and is a way for you to locate any errors in the data file that are identified as needing correction or adjustment to allow the program to read the file.

- A1 to A4 is the **Identifier** column and rows. The heading text is `Id` and then in the entries in rows A2 to A4 can be text or numbers, for example it might be an alloy name or another user-defined *<identifier>*.

> When the data file is imported into Thermo-Calc, there is also a **Row** column autogenerated by Thermo-Calc.

- B1 to B4 is the **Composition** column and rows for the element `Fe`. In this example, `Bal` indicates that the balance of the composition will be calculated for this column after the *<composition values>* for `C` and `Cr` are entered.
- C1 to C4 and D1 to D4 are the **Composition** columns each for `C` and `Cr` with the specific *<composition values>*, e.g. `0.000928` for `C` and `0.0149` for `Cr` in row 2.
- E1 to E4 and F1 to F4 are the **Experimental Value** columns and rows. The header starts with `Exp` and then user-defined *<keywords>* are added, e.g. `Ms C` and `Ms`. Then specific *<experimental values>* are entered, e.g. `529.85` for `Ms C` and `803` for `Ms` in row 2.
- G1 and H1 are the headings for the **Composition unit** and **Temperature unit** columns. No abbreviations allowed but it is NOT case sensitive. Then the rows G2 to G4 and H2 to H4 include an accepted text value e.g. `mole_frac` for the composition unit and `K` for the temperature unit.
- I1 is the **Parameter** heading where you need to enter `Param` followed by the parameter name `Critical radius`, which has numeric values entered in rows I2 to I4. The *<parameter name>* matches that on the GUI and is an available and selected Property Model parameter.



Critical radius: 2.88E-9
kp: 7.55E-6

Skip Validation of Data File

Select the **Skip validation of data file** checkbox to allow a calculation to perform using the data file even when certain criteria are not met.

When selected, the validation of the data file is skipped:

- If the **Composition** (elements) do not match the system composition entered on the GUI in the System Definer or Property Model Calculator.
- If one or more **Parameters** are not correctly entered, not selected for the specific Property Model, or are unavailable with the selected Property Model, then these are ignored in the calculation.

> If there are any data file validation error(s), a tooltip on the **Perform** button lists and describes these.

Skipping Composition Validation

If the **Composition** (elements) do not match the system composition entered on the GUI in the System Definer or Property Model Calculator then the default system composition is used for any missing elements after you select the **Skip validation of data file** checkbox.

This can occur when there are more elements included in the data file but not entered on the GUI, and then these are excluded from the calculation. For example, you might have too many or too few elements included in the data file compared to the composition entered on the System Definer, which is then further viewed under *Condition Definitions* on the Property Model Calculator **Configuration** window.

When configuring the System Definer, it is recommended you select the composition to match the composition in the data file. However, if this is not possible you can use this checkbox to override any differences of the composition included in the data file and use the GUI default.

Skipping Parameter Validation

If one or more **Parameters** are not correctly entered, not selected for the specific Property Model, or are unavailable with the selected Property Model, then these are ignored in the calculation after you select the **Skip validation of data file** checkbox.

For example, if a data file is uploaded and you are unable to perform the calculation, it means that one of the following criteria are not met for the `Param` columns and related to the *<parameter name>*.

- The parameter name is misspelled (does not match) the one on the GUI
- The parameter is not available with the selected Property Model.
- The parameter is not available with any Property Model.

It is best practice to use a data file that only includes available Property Model parameters. However, if this is not possible then use this checkbox to override the validation. Alternatives to skipping this validation, include removing the prefix `Param` from the data file (or delete this column), and confirming that the parameter you want to calculate is available and selected for the Property Model.

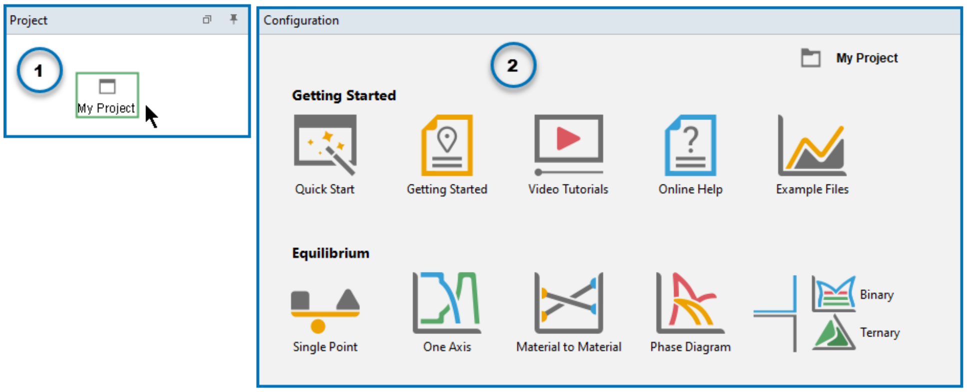
Plotting Experimental Data Against Simulation Results

You can plot experimental values loaded to the Property Model Calculator using the **Cross plot** *Plot type* available on the Plot Renderer. There are also additional options for this *Calculation Type*. See Plot Types for a list and also Plot Type: Cross Plot and Statistical.

Getting Started Links and Templates

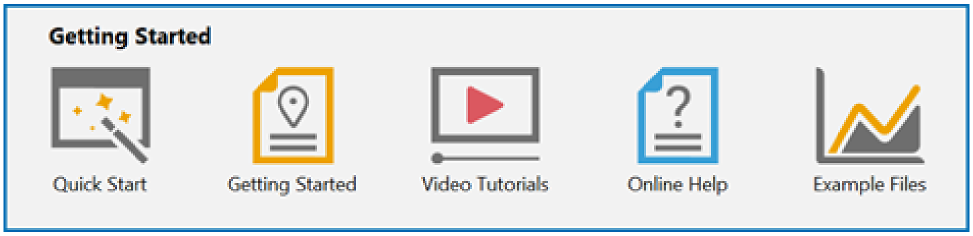
When you first open Thermo-Calc, the **My Project Configuration** window has a variety of links and templates available to get you started. From here, click any template button to add the relevant nodes to a Project tree. You can also right-click the **My Project** node and select a template from the **Create New Activity → Use Template** list.

1. In the **Project** window, click the **My Project** node.
2. The templates (plus additional links under **Getting Started**) are available to click in the **My Project Configuration** window.



Getting Started Links Including the Quick Start Wizard

Even before you understand how to work with Thermo-Calc projects or use the available templates, there are some links of interest available under **Getting Started**.



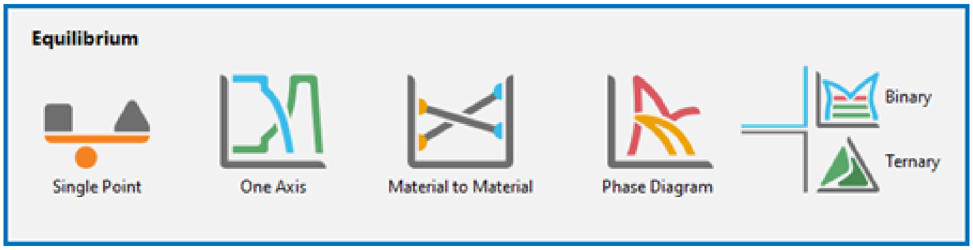
- Click Getting Started to go to the *Getting Started Guides* on the website.
- Click Video Tutorials to go to the Video Tutorials on the website.
- Click **Online Help** to open the help locally in a browser (or press F1).
- Click **Example Files** to open the Graphical Mode folder containing the installed example files.

In addition to the links above, click **Quick Start** to open the template wizard, which helps you set up a project and run calculations in Graphical Mode. You can set up, calculate and visualize any of the following:

- Single point equilibrium
- One axis equilibrium
- Phase diagram
- Scheil solidification simulation

? Creating a Project with the Quick Start Wizard

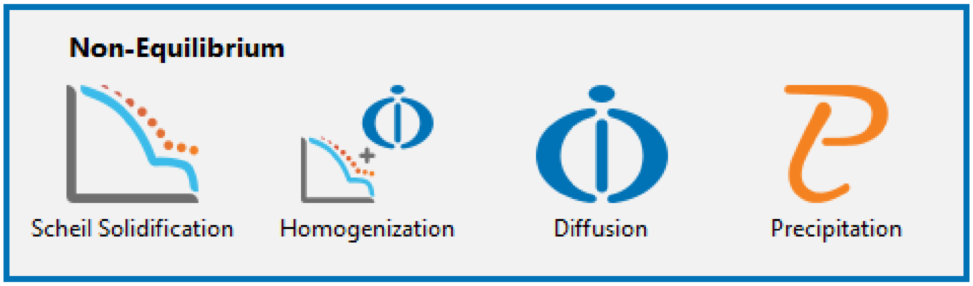
Equilibrium Templates



Under **Equilibrium**, click a template to create a project and add the applicable nodes to the **Project** window.

- **Single Point**: To calculate a single point equilibrium. The project consists of a System Definer, Equilibrium Calculator, and a Table Renderer.
- **One Axis**: To calculate a one axis diagram. The project consists of a System Definer, Equilibrium Calculator, and a Plot Renderer.
- **Material to Material**: To examine how materials transition into one another. The project consists of a System Definer, Material to Material Calculator, and a Plot Renderer.
- **Phase Diagram**: To calculate a phase diagram. The project consists of a System Definer, Equilibrium Calculator, and a Plot Renderer.
- **Binary**: To perform a binary calculation. The project consists of a Binary Calculator and a Plot Renderer.
- **Ternary**: To perform a ternary calculation. The project consists of a System Definer, Ternary Calculator, and a Plot Renderer.

Non-Equilibrum Templates

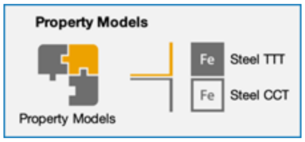


Under **Non-Equilibrium**, click a template to create a project and add the applicable nodes to the **Project** window.

- **Scheil Solidification**: To perform a Scheil calculation. The project consists of a System Definer, Scheil Calculator, and a Plot Renderer.
- **Homogenization**: To perform a Scheil solidification calculation followed by kinetic homogenization simulation of segregated composition profile. The project consists of a System Definer, a Scheil Calculator, a Diffusion Calculator, and two Plot Renderers.
- **Diffusion**: To calculate general diffusion simulations. The project consists of a System Definer, Diffusion Calculator, and a Plot Renderer.
- **Precipitation**: To simulate the evolution of particle size distributions. The project consists of a System Definer, Precipitation Calculator and a Plot Renderer.

> To run full calculations with the **Homogenization**, **Diffusion**, and **Precipitation** templates require additional licenses although you can run these in demo mode with up to three (3) components. See Available Graphical Mode Features and Available Options.

Property Models

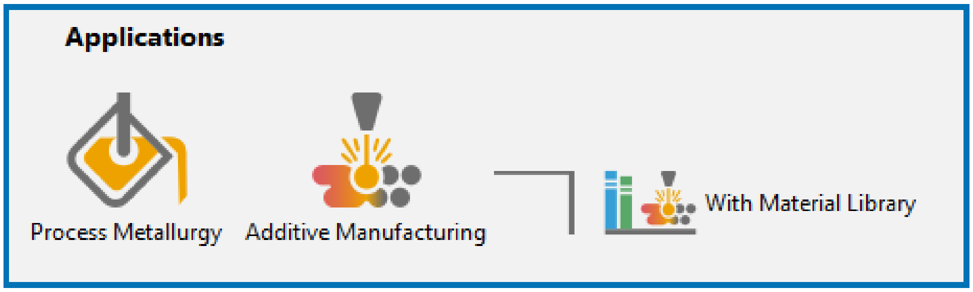


Under **Property Models**, click a template to create a project and add the applicable nodes to the **Project** window.

- **Property Models**: To choose from a variety of Property Models available on a Property Model Calculator. The project consists of a System Definer, Property Model Calculator, Plot Renderer, and a Table Renderer.
- **Steel TTT**: To use the **TTT Diagram** Property Model as part of the Steel Model Library and add all the activities for a Time-Temperature-Transformation (TTT) diagram calculation. The project consists of a System Definer, Property Model Calculator, and a Plot Renderer.
- **Steel CCT**: To use the **CCT Diagram** Property Model as part of the Steel Model Library and add all the activities for a Continuous-Cooling-Transformation (CCT) diagram calculation. The project consists of a System Definer, Property Model Calculator, and a Plot Renderer. Also see Steel Library TTT Diagram Template and Steel Library CCT Diagram Template.

> To run full calculations with the **Steel TTT** and **Steel CCT** templates (as part of the Steel Model Library) requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases.

Applications



Under **Applications**, click a template to create a project and add the applicable nodes to the **Project** window.

- **Process Metallurgy**: To allow for calculation and efficient setup of advanced calculations involving slag, metal, and gas. Also see Process Metallurgy Template.

> To run full calculations with the **Process Metallurgy** template requires both a valid Maintenance and Support Subscription (M&SS) and a license for the TCS Metal Oxide Solutions Database (TCOX8 or newer).

- **Additive Manufacturing** and **With Material Library**: These templates are to work with additive manufacturing. The Additive Manufacturing (AM) Module is used to better understand the laser powder bed fusion (LPBF) process by predicting the temperature distribution and melt pool geometry as a function of process parameters. Also see Additive Manufacturing Templates.

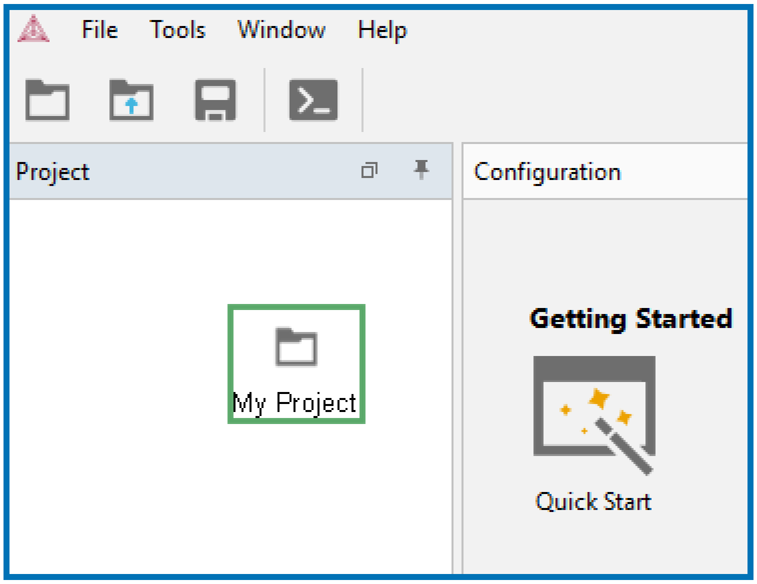
> To run full calculations with the **Additive Manufacturing** and **With Material Library** templates require a license for the Additive Manufacturing (AM) Module.

> When you also have licenses either for the Diffusion Module (DICTRA) and/or the Precipitation Module (TC-PRISMA), for transient simulations you can additionally include probe data from the AM Calculator in the set up of the thermal profile for diffusion and precipitation calculations, respectively.

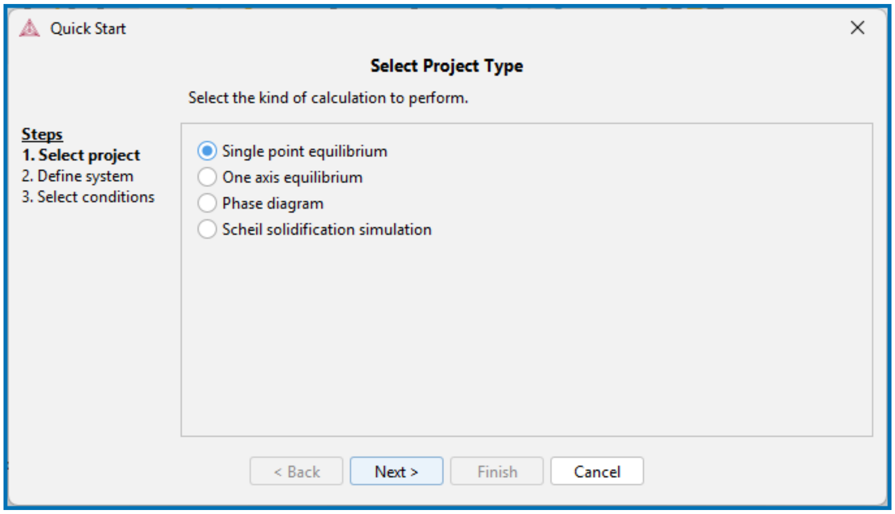
Creating a Project with the Quick Start Wizard

To set up, perform and visualize a calculation using the Quick Start wizard:

1. In the **Configuration** window click **Quick Start**. If you cannot see the **Quick Start** button, first click 🗀 **My Project** in the **Project** window.



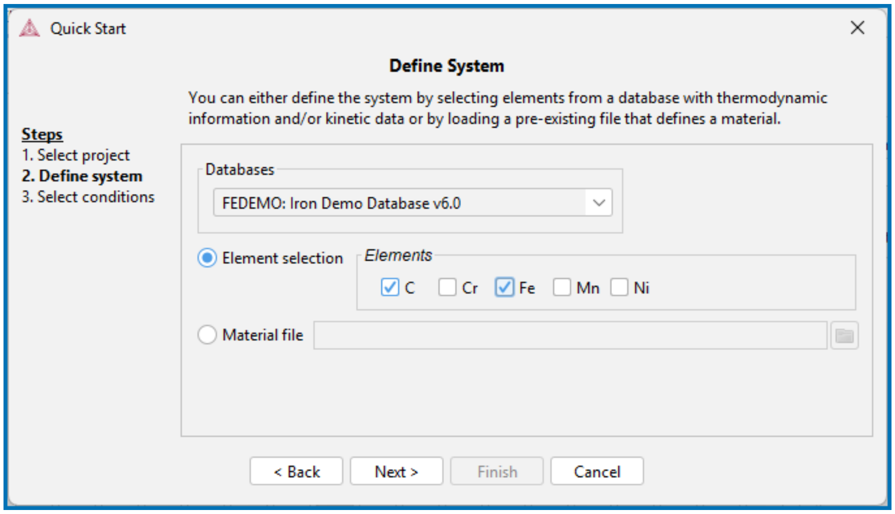
2. In the **Select Project Type** window click to select the type of calculation to perform. **Single point equilibrium**, **One axis equilibrium**, **Phase diagram**, or **Scheil solidification simulation** (a Classic Scheil simulation). Click **Next**.



Select the kind of calculation to perform.

● Single point equilibrium
○ One axis equilibrium
○ Phase diagram
○ Scheil solidification simulation

3. In the **Define Systems** window, choose an available **Database**.



Quick Start

Define System

You can either define the system by selecting elements from a database with thermodynamic information and/or kinetic data or by loading a pre-existing file that defines a material.

Steps
1. Select project
2. Define system
3. Select conditions

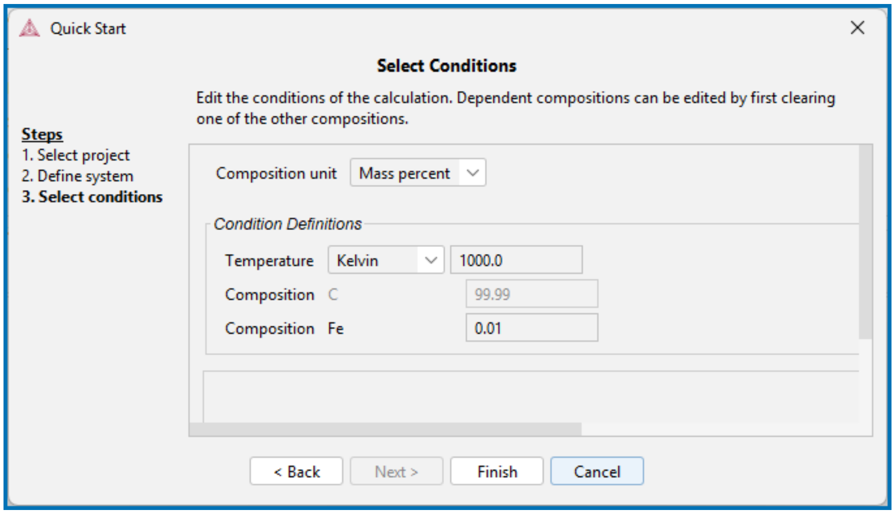
Databases: FEDEMO: Iron Demo Database v6.0

● Element selection — *Elements*: ☑ C ☐ Cr ☑ Fe ☐ Mn ☐ Ni

○ Material file

4. Click to select **Elements** checkboxes to include as system components. To add elements from an existing material file, click the **Material file** button to enter the file path to a material file or then click the **Select Material File** button (to the right of the field) to navigate to a file on the computer.
5. Click **Next**. The **Select Conditions** window has different options depending on the project type and the elements selected.

   In this example, using a **Single Point Equilibrium**, choose the **Composition unit** from the list and under *Condition Definitions* specify the values of the state variables in the system.



Quick Start

Select Conditions

Edit the conditions of the calculation. Dependent compositions can be edited by first clearing one of the other compositions.

Steps
1. Select project
2. Define system
3. Select conditions

Composition unit: Mass percent

Condition Definitions

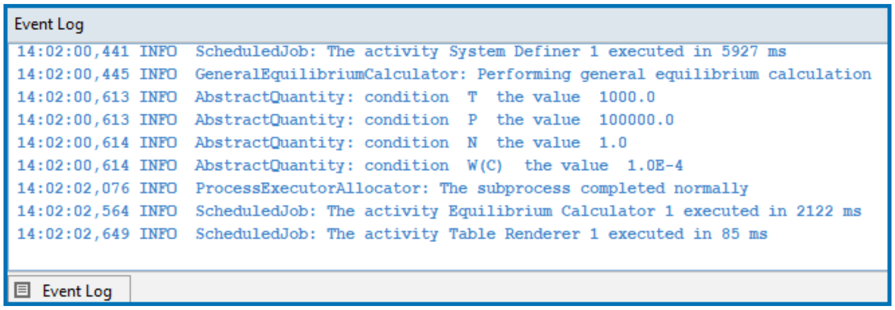
Temperature	Kelvin	1000.0
Composition	C	99.99
Composition	Fe	0.01

For **One axis equilibrium** or **Phase diagram** projects, specify the **Axis Definitions** of the stepping or mapping operation. Choose minimum and maximum values for the variable(s) (select **Linear – min no. of steps**, **Linear – max step size**, or **Logarithmic – scale factors**) and whether it is **Normal** or **Separate phases**.

For a **Scheil solidification simulation** project, and where applicable, select **Fast diffuser**.

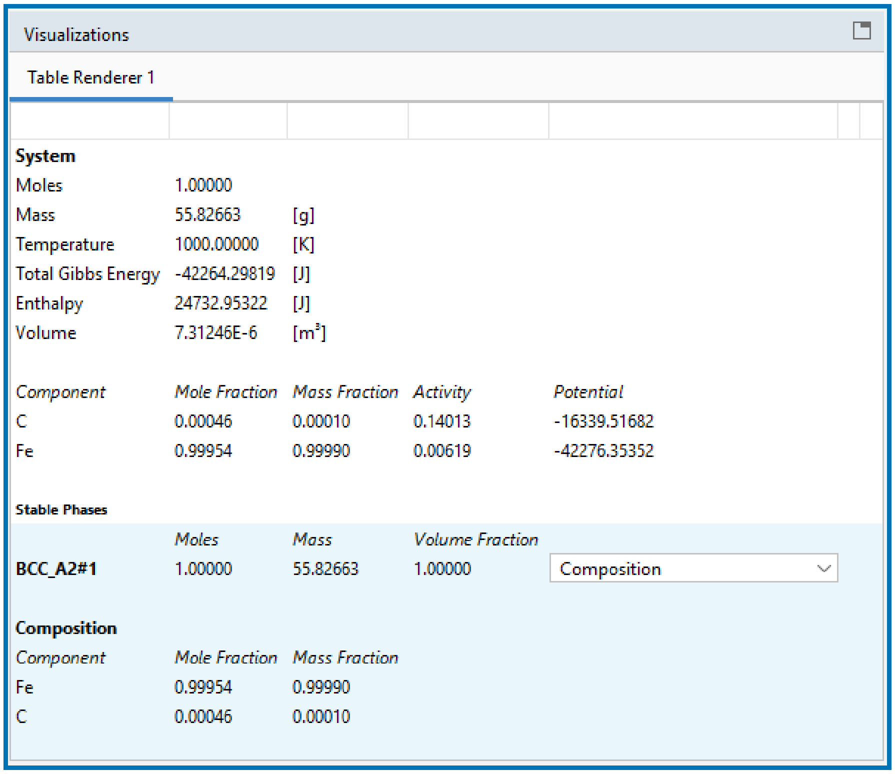
> After using this Quick Start Wizard to do a Classic Scheil calculation (or with fast diffuser components), a Scheil Calculator is added to the Project window. At this point you can review Scheil-Gulliver Solidification Calculations for details about all the options using the Scheil Calculator, i.e. back diffusion and solute trapping.

6. Click **Finish**. Click to expand the **Event Log** window to see information about the progress of the calculation.



```
14:02:00,441 INFO  ScheduledJob: The activity System Definer 1 executed in 5927 ms
14:02:00,445 INFO  GeneralEquilibriumCalculator: Performing general equilibrium calculation
14:02:00,613 INFO  AbstractQuantity: condition  T  the value  1000.0
14:02:00,613 INFO  AbstractQuantity: condition  P  the value  100000.0
14:02:00,614 INFO  AbstractQuantity: condition  N  the value  1.0
14:02:00,614 INFO  AbstractQuantity: condition  W(C)  the value  1.0E-4
14:02:02,076 INFO  ProcessExecutorAllocator: The subprocess completed normally
14:02:02,564 INFO  ScheduledJob: The activity Equilibrium Calculator 1 executed in 2122 ms
14:02:02,649 INFO  ScheduledJob: The activity Table Renderer 1 executed in 85 ms
```

The diagram is plotted in a **Plot Renderer** tab in the **Visualizations** window. If you have calculated a single-point equilibrium, then a **Table Renderer** tab shows information about the equilibrium.



System

Moles	1.00000	
Mass	55.82663	[g]
Temperature	1000.00000	[K]
Total Gibbs Energy	-42264.29819	[J]
Enthalpy	24732.95322	[J]
Volume	7.31246E-6	[m^3]

Component	*Mole Fraction*	*Mass Fraction*	*Activity*	*Potential*
C	0.00046	0.00010	0.14013	-16339.51682
Fe	0.99954	0.99990	0.00619	-42276.35352

Stable Phases

	Moles	*Mass*	*Volume Fraction*	
BCC_A2#1	1.00000	55.82663	1.00000	Composition

Composition

Component	*Mole Fraction*	*Mass Fraction*
Fe	0.99954	0.99990
C	0.00046	0.00010

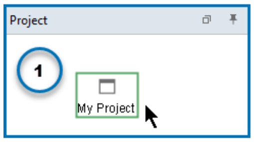
7. To save the project, click **Save** on the main toolbar. To save a diagram or table, right-click the diagram or table and select **Save As**.

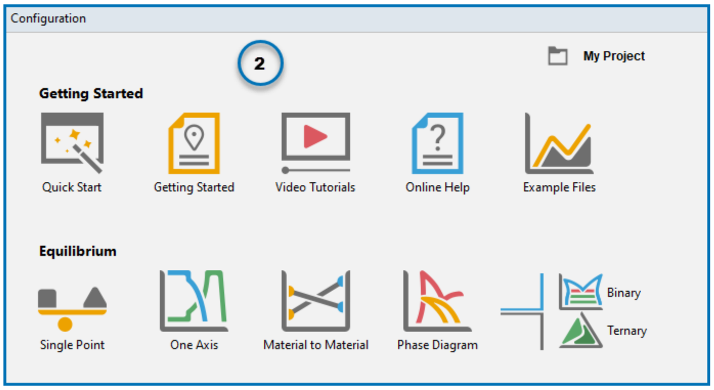
Creating a Project from a Template

Use a *Template* to create all the activities for a certain type of calculation.

Getting Started Links and Templates

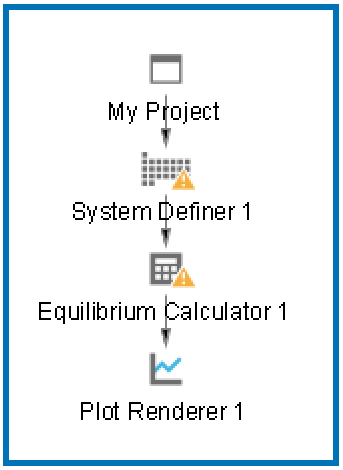
1. In the **Project** window, click the **My Project** node.
2. The templates (plus additional links under **Getting Started**) are available to click in the **My Project Configuration** window.



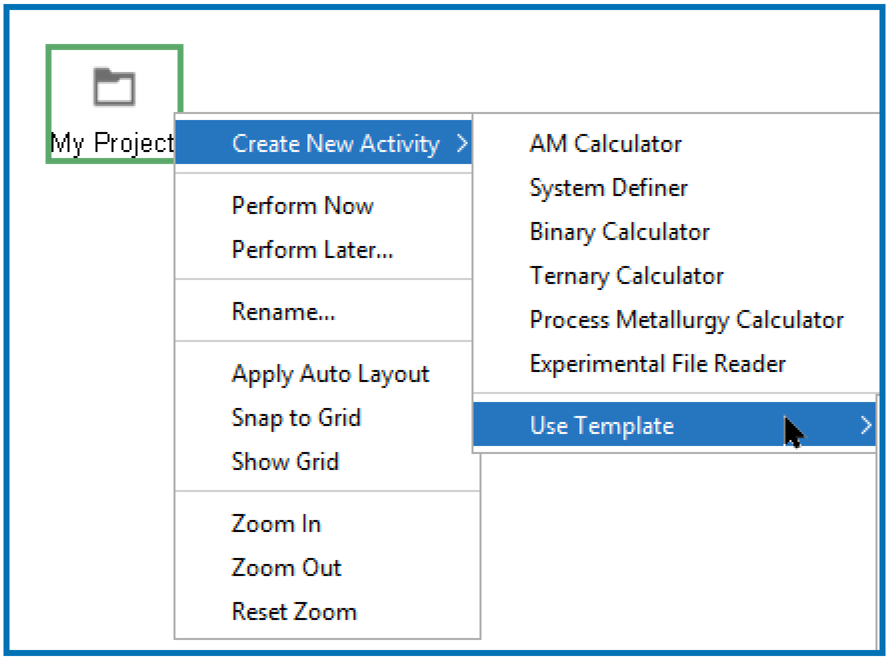


When you click a template, an activity tree is added to the **Project** window. You can then configure and perform the activities or the project.

For example, if under **Equilibrium** you click **One Axis**, a tree is added to the **My Project** node with **System Definer**, **Equilibrium Calculator**, and **Plot Renderer** nodes.



You can also add templates by right-clicking the **My Project** node and choosing an option from the **Create New Activity → Use Template** menu.



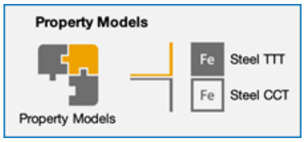
Steel Library TTT Diagram Template

The use of this Steel Model Library template requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases.

Use a **Steel TTT** template to add all the activities for a Time-Temperature-Transformation (TTT) diagram calculation. The **TTT Diagram** Property Model is automatically selected with all settings by default on the Property Model Configuration window. This makes it easy to add the project to the tree and examine the progress of transformation as a function of time at a fixed temperature.

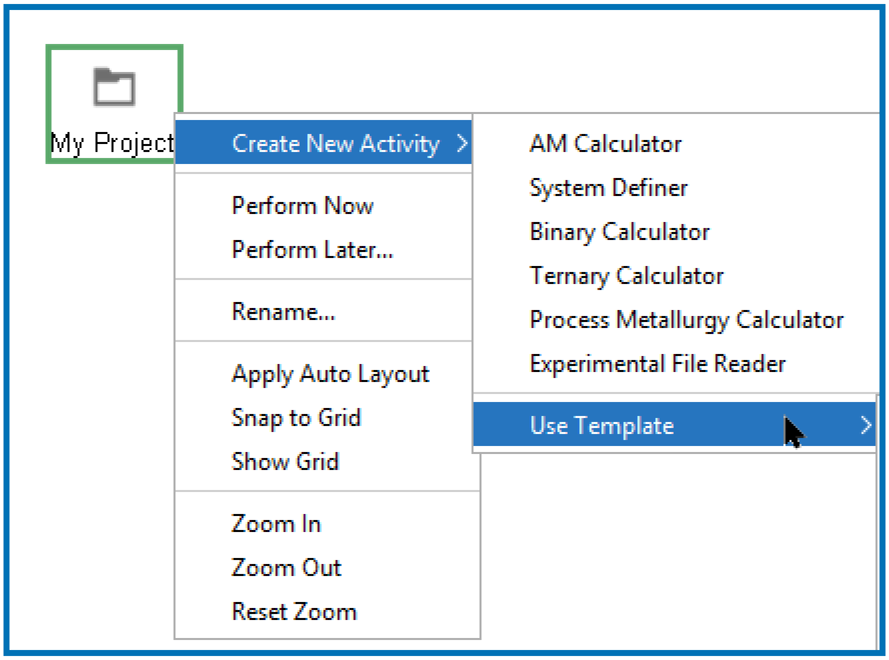
How to Add a Steel Library TTT Template to a Project

1. In the **Project** window click the **My Project** node to display the templates in the **Configuration** window.
2. Under **Property Models**, click the top icon **Steel TTT**.



A **System Definer**, *Property Model Calculator* (renamed to **Steel Models**) and a *Plot Renderer* (renamed to **TTT**) are added to the **Project** window. Also see Property Model Calculator and Plot Type: TTT Mode.

You can also add templates by right-clicking the **My Project** node and choosing an option from the **Create New Activity → Use Template** menu.



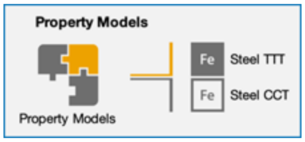
Steel Library CCT Diagram Template

> The use of this Steel Model Library template requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases.

Use a **Steel CCT** template to add all the activities for a Continuous-Cooling-Transformation (CCT) diagram calculation. The **CCT Diagram** Property Model is automatically selected on the Property Model Calculator with all settings by default. This makes it easy to add the project to the tree and examine the progress of transformation as a function of changing temperature.

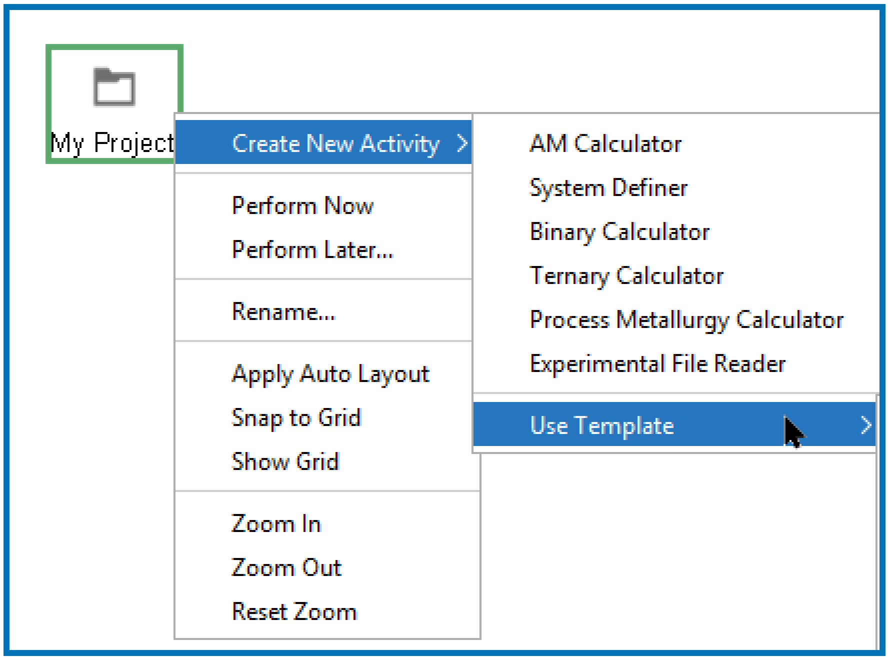
How to Add a Steel Library CCT Template to a Project

1. In the **Project** window click the 🗀 **My Project** node to display the templates in the **Configuration** window.
2. Under **Property Models**, click the bottom icon **Steel CCT**.



A **System Definer**, *Property Model Calculator* (renamed to **Steel Models**) and a *Plot Renderer* (renamed to **CCT**) are added to the **Project** window. Also see Property Model Calculator and Plot Type: CCT Mode.

You can also add templates by right-clicking the 🗀 **My Project** node and choosing an option from the **Create New Activity → Use Template** menu.



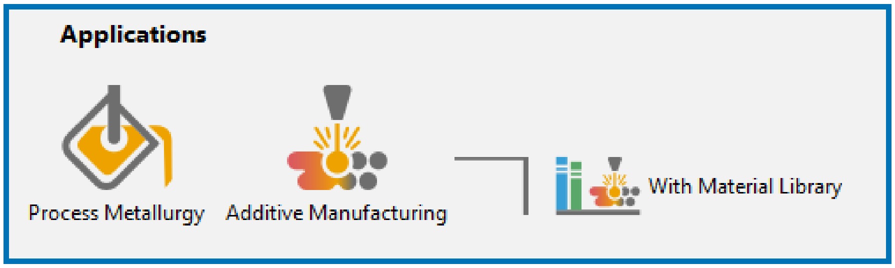
Process Metallurgy Template

Use a *Process Metallurgy* template to add the Process Metallurgy Calculator and a Plot Renderer to the **Project** window. The Process Metallurgy Calculator has several preconfigured settings making is easier to setup the different groups and materials needed to define a system for slag, metal and gas used in steelmaking.

? Process Metallurgy Calculator

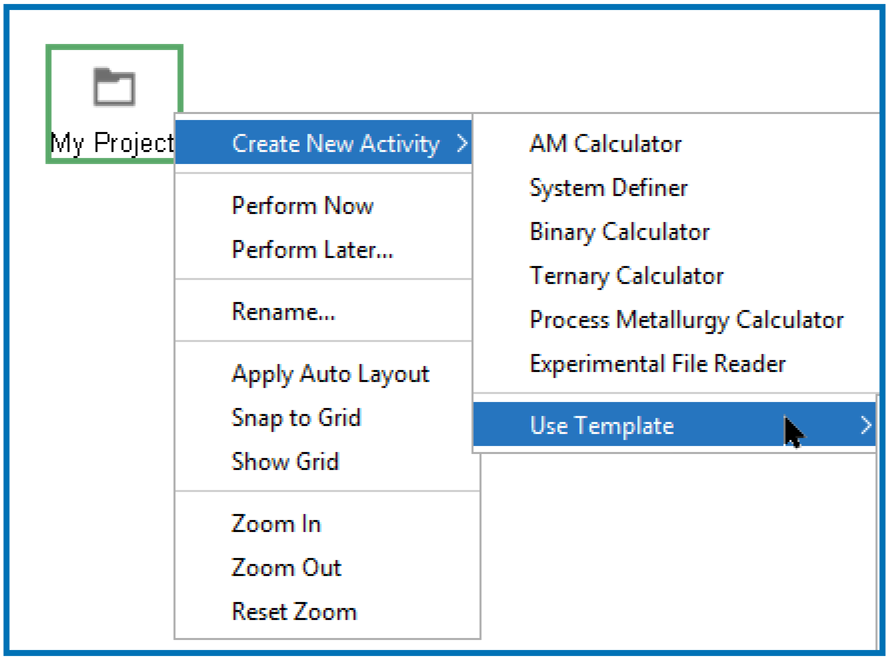
How to Add a Process Metallurgy Template to a Project

1. In the **Project** window click the 🗀 **My Project** node to display the templates in the **Configuration** window.
2. Under **Applications**, click **Process Metallurgy**.



A **System Definer**, **Process Metallurgy Calculator**, and a **Plot Renderer** are added to the **Project** window.

You can also add templates by right-clicking the 🗀 **My Project** node and choosing an option from the **Create New Activity → Use Template** menu.


My Project
Create New Activity
Perform Now
Perform Later...
Rename...
Apply Auto Layout
Snap to Grid
Show Grid
Zoom In
Zoom Out
Reset Zoom
AM Calculator
System Definer
Binary Calculator
Ternary Calculator
Process Metallurgy Calculator
Experimental File Reader
Use Template

Defining and Using the Activity Nodes

For information about the AM Calculator, see Additive Manufacturing (AM) Module

For information about the Process Metallurgy Calculator, see The Process Metallurgy Module.

In this section:

System Definer

In a **System Definer** activity, you select the database to use to retrieve thermodynamic data and define which elements the system has as components. You can also select the species to include as well as change the reference temperature and pressure for your components.

You can add the System Definer directly (right-click **My Project** and select it from the **Create New Activity** menu) or use a variety of the available templates to automatically add the node.

Many examples use the System Definer (see Graphical Mode Examples Listed by Product). For details about the templates, see Getting Started Links and Templates and Creating a Project from a Template.

Once you have added a System Definer, the **Configuration** window has these settings tabs:

- Elements
- Species
- Phases and Phase Constitution
- Components
- Data Sources
- Description

Define the System

This topic describes how to define a system, specifically how to select one or more databases and define the elements in the system with the **System Definer** activity node.

1. Right-click **My Project** and from the menu select **Create New Activity → System Definer**. For many templates a System Definer is also added to the Project tree.
2. In the **Project** window, click the **System Definer** activity node.
3. In the **Configuration** window, choose **Databases** from the list or a database **Package**.

About the Database Files

OPTIONS:

- From the **Databases** list, select **<User database>** to define your own.
- You can choose to add one or more databases by clicking the ⊕ **Add a database** button.

- From the **Package** list, choose a predefined database package to add multiple databases at a time. Depending on your license, there are predefined database packages available to select.

4. Select the **Elements** tab to choose the elements in the **Periodic Table** or use the **Alphabetic List** to choose elements for the system.
5. As required click the tabs to make edits: **Species**, **Phases and Phase Constitution**, and **Components**. The **Data Sources** and **Description** tabs provide information based on the database.

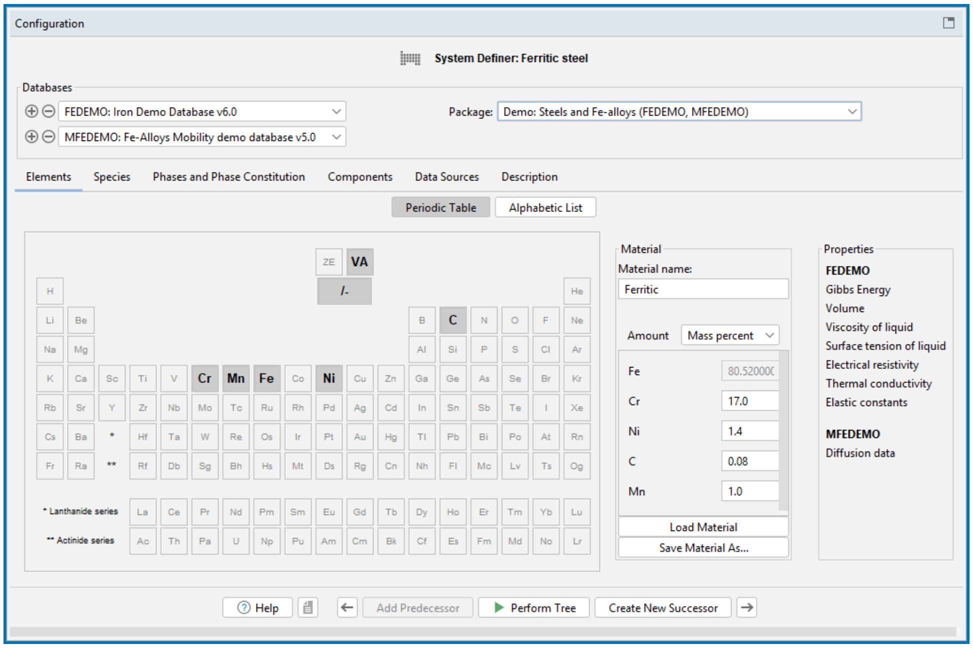
   Configuration Window Settings

6. Click **Perform** to start the System Definer activity immediately and retrieve data about the system. Click the **Event Log** window to watch the progress of the job.

Configuration Window Settings

The **System Definer** Configuration window has many settings available, which are briefly described below.

This uses PM_G_02: Coarsening and Interfacial Energy to show these features.



Configuration

System Definer: Ferritic steel

Databases

FEDEMO: Iron Demo Database v6.0

MFEDEMO: Fe-Alloys Mobility demo database v5.0

Package: Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)

Material name: Ferritic

Amount: Mass percent

Fe	80.52000
Cr	17.0
Ni	1.4
C	0.08
Mn	1.0

Properties

FEDEMO

Gibbs Energy

Volume

Viscosity of liquid

Surface tension of liquid

Electrical resistivity

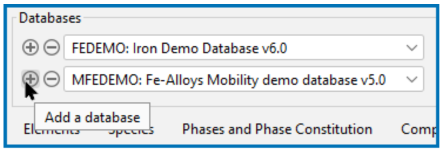
Thermal conductivity

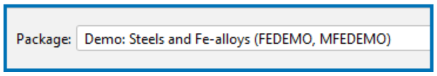
Elastic constants

MFEDEMO

Diffusion data

CHOOSE DATABASE(S) OR A DATABASE PACKAGE


Databases
FEDEMO: Iron Demo Database v6.0
MFEDEMO: Fe-Alloys Mobility demo database v5.0

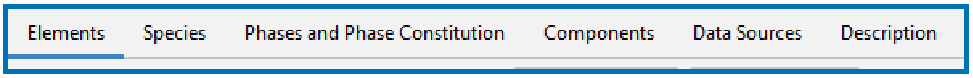

Package: Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)

At the top of the **Configuration** window you can choose to add one or more **Databases** by clicking the ⊕ **Add a database** button and choosing it from the list of available databases. You can also choose a predefined or custom database **Package** from the list. Depending on your license, there are predefined databases and packages available to select. After adding a database, click ⊖ **Remove this database** button as required for your simulation.

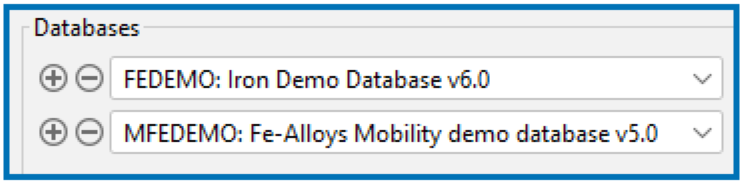
> If you have chosen a database package and then remove or change a database, a message displays *Selected databases and selected package may differ*. This means that the original package you selected, which added preset databases, does not match the databases you are using for the project. For information about how to clear the message, see Global Settings: System Definer.

Global Settings: System Definer

There are several settings tabs available for the System Definer activity.



The following example uses the FEDEMO and MFEDEMO databases and Graphical Mode example **PM_G_02**, which you can open from the **Help →** **Examples Files** menu or from the top **My Project** Configuration window.


Databases
FEDEMO: Iron Demo Database v6.0
MFEDEMO: Fe-Alloys Mobility demo database v5.0

ELEMENTS

On the **Elements** tab, and based on the databases or database package selected, you can select and review elements using a **Periodic Table** or **Alphabetic List** format. Unavailable elements, which are based on the selected database, are greyed out.

ELEMENTS: ADVANCED DATABASE OPTIONS

Also on the **Elements** tab, there three special elements used in the databases.

On the **Periodic Table** view, there are three buttons. For the **Alphabetic List**, the buttons are available each as a checkbox. In both cases you toggle ON (click to select the button or checkbox) or toggle OFF (click to deselect the button or checkbox, in other words, you are *rejecting* the phase).

From this tab, you are choosing to include or reject the *whole system of phases*. Click the **Phase and Phase Constituent** tab if you want to select specific phases to reject.

This is an advanced feature. The details of these options are described for Console Mode and generally in the *Database Manager User Guide*. For example, see ELEMENT and POURBAIX_DIAGRAM Module. For the purposes of Graphical Mode, the use of the buttons or checkboxes either include or reject (exclude) the vacancies (**VA**) or charged species (*I*-). It is recommended to keep the default after selecting the database(s). In general, these three special elements should not be rejected from the System Definer (Graphical Mode) or GES (Console Mode).

There is a training module related to this feature available via the Thermo-Calc online Learning Hub. Subscriptions also include access to live monthly office hours, where you can ask our experts about any of the content on the Learning Hub or your own design simulation challenges.

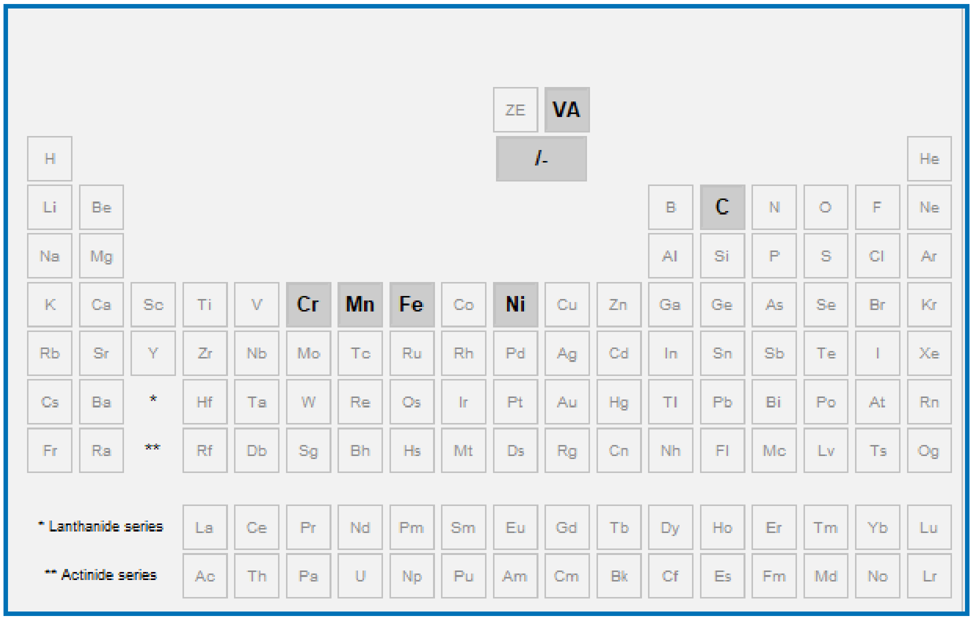
- **VA**. This allows a vacancy as a species. Toggled ON to include all vacancies or OFF to reject all vacancies in the phase constitution. VA itself is electrical neutral. It is usually a constituent of a phase. The element VA does not take any degree of freedom in an equilibrium calculation.
- */-*. This represents ELECTRON_GAS with -1 net charge. It is implemented in the database which includes ionic-modeled phases, i.e. with net-charged constituents. The charged species can be formed by combining /- (for negative charge) or /+ (for positive charge) with other ordinary elements, e.g. O-2 from O1/-2 or FE+2 from FE1/+2. The element /- does not take any degree of freedom in an equilibrium calculation. You can combine the elements VA and /- to model charged vacancies, e.g. VA-2 results from VA1/-2. To reject all charged species in the system, click to deselect (i.e. turn off). This is relevant to such databases as TCS Metal Oxide Solutions Database (TCOX), TCS Aqueous Solution Database (TCAQ), and the OXDEMO database.

  For most databases, there is an extensive list of all the phase models included with the technical information.

- The element **ZE** represents UNIT_CHARGE with +1 net charge. It is implemented and required only in the database that contains the AQUEOUS solution phase. ZE should never be rejected in GES. ZE itself is the only constituent of the phase REF_ELECTRODE, i.e. the reference electrode for ZE potential. This phase (REF_ELECTRODE) should always be suspended in the POLY module. Combining ZE with other ordinary elements forms aqueous species with net charge, e.g. the species H+1 results from H1ZE1 while OH-1 from H1O1ZE-1. The element ZE, like other ordinary elements, takes one degree of freedom in POLY in an equilibrium calculation. This is relevant to such databases as TCS Aqueous Solution Database (TCAQ) and when working with the Pourbaix module, which is only available with Console Mode and thus not available in Graphical Mode directly.

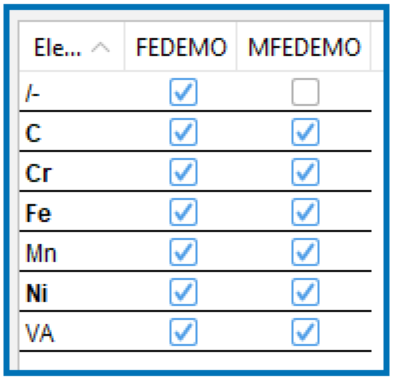
PERIODIC TABLE

In this example, using the demonstration databases FEDEMO and MFEDEMO, there are only a select number of elements to choose from when it is a DEMO database. These are selected for this example (Cr, Mn, Fe, Ni, C). The FEDEMO database is a subset of the main steel database TCS Steel and Fe-alloys Database (TCFE) and MFEDEMO is a subset of TCS Steels/Fe-Alloys Mobility Database (MOBFE).



ALPHABETIC LIST

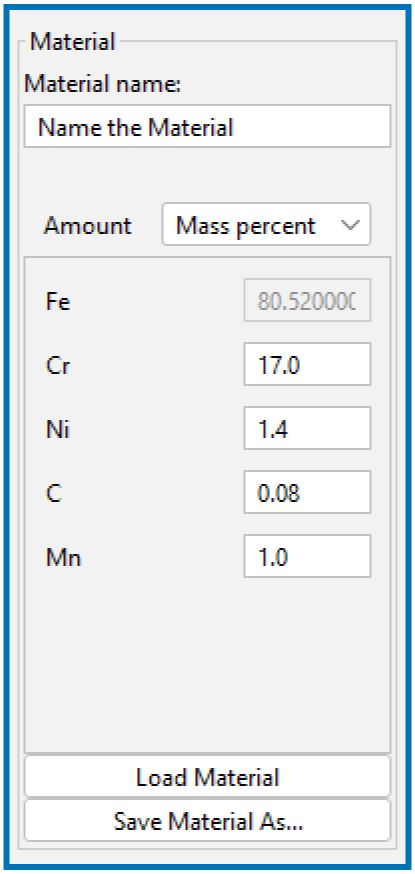
Click **Alphabetic List** to view a list of available and used elements.



Ele...	FEDEMO	MFEDEMO
/-	☑	☐
C	☑	☑
Cr	☑	☑
Fe	☑	☑
Mn	☑	☑
Ni	☑	☑
VA	☑	☑

MATERIAL COMPOSITION

After selecting the elements and in the **Periodic Table** view, under *Material*, you can enter a **Material name** and define the material composition **Amount** in **Mass percent**, **Mole percent**, **Mass fraction**, or **Mole fraction**.



Material name: Name the Material

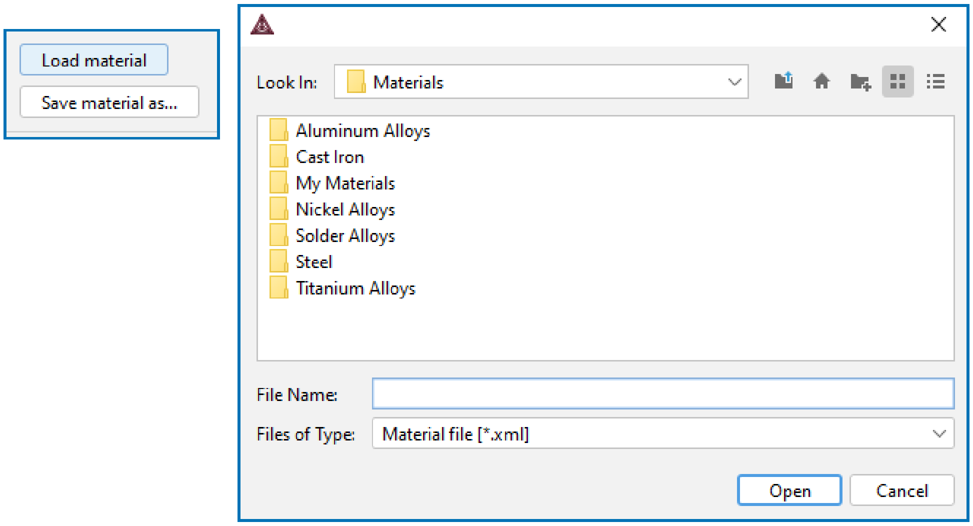
Amount: Mass percent

Fe	80.52000(
Cr	17.0
Ni	1.4
C	0.08
Mn	1.0

How To Load or Save a Material

Click **Load material** to open a material file. The default folder opens to the **Materials** folder included with your installation.

? About the Material Files and Installed Examples, Manuals, and Materials Folders



You can click **Save material as** to save the material you defined, for example **Ferritic**. Add your own folders as needed.

Global Settings: System Definer

For the **System Definer**, and if you load a material file and then change the composition, a message displays *The composition has changed*. This means that the original values/composition do not match the values you are using for the project. The message is cleared by either reloading the material file or editing the composition field to the original value.

PROPERTIES

After selecting the thermodynamic database and, when applicable, mobility database, the **Properties** section summarizes some of the key database properties.

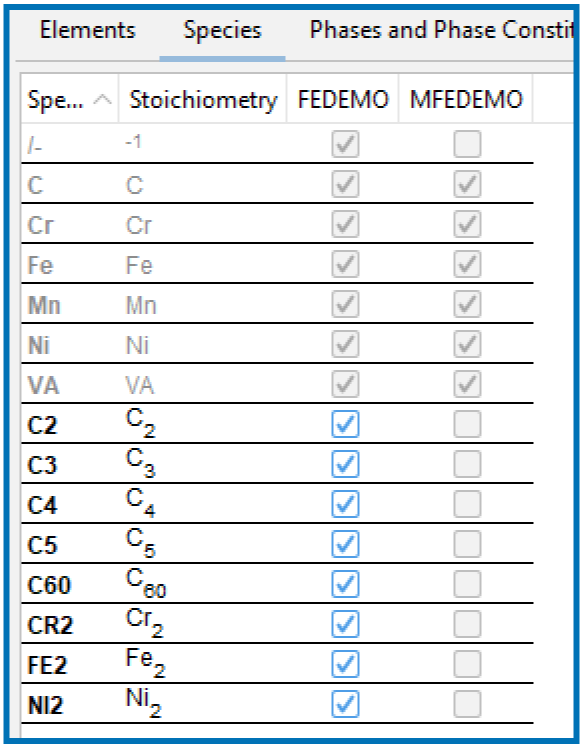
The software simulates many more properties than those listed.

The list includes some key database-specific properties, which are:

- **Physical properties**: Gibbs Energy, Volume, Viscosity of liquid, Surface tension of liquid, Electrical resistivity, Thermal conductivity
- **Elastic properties**: Elastic constants
- **Diffusion data** (for the mobility/kinetic databases)

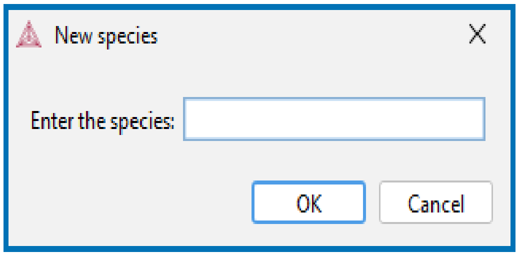
SPECIES

On the **Species** tab for each database you can select and edit the *Species* and view the *Stoichiometry* for the selected database species.

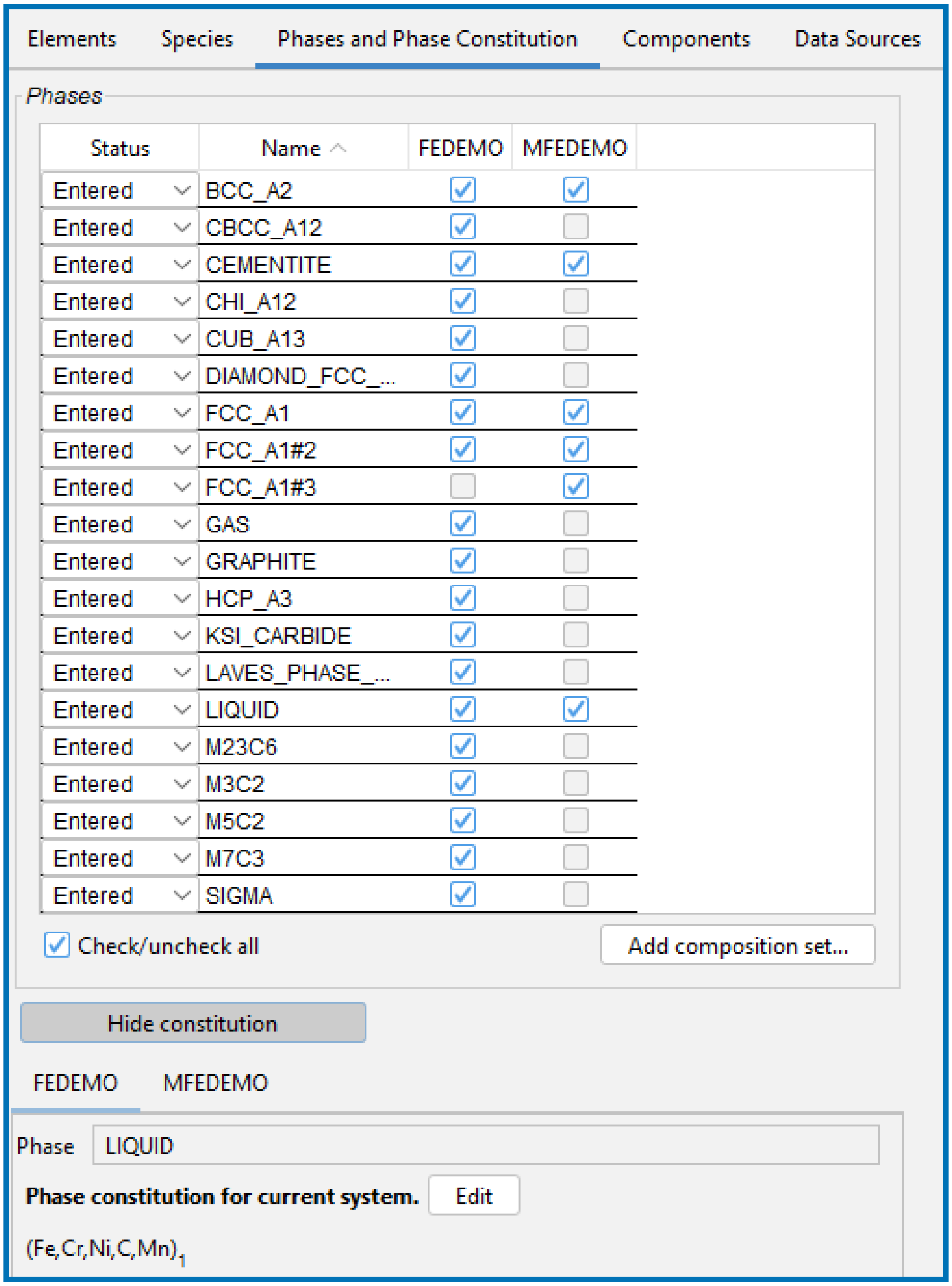


Spe...	Stoichiometry	FEDEMO	MFEDEMO
/-	-1	☑	☐
C	C	☑	☑
Cr	Cr	☑	☑
Fe	Fe	☑	☑
Mn	Mn	☑	☑
Ni	Ni	☑	☑
VA	VA	☑	☑
C2	C_2	☑	☐
C3	C_3	☑	☐
C4	C_4	☑	☐
C5	C_5	☑	☐
C60	C_{60}	☑	☐
CR2	Cr_2	☑	☐
FE2	Fe_2	☑	☐
NI2	Ni_2	☑	☐

At the bottom of the window, click **Add new species** and enter a **New species** name in the field.



PHASES AND PHASE CONSTITUTION



Phases

Status	Name	FEDEMO	MFEDEMO
Entered	BCC_A2	☑	☑
Entered	CBCC_A12	☑	☐
Entered	CEMENTITE	☑	☑
Entered	CHI_A12	☑	☐
Entered	CUB_A13	☑	☐
Entered	DIAMOND_FCC_...	☑	☐
Entered	FCC_A1	☑	☑
Entered	FCC_A1#2	☑	☑
Entered	FCC_A1#3	☐	☑
Entered	GAS	☑	☐
Entered	GRAPHITE	☑	☐
Entered	HCP_A3	☑	☐
Entered	KSI_CARBIDE	☑	☐
Entered	LAVES_PHASE_...	☑	☐
Entered	LIQUID	☑	☑
Entered	M23C6	☑	☐
Entered	M3C2	☑	☐
Entered	M5C2	☑	☐
Entered	M7C3	☑	☐
Entered	SIGMA	☑	☐

☑ Check/uncheck all

Phase: LIQUID

Phase constitution for current system.

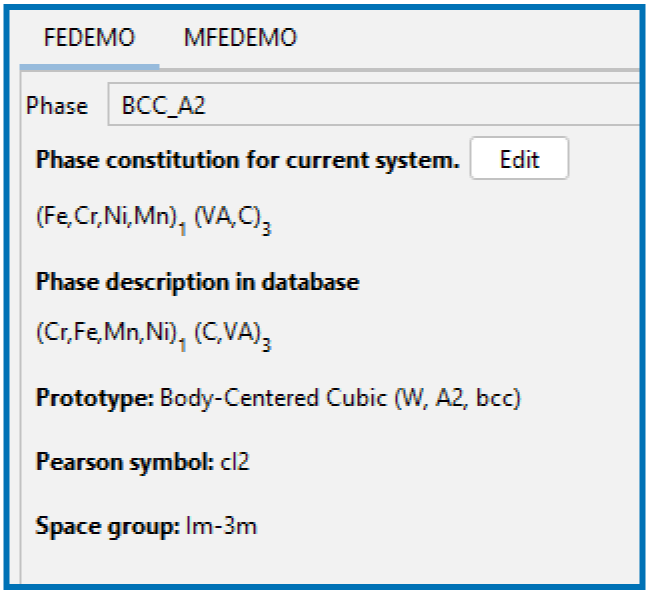
$(Fe,Cr,Ni,C,Mn)_1$

At the top of the **Phases and Phase Constitution** tab for each database you can review and edit the **Status** (**Entered** or **Dormant**) for the selected *Phases*.

Select the **Check/uncheck all** checkbox to toggle between the options.

From this tab, you can also choose specific phases to include or exclude the **VA** and */-* database species instead of doing it for the whole system as per Elements: Advanced Database Options.

To review the Phase constitution for a specific phase, click it in the *Phase* list (for example **BCC_A2**) and its details are displayed at the bottom of the window for the database selected. Click the relevant database tab to see its constitution by phase. Click **Edit** then click an element to select or reject a constituent. The last remaining constituent on a sublattice cannot be rejected.



Phase BCC_A2

Phase constitution for current system.

$(Fe,Cr,Ni,Mn)_1\ (VA,C)_3$

Phase description in database

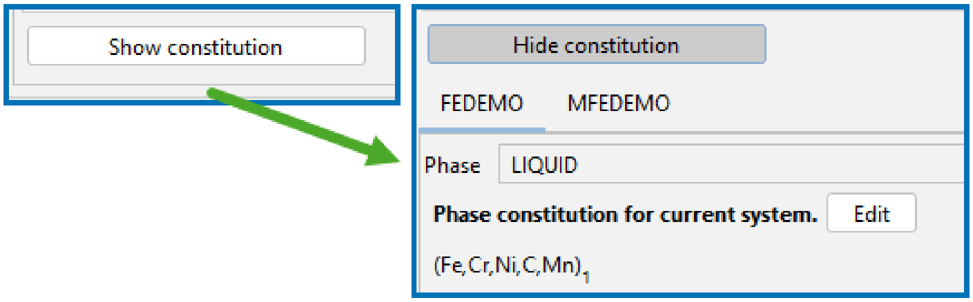
$(Cr,Fe,Mn,Ni)_1\ (C,VA)_3$

Prototype: Body-Centered Cubic (W, A2, bcc)

Pearson symbol: cI2

Space group: Im-3m

You can click the **Show constitution** or **Hide constitution** buttons found between the Phase table and Constitution details. Use this to toggle showing or hiding the details as needed. This is particularly useful when there is a long list and you are working on smaller displays where it may be difficult to scroll easily.



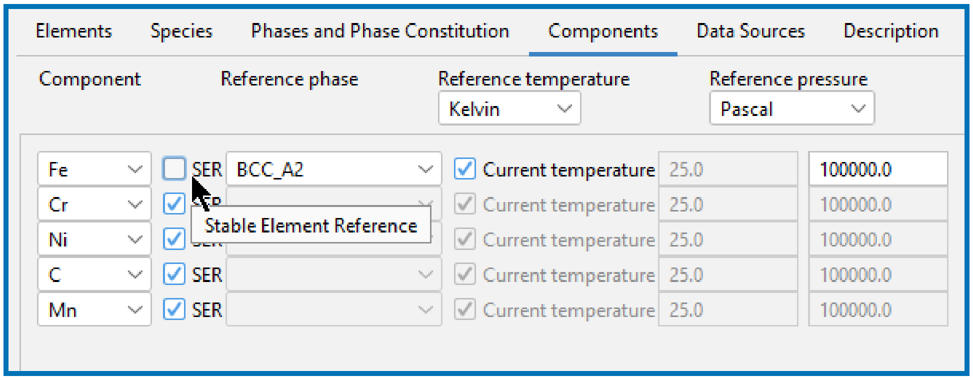
Phase: LIQUID

Phase constitution for current system.

$(Fe,Cr,Ni,C,Mn)_1$

COMPONENTS

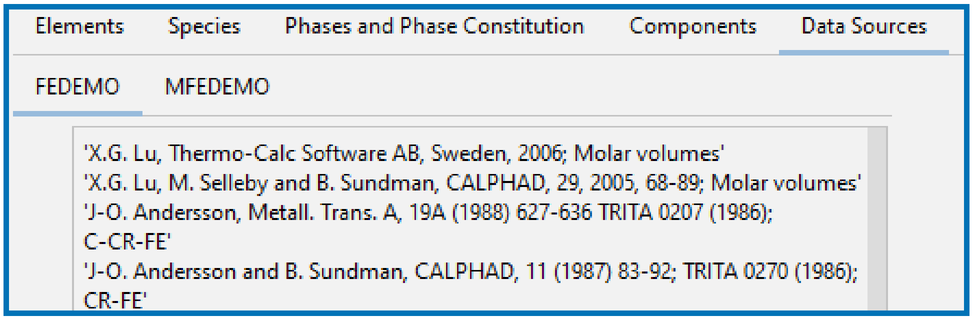
The **Components** tab is where you can review and edit the **Component**, **Reference phase**, **Reference temperature**, and **Reference pressure**. Click to toggle the **SER** (Stable Element Reference) checkbox on and off. Then choose a **Reference phase** from the list and edit accordingly. Choose a unit for the **Reference temperature**(**Kelvin**, **Celsius**, or **Fahrenheit**) and **Reference pressure** (**Pascal**, **Atmospheres**, or **Bar**).



Component	Reference phase		Reference temperature (Kelvin)		Reference pressure (Pascal)
Fe	☐ SER	BCC_A2	☑ Current temperature	25.0	100000.0
Cr	☑ SER		☑ Current temperature	25.0	100000.0
Ni	☑ SER		☑ Current temperature	25.0	100000.0
C	☑ SER		☑ Current temperature	25.0	100000.0
Mn	☑ SER		☑ Current temperature	25.0	100000.0

DATA SOURCES

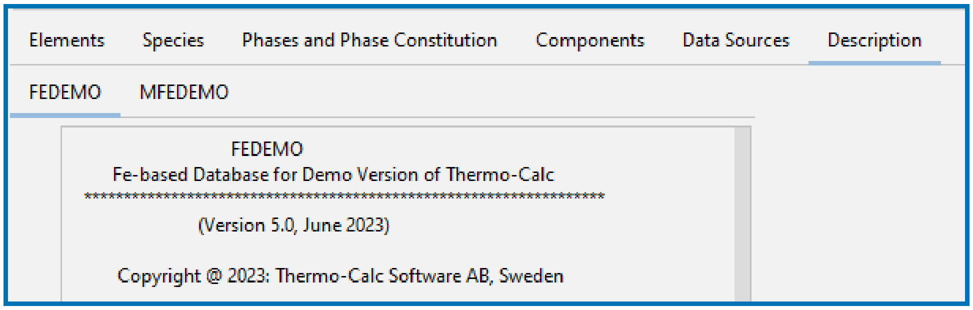
Data source references are shown after performing the activity. Click **Perform** or **Perform Tree** at the bottom of the window when your system is set up.



'X.G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'X.G. Lu, M. Selleby and B. Sundman, CALPHAD, 29, 2005, 68-89; Molar volumes'
'J-O. Andersson, Metall. Trans. A, 19A (1988) 627-636 TRITA 0207 (1986); C-CR-FE'
'J-O. Andersson and B. Sundman, CALPHAD, 11 (1987) 83-92; TRITA 0270 (1986); CR-FE'

DESCRIPTION

The **Description** tab displays a description of the selected database(s). In this example, **FEDEMO**, or click **MFDEMO** to view that information.

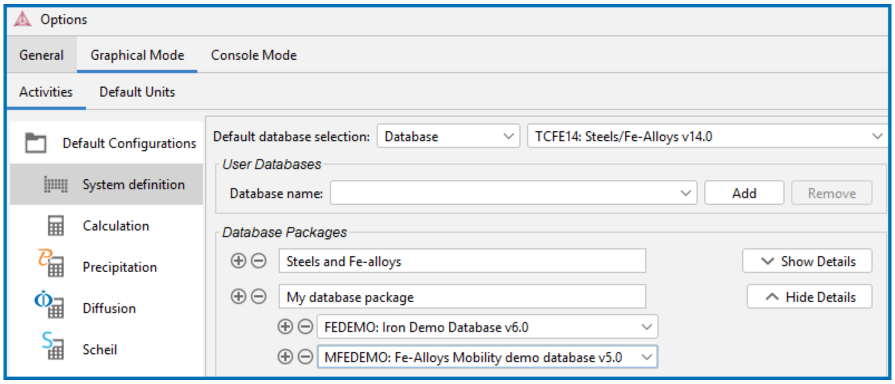


FEDEMO
Fe-based Database for Demo Version of Thermo-Calc
****
(Version 5.0, June 2023)

Copyright @ 2023: Thermo-Calc Software AB, Sweden

Creating a Database Package

1. From the main menu select **Tools → Options** .
2. Click the **Activities** tab and click **System definition**.
3. Under *Database Packages*, click the **Add a database package** ⊕ button.
4. Replace the default text *<Package #1>* with a name for the package, for example **My database package**.
5. Select a database from the **Choose database** list, for example, **FEDEMO Iron Demo Database**.
6. Click the ⊕ **Add a database** button and from the **Choose database** list, select another database.
7. Click **OK**. The software needs to relaunch for the Database Package to be available to choose as the default for new System Definer activities.



Default database selection: Database | TCFE14: Steels/Fe-Alloys v14.0

Database name:

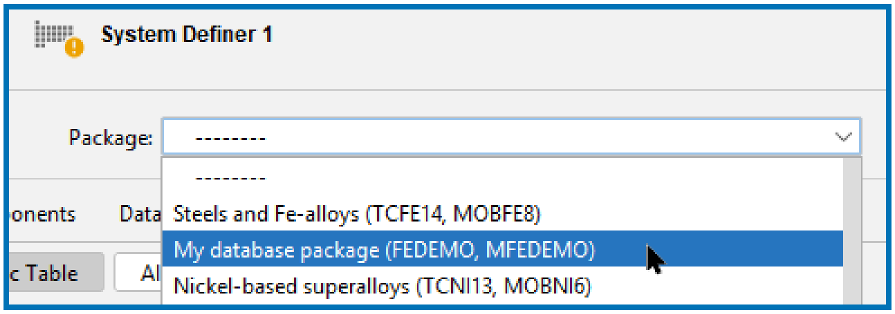
Steels and Fe-alloys

My database package

FEDEMO: Iron Demo Database v6.0

MFEDEMO: Fe-Alloys Mobility demo database v5.0

The package is available for new System Definer nodes defined after adding the package.



System Definer 1

Package: --------

- --------
- Steels and Fe-alloys (TCFE14, MOBFE8)
- My database package (FEDEMO, MFEDEMO)
- Nickel-based superalloys (TCNI13, MOBNI6)

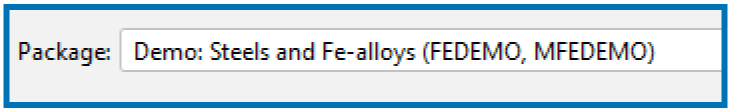
[Clearing a Database Package Message]() and [Global Settings: System Definer]()

Clearing a Database Package Message

Sometimes when working on the System Definer **Configuration** window, you may add or delete Databases. If you originally added a Database Package, the addition or removal of a database means that the original package you selected does not now match the databases you are using. To clear the message *Selected databases and selected package may differ* and reset the databases you need to either:

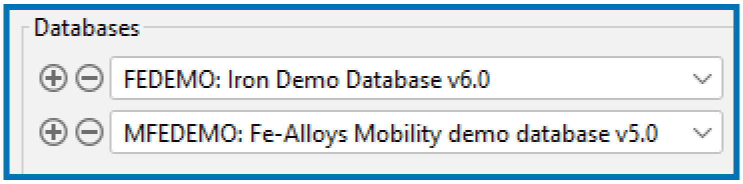
- Change the newly added database back to the one that matches the database package, or
- Choose another package from the **Package** list, then select the package you want.

For example, from the **Package** list you select **Demo: Steels and Fe-alloys**.



Package: Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)

This adds the **FEDEMO** and **MFEDEMO** databases.

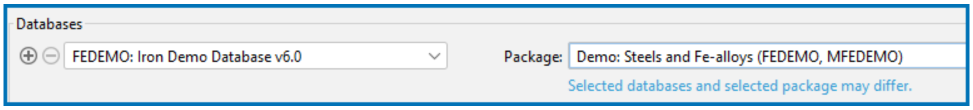


Databases

FEDEMO: Iron Demo Database v6.0

MFEDEMO: Fe-Alloys Mobility demo database v5.0

If you add or remove **Databases**, in this example **MFEDEMO** is removed, then this does not match the **Package** and the message displays:



Databases

FEDEMO: Iron Demo Database v6.0

Package: Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)

Selected databases and selected package may differ.

To clear the message, click the ⊕ **Add a database** button and from the **Choose database** list, select the database that belongs with the package, in this example, **MFEDEMO**. The message is cleared.

You can also choose another package from the list, which changes the databases, and then re-select the original package to reset the message.

? Creating a Database Package and Global Settings: System Definer

About the Material Files

When you are working with the System Definer or Material to Material Calculator in Graphical Mode you can open the default **Materials** folder included with your installation. The files are in .xml format and the data contained are from some common alloys. You can also save and create your own materials files or copy the xml files to the Materials folder.

? Installed Examples, Manuals, and Materials Folders

My Materials

This is where you can add your own material files to be able to load it to the System Definer or Material to Material Calculator. When you are in the System Definer **Configuration** window, you define your material then click **Save material as**. You can save the profile to this folder or create a folder with a new name.

Aluminum

- UNS_A95005
- UNS_A96053

Cast Iron

- UNS_F10007
- UNS_F33101

Nickel Alloys

- UNS_N06600
- UNS_N6600
- UNS_N06625
- UNS_N06690
- UNS_N07001
- UNS_N07718
- UNS_N08800
- UNS_N08825

Solder Alloys

- ASTM_25A
- ASTM_96TS
- UNS_L50134
- UNS_L54321

Steel

Austenitic Stainless Steel

- ASTM_304_(UNS_S30400)
- ASTM_304L_(UNS_S30403)
- ASTM_304LN_(UNS_S30453)
- ASTM_316_(UNS_S31600)
- ASTM_316L_(UNS_S31603)
- ASTM_316LN_(UNS_S31653)
- ASTM_317L_(UNS_S31703)
- UNS_J92710
- UNS_S30908

Duplex Stainless Steel

- UNS_S31803_A
- UNS_S32750_A
- UNS_S32750_B

High Speed Steel

- ASTM_M10_A5

High Temperature Steel

- UNS_S31008

HSLA Steel

- UNS_K12000

Low Carbon Steel

- UNS_H61180

Maraging Steel

- UNS_K92810

Martensitic Stainless Steel

- ASTM_420
- UNS_J82090
- UNS_J91639
- UNS_S44004

Tool Steel

- UNS_T30106
- UNS_T30109
- UNS_T51620

Training Steel

- Ferritic
- M7_Steel

Titanium Alloys

- UNS_R54520
- UNS_R56260

Equilibrium Calculator

An **Equilibrium Calculator** allows you to set the conditions for, and perform, a calculation. You can add the calculator to the System Definer directly (right-click and select it from the **Create New Successor** menu) or use a variety of the available templates.

Once you have added an Equilibrium Calculator, the **Configuration** window has these settings tabs. An Equilibrium Calculator that is the successor of another Equilibrium Calculator inherits all the settings of the predecessor.

- **Conditions**: Set the conditions for your calculation that define the stepping or mapping axis variables. Click the **Switch to Simplified Mode** and **Switch to Advanced Mode** buttons to toggle between those settings.
- **Functions**: Define your own quantities and functions, which you then can calculate and plot.
- **Options**: Modify numerical settings that determine how equilibria are calculated, as well as how stepping and mapping calculations are performed.

The **Options** tab is where you can locally define specific Equilibrium Calculator settings. These settings can also be applied globally. To open the **Options** window: From the main menu select **Tools** → **Options** and click the **Activities** tab. Then click **Calculation**.

There are these templates available under **Equilibrium** that use an Equilibrium Calculator: **Single Point**, **One Axis**, and **Phase Diagram**. Choose one of these to quickly set up a simulation. The **Quick Start** wizard is also an option. See Getting Started Links and Templates.

Define the Equilibrium Calculator

1. Add an Equilibrium Calculator node to the System Definer. If you used the **Single Point**, **One Axis**, or **Phase Diagram** templates (on the **My Projects Configuration** window under **Equilibrium**), click the **Equilibrium Calculator** node to display the **Configuration** settings window.

2. In the **Configuration** window, enter the settings described in Conditions Tab Settings. For the **Options** and **Functions** tab settings, see
   - Options Tab Settings
   - Calculating and Plotting Functions
3. Once you have finished defining the Equilibrium Calculator, you also choose settings on the Plot Renderer.

Calculating with a Fixed Phase

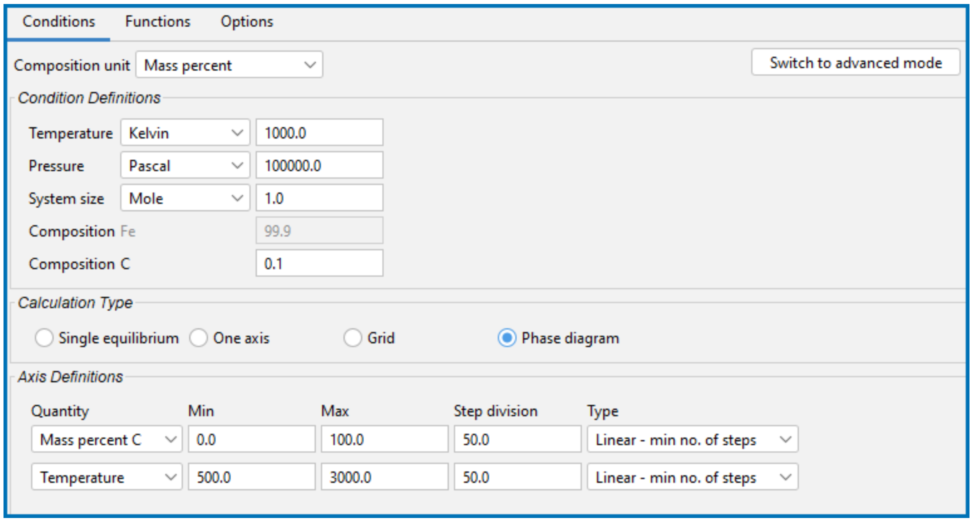
Examples

There are several examples that use an Equilibrium Calculator. As a start, see T_01: Calculating a Single-Point Equilibrium.

For an example of how serially coupled Equilibrium Calculators can be used, see T_06: Serially Coupled Equilibrium Calculators.

Conditions Tab Settings

Conditions and axis variables for the **Equilibrium Calculator** are set in the **Conditions** tab on the **Configuration** window. The tab can be viewed in two modes: **Simplified** (the default) or **Advanced** (see About Advanced Mode). The conditions to set depend on the type of calculation.



Composition unit: Mass percent

Condition Definitions

Temperature	Kelvin	1000.0
Pressure	Pascal	100000.0
System size	Mole	1.0
Composition Fe		99.9
Composition C		0.1

Calculation Type

○ Single equilibrium ○ One axis ○ Grid ● Phase diagram

Axis Definitions

Quantity	Min	Max	Step division	Type
Mass percent C	0.0	100.0	50.0	Linear - min no. of steps
Temperature	500.0	3000.0	50.0	Linear - min no. of steps

Examples

- T_01: Calculating a Single-Point Equilibrium
- T_02: Stepping in Temperature in the Fe-C System
- T_05: Stable and the Metastable Fe-C Phase Diagrams.

Options Tab Settings

Depending on the calculation type selected, there are also a variety of Plot Types to choose from.

Settings

The following outlines what you can set on the **Conditions** tab in simplified mode.

Click **Switch to Advanced Mode** for more options.

COMPOSITION UNIT

Select the **Composition unit**: **Mass percent**, **Mole percent**, **Mass fraction**, or **Mole fraction**.

CONDITION DEFINITIONS

Specify the values (and units) of the state variables: **Temperature**, **Pressure**, and **System size** or any other available lists under *Condition Definitions*.

CALCULATION TYPE

Click to select a *Calculation Type*:

- **Single equilibrium** (no axes): To calculate a single point. The results from this calculation are displayed in the **Event Log**.
- **One Axis**: To vary a quantity on the X-axis.
- **Grid**: Computes the equilibrium of each grid point in a two-dimensional grid.

- **Phase diagram**: To calculate in a defined multicomponent heterogeneous system, from one or more initial equilibria. A phase diagram is usually mapped within a specific space that is constructed by two (or more) defined independent mapping axis-variables.

For **Single equilibrium**, no additional settings are required. Add a **Table Renderer** to perform the calculation and view the details in the **Visualizations** window.

When you use the Equilibrium Property Model Settings with the **Property Model Calculator**, it is the same calculation result as when you are using an **Equilibrium Calculator** with the **Single equilibrium** calculation type.

AXIS DEFINITIONS

- **One Axis**: Define the axis variable using these fields and menus: **Quantity**, **Min**, **Max**, **Step division**, **Type**, and **Step Method**.
- **Grid**: Define the two axis variables using these fields and menus: **Quantity**, **Min**, **Max**, and **Number of steps**.
- **Phase diagram**: Define the two axis variables using these fields and menus: **Quantity**, **Min**, **Max**, **Step division**, and **Type**.

If the Calculator already has a Plot Renderer as a successor and you change the stepping/mapping quantities, then the quantities represented on the X- and Y-axis are automatically updated in the Plot Renderer.

Depending on the calculation type selected, there are also a variety of Plot Types to choose from.

STEP DIVISION AND TYPE (ONE AXIS AND PHASE DIAGRAM)

Enter a **Step division** and select a **Type**: **Linear - min no. of steps**, **Linear - max step size**, or **Logarithmic - scale factor**.

- For **Linear - min no. of steps**, the **Step division** value specifies a minimum number of steps that is calculated between the minimum and maximum value during the stepping/mapping operation.
- For **Linear - max step size**, the **Step division** sets the maximum size of each step. For **Logarithmic - scale factor**, **Step division** specifies the scale factor of a logarithmic function that distributes the steps from the initial equilibrium to the minimum and maximum values defined.

STEP METHOD (ONE AXIS)

From the **Step Method** list, choose **Normal** or **Separate phases**.

- **Normal** allows a stepping calculation with the chosen independently-varying equilibrium condition (axis-variable). Only the step axis value is changed between each step.
- **Separate phases** calculates how the Gibbs energy for a number of phases varies for different compositions. This is particularly useful to calculate Gibbs energies for complex phases with miscibility gaps and for an ordered phase that is never disordered (e.g. SIGMA-phase, G-phase, MU-phase, etc.).

NUMBER OF STEPS (GRID)

Set a fixed **Number of steps**. The number of steps along with the minimum and maximum values for the axes define a grid. For each grid point an equilibrium is calculated.

About Advanced Mode

Click **Switch to Advanced Mode** to add and remove conditions as well as set additional axis definitions. However, the number and types of conditions set must still conform to the Gibbs' phase rule. The **Number of missing conditions is** field, at the top of the tab shows how many conditions that you have left to set. If the number is negative, then that number of conditions need to be removed.

List of Advanced Mode Condition Definitions

When applicable, these quantities are grouped together as **Phase equilibria** on the Plot Renderer. See Quantities Groups Available for Plots and Tables.

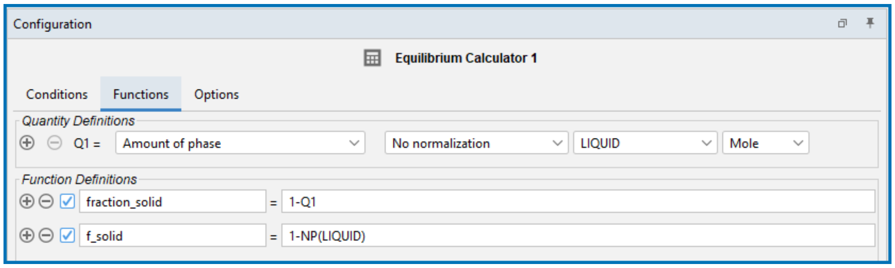
- Activity of component
- Activity referred to a phase
- Amount of component
- Amount of component in a phase
- Amount of phase
- Chemical potential of a component
- Chemical potential referred to a phase
- Composition
- Enthalpy
- Entropy
- Fix phase
- Gibbs energy
- Helmholtz energy
- Internal energy
- ln(activity of component)
- ln(activity referred to a phase)
- Pressure
- Site fraction
- System size
- Temperature
- User-defined
- Volume

Calculating and Plotting Functions

The **Functions** tab allows you to define your own functions that can be plotted in a Plot Renderer.

For an example of how you can use functions that you define, see T_07: User-Defined Functions.

1. Add an **Equilibrium Calculator** node and click it in the **Project** window.
2. In the **Configuration** window click the **Functions** tab.
3. Under **Quantity Definitions**, define **Q1**. Click the add ⊕ button to **Add a new quantity**. Then from the lists, choose the variable for each quantity to define. The quantities are called **Q1**, **Q2**, **Q3** and so on. In this example, the quantity **Q1** is defined as the **Amount of phase**, with **No normalization**, **LIQUID** in **Mole** units.



Quantity Definitions

⊕ ⊖ Q1 = Amount of phase | No normalization | LIQUID | Mole

Function Definitions

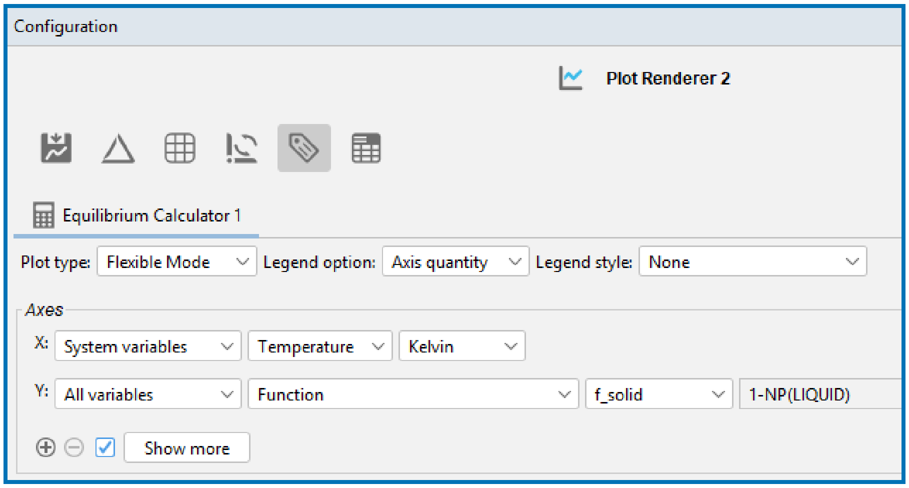
⊕ ⊖ ☑ fraction_solid = 1-Q1

⊕ ⊖ ☑ f_solid = 1-NP(LIQUID)

4. Under **Function Definitions**, click the add ⊕ button to add a new function. In the left field edit the default name of each function and enter the function itself in the right field after the equal sign. In this example, the quantity defined as Q1 is renamed to **fraction_solid**, which gives as its output the fraction of solid phase (**1-Q1**).

You can also use Console Mode syntax when entering the function. For example, the function above can be entered as `1-NP(LIQUID)`. See Parameters, Functions, and Variables for details.

5. To plot the defined function, right-click **Equilibrium Calculator** and choose **Create New Successor → Plot Renderer**.
6. Click the new **Plot Renderer** node.
   a. For the axis variable, which is grouped under an *Axes* section (**Flexible Mode**), or listed individually as *X*, *Y*, or *Z* (**Grouped Mode**), choose **All variables** from the first list.
   b. Select **Function** from the second list.
   c. From the third list, choose the function you defined on the Equilibrium Calculator Functions tab. In this example the Y axis is set to plot the value of the function **f_solid**.
   d. When run, the Plot Renderer plots the value of the function.



Configuration

Plot Renderer 2

Equilibrium Calculator 1

Plot type: Flexible Mode Legend option: Axis quantity Legend style: None

Axes

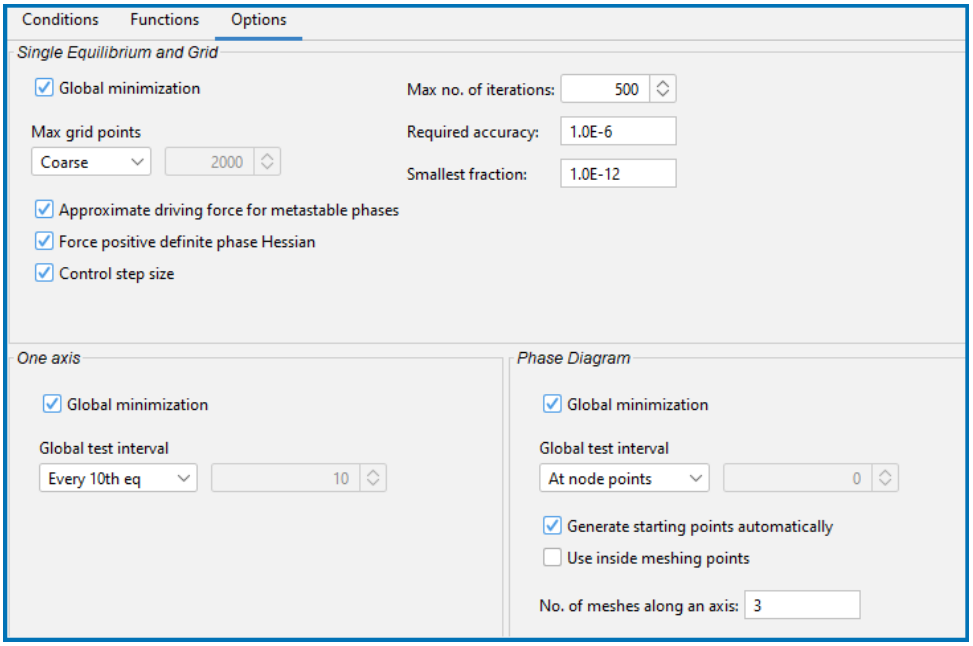
X: System variables Temperature Kelvin

Y: All variables Function f_solid 1-NP(LIQUID)

☑ Show more

Options Tab Settings

These settings are for the Equilibrium Calculator and are located on the **Configuration** window → **Options** tab.



Conditions Functions Options

Single Equilibrium and Grid

☑ Global minimization

Max no. of iterations: 500

Max grid points: Coarse 2000

Required accuracy: 1.0E-6

Smallest fraction: 1.0E-12

☑ Approximate driving force for metastable phases

☑ Force positive definite phase Hessian

☑ Control step size

One axis

☑ Global minimization

Global test interval: Every 10th eq 10

Phase Diagram

☑ Global minimization

Global test interval: At node points 0

☑ Generate starting points automatically

☐ Use inside meshing points

No. of meshes along an axis: 3

You can change these settings locally for a specific Calculator or globally for some defaults in the **Options** *window* (a different location than the tab).

To open the **Options** window:

- Windows: Select **Tools → ☰ Options**.
- Mac: Select **Thermo-Calc** *<version>* **→ Preferences** or **Settings** or press <⌘> on the keyboard.

then click the **Graphical Mode** tab and the **Calculation** node in the tree.

Single Equilibrium and Grid

Under *Single Equilibrium and Grid*, there are these *Calculation Type* setting options.

GLOBAL MINIMIZATION

The **Global minimization** checkbox is selected by default to ensure that the most stable minimum under the specified conditions is computed.

MAX GRID POINTS

For the **Max grid points**, the default is **Coarse** (2000 grid points), or choose **Medium** (20,000 grid points), **Fine** (200,000 grid points), or **Custom** to set your own number of grid points.

APPROXIMATE DRIVING FORCE FOR METASTABLE PHASES

The **Approximate driving force for metastable phases** checkbox is selected by default. Click to clear the checkbox to change the default as required and based on the options described below.

This setting involves the convergence of metastable phases and affects their driving forces. It can also have an effect on when an equilibrium is considered successful.

The default is to allow an equilibrium with metastable phases that have not converged, as long as the stable phases have converged. This is efficient but often causes approximate values of the driving forces for the metastable phases.

If you change the default, it enforces metastable phases to converge. This gives accurate driving forces for metastable phases as well as stable phases. It can however take a slightly longer time, and if metastable phases do not converge it causes the equilibrium calculation to fail.

FORCE POSITIVE DEFINITE PHASE HESSIAN

The **Force positive definite phase Hessian** checkbox is selected by default and this setting determines how to reach the minimum of an equilibrium state.

ADVANCED_OPTIONS

Control Stepsize

The **Control stepsize** checkbox is selected by default and this setting determines how to reach the minimum of an equilibrium state.

ADVANCED_OPTIONS

Max No of Iterations

Enter or choose a value for the **Max no. of iterations**. By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.

Required Accuracy

The default **Required accuracy** is `1.0E-6`. This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.

Smallest Fraction

The default **Smallest fraction** (or **Smallest fraction in a phase** for Property Models) is `1.0E-12`. This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions.

The default value for the smallest site-fractions is `1E-12` for all phases except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as `1E-30`.

In Console Mode, the default of 1E-30 for IDEAL phases is true unless you are using the command SET_NUMERICAL_LIMITS to reset an even-lower value (e.g. `1E-45`, that is naturally enforced to all the phases in the system.

One Axis

Under *One Axis*, there are these *Calculation Type* setting options.

GLOBAL MINIMIZATION

The **Global minimization** checkbox is selected by default to ensure that the most stable minimum under the specified conditions is computed.

ADVANCED_OPTIONS

GLOBAL TEST INTERVAL

The default **Every 10th eq** is the recommended **Global test interval** i.e. every tenth step and at each phase change during calculations. Or choose **Always** or **Custom**.

If you choose **Custom**, the integer number determines how often the global minimization should be used during step and mapping. Any other positive integer number, n, suggests it performs a global minimization test at every *n*-th step during calculations.

Phase Diagram

Under *Phase diagram*, there are these *Calculation Type* setting options.

GLOBAL MINIMIZATION

The **Global minimization** checkbox is selected by default to ensure that the most stable minimum under the specified conditions is computed.

GLOBAL TEST INTERVAL

The default **At node points**is the recommended **Global test interval** and is used only at node points during the calculations.

- If you choose **Every 10th eq**, this is every tenth step and at each phase change during calculations.
- If you choose **Custom**, the integer number determines how often the global minimization should be used during step and mapping. Any other positive integer number, n, suggests it performs a global minimization test at every *n*-th step during calculations.

GENERATE STARTING POINTS AUTOMATICALLY

The **Generate starting points automatically** checkbox is selected by default.

USE INSIDE MESHING POINTS

Click the **Use inside meshing points** checkbox as required. The initial mesh consists of initial equilibrium points added only along the edge/border of the diagram defined by the axis-variables. If you select the checkbox, then the initial equilibrium points added are also added to the inside edge.

NO OF MESHES ALONG AN AXIS

The default **No of meshes along an axis** is 3 , which represents how many intervals of initial equilibrium points are added along an edge in the diagram. For example, if set to 2 (two), initial equilibrium points are added at the beginning, center, and end of each axis-variable forming 2 intervals.

Calculating with a Fixed Phase

This describes how to use the advanced mode to set a phase to be fixed at a certain amount. This allows you to, for example, find out at what temperature a material starts to melt. If you set the phase to be fixed to liquid phase at zero amount, and do not define the temperature state variable, then you can calculate at what temperature the material enters a state where the liquid phase is no longer zero (that is, when it starts to melt).

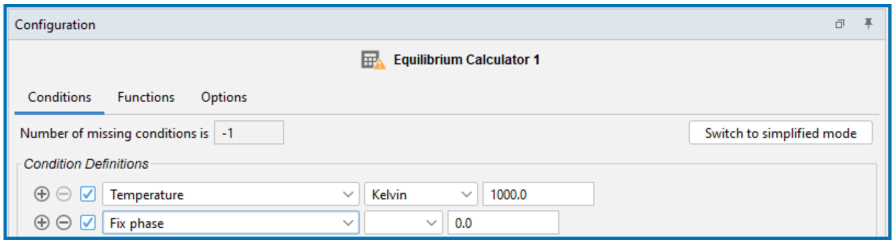
> For a fixed phase equilibrium calculation, it is recommended to serially couple the Equilibrium Calculators. This is where one Equilibrium Calculator activity is the successor to another Equilibrium Calculator activity that performs an ordinary equilibrium calculation, and then, for the condition you are interested in, you make a rough estimate of the value. This gives the fixed phase calculation better starting values.

1. Right-click a node that can add an **Equilibrium Calculator** to your project.
2. In the **Project** window, click the **Equilibrium Calculator** activity node.
3. In the **Configuration** window, click **Switch to Advanced Mode**.

> If the **Default calculation mode** is globally set to **Advanced** then by default the Configuration window is already in advanced mode.

[Global Settings](#)

4. Under *Condition Definitions*, click the ⊕ **Add quantity** button.
5. Select **Fix phase** from the first menu.
6. Select the phase that you want to fix in the second menu, and set the amount of that phase you want to fix the phase to. For example, if you want to know when your material starts to melt, set the phase to **LIQUID** and the value to **0.0**:



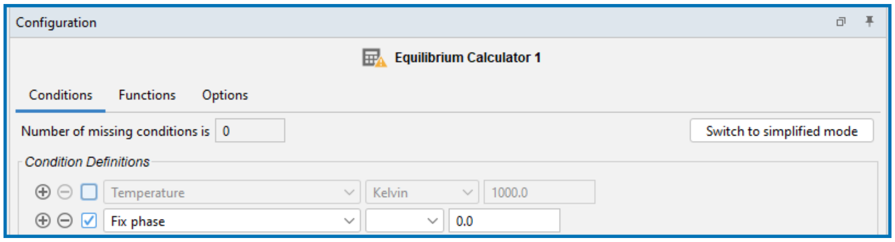
Number of missing conditions is -1

⊕ ⊖ ☑ Temperature Kelvin 1000.0

⊕ ⊖ ☑ Fix phase 0.0

Above the *Condition Definitions*, the **Number of missing conditions is** field is probably **-1**. This means that you must remove one condition.

7. To remove a condition, either click the ⊖ **Remove** button, or click to clear the checkbox. For example, if you want to know at what temperature your material starts to melt, then you cannot have a fixed temperature, in which case the temperature condition is not selected:



Number of missing conditions is 0

⊕ ⊖ ☐ Temperature Kelvin 1000.0

⊕ ⊖ ☑ Fix phase 0.0

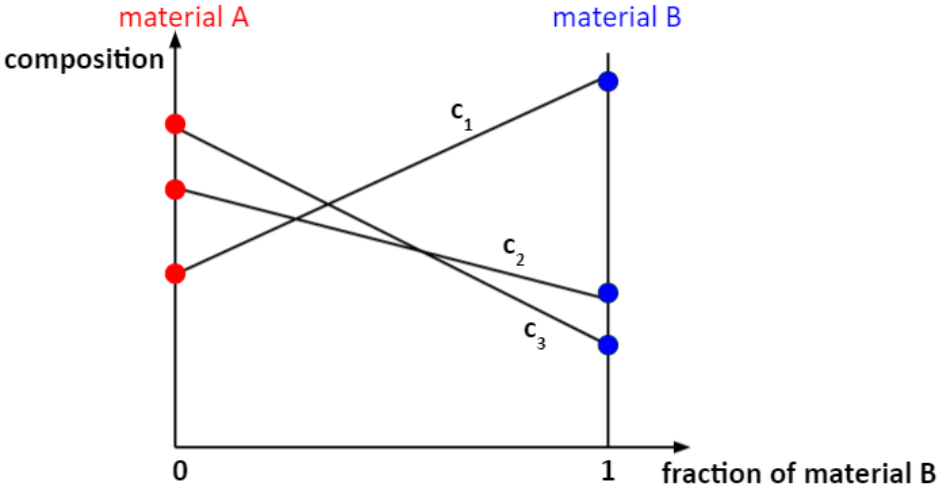
The **Number of missing conditions is** field displays **0**. When you have set all your conditions, you can perform the Equilibrium Calculator (now or later).

Material to Material Calculator

A **Material to Material Calculator** allows you to set the conditions for, and perform, a calculation to examine how materials transition from one into the other. Typical applications are for graded materials, non-similar material joints (without requiring a diffusion calculation), or a reaction of two materials, e.g. influence of volcanic ash on a turbine component in an engine.

For example, you can look at the transitions of phase compositions (c_1, c_2, c_3 in the diagram) for two materials, A and B and then calculate an equilibrium, one axis (similar to a property diagram), or phase diagram to examine, for example, what phases are forming at the interfaces or to see what kinds of reactions there are at specific points in the transition.

Composition of the elements is evolving versus the fraction of the second material.



You can add the calculator to the System Definer directly (right-click and select it from the **Create New Successor** menu).

There is also a **Material to Material** template available under **Equilibrium** that you can use to quickly set up a simulation. See Getting Started Links and Templates.

Once you have added a Material to Material Calculator, the **Configuration** window has these settings tabs.

- **Conditions**: Set the conditions for your calculation that define the stepping or mapping axis variables.
- **Functions**: Define your own quantities and functions, which you then can calculate and plot.
- **Options**: Modify numerical settings that determine how equilibria are calculated, as well as how stepping and mapping calculations are performed.

Read more on our website about the Material to Material Calculator. If you are in Thermo-Calc, press F1 to search the help.

Define the Material to Material Calculator

1. Add a Material to Material Calculator node to the System Definer. If you used the **Material to Material** template (on the **My Projects Configuration** window under **Equilibrium**), click the **Material to Material Calculator** node to display the **Configuration** settings window.
2. In the **Configuration** window, enter the settings described in Material to Material Calculator Conditions Tab Settings.

   For the **Options** and **Functions** tabs, the settings are the same as the Equilibrium Calculator. See Options Tab Settings and Calculating and Plotting Functions.

3. Once you have finished defining the Material to Material Calculator, you also choose settings on the Plot Renderer.

Example

For an example, see T_14: Fe-Cr-Ni Transition Comparison Using the Material to Material Calculator.

Material to Material Calculator Conditions Tab Settings

Conditions and axis variables for the Material to Material Calculator are set in the **Conditions** tab on the **Configuration** window. The conditions to set depend on the type of calculation.

Example

For an example, see T_14: Fe-Cr-Ni Transition Comparison Using the Material to Material Calculator.

The **Material to Material** template (on the **My Projects Configuration** window under **Equilibrium**) creates a project to perform calculations to examine how materials transition from one into the other. The project consists of a System Definer, Material to Material Calculator, and a Plot Renderer.

Functions: This is the same as the Equilibrium Calculator. See Calculating and Plotting Functions

Options: This is the same as the Equilibrium Calculator. See Options Tab Settings

Settings

The following outlines what you can set on the **Conditions** tab.

COMPOSITION UNIT

Select the **Composition unit**: **Mass percent**, **Mole percent**, **Mass fraction**, or **Mole fraction**.

CONDITION DEFINITIONS

Under *Condition Definitions*:

- For both the **First material** and **Second material**, define the values (and units) of the state variables **Temperature** and **Pressure**.
- Enter a **Fraction of second material**.
  - For a **Single equilibrium** calculation this is used as condition for the calculation.
  - For a **One Axis** calculation this is used as the start value for the calculation.
  - For a **One Axis** or **Phase diagram** calculation, and if the **Fraction of second material** is chosen as the *Axis Definition>Quantity*, then it is stepping between the *Min* and *Max*.
- For both materials, select the **Dependent component**.
- Select the **Activity conditions** checkbox to define the **Activity of component** for one or more components. By default this is not selected. Click the ⊕ **Add quantity** and ⊖

Remove quantity buttons to add and remove conditions.

- The reference state is defined on the System Definer.

CONDITION DEFINITIONS > DEFINE THE FIRST AND SECOND MATERIALS

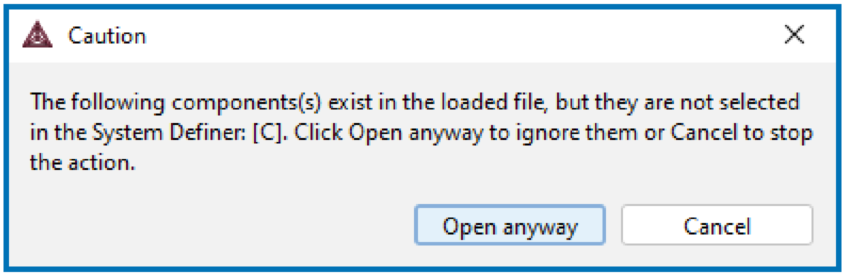
For each **First material** and **Second material** component there are individual settings to define as follows.

Enter a unique **Material name** for each. This name is used on the plots and in the quantity definitions so it is good to use as concise a name as possible that clearly identifies each material. For example, `Martensitic Steel` for the **First material** and `Alloy 800` for the **Second material**.

For each **Composition** field, enter numeric values for each material.

- Click **Save material as** after defining a composition to add it for reuse in other projects and calculations.
- Click **Load material** to add the composition of a predefined material from an xml file. Also see How To Load or Save a Material

If the user-defined material file includes one or more components not defined on the System Definer, then you are prompted to make a decision:



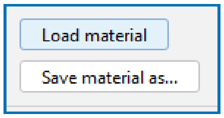
The following components(s) exist in the loaded file, but they are not selected in the System Definer: [C]. Click Open anyway to ignore them or Cancel to stop the action.

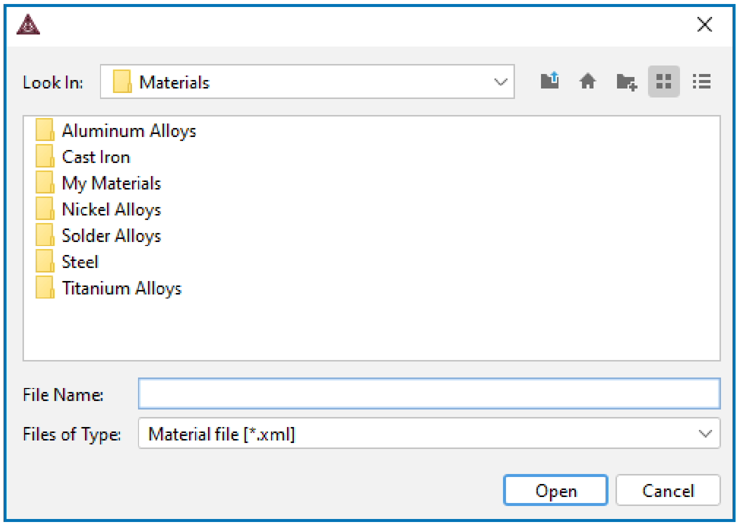
Click **Open anyway** to continue to load the material file even with the undefined component(s). However, this means the undefined component is excluded at first from calculations until it is further defined on the System Definer. Once the material is defined then it is automatically included the next time calculations are run. Otherwise, click **Cancel** to stop the action and either edit the material file or manually define the component(s) in the System Definer.

How To Load or Save a Material

Click **Load material** to open a material file. The default folder opens to the **Materials** folder included with your installation.

About the Material Files and Installed Examples, Manuals, and Materials Folders





Look In: Materials

Files of Type: Material file [*.xml]

You can click **Save material as** to save the material you defined, for example **Ferritic**. Add your own folders as needed.

Global Settings: System Definer

For the **System Definer**, and if you load a material file and then change the composition, a message displays *The composition has changed*. This means that the original values/composition do not match the values you are using for the project. The message is cleared by either reloading the material file or editing the composition field to the original value.

CALCULATION TYPE

Click to select a *Calculation Type*:

- **Single equilibrium** (no axes): To calculate a single point. The results from this calculation are displayed in the **Visualizations** window if a Table Renderer is used.
- **One Axis**: To vary a quantity on the *X*-axis; the fraction of one of the materials or temperature.
- **Phase diagram**: To calculate a section in a multicomponent system between two materials, transitioning from one into the other. The phase diagram is mapped within a specific space that is constructed by the two mapping axis-variables; the fraction of one of the materials and temperature.

AXIS DEFINITIONS

- **One Axis**: Define the axis variable using these fields and menus: **Quantity**, **Min**, **Max**, **Step division**, **Type**, and **Step Method**.
- **Phase diagram**: Define the two axis variables using these fields and menus: **Quantity**, **Min**, **Max**, **Step division**, and **Type**.

Also see additional setting details for **Step division**, **Type**, and **Step Method**.

If the Calculator already has a Plot Renderer as a successor and you change the stepping/mapping quantities, then the quantities represented on the X- and Y-axis are automatically updated in the Plot Renderer.

STEP DIVISION AND TYPE (ONE AXIS AND PHASE DIAGRAM)

Enter a **Step division** and select a **Type**: **Linear - min no. of steps**, **Linear - max step size**, or **Logarithmic - scale factor**.

- For **Linear - min no. of steps**, the **Step division** value specifies a minimum number of steps that is calculated between the minimum and maximum value during the stepping/mapping operation.
- For **Linear - max step size**, the **Step division** sets the maximum size of each step. For **Logarithmic - scale factor**, **Step division** specifies the scale factor of a logarithmic function that distributes the steps from the initial equilibrium to the minimum and maximum values defined.

STEP METHOD (ONE AXIS)

From the **Step Method** list, choose **Normal** or **Separate phases**.

- **Normal** allows a stepping calculation with the chosen independently-varying equilibrium condition (axis-variable).
- **Separate phases** calculates how the Gibbs energy for a number of phases varies for different compositions. This is particularly useful to calculate Gibbs energies for complex phases with miscibility gaps and for an ordered phase that is never disordered (e.g. SIGMA-phase, G-phase, MU-phase, etc.).

Binary Calculator

A Binary Calculator can be used for some calculations involving two components. You can think of this activity as a combination of a System Definer and an Equilibrium Calculator, but designed to simplify setting up and performing calculations on binary systems.

The Binary Calculator relies on some specifications that are not supported by all databases. You need a specially designed database for the Binary Calculator such as the TCBIN database.

Template

There is a **Binary** template available on the **My Projects Configuration** window under **Equilibrium** that you can use to quickly set up a simulation. See Getting Started Links and Templates.

Configuration Settings

See Configuration Window Settings.

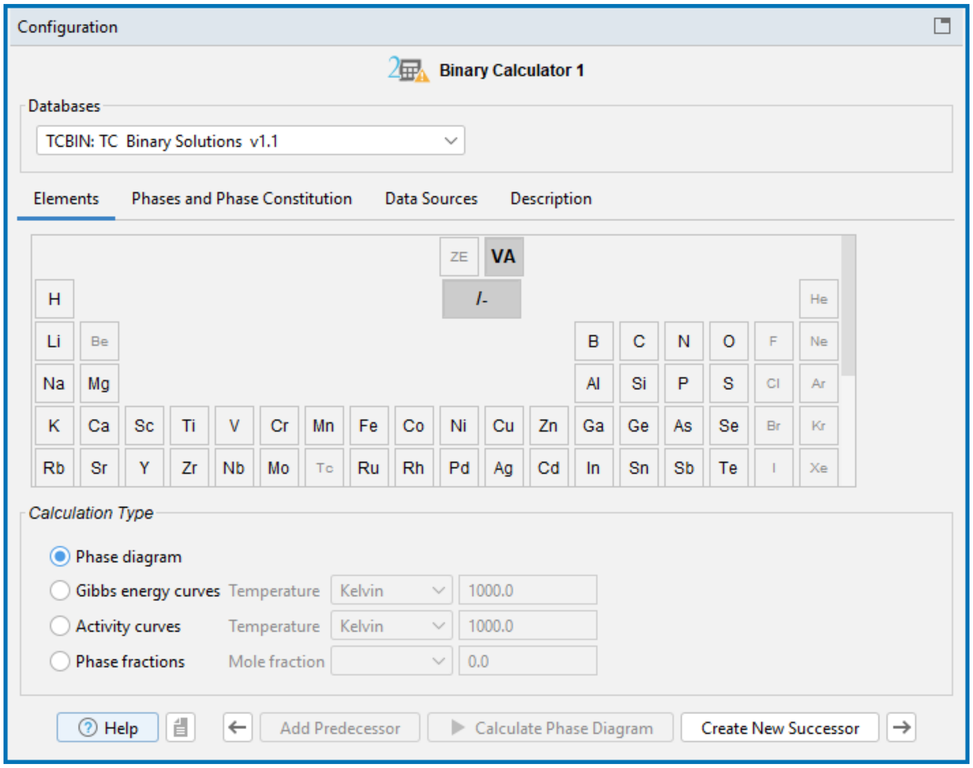
Example

For an example see T_03: Fe-C Phase Diagrams.

Configuration Window Settings

The Binary Calculator **Configuration** settings window and the associated tabs are similar to what you see on a System Definer. The database TCBIN is added by default when you use the **Binary** template (on the **My Projects Configuration** window under **Equilibrium**), but you can choose an installed and licensed database from the list.

> The various versions of the TCFE (Thermo-Calc Steels and Fe-Alloys) databases are not compatible with the Binary Calculator.



Databases: TCBIN: TC Binary Solutions v1.1

● Phase diagram

○ Gibbs energy curves Temperature Kelvin 1000.0

○ Activity curves Temperature Kelvin 1000.0

○ Phase fractions Mole fraction 0.0

Settings

ELEMENTS

On the **Elements** tab, and based on the database selected, select and review elements from the periodic table. Unavailable elements, which are based on the selected database, are greyed out.

PHASES AND PHASE CONSTITUTION

At the top of the **Phases and Phase Constitution** tab, and based on the selected database, you can review the *Status* for the selected *Phases*. Select the **Check/uncheck all** checkbox to toggle between the options.

To review the **Phase constitution** for a specific phase, click it in the *Phase* list (for example **BCC_A2**) and its details are displayed below the *Phases* list. Click **Edit** then click an element to select or reject a constituent. The last remaining constituent on a sublattice cannot be rejected.

DATA SOURCES

Data sources are not available until the activity is performed. Click **Perform Tree** at the bottom of the window to display available data sources.

DESCRIPTION

The **Description** tab displays a description of the selected database.

CALCULATION TYPE

Click to choose a *Calculation Type*.

- **Phase diagram**: To calculate in a defined multicomponent heterogeneous system, from one or more initial equilibria. A phase diagram is usually mapped within a specific space that is constructed by two (or more) defined independent mapping axis-variables.
- **Gibbs energy curves**: To calculate at a constant temperature over the whole composition range.
- **Activity curves**: To calculate at a constant temperature over the whole composition range.
- **Phase fractions**: To calculate as a function of temperature at a constant composition.

Then:

- For **Gibbs energy curves** and **Activity curves**, select a unit from the **Temperature** list: **Kelvin**, **Celsius**, or **Fahrenheit** and enter a value in the field.
- For **Phase fractions**, select and enter the **Mole fraction** component and enter a value in the field.

For the Plot Renderer, there is an option to use the **Table View** button to convert plots to table data for all calculation types and calculators. See Plot Renderer: Convert a Plot to a Table and Export the Data.

Ternary Calculator

A **Ternary Calculator** is used for some calculations involving three components. You can think of this activity as a combination of a System Definer and an Equilibrium Calculator, but designed to simplify setting up and performing calculations on ternary systems.

Template

There is a **Ternary** template available under **Equilibrium** that you can use to quickly set up a simulation. See Getting Started Links and Templates.

Configuration Settings

See Configuration Window Settings.

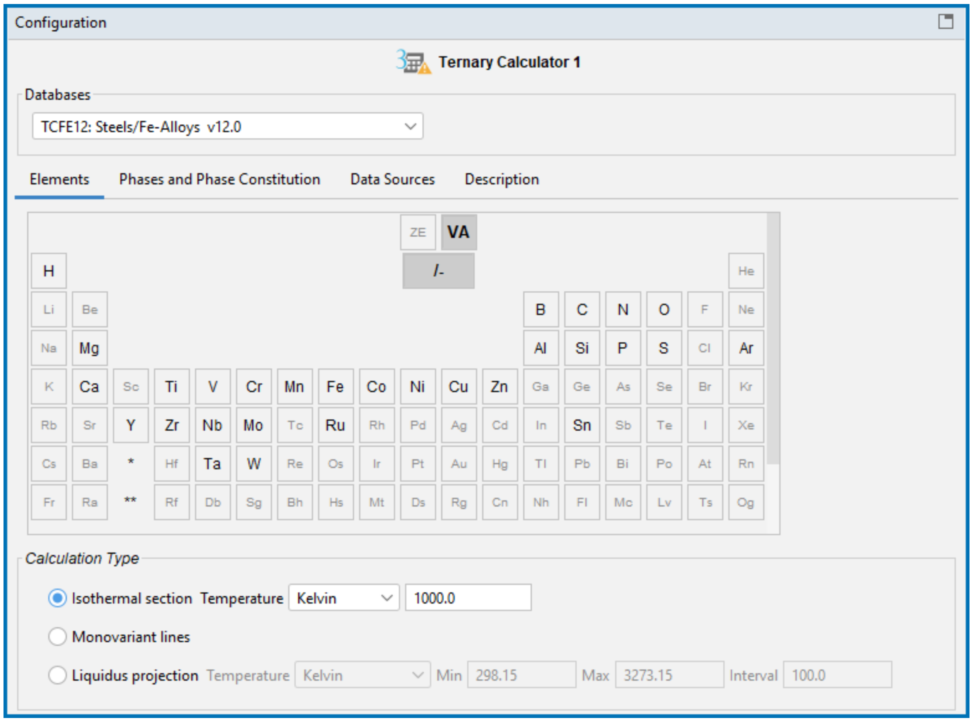
Examples

For examples, see

- T_04: Fe-Cr-C Ternary Phase Diagram at 1000 K
- T_20: Ternary Diagram with Clockwise Plot Axes

Configuration Window Settings

The Ternary Calculator **Configuration** settings window is described in this section that lists the available settings that must be configured before performing the calculation.



Ternary Calculator 1

Databases: TCFE12: Steels/Fe-Alloys v12.0

Calculation Type

● Isothermal section Temperature Kelvin 1000.0

○ Monovariant lines

○ Liquidus projection Temperature Kelvin Min 298.15 Max 3273.15 Interval 100.0

Settings

DATABASES

Select a database that contains specifications dedicated to the Ternary Calculator.

ELEMENTS

On the **Elements** tab, and based on the database selected, select and review elements from the periodic table. Unavailable elements, which are based on the selected database, are greyed out.

PHASES AND PHASE CONSTITUTION

At the top of the **Phases and Phase Constitution** tab, and based on the selected database, you can review the *Status* for the selected *Phases*. Select the **Check/uncheck all** checkbox to toggle between the options.

To review the **Phase constitution** for a specific phase, click it in the *Phase* list (for example **BCC_A2**) and its details are displayed below the *Phases* list. Click **Edit** then click an element to select or reject a constituent. The last remaining constituent on a sublattice cannot be rejected.

DATA SOURCES

Data sources are not available until the activity is performed. Click **Perform Tree** at the bottom of the window to display available data sources.

DESCRIPTION

The **Description** tab displays a description of the selected database.

CALCULATION TYPE

Click to choose a *Calculation Type*.

- **Isothermal section**: To calculate the ternary system for the whole composition range.
- **Monovariant lines**: To calculate the variation of the liquid compositions with temperature.
- **Liquidus projection**: The projection liquid surface and the monovariant lines are calculated over the given temperature range.

Then for **Isothermal section** and **Liquidus projection**, select a unit from the **Temperature** list: **Kelvin**, **Celsius**, or **Fahrenheit** and enter a value in the field.

For the Plot Renderer, there is an option to use the **Table View** button to convert plots to table data for all calculation types and calculators. See Plot Renderer: Convert a Plot to a Table and Export the Data.

Scheil-Gulliver Solidification Calculations

In Graphical Mode, you use the Scheil Calculator activity node to simulate the various models available in Thermo-Calc or with the Add-on Modules or additional databases.

Read more about Scheil Solidification Simulations on our website, including how to select the right model for your simulation. If you are in Thermo-Calc, press F1 to search the help to learn about using Scheil.

Thermo-Calc is often used to perform equilibrium calculations, but some non-equilibrium transformations or partial-equilibrium transformations can also be simulated.

A well-known example of a non-equilibrium calculation is the *Scheil-Gulliver solidification simulation*. In Thermo-Calc, the available Scheil-Gulliver solidification simulations are *classic* Scheil, Scheil with *back diffusion* in the primary phase, or Scheil with *solute trapping*. There are also configuration options available with *fast diffusers* for the classic and back diffusion models.

Classic Scheil Simulation

This is a Scheil simulation based on the well-known *Scheil-Gulliver* model. If this model is used without "fast diffusers" it is *Classic Scheil* simulation with the following assumptions:

- Diffusion in the liquid phase is assumed to be very fast, that is, infinitely fast.
- Diffusion in the solid phases is so slow that it can be ignored, that is, diffusion is assumed to be zero.
- The liquid/solid interface is in thermodynamic equilibrium.

In this Classic Scheil simulation the temperature is decreased step-by-step. When the temperature drops below the liquidus temperature the equilibrium amount and composition of solid and liquid phase is calculated. The solid phase is removed from the system and only the amount and composition of the liquid phase is used for the next calculation step at a lower temperature. Again, the equilibrium amount and composition of solid and liquid phase is calculated and again the solid phase is removed from the system for the next step. This procedure is repeated until the last liquid disappears.

This calculation procedure is equivalent to assuming that there is no diffusion in the solid phase and infinitely fast diffusion of all elements in the liquid phase. It has been shown to be a good approximation of the solidification of most alloys such as Ni-superalloys, Cu alloys, Al alloys, Mg alloys, and others. However, in materials with interstitial elements, such as carbon, ignoring diffusion in the solid causes discrepancies with experimental results. Interstitial elements have much faster diffusion rates. The assumption of no diffusion in the solid phase during solidification is thus not correct at most industrial or lab-scale solidification rates.

For this reason, a variant of the Scheil simulation was developed and implemented in Thermo-Calc, where one or more elements can be defined as *fast diffusers*. See Other Options: Fast Diffusers and Scheil Simulations.

Scheil Simulation with Back Diffusion in Primary Phase

The *Scheil simulation with back diffusion in primary phase* kinetic model quantitatively takes into account the real back diffusion of all elements in the primary solid phase (typically the FCC or BCC phase). This model requires the use of both a thermodynamic and mobility database. The calculation also requires the cooling rate to be specified; a fast cooling rate allows for less time for back diffusion and the simulation result is similar to the classic Scheil-Gulliver solidification simulation. A very slow cooling rate allows for almost complete back diffusion, the solidification simulation is then close to an equilibrium calculation. It also requires that the size of the solidification domain is specified. In most cases this domain size corresponds to the secondary arm spacing, as this is where typically the liquid is trapped during solidification.

The secondary arm spacing also depends on the cooling rate. For this reason, a simple empirical relation between cooling rate and secondary arm spacing is predefined in Thermo-Calc.

For the *Scheil simulation with back diffusion in primary phase* model the following assumptions are made.

- Diffusion of all elements in the liquid phase is infinitely fast.
- Diffusion of all elements in the primary solid phase are quantitatively calculated using mobility data, a cooling rate and a domain size (typically this is the secondary arm spacing).
- The liquid/solid interface is in thermodynamic equilibrium.

Also see Other Options: Fast Diffusers and Scheil Simulations.

Scheil with Solute Trapping

The *Scheil with solute trapping* model simulates deviation from local equilibrium for the primary phase. It is useful for high solidification speeds, such as those seen in additive manufacturing applications.

For equilibrium- and classical Scheil-type solidification simulations thermodynamic equilibrium is established at the solid-liquid interface. This means that solutes are partitioned between the solid and liquid phases according to solidus and liquidus lines of the phase diagram. The assumption of thermodynamic equilibrium at the solid-liquid interface however, is invalid for very fast solidification rates, as encountered for example during additive manufacturing. The faster the solidification rate, the less the partitioning at the interface, which can be perceived as that solutes in the liquid are trapped in the advancing solid phase, hence the term *solute trapping*.

The *Scheil with solute trapping* model calculates the solute partitioning between liquid and primary solid that deviates from thermodynamic equilibrium due to solidification speed.

The following assumptions are made:

- Only one primary solid phase forms dendrite, NOT necessarily the first solid phase.
- Solute trapping in primary solid phase only. Other solid phases have equilibrium compositions following Scheil model.
- Dynamic liquidus for primary solid phases is dependent on solute trapping and solidification speed.
- Amounts of solid phases are dependent on solute trapping and solidification.

More theory details are in About Scheil with Solute Trapping.

Other Options: Fast Diffusers and Scheil Simulations

If a *Classic Scheil* or *Scheil simulation with back diffusion in primary phase* model is selected plus one or more *Fast diffuser* checkboxes selected, then Thermo-Calc takes into account the concept of the *fast diffuser*. Typically, C is defined as a fast diffuser, but also other elements such as N, O, or others can also be defined.

Fast diffuser does not quite define this since diffusion is not actually simulated. It is simply assumed that the “fast diffusers” distribute throughout the solid and liquid phase according to thermodynamic equilibrium. This corresponds to *infinitely fast diffusion* for the selected elements.

For a *Classic Scheil* model with the compositions defined with *Fast diffuser* the following assumptions are made.

- Diffusion of all elements in the liquid phase is infinitely fast.
- Diffusion of all elements in the solid phases, except the ones defined as “fast diffusers”, is zero.
- Diffusion of the elements defined as “fast diffusers” is infinitely fast in the solid phase.
- The liquid/solid interface is in thermodynamic equilibrium.

For a *Scheil simulation with back diffusion in primary phase* model with the compositions defined with *Fast diffuser* the following assumptions are made.

- Diffusion of all elements in the liquid phase is infinitely fast.
- Diffusion of all elements in the primary solid phase are quantitatively calculated using mobility data, a cooling rate and a domain size (typically this is the secondary arm spacing).
- Diffusion of the elements defined as “fast diffusers” is infinitely fast in the solid phase.
- The liquid/solid interface is in thermodynamic equilibrium.

The Classic Scheil simulation and Classic Scheil simulation with fast diffuser models can be considered *thermodynamic* models. There are clear limitations as a certain amount of back diffusion always takes place in the solid phase at real solidification.

You can also use the more sophisticated *Scheil simulation with back diffusion in primary phase* kinetic model. Adding the fast diffuser option to this can be useful, for example for interstitials like C in steels where these then equilibrate in all phases and not just the primary phase.

Homogenization, Segregation Profiles, and the Diffusion Module

Scheil calculations can be used in diffusion simulations with the Diffusion Module (DICTRA).

Homogenization is a process were you want to get rid of the composition segregation from solidification with a homogenization heat treatment. This composition segregation can be simulated with Scheil. Then with the Diffusion Module (DICTRA), you input the secondary dendrite arm spacing to get the right diffusion distances. With composition profile from file the idea is that you should be able to input for example a measured composition profile (from EDS/WDS, micro-probe etc). This could also be a segregation profile but also composition profiles over a weld, substrate/coating, diffusion couple, and so forth.

Summary

The available Scheil-Gulliver solidification simulations are *classic* Scheil, Scheil with *back diffusion* in the primary phase, or Scheil with *solute trapping*. There are also configuration options available with *fast diffusers* for the classic and back diffusion models.

There is also connectivity to the Diffusion Module (DICTRA) and *homogenization* where you collect data from a Scheil solidification calculation, which is then used as part of the kinetic homogenization simulation of segregated composition profiles.

Scheil in Graphical Mode vs Console Mode

The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. this model requires the use of a mobility database.

In Thermo-Calc, the Scheil calculation allows the calculation of:

- The solidification range of an alloy.
- Depression of the solidus temperature due to segregation.
- Composition of the last liquid to disappear in segregation pockets.
- Phases formed on final solidification in segregation pockets.
- The composition gradient in the primary solid phase(s) (segregation profile).
- Solute trapping to simulate deviation from local equilibrium for the primary phase
- Kinetic homogenization simulation of segregated composition profile (diffusion calculations)

Scheil in Graphical Mode vs Console Mode

Type of Calculation	*Console Mode*	*Graphical Mode*
Classic Scheil	Use the START_WIZARD command to answer prompts	Scheil Calculator > click the **Classic Scheil** button on the Configuration window. On the My Project Configuration window under Getting Started, click **Quick Start** and select **Scheil solidification simulation**.
Scheil with back diffusion in the primary phase	USE_BACK DIFFUSION command (turn on) then use the START_WIZARD command to answer prompts	Scheil Calculator > click the **Scheil with back diffusion in the primary phase** button on the Configuration window then enter the settings as needed. A mobility database is required.
Scheil with solute trapping	SOLUTE_TRAPPING command (turn on) then use the START_WIZARD command to answer prompts	Scheil Calculator > click the **Scheil with solute trapping** button on the Configuration window then enter the settings as needed.
Fast diffusers and Classic Scheil	Use the START_WIZARD command to answer the prompt`Fast diffusing components`where you enter the elements that diffuse fast in solid phases and can assume to be in equilibrium in the whole phase. E.g. C in a steel.	Scheil Calculator > click the **Classic Scheil** button plus one or more of the **Fast diffuser** checkboxes next to the composition(s) on the Configuration window then enter the settings as needed.
Fast diffusers and Scheil with back diffusion in the primary phase	USE_BACK DIFFUSION command (turn on) then use the START_WIZARD command to answer the prompt `Fast diffusing components`where you enter the elements that diffuse fast in solid phases and can assume to be in equilibrium in the whole phase. E.g. C in a steel.	Scheil Calculator > click the **Scheil with back diffusion in the primary phase** button plus one or more of the **Fast diffuser** checkboxes next to the composition(s) on the Configuration window then enter the settings as needed. A mobility database is required.
Homogenization	Use the EVALUATE_SEGREGATION_PROFILE command before START_WIZARD to generate the segregation profile to file. In DICTRA_MONITOR use INPUT_SCHEIL_PROFILE for use of segregated profile in simulation. An additional license to the Diffusion Module (DICTRA) is needed to work with more than three components.	Use the **Homogenization** template under **Non-Equilibrium** to automatically set up the project tree with the defaults needed to work with this. An additional license to the Diffusion Module (DICTRA) is needed to work with more than three components.

About Scheil with Solute Trapping

The *Scheil with solute trapping* model simulates deviation from local equilibrium for the primary phase. It is useful for high solidification speeds, such as those seen in additive manufacturing applications.

For equilibrium- and classical Scheil-type solidification simulations thermodynamic equilibrium is established at the solid-liquid interface. This means that solutes are partitioned between the solid and liquid phases according to solidus and liquidus lines of the phase diagram. The assumption of thermodynamic equilibrium at the solid-liquid interface however, is invalid for very fast solidification rates, as encountered for example during additive manufacturing. The faster the solidification rate, the less the partitioning at the interface, which can be perceived as that solutes in the liquid are trapped in the advancing solid phase, hence the term *solute trapping*.

The *Scheil with solute trapping* model calculates the solute partitioning between liquid and primary solid that deviates from thermodynamic equilibrium due to solidification speed.

The following assumptions are made:

- Only one primary solid phase forms dendrite, NOT necessarily the first solid phase.
- Solute trapping in primary solid phase only. Other solid phases have equilibrium compositions following Scheil model.
- Dynamic liquidus for primary solid phases is dependent on solute trapping and solidification speed.
- Amounts of solid phases are dependent on solute trapping and solidification.

The model is based on Aziz [1982Azi; 1988Azi] and Hillert [1999Hil], and extends to multicomponent systems. The motion of liquid/solid interface is regarded as two concurrent processes, trans-interface diffusion (solute transport across the interface leading to solute partitioning) and migration (liquid to solid transformation without changing composition).

Aziz and Hillert used slightly different formulations to describe the trans-interface diffusion. Aziz [1982Azi; 1988Azi] formulated the expression in terms of chemical reaction theory, describing the diffusion of the i th solute element (the dependent element being labeled as $n$in a n-component system) with respect to chemical potential gradient and interface velocity $v$as:

[Eq. 1]

$$\left(X_i^L - X_i^S\right) \frac{v}{v_i^D} = X_i^S X_n^L \left(1 - \psi_i^e\right) \quad (i = 1, 2, \ldots, n-1)$$

Where X_i^s and X_i^L are compositions (mole fractions) of primary solid and liquid at the interface, respectively. v_i^D is the diffusion velocity defined as:

[*Eq. 2*]

$$v_i^D = \frac{D_i}{\lambda}$$

Where D_i is the trans-interface diffusivity and λ is the interface thickness. In the software, λ is treated as a constant of 1×10^{-9} m.

In Eq. 1 ψ_i^e is an activation term for diffusion:

[*Eq. 3*]

$$\psi_i^e = exp\left[-\frac{\Delta\tilde{\mu}_i}{RT}\right]$$

Where $\Delta\tilde{\mu}_i$ is the diffusion potential difference:

[*Eq. 4*]

$$\Delta\tilde{\mu}_i = \left(\mu_i^S - \mu_n^S\right) - \left(\mu_i^L - \mu_n^L\right)$$

Where $\mu_i^{\S}$ and μ_i^L are chemical potentials of i th element in the primary solid and liquid at the interface.

Hillert [1999Hil], on the other hand, formulated the expression based on diffusion theory as:

[*Eq. 5*]

$$\left(X_i^L - X_i^S\right)\frac{v}{v_i^D} = -K_i\Delta\tilde{\mu}_i$$

Where:

[*Eq. 6*]

$$K_i = \frac{X_n^L X_i^S}{RT}\exp\left(-\frac{\Delta\tilde{\mu}_i}{RT}\right)$$

For migration process, the formulation relates the free energy change, or driving force that is opposite to free energy change, to the interface velocity. The overall free energy change (termed as *driving energy*), including both trans-interface diffusion and migration processes, is defined as:

[*Eq. 7*]

$$\Delta G^{DE} = \sum_{i=1}^{n} X_i^S\left[\mu_i^S - \mu_i^L\right]$$

The free energy change for migration process (termed as *migration energy*) is:

[*Eq. 8*]

$$\Delta G^{ME} = \sum_{i=1}^{n} X_i^L\left[\mu_i^S - \mu_i^L\right]$$

The interface velocity is then related to the free energy change as:

[*Eq. 9*]

$$v = v_0\left[1 - \exp\left(\frac{\Delta G^E}{RT}\right)\right]$$

Where:

- ΔG^{e} can be either ΔG^{DE} or ΔG^{ME} defined in Eq. 7 and Eq. 8.
- v_0 is the maximum velocity limit when the free energy change becomes infinitely negative.

Additionally, the mass conservation within the interface is assumed:

[*Eq. 10*] $$\frac{X_i^0 - X_i^L}{X_i^S - X_i^L} = \frac{X_j^0 - X_j^L}{X_j^S - X_j^L} \quad (i \neq j, i, j = 1, 2, \ldots n-1)$$

Where X_i^0 is the far-field liquid composition.

Eq. 1 (for Aziz model) or Eq. 5 (for Hillert model), together with Eq. 9 and Eq. 10 are then used to calculate the solute partitioning at the interface between primary solid and liquid for multicomponent systems. Likewise, if replacing X_i^L with the initial alloying compositions, Eq. 1 (Eq. 5) and Eq. 9 are used to calculate the dynamic liquidus of the primary solid phase.

Solute trapping also reduces the volume fraction of other solid precipitates. The reduction factor is estimated by employing the effect of the solute trapping on the heat of fusion, which can be manifested by the liquid + primary solid phase boundaries in the phase diagrams by [1998Hil]:

[*Eq. 11*] $$\sum_{i=1}^{n} X_i^S \left(H_i^S - H_i^L\right) = -\frac{T}{dT} \sum_{i=1}^{n-1} \sum_{j=1}^{n-1} \left(X_i^S - X_i^L\right) g_{ji}^L dX_j^L$$

Where all values are determined at phase boundaries. g_{ij}^L is the second partial derivative of Gibbs free energy of liquid phase with respect to mole fraction. The left side of Eq. 11 is the enthalpy change when one (1) mole of primary solid with composition X_i^S is melted into a reservoir of liquid. Since we are interested in a ratio, the term that needs to be considered is:

[*Eq. 12*] $$H_f = \sum_{i=1}^{n-1} \sum_{j=1}^{n-1} \left(X_i^S - X_i^L\right) g_{ji}^L dX_j^L$$

The reduction factor is then obtained by comparing solute trapping with equilibrium values:

[*Eq. 13*] $$f = \frac{H_f^{ST}}{H_f^{eq}}$$

Scheil Calculator Configuration Settings

The Graphical Mode settings are described in Configuration Window Settings.

T_13: Scheil Solidification with Solute Trapping

On the **Configuration** window, these are the relevant settings related to solute trapping:

- **Trans-interface diffusivity** (D_i): Smaller value leads to larger solute trapping effect. Be cautious that $D_i < 2.0 \times 10^{-9} \frac{m^2}{s}$ may result in complete solute trapping and possibly numerical errors.
- **Maximum velocity for infinite driving force** (v_0): Smaller values lead to a larger solute trapping effect.
- Choose the solute trapping **Model** (**Aziz** or **Hillert**): **Hillert** model usually leads to a larger solute trapping effect, though **Aziz** model is recommended for overall numerical performance including calculating the amount of non-primary solid phases.
- **Interface driving force**: **Driving energy** ΔG^{DE} or **Migration energy**ΔG^{ME}. Using migration energy option leads to larger solute trapping effect, while using driving energy option is numerically more stable. It is recommended to using driving energy option and adjusting other parameters (e.g., trans-interface diffusivity) for desired solute trapping effect.

References

[1982Azi] M. J. Aziz, Model for solute redistribution during rapid solidification. J. Appl. Phys. 53, 1158–1168 (1982).

[1988Azi] M. J. Aziz, T. Kaplan, Continuous growth model for interface motion during alloy solidification. Acta Metall. 36, 2335–2347 (1988).

[1998Hil] M. Hillert, Phase Equilibria, Phase Diagrams and Phase Transformations: A Thermodynamic Basis (Cambridge University Press, 1998), 596 pp.

[1999Hil] M. Hillert, Solute drag, solute trapping and diffusional dissipation of Gibbs energy, Acta Mater., 47(18)4481-45-5(1999)

Scheil Calculator

In Graphical Mode, you use the **Scheil Calculator** to set up the various Scheil solidification simulations outlined in more detail in Scheil-Gulliver Solidification Calculations.

The Scheil Calculator is also used in combination with the specialized Add-on Modules such as the Diffusion Module (DICTRA) and Additive Manufacturing (AM) Module.

The available Scheil-Gulliver solidification simulations are *classic* Scheil, Scheil with *back diffusion* in the primary phase, or Scheil with *solute trapping*. There are also configuration options available with *fast diffusers* for the classic and back diffusion models.

There is also connectivity to the Diffusion Module (DICTRA) and *homogenization* where you collect data from a Scheil solidification calculation, which is then used as part of the kinetic homogenization simulation of segregated composition profiles.

Scheil in Graphical Mode vs Console Mode

The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. this model requires the use of a mobility database.

In Thermo-Calc, the Scheil calculation allows the calculation of:

- The solidification range of an alloy.
- Depression of the solidus temperature due to segregation.
- Composition of the last liquid to disappear in segregation pockets.
- Phases formed on final solidification in segregation pockets.
- The composition gradient in the primary solid phase(s) (segregation profile).
- Solute trapping to simulate deviation from local equilibrium for the primary phase
- Kinetic homogenization simulation of segregated composition profile (diffusion calculations)

There are several options to get started with a Scheil simulation using the Scheil Calculator.

- On the **My Project** window under **Getting Started**, use the **Quick Start → Scheil Solidification Simulation** option to set up a Classic Scheil simulation. This adds a tree of nodes where you can then choose to simulate using the other options on the Scheil Calculator. See Creating a Project with the Quick Start Wizard.
- Use the **Scheil Solidification** template under **Non-Equilibrium** to add a project tree consisting of **System Definer**, **Scheil Calculator**, and **Plot Renderer** nodes. See Getting Started Links and Templates.
- Use the **Homogenization** template under **Non-Equilibrium** to add a project tree consisting of **System Definer**, **Scheil Calculator**, **Diffusion Calculator**, and two **Plot Renderer** nodes. See Getting Started Links and Templates.

When working with the **Homogenization** template, this also includes a **Diffusion Calculator**, which may require additional licenses to run with more than three components. Information, such as the Scheil segregation profiles available with the Diffusion Calculator, is described with that content.

- Build your own tree by right-clicking and adding nodes from **My Project**. Then go to Configuration Window Settings to enter settings directly.
- Open an example and use this as a template.
- When you are working with the Additive Manufacturing (AM) Module, a **Scheil Calculator** is also included with one of the Additive Manufacturing Templates or can be added as a predecessor to the **AM Calculator**, where it is used to generate the materials property data required for these simulations.

By default, a Plot Renderer successor to a Scheil Calculator has the plot axes defined as **Mole fraction of solid** (X-axis) and **Temperature Celsius** (Y-axis). When these default axes are used and the setting **Include one axis equilibrium calculation** is enabled (see Advanced Options), the results of solidification under equilibrium conditions are automatically plotted in the same diagram as the Scheil calculations.

Define the Scheil Calculator

1. Add a **Scheil Calculator** node to the System Definer. If you used the **Scheil Solidification** or **Homogenization** templates on the **My Projects Configuration** window under **Non-Equilibrium** (or opened an example), click the node to display the **Configuration** settings window.
2. Enter the settings described in Configuration Window Settings. The **Configuration** tab as all the main settings and the permutations related to the types of Scheil simulations available such as back diffusion and solute trapping.

   When working with the **Homogenization** template, this also includes a **Diffusion Calculator**, which may require additional licenses to run with more than three components. Information, such as the Scheil segregation profiles available with the Diffusion Calculator, is described with that content.

3. As needed you can also change default settings from the **Advanced Options** tab (see Advanced Options).

4. Once you have finished defining the Scheil Calculator, you also choose settings and variables on the Plot Renderer. For a list of available variables see Scheil Calculator Available Plot Variables.

Examples

For examples using the Scheil Calculator, see:

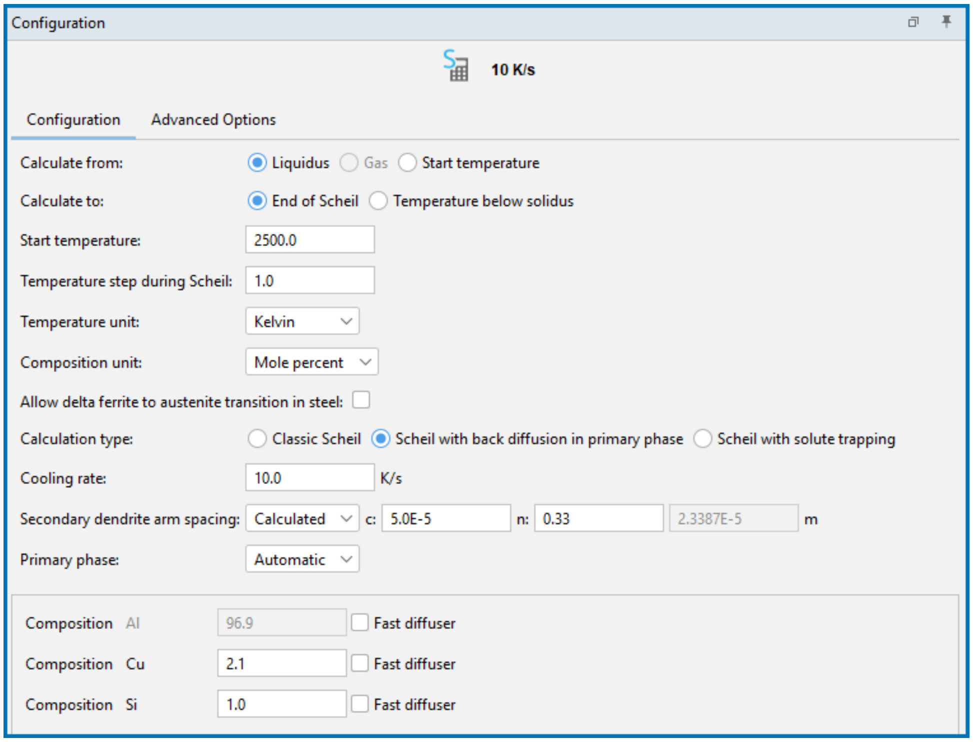
- T_08: Scheil and Equilibrium Solidification
- T_10: Scheil Solidification with Back Diffusion
- T_13: Scheil Solidification with Solute Trapping

There are also Console Mode, TC-Python, and Diffusion Module (DICTRA) examples described elsewhere in the content.

Configuration Window Settings

An example of the main **Configuration** window of a **Scheil Calculator** activity is shown below using the T_10: Scheil Solidification with Back Diffusion example.

> Scheil-Gulliver Solidification Calculations is a general overview of the Scheil options. For more details about the *solute trapping* related settings, see the theory in About Scheil with Solute Trapping.



Calculate from: ● Liquidus ○ Gas ○ Start temperature

Calculate to: ● End of Scheil ○ Temperature below solidus

Start temperature: 2500.0

Temperature step during Scheil: 1.0

Temperature unit: Kelvin

Composition unit: Mole percent

Allow delta ferrite to austenite transition in steel: ☐

Calculation type: ○ Classic Scheil ● Scheil with back diffusion in primary phase ○ Scheil with solute trapping

Cooling rate: 10.0 K/s

Secondary dendrite arm spacing: Calculated c: 5.0E-5 n: 0.33 2.3387E-5 m

Primary phase: Automatic

Composition Al 96.9 ☐ Fast diffuser

Composition Cu 2.1 ☐ Fast diffuser

Composition Si 1.0 ☐ Fast diffuser

An example of the Scheil Calculator Configuration window with the back diffusion option selected. There are different settings available and described below based on the calculation type selected.

Settings

There are additional settings found on the **Advanced Options** tab and based on the type of Scheil calculation. See Advanced Options.

CALCULATE FROM

Use the **Calculate from** setting to choose from where the calculation should start. With this setting it is possible to obtain properties of the gas and/or liquid phase before the solidification starts.

Some of the temperature definitions related to these choices are:

- *Liquidus*, the temperature where solidification starts.
- *Gas / Liquid*, the temperature above which the liquid phase is no longer stable.
- *Liquid / Gas*, the temperature below which the gas phase is no longer stable.

Click a button to choose **Liquidus**, **Gas**, or **Start temperature**.

> Depending on the choice for this setting (**Liquidus**, **Gas**, or **Start temperature**), one or more of the following temperature values is calculated and collected in the **Event Log** at the end of the calculation: *Liquidus*, *Gas / Liquid*, or *Liquid / Gas*.

By default, **Liquidus** is selected. The results are calculated from the start of the solidification.

Select **Gas** (after a gas phase is selected on the System Definer) to perform single equilibrium calculations from the *Gas / Liquid* temperature.

- The equilibrium calculations are performed at 5 Kelvin (K) intervals in the two-phase region between the *Gas/ Liquid* temperature and the *Liquid / Gas* temperature.
- In the fully liquid region below the *Liquid / Gas* temperature single equilibrium calculations are performed at 50 K intervals until the *Liquidus* temperature is reached. After that the Scheil solidification calculation proceeds as usual.

Select **Start temperature** if you want to obtain properties of the liquid phase (and gas phase if selected) before the solidification starts.

- Ordinarily the start temperature is only used as a start point in the search of the liquidus temperature, as the Scheil calculation starts from the *Liquidus* temperature.
- For this choice, single equilibrium calculations are performed at specific intervals from the temperature entered in the start temperature field, down to the *Liquidus* temperature, and after that the Scheil solidification calculation proceeds as usual.
- The equilibrium calculations are performed at 50 Kelvin (K) intervals in the fully liquid region and at 5 K intervals in a possible two-phase (*Liquid / Gas*) region.

CALCULATE TO

Use the **Calculate to** setting to choose from where the calculation should end, **End of Scheil** or **Temperature below solidus**, where a frozen structure is assumed below solidus.

- **End of Scheil** stops the calculation when the Scheil calculation is finished.

- **Temperature below solidus** calculates the properties in the solid state, for the phase compositions and fractions at the end of the Scheil calculation. The default **Final temperature** is room temperature. Click **Show advanced options** to adjust the *Temperature below solidus settings*: Change the **Final temperature** and/or define the **No. of points**.

See Advanced Options.

START TEMPERATURE

Enter a **Start temperature** that is higher than the liquidus temperature of the alloy, in other words, the temperature at which the alloy is completely melted.

TEMPERATURE STEP DURING SCHEIL

Enter a **Temperature step during Scheil**. The temperature step is given in the same unit as **Start temperature**. Decreasing the temperature step increases the accuracy, but the default value is usually adequate.

TEMPERATURE UNIT

Select the **Temperature unit**: **Kelvin**, **Celsius** or **Fahrenheit**.

COMPOSITION UNIT

Select the **Composition unit**: **Mass percent**, **Mole percent**, **Mass fraction**, or **Mole fraction**.

ALLOW DELTA FERRITE TO AUSTENITE TRANSITION IN STEEL

Select the **Allow delta ferrite to austenite transition in steel** checkbox to enable BCC to FCC transition.

This feature should only be used for such steels for which it is reasonable to assume infinitely fast diffusion (equilibrium conditions) when delta ferrite is present. When the **Allow delta ferrite to austenite transition in steel** checkbox is selected in Graphical Mode or the DELTA_FERRITE_AUSTENITE_TRANSITION command used in Console Mode, this essentially assumes that diffusion can be considered (infinitely) fast when delta ferrite is present as a solid phase, i.e assumes an equilibrium condition. After delta ferrite is no longer stable, the usual Scheil assumptions for the selected calculation type are in effect. This setting is therefore not suitable for steels where you DO NOT have a complete BCC to FCC transition during solidification. This setting is also NOT available in combination with solute trapping.

CALCULATION TYPE: CLASSIC, BACK DIFFUSION, SOLUTE TRAPPING

The available settings are based on the chosen model. See Scheil-Gulliver Solidification Calculations for descriptions.

Click to select a **Calculation type**: **Classic Scheil**, **Scheil with back diffusion in primary phase**, or **Scheil with solute trapping**. Then based on this selection, additional settings are made available as indicated.

The back diffusion and solute trapping options are available to select after adding a mobility database and once components are defined on the System Definer.

COMPOSITION

The **Composition** settings display after you add components to the **System Definer**.

FAST DIFFUSER

The **Fast diffuser** checkboxes are available after you add components to the System Definer. Click the checkbox to allow redistribution of this component in both the solid and liquid parts of the alloy.

COOLING RATE (BACK DIFFUSION)

This field is available when **Scheil with back diffusion in primary phase** is selected.

Specify the **Cooling rate** in Kelvin per second (K/s). An increased value moves the result from equilibrium toward a Scheil-Gulliver calculation.

SECONDARY DENDRITE ARM SPACING (BACK DIFFUSION)

This field is available when **Scheil with back diffusion in primary phase** is selected.

The **Secondary dendrite arm spacing** is the distance in meters between two secondary dendrite arms. It can be either a **Constant** or **Calculated** from the cooling rate as c*(cooling rate)$^{-n}$ where c and n are entered in these fields.

Select **Calculated** or **Constant**.

- For **Calculated**, enter values for **c** and **n**.
- For **Constant**, enter a value (unit = m) in the field.

PRIMARY PHASE (BACK DIFFUSION AND SOLUTE TRAPPING)

This field is available when **Scheil with back diffusion in primary phase** or **Scheil with solute trapping** is selected.

The primary solidified phase is the phase where the back diffusion or solute trapping takes place.

If **Automatic** (Scheil Calculator) or **Any phase** (Property Models) is selected (or kept as the default), the program tries to find the phase which gives the most back diffusion or solute trapping.

To override this setting, choose a specific primary phase from the list:

- For back diffusion, only phases with diffusion data can be used as primary phases.
- For solute trapping, only phases that dissolve all elements in the system can be used as primary phases.

SCANNING SPEED, ALPHA, AND CALCULATED SOLIDIFICATION SPEED (SOLUTE TRAPPING)

These fields are available when **Scheil with solute trapping** is selected.

As needed, enter **Scanning speed** and **α**to define the **Calculated solidification speed**.

On the Scheil Calculator, the **Calculated solidification speed** is shown. For Property Models, below is how the values are calculated from the **Scanning speed** and **α** values entered.

The **Calculated Solidification Speed** is $Vs = V_{scanning} * \cos(\alpha)$ m/s, where $V_{scanning}$ is the user specified **Scanning speed** in m/s and **α** is the alpha angle, α, between the solid/liquid boundary and scanning direction.

TRANS-INTERFACE DIFFUSIVITY (SOLUTE TRAPPING)

These fields are available when **Scheil with solute trapping** is selected.

Select a **Trans-inteface Diffusivity** option: **Same for all elements** or **Per element**.

Smaller value leads to larger solute trapping effect. Be cautious that $D_i < 2.0 \times 10^{-9} \frac{m^2}{s}$ may result in complete solute trapping and possibly numerical errors.

- For **Same for all elements**, enter one **Pre-exponential factor**(default `5.0E-9` m^2/s) and **Activation energy** (default `0` J/mol) in the fields for the solute diffusivity across the interface between liquid and primary dendrite phase.
- For **Per element**, enter individual values for each one in the provided fields for **Pre-exponential factor**(default `5.0E-9` m^2/s) and **Activation energy** (default `0` J/mol) for the solute diffusivity across the interface between liquid and primary dendrite phase.

MAXIMUM VELOCITY FOR INFINITE DRIVING FORCE (SOLUTE TRAPPING)

This field is available when **Scheil with solute trapping** is selected.

Enter a **Maximum velocity for infinite driving force**. The default is `2000` m/s. This is the maximum migration speed of the liquid/primary solid interface when the driving force is infinite. Smaller values lead to a larger solute trapping effect.

MODEL (SOLUTE TRAPPING)

This option is available when **Scheil with solute trapping** is selected.

Choose a **Model**to calculate the relation between migration speed and solute partitioning at the liquid/primary solid interface, developed by either **Aziz** or **Hillert**.

> The **Hillert** model usually leads to a larger solute trapping effect, though **Aziz** model is recommended for overall numerical performance including calculating the amount of non-primary solid phases.

INTERFACE DRIVING FORCE (SOLUTE TRAPPING)

This option is available when **Scheil with solute trapping** is selected.

Choose the **Interface driving force**, where this driving force (free energy change at the liquid/primary solid interface) is used to evaluate the migration speed in comparison with the maximum velocity.

- **Driving energy**: Uses the overall free energy change.
- **Migration energy**: Uses free energy change due to migration, i.e. the overall free energy change excluding that contributes to diffusion.

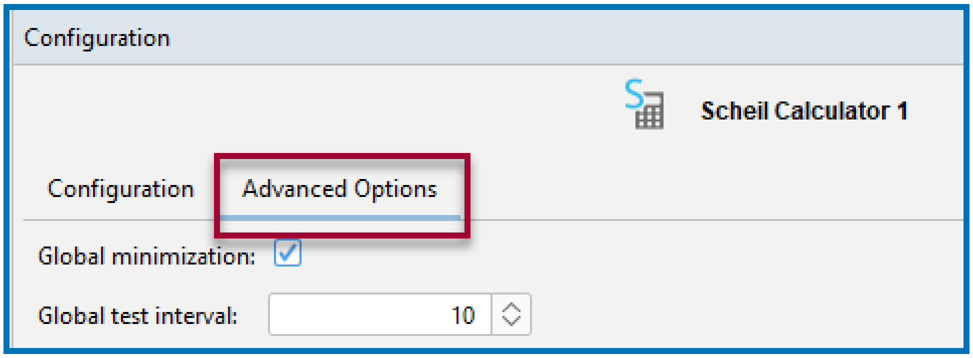
> Selecting **Migration energy** leads to a larger solute trapping effect. It is generally recommended to select **Driving energy** as this is numerically more stable, and then adjust the other settings (e.g., **Trans-interface diffusivity**) for the desired solute trapping effect.

Advanced Options

This topic has advanced settings information for the **Scheil Calculator Configuration** window. The main settings are on the **Configuration** tab.

Configuration Window Settings

Click the **Advanced Options** tab to adjust the following default settings as needed.


Configuration

Scheil Calculator 1

Global minimization: ☑

Global test interval: 10

To make global default setting changes, see Global Settings: Scheil Calculator.

GLOBAL MINIMIZATION

Global minimization is enabled by default i.e. the **Global minimization** checkbox is selected.

It is recommended to keep global minimization on as it makes the calculation more accurate. However, turn it off if you find that the calculation is taking too long for any particular system, and accuracy is not the highest priority.

For this setting, a global equilibrium test is performed at selected intervals when an equilibrium is reached. By default it is at every 10 th Scheil step but this can be changed using the **Global test interval** setting. The global equilibrium test is also done every time the set of stable phases tries to change. This costs more computer time but the calculations are more robust.

GLOBAL TEST INTERVAL

Use the **Global test interval** setting to change the interval at which a global equilibrium test is done, which by default is every 10th step as long as there are no changes in the set of stable phases. Every time the set of stable phases tries to change, a global equilibrium test is also done regardless of the test interval value chosen. A global equilibrium test means that the calculated equilibrium state obtained by the ordinary minimization calculation is tested against the Global Minimization Technique, and if the result is found unstable then the full global minimization calculation is performed instead.

MAX GRID POINTS

Use the **Max grid points** to set the maximum number of grid points per phase for global minimization. The default is 2000.

LIQUID PHASE

The default in the list is the **LIQUID** phase already defined in the chosen database.

GAS PHASE

The default in the list is the **Gas phase** already defined in the database

CALCULATE EVAPORATION PROPERTIES

Select the **Calculate evaporation properties** checkbox to calculate the **Molar mass of gas**, **Driving force for evaporation**, and **Evaporation enthalpy** properties.

A gas phase is required to calculate these properties.

This option sets the gas phase to dormant, meaning that the thermodynamic properties of the gas are evaluated, without the gas being allowed to form. This enables the calculation of the following properties: **Molar mass of gas**, **Evaporation enthalpy**, and **Driving force** for evaporation. Driving force for evaporation is positive when the gas is stable (temperature above evaporation temperature). A negative driving force means the gas is metastable.

TERMINATE SCHEIL ON

This setting controls when a Scheil calculation should terminate. From the **Terminate Scheil on** list, choose **Fraction of liquid phase** (unit = mole fraction) or **Temperature** and enter a value in the field.

MAX NO. OF ITERATIONS

Enter or choose a value for the **Max no. of iterations**. By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.

REQUIRED ACCURACY

The default **Required accuracy** is `1.0E-6`. This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.

SMALLEST FRACTION

The default **Smallest fraction** (or **Smallest fraction in a phase** for Property Models) is `1.0E-12`. This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions.

The default value for the smallest site-fractions is `1E-12` for all phases except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as `1E-30`.

In Console Mode, the default of 1E-30 for IDEAL phases is true unless you are using the command SET_NUMERICAL_LIMITS to reset an even-lower value (e.g. `1E-45`, that is naturally enforced to all the phases in the system.

APPROXIMATE DRIVING FORCE FOR METASTABLE PHASES

The **Approximate driving force for metastable phases** checkbox is selected by default. Click to clear the checkbox to change the default as required and based on the options described below.

This setting involves the convergence of metastable phases and affects their driving forces. It can also have an effect on when an equilibrium is considered successful.

The default is to allow an equilibrium with metastable phases that have not converged, as long as the stable phases have converged. This is efficient but often causes approximate values of the driving forces for the metastable phases.

If you change the default, it enforces metastable phases to converge. This gives accurate driving forces for metastable phases as well as stable phases. It can however take a slightly longer time, and if metastable phases do not converge it causes the equilibrium calculation to fail.

INCLUDE ONE AXIS EQUILIBRIUM CALCULATION

The **Include one axis equilibrium calculation** checkbox is selected by default and a **One Axis** (also called *step*) calculation is performed before the actual Scheil calculation. It produces the solidification curve under equilibrium conditions and it is shown on the plot if the default axis variables are used. This is sometimes referred to as the *equilibrium line*.

If a comparison to equilibrium is not necessary, change the default setting and then only a Scheil calculation is performed. This results in a much faster calculation, which for a complex system may be preferable.

TEMPERATURE BELOW SOLIDUS SETTINGS

The **Temperature below solidus settings** are available when **Temperature below solidus** is selected for **Calculate to**. This calculates the properties for the given number of temperatures, down to the final temperature for the phase compositions and fractions at the solid phases at the end of the Scheil calculation.

- Enter the **No. of points**. The default is 50.
- Enter the **Final temperature**. The default is room temperature (298.15 K).

Scheil Calculator Available Plot Variables

When working with Scheil calculations in Graphical Mode, there are several plot variables available with the Plot Renderer that is a successor to the Scheil Calculator.

For a comparable list in Console Mode, see State Variables for Scheil.

The following list is specific to a Plot Renderer that is a successor to a Scheil Calculator. The software includes relevant variables in the *Axis variable* list based on the set up of the Scheil Calculator.

There may be some additional variables available if the calculation involves the Diffusion Module (DICTRA) and/or other specialized databases are used.

When certain variables are selected (i.e. electric or thermal conductivity, electric or thermal resistivity, or thermal diffusivity), there are additional settings related to these described in Configuration Settings.

Quantities Groups Available for Plots and Tables

Quantities	
Apparent heat capacity per gram	Apparent heat capacity per mole
Apparent volumetric CTE	Average composition of solid phases
Composition of a phase	Density
Distribution of component in phase	Driving force for evaporation per mole
Dynamic viscosity	Electric conductivity
Electric resistivity	Evaporation enthalpy per mole
Heat per gram	Heat per mole
Kinematic viscosity	Latent heat per gram
Latent heat per mole	Mass fraction of liquid
Mass fraction of solid	Mass fraction of solid phase
Molar mass of gas	Molar volume
Molar volume of phase	Mole fraction of liquid
Mole fraction of solid	Mole fraction of solid phase
Site fraction	Surface tension
Temperature	Thermal conductivity
Thermal diffusivity	Thermal resistivity
Volume fraction of liquid	Volume fraction of solid
Volume fraction of solid phase	

Scheil Calculations Frequently Asked Questions

Below are some frequently asked questions (FAQs) related to Scheil calculations in Thermo-Calc. It is not intended to cover all the scenarios that can occur with such complex calculations. A particular focus is on the use and definition of variables available for plotting latent heat, heat, and apparent heat capacity, and the differences between Graphical Mode and Console Mode.

What is the latent heat evolution for a Scheil solidification simulation?

Theory usually defines the latent heat as the isothermal enthalpy change of phase transformation at any chosen temperature. It is called *latent* because it is regarded as a potential heat release or uptake. Usually this is the transformation from liquid to solid.

However, most alloys, if not all, solidify non-isothermally. In the Scheil calculation the plotted quantity called *latent heat* might not follow the theoretical definition of latent heat. It is the cumulative enthalpy change of phase transformation.

There is no contribution from heat capacity, only from phase transformation.

How can I plot the latent heat evolution after a Scheil simulation?

In Graphical Mode, on the Plot Renderer node, select one of the **Axis variables**—**Latent heat per mole** or **Latent heat per gram**—to plot the quantity.

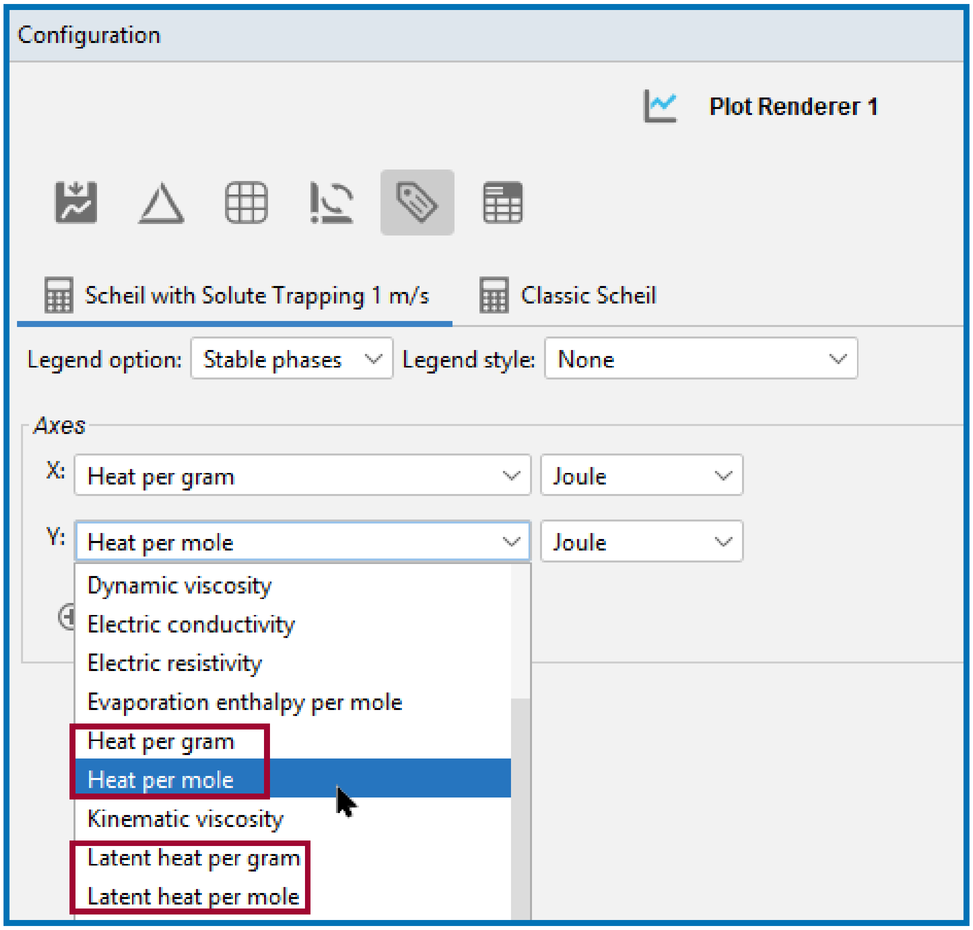
In Console Mode, the corresponding quantities are `NHR` or `BHR`. If you plot NH in Console Mode, you get two curves. The bottom curve is NHR, or the latent heat. See State Variables for Scheil for a list of the other variables.

For more detail, see Why in Console Mode are there two curves when plotting heat evolution after a Scheil simulation?

What is the difference between the Latent heat per mole or gram and just Heat per mole or gram?

In Graphical Mode, on the Plot Renderer node, in addition to **Latent heat per mole** and **Latent heat per gram** you can also select one of the variables for each **Axes**—**Heat per mole** or **Heat per gram**. What is the difference?

Heat per mole or **Heat per gram** is the total molar (or specific) enthalpy of the system. This includes both the enthalpy change from phase transformations, and from the temperature change, which comes from the heat capacity.



Legend option: Stable phases

Legend style: None

X: Heat per gram Joule

Y: Heat per mole Joule

Why in Console Mode are there two curves when plotting heat evolution after a Scheil simulation?

The following is applicable to Console Mode.

The top curve is the total heat evolution and it is plotted with the quantity `NHV`. This is the total molar or specific enthalpy, including the contribution from both phase transformations and form heat capacity of the phases. The contribution from the solid phases are averaged.

The bottom curve is the axis quantity and it is plotted with the quantity `NHR`. This means that this is only the contribution of enthalpy changes from phase transformation from liquid; therefore it starts at 0 at the onset of melting.

How do you plot the distribution of component in phase?

In Graphical Mode the axis quantity is called **Distribution of component in phase**. This gives the distribution of that element as a fraction of the total molar inventory of that element, from 0 to 1 (0 to 100 % of the overall composition). For example, the total amount of Fe in all phases should then sum up to 1.

Be aware that if using the fast diffuser option there may be issues summing up to 1.

In Console Mode, `NN(Phase,Element)` shows the fraction of this element relative to its total amount in the system, residing in that phase. Here a value of 0.3 means 30 % of all the Fe in the system is in that particular phase.

You can also use wildcards, e.g. `NN(Phase,*)`, which shows all elements’ respective fractions of the total in that phase (this does not sum up to 1). This is useful to get an overview of preferential partitioning of elements during the solidification process.

Also useful is plotting `NN(*,Element)`, where you see the distribution of the element over all phases in the system; these curves should all sum up to 1. Here, 0.3 of Fe in Liquid and 0.7 in FCC, would mean that 30 % of the total Fe-content in this alloy is still in the liquid, etc.

Due to calculation issues when working with fast diffusers, this command is not available in Console Mode.

What is the apparent heat capacity?

The apparent heat capacity is what is going to be measured experimentally; heat capacity is theoretically the derivative of enthalpy with respect to temperature. This apparent heat capacity includes both contributions from phase transformation and from temperature change.

Scheil Resources: Installed Examples

For Graphical Mode examples, see T_08: Scheil and Equilibrium Solidification, T_10: Scheil Solidification with Back Diffusion, and T_13: Scheil Solidification with Solute Trapping.

For Console Mode examples see Scheil-Gulliver Examples.

Scheil Resources: Website Video Tutorials and Application Example

Link to more information about Scheil Solidification Simulations on our website. There are also video tutorials related to some Scheil examples as part of a playlist on our YouTube channel and an application example using the Diffusion Module (DICTRA).

Scheil Resources: Self-paced Learning Hub

The Thermo-Calc Learning Hub has a module dedicated to Scheil Calculations.

Learn about Thermo-Calc and the Add-on Modules at your own pace with our comprehensive online Learning Hub. The Learning Hub includes courses for Thermo-Calc, the Diffusion Module (DICTRA), the Precipitation Module (TC-PRISMA), and the TC-Python SDK. In addition to introductory lectures, instructors walk through and discuss real world examples that correlate calculations with microstructures and other metallurgical concepts, spanning a wide range of material types.

Subscriptions also include access to live monthly office hours, where you can ask our experts about any of the content on the Learning Hub or your own materials challenges.

Property Model Calculator

A **Property Model Calculator** enables you to predict and optimize material properties based on their chemical composition and temperature. The available calculation types are **Single**, **One Axis**, **Grid**, **Min/Max**, **Uncertainty**, and **Batch**.

Using these, you can evaluate models simultaneously over a range of compositions and temperature and cross plot the results, then conduct an uncertainty analysis and plot the results as either a histogram or a probability plot. The **Batch** calculation further enables you to read input from a file, such as a spreadsheet.

There are **General Models** plus material specific Model Libraries for **Nickel Models**, **Noble Metal Alloys Models**, **Steel Models**, and **Titanium Models** available. For more information start with the section About the Property Models.

Property Model Calculator Workflow

At the start when you are designing a project, it is recommended you first test it by performing a **Single** calculation type. This verifies that the configuration of the model is valid, otherwise you will get a *Not a Number* result in the Event Log Window, which indicates the calculation did not work correctly.

Once the Single calculation performs successfully, you can experiment with other calculation types such as **Grid**, **Min/Max**, **Uncertainty**, or **Batch**. Best practice for both Grid and Uncertainty is to start with a small number of steps (Grid) or samples (Uncertainty) to confirm that it works before increasing the number of steps or samples. For Batch calculations, it is good practice to first review the data file requirements described in Working with Batch Calculations.

For a Grid calculation, you can additionally plot a *Heat map*, *Contour*, or *3D* diagram. This setting is done on the Plot Renderer, which has several Plot Types, Plotting Options, and Plot Types available.

In general, the workflow for each model differs. A recommended start point is to do a **One Axis** calculation (using the Equilibrium Calculator) to determine what phases you get and where the transitions are before setting up the Property Model Calculator.

Templates

There are a variety of related templates both for the equilibrium One Axis calculations and to add a **Property Model** node structure.

In addition there are **Steel TTT** and **Steel CCT** templates that you can use to quickly set up a simulation for the Steel Model Library. For details, see Getting Started Links and Templates.

Configuration Settings

Each Property Model has its own set of configuration parameters. There are some standard ones entered starting with the Configuration Window Settings topic.

Custom Property Models

You can also create custom Property Models. Search the TC-Python help on the website for details about creating custom models. In general go to the **Property Model Framework → Best Practices** section.

About the Property Models

Property Models are used to predict and optimize properties of materials using models stored within the software where the calculations are set up in the Property Model Calculator.

General Models

The following General Property Models are available with the Property Model Calculator.

The **General Models** are available to all users.

To run calculations with the Add-on Property Model Libraries all require a valid maintenance license plus a license for the specific database version: **Nickel Models** (TCNI11 and newer and MOBNI5 and newer; **Noble Metal Alloys Models** (TCNOBL3 and newer); **Steel Models** (TCFE9 and newer + MOBFE4 and newer); **Titanium Models** (TCTI6 and newer).

About the Steel Model Library Property Models, About the Nickel Model Library Property Models, and About the Titanium Model Library Property Models, and About the Noble Metal Alloys Model Library Property Models.

Coarsening

The **Coarsening** Property Model calculates the coarsening rate coefficient K (m^3/s) of a spherical precipitate phase in a matrix phase.

See About the Coarsening Property Model and Coarsening Property Model Settings for background theory and input parameter details.

Columnar to Equiaxed Transition (CET)

The **Columnar to Equiaxed Transition** Property Model calculates the fraction of equiaxed grains that correlates with a certain solidification condition, specifically thermal gradient (G) and solidification growth rate (v).

See About the Columnar to Equiaxed Transition (CET) Property Model and Columnar to Equiaxed Transition (CET) Property Model Settings for background theory and input parameter details.

Crack Susceptibility Coefficient

The **Crack Susceptibility Coefficient** Property Model calculates the hot tearing tendency during solidification.

See About the Crack Susceptibility Coefficient Property Model and Crack Susceptibility Coefficient Property Model Settings for background theory and input parameter details.

Driving Force

The **Driving Force** Property Model calculates the thermodynamic driving force for a phase.

See Driving Force Property Model Settings for input parameter details.

Equilibrium

The **Equilibrium** Property Model calculates the equilibrium for the given conditions. Optionally define additional function definitions.

See Equilibrium Property Model Settings for input parameter details.

Equilibrium with Freeze-in Temperature

The **Equilibrium with Freeze-in Temperature** Property Model calculates equilibrium at the freeze-in temperature and evaluates the properties at a different temperature. The assumption is that diffusion and phase transformations are negligible when changing from the freeze-in-temperature and, therefore, that the phase amounts and compositions of phases are kept at all other temperatures.

See About the Equilibrium with Freeze-in Temperature Property Model and Equilibrium with Freeze-in Temperature Property Model Settings for background information and input parameter details.

Interfacial Energy

The **Interfacial Energy** Property Model estimates the interfacial energy between a matrix phase and a precipitate phase using thermodynamic data from a CALPHAD database.

? See About the Interfacial Energy Property Model and Interfacial Energy Property Model Settings for background information and input parameter details.

Liquid and Solidus Temperature

The **Liquid and Solidus Temperature** Property Model is for doing a common calculation. For example, you can easily use uncertainty calculations, vary one or more conditions, and see how that affects the liquidus and solidus temperatures.

? See Liquid and Solidus Temperature Property Model Settings for input parameter details.

Phase Transition

The **Phase Transition** Property Model can be used to vary which condition to relax, and then it calculates the point when a new phase may form. It is useful to determine melting temperature, boiling temperature or solubility limits. It returns the phase transformation temperature, or composition, depending on the relaxed condition.

? See Phase Transition Property Model Settings for input parameter details.

Scheil

The **Scheil** Property Model is used to calculate solidification under the Scheil assumption. The majority of the Model input parameters are pulled from the Scheil Calculator to offer the outputs of the liquidus/solidus/solidification range so you can explore these in the calculation types of the Property Models.

? See Scheil Property Model Settings, and Scheil Advanced Options: Property Models.

Spinodal

The **Spinodal** Property Model calculates the spinodal line.

? See About the Spinodal Property Model and Spinodal Property Model Settings for background information and input parameter details.

T-Zero Temperature

The **T-Zero Temperature** Property Model calculates the so-called T_0 line.

See About the T0 Temperature Property Model and T0 Temperature Property Model Settings for background information and input parameter details.

Yield Strength

The **Yield Strength** Property Model calculates yield stress. It returns the calculated yield strength at room temperature for the specified material using the equilibrium values calculated at temperature T (i.e. T is the freeze-in temperature). Then you can further define the following contributions to the total yield stress: precipitation strengthening, solid solution, grain boundary strengthening, and constant addition of strength.

See About the Yield Strength Property Model and Yield Strength Property Model: Simplified Mode Settings or Yield Strength Property Model: Advanced Mode Settings for background information and input parameter details.

Calculation Types

The Property Model Calculator includes these calculation types:

- **Single**: Calculates a single point.
- **One Axis**: Varies a quantity on the X-axis.
- **Grid**: Evaluates two axis variables of the selected quantities in the specified range and number of steps. You can then select to create heat map, contour and 3D plots on the Plot Renderer.
- **Min/Max**: Evaluates the Property Model(s) for all variations of the selected quantities at the given limits. The Mean field is as defined under *Condition Definitions* for the respective quantity. The total minimum and maximum of the Model(s) results are shown in the Event log.
- **Uncertainty**: Evaluates the Property Model(s) where the values of the quantities are sampled from Gaussian distributions. The Mean field is as defined under *Condition Definitions* for the respective quantity. The result is visualized as a histogram or normal probability plot by adding a Plot Render activity.
- **Batch**: Use this to allow for high throughput calculations and read data from a file, such as a spreadsheet. You can include experimental results in the data file, which then can be used to compare to the batch calculation results.

About the Uncertainty Calculations and Plot Types

Examples and Video Tutorials

Thermo-Calc General Property Models Examples Collection

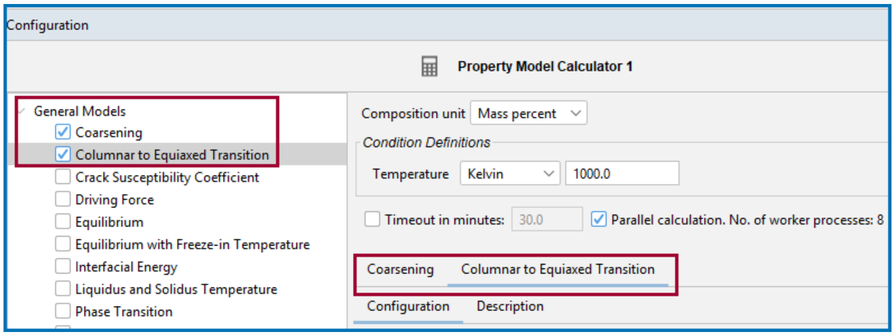
For tutorials about this feature, go to our website or browse the Property Model Calculator playlist on our YouTube channel.

Define the Property Model Calculator

1. Add a **Property Model Calculator** node to the System Definer. If you used the **Property Models** template, click the node to display the **Configuration** settings window.
2. From the left side of the **Configuration** window, click to select one or more of the checkboxes under the **General Models**. If you have licenses for the material specific libraries, you can also select and run the Property Models from the **Nickel Models**, **Noble Metal Alloys Models**, **Steel Models**, or **Titanium Models** folders.

   > For the material specific libraries these are only available if you have the applicable licenses. If you are interested in learning more about the available models, go to our website.

   A tab with the same name as the Property Model opens in the right side of the window under *Condition Definitions*. When you select more than one Model at a time, a matching tab is added in the same order that the checkbox is selected.



Configuration

Property Model Calculator 1

General Models
- ☑ Coarsening
- ☑ Columnar to Equiaxed Transition
- ☐ Crack Susceptibility Coefficient
- ☐ Driving Force
- ☐ Equilibrium
- ☐ Equilibrium with Freeze-in Temperature
- ☐ Interfacial Energy
- ☐ Liquidus and Solidus Temperature
- ☐ Phase Transition

Composition unit: Mass percent

Condition Definitions

Temperature: Kelvin 1000.0

☐ Timeout in minutes: 30.0 ☑ Parallel calculation. No. of worker processes: 8

3. For each Model on the **Configuration** tab, select or enter settings described in Configuration Window Settings and based on the *Calculation Type* chosen.

   > When working in the **Configuration** window, click the **Description** tab for

more information about the Model.

4. Once you have finished defining the Property Model Calculator, you also choose settings on the Plot Renderer.

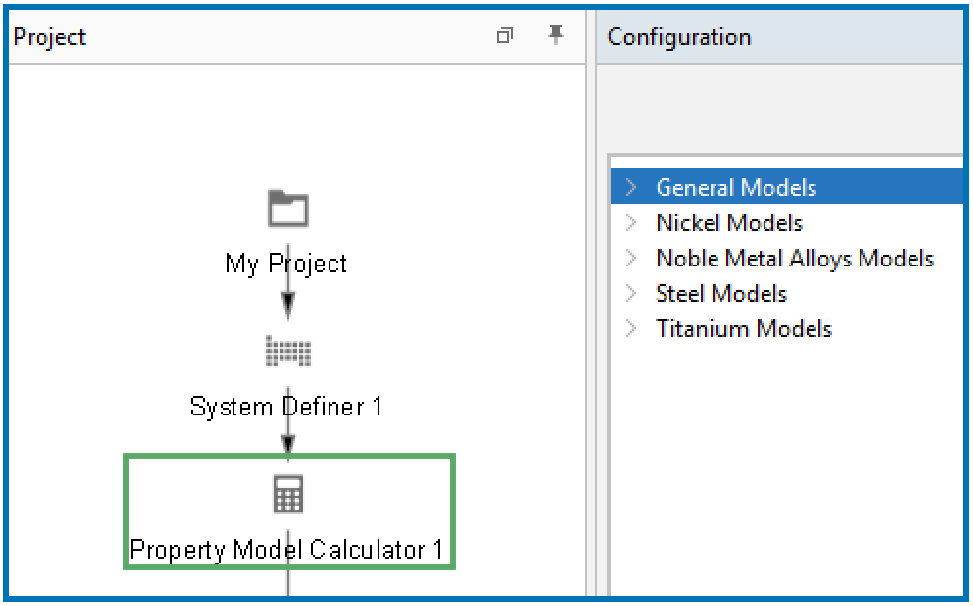
Examples and Video Tutorials

Thermo-Calc General Property Models Examples Collection

For tutorials about this feature, go to our website or browse the Property Model Calculator playlist on our YouTube channel.

Configuration Window Settings

Click the **Property Model Calculator** node in the **Project** window to view the **Configuration** window. The settings available vary based on such choices as the Property Model and calculation type selected.



Depending on your license, there are many Property Models available and the available options on the Configuration window vary. The General Models are available to all users.

General Configuration Settings

COMPOSITION UNIT

Select the **Composition unit**: **Mass percent**, **Mole percent**, **Mass fraction**, or **Mole fraction**.

CONDITION DEFINITIONS

Choose a unit (**Kelvin**, **Celsius** or **Fahrenheit**) and then enter a value for the **Temperature** and **Composition** for each component.

The values entered in *Condition Definitions* are used as the start values for the different calculation types.

TIMEOUT IN MINUTES

Select the **Timeout in minutes** checkbox to enter a time when a calculation will stop trying to complete the evaluation. This is useful if it is a complex or unknown calculation outcome and you want to prevent it from taking too much computer time or resources. The number entered in the field means that this is the maximum amount of time that each line can take for an individual calculation. This is useful in particular for Batch or Uncertainty calculations.

PARALLEL CALCULATION

By default, the **Parallel calculation** (Property Model Calculator Configuration window) and **Parallel calculation for Property Model Calculator** (Options window for a Global setting) checkbox is selected.

The number of parallel branches (the **No. of worker processes**) can only be changed globally via the Options window. The default number of worker processes is based on the number of physical cores available on the computer. You can adjust the number of worker processes as needed, however it is still dependent on the available cores on the computer.

This checkbox is used for all the calculation types available with the Property Model Calculator in Graphical Mode. When you click **Perform**, the grid points calculated are distributed among these worker processes, which enables parallel calculations and speeds up the calculation. Click to deselect the checkbox as needed to not use these worker processes.

DEFINE THE PROPERTY MODEL

For each Property Model chosen, select or enter **Configuration** settings as required.

For links to each Model with the settings details, see About the Property Models.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

CALCULATION TYPE

Click to select a *Calculation Type*:

- **Single** to calculate a single point. Any model can use this calculation type and no additional settings are required. The results from this calculation are displayed in the **Event Log** or if a **Table Renderer** is used, in the **Visualizations** window.
- **One Axis**: To vary a quantity on the *X*-axis.
- **Grid**: Evaluates two axis variables of the selected quantities in the specified range and number of steps.
- **Min/Max**: Evaluates the Property Model(s) for all variations of the selected quantities at the given limits. The **Mean** field is as defined under *Condition Definitions* for the respective quantity. The total minimum and maximum of the model(s) results are shown in the **Event** log.
- **Uncertainty**: Evaluates the Property Model(s) where the values of the quantities are sampled from Gaussian distributions. The **Mean** field is as defined under *Condition Definitions* for the respective quantity. The result is visualized as a histogram or normal probability plot by adding a Plot Renderer activity.
- **Batch**: Use this to allow for high throughput calculations and read data from a file, such as a spreadsheet, rather than, for example, having a fixed grid or random values. Results from these batch calculations can then be compared to experimental values (as long as this data is included), using a **Cross plot** on the Plot Renderer.

AXIS DEFINITION

For **One Axis**, select a **Quantity** to vary along the X-axis, for example, **Temperature** then enter a **Min**, **Max** and **Number of steps**.

GRID DEFINITIONS

For the **Grid** calculation type, define the two axes variables using the fields and menus: **Quantity**, **Min**, **Max**, and **Number of steps**. The number of steps along with the minimum and maximum values for the axes define a grid. For each grid point the selected models are evaluated.

> For a **Grid**, on the Plot Renderer, you can choose to plot a *Heat map*, *Contour*, or *3D* diagram.

Plot Type: Heat Map, Contour, and 3D

MIN/MAX DEFINITIONS

For the **Min/Max** calculation type, click to select the applicable checkboxes under **Quantity to enable or disable an axis**. The **Mean** field is as defined under *Condition Definitions* for the respective quantity.

Enter numerical values in the Δ **Min/Max** fields to evaluate the change to the quantity. The highest and lowest value of each selected model results are shown in the **Event Log**.

SAMPLING OF DATA FROM GAUSSIAN DISTRIBUTIONS

For the **Uncertainty** calculation type, click to select the applicable checkboxes under **Quantity to vary this quantity**. The **Mean** field is for the distribution function as defined under *Condition Definitions* for the respective quantity. The default ΔMin/Max is a 95% confidence interval.

About the Uncertainty Calculations

SAMPLING PARAMETERS

For the **Uncertainty** calculation type, choose a number of **Standard deviations** where you want to **Truncate the distribution**. Choose the **Total number of samples**.

About the Uncertainty Calculations

BATCH CONTROLS

For more details about the format of a data file used to define the compositions, parameters, experimental data, or skipping validation, see Working with Batch Calculations.

In the **Data file** field, either enter a file path or click the load data file button (📁) to navigate to a data file such as an Excel spreadsheet (with `*.xls` or `*.xlsx` extensions) or a `*.csv` file. You can also use other programs (e.g. Google Sheets) to enter data and export to a CSV format that can be read by the software.

Click **Open** to import the data. In the **Data file** field you can see the file path to the selected file. The next time you click the load data file button (📁) the program remembers the last location from where the file is opened.

Choose the delimiter—**Comma** (`,`), **Colon** (`:`), **Equals sign** (`=`), **Semicolon** (`;`), or **Tab**—that matches the delimiter in the data file and click the **Reload** (🔄) button.

The data is imported and displays on the Property Model Calculator:

- The data are used for the applicable fields that must match what already exists as a Property Model parameter (e.g. critical radius, grain size, etc.) as well as the composition, temperature, and units that you want to run the calculation for. Also, if the dependent element composition is not included in the data file, the batch calculation then sets the dependent element to be the same as defined in the user interface.
- The calculation runs once for every row of data included in the file.

When the data file is imported into Thermo-Calc, there is also a **Row** column autogenerated by Thermo-Calc.

Select the **Set zero amount to value (in mole-/mass-fraction)** to enter a small value for the mole/mass-fraction in cases where a Property Model has problems calculating zero amounts of elements.

Select the **Skip validation of data file** checkbox to allow a calculation to perform using the data file even when certain criteria are not met.

When selected, the validation of the data file is skipped:

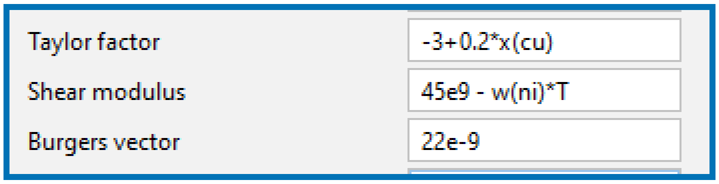
- If the **Composition** (elements) do not match the system composition entered on the GUI in the System Definer or Property Model Calculator.
- If one or more **Parameters** are not correctly entered, not selected for the specific Property Model, or are unavailable with the selected Property Model, then these are ignored in the calculation.

If there are any data file validation error(s), a tooltip on the **Perform** button lists and describes these.

Entering Model Parameters as Functions

For many model parameters that are defined as a numeric value this can be entered in number format or as a user-defined function (an expression).

An exception to this is the Yield Strength Model *Advanced Mode* setting for *Solid solution strengthening* and when entering the **Solid solution strengthening temperature**. This field must be entered in number format i.e. it does not accept a user-defined function.



Taylor factor	-3+0.2*x(cu)
Shear modulus	45e9 - w(ni)*T
Burgers vector	22e-9

GUIDELINES FOR ENTERING FUNCTIONS

- The user-defined function can contain the operators for multiplication (`*`), division (`/`), addition (`+`), subtraction (`-`), and exponentiation (`**` or (`^`).
- If an invalid function is entered, the **Event Log** warns you of the error.
- If an expression is entered as a parameter/function value, then that parameter is not available to select as a quantity on the Plot Renderer, i.e. as an axis quantity.

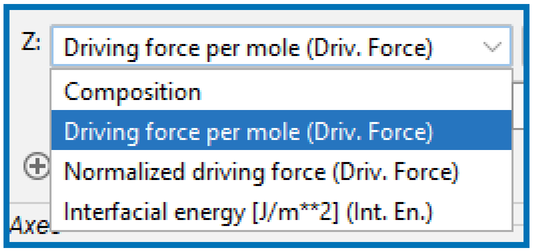
Only the thermodynamic quantities for composition (mole fraction and weight fraction) and temperature can be used in functions and these must be entered using a specific syntax (which uses Console Mode format). An example of a valid function for composition (mole fraction) and temperature is `x(Fe)*2 - T^(1.0/3.0)`.

Quantity	***Syntax***
Mole fraction	`x(element)`
Weight fraction	`w(element)`
Temperature	`T`

Result Quantities: Property Model Abbreviations

When selecting quantities on the Plot Renderer or Table Renderer, the quantity names include an abbreviated name for the Property Model it is associated to. This is useful in particular when you are calculating two or more Property Models that share names for the quantities. The short name identifying the specific Property Model is included in parentheses after the name of the quantity. Below are the full and abbreviated names for each Property Model.

This is not applicable to the **Equilibrium** Property Model.



An example of the short names included in parentheses for the Driving Force and Interfacial Energy Property Model quantities. This is from example PM_G_03.

Full Name	***Abbreviation***	***Model Library***
Columnar to Equiaxed Transition (CET)	Col. Eq. Trans.	General
Coarsening	Coarsening	General
Crack Susceptibility Coefficient	Crack Susc. Coeff.	General
Driving Force	Driv. Force	General
Equilibrium with Freeze-in Temperature	Eq. Freeze-in Temp.	General

Full Name	***Abbreviation***	***Model Library***
Interfacial Energy	Int. En.	General
Liquid and Solidus Temperature	Liq. & Sol. Temp	General
Phase Transition	Phase Trans.	General
Scheil	Scheil	General
Spinodal	Spinodal	General
T-Zero Temperature	T-Zero Temp.	General
Yield Strength	Yield Strength	General
Antiphase Boundary Energy	Ant. Bound En. - Ni	Nickel
Coarsening Nickel	Coars. -Ni	Nickel
Equilibrium with Freeze-in Temperature Nickel	Eq. Freeze-in Temp. - Ni	Nickel
Solvus for Ordered Phase	Solv. Ord. Phase - Ni	Nickel
Strain-Age Cracking	Strain-Age Crack. - Ni	Nickel
Optical Properties	Opt.Prop.- Noble	Noble Metal Alloys
Bainite	Bainite	Steel
CCT Diagram	CCT Diagr.	Steel
Critical Transformation Temperatures	Crti. Transf. Temp.	Steel
Ferrite	Ferrite	Steel
Martensite Fractions	Mart. Fract.	Steel
Martensite Temperatures	Mart. Temp.	Steel
Martensitic Steel Strength	Mart. Steel Strength	Steel
Pearlite	Pearlite	Steel

Full Name	*Abbreviation*	*Model Library*
TTT Diagram	TTT Diagr.	Steel
Alloy Strength - Ti	All. Strength - Ti	Titanium
Martensite Temperatures - Ti	Mart. Temp. - Ti	Titanium

Diffusion Calculator

The Diffusion Calculator is available with three elements if you do not have the additional Diffusion Module (DICTRA) license. With the Add-on Module you can use all available elements as per the licensed database selected. See Available Graphical Mode Features for details about this and other options available with additional licenses.

A **Diffusion Calculator** allows you to set the conditions for, and perform, a diffusion calculation. You can add the calculator to the System Definer directly (right-click and select it from the **Create New Successor** menu).

There are also templates available under **Non-Equilibrium** that you can use to quickly set up a simulation. See Getting Started Links and Templates.

Once you have added a Diffusion Calculator, the **Configuration** window has **Conditions** and **Options** settings tabs where there are many available conditions to set and then continue the settings with the specialized **Plot Renderer**.

- **Conditions**: Set the conditions for your calculation that define the geometry, regions, phases, grids, composition profiles, and thermal profile.

  The **Composition Profiles** and **Thermal Profile** are both set up on the **Configuration** window for a Diffusion Calculator. These are previewed in the **Visualizations** window.

- **Options**: Modify the simulation conditions such as the choosing the default solver (automatic or homogenization) and the time integration method. Also define the time step controls and if you choose homogenization as the solver, define further settings such as the interpolation scheme and whether to use global minimization or not.
- **Plot Renderer**: There are also unique settings available for this calculator once you add a Diffusion Calculator Plot Renderer.

Working with these simulations is an advanced topic. It is recommended you review the documentation and videos available or search for a specific topic.

Available Graphical Mode Features

The Diffusion Module is an Add-on Module to the core Thermo-Calc software.

A separate license is required to perform calculations for more than three elements. Without it you are able to use the module in *Demo Mode*. This is not available in Console Mode.

Diffusion Templates

Under **Non-Equilibrium Calculations**, the **Homogenization** and **Diffusion** templates are available to all Thermo-Calc users when in Graphical Mode.

If you are using the Diffusion Module in Demo Mode, see Demonstration (Demo) Mode for what is available to you. Even if you have a license, you may find yourself in Demo Mode if you have a network license and all the licenses are checked out.

USING THE TEMPLATES

After opening Thermo-Calc in Graphical Mode, in the templates section under **Non-Equilibrium Calculations** click:

- **Homogenization** to add a *System Definer*, *Scheil Calculator*, *Diffusion Calculator*, and two *Plot Renderer* nodes to the **Project** tree.
- **Diffusion** to add a *System Definer*, *Diffusion Calculator*, and *Plot Renderer* to the **Project** tree.

Creating a Project from a Template

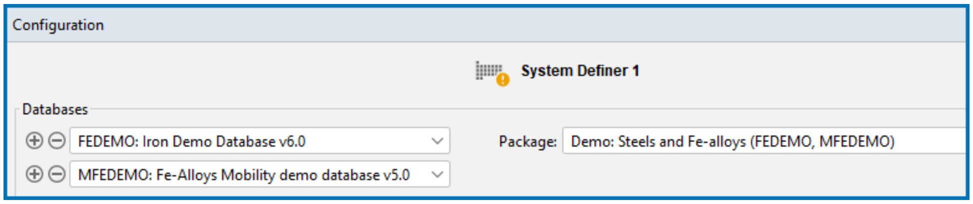
Diffusion Calculator

A Diffusion Calculator allows you to set the conditions for your calculation that define the geometry, regions, phases, grids, composition profiles, and the thermal profile, plus additional options. Many of the settings are automatically set as you define your system. Details about this activity are described in Diffusion Calculator.

Demo Database Packages for the Examples Collection

Both a thermodynamic and mobility database are required to run the Diffusion Module simulation. If you have a Diffusion Module (DICTRA) license you can run all the examples because the demonstration database packages are included with your installation.

Select the database packages from the **System Definer Configuration** window to run a simulation.



FEDEMO: Iron Demo Database v6.0

MFEDEMO: Fe-Alloys Mobility demo database v5.0

Package: Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)

Demonstration (Demo) Mode

The Diffusion Module and some examples are available to all Thermo-Calc users but only for simulations with three elements. If you do not have a license then you are in *Demo Mode* when using the Diffusion Calculator, or either of the templates.

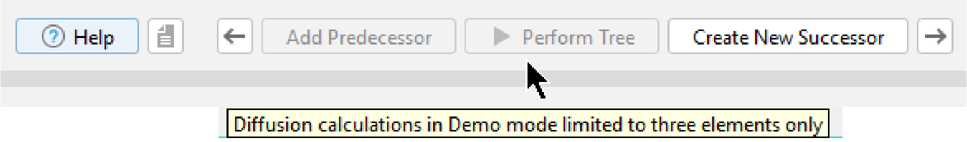
DIFFUSION TEMPLATES

If you are in DEMO mode then this is indicated by the addition of **DEMO** text under the button.

DIFFUSION CALCULATOR

If you are experimenting with the Diffusion Calculator in Demo Mode then you may have access to a variety of databases based on your license. However, you can only define three elements for a demo simulation.

If you define more than three elements on the System Definer, when you go to the Diffusion Calculator, the **Perform** button is unavailable and the tooltip explains why.



Diffusion calculations in Demo mode limited to three elements only

Even if you have more than three elements, the Plot Renderer **Perform** button is still available. However, if you click the button and try to run the simulation the **Event Log** displays an error message.

Additive Manufacturing (AM) Module

There is connectivity between the Diffusion Module (DICTRA) or the Precipitation Module (TC-PRISMA) and the Additive Manufacturing (AM) Module when you have full licenses available for all relevant Add-on Modules and databases.

You can add a Diffusion Calculator or Precipitation Calculator as a successor to the AM Calculator and then when probes are included with the AM Calculator this data can be further used with the thermal profile.

Details are in the AM Module documentation. See AM Calculator: Working with Probe Data.

Define the Diffusion Calculator

Working with diffusion simulations is an advanced topic. It is recommended you review the Diffusion Module (DICTRA) documentation and videos available or search for a specific topic.

1. Add a **Diffusion Calculator** node to the **System Definer**. If you used the **Diffusion** template (on the **My Projects Configuration** window under **Non-Equilibrium**), click the node to display the **Configuration** settings window.

2. In the Diffusion Calculator **Configuration** window, enter the settings described in Conditions Tab Settings and Options Tab Settings.

The **Composition Profiles** and **Thermal Profile** are both set up on the **Configuration** window for a Diffusion Calculator. These are previewed in the **Visualizations** window.

When you also have licenses either for the Diffusion Module (DICTRA) and/or the Precipitation Module (TC-PRISMA), for transient simulations you can additionally include probe data from the AM Calculator in the set up of the thermal profile for diffusion and precipitation calculations, respectively.

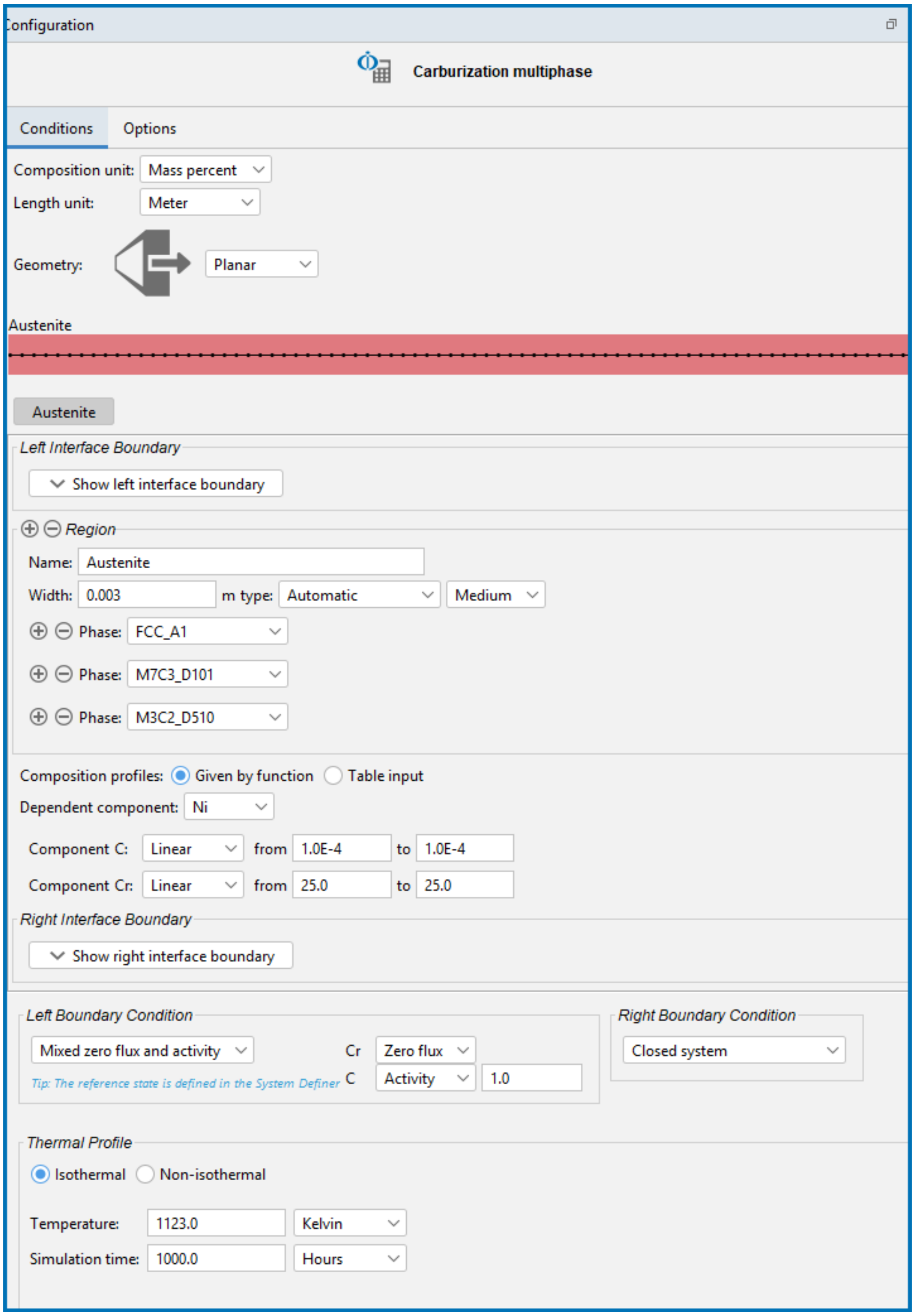
3. Once you have finished defining the Diffusion Calculator, you also choose settings on the Plot Renderer. Some additional settings are specific to the Diffusion Calculator Plot Renderer.

Available Graphical Mode Features

Diffusion Module (DICTRA) Examples Collection

Conditions Tab Settings

The following **Configuration** window is from the *Graphical Mode Quick Start Guide*. It is using project example file *D_07: Diffusion Carburization Multiphase*.



Composition unit: Mass percent
Length unit: Meter
Geometry: Planar

Left Interface Boundary

Region

Name: Austenite
Width: 0.003 m type: Automatic Medium
Phase: FCC_A1
Phase: M7C3_D101
Phase: M3C2_D510

Composition profiles: ● Given by function ○ Table input
Dependent component: Ni

Component C: Linear from 1.0E-4 to 1.0E-4
Component Cr: Linear from 25.0 to 25.0

Right Interface Boundary

Left Boundary Condition

Mixed zero flux and activity
Cr Zero flux
C Activity 1.0
Tip: The reference state is defined in the System Definer

Right Boundary Condition

Closed system

Thermal Profile

● Isothermal ○ Non-isothermal

Temperature: 1123.0 Kelvin
Simulation time: 1000.0 Hours

These are the settings available from the **Conditions** tab. To edit the global defaults for some settings, go to the **Options** window (different from the tab). See Global Settings: Diffusion Calculator.

The Diffusion Module (DICTRA) in Console Mode has commands to perform some of the settings also available on the Diffusion Calculator. Where possible the name of the command is indicated and includes a link to the topic.

General

COMPOSITION UNIT

Choose a **Composition unit** from the list: **Mass percent**, **Mole percent**, **Mass fraction**, or **Mole fraction**.

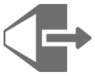
LENGTH UNIT

Choose a **Length unit** from the list: **Meter**, **Millimeter**, **Micrometer**, **Nanometer**, or **Ångström**.

GEOMETRY

Choose a **Geometry**: **Planar**, **Spherical**, or **Cylindrical**. For **Cylindrical**, also enter a value for the **First interface position**.

With a cylindrical or spherical geometry, the system's zero coordinate (left boundary) is at the center of the cylinder or sphere. The highest coordinate (right boundary) is defined by the cylinder or sphere radius.

Geometry	***Graphic***
Planar	
Spherical	
Cylindrical	

The **Composition Profiles** and **Thermal Profile** are both set up on the **Configuration** window for a Diffusion Calculator. These are previewed in the **Visualizations** window.

Region Settings

There should be one unique phase in each region.

LEFT AND RIGHT INTERFACE BOUNDARY

Toggle between hiding and showing the **Left interface boundary** or **Right interface boundary**.

Click the ⊕ **Add quantity** or ⊖ **Remove quantity** buttons as required to add a **Phase** and then enter a value for the **Driving force** as required. The default driving force is `1.0E-5`.

NAME

Enter a **Name** for the region in the field. For example, enter `Austenite`. This name is automatically updated on the tab and above the grid points graphic.

WIDTH

Enter a numerical value in the **Width** field. The unit is the one selected for the **Length unit**.

TYPE (OF GRID)

Select a type of grid:

Automatic is not available when the **Composition profiles: Table input** is selected. See Composition Profiles.

- **Automatic** for an automatic grid point distribution. An appropriate grid is generated at the start of the simulation where the grid points are automatically distributed according to the entered composition profile and boundary conditions.
- **Linear** for an equally spaced grid.
- **Geometric** for a grid that yields a varying density of grid points in the region.
- **Double geometric** to have a high number of grid points in the middle or at both ends of a region.

AUTOMATIC GRID TYPE SETTINGS

For an **Automatic** grid type, also choose a grid accuracy level: **Coarse**, **Medium**, **Fine**, or **Custom**.

> The values for the Grid Accuracy settings for each option differ when calculated by Thermo-Calc based on whether it is the Classic or Homogenization model.

- If you are using a Classic model: Fine 75/1.25, Medium 50/1.2, Coarse 25/1.15 (Number of points/Max geometric factor)
- If you are using the Homogenization model: Fine 100/1.03, Medium 80/1.02, Coarse 60/1.01 (Number of points/Max geometric factor)

For **Custom**, also enter values for:

- **max number of points**: the maximum number of equidistant points in a region.
- **max geometric factor**: Value in the geometrical factor in the series determining the distribution of the grid points. A geometrical factor larger than one yields a higher density of grid points at the lower end of the region and a factor is smaller than one yields a higher density of grid points at the upper end of the region.

POINTS (LINEAR, GEOMETRIC, AND DOUBLE GEOMETRIC GRIDS)

For **Linear**, **Geometric**, or **Double geometric** grids, enter a numerical value in the **points** field. The default is 50.

RATIO (GEOMETRIC GRID)

For a **Geometric** grid, choose or enter a number for the **Ratio** to determine the distribution. A geometrical factor larger than one yields a higher density of grid points at the lower end of the region and a factor smaller than one yields a higher density of grid points at the upper end of the region.

LOWER RATIO AND UPPER RATIO (DOUBLE GEOMETRIC GRID)

For a **Double geometric** grid, specify two geometrical factors. Enter a **Lower ratio** for the distribution in the lower (left) part of a region, and an **Upper ratio** for the distribution in the upper (right) part of a region.

PHASE

Choose a **Phase** from the list. The available options are defined in the System Definer. At least one phase that dissolves all system elements must be selected.

Click the ⊕ **Add phase** or ⊖ **Remove phase** buttons as required.

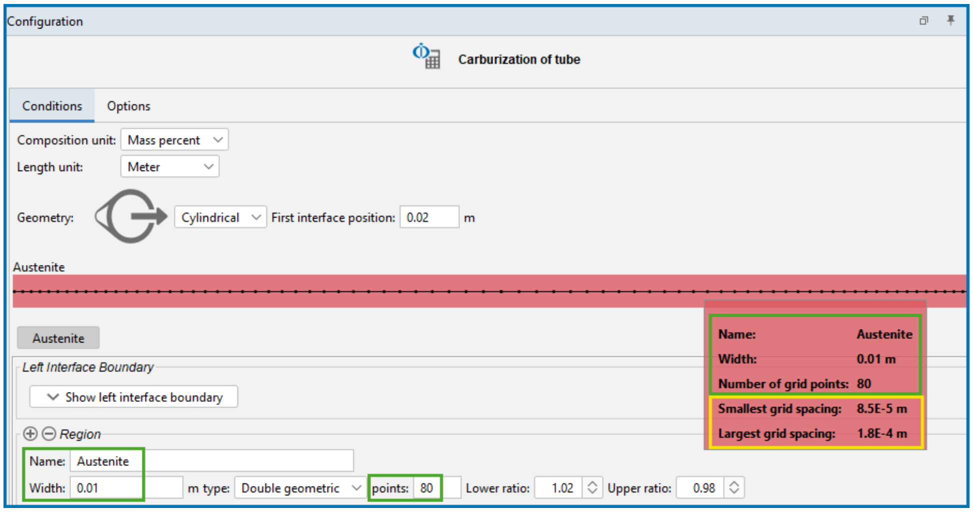
The **Composition Profiles** and **Thermal Profile** are both set up on the **Configuration** window for a Diffusion Calculator. These are previewed in the **Visualizations** window.

TIP: View a Summary of the Region Grid Point Settings

When working with the **Diffusion Calculator** in Graphical Mode, you can hover over the grid points on the **Configuration** window to view additional tooltip details about the region.

The settings information includes the **Name** of the region (in the example it is renamed to **Austenite**), the **Width** of the region, and the number of grid **points**.

For all types of grids, useful calculated information is included about the **Smallest grid spacing** and **Largest grid spacing** points. The information is available to prevent you from setting a combination with too many grid points and a high geometric factor that could lead to unusable grid point spacings.



Composition unit: Mass percent
Length unit: Meter
Geometry: Cylindrical First interface position: 0.02 m

Name: Austenite
Width: 0.01 m
Number of grid points: 80
Smallest grid spacing: 8.5E-5 m
Largest grid spacing: 1.8E-4 m

Name: Austenite
Width: 0.01 m type: Double geometric points: 80 Lower ratio: 1.02 Upper ratio: 0.98

An example of a Diffusion Calculator Configuration window. The Region settings (in the green boxes) are taken directly from the settings. The Smallest and Largest grid spacing details (in the yellow box) are taken from the grid point placement information calculation. This is using example D_06.

Boundary Conditions

Boundary conditions are conditions that define how matter behaves at the boundaries of your system. By default, matter is not allowed to cross the system boundaries.

You can change the setting for both the lower boundary (left side/centre) and the upper boundary (right side/surface) of the system.

Examples D_06 and D_07 use boundary conditions, as described in Diffusion Module (DICTRA) Examples Collection.

The boundary condition settings are done on the **Diffusion Calculator**. The following describes the options available for the *Left boundary* and *Right boundary* conditions.

CLOSED SYSTEM

By default it is a **Closed system**. Choose **Mixed zero flux and activity** or **Composition** if the system is not closed. Corresponds to a fix flux value, which is set to zero at all times. This is the default boundary condition.

COMPOSITION

Allows you to set a fix composition at the boundary.

In Console Mode this is similar to the command STATE_VARIABLE_VALUE, but in Graphical Mode this condition is limited to setting a fixed composition.

MIXED ZERO FLUX AND ACTIVITY

The flux of selected components is either set to zero or a prescribed activity value.

For **Mixed zero flux and activity**, and for each independent element selected in the **Composition profile**, choose either **Zero flux** or **Activity** from the lists and enter a value in the field when **Activity** is selected. The reference state for the components are taken from the System Definer **Components** tab.

In the field for **Activity**, enter a formula that the software evaluates during the calculation.

The formula can be:

- A function of the variable TIME
- A constant

The formula must be written with these rules:

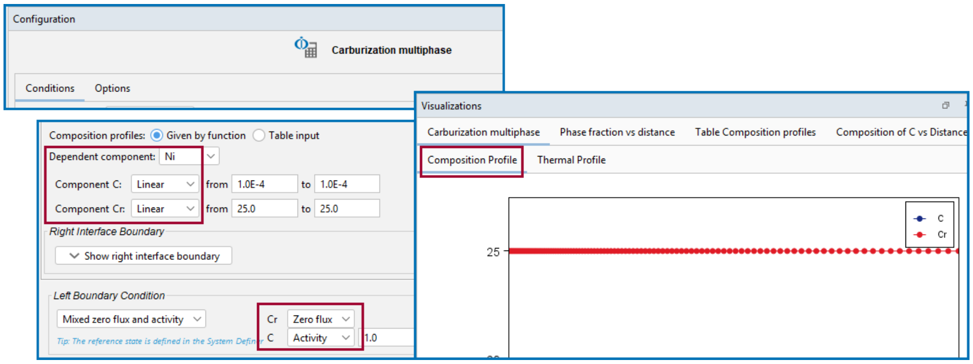
- A number must begin with a number (not a dot)
- A number must have a dot or an exponent (E)

The operators + , - , * , / , ** (exponentiation) can be used and with any level of parenthesis.

As shown, the following operators must be followed by `()` i.e. open and closed parentheses:

- SQRT(X) is the square root
- EXP(X) is the exponential
- LOG(X) is the natural logarithm
- LOG10(X) is the base 10 logarithm
- SIN(X), COS(X), TAN(X), ASIN(X), ACOS(X), ATAN(X)
- SINH(X), COSH(X), TANH(X), ASINH(X), ACOSH(X), ATANH(X)
- SIGN(X)
- ERF(X) is the error function

This is from example *D_07: Diffusion Carburization Multiphase*.



Composition profiles: ● Given by function ○ Table input

Dependent component: Ni

Component C: Linear from 1.0E-4 to 1.0E-4

Component Cr: Linear from 25.0 to 25.0

Left Boundary Condition: Mixed zero flux and activity

Cr: Zero flux

C: Activity 1.0

Tip: The reference state is defined in the System Defin

Composition Profiles

The **Composition Profiles** are set up on the **Configuration** window for a Diffusion Calculator. These are viewed in the **Visualizations** window.

For most calculations, you can include data as follows.

- *Given by function* (linear, step, or function). See Composition Profiles: Given by Function. The grid types available to select are **Automatic**, **Linear**, **Geometric**, or **Double geometric**.
- *Table input* that can be either directly entered or imported. See Composition Profiles: Table Input (i.e. Data File Import). The grid types available to select are **Linear**, **Geometric**, or **Double geometric**.
- *Solidification data*. For a **Diffusion Calculator** that is a successor to the **Scheil Calculator**, you can perform a Scheil solidification calculation followed by kinetic homogenization simulation of segregated composition profile. In this case, there are different options on the **Configuration** window for this section. The profile then uses information from the Scheil Calculator. See Composition Profiles: Scheil Segregation Profiles.

When using the **Table input** setting, you can directly enter data in the table or you can import a **Data file**. If you import a data file, even though it is a simple set of data, first prepare it based on the Guidelines for Importing Data Files to Composition Profiles.

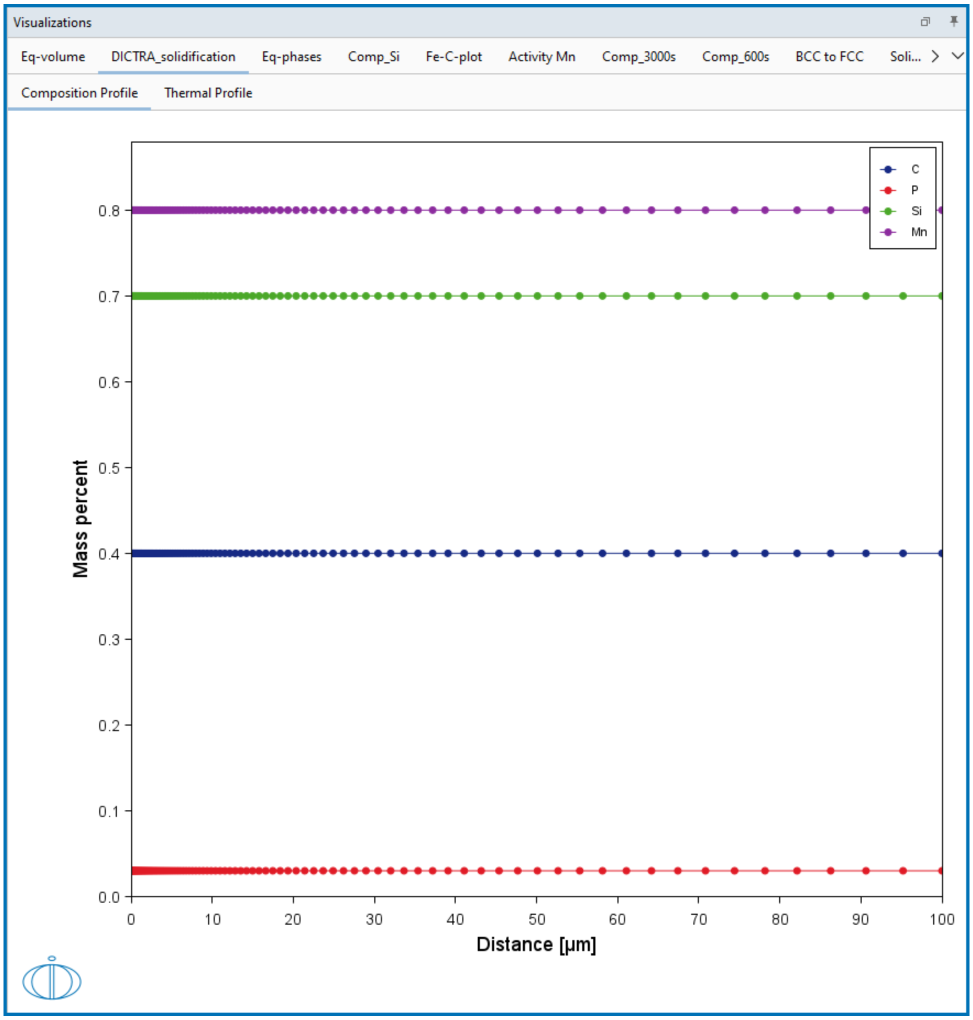


Figure 1: This composition profile is from example D_08 Microsegregation During Solidification. Other examples using this feature are D_04_Diffusion_Fe-C_Moving_Boundary_Austenite_to_Ferrite and D_09 Ni_Post_Weld_Heat_Treatment_From_File, which are all included with your installation.

Composition Profiles: Given by Function

1. On the Diffusion Calculator **Configuration** window, first enter the required settings described in Conditions Tab Settings including the Region Settings and Boundary Conditions.
2. Click to select the **Composition profiles** → **Given by function** option.
3. Select a **Dependent component** for which the composition does not need to be given. The available options depend on the phase description.

4. For each **Component** choose one of these options:
    - **Linear**: Enter numerical values in the **from** and **to** fields.
    - **Step**: Enter numerical values in the **from**, **to**, and **step at** fields. The unit is the same as the **Length unit** selected at the top of the Configuration window.
    - **Function**: Enter a composition function in the field using SI units. The syntax to use for writing functions is a Python syntax (a programming language). Any valid Python expression that is a function of the distance variable *x* will work.

    > You can use the standard Jython math library but you must prefix these functions with the text "math" For example: `10 + math.sin(x*2)`. The Jython math library is available here: https://www.jython.org/.

    - The error function `erf(X)` is also available in the Jython math library and can be called with `math.erf(x)`.
    - Another useful function is the Heaviside step-function `hs(X)`. For example, `3+2hs(x-1e-4)` provides a concentration of 3 at the left side and 5 at the right side with a sharp step in the concentration profile at 1e-4m=100 mm.
5. The **Composition Profile** is previewed in the **Visualizations** window as in Figure 1. Make adjustments to the settings as needed and watch it dynamically change in the window.
6. After completing this section, also continue with Boundary Conditions and the Diffusion Calculator Thermal Profile.

Composition Profiles: Table Input (i.e. Data File Import)

1. On the Diffusion Calculator **Configuration** window, first enter the required settings described in Conditions Tab Settings including the Region Settings and Boundary Conditions.
2. Click to select the **Composition profiles** → **Table input** option.
3. Select a **Dependent component** for which the composition does not need to be given (i.e. it is excluded from the table). The available options depend on the phase description. The **Composition unit** and **Length unit** are taken from the settings already entered.

4. To enter data directly into the table:
   a. Click in each cell under the applicable columns, e.g. **Distance** and then each individual component such as **Fe**, **Al**, etc.
   b. Directly enter the values in the table. Press `<Enter>` to add rows and use the scroll bars to navigate the table.
5. To import a data file:
   a. It is important to first prepare the data file as in Guidelines for Importing Data Files to Composition Profiles.
   b. When the data file is ready, to the right of the **Data file** field, click the file 📁 button to load the file.
   c. Navigate to a data file such as an MS Excel spreadsheet (with ***.xls** or ***.xlsx** extensions) or a ***.csv** file. You can also use other programs (e.g. Google Sheets) to enter data and export to a CSV format that can be read by the software. Click **Open** to import the data to the **Configuration** window table.
   d. If there are issues with the above import, experiment with choosing the delimiter type that corresponds to the data in the file: **Comma** (`,`), **Colon** (`:`), **Equals sign** (`=`), **Semicolon** (`;`), or **Tab**—that matches the delimiter in the data file. Click the **Reload** button ↻. The data is imported to the **Configuration** window table.
6. The **Composition Profile** is previewed in the **Visualizations** window as in Figure 1. Make adjustments to the settings as needed and watch it dynamically change in the window.
7. After completing this section, also continue with Boundary Conditions and the Diffusion Calculator Thermal Profile.

Composition Profiles: Scheil Segregation Profiles

This section is specific to when the **Homogenization** template is used, or generally when a **Diffusion Calculator** is a successor to the **Scheil Calculator**.

When this is the case, the *Composition profiles* take information from the Scheil calculation, and then you can choose to **Average over all solidified phases** (the default), where **All solidified phases** is further selected by default or you can define by **Custom phases**.

Alternatively, choose **Primary dendrite phase**, where it is assumed that other phases formed during solidification will not dissolve during homogenization. The **Primary dendrite phase** can only be BCC, FCC, or HCP.

Also when **Primary dendrite phase** is selected, the Scheil segregation profiles for fast diffusers are not available. The alloy composition for fast diffusers that is defined on the **Scheil Calculator Configuration** window next to the **Fast diffusers** checkbox is used instead.

The segregated composition profile can be assumed to be equal to a concentration profile for regular Scheil assumptions. i.e. the segregated composition profile as a function of solidified material can be directly mapped to a concentration profile given the secondary arm spacing. This direct relation between segregated and concentration profiles is no longer valid when fast diffusers are used. Then the fast diffusers equilibrate at all temperatures during the Scheil solidification and the concentration profiles for fast diffusers therefore change at every temperature. The average segregated profile for all elements (also fast diffusers) as a function of solidified material represent the composition profile at the final temperature at the end of solidification.

To learn about the **Homogenization** template, see Getting Started Links and Templates.

Example D_10: Iron (Fe) Homogenization in Scheil uses the **Homogenization** template to demonstrate the use of the Scheil data with a diffusion calculation.

Guidelines for Importing Data Files to Composition Profiles

The **Composition Profiles** settings are done on the **Configuration** window for a **Diffusion Calculator**. The profile is then previewed in the **Visualizations** window.

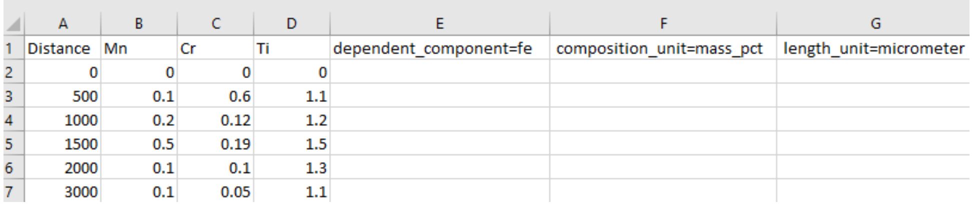
You can import data from a file. There are specific guidelines needed to correctly prepare the data in the file to ensure it imports without errors.

Data File Requirements

The following are instructions about setting up the data file when **Table input** is selected for the Composition Profiles.

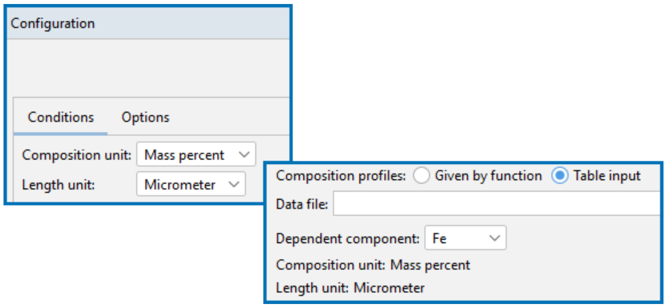
The data in the spreadsheet or csv file can include the distance and the compositions, plus the parameters defining the dependent component, composition unit, and length unit. In order for the data to be included in the calculation, the column and row definitions in the file must adhere to certain rules of entry.

Only the columns described here are read / used in the calculation. It is important to enter the information exactly as described. It is recommended that the data file is cleaned up before importing / loading it and performing calculations.



	A	B	C	D	E	F	G
1	Distance	Mn	Cr	Ti	dependent_component=fe	composition_unit=mass_pct	length_unit=micrometer
2	0	0	0	0			
3	500	0.1	0.6	1.1			
4	1000	0.2	0.12	1.2			
5	1500	0.5	0.19	1.5			
6	2000	0.1	0.1	1.3			
7	3000	0.1	0.05	1.1			

Figure 2: This is an example of data entered into an Excel spreadsheet (which is then converted to csv format). Columns A to D show the data entered to create the Composition Profile itself. Columns E, F, and G are to define default settings although these can also be defined on the Configuration window.



Composition unit: Mass percent

Length unit: Micrometer

Composition profiles: ○ Given by function ● Table input

Data file:

Dependent component: Fe

Composition unit: Mass percent

Length unit: Micrometer

Figure 3: Three columns in the spreadsheet correspond to settings that can either be entered on the Configuration window, or defined in the data file. This is for the dependent component (column E), composition unit (column F), and length unit (column G). When this information is not specified in the data file, the default is taken from the settings defined on the Configuration window.

Distance and Composition/Components Plus Values

General Rules

- No abbreviations are allowed.
- All header text must be in English, i.e. no translations into other languages will be read correctly by the data file.
- The composition columns MUST match what is already entered on the System Definer or the file will not load.

In the table, `code font` indicates something entered into the data file (or it is an example) and any *<text in italic with angle brackets>* is a generic name for an entry.

Column Heading Requirements and Options	*Row Cell Requirements and Options*
Distance This is column A as in Figure 2 Enter the text `Distance`. No abbreviations allowed but it is not case sensitive.	Valid format and entries for each row in this column: • Any numerical input for the distance e.g. `500`, `0.15`, `8.7`, `1.00E-05`, etc.
<Components / Composition> These are columns B to D as in Figure 2 Each element of the composition is in a separate heading column using the *<element short name>* This is already included in the table header on the **Configuration** window and based on the entries selected on the System Definer. Enter an *<element short name>* into each column, row 1. e.g. in this example, `Mn`, `Cr`, and `Ti` are entered in columns B, C, and D, respectively. Entries are not case sensitive, so alternatives in this example for Mn can be `mn` or `MN`.	Valid format and entries for each row in these columns: • A number for the composition e.g. `0.15`, `8.7`, `1.00E-05`, etc. The elements in the file must match what is selected on the System Definer. (1) If it is in the file but not selected on the System Definer, then it is not added to the table, and (2) if the opposite is true, that an element is selected on the System Definer but not included in the file, then an empty column is added and manually you must enter the details.

Composition Unit, Length Unit, and Dependent Component

General Rules

- The defaults can be selected on the **Configuration** window, or can be entered in its own column in the data file. When this is not specified in the data file, the default is taken from the settings defined on the Configuration window. See Figure 3.
- No abbreviations allowed but it is not case sensitive. For example, it is acceptable to enter `composition_unit` or `Composition_Unit`, or `COMPOSITION_UNIT`, etc.

- All header text must be in English, i.e. no translations into other languages will be read correctly by the data file. For example, do not add the accents to the A and O in the word Angstrom, e.g. Ångström cannot be read correctly.
- Do not enter anything in the rows in each of these columns.

> In the table, `code font` indicates something entered into the data file (or it is an example) and any *<text in italic with angle brackets>* is a generic name for an entry.

Column Heading Description	*Column Heading Requirements and Options*
The **Dependent component** in the data file is defined with the heading `dependent_component=`*`<element>`* In Figure 3, this is in column E. i.e. `dependent_component=fe`. Add the heading to its own column to set the **Dependent component** to **Fe**.	Valid format and entries of the *<dependent_ component>* (the text is added after the = sign): • Any of the components/elements selected already on the System Definer can be entered.
The **Composition unit** in the data file is defined with the heading `composition_unit=`*`<unit>`*. In Figure 3, this is in column F. i.e. `composition_unit=mass_pct`. Add the heading to its own column to set the **Composition unit** to **Mass percent**.	Valid format and entries of the *<composition_ unit>* (the text is added after the = sign): • `mass_pct` • `mass_frac` • `mole_pct` • `mole_frac`
The **Length unit** for the distance in the data file is defined with the heading `length_unit=`*`<unit>`*. In Figure 3, this is in column G. i.e. `length_unit=micrometer`. Add the heading to its own column to set the **Length unit** for the distance to **Micrometer**.	Valid format and entries of the *<length_unit>* (the text is added after the = sign): • `Meter` • `Millimeter` • `Micrometer` • `Nanometer` • `Angstrom` Enter `Angstrom` without the accents on A and O, e.g. Ångström will not be read correctly.

Diffusion Calculator Thermal Profile

The **Thermal Profile** is set up on the **Configuration** window for a **Diffusion Calculator**. The isothermal or non-isothermal profile is viewed in the **Visualizations** window. Choose **Isothermal** to do a simulation at constant temperature. Choose **Non-isothermal** to enter or import data for a user-defined temperature profile.

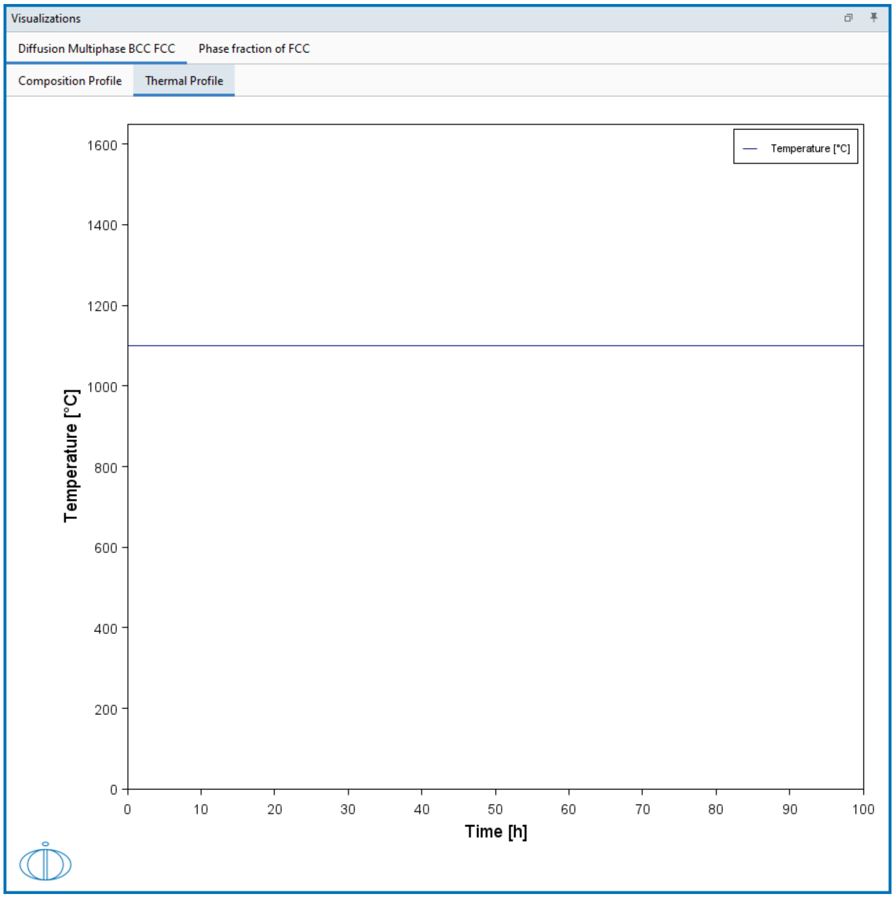
When connected to an AM Calculator (see Including Probe Data from an AM Calculator) the **Isothermal** and **Non-isothermal** options are not visible as it is not relevant to that view.

Isothermal Calculations

Many of the Graphical Mode examples for this Add-on Module are isothermal calculations, e.g. *D_03_Diffusion_Multiphase*.

1. On the Diffusion Calculator **Configuration** window, first enter the required settings described in Conditions Tab Settings including the Region Settings, Boundary Conditions, and Composition Profiles.
2. Under **Thermal Profile** click to choose **Isothermal** to do a simulation at constant temperature.
3. Enter a **Temperature** and choose a unit (**Kelvin**, **Celsius**, or **Fahrenheit**.
4. Enter a **Simulation time** and choose a unit: **Seconds**, **Minutes**, **Hours**, or **Days**.

   The **Thermal Profile** is displayed in the **Visualizations** window showing the constant temperature entered.

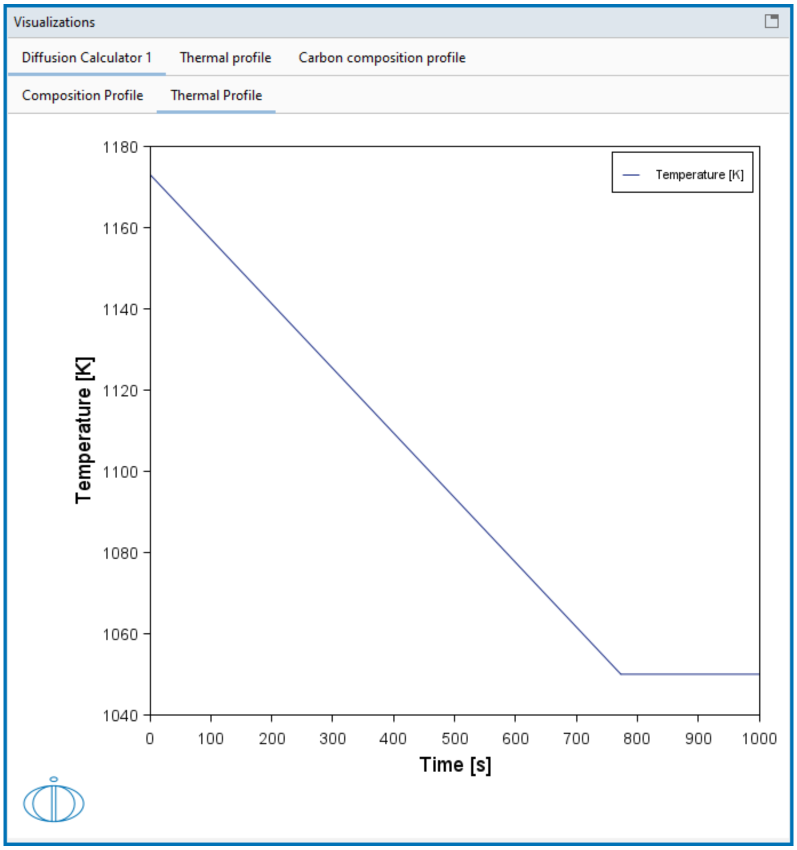


5. For this calculation type this completes the settings you need to enter for the Thermal Profile.

Non-isothermal Calculations

1. On the Diffusion Calculator **Configuration** window, first enter the required settings described in Conditions Tab Settings including the Region Settings, Boundary Conditions, and Composition Profiles.
2. Under **Thermal Profile** click to choose **Non-isothermal** to enter or import data for a user-defined temperature profile.
3. Select a **Temperature unit**: **Kelvin**, **Celsius**, or **Fahrenheit**.
4. Enter an **End time** and choose a unit: **Seconds**, **Minutes**, **Hours**, or **Days**. The *Simulation time* is displayed as text.
5. You can next either directly enter **Time** and **Temperature** coordinates into the table or import the information from a file. A minimum of two points is required.

6. To enter data directly into the table:
    a. Click in each cell under the applicable columns, **Time** and **Temperature** then directly enter the values in the table.
    b. Press `<Enter>` to add rows and use the scroll bars to navigate the table.
7. To import from a file:
    a. Although it is a simple set of data, prepare the data file as in Guidelines for Importing Data Files to Thermal Profiles.
    b. When the data file is ready, to the right of the **Import from file** field, click the file 📁 button.
    c. Navigate to a data file such as an MS Excel spreadsheet (with ***.xls** or ***.xlsx** extensions) or a ***.csv** file. You can also use other programs (e.g. Google Sheets) to enter data and export to a CSV format that can be read by the software. Click **Open** to import the data to the **Configuration** window table.
    d. If there are issues with the above import, experiment with choosing the delimiter type that corresponds to the data in the file: **Comma** (`,`), **Colon** (`:`), **Equals sign** (`=`), **Semicolon** (`;`), or **Tab**. Click the **Reload** button 🔄. The data is imported to the **Configuration** window table.
8. For this calculation type this completes the settings you need to enter for the **Thermal Profile**, which is displayed in the **Visualizations** window. Make adjustments to the settings as needed and watch it dynamically change in the window.



This is from example *D_04: Diffusion Fe-C Moving Boundary Austenite to Ferrite*.

Including Probe Data from an AM Calculator

> When you also have a license for the Additive Manufacturing (AM) Module you can include probe data from the AM Calculator in the set up of the thermal profile.

There is connectivity between the Diffusion Module (DICTRA) or the Precipitation Module (TC-PRISMA) and the Additive Manufacturing (AM) Module when you have full licenses available for all relevant Add-on Modules and databases.

You can add a Diffusion Calculator or Precipitation Calculator as a successor to the AM Calculator and then when probes are included with the AM Calculator this data can be further used with the thermal profile.

Details are in the AM Module documentation. See AM Calculator: Working with Probe Data.

Guidelines for Importing Data Files to Thermal Profiles

The **Thermal Profile** settings are done on the **Configuration** window for a **Diffusion Calculator**. The profile is then previewed in the **Visualizations** window.

You can import data from a file. There are specific guidelines needed to correctly prepare the data in this file to ensure it imports without errors.

Data File Requirements

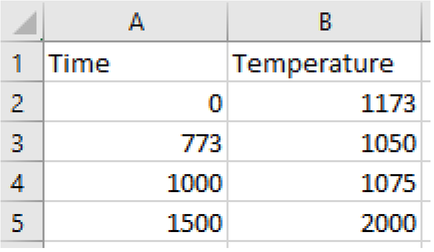
For a Thermal Profile you can either directly enter **Time** and **Temperature** coordinates into the table on the **Configuration** window, or import the data from a file. A minimum of two points is required.

Although there are only two columns to define, it is still important to ensure the file is set up correctly. In order for the data to be included in the calculation, the column and row definitions in the file must adhere to certain rules of entry.

GENERAL RULES

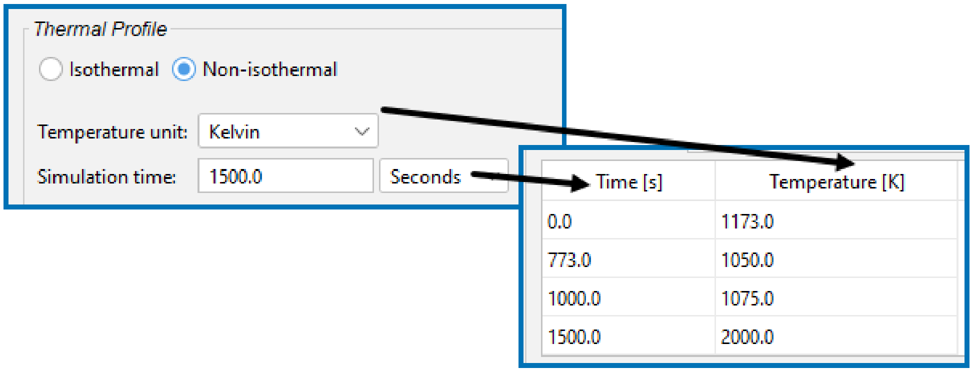
- No abbreviations are allowed in the header.
- A header is not actually required in this file but in order to know which column is which, it is recommended to include it.
- All header text must be in English, i.e. no translations into other languages will be read correctly by the data file.

Only the columns described here are read / used in the calculation. It is important to enter the information exactly as described. It is recommended that the data file is cleaned up before importing / loading it and performing calculations.



	A	B
1	Time	Temperature
2	0	1173
3	773	1050
4	1000	1075
5	1500	2000

Figure 4: This is an example of data entered into an Excel spreadsheet (which is then converted to csv format). Columns A and B show the data entered to create the Thermal Profile.



Thermal Profile

○ Isothermal ● Non-isothermal

Temperature unit: Kelvin

Simulation time: 1500.0 Seconds

Time [s]	Temperature [K]
0.0	1173.0
773.0	1050.0
1000.0	1075.0
1500.0	2000.0

Figure 5: The units shown on the Configuration window for the Time and Temperature correspond to settings that can ONLY be selected on the Configuration window. The data file does not contain any information about the units.

Column Heading Requirements and Options	***Row Cell Requirements and Options***
Time This is column A as in Figure 4 Enter the text `Time`. No abbreviations allowed but it is not case sensitive. It is also not required but recommended to include so you know which column of data it applies to.	Valid format and entries for each row in this column: • Any numerical input for the time that corresponds to the unit selected on the Configuration window e.g. `0.0`, `773`, `1000`, `1500`, are times in seconds, which is the unit chosen in the example shown in Figure 5.
Temperature This is column B as in Figure 4 Enter the text `Temperature`. No abbreviations allowed but it is not case sensitive. It is also not required but recommended to include so you know which column of data it applies to.	Valid format and entries for each row in these columns: • Any numerical input for the temperature that corresponds to the unit selected on the Configuration window e.g. `1173`, `1050`, `1075`, are temperatures in Kelvin, which is the unit chosen in the example shown in Figure 5

Options Tab Settings

The following settings are available on the **Options** tab for a Diffusion Calculator.

You can change these settings locally for a specific Calculator or globally for some defaults in the **Options** *window* (a different location than the tab).

To open the **Options** window:

- Windows: Select **Tools** → **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

then click the **Graphical Mode** tab and the **Diffusion** node in the tree.

Global Settings: Diffusion Calculator.

The Diffusion Module (DICTRA) in Console Mode has commands to perform some of the settings also available on the Diffusion Calculator. Where possible the name of the command is indicated and includes a link to the topic.

Simulation Conditions

DEFAULT SOLVER

Choose the *Default solver*: **Automatic** or **Homogenization**. Select **Homogenization** to define the *Homogenization Model Specific* sections.

Classic and Homogenization Model Settings

The homogenization solver (called the homogenization model in Console Mode) is useful when you want to simulate long-range diffusion through a multiphase mixture, under the assumption that local equilibrium holds at each node point.

TIME INTEGRATION METHOD

Automatic , **Trapezoidal**, or **Euler backwards**.

The default is **Automatic** where the default degree of implicity corresponds to trapezoidal (0.5) for classic and Euler Backward (1.0) for the homogenization model. If large fluctuations occur in the profiles it may be necessary to use the more stable but less accurate *Euler backwards*.

SAVE RESULTS ON FILE

Yes, **No**, or **Every nth.**. Select **Every nth** to enter a value in the field.

This setting determines if the results are to be saved on file during the course of the simulation. Select:

- **Yes** to always save on file.
- **No** to never save on file.
- **Every nth.** to save every n^{th} time to file. Then enter an integer value ranging from 0 to 99.

USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATIONS

The default, **Automatic**, allows the software program to automatically use forced starting values to perform the equilibrium calculations. When a phase with an ordering contribution is entered into the simulation, for example the gamma-prime/FCC_l12 phase in Ni-base superalloys, forced starting values are automatically turned on. Or choose **Yes** or **No**.

DEFAULT DRIVING FORCE FOR PHASES ALLOWED TO FORM AT INTERFACES

Enter a value in the field. The required driving force (evaluated as `DGM (ph)`) to be used for determining whether an inactive phase is stable. DGM is the variable for the driving force that is already divided by RT, and it is dimensionless. The default is `1E-5`.

? Suffixes

Timestep Control

MAX RELATIVE ERROR

Enter a value in the field. The default is `0.05`.

MAX ABSOLUTE ERROR

Enter a value in the field. The default is `1.0E-5`.

TIMESTEP

Enter values in the fields.

> ❗ This value is always in seconds.

- **Initial**: What is used as the initial time step. The default is `1.0E-7`.
- **Smallest allowed**: The smallest time step allowed during the simulation. This is required when using the automatic procedure to determine the time step. The default is `1.0E-7`.
- **Max % of simulation time**: The default is `10`.

FACTOR SPECIFYING THE MAXIMUM INCREASE IN THE TIME STEP TAKEN FROM ONE TIME STEP TO ANOTHER

For example, if 2 is entered the maximum time step is twice as long as the previous time step taken. Enter a value in the field. The default is 2.

THE TIMESTEP IS TO BE CONTROLLED BY THE PHASE INTERFACE DISPLACEMENT DURING THE SIMULATION

The default is **Automatic**. When a liquid phase is entered in a simulation this option is automatically turned on. Optionally choose **Yes** or **No** to set whether the time step is to be controlled by the phase interface displacement during the simulation.

Classic and Homogenization Model Settings

Classic Model Specific

ACTIVITY OR POTENTIAL

Use the [**activity** or **potential**] of a component in order to find the correct tieline at the phase interface.

Determines whether the program should use the potential or the activity of a component in order to find the correct tie-line at the phase interface. The potential or the activity is varied by the program and is set in order to reduce the degrees of freedom at the local equilibrium.

FLUX BALANCE EQUATION ACCURACY

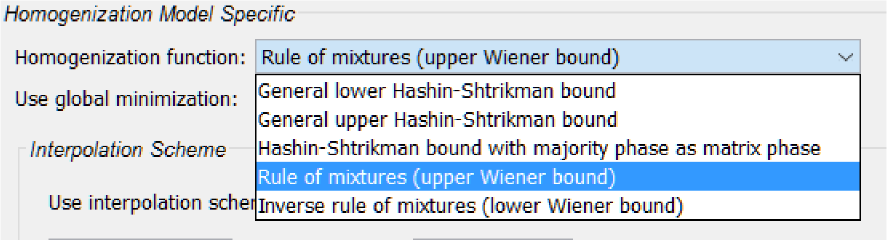
Required accuracy during the solution of the flux balance equations. The default is `1.0E-16`.

Homogenization Model Specific

This section is available when **Homogenization** is selected (or automatically selected) as the **Default solver**. These settings are available on the **Options** tab.

HOMOGENIZATION FUNCTION

Several functions are available. The default is **Rule of mixtures (upper Wiener bound)**. See About the Homogenization Functions.



USE GLOBAL MINIMIZATION

Select the checkbox for global minimization used in equilibrium calculations. In general, using global minimization significantly increases the simulation time, but there is also a significantly reduced risk for non-converged equilibrium calculations.

INTERPOLATION SCHEME

When the homogenization model is used, simulations are run using an implicit finite volume method to increase numerical stability. Because of this, and other factors, homogenization model simulations generally run slower than other comparable simulations. You can reduce simulation time with the **Use Interpolation scheme** checkbox. The checkbox is selected by default.

DISCRETIZATION

[**Logarithmic** or **Linear**] discretization with *[number of]* steps in each dimension.

- For the linear discretization the scheme is not used at node points where the content of one or more solutes fall below a certain critical value. For such cases, where composition span many orders of magnitude, the logarithmic discretization can be tried.
- Enter the number of steps in composition space. In the limit where an infinite number of steps are used, exactly the same solution is obtained as without the interpolation scheme. However, excellent results can be obtained with a reasonable discretization. The default is `10000` steps.

MEMORY TO USE

This is the fraction of free physical memory to be used by the interpolation scheme.

Select **Megabyte** or **Fraction of free** and then enter a value in the field.

About the Homogenization Functions

The geometrical interpretation of the Hashin-Shtrikman bounds are concentric spherical shells of each phase. For the general lower Hashin-Shtrikman bound the outermost shell consists of the phase with the most sluggish kinetics and vice versa for the general upper bound. The geometrical interpretation of the Hashin-Shtrikman bounds suggest further varieties of the bounds, viz. *Hashin-Shtrikman bound with prescribed matrix phase* and *Hashin-Shtrikman bound with majority phase as matrix phase*, where the outermost shell consist of a prescribed phase or the phase with highest local volume fraction, respectively.

The geometrical interpretation of the Wiener bounds are continuous layers of each phase either parallel with (upper bound) or orthogonal to (lower bound) the direction of diffusion.

The labyrinth factor functions (described below) are available in Console Mode and when using TC-Python.

The labyrinth factor functions implies that all diffusion takes place in a single continuous matrix phase. The impeding effect on diffusion by phases dispersed in the matrix phase is taken into account by multiplying the flux with either the volume fraction (*Labyrinth factor f with prescribed matrix phase*), or the volume fraction squared (*Labyrinth factor f**2 with prescribed matrix phase*), of the matrix phase.

The varieties with excluded phases (described below) are available in Console Mode and when using TC-Python.

The varieties with excluded phases are useful in several respects. First, if a phase is modeled as having zero solubility for a component, the mobility of that component in that phase is undefined, which causes a (non-terminal) error. Setting a phase as excluded causes the mobility of all components in that phase to be set to zero. Second, often there are some major matrix solid solution phases and some minor precipitate phases. If the mobilities in the minor precipitate phases are zero the lower Hashin-Shtrikman bound is useless as it produces a kinetic coefficient of zero. However, using *General lower Hashin-Shtrikman bound with excluded phase(s)*the excluded phases are not considered when evaluating what phase has the most sluggish kinetics.

Pause, Resume, and Cancel Diffusion Calculations

Diffusion calculations are often complex simulations that take some time to complete. Sometimes you may want or need to pause or resume a calculation, or make adjustments to your compositions and start again.

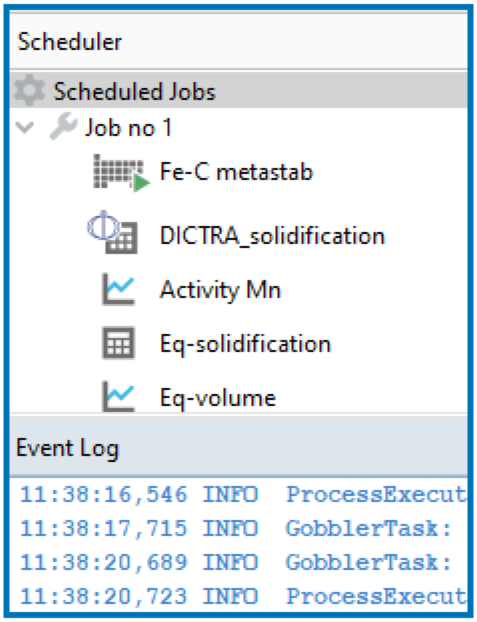
Graphical Mode

In Graphical Mode, you pause and resume when you are on the Diffusion Calculator **Configuration** window. When pausing a Diffusion Calculator calculation, you can make changes to the **Simulation time**, **Left Boundary Condition**, and **Right Boundary Condition**. This is useful, for example, when simulating carburization, where it is common to first have a step with high carbon activity in the furnace for the actual carburization, and then lower it and allow the carbon in the specimen to diffuse without further increased carbon content.

This is also available for the Precipitation Calculator (but not any other calculators). See Pause, Resume, and Cancel Precipitation Calculations.

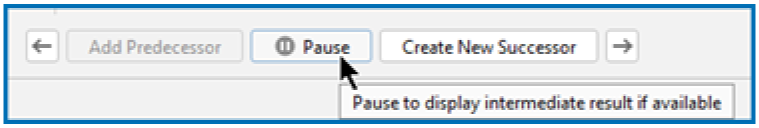
HOW TO PAUSE AND RESUME A JOB

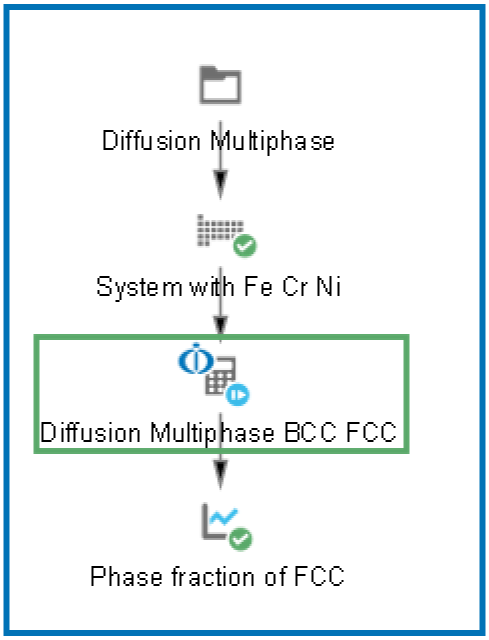
1. Run the job (i.e. click **Perform Tree**). In the **Scheduler** you can see the job listed and in the **Event Log** you can follow the progress of the calculation.



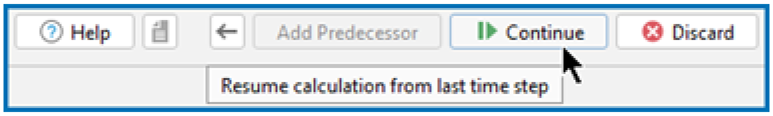
```
11:38:16,546 INFO  ProcessExecut
11:38:17,715 INFO  GobblerTask:
11:38:20,689 INFO  GobblerTask:
11:38:20,723 INFO  ProcessExecut
```

2. In the **Project** window, click the **Diffusion Calculator** node.
3. In the **Configuration** window at the bottom, click **Pause**. Observe that the **Diffusion Calculator** in the **Project** window has a pause indicator. If there are intermediate results available these are listed in the **Event Log**.



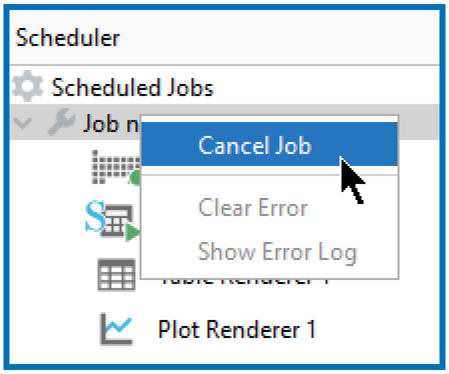


4. As required, make changes to the settings: *Left Boundary Condition*, *Right Boundary Condition*, *Temperature*, and/or *Simulation time*. The rest of the **Configuration** window settings are grayed out and no other editing can be done while paused.
5. When ready, click ▶ **Continue** to resume your calculations from the last time step or click ⊗ **Discard** to discard the calculation (then click **Yes** or **No** on the window that opens).



HOW TO CANCEL A JOB

In the **Scheduler** window, right-click the job you want to cancel and select **Cancel Job**.



Console Mode

In response to a command or a lengthy calculation, Thermo-Calc may display a lot of text in the Console window. Use these keyboard shortcuts to pause, resume, or stop a process.

- To pause the text on printing press <Ctrl+S>.
- To resume the printing on screen, press <Ctrl+Q>.
- When Thermo-Calc is performing a stepping or mapping operation, the results are continuously printed in the Console window. To stop the calculation of the current region of the mapping and stop the output, press <Ctrl-A> (Windows) or <Ctrl-C> (Linux).

Diffusion Calculator Plot Renderer

The following is information about the settings available in both Simplified and Advanced Mode for a Plot Renderer when it is a successor to a **Diffusion Calculator**.

Conditions Tab Settings and Configuration Settings

See Quantities Groups Available for Plots and Tables for a general list of quantities. However, for the Diffusion Calculator Plot Renderer Advanced Mode and Simple Mode plot types, there are no defined groups to choose from.

When you select **Advanced Mode** as the *Plot type*, this expands the variable options available from both the *X* and *Y Axes* lists. Otherwise the axis variables default to the most logical combination.

Simple Mode

When you open the Diffusion Calculator Plot Renderer, it defaults to **Simple Mode**. Use the **Advanced Mode** to have more flexibility.

Use **Simple Mode** to define the most common axis variables. The software automatically sets the correct **Plot condition** and **Independent variable**.

X-AXIS VARIABLE

Select the variable for the *X*-axis: **Distance** or **Time**.

- For **Distance** also choose a unit (**Meter**, **Millimeter**, **Micrometer**, **Nanometer**, or **Ångström**) and what **Region** to include. The list contains the regions defined on the Diffusion Calculator or you can choose **All regions**.
- For **Time** choose a unit (**Seconds**, **Minutes**, **Hours**, or **Days**).

Y-AXIS VARIABLE

Select the variable to plot on the *Y*-axis. The available options are based on choices such as whether **Distance** or **Time** is chosen for the *X*-axis, whether isothermal or non-isothermal is selected, whether there is a homogenization solver, or if there is one or more regions.

DISTANCE ALONG THE X-AXIS

If **Distance** is plotted along the *X*-axis, then by default the **Composition** is plotted along the *Y*-axis.

- From the list in the middle, choose the component to plot, or select **All**.
- From the next list, choose the unit to be **Mass percent**, **Mole percent**, **Mass fraction**, **Mole fraction**, or **u-fraction**.

TIME ALONG THE X-AXIS (ONE REGION)

If **Time** is plotted along the *X*-axis, then choose the *Y*-axis variable to plot plus the additional settings:

- **Total phase fraction**: **By volume** or **By mass**. Then select a phase from the list.
- **Total fraction of component**: **By mole** or **By mass**. Then select a component from the list.
- **Total fraction of component in phase**: **By mole** or **By mass**. Then select a component and a phase from the lists.

DISTANCE ALONG THE X-AXIS (HOMOGENIZATION)

If **Distance** is plotted along the *X*-axis and a homogenization solver is being used, then choose **Composition** or **Phase fraction** to plot on the *Y*-axis. Then select the applicable settings.

- Choose the component to plot, or select **All** and the unit **Mass percent**, **Mole percent**, **Mass fraction**, **Mole fraction**, or **u-fraction**.
- Choose **By mole** or **By mass** then select a component from the list.

TIME ALONG THE X-AXIS (TWO OR MORE REGIONS)

If **Time** is plotted along the *X*-axis, then choose the *Y*-axis variable to plot plus the additional settings:

- **Total phase fraction**: **By volume** or **By mass**. Then select a phase from the list.
- **Total fraction of component**: **By mole** or **By mass**. Then select a component from the list.
- **Total fraction of component in phase**: **By mole** or **By mass**. Then select a component and a phase from the lists.
- **Composition at interface**: **Mass percent**, **Mole percent**, **Mass fraction**, or **Mole fraction**. Then choose a **Region** and whether it is **Upper** or **Lower** and a component.
- **Position of interface**: Choose a unit (**m**, **µm**, or **nm**) and the interface.
- **Velocity of interface**: Choose a unit (**m**, **µm**, or **nm**) and the interface.
- **Width of region**: Choose a unit (**m**, **µm**, or **nm**) and the interface.
- For a **Non-isothermal** profile, **Temperature** is available. Choose a unit **Kelvin**, **Celsius**, or **Fahrenheit**.

AXIS TYPE

Click **Show more**. Select the type of axis scale: **Linear**, **Logarithmic**, **Logarithmic 10**, or **Inverse**.

LIMITS

Click **Show more**. Specify the range along the axis to show in the plot. In the fields, enter the minimum and maximum values of the axis variable. You can also determine the **step** size between the tick marks along each axis.

Select the **Automatic scaling** checkbox to allow the program to set the limits.

ADD AND REMOVE AXES

Use the ⊕ **Add an axis** and ⊖ **Remove this axis** buttons to add additional *X*- and/or *Y*-axes to a plot or to merge plots (to overlay one plot with another in the same diagram).

Advanced Mode

Use **Advanced Mode** to select any combination of axis variables, and then access further settings such as the **Plot condition**, **Region**, and **Independent variable**. Examples of advanced plot options are activity of a component at an interface, diffusivities, and diffusion paths. Also user-defined functions can be used as plot variables where Console Mode syntax is used to define functions. In some cases, sensible default values are selected, but they can be changed according to your needs.

DISTANCE ALONG X-AXIS - ADVANCED TIME SETTING

An alternative **Time** setting is available in **Advanced Mode**.

When the *X*-axis variable is **Distance**, for the Y-axis choose a **Time** unit (**Seconds**, **Minutes**, **Hours**, or **Days**). Enter a numerical value.

PLOT CONDITION AND INDEPENDENT VARIABLE

- If any plot axis variable of the type **Integral** is selected, then the plot condition is set to **Integral** and the independent variable is set to **Time**.
- If a plot axis variable is set to **Time** then the plot condition is set to **Time** and the Independent variable is also set to **Time**.
- If a plot axis variable is set to **Distance** then the plot condition is set to **Distance** or **Interface** and the Independent variable is set to **Distance**.

Plot Condition	*Independent Variable settings based on the Plot Condition*
Time: Choose a unit (**Seconds**, **Minutes**, **Hours**, or **Days**). Enter	The default is **Distance**: Choose a **Global** or **Local** distance. A **Global** distance is counted from the rightmost interface of the system. A **Local** distance is counted

Plot Condition	*Independent Variable settings based on the Plot Condition*
a numerical value.	from the lower interface of the Region selected. You can also choose **Time**, which requires no further settings.
Distance: Choose a specific **Region** from the list or use the default **All regions**.	The default is **Time** and there are no further settings. You can also choose a **Global** or **LocalDistance**. A **Global** distance is counted from the rightmost interface of the system. A **Local** distance is counted from the lower interface of the Region selected.
Interface: From the lists choose a **Region**and whether it is the **Upper** or **Lower** region.	The default is **Distance**: Choose a **Global** or **Local** distance. A **Global** distance is counted from the rightmost interface of the system. A **Local** distance is counted from the lower interface of the Region selected. You can also choose **Time**, which requires no further settings.
Integral	The default is **Time** and there are no further settings. You can also choose a **Global** or **LocalDistance**. A **Global** distance is counted from the rightmost interface of the system. A **Local** distance is counted from the lower interface of the Region selected.

Precipitation Calculator

The Precipitation Calculator is available with three elements if you do not have the additional Precipitation Module (TC-PRISMA) license. With the Add-on Module you can use all available elements. See Available Options for details about this and other options available with additional licenses.

A **Precipitation Calculator** allows you to set the conditions for, and perform, a precipitation calculation. You can add the calculator to the System Definer directly (right-click and select it from the **Create New Successor** menu)

There is also a **Precipitation** template available under **Non-Equilibrium** that you can use to quickly set up a simulation. See Getting Started Links and Templates.

Once you have added a Precipitation Calculator, the **Configuration** window has **Conditions** and **Options** settings tabs where there are many available conditions to set and then continue the settings with the specialized **Plot Renderer**.

Conditions

Set the conditions for your calculation that define the *Matrix phase* and *Precipitate phase*. Choose the *Calculation Type*.

- Matrix Phase Settings
- Precipitate Phase Settings
- Calculation Type Settings

Options

Modify *Numerical Parameters* that determine how the conditions are calculated.

- Options Tab

Plot Renderer

There are also unique settings available for this calculator once you add a Precipitation Calculator Plot Renderer.

Working with these simulations is an advanced topic. It is recommended you review the documentation and videos available or search for a specific topic.

Precipitation Module (TC-PRISMA) Examples Collection

Available Options

The Precipitation Module, previously referred to as TC-PRISMA, is an Add-on Module to the core Thermo-Calc software.

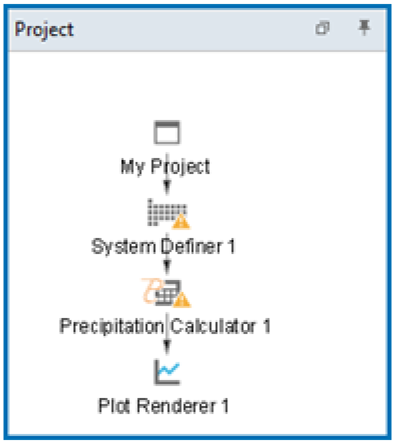
A separate license is required to perform calculations for more than three elements. Without it you are able to use the module in *Demo Mode*.

Precipitation Template

A **Precipitation** template under **Non-Equilibrium Calculations** is available to all Thermo-Calc users when in Graphical Mode. If you are in DEMO mode then this is indicated by the addition of **DEMO** text.

USING THE TEMPLATE

After opening Thermo-Calc in Graphical Mode, in the templates section under **Non-Equilibrium**, click the **Precipitation** button to add a *System Definer*, *Precipitation Calculator*, and *Plot Renderer* to the **Project** tree.



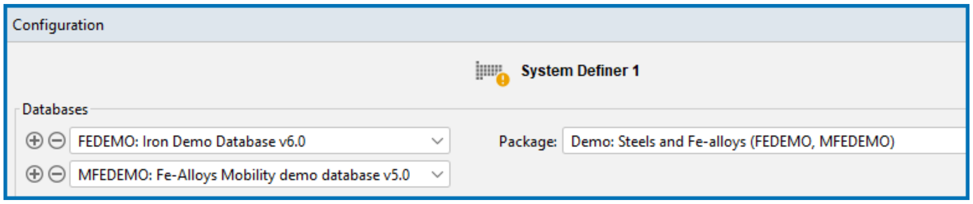
Creating a Project from a Template

Precipitation Calculator

A Precipitation Calculator allows you to set the conditions for, and perform, a precipitation calculation.

Demo Database Packages for the Examples Collection

Both a thermodynamic and mobility database are required to run the Precipitation Module simulation. If you have a Precipitation Module (TC-PRISMA) license you can run all the examples as the demonstration database packages are included with your installation. Select the database packages from the **System Definer** → **Configuration** window to run a simulation.



Databases

FEDEMO: Iron Demo Database v6.0

MFEDEMO: Fe-Alloys Mobility demo database v5.0

Package: Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)

Demonstration (Demo) Mode

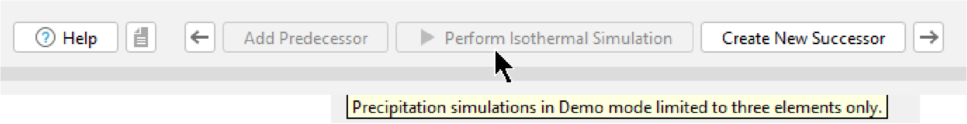
The Precipitation Module, and some examples, are available to all Thermo-Calc users but only for simulations of alloys with up to three elements. If you do not have a license for the Precipitation Module then you are in *Demonstration Mode* when using the Precipitation Calculator or Precipitation Simulation template.

A **Precipitation** template under **Non-Equilibrium Calculations** is available to all Thermo-Calc users when in Graphical Mode. If you are in DEMO mode then this is indicated by the addition of **DEMO** text.

PRECIPITATION CALCULATOR

If you are experimenting with the Precipitation Calculator in Demo Mode, you may have access to a variety of databases based on your license. However, you can only define up to three elements for a demo simulation.

If you define more than three elements on the System Definer, when you go to the Precipitation Calculator, the **Perform** button is unavailable and the tooltip explains why. In this case one of the chosen elements needs to be removed and then the Perform button is made available.



Precipitation simulations in Demo mode limited to three elements only.

> Even if you have more than three elements, the Plot Renderer or Table Renderer **Perform** button is still available. However, if you click the button and try to run the simulation the Event Log displays an error message.

Additive Manufacturing (AM) Module

There is connectivity between the Diffusion Module (DICTRA) or the Precipitation Module (TC-PRISMA) and the Additive Manufacturing (AM) Module when you have full licenses available for all relevant Add-on Modules and databases.

You can add a Diffusion Calculator or Precipitation Calculator as a successor to the AM Calculator and then when probes are included with the AM Calculator this data can be further used with the thermal profile.

Details are in the AM Module documentation. See AM Calculator: Working with Probe Data.

Define the Precipitation Calculator

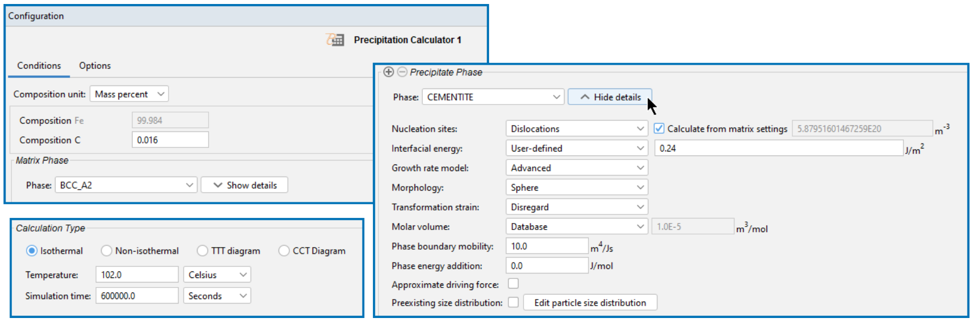
1. Add a **Precipitation Calculator** node to the System Definer. If you used the **Precipitation** template (on the **My Projects Configuration** window under **Non-Equilibrium**), click the node to display the **Configuration** settings window.

2. In the Precipitation Calculator **Configuration** window, enter the settings on the **Conditions** and **Options** tabs. These are described separately:
    - Matrix Phase
    - Precipitate Phase
    - Calculation Type and Precipitation Calculator Thermal Profile
    - Options Tab Advanced Settings
3. Once you have finished defining the Precipitation Calculator, you also choose settings on the **Plot Renderer**. Some additional settings are specific to the Precipitation Calculator Plot Renderer.

Matrix Phase Settings

Below are details about the settings available for the *Composition* and *Matrix Phase*, which is selected from the **Conditions** tab on the calculator **Configuration** window.

There are additional **Conditions** tab settings described for the Precipitate Phase and Calculation Type.



Composition unit: Mass percent

Composition Fe: 99.984

Composition C: 0.016

Matrix Phase

Phase: BCC_A2

Calculation Type

● Isothermal ○ Non-isothermal ○ TTT diagram ○ CCT Diagram

Temperature: 102.0 Celsius

Simulation time: 600000.0 Seconds

Precipitate Phase

Phase: CEMENTITE

Nucleation sites: Dislocations ☑ Calculate from matrix settings 5.87951601467259E20 m^{-3}

Interfacial energy: User-defined 0.24 J/m^2

Growth rate model: Advanced

Morphology: Sphere

Transformation strain: Disregard

Molar volume: Database 1.0E-5 m^3/mol

Phase boundary mobility: 10.0 m^4/Js

Phase energy addition: 0.0 J/mol

Approximate driving force: ☐

Preexisting size distribution: ☐

There are three distinct settings areas for the Configuration window for example P_04_Precipitation_Fe-C_Cemetite. In this case, Show Details is expanded to show the Precipitate Phase settings.

You can change these settings locally for a specific Calculator or globally for some defaults in the **Options** *window* (a different location than the tab).

To open the **Options** window:

- Windows: Select **Tools** → **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

then click the **Graphical Mode** tab and the **Precipitation** node in the tree.

SHOW OR HIDE DETAILS

Click **Show Details** to view some of the additional settings listed below. You can also set the default to display in **Phase view mode** on the **Options** window then click the **Graphical Mode** tab and the **Precipitation** node in the tree. Click **Hide Details** to hide the information.

Composition Settings

COMPOSITION UNIT

Select the **Composition unit**: **Mass percent**, **Mole percent**, **Mass fraction**, or **Mole fraction**.

Matrix Phase Settings

Selecting the Disordered Phase as a Matrix Phase

PHASE

> Only phases with kinetic data can be selected as the matrix phase. If the list is empty, go to the System Definer to confirm that both thermodynamic and kinetic databases are selected and defined.

Choose a **Phase** from the list. The list is based on the settings for the System Definer. When setting up a system, choose a matrix phase with kinetic data available in the database.

ELASTIC PROPERTIES

Choose **Disregard** to ignore the elastic properties.

Default elastic constants for **Isotropic** or **Cubic** are based on the major element of the alloy system. The elastic properties can affect nucleation rate, nuclei size, and particle shape.

- For **Isotropic**, enter values for **Shear modulus** (in GPa) and **Poisson's ratio** as required.
- For **Cubic**, enter values for **c11**, **c12**, and **c44** as required. c_{11}, c_{12}, c_{44} are the elastic constants.

MOLAR VOLUME

Use the **Database** value (if the molar volume for the phase is defined in the thermodynamic database) or select **User-defined** to enter another value in m^3/mol.

If you select the **Grain growth** checkbox, see the separate Grain Growth Settings section for details.

GRAIN SIZE

If the **Grain growth** checkbox is NOT selected then this version of the **Grain size** section is available in order for the **Average diameter** of the grain size to be entered.

Grain size is the "diameter" of a grain. The **Grain size** value changes the available nucleation sites when **Grain boundaries**, **Grain edges**, or **Grain corners** is selected along with **Calculate from matrix settings** in the *Precipitate Phase*. Enter a numerical value and choose a unit from the list. The default is `1.0E-4` m.

GRAIN ASPECT RATIO

For an elongated grain with a minor axis and a major axis, one may use the minor axis as grain size and the major/minor ratio as the grain aspect ratio to characterize the grain. The **Grain aspect ratio** value also changes the available nucleation sites when **Grain boundaries**, **Grain edges**, or **Grain corners** is selected along with **Calculate from matrix settings** in the *Precipitate Phase*. Enter a numerical value. The default is 1.0.

If the **Grain growth** checkbox is selected, the aspect ratio is fixed at 1.0 and can not be changed. See Grain Growth Settings.

DISLOCATION DENSITY

The **Dislocation density** value changes the available nucleation sites when **Dislocations** is selected along with **Calculate from matrix settings** in the *Precipitate Phase*. Enter a numerical value. The default is 5.0E12 m^{-2}.

MOBILITY ADJUSTMENT

The **Mobility adjustment** parameters modify the atomic mobility data from a database.

Choose **Same for all elements**, which applies the adjustment to all elements, or **Per element** to adjust to each individual element. Then for the following settings, enter one set of values for **Same for all elements**, or individually for **Per element**.

- **Prefactor** (unitless) is a parameter that multiplies to the mobility data from a database. This value scales the mobility by a constant amount. This can be useful, for example, when the material has a higher than normal vacancy concentration at the start of the precipitation simulation. (e.g. from a prior solutionizing and quenching treatment).
- The **Activation energy** (J/mol) is a value that adds to the activation energy of mobility data from a database. This value scales the mobility by a temperature-dependent amount. Similar usage as the **Mobility adjustment >Prefactor** setting.

Grain Growth Settings

GRAIN GROWTH

Select the **Grain growth** checkbox to use this to calculate the temporal evolution of grain size distribution (GSD). The grains are assumed of spherical morphology when modeling the growth rates. Nucleation is not considered, thus an initial GSD is necessary to start the simulation.

After selecting the checkbox, there are additional settings made available as described in this section.

> This checkbox is not available when a **TTT diagram** or **CCT diagram** *Calculation Type* is selected.

GRAIN SIZE >> GRAIN SIZE DISTRIBUTION

When the **Grain growth** checkbox is selected, then this version of the **Grain size** settings section is available. This is where you access the grain *Size distribution* settings.

Click **Edit grain size distribution** to open the *Size distribution* settings window. In this window, you can edit the parameters and generate a graph comparing the radius and number density for initial grains.

Select a **Length unit**: **Meter**, **Micrometer**, **Nanometer**, or **Ångström**.

Select a **Distribution**: **Normal**, **Log normal**, or **From file**.

- If **Normal** or **Log normal** is selected, enter values for **Mean radius** and **Std** (standard deviation). The default Std is different for each choice.
- If **Hillert** is selected, enter a value for the **Mean radius**.
- If **From file** is selected, click **Import** and navigate to the file containing the required information and click **Open**. This file can be in .xls, .xlsx, .csv or .txt formats. The file should consist of two columns with values where the first column contains **radius** data and the second contains **number density** data.

A similar setup can also be found in the Particle Size Distribution (PSD).

Once the size distribution is defined, click **Generate** to view or update the graph comparing the radius and number density for initial grains.

GRAIN BOUNDARY ENERGY

This setting is available when the **Grain growth** checkbox is selected.

Enter a value for the **Grain boundary energy**. The default is 0.5 J/m^2.

GRAIN BOUNDARY MOBILITY

This setting is available when the **Grain growth** checkbox is selected.

The **Prefactor** (m^4/Js) is a parameter that represents the magnitude of the grain boundary motion.

The **Activation energy** (J/mol) is a parameter that describes the temperature dependence of the grain boundary mobility.

ZENER PINNING

This setting is available when the **Grain growth** checkbox is selected.

Select the **Zenner pinning** checkbox to consider the effect of precipitates on inhibiting normal grain growth. When this checkbox is selected, there are additional settings available in the **Precipitate Phase** section.

P_14: Grain Growth and the Zener Pinning Effect

Selecting the Disordered Phase as a Matrix Phase

The following information is about using disordered FCC as a matrix phase with the following thermodynamic and mobility database packages:

- TCCU and MOBCU (Cu-based alloys)
- TCNI and MOBNI (Ni-based alloys)

In the TCNI/MOBNI and TCCU/MOBCU packages, the well-known order/disorder two-sublattice model is used to describe the Gibbs energy of both FCC_A1 and FCC_L12. With this treatment, FCC_L12 is becoming FCC_A1 if the site fractions of each element on both sublattices are identical, which means that FCC_A1 is only a special case of FCC_L12. Therefore, FCC_A1 is not shown in the phase list on the *Phases and Phase Constitution* tab on the System Definer activity and in subsequent equilibrium calculation results. Instead it is shown only as FCC_L12. The real ordered FCC_L12 is shown as FCC_L12#2.

In precipitation simulations, the matrix phase is quite often the disordered FCC phase. You can directly select FCC_L12 as the matrix phase and run a simulation. However, the speed is not optimal due to the sophisticated model used for both Gibbs energy and atomic mobilities. A better and more convenient way is to deselect FCC_L12 and FCC_L12#2 from the phase list on the *Phases and Phase Constitution* tab on the **System Definer** if the ordered phase is irrelevant in the alloy under investigation, such as in most Cu alloys. Once these are unchecked (i.e. not selected), the FCC_A1 phase is available and can later be selected as the matrix phase.

For Ni-based superalloys using the TCNI/MOBNI package, the ordered FCC_L12#2 (gamma prime) has to be included as the precipitate phase in most of calculations. In this case, you can select DIS_FCC_A1 from the phase list on the *Phases and Phase Constitution* tab and then select it as the matrix phase in the **Precipitation Calculator**.

Precipitate Phase Settings

Below are details about the settings for the *Precipitate Phase*, which is selected from the **Conditions** tab on the Precipitation Calculator **Configuration** window.

There are additional **Conditions** tab settings described for the Matrix Phase and Calculation Type.

To open the **Options** window:

- Windows: Select **Tools** → **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

then click the **Graphical Mode** tab and the **Precipitation** node in the tree.

SHOW OR HIDE DETAILS

Click **Show Details** to view some of the additional settings listed below. You can also set the default to display in **Phase view mode** on the **Options** window then click the **Graphical Mode** tab and the **Precipitation** node in the tree. Click **Hide Details** to hide the information.

PHASE

The phases available to choose have both thermodynamic and kinetic data. If the list is empty, go to the System Definer to confirm that both types of databases are selected and defined.

Choose a **Phase** from the list. The list is based on the System Definer settings.

NUCLEATION SITES

The number of different nucleation sites is dependent on the shape and size of grains in the matrix. Grain size is the "diameter" of a grain. Choose one of the following from the list.

- **Bulk**, **Grain boundaries**, **Grain edges**, **Grain corners**, or **Dislocations**.
- For **Grain boundaries**, **Grain edges**, and **Grain corners**, enter the **Wetting angle (0-90)** in addition to the matrix settings. **Wetting angle** defines the deviation from spherical shape (or dihedral angle).

Click to select the **Calculate from matrix settings** checkbox to calculate the initial number density of sites from the matrix grain size or dislocation density.

To enter a specific value for the number of **Nucleation sites**, click to clear the checkbox.

INTERFACIAL ENERGY

Choose **Calculated** to use the estimated value. To adjust the estimate, enter a different **prefactor** or choose **User-defined** to enter a value in J/m^2. For the User-defined option, you can also enter it as a function of radius (r) and temperature (T).

GROWTH RATE MODEL

Select **Simplified**, **General**, **Advanced**, **Para-eq**, **NPLE**, or **PE Automatic** (where Para-eq and PE are both abbreviations for *paraequilibrium*).

All models treat a particle (precipitate) of stoichiometric composition or with negligible atomic diffusivity. Except for the **PE Automatic** model, local equilibrium or paraequilibrium at the precipitate-matrix interface is assumed. The **PE Automatic** model enables smooth transition from paraequilibrium to local equilibrium.

In the documentation and on the GUI, the abbreviations *Para-eq* and *PE* are both used for paraequilibrium. There is also the use of OE as an abbreviation for *ortho-equilibrium* and LE for *local equilibrium*.

MORPHOLOGY

Choose the particle shape: **Sphere** (default), **Cuboid**, **Plate**, or **Needle**. Options are based on the **Elastic properties** selected for the **Matrix** phase:

- For a **Cubic** elastic property, **Sphere**, **Plate**, **Needle**, and **Cuboid** are available.
- For an **Isotropic**elastic property, **Sphere**, **Plate** and **Needle** are available.

For **Plate** or **Needle**, select the **Calculate aspect ratio from elastic energy** checkbox or enter a numerical value in the **Aspect ratio** field to provide a constant aspect ratio.

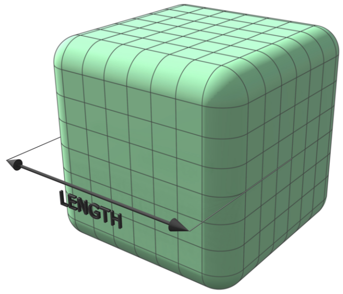


Figure 6: The cuboid shape is described by a supersphere. Cuboids have six faces, which form a convex polyhedron.

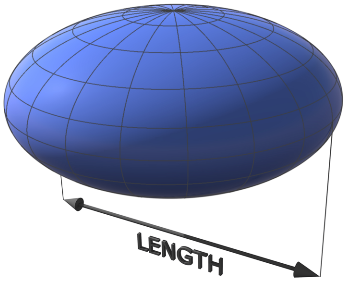


Figure 7: The plate is described as oblate spheroid. Oblate spheroids have rotational symmetry around an axis from pole to pole.

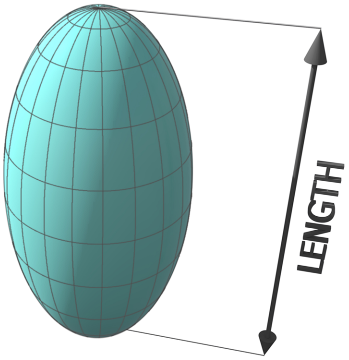


Figure 8: The needle shape is described as prolate spheroid. A prolate spheroid is a surface of revolution obtained by rotating an ellipse about its major axis.

TRANSFORMATION STRAIN

Choose **Disregard** to ignore the transformation strain. When **Isotropic** or **Cubic** is chosen in **Elastic properties** in Matrix Phase, you can also choose **Calculated from molar volume** to obtain a purely dilatational strain. If **Plate** or **Needle** is selected as the **Morphology**, you can alternatively choose **User-defined** and enter the properties for **ε11**, **ε12**, **ε13**, **ε22**, **ε23**, and **ε33**.

MOLAR VOLUME

Use the **Database** value (if the phase molar volume is defined in the thermodynamic database) or select **User-defined** to enter another value.

ZENER PINNING PARAMETERS

These parameters are available when the **Zener pinning** checkbox is selected under the **Matrix Phase** settings. These settings are to consider the effect of precipitates on inhibiting normal grain growth.

- **Cutoff size**: Precipitates with radius smaller than this value are neglected in pinning force calculation. Default value : 7 x 10^{-7} m.
- **Kinetic prefactor**: Dimensionless kinetic coefficient in Zener equation. Default value: 0.5.
- **Exponent**: Exponent of precipitate volume fraction in Zener equation. Default value: 0.93.

P_14: Grain Growth and the Zener Pinning Effect

PHASE BOUNDARY MOBILITY

A parameter that accounts for interface-controlled growth. Only effective if a very small, positive value is used. Use with caution due to a tentative treatment.

TRANS-INTERFACE MOBILITY ADJUSTMENT

This setting is available when **PE Automatic Growth rate model** is selected.

The **Trans-Interface mobility adjustment** parameters modify the atomic mobility data from a database.

Choose **Same for all elements**, which applies the adjustment to all elements, or **Per element** to adjust to each individual element.

> The transition kinetics from Para-Equilibrium (PE) to Ortho-Equilibrium (OE) is controlled by the ratio of atomic mobility of substitutional elements to that of interstitial elements. This implies that the option of **Same for all elements**—while useful to the case that the atomic mobility data for all elements are needed to be scaled with the same factor to match experimental trans-interface mobility data—does not change the PE-OE transition kinetics. Therefore, the change of transition kinetics separately requires adjustment of individual elements, which is when the **Per element** setting is useful.

Then for the following settings, enter one set of values for **Same for all elements**, or individually for **Per element**:

- **Prefactor** (unitless) is a parameter that multiplies to the mobility data from a database. This value scales the mobility by a constant amount. This results in the trans-interface mobility that controls the kinetics of Para-Equilibrium (PE) to Ortho-Equilibrium (OE) transition.
- The **Activation energy** (J/mol) is a value that adds to the activation energy of mobility data from a database. This value scales the mobility by a temperature-dependent amount. Similar usage as the **Trans-Interface mobility adjustment >Prefactor** setting.

PHASE ENERGY ADDITION

An energy value that adds to the Gibbs free energy of the precipitate phase from a database.

APPROXIMATE DRIVING FORCE

Select the checkbox to include this if simulations with several compositions sets of the same phase create problems.

PREEXISTING SIZE DISTRIBUTION

Select the checkbox to include this. Click **Edit particle size distribution** to open the **Preexisting Particle Size Distribution** window where you can edit the parameters and view a graph comparing the radius and number density for the selected component.

Press F1 and search for "Particle Size Distribution (PSD)" for detailed instructions.

Precipitation Calculator Thermal Profile

The **Thermal Profile** is set up on the **Configuration** window for a **Precipitation Calculator**. The isothermal or non-isothermal profile is viewed in the **Visualizations** window. Choose **Isothermal** to do a simulation at constant temperature. Choose **Non-isothermal** to enter or import data for a user-defined temperature profile.

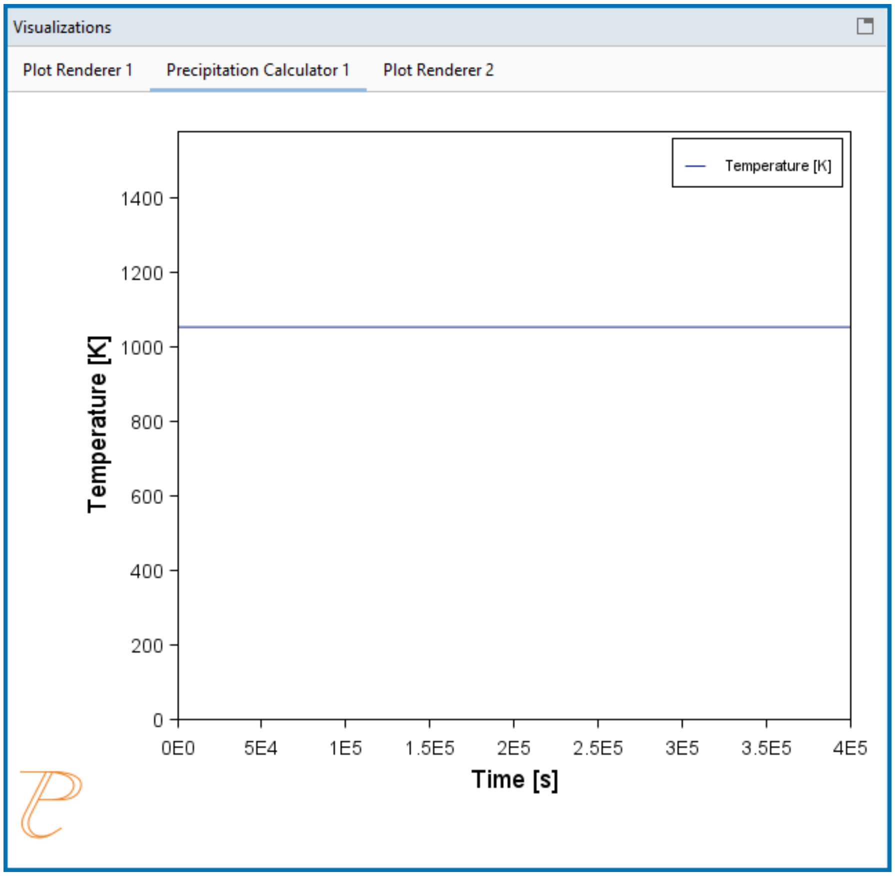
When connected to an AM Calculator (see Including Probe Data from an AM Calculator) the **Isothermal** and **Non-isothermal** options are not visible as it is not relevant to that view.

Isothermal Calculations

Many of the Graphical Mode examples for this Add-on Module are isothermal calculations, e.g. *P_02_Precipitation_Fe-C-Cr_Cementite-M7C3-M23C6*.

1. On the Precipitation Calculator **Configuration** window, first enter the required *Matrix Phase* and *Precipitate Phase* settings.
2. Under **Calculation Type**, click to choose **Isothermal** to do a simulation at constant temperature.
3. Enter a **Temperature** and choose a unit (**Kelvin**, **Celsius**, or **Fahrenheit**).
4. Enter an **End time** and choose a unit: **Seconds**, **Minutes**, **Hours**, or **Days**. The *Simulation time* is displayed as text.

   The profile is displayed on the **Precipitation Calculator** tab in the **Visualizations** window showing the constant temperature entered.



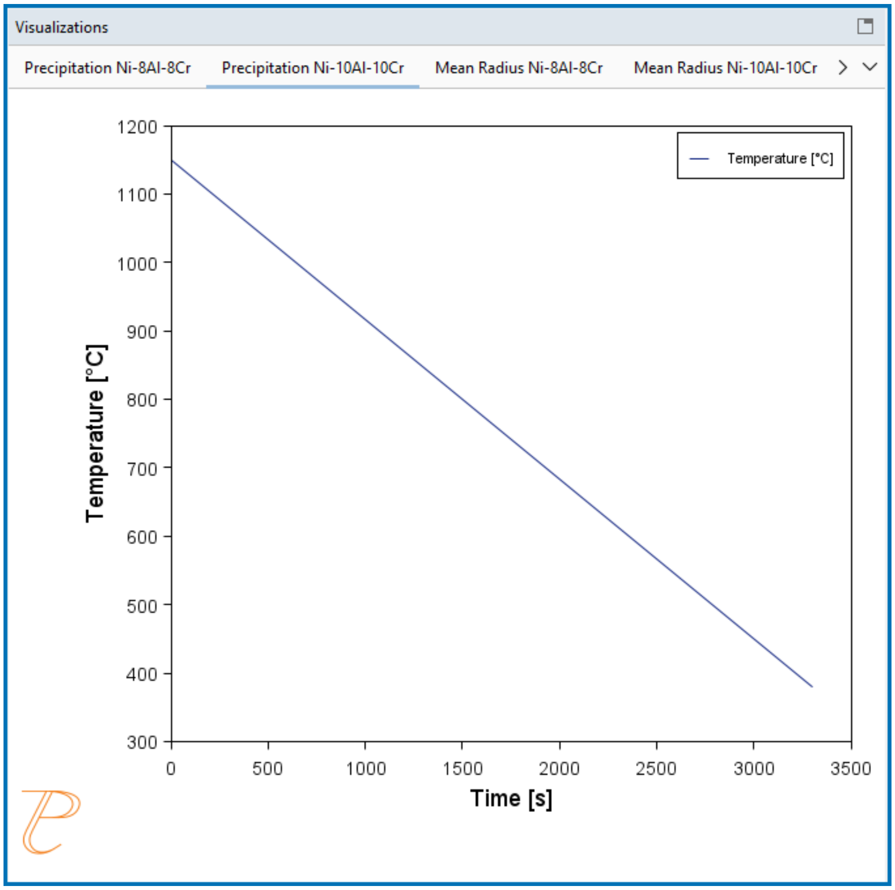
5. For this calculation type this completes the settings you need to enter for the Thermal Profile.

Non-isothermal Calculations

1. On the Precipitation Calculator **Configuration** window, first enter the required *Matrix Phase* and *Precipitate Phase* settings.
2. Under **Calculation Type**, click to choose **Non-isothermal** to enter or import data for a user-defined temperature profile.
3. Select a **Temperature unit**: **Kelvin**, **Celsius**, or **Fahrenheit**.
4. Enter an **End time** and choose a unit: **Seconds**, **Minutes**, **Hours**, or **Days**. The *Simulation time* is displayed as text.

   You can next either directly enter **Time** and **Temperature** coordinates into the table or import the information from a file. A minimum of two points is required.

5. To enter directly into the table:
    a. Click in each cell under the applicable columns, **Time** and **Temperature** then directly enter the values in the table.
    b. Press `<Enter>` to add rows and use the scroll bars to navigate the table.
6. To import a data file:
    a. Although it is a simple set of data, prepare the data file as in Guidelines for Importing Data Files to Thermal Profiles.
    b. When the data file is ready, to the right of the **Import from file** field, click the file 📁 button.
    c. Navigate to a data file such as an MS Excel spreadsheet (with ***.xls** or ***.xlsx** extensions) or a ***.csv** file. You can also use other programs (e.g. Google Sheets) to enter data and export to a CSV format that can be read by the software. Click **Open** to import the data to the **Configuration** window table.
    d. If there are issues with the above import, experiment with choosing the delimiter type that corresponds to the data in the file: **Comma** (`,`), **Colon** (`:`), **Equals sign** (`=`), **Semicolon** (`;`), or **Tab**. Click the **Reload** button 🔄. The data is imported to the **Configuration** window table.
7. For this calculation type this completes the settings you need to enter for the profile, which is displayed on the **Precipitation Calculator** tab in the **Visualizations** window. Make adjustments to the settings as needed and watch it dynamically change in the window.



This is from the non-isothermal calculation example, *P_06_Precipitation_ Ni-Al-Cr_Non-isothermal_Gamma-Gamma_prime*.

Including Probe Data from an AM Calculator

When you also have a license for the Additive Manufacturing (AM) Module you can include probe data from the AM Calculator in the set up of the thermal profile.

There is connectivity between the Diffusion Module (DICTRA) or the Precipitation Module (TC-PRISMA) and the Additive Manufacturing (AM) Module when you have full licenses available for all relevant Add-on Modules and databases.

You can add a Diffusion Calculator or Precipitation Calculator as a successor to the AM Calculator and then when probes are included with the AM Calculator this data can be further used with the thermal profile.

Details are in the AM Module documentation. See AM Calculator: Working with Probe Data.

Guidelines for Importing Data Files to Thermal Profiles

The **Thermal Profile** settings are done on the **Configuration** window for a Precipitation Calculator. The profile is then previewed in the **Visualizations** window.

You can import data from a file. There are specific guidelines needed to correctly prepare the data in this file to ensure it imports without errors.

Data File Requirements

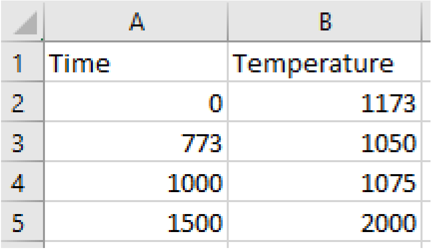
For a Thermal Profile you can either directly enter **Time** and **Temperature** coordinates into the table on the **Configuration** window, or import the data from a file. A minimum of two points is required.

Although there are only two columns to define, it is still important to ensure the file is set up correctly. In order for the data to be included in the calculation, the column and row definitions in the file must adhere to certain rules of entry.

GENERAL RULES

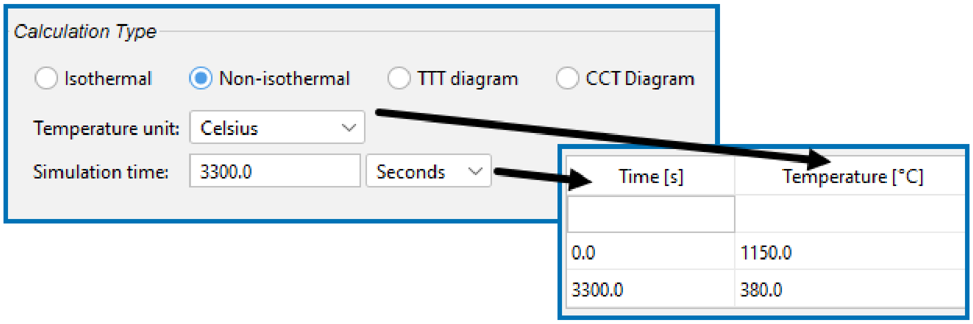
- No abbreviations are allowed in the header.
- A header is not actually required in this file but in order to know which column is which, it is recommended to include it.
- All header text must be in English, i.e. no translations into other languages will be read correctly by the data file.

> Only the columns described here are read / used in the calculation. It is important to enter the information exactly as described. It is recommended that the data file is cleaned up before importing / loading it and performing calculations.



	A	B
1	Time	Temperature
2	0	1173
3	773	1050
4	1000	1075
5	1500	2000

Figure 9: This is an example of data entered into an Excel spreadsheet (which is then converted to csv format). Columns A and B show the data entered to create the Thermal Profile.



Calculation Type

○ Isothermal ● Non-isothermal ○ TTT diagram ○ CCT Diagram

Temperature unit: Celsius

Simulation time: 3300.0 Seconds

Time [s]	Temperature [°C]
0.0	1150.0
3300.0	380.0

Figure 10: The units shown on the Configuration window for the Time and Temperature correspond to settings that can ONLY be selected on the Configuration window. The data file does not contain any information about the units.

Column Heading Requirements and Options	***Row Cell Requirements and Options***
Time This is column A as in Figure 9 Enter the text `Time`. No abbreviations allowed but it is not case sensitive. It is also not required but recommended to include so you know which column of data it applies to.	Valid format and entries for each row in this column: • Any numerical input for the time that corresponds to the unit selected on the Configuration window e.g. `0.0`, `773`, `1000`, `1500`, are times in seconds, which is the unit chosen in the example shown in Figure 10.
Temperature This is column B as in Figure 9 Enter the text `Temperature`. No abbreviations allowed but it is not case sensitive. It is also not required but recommended to include so you know which column of data it applies to.	Valid format and entries for each row in these columns: • Any numerical input for the temperature that corresponds to the unit selected on the Configuration window e.g. `1173`, `1050`, `1075`, are temperatures in Celsius, which is the unit chosen in the example shown in Figure 10

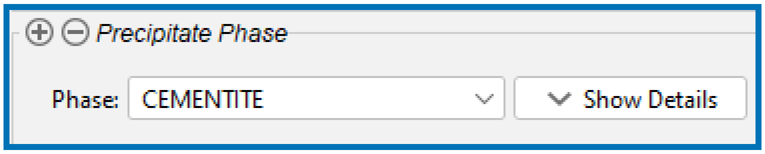
Particle Size Distribution (PSD)

P_10: Initial Particle Size Distribution of Fe-Cr-C

On the Precipitation Calculator you can set the pre-exisiting particle size distribution (PSD) parameters in the **Show Details** section. The size distribution can be generated from a probability distribution function, by importing a file, calibrating a probability distribution function to experimental data, or by manually entering information into a table. Uni-modal distributions can be created within the Graphical Mode interface. Pre-existing multimodal distributions can be loaded from a file.

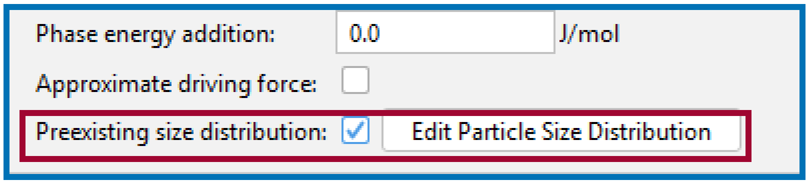
Accessing the 'Preexisting Size Distribution' Settings

1. To the right of the *Precipitate Phase* settings fields, click **Show Details**.



Phase: CEMENTITE

2. At the bottom of the *Precipitate Phase* section, click to select the **Preexisting size distribution** checkbox. Then click **Edit Particle Size Distribution**.

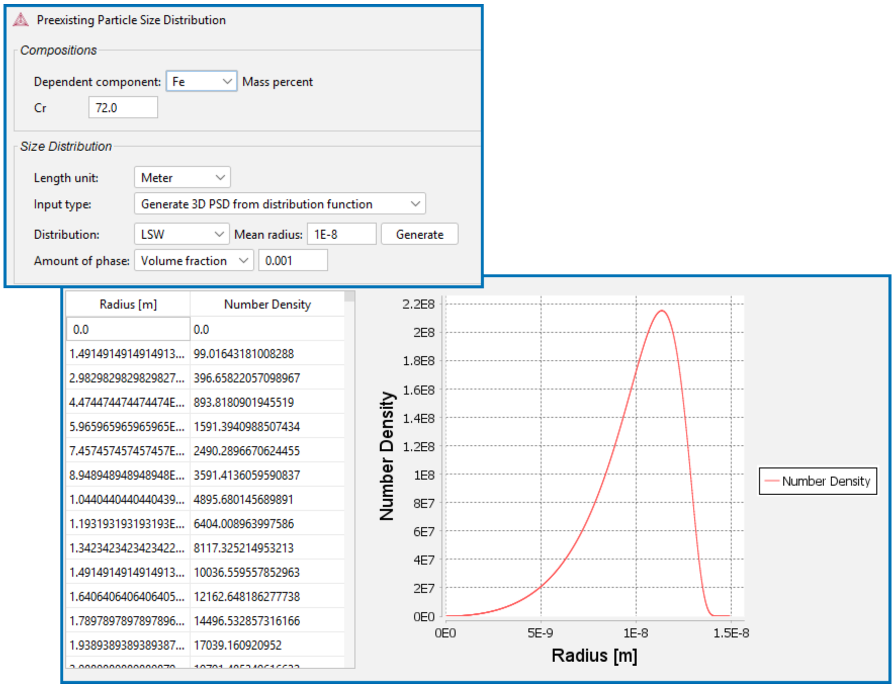


Phase energy addition: 0.0 J/mol

Approximate driving force: ☐

Preexisting size distribution: ☑

3. The **Preexisting Particle Size Distribution** window opens as shown for example P_10 CEMENTITE phase.



Dependent component: Fe Mass percent

Cr 72.0

Length unit: Meter

Input type: Generate 3D PSD from distribution function

Distribution: LSW Mean radius: 1E-8

Amount of phase: Volume fraction 0.001

Radius [m]	Number Density
0.0	0.0
1.4914914914914913...	99.01643181008288
2.9829829829829827...	396.65822057098967
4.474474474474474E...	893.8180901945519
5.965965965965965E...	1591.3940988507434
7.457457457457457E...	2490.2896670624455
8.948948948948948E...	3591.4136059590837
1.0440440440440439...	4895.680145689891
1.193193193193193E...	6404.008963997586
1.3423423423423422...	8117.325214953213
1.4914914914914913...	10036.559557852963
1.6406406406406405...	12162.648186277738
1.7897897897897896...	14496.532857316166
1.9389389389389387...	17039.160920952

Defining the Preexisting Size Distribution

Compositions

Choose a **Dependent component** from the list and enter the composition for the other component.

Length Unit

Choose a **Length unit**: **Meter**, **Micrometer**, **Nanometer**, or **Ångström**.

Amount of Phase

For all options, choose an **Amount of phase**: **Volume percent** or **Volume fraction** and then enter a number in the field.

Input Type

Choose an **Input type**: **Generate 3D PSD from distribution function**, **From File**, or **Approximate the 3D PSD from experimental data**. See the following sections for the details about each setting.

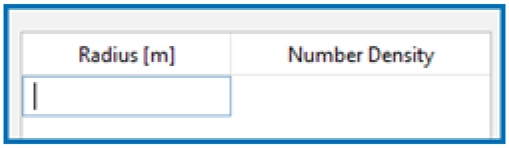
Generate 3D PSD from Distribution Function

This option allows the generation of the size distribution from a list of probability distribution functions. The **Distribution** types include **LSW**, **Normal**, **Log normal**, and **Weibull**.

- **Mean radius** The mean particle radius.
- **Sigma** The standard deviation for the chosen length unit.
- **Alpha** A dimensionless shape factor that should vary between 1.5 and 10.
- **Fraction offset** The fraction offset applied to the mean radius to shift the start of the distribution. This must be greater than or equal to zero, and less than 0.95.

Once the **Distribution** is defined, click **Generate** to create the size distribution.

You can also click in the table to manually enter numbers into the cells rather than use one of the provided probability distribution functions. The radius values must monotonically increase in size.



Radius [m]	Number Density

From File

This option lets you load the initial size distribution from a file. Click **Import** and navigate to the file containing the required information and click **Open**. This file can be in .xls, .xlsx, .csv, or .txt formats. The file should consist of two columns with values where the first column contains **radius** data and the second contains **number density** data.

The example `P_10` (available from the **Example files** → **Precipitation Module - TC-PRISMA**folder) shows this for the precipitate phase M23C6. There is also a file in this folder called `P_10_Precipitation_Initial_PSD_FeCrC_psd_3D_M23C6.csv` that is an example of a correctly formatted text file.

The imported size distribution is normalized into a probability distribution function by ensuring that the zeroth moment is unity. If you wish to import a histogram that has un-even bin spacing, it is necessary to convert the Y-axis counts of the histogram to a count density first to avoid changes to the shape of the distribution. The count density is obtained simply by dividing the count of a bin by the bin's width.

Approximate the 3D PSD from Experimental Data

The **Approximate the 3D PSD from experimental dataInput type** allows you to calibrate a continuous probability distribution function to an experimentally measured size distribution, and account for stereological considerations. There are additional settings related to this.

DIMENSIONALITY OF EXP. DATA AND IMPORT EXP. DATA

The **Dimensionality of exp. data** setting must be defined.

- For precipitate radius measurements that are a good approximation of the 3D size of the particles, select **3D**. Measurements from quantitative image analysis of Transmission Electron Micrographs (TEM) provide **3D** size data, however the precipitates can still be truncated within the TEM sample foil thickness.

- **2D** data is obtained from a cross section taken through the microstructure. Examples include micrographs taken from Scanning Electron Microscopy (SEM), and Optical Microscopy (OM). The radius measurements are obtained from calculating the equivalent radius of a circle from the areas of identified objects from quantitative image analysis of the micrographs. It is possible that the samples of interest are over-etched, revealing the full size of the precipitates. In this case the data may be more descriptive of the **3D** size, however smaller particles are removed by the etching, distorting the obtained size distribution.
- **1D** data is obtained from applying the linear intercept method to micrographs descriptive of a cross section through the dispersion. A half-linear intercept is used in this calculation, which is analogous to the radius of the particle, opposed to the diameter.

Click **Import exp. data** to import the experimental data. Navigate to the file containing the required information and click **Open**. This file can be in .xls, .xlsx, .csv, or .txt formats. The file should consist of two columns with values where the first column contains **radius** data and the second contains **number density** data.

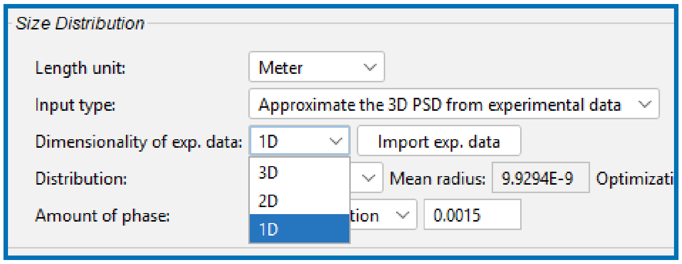
The example `P_10` (available from the **Example files → Precipitation Module - TC-PRISMA**folder) shows this for the precipitate phase M7C3. There is also a file in this folder called `P_10_Precipitation_Initial_PSD_FeCrC_psd_1D_M7C3.csv` that is an example of a correctly formatted text file.

DISTRIBUTION

Choose a **Distribution**: **LSW** (Lifshitz-Slyozov-Wagner), **Normal**, **Log normal**, or **Weibull**.

Click **Generate** to calibrate the chosen **Distribution** to capture the **Import exp. data** accounting for the chosen stereological **Dimensionality of exp. data**.

For 3D data, there are two datasets shown in the preview; the experimental data and the 3D model data. For 2D and 1D data, the sectioned model data is also shown and compared with the experimental data



Size Distribution

Length unit: Meter

Input type: Approximate the 3D PSD from experimental data

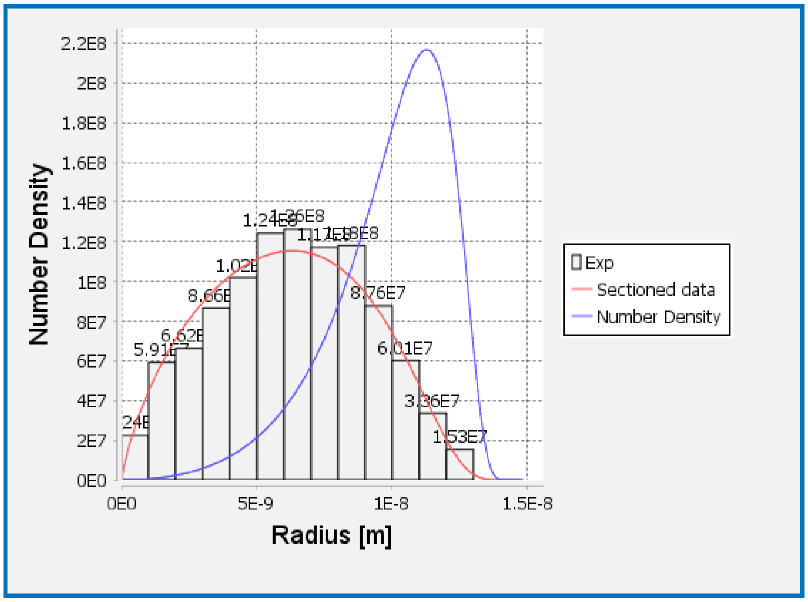
Dimensionality of exp. data: 1D

Distribution:

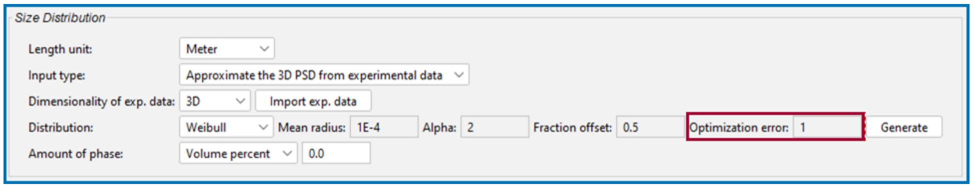
Mean radius: 9.9294E-9

Optimizati

Amount of phase: tion 0.0015



The Optimization error is output into the text-field highlighted below. This can be used to determine the best distribution type to use for a given dataset.



Size Distribution

Length unit: Meter

Input type: Approximate the 3D PSD from experimental data

Dimensionality of exp. data: 3D

Distribution: Weibull Mean radius: 1E-4 Alpha: 2 Fraction offset: 0.5 Optimization error: 1

Amount of phase: Volume percent 0.0

Calculation Type Settings

Below are details about the settings for the *Calculation Type*, which is selected from the **Conditions** tab on the Precipitation Calculator **Configuration** window.

There are additional **Conditions** tab settings described for the Matrix Phase and Precipitate Phase.

ISOTHERMAL

Use an **Isothermal** calculation type to do a simulation at constant temperature.

These settings are described in the section for the Precipitation Calculator Thermal Profile.

NON-ISOTHERMAL

Use a **Non-isothermal** calculation type to do a simulation with a user-defined temperature profile. You can enter information directly or import a data file.

These settings are described for the Precipitation Calculator Thermal Profile including information about importing data files.

When you also have a license for the Additive Manufacturing (AM) Module you can include probe data from the AM Calculator in the set up of the thermal profile.

TTT DIAGRAM

Use a **TTT-diagram** to calculate the time-temperature-transformation (TTT) curve for the formation of the precipitate phase.

- **Temperature**: Enter **Min**, **Max**, and **Step** numerical values and choose a temperature **Unit**.
- **Max annealing time**: Enter a numerical value and choose a time **Unit**.
- **Stop criteria**: Choose **Volume fraction of phase** or **% of equilibrium fraction** and then enter a numerical value. For each temperature, the simulation stops when the stop criteria is fulfilled or if the maximum annealing time is reached, whichever happens first.

See example P_03: Stable and Metastable Carbides - TTT Diagram

CCT DIAGRAM

Use a **CCT-diagram** to calculate the continuous-cooling-transformation (CCT) curve for precipitation.

- **Temperature**: Enter **Min** and **Max** numerical values and choose a temperature **Unit**.
- **Cooling rate(s)**: Enter a range of values in the field, e.g..`01 .1 1 10 100`. These values are equal to **K/s**, **°C/s** or **°F/s** per second based on the temperature **Unit** selected.
- **Stop criteria**: Enter a numerical value for the **Volume fraction of phase**. For each temperature, the simulation stops when the stop criteria is fulfilled.

See example P_07: Continuous Cooling Transformation (CCT) Diagram of Ni-Al-Cr γ-γ'.

Precipitation Calculator Thermal Profile

The **Thermal Profile** is set up on the **Configuration** window for a **Precipitation Calculator**. The isothermal or non-isothermal profile is viewed in the **Visualizations** window. Choose **Isothermal** to do a simulation at constant temperature. Choose **Non-isothermal** to enter or import data for a user-defined temperature profile.

When connected to an AM Calculator (see Including Probe Data from an AM Calculator) the **Isothermal** and **Non-isothermal** options are not visible as it is not relevant to that view.

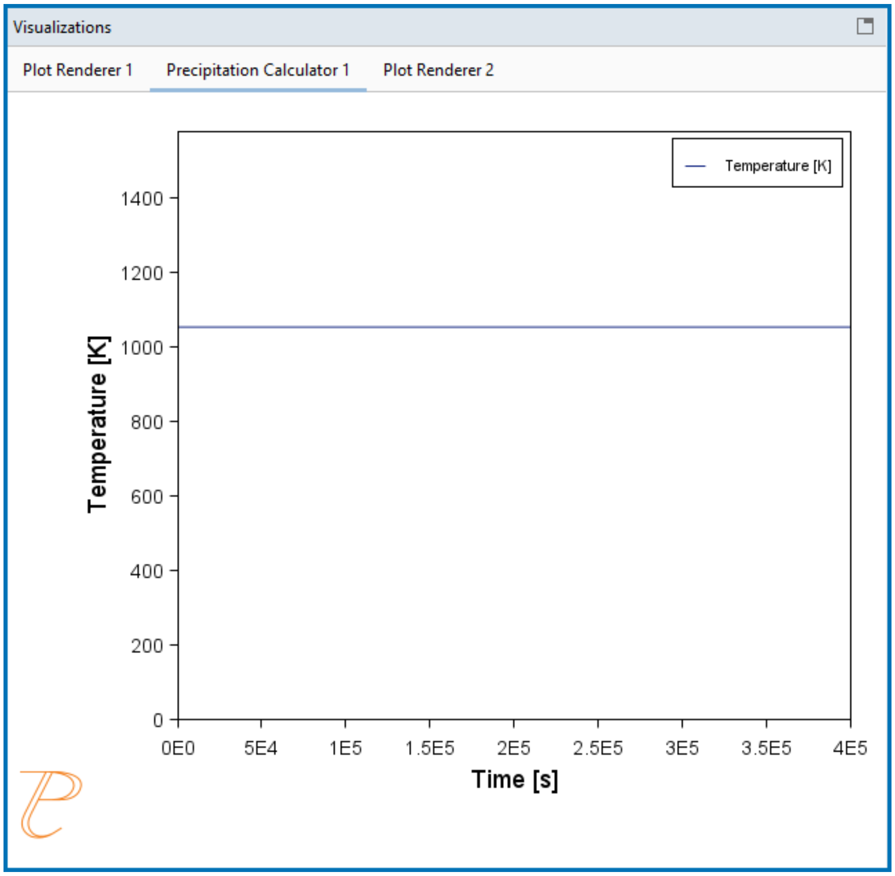
Isothermal Calculations

Many of the Graphical Mode examples for this Add-on Module are isothermal calculations, e.g. *P_02_Precipitation_Fe-C-Cr_Cementite-M7C3-M23C6*.

1. On the Precipitation Calculator **Configuration** window, first enter the required *Matrix Phase* and *Precipitate Phase* settings.
2. Under **Calculation Type**, click to choose **Isothermal** to do a simulation at constant temperature.
3. Enter a **Temperature** and choose a unit (**Kelvin**, **Celsius**, or **Fahrenheit**).

4. Enter an **End time** and choose a unit: **Seconds**, **Minutes**, **Hours**, or **Days**. The *Simulation time* is displayed as text.

   The profile is displayed on the **Precipitation Calculator** tab in the **Visualizations** window showing the constant temperature entered.



5. For this calculation type this completes the settings you need to enter for the Thermal Profile.

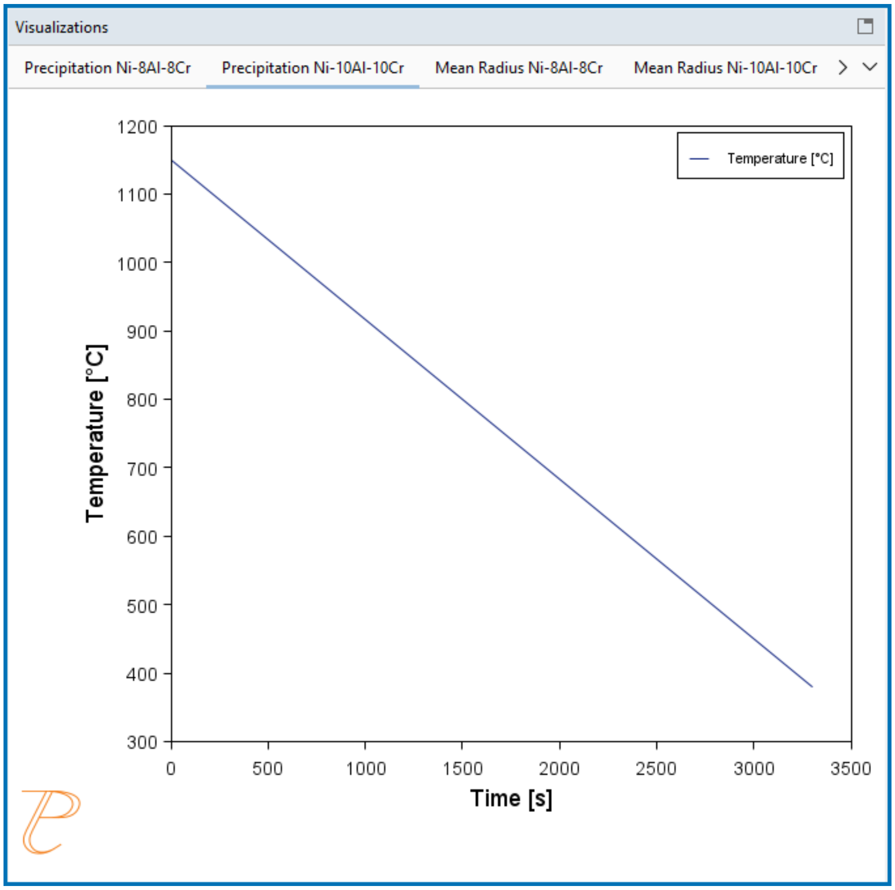
Non-isothermal Calculations

1. On the Precipitation Calculator **Configuration** window, first enter the required *Matrix Phase* and *Precipitate Phase* settings.
2. Under **Calculation Type**, click to choose **Non-isothermal** to enter or import data for a user-defined temperature profile.
3. Select a **Temperature unit**: **Kelvin**, **Celsius**, or **Fahrenheit**.

4. Enter an **End time** and choose a unit: **Seconds**, **Minutes**, **Hours**, or **Days**. The *Simulation time* is displayed as text.

   You can next either directly enter **Time** and **Temperature** coordinates into the table or import the information from a file. A minimum of two points is required.

5. To enter directly into the table:
   a. Click in each cell under the applicable columns, **Time** and **Temperature** then directly enter the values in the table.
   b. Press `<Enter>` to add rows and use the scroll bars to navigate the table.
6. To import a data file:
   a. Although it is a simple set of data, prepare the data file as in Guidelines for Importing Data Files to Thermal Profiles.
   b. When the data file is ready, to the right of the **Import from file** field, click the file 📁 button.
   c. Navigate to a data file such as an MS Excel spreadsheet (with ***.xls** or ***.xlsx** extensions) or a ***.csv** file. You can also use other programs (e.g. Google Sheets) to enter data and export to a CSV format that can be read by the software. Click **Open** to import the data to the **Configuration** window table.
   d. If there are issues with the above import, experiment with choosing the delimiter type that corresponds to the data in the file: **Comma** (`,`), **Colon** (`:`), **Equals sign** (`=`), **Semicolon** (`;`), or **Tab**. Click the **Reload** button ↻. The data is imported to the **Configuration** window table.
7. For this calculation type this completes the settings you need to enter for the profile, which is displayed on the **Precipitation Calculator** tab in the **Visualizations** window. Make adjustments to the settings as needed and watch it dynamically change in the window.



This is from the non-isothermal calculation example, *P_06_Precipitation_Ni-Al-Cr_Non-isothermal_Gamma-Gamma_prime*.

Including Probe Data from an AM Calculator

When you also have a license for the Additive Manufacturing (AM) Module you can include probe data from the AM Calculator in the set up of the thermal profile.

There is connectivity between the Diffusion Module (DICTRA) or the Precipitation Module (TC-PRISMA) and the Additive Manufacturing (AM) Module when you have full licenses available for all relevant Add-on Modules and databases.

You can add a Diffusion Calculator or Precipitation Calculator as a successor to the AM Calculator and then when probes are included with the AM Calculator this data can be further used with the thermal profile.

Details are in the AM Module documentation. See AM Calculator: Working with Probe Data.

Options Tab

The Precipitation Calculator settings including the section *Numerical Parameters* are located on the **Configuration** window → **Options** tab.

You can change these settings locally for a specific Precipitation Calculator or globally for some defaults in the **Options** window settings.

Preprocess Equilibrium Data

Select the **Preprocess equilibrium data** checkbox to calculate the required phase equilibrium properties as a function of temperature for stable and metastable conditions. This speeds up the computation time of non-isothermal simulations or isothermal simulations where there is difficulty with losing precipitate phases during the calculation.

When the checkbox is selected, the stable and meta-stable property diagram data for all simulated precipitate phases is preprocessed. This preprocessing avoids repeating global equilibrium calculations, and speeds up computational time. It also allows for an improved description of precipitate kinetics under severe dissolution conditions. This can occur when temperatures are too high, where the phase is no longer detected in equilibrium calculations, or if the matrix is depleted of precipitate forming species, and the precipitate phase is lost when calculating the driving force.

This feature is used primarily for non-isothermal simulations. For isothermal simulations it can be used when there is difficulty losing precipitate phases during the calculation. In this case, it alters the predicted dissolution kinetics in certain conditions where the precipitation phase is lost and then it also speeds up these calculations.

Include Incipient Melting

> To use the **Include incipient melting** checkbox requires that the thermodynamic database (i.e. TCFE, TCNI, and so on) includes the liquid phase. If the liquid phase is not included, then the **Perform** button is not available (it is grayed out with a message explaining why) until either a liquid phase is included or this checkbox is deselected.

This is available when the **Preprocess equilibrium data** checkbox is selected.

Select the **Include incipient melting** checkbox to approximate the melting temperature of precipitate phases. The precipitates are removed upon exceeding this temperature.

Incipient melting is a phenomenon where, due to rapid heating rates, a solid-state precipitate is in solution at temperatures where it would normally dissolve. It liquidates rather than dissolves into the matrix. Being able to include (or exclude) the incipient melting is relevant to simulations involving welding and AM. Including incipient melting in AM calculations is useful to avoid excessive computation time modeling the dissolution of precipitates which would melt. The precipitates are assumed to melt instantaneously upon reaching their incipient melting temperature.

Max Time Step Fraction

The **Max time step fraction** is the maximum time step allowed for time integration as fraction of the simulation time. The default is 0.1.

No. of Grid Points Over One Order of Magnitude in Radius

The default number of grid points for every order of magnitude in size space. The default is 150.0.

Max No. of Grid Points Over One Order of Magnitude in Radius

The maximum allowed number of grid points in size space. The default is 200.0.

Min No. of Grid Points Over One Order of Magnitude in Radius

The minimum allowed number of grid points in size space. The default is 100.0.

MAX RELATIVE VOLUME FRACTION OF SUBCRITICAL PARTICLES ALLOWED TO DISSOLVE IN ONE TIME STEP

The portion of the volume fraction that can be ignored when determining the time step. The default is 0.01.

MAX RELATIVE RADIUS CHANGE

The maximum value allowed for relative radius change in one time step. The default is 0.01.

RELATIVE RADIUS CHANGE FOR AVOIDING CLASS COLLISION

Set a limit on the time step. The default is 0.5.

MAX OVERALL VOLUME CHANGE

This defines the maximum absolute (not ratio) change of the volume fraction allowed during one time step. The default is 0.001.

MAX RELATIVE CHANGE OF NUCLEATION RATE IN LOGARITHMIC SCALE

This parameter ensures accuracy for the evolution of effective nucleation rate. The default is 0.5.

MAX RELATIVE CHANGE OF CRITICAL RADIUS

Used to place a constraint on how fast the critical radium can vary, and thus put a limit on time step. The default is 0.1.

MIN RADIUS FOR A NUCLEUS TO BE CONSIDERED AS A PARTICLE

The cut-off lower limit of precipitate radius. The default is 5.0E-10 m.

MAX TIME STEP DURING HEATING STAGES

The upper limit of the time step that has been enforced in the heating stages. The default is 1.0 s.

MAXIMUM RELATIVE SOLUTE COMPOSITION CHANGE AT EACH TIME STEP

Set a limit on the time step by controlling solute depletion or saturation, especially at the isothermal stage. The default is 0.01.

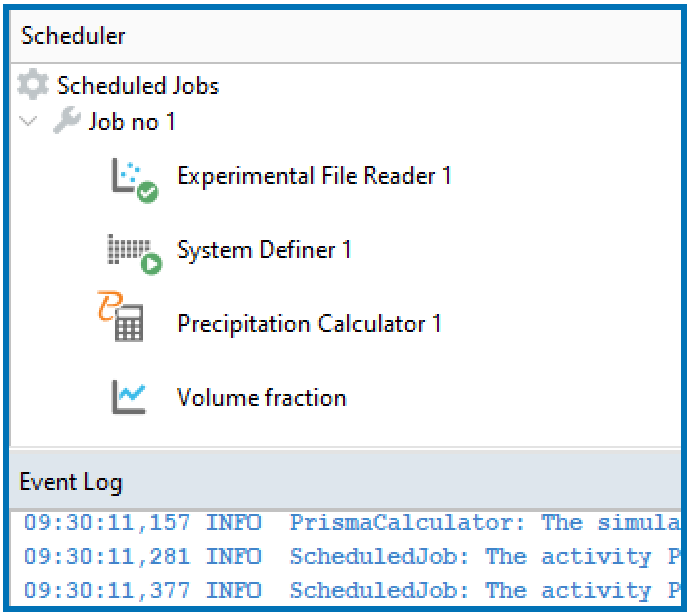
Pause, Resume, and Cancel Precipitation Calculations

Precipitation calculations are often complex simulations that take some time to complete. Sometimes you may want or need to pause or resume a calculation, or make adjustments to your compositions and start again. You pause and resume from the Precipitation Calculator **Configuration** window.

This is also available for the Diffusion Calculator (but not any other calculators). See Pause, Resume, and Cancel Diffusion Calculations.

To Pause and Resume a Job

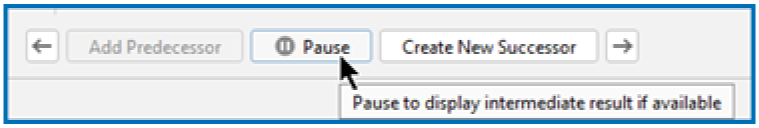
1. Run the job (i.e. click **Perform Tree**). In the **Scheduler**, you can see the job listed and in the **Event Log** you can follow the progress of the calculation.

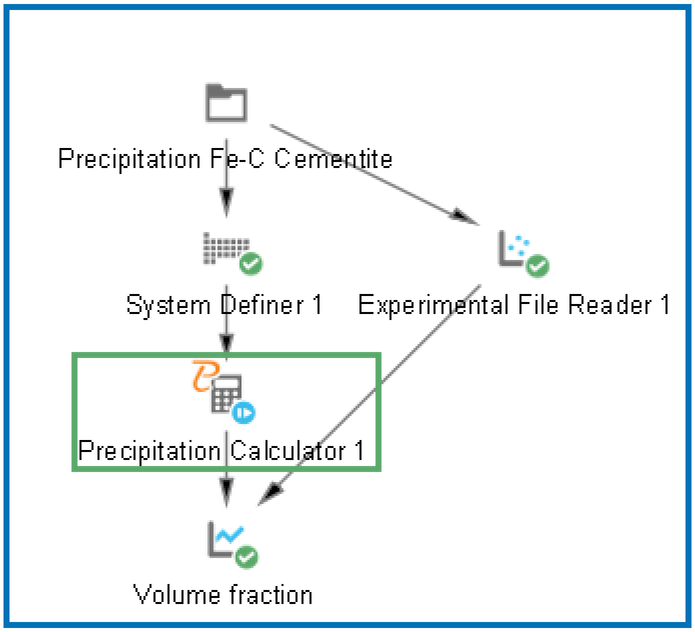


```
09:30:11,157 INFO  PrismaCalculator: The simula
09:30:11,281 INFO  ScheduledJob: The activity P
09:30:11,377 INFO  ScheduledJob: The activity P
```

2. In the **Project** window, click the **Precipitation Calculator** node.

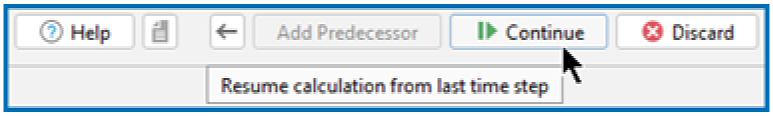
3. In the **Configuration** window at the bottom, click **Pause**. Observe that the **Precipitation Calculator** in the **Project** window has a pause indicator. If there are intermediate results available these will be listed in the **Event Log**.





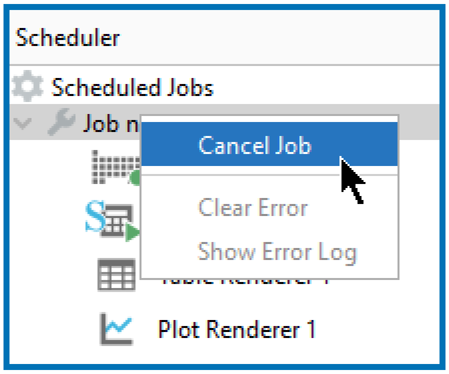
4. When pausing the calculation, you can make changes to a variety of settings under the *Matrix Phase* or *Precipitate Phase* sections (click **Show Details**), plus the **Interfacial energy**, **Temperature** (for non-isothermal calculations), and **Simulation time**. The rest of the **Configuration** window settings are grayed out and no other editing can be done while paused.

5. When ready, click ▶ **Continue** to resume your calculations from the last time step or click ⊗ **Discard** to discard the calculation (then click **Yes** or **No** on the window that opens).



To Cancel a Job

- In the **Scheduler** window, right-click the job you want to cancel and select **Cancel Job**.



Precipitation Calculator Plot Renderer

The following is information about the settings available for a **Plot Renderer** when it is a successor to a **Precipitation Calculator**.

ⓘ [Quantities Groups Available for Plots and Tables](#) for a general list of quantities. However, for the Precipitation Calculator Plot Renderer there are no defined groups to choose from.

Plot Settings

LEGEND OPTION

Select whether the diagram's legend displays **On** or **Off**.

Y- AND X-AXES VARIABLES

Set the state variable you want plotted along the X-axis and the Y-axis. The available variables in the list are based on how your system is set up.

Below are additional details related to the axis variable chosen.

- **Separate Multimodal PSD:** If you select **Mean radius**, **Number density**, **Volume fraction**, **Size distribution**, **Number density distribution**, or **Normalized number density distribution** then the **Separate multimodal PSD** checkbox is available. For variables with time for the X-axis, the number of **Points** used to sample the results can be modified. The **Inflection neighbors** and **Smoothing iterations** are used to identify individual particle populations. See Separate Multimodal PSD below for more detail.

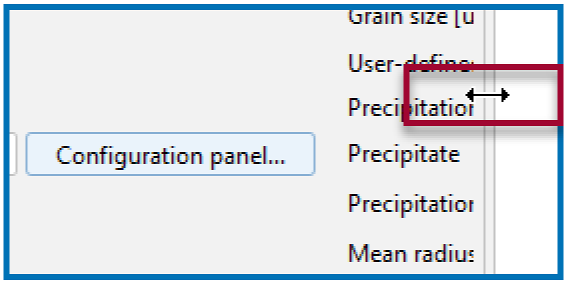
- **3D → 2D:** For a spherical morphology, and if you select **Mean radius**, **Number density**, **Volume fraction**, **Size distribution**, **Number density distribution**, or **Normalized number density distribution** as an axis variable, you can also select the **3D → 2D** checkbox to convert the 3D property to the corresponding 2D property considering the resulting 2D size distribution obtained from sectioning a 3D spherical dispersion. See 3D to 2D Conversion below for more detail.
- **Yield Strength**: If you select this as an axis variable there are additional settings. See Yield Strength below for more detail.

Yield Strength

If you choose **Yield strength** as an *Axis variable*, you can further define the model. Click to expand the drop down list to the right of the *Axis variable*, then select any or all of the checkboxes listed below to plot the respective contributing elements to the yield strength.

Click **Configuration Panel** toggle between the settings options and to further fine-tune the model. These options are described for the Yield Strength Property Model: Simplified Mode Settings and Yield Strength Property Model: Advanced Mode Settings. The greyed out sections (e.g. the **Matrix**, **Precipitate** phases, and **Grain size**) are defined on the **Precipitation Calculator** and cannot be changed.

> To see these settings after clicking **Configuration Panel**, you need to expand the **Plot Renderer Configuration** window to the right. Either detach the window to resize, or hover with the mouse until you see the double arrow, then click and drag to expand the window.



- Total yield strength
- Intrinsic strength
- Solid solution strengthening
- Solid solution strengthening FCC
- Solid solution strengthening BCC
- Solid solution strengthening HCP
- Grain boundary strengthening
- Total precipitation strengthening
- Precipitation strengthening per phase
- Constant strength addition

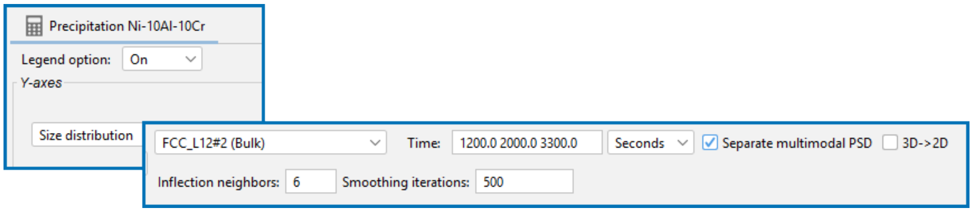
The **P_01: Isothermal Precipitation of Al3Sc** example demonstrates the use of this Yield Strength Model.

Separate Multimodal PSD

This setting is available if you select **Mean radius**, **Number density**, **Volume fraction**, or **Size distribution** as the *Axis Variable*.

When the **Separate multimodal PSD** checkbox is selected on a **Plot Renderer** activity for the **Precipitation Calculator**, the size distribution is evaluated at the given time steps and results for individual particle populations are identified and presented. These are separated and used to calculate the specified property.

P_06: Precipitation of γ’ in Ni Superalloys - Non-isothermal



Precipitation Ni-10Al-10Cr

Legend option: On

Y-axes

Size distribution

FCC_L12#2 (Bulk) Time: 1200.0 2000.0 3300.0 Seconds ☑ Separate multimodal PSD ☐ 3D->2D

Inflection neighbors: 6 Smoothing iterations: 500

POINTS

This field is available when the **Separate multimodal PSD** checkbox is selected. It is not available with the **Size distribution** variable.

Since the evaluation of multimodality at each time step is costly, you can specify how many evaluation **Points** to use. The points are geometrically distributed over the time scale where nucleated particles are found. The default is 40 points.

INFLECTION NEIGHBORS

This field is available when the **Separate multimodal PSD** checkbox is selected.

Enter the **Inflection neighbors**, which are the number of neighboring points with consistent gradient direction to identify inflection points. The default is 6. As a guide, too low a number is sensitive to noise and too high a number can fail to detect particle populations.

SMOOTHING ITERATIONS

This field is available when the **Separate multimodal PSD** checkbox is selected.

Enter the number of **Smoothing iterations** performed to reveal significant particle populations. The default is 500. As a guide, too small a number can fail to remove noise, and too high a number can remove the particle populations of interest.

3D to 2D Conversion

When the *Precipitate Phase* **Morphology** is set to **Sphere** on the Precipitation Calculator, the following options are available when certain axis variables are also selected.

Select the **3D → 2D** checkbox if you want to make a direct comparison between the predicted three-dimensional (3D) radius of the precipitates and the two-dimensional (2D) data obtained from a cross-section taken through the dispersion.

> The stereological conversion is described in the theory for spherical particles.

These variables can be converted to 2D:

- **Mean radius**: The average circular radius of cross sections of particles obtained by taking a section through the dispersion, assuming spherical precipitates.
- **Number density** The number concentration of precipitates found on a 1 m^2 cross-section through the microstructure.
- **Volume fraction** The area fraction of precipitates found on a cross-section taken through the microstructure.
- **Size distribution**: The number density of particle cross sections that have a radius varying within a given size class in a unit area.
- **Number density distribution**: The number of particle cross sections that have a radius varying within a given size class in a unit area.
- **Normalized number density distribution**: The probability of finding particle cross sections with a cross sectional radius varying within the size class. The radius is normalized by the volumetric mean of the dispersion.

AXIS TYPE

Select the type of axis scale: **Linear**, **Logarithmic**, **Logarithmic 10**, or **Inverse**.

LIMITS

Specify the range along the axis to show in the plot. In the fields, enter the minimum and maximum values of the axis variable. You can also determine the **step** size between the tick marks along each axis.

Select the **Automatic scaling** checkbox to allow the program to set the limits.

UNIT (*TIME X-AXIS*)

Choose a **Unit**: **Seconds**, **Hours**, or **Days**.

ADD AN AXIS AND REMOVE THIS AXIS BUTTON

Use the ⊕ **Add an axis** and ⊖ **Remove this axis** buttons to add additional *X*- and/or *Y*-axes to a plot or to merge plots (to overlay one plot with another in the same diagram). When merging plots, you define this variable as the *Z*-axis.

AVAILABLE AXIS VARIABLES

Quantities Groups Available for Plots and Tables for a general list of quantities. However, for the Precipitation Calculator Plot Renderer there are no defined groups to choose from.

- **Mean radius**: Spherical radius of average volume of all particles for a specific phase and nucleation type, regardless of their actual shapes. If the matrix phase is selected, it outputs the average grain radius.
- **Critical radius**: Spherical radius of critical nuclei for a specific phase and nucleation type. If the matrix phase is selected, it outputs critical grain radius.
- **Yield strength**: To use the Yield Strength Property Model to calculate yield stress. For more information see About the Yield Strength Property Model.
- **Matrix composition**: Instantaneous compositions of the matrix phase.
- **Precipitate composition**: To track the instantaneous composition of precipitate particles. In particular, it is useful to distinguish different composition sets of the same phase (for example, FCC_A1#2 and FCC_A1#3). Further choose **Solutes** or **All**.
- **Number density**: Instantaneous number of particles per unit volume for a specific phase and nucleation type. If the matrix phase is selected, it outputs instantaneous number of grains per unit volume.
- **Size distribution**: Number of particles, or grains if the matrix phase is selected, varying with their sizes per unit volume per unit length, for a specific phase and nucleation type, at a specific time.
- **Number density distribution**: Retrieve the number density (number of particles per unit volume) of precipitates, or grains if the matrix phase is selected, distributed in different particle sizes.
- **Normalized Number density distribution**: Retrieve the number density (number of particles per unit volume) of precipitates, or grains if the matrix phase is selected, normalized by total number of particles or grains per unit volume, distributed in different particle sizes normalized by average size.
- **Volume fraction**: Instantaneous volume fraction for a specific phase and nucleation type.
- **Nucleation rate**: Instantaneous number of nuclei per unit volume per unit time for a specific phase and nucleation type.
- **Normalized driving force**: Instantaneous nucleation driving force per unit mole of elements for a specific phase and nucleation type. It is normalized with RT and therefore, dimensionless.

- **Temperature**
- **Mean cubic factor**: Average cubic factor of cuboid particles. Available only when cuboid is selected as the **Morphology**.

The following settings area available as indicated when **Needle**, **Plate**, or **Cuboid** are selected as the **Morphology** in the *Precipitate Phase* section on the Precipitation Calculator.

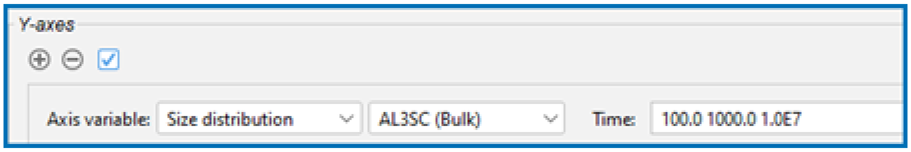
- **Cubic factor distribution**: Variation of cubic factor with particle size at a specific time. Available with a cuboid morphology.
- **Mean aspect ratio**: Average aspect ratio of non-spherical particles. Available with a needle or plate morphology. Note that this is always larger than 1, where 1 = a sphere.
- **Mean particle length**: Diameter of non-spherical particles along the longer axis. Available with a needle or plate morphology.
- **Aspect ratio distribution**: Variation of aspect ratio with particle size at a specific time. Available with a needle or plate morphology.

TIME (Y-AXES)

This field is available when **Size distribution** or **Number density distribution** is selected as the Y-axes variable. Enter one or a series of numbers in the field, separated by a space.

P_09: Precipitation of Al-Sc AL3SC with Assumption of Sphere and Cuboid Morphologies

If you open the example P_09, then change the **Time** settings on the **PSD** Plot Renderer to be `100.0 1000.0 1.0E7`:



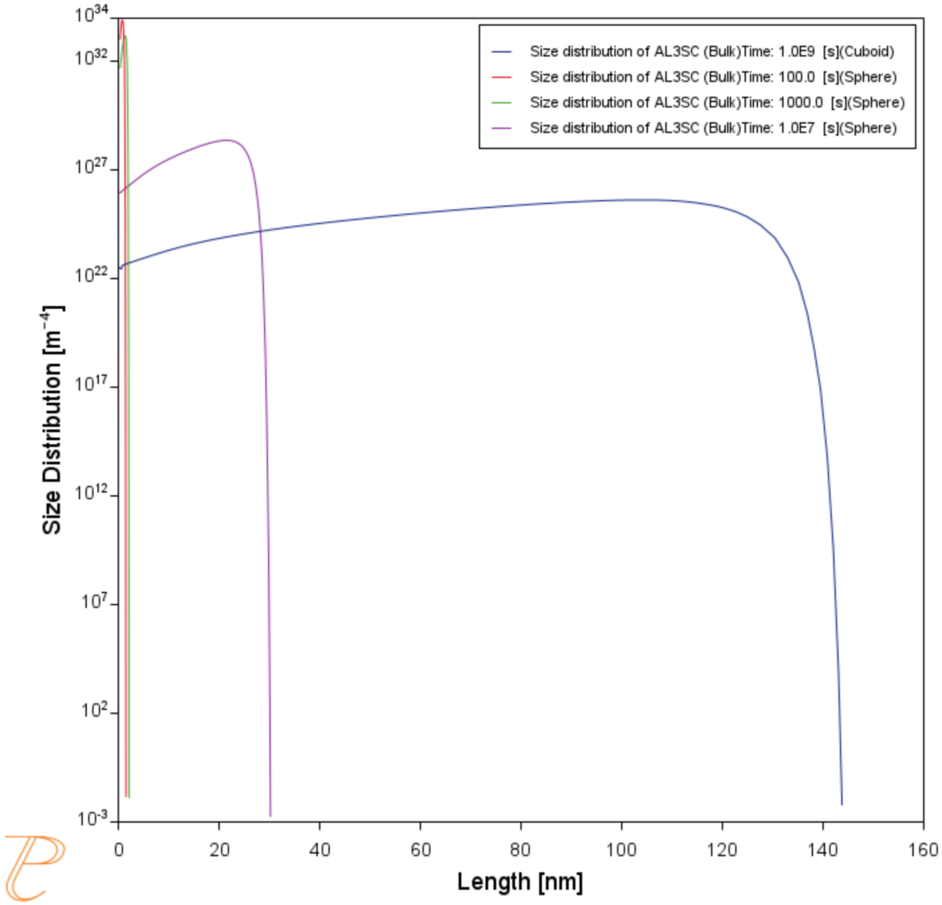
Y-axes

Axis variable: Size distribution

AL3SC (Bulk)

Time: 100.0 1000.0 1.0E7

When you click **Perform** the series of times are plotted:



Size distribution of AL3SC (Bulk)Time: 1.0E9 [s](Cuboid)
Size distribution of AL3SC (Bulk)Time: 100.0 [s](Sphere)
Size distribution of AL3SC (Bulk)Time: 1000.0 [s](Sphere)
Size distribution of AL3SC (Bulk)Time: 1.0E7 [s](Sphere)
Size Distribution [m^{-4}]
10^{34}
10^{32}
10^{27}
10^{22}
10^{17}
10^{12}
10^{7}
10^{2}
10^{-3}
0
20
40
60
80
100
120
140
160
Length [nm]

Plot Renderer

The Plot Renderer is where you define the settings and output results in a diagram that displays in the **Visualizations** window. The available Plot Renderer settings are based on the System Definer and/or calculator activity node predecessor (i.e. Equilibrium Calculator, Scheil Calculator, Property Model Calculator, and so forth). Settings availability is also determined by the *Calculation Type* as well as if you have an Add-on Module. If you used any of the templates, the Plot Renderer is automatically added to the Project tree.

Configuration Settings

For the standard plot settings, see Configuration Settings.

There are additional details for more advanced settings in Plotting Options.

There are additional details for the Add-on Modules:

- Diffusion Calculator Plot Renderer
- Precipitation Calculator Plot Renderer
- AM Calculator: Plot Renderer Settings

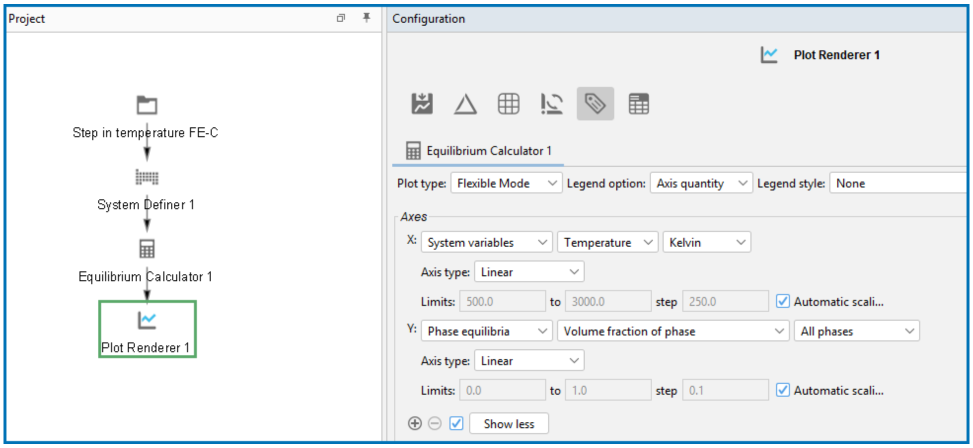
Plot Toolbar

For any Plot Renderer, there is a toolbar available.

Button	*Name*	*Description*
	Save Diagram	Save the plot diagram. From the **Save** window, choose the file type–png (the default), jpg, ps, pdf, gif, svg, or emf. For PNG and JPG files you can also change the image quality. ? Saving and Printing the Output in Graphical Mode
△	Toggle Triangular/Regular Diagram	Display the diagram in triangular form, with the X-axis along the base and the Y-axis along the left side. Such a diagram is often useful if you want to plot the fractions of two components in a ternary diagram.
⊞	Show Grid	Overlay a grid on the diagram.
	Switch Axes	Show the plotting X-axis variable on the diagram's Y-axis, and the Y-axis variable on the diagram's X-axis.
🏷	Retain Labels	The default is to keep labels displaying, i.e. retained, on the plot. This keeps all labels on the plot each time you click **Perform** or **Perform Tree**. If the **Retain Labels** button is clicked to turn this off, then it clears all labels fully and the label needs to be added again before performing.
▦	Table View	Toggle to switch between displaying a Plot or the results of a Table in the **Visualizations** window. This is available for single equilibrium or stepping calculations. When you click to toggle ON, click **Perform** to regenerate as a Table. When you click to toggle OFF, click **Perform** to regenerate the Plot. For example, set up the Plot Renderer and click **Perform** to display the Plot. Then click **Table View** and **Perform** to see the results in a Table format in the **Visualizations** window. When toggled ON, click **Save table** to export the table data. Choose the **Decimal digits** and **Number format** (**Auto**, **Decimal**, or **Scientific**). ? Saving and Printing the Output in Graphical Mode

Configuration Settings

Click the **Plot Renderer** node in the **Project** window to view the **Configuration** window. The settings available vary based on such choices as the specific calculator used and calculation type selected.



Plot type: Flexible Mode Legend option: Axis quantity Legend style: None

Axes

X: System variables Temperature Kelvin

Axis type: Linear

Limits: 500.0 to 3000.0 step 250.0 ☑ Automatic scali...

Y: Phase equilibria Volume fraction of phase All phases

Axis type: Linear

Limits: 0.0 to 1.0 step 0.1 ☑ Automatic scali...

☑ Show less

Working with Plots and Tables

For the Add-on Modules with additional specialized functionality also see:

- Diffusion Calculator Plot Renderer
- Precipitation Calculator Plot Renderer
- AM Calculator: Plot Renderer Settings

Settings

The options along the top of the window are available depending on the calculation type.

PLOT TYPE

There are a variety of combinations of Calculator and *Calculation Type* that offer different Plot Types. These are described in separate topics:

- Plot Type: Cross Plot and Statistical
- Plot Type: Heat Map, Contour, and 3D
- Plot Type: Parallel Coordinates
- Plot Type: Flexible Mode and Grouped Mode

- Plot Type: CCT Mode
- Plot Type: TTT Mode
- Plot Type: Simple Mode and Advanced Mode

TIE-LINES

Select how many tie-lines to be plotted in the diagram. Every n^{th} number of tie-line is plotted, where *n* is the number set here. Consequently, the higher the number, the fewer the number of plotted tie-lines in the diagram.

> This setting is not available if the Plot Renderer is a successor to an Equilibrium Calculator where only one axis is defined and varied (that is, an Equilibrium Calculator that has performed a stepping calculation).

LEGEND OPTION

Select whether the diagram's legend displays the **Stable phases**, the **Axis quantity**, or choose **Off** for no legend.

LEGEND STYLE

You can select a **Legend style** for the **Stable phases** or **Axis quantity** selected for **Legend option**. Choose **None**, **All**, **Constitution description**, or **Ordering description**.

? About Legend Styles

FILTER

This is available with the **Property Model Calculator** and **Process Metallurgy Calculator**.

Use the **Filter** checkbox to add various filters to the plot or table based on the set up of the calculation. When selected, click the ⊕ **Add quantity** and ⊖ **Remove quantity** buttons to add filters. For example, enter a **Min** and **Max** and choose an axis variable such as **Ms Temperature** and the unit **Kelvin** to adjust the output in the **Visualizations** window. Click **Perform** each time you add or remove a filter for the results to update.

SHOW LIMITS (BATCH)

This is available for the **Batch** calculation type, **Cross plot**.

Click the **Show limits** checkbox and then choose **RMS** (root mean squared), **Absolute**, or **Relative in % limits**. For **Absolute** or **Relative in %** enter a value in the field (the default is 15.0). A "perfect fit" line is added (solid line) to the plot and then the upper and lower limits shown on the plot are based on the type of limit selected.

- When **RMS** is selected, a "perfect fit" line is added (solid line) plus the upper and lower limits (dashed lines), which are calculated for the experimental data points (read from the data file). The RMS error value is shown in the plot legend. The upper and lower limits are then this calculated value plus and minus from the perfect fit line.
- When **Absolute** is selected, the value entered (e.g. the default is 15), then this is the plus or minus value from the perfect fit line.
- When **Relative in %** is selected, the value entered (e.g. the default is 15%), then this is the upper and lower limit that is plotted and this value is plus or minus percent from the perfect fit line as is calculated and shows in the plot legend.

SHOW CALCULATION FAILURES AT VALUE (BATCH)

This is available for the **Batch** calculation type, **Cross plot**.

Click the **Show calculation failures at value** checkbox and enter a value in the field. Use this checkbox to include any values that failed in the calculation and you want to see these on the plot. The value entered in the field replaces the non-existing calculated value(s) and can be cross plotted against experimental results from that data file.

INTERPOLATE (GRID)

From the **Interpolate** list, choose to interpolate data **Never** (the default), **Once**, **Twice** or **3 times**. This means points are put in between calculated points in the grid and interpolated instead of calculated in the calculation engine.

Choose how many points of data to interpolate to improve curve smoothness – **Never**, **20x20**, **50x50**, or **100x100**. Try different settings for your own set of data.

LABEL DECIMAL DIGITS

Choose the number of decimal digits to display in the plot label. The default is **2**.

LABEL NUMBER FORMAT

Choose from **Auto** (the default), **Decimal**, or **Scientific**.

AXES DEFINITIONS

Set the state variable you want plotted along the *X*-axis and the *Y*-axis (and *Z*-axis for **Grid** calculations).

The quantities are sometimes grouped into categories on the Plot Renderer or Table Renderer. Availability of the list and the variables themselves, is based on several factors, including the database selected, the Calculator used, and the type of calculation being performed. Other differences are based on the *Plot type* selected, e.g. what you see on the **Configuration** window changes if you use **Flexible Mode** or **Grouped Mode**. Other plot types do not group the quantities and each Calculator handles the information differently.

When working on a Plot Renderer (e.g. associated to the *Axes* X, Y, and Z) or Table Renderer (associated to *Columns*), there is sometimes the option to choose a quantity group from a list. When applicable, these are the categories:

- All variables
- System variables
- Phase equilibria
- Physical properties
- Kinetic properties
- Elastic properties

After selecting the group, you next choose from the available variables and continue to define each based on the additional settings specifically available, i.e. select a unit or a phase, and many other options that are only displayed when relevant.

Quantities Groups Available for Plots and Tables

There are various items to note regarding the **Axes**.

- If the stepping/mapping variables are changed in the Equilibrium Calculator that precedes the Plot Renderer, then the variables to be plotted along the diagram's *X*- and *Y*-axes are automatically updated to the appropriate quantities.
- For a **Grid** *Calculation Type*, the *X*- and *Y*-axes always represent the quantities that define the calculation axes, but you need to set a variable for the *Z-axis* (the axis perpendicular to the plane defined by the *X*- and *Y*-axes).
- For a **Batch** *Calculation Type*, the available options from the *X*- and *Y*- axes lists are based on the data file contents, i.e. if experimental data is included, then these are listed. See Working with Batch Calculations for details. Additional Plot Types are also available.

- For a **Parallel coordinates** *Plot type*, and only for parameterized result quantities, you can choose to show all or one specific quantity on the plot. By default, and when you first choose these types of results quantities, **All** quantities are plotted in the **Visualizations** window output after performing the first calculation. Once the secondary list is available you can then choose to plot only one of the quantities at a time. The availability of the filter list is dependent on the result of the initial calculation. See Plot Type: Parallel Coordinates for details.

AXIS TYPE

Select the type of axis scale: **Linear**, **Logarithmic**, **Logarithmic 10**, or **Inverse**.

AUTOMATIC SCALING

The **Automatic scaling** checkbox is selected by default to allow the program to set the limits.

LIMITS

This setting is available when the **Automatic scaling** checkbox is cleared (the scaling is turned off).

Enter the lower and upper **Limits** of the variables to display on the axis. You can also determine the **step** size between the tick marks along each axis.

If the **Automatic scaling** is turned off (i.e. the checkbox is not selected) then it is important to enter a large enough number in the *step* field for the numerical values to display correctly on the axis. That is, if the step size is too small, the program ignores this setting and the axis labels will not be as expected.

For logarithmic axes, the step size is related to the exponent. For example, if the step entered is 1.0, then the exponent increases by one each time (10^{-9}, 10^{-8}, 10^{-7} and so forth).

CONTOUR VALUES AND USE CUSTOM CONTOUR VALUES (Z-AXIS, CONTOUR PLOTS)

The **Use custom contour values** checkbox is available when **Contour** is selected as the **Plot type**. Select this checkbox to enter one or a series of numbers in the **Contour values** field. Numbers can only be separated by a space.

ADD AN AXIS AND REMOVE THIS AXIS BUTTONS

Use the ⊕ **Add an axis** and ⊖ **Remove this axis** buttons to add additional *X*- and/or *Y*-axes to a plot or to merge plots (to overlay one plot with another in the same diagram). When merging plots, you define this variable as the *Z*-axis.

Plotting Options

SLAG PROPERTY OPTIONS (PROCESS METALLURGY)

For the **Process Metallurgy Calculator** when you are selecting axis variables on the Plot Renderer, there is the option to choose **Slag property**. The associated quantity that you select from the next drop-down list has these options to choose: **All**, **B2**, **B3**, **B4**, **Bas2**, **Bells ratio**, **Ls**, or **Log10 (Sulphur capacity)**.

Also choose **In liquid slag only**, **In solid slag only**, or **In all slag**.

References and equations for these properties are described in Process Metallurgy Slag Properties.

UNIT (PROCESS METALLURGY)

For the **Process Metallurgy Calculator** select a **Unit** for the quantity to plot: **Tonne**, **Kilogram**, **Gram**, or **Pound**

ACCOUNT FOR INTERFACE SCATTERING (SCHEIL)

Scheil Calculator Available Plot Variables

The **Account for interface scattering** checkbox is available when any of the following quantities are selected for an axis for a Scheil Calculator:

- Electric conductivity
- Electric resistivity
- Thermal conductivity
- Thermal diffusivity
- Thermal resistivity

The electrical resistivity due to phase interface scattering is evaluated as the scattering constant times sum of the interaction between the volume fraction of all the phases. The default value for the **Phase interface scattering constant** is found to be `4.0e-8` Ωm for aluminum alloys produced with conventional methods. A higher value could be required for the AM process where the rapid solidification results in a very fine microstructure with a large amount of phase interfaces.The contribution to thermal conductivity is assumed to be related to that to electrical resistivity, following the Wiedemann-Franz law.

Either keep the default **Phase interface scattering constant**, which is a constant for evaluating thermal conductivity due to scattering at phase interfaces, or enter another value.

Table Renderer

A **Table Renderer** visualizes calculation results in a table. Several Table Renderer activities (as well as Plot Renderer activities) can be shown in the **Visualizations** window as different tabs.

You can add the Table Renderer directly (right-click a calculator node and select it from the **Create New Successor** menu) or use a variety of the available templates to automatically add the node. For example, on the **My Projects Configuration** window under **Equilibrium**, choose the **Single Point** or **One Axis** templates.

For details about the templates, see Getting Started Links and Templates and Creating a Project from a Template.

You can only successfully tabulate the results of a single equilibrium calculation or a stepping (i.e. property diagram) operation. The tabulated data from an equilibrium calculation is different from the tabulated data from a stepping calculation.

The settings are described in the section Configuration Settings.

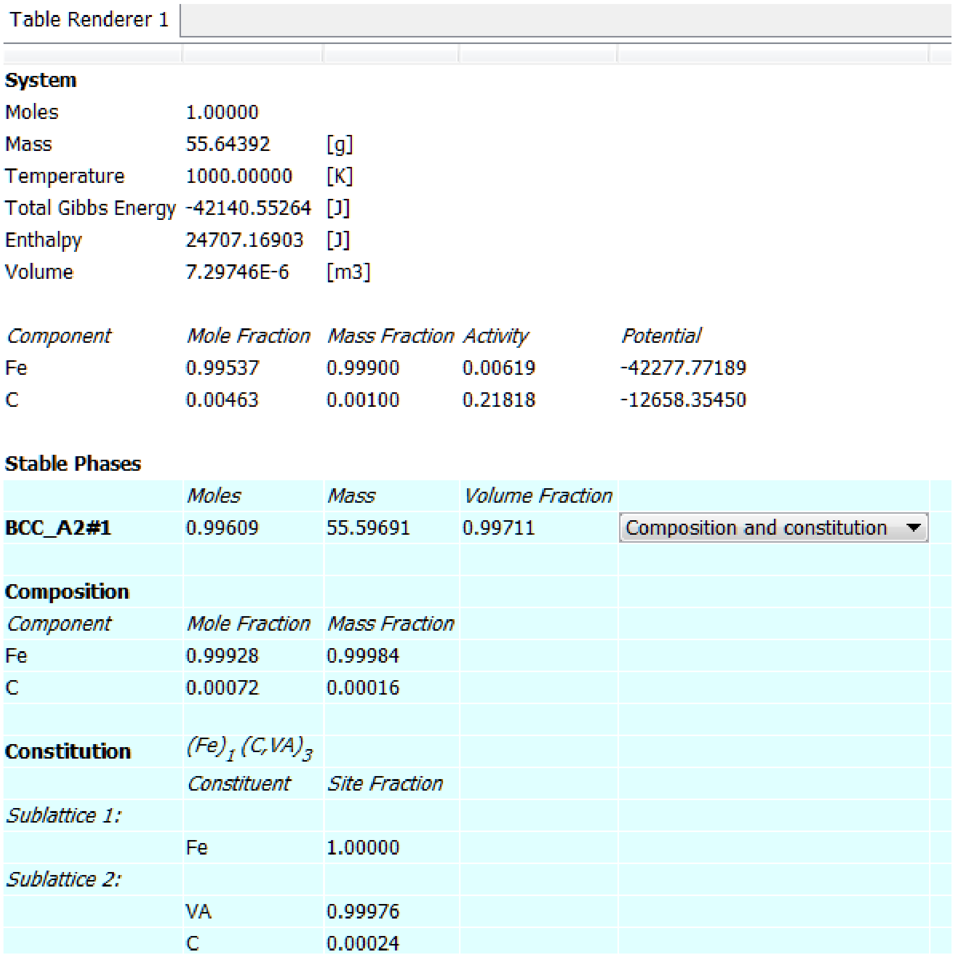
Table Button

Button	*Name*	*Description*
	Save Table	Once a calculation is performed and there is data in the table, click to save it. Saving and Printing the Output in Graphical Mode

For the Plot Renderer, there is an option to use the **Table View** button to convert plots to table data for all calculation types and calculators. See Plot Renderer: Convert a Plot to a Table and Export the Data.

Results from an Equilibrium Calculation

The following tab shows the result of an equilibrium calculation (from example T_01: Calculating a Single-Point Equilibrium).



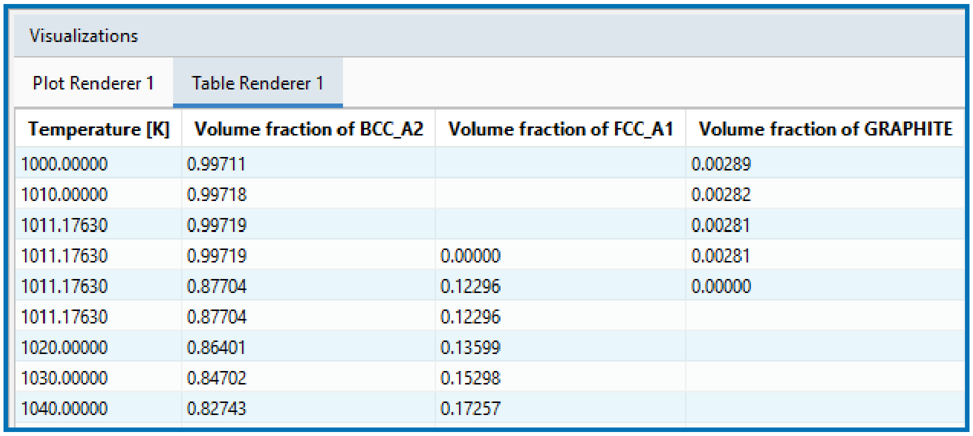
System				
Moles	1.00000			
Mass	55.64392	[g]		
Temperature	1000.00000	[K]		
Total Gibbs Energy	-42140.55264	[J]		
Enthalpy	24707.16903	[J]		
Volume	7.29746E-6	[m3]		
Component	*Mole Fraction*	*Mass Fraction*	*Activity*	*Potential*
Fe	0.99537	0.99900	0.00619	-42277.77189
C	0.00463	0.00100	0.21818	-12658.35450
Stable Phases				
	Moles	*Mass*	*Volume Fraction*	
BCC_A2#1	0.99609	55.59691	0.99711	Composition and constitution ▼
Composition				
Component	*Mole Fraction*	*Mass Fraction*		
Fe	0.99928	0.99984		
C	0.00072	0.00016		
Constitution	*$(Fe)_1(C,VA)_3$*			
	Constituent	*Site Fraction*		
Sublattice 1:				
	Fe	1.00000		
Sublattice 2:				
	VA	0.99976		
	C	0.00024		

For each stable phase listed, from the **Composition and constitution** menu you can select the information to view. In this example, the maximum amount of information is shown and includes details about both composition and constitution for **BCC_A2#1**.

> The default for the Phase description detail can be changed globally from the **Options** window.

Results from a Stepping Operation

The **Table Render 1** tab in the example shows the results of a stepping calculation (where a Table Renderer is added to the example in T_02: Stepping in Temperature in the Fe-C System).

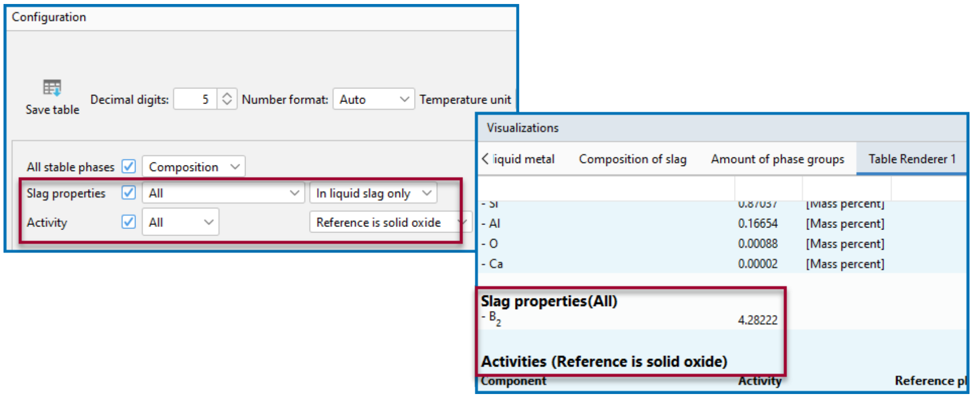


Temperature [K]	Volume fraction of BCC_A2	Volume fraction of FCC_A1	Volume fraction of GRAPHITE
1000.00000	0.99711		0.00289
1010.00000	0.99718		0.00282
1011.17630	0.99719		0.00281
1011.17630	0.99719	0.00000	0.00281
1011.17630	0.87704	0.12296	0.00000
1011.17630	0.87704	0.12296	
1020.00000	0.86401	0.13599	
1030.00000	0.84702	0.15298	
1040.00000	0.82743	0.17257	

Process Metallurgy Module Single Equilibrium

When you use a **Process Metallurgy Calculator** with a **Single** equilibrium calculation, there is a variety of additional information you can display in the table such as the **Slag properties** (see Process Metallurgy Slag Properties for equations and references) and the **Activities**.

PMET_01: Basic Oxygen Furnace (BOF). Using version 01b, added a Table Renderer and did a **Single** calculation.



Decimal digits: 5

Number format: Auto

All stable phases ☑ Composition

Slag properties ☑ All · In liquid slag only

Activity ☑ All · Reference is solid oxide

- Si
- Al 0.16654 [Mass percent]
- O 0.00088 [Mass percent]
- Ca 0.00002 [Mass percent]

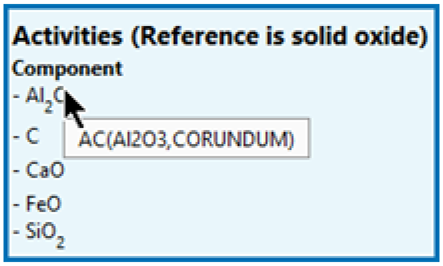
Slag properties(All)

- B_2 4.28222

Activities (Reference is solid oxide)

Component **Activity** **Reference pl**

For the activities in the table, you can hover over the Component and the syntax of the activity displays.



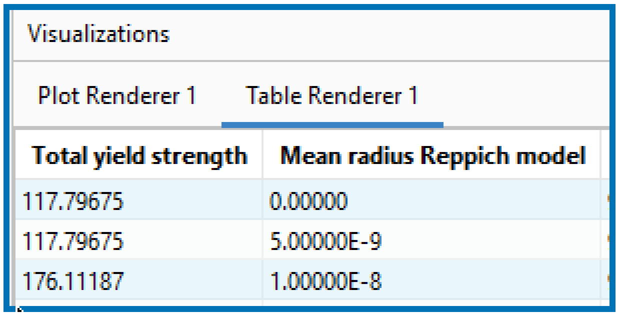
Activities (Reference is solid oxide)
Component
- Al_2O_3
- C
- CaO
- FeO
- SiO_2

Yield Strength Property Model

The Yield Strength Property Model: Simplified Mode Settings is available with the Property Model Calculator. After defining the Model and adding a Table or Plot, all yield strength quantities are available to select from this list. These yield strength quantities are also accessible via a Table Renderer (or Plot Renderer) that is a successor to the Precipitation Calculator.

For details about the quantities, see About the Yield Strength Property Model.

This uses the PM_G_05: Yield Strength NiAlCr example and then a Table Renderer is added. Alternatively, you can click the **Table View** button and reperform the Plot Renderer for the same results.



Total yield strength	Mean radius Reppich model
117.79675	0.00000
117.79675	5.00000E-9
176.11187	1.00000E-8

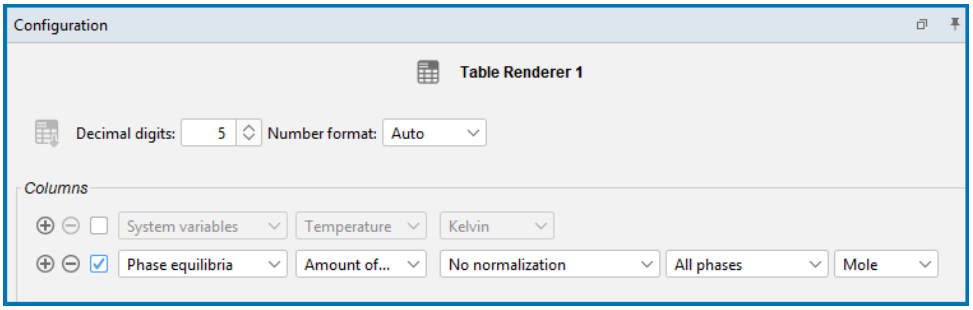
An example of the results when yield strength is chosen as the Axis variable for a Table Renderer that is a successor to the Property Model Calculator.

Precipitation Calculator Multimodal PSD and 3D --> 2D Settings

These settings are described in the Precipitation Calculator Plot Renderer.

Configuration Settings

The **Table Renderer** settings are done on the **Configuration** window. Depending on what calculator node the table is a successor to, you can have different settings available. For most tables, this is where you set the level of detail for the columns.



Decimal digits: 5 Number format: Auto

Columns

☐ System variables Temperature Kelvin

☑ Phase equilibria Amount of... No normalization All phases Mole

SAVE THE TABLE

To save all the data in a table as a Character separated (`.csv`), Hyper Text Markup (`.html`), or Excel (`.xls`), in the **Configuration** window click **Save Table** or in the **Visualizations** window right-click in the table and select **Save As**.

To copy the data from a single cell of a table to the clipboard, right-click the cell and select **Copy**. To copy the whole table to the clipboard, select **Copy all**.

The data saved is what is shown in the **Table Renderer** tab on the **Visualizations** window. If data is calculated (and not displayed) it is not saved.

NUMBER OF DECIMAL DIGITS AND NUMBER FORMAT

The table results can be presented in ordinary decimal number format or with normalized scientific notion. Choose **Scientific** or **Decimal** to increase or decrease the number of **Decimal digits** used in the table. The default is 5 digits. The **Number format** defaults to **Auto** to use the most appropriate format based on the tabulated data.

The defaults for these settings can be changed globally.

To open the **Options** window:

- Windows: Select **Tools** → **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

then click the **Activities** tab and the **Tabulation** node in the tree.

About Quantity Categories

The quantities are sometimes grouped into categories on the Plot Renderer or Table Renderer. Availability of the list and the variables themselves, is based on several factors, including the database selected, the Calculator used, and the type of calculation being performed. Other differences are based on the *Plot type* selected, e.g. what you see on the **Configuration** window changes if you use **Flexible Mode** or **Grouped Mode**. Other plot types do not group the quantities and each Calculator handles the information differently.

When working on a Plot Renderer (e.g. associated to the *Axes* X, Y, and Z) or Table Renderer (associated to *Columns*), there is sometimes the option to choose a quantity group from a list. When applicable, these are the categories:

- All variables
- System variables
- Phase equilibria
- Physical properties
- Kinetic properties
- Elastic properties

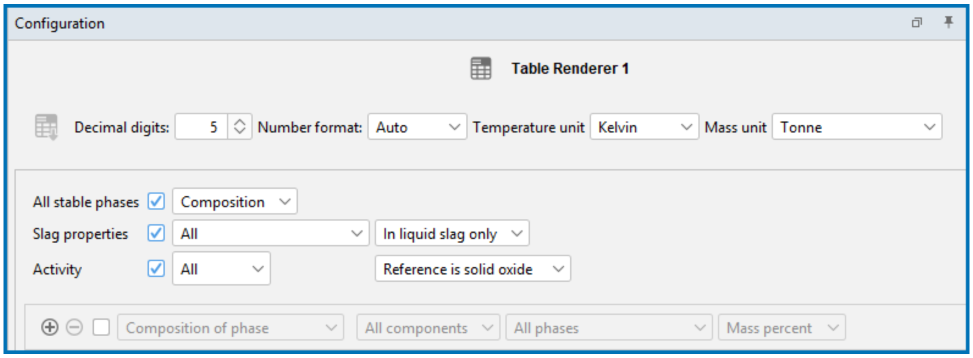
After selecting the group, you next choose from the available variables and continue to define each based on the additional settings specifically available, i.e. select a unit or a phase, and many other options that are only displayed when relevant.

Quantities Groups Available for Plots and Tables

Process Metallurgy Settings

For the **Process Metallurgy Calculator** there are additional settings available.

PMET_01: Basic Oxygen Furnace (BOF). Using version 01b, a Table Renderer is added and on the Process Metallurgy Calculator, changed the *Calculation Type* to **Single**.



Configuration

Table Renderer 1

Decimal digits: 5 Number format: Auto Temperature unit Kelvin Mass unit Tonne

All stable phases ☑ Composition

Slag properties ☑ All In liquid slag only

Activity ☑ All Reference is solid oxide

⊕ ⊖ ☐ Composition of phase All components All phases Mass percent

- Choose a **Temperature unit**: **Kelvin**, **Celsius** or **Fahrenheit**.
- Choose a **Mass unit**: **Tonne**, **Kilogram**, **Gram**, or **Pound**.
- Select the **All stable phases** checkbox and choose **Composition** or **Condensed** from the list.
- Select the **Slag properties** checkbox and choose the associated quantity from the next drop-down list: **All**, **B2**, **B3**, **B4**, **Bas2**, **Bells ratio**, **Ls**, or **Log10 (Sulphur capacity)**.
- Also choose **In liquid slag only**, **In solid slag only**, or **In all slag**.

  Details, including references and equations, are described in Process Metallurgy Slag Properties.

- Select the **Activity** checkbox then from the first list choose a component (or keep the default **All**). Then from the second list select **Reference solid oxide** or **Reference liquid slag**.

  The activity is always given relative to a phase. The liquid slag is always the IONIQ_LIQ phase. The composition set of ION_LIQ depends on the calculation and the slag always contains a high amount of oxygen. The reference phase for the solid oxides depends on the components and it is always listed in the table.

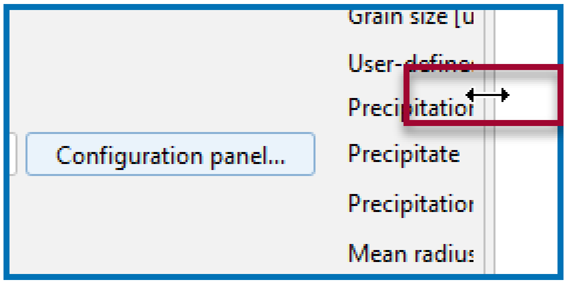
PRECIPITATION CALCULATOR WITH YIELD STRENGTH

When you use a **Precipitation Calculator** and choose **Yield strength** as an *Axis variable*, there are additional settings available.

If you choose **Yield strength** as an *Axis variable*, you can further define the model. Click to expand the drop down list to the right of the *Axis variable*, then select any or all of the checkboxes listed below to plot the respective contributing elements to the yield strength.

Click **Configuration Panel** toggle between the settings options and to further fine-tune the model. These options are described for the Yield Strength Property Model: Simplified Mode Settings and Yield Strength Property Model: Advanced Mode Settings. The greyed out sections (e.g. the **Matrix**, **Precipitate** phases, and **Grain size**) are defined on the **Precipitation Calculator** and cannot be changed.

To see these settings after clicking **Configuration Panel**, you need to expand the **Plot Renderer Configuration** window to the right. Either detach the window to resize, or hover with the mouse until you see the double arrow, then click and drag to expand the window.



- Total yield strength
- Intrinsic strength
- Solid solution strengthening
- Solid solution strengthening FCC
- Solid solution strengthening BCC
- Solid solution strengthening HCP
- Grain boundary strengthening
- Total precipitation strengthening
- Precipitation strengthening per phase
- Constant strength addition

The **P_01: Isothermal Precipitation of Al3Sc** example demonstrates the use of this Yield Strength Model.

Yield Strength Property Model: Simplified Mode Settings

PRECIPITATION CALCULATOR SEPARATE MULTIMODAL PSD AND 3D > 2D

When certain axis variables are selected on the Plot Renderer or Table Renderer that is a successor to the Precipitation Calculator, the **Separate multimodal PSD** and **3D > 2D** checkboxes are available for the Precipitation Module (TC-PRISMA).

Another requirement is that the *Precipitate Phase* **Morphology** is set to **Sphere** on the Precipitation Calculator.

See the specialized section for the Plot Renderer for details.

Precipitation Calculator Plot Renderer

Experimental File Reader

The **Experimental File Reader** activity node is added as a predecessor from the top 🗀 **My Project** node. This allows you to use (or "read") the data contained in an experimental data file (with the file extension `*.EXP`) and then plot the data on one or more Plot Renderers.

> See the Tips and Tricks: How to Plot Experimental Data blog post on our website for useful guidance about this topic.

If you are a Console Mode user, this is the same concept as using the Experimental Data Files (*.POP, *.DOP).

The `EXP` file is a type of data file with information specifying a plotted diagram and it is written in the DATAPLOT graphical language. From this activity node you can plot the EXP file or save a copy of the file to another location.

Creating Activities and Successors and Plotting Experimental Data Files in the *DATPLOT User Guide* included with this documentation set.

How to Plot Using an Experimental Data File

1. Right-click 🗀 **My Project** and from the **Create New Activity** submenu choose **Experimental File Reader**.
2. In the **Configuration** window in the *EXP file* field, enter the name of the EXP file to plot. Or click the **Select Exp file** 🗀 button to navigate to a location on the computer to add the dataset.
3. Once the .EXP file is added, under **Dataset Selection** you can choose to include or exclude specific datasets. Use the **Select/Deslect all datasets** checkbox as required.
4. Right-click the **Experimental File Reader** node and from the **Create New Successor** submenu choose **Plot Renderer**.

   If the source EXP file is changed, you can also click the **Reload the selected EXP file from disk** ⟳ button to refresh the data. If you want to save or export the loaded file, click the **Save EXP file** 🖫 button, then navigate to where you want to save it and give it a file name.

5. In the **Configuration** window click **Perform** or right-click the **Plot Renderer** node and select **Perform**.

General Property Models

? Property Model Calculator

In this section:

About the Property Models

Property Models are used to predict and optimize properties of materials using models stored within the software where the calculations are set up in the Property Model Calculator.

General Models

The following General Property Models are available with the Property Model Calculator.

The **General Models** are available to all users.

To run calculations with the Add-on Property Model Libraries all require a valid maintenance license plus a license for the specific database version: **Nickel Models** (TCNI11 and newer and MOBNI5 and newer; **Noble Metal Alloys Models** (TCNOBL3 and newer); **Steel Models** (TCFE9 and newer + MOBFE4 and newer); **Titanium Models** (TCTI6 and newer).

About the Steel Model Library Property Models, About the Nickel Model Library Property Models, and About the Titanium Model Library Property Models, and About the Noble Metal Alloys Model Library Property Models.

Coarsening

The **Coarsening** Property Model calculates the coarsening rate coefficient K (m^3/s) of a spherical precipitate phase in a matrix phase.

See About the Coarsening Property Model and Coarsening Property Model Settings for background theory and input parameter details.

Columnar to Equiaxed Transition (CET)

The **Columnar to Equiaxed Transition** Property Model calculates the fraction of equiaxed grains that correlates with a certain solidification condition, specifically thermal gradient (G) and solidification growth rate (v).

See About the Columnar to Equiaxed Transition (CET) Property Model and Columnar to Equiaxed Transition (CET) Property Model Settings for background theory and input parameter details.

Crack Susceptibility Coefficient

The **Crack Susceptibility Coefficient** Property Model calculates the hot tearing tendency during solidification.

See About the Crack Susceptibility Coefficient Property Model and Crack Susceptibility Coefficient Property Model Settings for background theory and input parameter details.

Driving Force

The **Driving Force** Property Model calculates the thermodynamic driving force for a phase.

See Driving Force Property Model Settings for input parameter details.

Equilibrium

The **Equilibrium** Property Model calculates the equilibrium for the given conditions. Optionally define additional function definitions.

See Equilibrium Property Model Settings for input parameter details.

Equilibrium with Freeze-in Temperature

The **Equilibrium with Freeze-in Temperature** Property Model calculates equilibrium at the freeze-in temperature and evaluates the properties at a different temperature. The assumption is that diffusion and phase transformations are negligible when changing from the freeze-in-temperature and, therefore, that the phase amounts and compositions of phases are kept at all other temperatures.

See About the Equilibrium with Freeze-in Temperature Property Model and Equilibrium with Freeze-in Temperature Property Model Settings for background information and input parameter details.

Interfacial Energy

The **Interfacial Energy** Property Model estimates the interfacial energy between a matrix phase and a precipitate phase using thermodynamic data from a CALPHAD database.

See About the Interfacial Energy Property Model and Interfacial Energy Property Model Settings for background information and input parameter details.

Liquid and Solidus Temperature

The **Liquid and Solidus Temperature** Property Model is for doing a common calculation. For example, you can easily use uncertainty calculations, vary one or more conditions, and see how that affects the liquidus and solidus temperatures.

See Liquid and Solidus Temperature Property Model Settings for input parameter details.

Phase Transition

The **Phase Transition** Property Model can be used to vary which condition to relax, and then it calculates the point when a new phase may form. It is useful to determine melting temperature, boiling temperature or solubility limits. It returns the phase transformation temperature, or composition, depending on the relaxed condition.

See Phase Transition Property Model Settings for input parameter details.

Scheil

The **Scheil** Property Model is used to calculate solidification under the Scheil assumption. The majority of the Model input parameters are pulled from the Scheil Calculator to offer the outputs of the liquidus/solidus/solidification range so you can explore these in the calculation types of the Property Models.

See Scheil Property Model Settings, and Scheil Advanced Options: Property Models.

Spinodal

The **Spinodal** Property Model calculates the spinodal line.

See About the Spinodal Property Model and Spinodal Property Model Settings for background information and input parameter details.

T-Zero Temperature

The **T-Zero Temperature** Property Model calculates the so-called T_0 line.

See About the T0 Temperature Property Model and T0 Temperature Property Model Settings for background information and input parameter details.

Yield Strength

The **Yield Strength** Property Model calculates yield stress. It returns the calculated yield strength at room temperature for the specified material using the equilibrium values calculated at temperature T (i.e. T is the freeze-in temperature). Then you can further define the following contributions to the total yield stress: precipitation strengthening, solid solution, grain boundary strengthening, and constant addition of strength.

See About the Yield Strength Property Model and Yield Strength Property Model: Simplified Mode Settings or Yield Strength Property Model: Advanced Mode Settings for background information and input parameter details.

Calculation Types

The Property Model Calculator includes these calculation types:

- **Single**: Calculates a single point.
- **One Axis**: Varies a quantity on the X-axis.
- **Grid**: Evaluates two axis variables of the selected quantities in the specified range and number of steps. You can then select to create heat map, contour and 3D plots on the Plot Renderer.
- **Min/Max**: Evaluates the Property Model(s) for all variations of the selected quantities at the given limits. The Mean field is as defined under *Condition Definitions* for the respective quantity. The total minimum and maximum of the Model(s) results are shown in the Event log.
- **Uncertainty**: Evaluates the Property Model(s) where the values of the quantities are sampled from Gaussian distributions. The Mean field is as defined under *Condition Definitions* for the respective quantity. The result is visualized as a histogram or normal probability plot by adding a Plot Render activity.

- **Batch**: Use this to allow for high throughput calculations and read data from a file, such as a spreadsheet. You can include experimental results in the data file, which then can be used to compare to the batch calculation results.

About the Uncertainty Calculations and Plot Types

Examples and Video Tutorials

Thermo-Calc General Property Models Examples Collection

For tutorials about this feature, go to our website or browse the Property Model Calculator playlist on our YouTube channel.

Scheil Advanced Options: Property Models

This topic has advanced settings information for the **Show advanced Scheil options** checkbox that is available for a Property Model **Configuration** windows. The main settings are on the **Configuration** tab.

These settings are based on the Scheil Calculator settings with minor differences in wording or application. See Advanced Options.

For theory or background details about Scheil, start by reviewing Scheil-Gulliver Solidification Calculations.

To view all of these settings, click the **Show advanced Scheil options** checkbox.

TEMPERATURE STEP DURING SCHEIL

Enter a **Temperature step during Scheil** for the Scheil simulation. Temperature step is given in the same unit as the temperature in the **Condition Definitions**.

GLOBAL MINIMIZATION

Global minimization is enabled by default i.e. the **Global minimization** checkbox is selected.

It is recommended to keep global minimization on as it makes the calculation more accurate. However, turn it off if you find that the calculation is taking too long for any particular system, and accuracy is not the highest priority.

For this setting, a global equilibrium test is performed at selected intervals when an equilibrium is reached. By default it is at every 10 th Scheil step but this can be changed using the **Global test interval** setting. The global equilibrium test is also done every time the set of stable phases tries to change. This costs more computer time but the calculations are more robust.

GLOBAL TEST INTERVAL

Use the **Global test interval** setting to change the interval at which a global equilibrium test is done, which by default is every 10th step as long as there are no changes in the set of stable phases. Every time the set of stable phases tries to change, a global equilibrium test is also done regardless of the test interval value chosen. A global equilibrium test means that the calculated equilibrium state obtained by the ordinary minimization calculation is tested against the Global Minimization Technique, and if the result is found unstable then the full global minimization calculation is performed instead.

LIQUID PHASE

The default in the list is the **LIQUID** phase already defined in the chosen database.

SOLID FRACTION FOR EVALUATING LIQUIDUS TEMPERATURE

Enter a value for the **Solid fraction for evaluating liquidus temperature**. A small fraction larger than zero can be used to avoid small amounts of high temperature stable phases for the evaluation of liquidus temperature.

TERMINATE AT FRACTION OF LIQUID PHASE AMOUNT

Enter a value in the field for **Terminate at fraction of liquid phase amount**.

> For **Crack Susceptibility Coefficient** model, the value should not be larger than the setting **Liquid fraction: Smallest for vulnerability**.

MAX NO. OF ITERATIONS

Enter or choose a value for the **Max no. of iterations**. By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.

REQUIRED ACCURACY

The default **Required accuracy** is `1.0E-6`. This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.

SMALLEST FRACTION IN A PHASE

The default **Smallest fraction** (or **Smallest fraction in a phase** for Property Models) is `1.0E-12`. This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions.

The default value for the smallest site-fractions is `1E-12` for all phases except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as `1E-30`.

This default setting is used as a start value in the Scheil Calculator. During simulation, and if there are convergence issues, the value can be decreased.

SMALLEST FRACTION FOR ALLOY COMPOSITION

The default **Smallest fraction for alloy composition** is 1.0E-7. A smallest value assigned to alloy mole/mass fraction in case a smaller input value for an element is entered.

APPROXIMATE DRIVING FORCE FOR METASTABLE PHASES

The **Approximate driving force for metastable phases** checkbox is selected by default. Click to clear the checkbox to change the default as required and based on the options described below.

This setting involves the convergence of metastable phases and affects their driving forces. It can also have an effect on when an equilibrium is considered successful.

The default is to allow an equilibrium with metastable phases that have not converged, as long as the stable phases have converged. This is efficient but often causes approximate values of the driving forces for the metastable phases.

If you change the default, it enforces metastable phases to converge. This gives accurate driving forces for metastable phases as well as stable phases. It can however take a slightly longer time, and if metastable phases do not converge it causes the equilibrium calculation to fail.

About the Coarsening Property Model

Coarsening is a Property Model available when using the Property Model Calculator in Thermo-Calc.

In the coarsening regime where the driving force is capillarity, the change of mean particle radius evolves according to the equation:

$$\bar{r}^3 - \bar{r}_0^3 = Kt$$

Following Morral and Purdy [1994Mor], the rate constant of precipitating β phase in a multicomponent α phase is

$$K = \frac{8\sigma V_m^\beta}{9}\left[\left[c_i^\beta - c_i^\alpha\right]^T [M]^{-1}\left[c_k^\beta - c_k^\alpha\right]\right]^{-1}$$

The mobility matrix *M* is not the same as the mobilites that can be obtained directly from the Diffusion Module (DICTRA). The *M* matrix instead corresponds to the L’’ matrix as defined by Andersson and Ågren [1992And].

Using the u-fractions that is defined as

$$u_k = \frac{x_k}{\sum\limits_{j\in S} x_j}$$

where the summation only is performed over the substitutional elements give the final equation for the coarsening rate coefficient.

$$K = \frac{8\sigma V_m^\beta}{9}\left[\left[u_i^\beta - u_i^\alpha\right]^T [L''^{\alpha}_{jk}]^{-1}\left[u_k^\beta - u_k^\alpha\right]\right]^{-1}$$

The interfacial energy, σ, is calculated using the extended Becker’s model (also available as the **Interfacial Energy** Property Model).

Configuration Settings

The settings are entered on the **Configuration** window for the Property Model Calculator and described in Coarsening Property Model Settings.

Example

For an example, see PM_G_02: Coarsening and Interfacial Energy.

References

[1992And] J.-O. Andersson, J. Ågren, Models for numerical treatment of multicomponent diffusion in simple phases. J. Appl. Phys. 72, 1350–1355 (1992).

[1994Mor] J. E. Morral, G. R. Purdy, Particle coarsening in binary and multicomponent alloys. Scr. Metall. Mater. 30, 905–908 (1994).

Coarsening Property Model Settings

Coarsening is a General Property Model available when using the Property Model Calculator in Thermo-Calc and it calculates the coarsening rate coefficient *K* (m^3/s) of a spherical precipitate phase in a matrix phase.

The output using this Model is the coarsening rate coefficient [m^3/s] for the precipitate phase and the interfacial energy [J/m^2] between matrix and the precipitate phase.

> This Model requires that the thermodynamic database used includes descriptions of molar volume of the matrix and precipitates phases as well as a kinetic database with mobilities for the matrix phase.

Theory and Example

About the Coarsening Property Model

For an example, see PM_G_02: Coarsening and Interfacial Energy.

Configuration Settings

The settings are found on the Property Model Calculator when **Coarsening** is selected under **General Models**.

> When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

MATRIX PHASE

Choose a **Matrix phase**.

PRECIPITATE PHASE

Choose a **Precipitate phase** to calculate its coarsening rate. Click the ⊕ **Add phase** button to add another Precipitate phase. Click the ⊖ **Remove phase** button to remove a phase.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

When selecting quantities on the Plot Renderer or Table Renderer, the quantity names include an abbreviated name for the Property Model it is associated to. This is useful in particular when you are calculating two or more Property Models that share names for the quantities. The short name identifying the specific Property Model is included in parentheses after the name of the quantity. Below are the full and abbreviated names for each Property Model.

For a list of the abbreviations associated to a Property Model, see Result Quantities: Property Model Abbreviations.

Select from these plot quantities:

- **Temperature**
- **Coarsening rate coefficient Ni [m^3/s]** for the precipitate phase.
- **Interfacial energy Ni [J/m^2]** for it to be between the matrix and precipitate phase.

About the Columnar to Equiaxed Transition (CET) Property Model

The **Columnar to Equiaxed Transition** Property Model calculates the fraction of equiaxed grains that correlates with a certain solidification condition, specifically thermal gradient (G) and solidification growth rate (v) (defined as the migration rate of the interface between liquid and primary solid), so that valuable information on the solidification microstructure can be obtained.

This General Model is available when using the Property Model Calculator in Thermo-Calc. The Model formulation consists of two essential steps (1) to determine the dendrite tip radius and tip undercooling, and (2) to apply the calculated undercooling to the CET Model. These are discussed below.

> ❗ Use of this Property Model requires mobility data of liquid for the calculations. For all simulations both a thermodynamic and a mobility (kinetic) database must be selected on the System Definer.

Determine the Dendrite Tip Radius and Tip Undercooling

The first step determines the dendrite tip radius and tip undercooling, which is strongly dependent on v while slightly on G. For this Model, only primary solid is assumed to be stable while other secondary solid phases are ignored. Mullins and Sekerka instability analysis [1964Mul] and marginal stability criterion [1978(a)Lan; 1978(b)Lan; 1978Mül] are used to determine the tip radius. Meanwhile, tip undercooling, ΔT, is also calculated due to constitutional, curvature, and solute trapping effects. The multicomponent extension of this framework is achieved based on the approach developed by Hunziker [2001Hun]. It integrates with both thermodynamic and mobility databases so that key thermodynamic and kinetic properties for multicomponent alloy systems, such as liquidus, liquidus slope, solute partitioning coefficients, and diffusivities of liquid, etc., can be obtained directly from the databases. Solute trapping effects on liquidus, liquidus slope, and solute partitioning are also considered based on the model developed by Aziz [1982Azi] and extended to multicomponent systems.

Apply the Undercooling to the CET Model

The second step is to apply the calculated undercooling, ΔT, to the CET Model. The model developed by Gäumann et al. [2001Gäu] is used, which extended Hunt's model [1984Hun] to include high solidification rate. A slight modification [2018Hai] enables elimination of an adjustment parameter by directly using ΔT. The model correlates G, ΔT(mostly in terms of v), and the fraction of equiaxed grains, ϕ, as

$$G = \frac{1}{n+1}\sqrt[3]{\frac{-4\pi N_0}{3\ln(1-\phi)}}\Delta T\left(1 - \frac{\Delta T_n^{n+1}}{\Delta T^{n+1}}\right)$$

Where three materials related parameters are introduced:

- N_0: number of nucleation sites per unit volume, in the unit of 1/m^3
- ΔT_n: nucleation undercooling, in the unit of K
- n: exponent

Configuration Settings

The settings are entered on the **Configuration** window for the Property Model Calculator and described in Columnar to Equiaxed Transition (CET) Property Model Settings.

Examples

- PM_G_15: Columnar to Equiaxed Transition (CET) of a NiAlCr Alloy
- PM_G_16: Columnar to Equiaxed Transition of a CMSX-4 Alloy
- PM_G_17: Columnar to Equiaxed Transition of an IN718 Alloy

References

[1964Mul] W. W. Mullins, R. F. Sekerka, Stability of a Planar Interface During Solidification of a Dilute Binary Alloy. J. Appl. Phys. 35, 444–451 (1964).

[1978(a)Lan] J. S. Langer, H. Müller-Krumbhaar, Theory of dendritic growth—I. Elements of a stability analysis. Acta Metall. 26, 1681–1687 (1978).

[1978(b)Lan] J. S. Langer, H. Müller-Krumbhaar, Theory of dendritic growth—II. Instabilities in the limit of vanishing surface tension. Acta Metall. 26, 1689–1695 (1978).

[1978Mül] H. Müller-Krumbhaar, J. S. Langer, Theory of dendritic growth—III. Effects of surface tension. Acta Metall. 26, 1697–1708 (1978).

[1982Azi] M. J. Aziz, Model for solute redistribution during rapid solidification. J. Appl. Phys. 53, 1158–1168 (1982).

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[2001Gäu] M. Gäumann, C. Bezençon, P. Canalis, W. Kurz, Single-crystal laser deposition of superalloys: processing–microstructure maps. Acta Mater. 49, 1051–1062 (2001).

[2001Hun] O. Hunziker, Theory of plane front and dendritic growth in multicomponent alloys. Acta Mater. 49, 4191–4203 (2001).

[2018Hai] M. Haines, A. Plotkowski, C. L. Frederick, E. J. Schwalbach, S. S. Babu, A sensitivity analysis of the columnar-to-equiaxed transition for Ni-based superalloys in electron beam additive manufacturing. Comput. Mater. Sci. 155, 340–349 (2018).

Columnar to Equiaxed Transition (CET) Property Model Settings

The **Columnar to Equiaxed Transition** Property Model calculates the fraction of equiaxed grains that correlates with a certain solidification condition, specifically thermal gradient (G) and solidification growth rate (v).

This **General Model** is available when using the Property Model Calculator in Thermo-Calc.

Theory and Examples

For theory, see About the Columnar to Equiaxed Transition (CET) Property Model.

For examples see:

- PM_G_15: Columnar to Equiaxed Transition (CET) of a NiAlCr Alloy
- PM_G_16: Columnar to Equiaxed Transition of a CMSX-4 Alloy,
- PM_G_17: Columnar to Equiaxed Transition of an IN718 Alloy

System Definer Configuration Settings

Use of this Property Model requires mobility data of liquid for the calculations. For all simulations both a thermodynamic and a mobility (kinetic) database must be selected on the System Definer.

Property Model Calculator Configuration Settings

The settings are found on the Property Model Calculator when the **Columnar to Equiaxed Transition** Model is selected under **General Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

PRIMARY PHASE

Select the **Primary phase** from the list. This is the primary solid phase to form the dendrite.

INTERFACIAL ENERGY

Enter a value for the **Interfacial energy [J/m^2]**, which is between the liquid and primary phase. The default is `0.25` J/m^2.

NUMBER OF NUCLEATION SITES

Enter a value for the **Number of nucleation sites [/m^3]** for equiaxed grains per cubic meter. The default is `2.0E15` / m^3.

NUCLEATION UNDERCOOLING

Enter a value for the **Nucleation undercooling [K]**, which is the critical undercooling for nucleation of equiaxed grains. The default is `2.5` K.

EQUIAXED EXPONENT

Enter a value for the **Equiaxed exponent**. The Equiaxed exponent is used in the equation that calculates the fraction of equiaxed grains. This is usually a value between 3 and 5.

SOLVE FOR, TEMPERATURE GRADIENT, AND EQUIAXED FRACTIONS

Select an option from the **Solve for** list (**Equiaxed fraction** or **Thermal gradient**) and then enter the required secondary information as indicated.

- **Equiaxed fraction**: Solve for the equiaxed fraction given the thermal gradient. When **Equiaxed fraction** is selected, then enter a value for the **Temperature gradient**, which is the temperature gradient of the liquid ahead of the dendrite tip. The default is `1000` K/m.
- **Thermal gradient** [K/m]: Solve for the thermal gradient given the equiaxed fraction (s). When **Thermal gradient** is selected, then enter a value for the **Equiaxed fractions**. This finds the thermal gradient for the given equiaxed fractions. The values entered should be between 0.001 and 0.99. If more than one fraction, separate the values with a space. The default is `0.0066 0.49 0.99`.

GROWTH RATE

Select a **Growth rate** from the list then enter a value in the field.

- If **v** is selected, then enter a value for the solidification growth rate, **v**. The default is `0.1` m/s.
- If **log10(v)** is selected, then enter a value for the logarithm of growth rate, **log10(v)**. The default is `-1.0` m/s.

SOLUTE TRAPPING

Select the **Solute trapping** checkbox to enable solute trapping at the tip interface. By default this is not selected.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

When selecting quantities on the Plot Renderer or Table Renderer, the quantity names include an abbreviated name for the Property Model it is associated to. This is useful in particular when you are calculating two or more Property Models that share names for the quantities. The short name identifying the specific Property Model is included in parentheses after the name of the quantity. Below are the full and abbreviated names for each Property Model.

For a list of the abbreviations associated to a Property Model, see Result Quantities: Property Model Abbreviations.

Select from these plot quantities:

- **log10(v) [m/s]**
- **Liquidus**
- **Fraction of equiaxed grains**
- **Tip radius**
- **Thermal gradient**
- **Solidification rate**
- **Dendrite tip undercooling [K]**

About the Crack Susceptibility Coefficient Property Model

The **Crack Susceptibility Coefficient** is a Property Model available when using the Property Model Calculator in Thermo-Calc. It is used to calculate the hot tearing tendency during solidification. The model is based on the publication by Yan and Lin [2006Yan].

Hot tearing is one of the most common and serious defects encountered during the casting of, for example, aluminum alloys. In general, it is defined by the formation of a macroscopic fissure in a casting as a result of stress and the associated strain, generated during cooling, at a temperature above the non-equilibrium solidus.

Crack susceptibility is also referred to as solidification cracking, hot cracking, hot shortness, supersolidus cracking, and shrinkage brittleness [2006Yan].

The Crack Suscebility Coefficient (CSC) is calculated using Scheil results with three different models; Clyne and Davies [1981Cly; 2006Yan] , Kou [2015Kou], and Easton [2014Eas].

Input Parameters, Scheil Settings, and CSC Model Selection

There are these models to choose from as the Crack Susceptibility Coefficient (CSC) Model: **Clyne and Davies**, **Kou**, or **Easton**.

There are also several Scheil settings, including advanced options to choose from. Some additional theory and background is included below to supplement the settings input choices.

Clyne and Davis CSC Model Theory and Background

The original model assumptions are from Clyne and Davis [1981 Clyne]. Later, the experimental hot cracking susceptibility was collected from several sources by Yan and Lin [2006 Yan] and given as a probability 0-100%. The CSC calculated with the current model cannot be compared by absolute values with the experimental number; instead it is best to compare the trends, to see if it is increasing or decreasing. The experimental values are therefore given with relative coordinates and do not map directly to the calculated plot axes.

The following information describes the background when **Clyne and Davies** is chosen as the **CSC Model**.

The **Crack Susceptibility Coefficient** (CSC) was originally proposed by Clyne and Davies [1981Cly] to describe the effects of alloy composition on hot tearing.

The current model is based on the publication by Yan and Lin [2006Yan]. In Thermo-Calc, the CSC is calculated using Scheil and uses assumptions of cooling rates under the thermal conditions that the heat flow is proportional to $\frac{1}{\sqrt{time}}$.

The CSC is defined as $CSC = \frac{tV}{tR}$ where:

- tV is the time during solidification where the casting is vulnerable to cracking, and
- tR is the time available for the stress relief process.

The values for tV and tR are given by the thermal condition, the Scheil results, and the input parameters for the liquid fraction (defined on the **Configuration** window):

- Start of relaxation
- Transition to vulnerability
- Smallest for vulnerability

These liquid fraction parameters are elaborated on next using the results from a simulation using the TCS Al-based Alloy Database (TCAL) and the alloy Al-0.9Cu-10Mg-0.9Ni-12.2Si mass%.

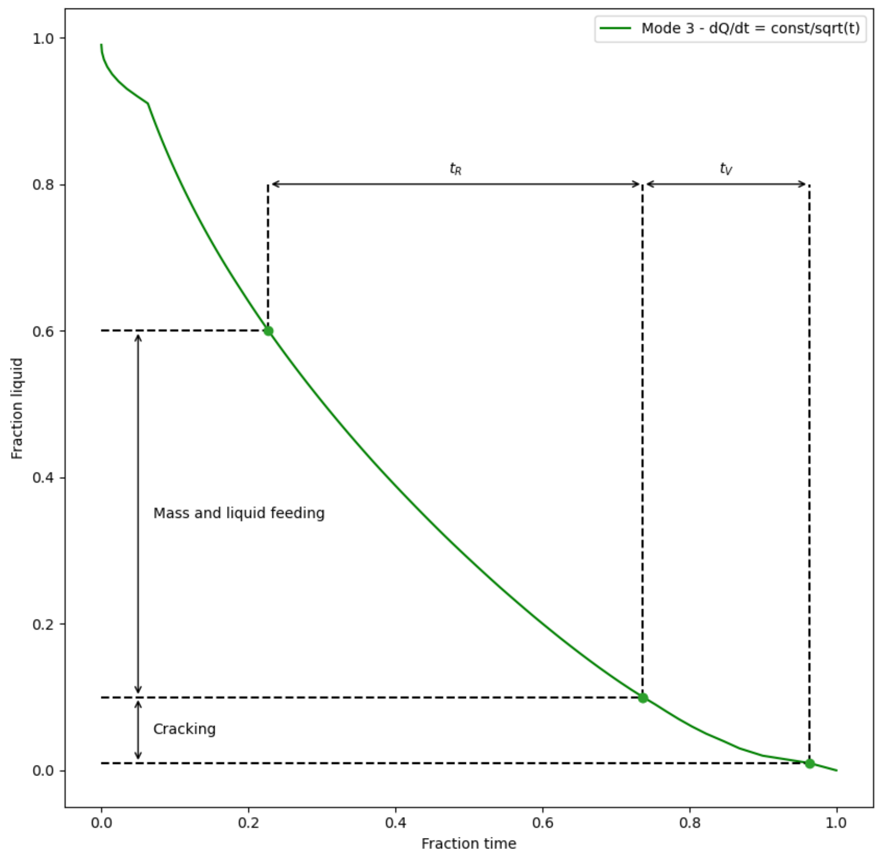


Figure 11: The results of the thermal condition in Mode 3, fraction of liquid, including the addition of lines and arrows to the plot for clarity. See the text for more detail.

Liquid Fraction Parameters

The **Crack Susceptibility Coefficient** Model is based on the concept of the existence of critical time periods during the solidification process when the structure is most vulnerable to cracking.

Clyne and Davies concluded that the mass and liquid feeding readily occurs at liquid volume fractions between about 0.6 and 0.1, so the time spent in these ranges was defined as time-relaxation (tR). At very low volume fractions of liquid, the material is too strong to crack. The authors chose a fraction of liquid between 0.1 and 0.01 as the vulnerable regime, and the time spent defined as tV. See Figure 11 for the results from a simulation using the TCS Al-based Alloy Database (TCAL) and the alloy Al-0.9Cu-10Mg-0.9Ni-12.2Si mass%.

The Scheil simulation takes temperature steps and does not regard time at all. See Figure 12 for the typical Scheil results of amount of solid phases as function of temperature. The simulation is made with the TCS Al-based Alloy Database (TCAL) and the alloy Al-0.9Cu-10Mg-0.9Ni-12.2Si mass%.

A thermal condition is assumed to connect the amount of liquid fraction to fraction of time.

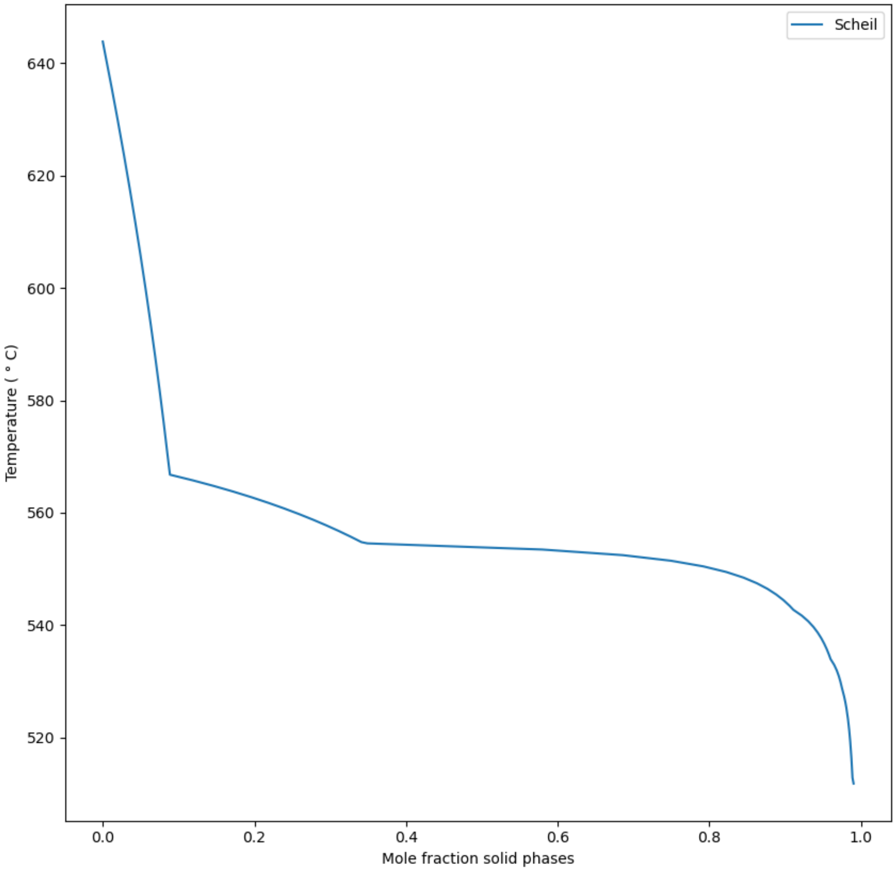


Figure 12: A Scheil simulation result of the mole fraction solid phases vs temperature (°C). See the text for more detail.

Following Clyne and Davies' approach, the cooling rates were then estimated under three different thermal conditions:

- Mode 1 with a constant cooling rate, dT/dt = constant
- Mode 2 with a constant heat flow, , dQ/dt = constant, and
- Mode 3 with a heat flow proportional to 1/sqrt(time)

Then:

- Liquid fraction: Start of relaxation
- Liquid fraction: Transition to vulnerability
- Liquid fraction: Smallest for vulnerability

The crack index can then be obtained from the Scheil simulation results: fraction liquid vs T curve and the thermal condition.

1-fraction solid phases = fraction liquid phase.

Figure 13 can be thought of as the 'master curve' for the connection between fraction of liquid and fraction of time. The limits of the amount of liquid 0.01, 0.1, and 0.6 and the corresponding fraction time are shown for each thermal condition. In Figure 11 , which is a less cluttered plot, the time spent in the relaxation and in the vulnerable regions are marked with lines and arrows for a single thermal mode.

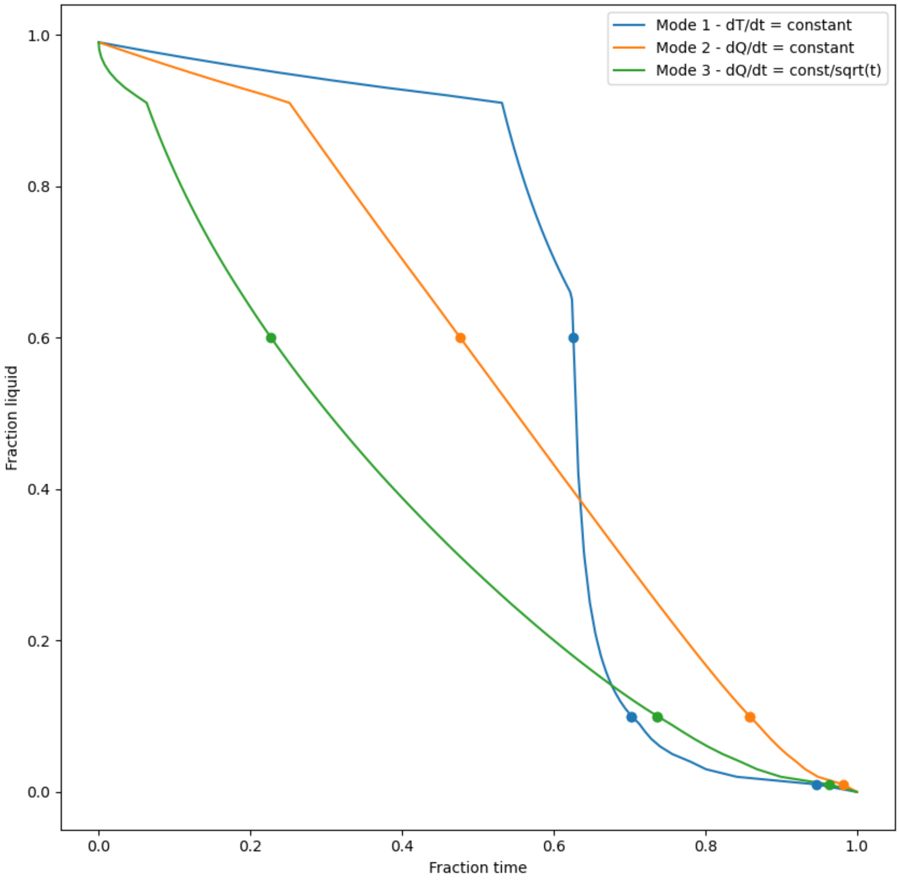


Figure 13: The results of the thermal condition in Modes 1-3, the fraction of time vs the fraction of liquid. See the text for more detail.

Kou CSC Model

When **Kou** is chosen as the **CSC Model**[2015Kou], the cracking susceptibility coefficient is defined as the absolute value of the derivative of the T vs $fs^{0.5}$ curve at the end of the solidification, where

- T = Temperature
- fs = fraction solid

Easton CSC Model

When **Easton** is chosen as the **CSC Model** [2014Eas], the cracking susceptibility coefficient is defined as the integral of $fs(T)$ between $T0$ and Tco where

- fs = fraction solid
- $T0$ = temperature for the solid fraction of a coherent dendrite structure.
- Tco = The temperature for the solid fraction of coalescence of dendrite structure. The user inputs are the solid fraction for coherency and coalescence.

Configuration Settings

The settings are entered on the **Configuration** window for the Property Model Calculator and described in Crack Susceptibility Coefficient Property Model Settings.

Example

For an example, see PM_G_07: Hot Crack Susceptibility.

References

[1981Cly] T. W. Clyne, G. J. Davies, The Influence of Composition on Solidification Cracking Susceptibility in Binary Alloy Systems. Br. Foundrym. 74, 65–73 (1981).

[2006Yan] X. Yan, J. C. Lin, Prediction of hot tearing tendency for multicomponent aluminum alloys. Metall. Mater. Trans. B. 37, 913–918 (2006).

[2014Eas] M. A. Easton, M. A. Gibson, S. Zhu, T. B. Abbott, An A Priori Hot-Tearing Indicator Applied to Die-Cast Magnesium-Rare Earth Alloys. Metall. Mater. Trans. A. 45, 3586–3595 (2014).

[2015Kou] S. Kou, A criterion for cracking during solidification. Acta Mater. 88, 366–374 (2015).

Crack Susceptibility Coefficient Property Model Settings

The **Crack Susceptibility Coefficient** Property Model calculates the hot tearing tendency during solidification.

This General Model is available when using the Property Model Calculator in Thermo-Calc.

When the default **Clyne and Davies** is selected as the **CSC Model**, the calculations use Scheil and assumptions of cooling rates under three different thermal conditions:

- Constant cooling rate, dT/dt = constant
- Constant heat flow, dQ/dt = constant
- Heat flow proportional to 1/sqrt(time)

Theory and Example

For details about this more advanced model, see About the Crack Susceptibility Coefficient Property Model.

For an example, see PM_G_07: Hot Crack Susceptibility.

Configuration Settings

These settings are found on the Property Model Calculator when **Crack Susceptibility Coefficient** is selected under **General Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

Scheil Parameters

These parameters are the same as those used for the Scheil Calculator although some setting names are slightly different.

The advanced Scheil settings are described with Scheil Advanced Options: Property Models.

SCHEIL START TEMPERATURE

Enter a **Scheil start temperature** for the Scheil simulation that is higher than the liquidus temperature of the alloy. Is given in the same unit as the temperature in the **Condition Definitions**.

SCHEIL CALCULATION TYPE

Click to select a **Calculation type**: **Classic Scheil**, **Scheil with back diffusion in primary phase**, or **Scheil with solute trapping**. Then based on this selection, additional settings are made available as indicated.

See Additional Scheil Calculation Type Settings

The back diffusion and solute trapping options require the selection of a mobility database on the System Definer.

FAST DIFFUSERS

Enter the element/component to make as **Fast diffusers**. Include a space between each entry, `C N`, for example, is the default entered for Carbon and Nitrogen to be fast diffusers.

ALLOW DELTA FERRITE TO AUSTENITE TRANSITION IN STEEL

This is available when **Classic Scheil** or **Scheil with back diffusion in primary phase** is selected.

Select the **Allow delta ferrite to austenite transition in steel** checkbox to enable BCC to FCC transition.

This feature should only be used for such steels for which it is reasonable to assume infinitely fast diffusion (equilibrium conditions) when delta ferrite is present. When the **Allow delta ferrite to austenite transition in steel** checkbox is selected in Graphical Mode or the DELTA_FERRITE_AUSTENITE_TRANSITION command used in Console Mode, this essentially assumes that diffusion can be considered (infinitely) fast when delta ferrite is present as a solid phase, i.e assumes an equilibrium condition. After delta ferrite is no longer stable, the usual Scheil assumptions for the selected calculation type are in effect. This setting is therefore not suitable for steels where you DO NOT have a complete BCC to FCC transition during solidification. This setting is also NOT available in combination with solute trapping.

SHOW ADVANCED SCHEIL OPTIONS

Click the **Show advanced Scheil options** checkbox to enter several settings related to Scheil calculations. See Scheil Advanced Options: Property Models.

CSC Model Selection

CSC MODEL

Choose a **CSC Model**: **Clyne and Davies** (the default), **Kou**, or **Easton**.

Then continue with these additional settings:

- For **Clyne and Davies** go to Thermal Mode and Liquid Fraction Parameters (Clyne and Davies).
- For **Easton**, go to Solid Fraction for Coherency and Solid Fraction for Coalescence (Easton)

For details and references about these models, see About the Crack Susceptibility Coefficient Property Model.

Additional Scheil Calculation Type Settings

COOLING RATE (BACK DIFFUSION)

This field is available when **Scheil with back diffusion in primary phase** is selected.

Specify the **Cooling rate** in Kelvin per second (K/s). An increased value moves the result from equilibrium toward a Scheil-Gulliver calculation.

SECONDARY DENDRITE ARM SPACING (BACK DIFFUSION)

This field is available when **Scheil with back diffusion in primary phase** is selected.

The **Secondary dendrite arm spacing** is the distance in meters between two secondary dendrite arms. It is calculated from the cooling rate as c*(cooling rate)$^{-n}$ where c and n are entered in these fields.

Enter values for **Secondary dendrite arm spacing c** and **Secondary dendrite arm spacing n**.

PRIMARY PHASE (BACK DIFFUSION AND SOLUTE TRAPPING)

This field is available when **Scheil with back diffusion in primary phase** or **Scheil with solute trapping** is selected.

The primary solidified phase is the phase where the back diffusion or solute trapping takes place.

If **Automatic** (Scheil Calculator) or **Any phase** (Property Models) is selected (or kept as the default), the program tries to find the phase which gives the most back diffusion or solute trapping.

To override this setting, choose a specific primary phase from the list:

- For back diffusion, only phases with diffusion data can be used as primary phases.
- For solute trapping, only phases that dissolve all elements in the system can be used as primary phases.

SCANNING SPEED AND A (SOLUTE TRAPPING)

These fields are available when **Scheil with solute trapping** is selected.

As needed, enter **Scanning speed** and **α**to define the **Calculated solidification speed**.

On the Scheil Calculator, the **Calculated solidification speed** is shown. For Property Models, below is how the values are calculated from the **Scanning speed** and **α** values entered.

The **Calculated Solidification Speed** is Vs = $V_{scanning}$ * cos(α) m/s, where $V_{scanning}$ is the user specified **Scanning speed** in m/s and **α** is the alpha angle, α, between the solid/liquid boundary and scanning direction.

Thermal Mode and Liquid Fraction Parameters (Clyne and Davies)

These settings are available when **Clyne and Davies** is selected as the **CSC Model**.

THERMAL MODE

Select a **Thermal mode** for the solidification simulation:

- **Constant cooling rate, dT/dt = constant**
- **Constant heat flow, dQ/dt = constant**
- **Heat flow proportional to 1/sqrt(time)** (i.e. heat flow is proportional to $\frac{1}{\sqrt{time}}$)

LIQUID FRACTION FOR START OF RELAXATION

Enter a value for the **Liquid fraction for start of relaxation**.

LIQUID FRACTION TRANSITION TO VULNERABILITY

Enter a value for the **Liquid fraction transition to vulnerability**.

LIQUID FRACTION SMALLEST TO VULNERABILITY

Enter a value for the **Liquid fraction smallest to vulnerability**.

Solid Fraction for Coherency and Solid Fraction for Coalescence (Easton)

These settings are available when **Easton** is selected as the **CSC Model**.

SOLID FRACTION FOR COHERENCY

Enter a value in the **Solid fraction for coherency** field, which is the solid fraction for a coherent dendrite structure. The default is 0.7.

SOLID FRACTION FOR COALESCENCE

Enter a value in the **Solid fraction for coalescence** field, which is the solid fraction for coalescence of a dendrite structure. The default is 0.98.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

When selecting quantities on the Plot Renderer or Table Renderer, the quantity names include an abbreviated name for the Property Model it is associated to. This is useful in particular when you are calculating two or more Property Models that share names for the quantities. The short name identifying the specific Property Model is included in parentheses after the name of the quantity. Below are the full and abbreviated names for each Property Model.

For a list of the abbreviations associated to a Property Model, see Result Quantities: Property Model Abbreviations.

Select from these plot quantities:

- **Composition**
- **Crack Susceptibility coefficient**. The tendency for the material to crack during solidification.
- **Liquidus temperature**
- **Solidus temperature**
- **Freezing range [K]**. The solidification freezing range (Liquidus - Solidus) given in Kelvin.

Driving Force Property Model Settings

Driving Force is a General Property Model available when using the Property Model Calculator in Thermo-Calc and it calculates the thermodynamic driving force for a phase divided by RT.

Example

For an example, see PM_G_03: Driving Force and Interfacial Energy.

Configuration Settings

The settings are found on the Property Model Calculator when **Driving force** is selected under **General Models**.

> When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

MATRIX PHASE

Choose a **Matrix phase**, the single phase region to start in. Select **Any phase** to use the phases that take part of the initial equilibrium or choose a specific phase.

PRECIPITATE PHASE

Choose a **Precipitate phase** to calculate its driving force. Click the plus ⊕ and minus ⊖ buttons to add or remove **Precipitate phases** as needed.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

When selecting quantities on the Plot Renderer or Table Renderer, the quantity names include an abbreviated name for the Property Model it is associated to. This is useful in particular when you are calculating two or more Property Models that share names for the quantities. The short name identifying the specific Property Model is included in parentheses after the name of the quantity. Below are the full and abbreviated names for each Property Model.

For a list of the abbreviations associated to a Property Model, see Result Quantities: Property Model Abbreviations.

Select from these plot quantities:

- **Composition**
- **Interfacial energy Ni [J/m^2]**
- **Driving force per mole** and then choose a unit: **Joule**, **Calorie**, **Electron volt**, **Gigajoule**, **Watt hour**, or **Kilowatt hour**.
- **Normalized driving force**

About the Equilibrium with Freeze-in Temperature Property Model

The **Equilibrium with Freeze-in Temperature** Property Model calculates equilibrium at the freeze-in temperature and evaluates the properties at a different temperature.

The assumption is that diffusion and phase transformations are negligible when changing from the freeze-in-temperature and, therefore, that the phase amounts and compositions of phases are kept at the evaluation temperatures.

Typically, the freeze-in occurs during cooling where equilibrium can be assumed above the freeze-in temperature. This is the default setting and the **Equilibrium above freeze-in temperature** checkbox is automatically selected for this model. Change this default setting (i.e. click to clear the checkbox) when the frozen structure should be evaluated at a higher temperature than the freeze-in temperature.

The electrical resistivity due to phase interface scattering is evaluated as the scattering constant times sum of the interaction between the volume fraction of all the phases. The default value for the constant is 4.0e-8 Ωm. The contribution to thermal conductivity is assumed to be related to that of electrical resistivity, following the Wiedemann-Franz law.

A selection of homogenization functions is available for the evaluation of thermal- and electric-properties. Thermal and electric properties depend on the microstructure and the geometrical representation of phases in the microstructure can be linked to different homogenization functions. The homogenization function is applied on thermal- and electrical-resistivity. The electric conductivity, thermal conductivity, and thermal diffusivity are evaluated from the resistivities.

This Property Model uses thermophysical properties that are included with some Thermo-Calc databases such as the TCS Al-based Alloy Database (TCAL), which is used in the two examples included with your installation. For more information about the availability and the theory, see About Thermophysical Properties Data Parameters, Electrical Resistivity Model, and Thermal Conductivity Model.

Configuration Settings

The settings are entered on the **Configuration** window for the Property Model Calculator and described in Equilibrium with Freeze-in Temperature Property Model Settings.

Examples

For examples, see PM_G_10: Freeze-in Thermal Conductivity and PM_G_11: Freeze-in Electrical Resistivity.

Equilibrium with Freeze-in Temperature Property Model Settings

The **Equilibrium with Freeze-in Temperature** Property Model calculates equilibrium at the freeze-in temperature and evaluates the properties at a different temperature. The assumption is that diffusion and phase transformations are negligible when changing from the freeze-in-temperature and, therefore, that the phase amounts and compositions of phases are kept at all other temperatures.

Theory and Examples

For theory, see About the Equilibrium with Freeze-in Temperature Property Model.

For examples, see:

- PM_G_10: Freeze-in Thermal Conductivity
- PM_G_11: Freeze-in Electrical Resistivity

Configuration Settings

The settings are found on the Property Model Calculator when the **Equilibrium with Freeze-in Temperature** Model is selected under **General Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

FREEZE-IN TEMPERATURE

Enter a **Freeze-in temperature** value in the field. The unit matches those selected under *Condition Definitions*. This is the temperature where the equilibrium is calculated.

The default is 623.15 K (350 °C).

EQUILIBRIUM ABOVE FREEZE-IN TEMPERATURE

The **Equilibrium above freeze-in temperature** checkbox is selected by default and it calculates equilibrium above freeze-in temperature. Click to clear the checkbox when evaluating the frozen-in structure at higher temperatures than the freeze-in temperature.

EVALUATE FOR SINGLE PHASE ONLY

Select the **Evaluate for a single phase only** checkbox to evaluate the properties of a specific phase or deselect to evaluate the properties for the entire system.

PHASE FOR EVALUATION

This setting is available when the **Evaluate for a single phase only** checkbox is selected.

From the **Phase for evaluation** list, select any available phase or **None**.

EQUILIBRIUM MINIMIZATION STRATEGY

Select an **Equilibrium minimization strategy**. The default uses the **Local minimization preferred** option.

The **Minimization Strategy** setting is used to ensure that the most stable minimum under the specified conditions is computed.

With either the *Global test preferred* or *Local minimization preferred* setting, the program cycles through options before it gives up:

- For **Global test preferred** the minimization starts with a global test and if that fails it runs full global minimization.
- For **Local minimization preferred**the minimization starts with a local minimization, in case of failure it tries a global test and finally a full global minimization.

If you choose **Local minimization only** or **Global minimization only**, the program just tries the one setting and gives up if it fails.

For general information about global minimization, see the topic related to the Console Mode command, GLOBAL_MINIMIZATION.

HOMOGENIZATION FUNCTION

The **Homogenization function** is used for the evaluation of the systems thermal and electric properties. The function is applied on thermal- and electrical-resistivity. The electric conductivity, thermal conductivity, and thermal diffusivity are evaluated from the resistivities.

The geometrical interpretation of the Hashin-Shtrikman bounds are concentric spherical shells of each phase.

- **Rule of mixtures (upper Wiener bound)**: the geometrical interpretation are continuous layers of each phase parallel with the direction of evaluation of the property.
- **Inverse rule of mixtures (lower Wiener bound)**: The geometrical interpretation are continuous layers of each phase orthogonal to the direction of evaluation of the property.
- **General lower Hashin-Shtrikman bound**: The outermost shell consists of the phase with the most sluggish property.
- **General upper Hashin-Shtrikman bound**: The innermost shell consists of the phase with the most sluggish property.
- **Hashin-Shtrikman bound with majority phase as matrix phase**: The outermost shell consists of the phase with the highest local volume fraction.

ACCOUNT FOR PHASE INTERFACE SCATTERING

The **Account for phase interface scattering** checkbox is selected by default.

The electrical resistivity due to phase interface scattering is evaluated as the scattering constant times sum of the interaction between the volume fraction of all the phases. The default value for the constant is 4.0e-8 Ωm. The contribution to thermal conductivity is assumed to be related to that of electrical resistivity, following the Wiedemann-Franz law.

PHASE INTERFACE SCATTERING CONSTANT

This setting is available when the **Account for phase interface scattering** checkbox is selected.

The **Phase interface scattering constant** default value is 4.0e-8 Ωm.

SET REFERENCE TEMPERATURE FOR TECHNICAL CTE

This setting is available when the **Account for phase interface scattering** checkbox is selected.

In the field, enter the **Reference temperature for technical CTE**, where CTE is the coefficient of thermal expansion. Typically room temperature is used as the default 293.15 K (20 °C).

DEFINE USER FUNCTIONS

Select the **Define user functions** checkbox to enter up to two **User-defined functions** using the Console Mode syntax.

For an example of user-defined functions, see T_07: User-Defined Functions.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

When selecting quantities on the Plot Renderer or Table Renderer, the quantity names include an abbreviated name for the Property Model it is associated to. This is useful in particular when you are calculating two or more Property Models that share names for the quantities. The short name identifying the specific Property Model is included in parentheses after the name of the quantity. Below are the full and abbreviated names for each Property Model.

For a list of the abbreviations associated to a Property Model, see Result Quantities: Property Model Abbreviations.

Select from these plot quantities:

- **Temperature**
- **Electric resistivity (ohm m)** (Ωm)
- **Electric conductivity (S/m)**
- **Thermal conductivity (W/(mK))**
- **Thermal resistivity (mK/W)**
- **Thermal diffusivity (m^2/s)**
- **Heat capacity (J/mol K))**

- **Volume (m^3/mol)**
- **Density (g/cm^3)**
- **Linear CTE (technical) (1/K)**: Fractional change of length per unit temperature change. Calculated as (L1-L0)/(T1-T0)/L0, where L0 is the length at a reference temperature T0. T0 is by default equal to room temperature. Assumed Isotropic material.
- **Linear CTE (physical) (1/K)**: Fractional change of length per unit temperature change. Assumed Isotropic material.
- **Volumetric CTE (physical) (1/K)**: Fractional change of volume per unit temperature change.
- **User-defined function** and **2nd user-defined function**: Available when the **Define user functions** checkbox is selected and the functions are defined.

Elastic moduli is available to plot when the thermodynamic database selected includes elastic properties. However, even if the database does not have elastic constants, the quantity is visible to select from the list even. In this case there is a message in the Event Log to indicate there is no elastic data and the value will be NaN.

Equilibrium Property Model Settings

Equilibrium is a General Property Model available when using the Property Model Calculator in Thermo-Calc and it calculates the equilibrium for the given conditions.

When you use this Model with the **Property Model Calculator**, it is the same calculation result as when you are using an **Equilibrium Calculator** with the **Single equilibrium** calculation type.

Configuration Settings

The settings are found on the Property Model Calculator when **Equilibrium** is selected under **General Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

EQUILIBRIUM MINIMIZATION STRATEGY

Select an **Equilibrium minimization strategy**. The default uses the **Global test preferred** option. For this Property Model, and for either Global option, also enter the **Max number of global gridpoints**, where the default is 2000.

The **Minimization Strategy** setting is used to ensure that the most stable minimum under the specified conditions is computed.

With either the *Global test preferred* or *Local minimization preferred* setting, the program cycles through options before it gives up:

- For **Global test preferred** the minimization starts with a global test and if that fails it runs full global minimization.
- For **Local minimization preferred**the minimization starts with a local minimization, in case of failure it tries a global test and finally a full global minimization.

If you choose **Local minimization only** or **Global minimization only**, the program just tries the one setting and gives up if it fails.

For general information about global minimization, see the topic related to the Console Mode command, GLOBAL_MINIMIZATION.

QUANTITY DEFINITIONS

For *Quantity Definitions* define **Q1**. Click the ⊕ **Add** button to define additional items and the ⊖ **Remove** button to delete items.

Then from the lists, choose the variable for each quantity to define. The quantities are called **Q1**, **Q2**, **Q3** and so on.

All quantities that normally can be obtained from an equilibrium calculation can also be obtained when plotting the results.

FUNCTION DEFINITIONS

For *Function Definitions*, define **Function 1**. Click the ⊕ **Add** button to define additional items and the ⊖ **Remove** button to delete items. In the left field edit the default name of each function and enter the function itself in the right field after the equal sign.

To learn about using variables and functions, in Graphical Mode, see T_07: User-Defined Functions and in Console Mode, see example 44.

You can also use Console Mode syntax when entering the function. See Parameters, Functions, and Variables for details.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

All quantities that normally can be obtained from an equilibrium calculation can also be obtained when plotting the results as well as the defined functions.

Conditions Tab Settings

About the Interfacial Energy Property Model

Interfacial Energy is a Property Model available when using the Property Model Calculator in Thermo-Calc.

Interfacial energy is an important parameter used in precipitation simulations to calculate the rates of nucleation, growth/dissolution, and coarsening. The value of interfacial energy can vary dramatically (usually between 0.01 to 2.0 J/m^2).

The extended Becker's model functions to estimate coherent interfacial energy by using thermodynamic data from existing CALPHAD thermodynamic databases:

$$\sigma_c = \frac{n_s z_s}{N_A z_l} \Delta E_s$$

where σ_c is the coherent interfacial energy, n_s is the number of atoms per unit area at the interface, z_s is the number of cross bonds per atom at the interface, z_l is the coordination number of an atom within the bulk crystal lattice, and ΔE_s is the energy of solution in a multicomponent system involving the two phases being considered [1938Bec].

Reference

[1938Bec] R. Becker, Die Keimbildung bei der Ausscheidung in metallischen Mischkristallen. Ann. Phys. 424, 128–140 (1938).

Configuration Settings

The settings are entered on the **Configuration** window for the Property Model Calculator and described in Interfacial Energy Property Model Settings.

Example

For an example, see PM_G_03: Driving Force and Interfacial Energy.

Interfacial Energy Property Model Settings

Interfacial Energy is a Property Model available when using the Property Model Calculator in Thermo-Calc and is used to estimate the interfacial energy between a matrix phase and a precipitate phase using thermodynamic data from a CALPHAD database. The approximation model is based on Becker's bond energy approach and is also available in Precipitation Module (TC-PRISMA).

> In the actual calculation, the coefficients taken distinguish between only bcc and fcc structure for the (110) and (111) lattice plane, respectively.

For other planes and/or other phases, the estimate is approximate. In most situations, it is recommended to perform calibrations against some experimental data because the interfacial energy is dependent on so many factors that are ignored in the estimation, for example entropy, incoherency, orientation, and curvature, etc. Uncertainty factors must also be considered as thermodynamic data in CALPHAD databases are not always accurate.

Theory and Example

For theory see About the Interfacial Energy Property Model. For an example, see PM_G_03: Driving Force and Interfacial Energy.

Configuration Settings

The settings are found on the Property Model Calculator when **Interfacial energy** is selected under **General Models**.

> When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

MATRIX PHASE

Choose a **Matrix phase** to calculate the interfacial energy [J/m^2].

PRECIPITATE PHASE

Choose a **Precipitate phase** to calculate the interfacial energy [J/m^2].

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

When selecting quantities on the Plot Renderer or Table Renderer, the quantity names include an abbreviated name for the Property Model it is associated to. This is useful in particular when you are calculating two or more Property Models that share names for the quantities. The short name identifying the specific Property Model is included in parentheses after the name of the quantity. Below are the full and abbreviated names for each Property Model.

For a list of the abbreviations associated to a Property Model, see Result Quantities: Property Model Abbreviations.

Select from these plot quantities:

- **Temperature**
- **Interfacial energy Ni [J/m^2]** for it to be between the matrix and precipitate phase.

Liquid and Solidus Temperature Property Model Settings

Liquidus and solidus temperature is a Property Model available when using the Property Model Calculator in Thermo-Calc. It calculates the equilibrium solidification range in terms of temperature. If only the liquidus temperature is required, the calculation times are reduced.

Configuration Settings

The settings are found on the Property Model Calculator when **Liquidus and solidus temperature** is selected under **General Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

ONLY CALCULATE LIQUIDUS TEMPERATURE

Select the **Only calculate liquidus temperature** checkbox as required. When selected, this improves the calculation speed but the solidus is not calculated.

LIQUID PHASE

Choose the **Liquid phase** of the system. This is a fallback choice. Normally this should be handled automatically, even if multiple liquid phases are present.

UPPER TEMPERATURE SEARCH LIMIT

Enter an **Upper temperature search limit** to calculate for a temperature above liquidus for any of the considered compositions. This needs to be in the fully liquid state.

MAX. NUMBER OF ITERATIONS

Enter a **Max. number of iterations**, which is the maximum number of phase transformation iterations performed. The default is 10.

GLOBAL MINIMIZATION (LIQUIDUS AND SOLIDUS)

Select the **Global minimization for liquidus** and/or **Global minimization for solidus** checkboxes to find all phases present in the equilibria.

> Selecting one or both checkboxes can significantly slow down the calculations but ultimately it produces more reliable results.

> Global minimization recommendation: First try to calculate without global minimization, then if inaccuracies occur, switch global minimization on. Problems mostly occur if many phases are present at a given temperature.

SUSPEND GAS PHASE

Select the **Suspend gas phase** checkbox as required. The occurrence of a gas phase may mislead the liquidus temperature determination. If the presence of the gas phase is absolutely required, you can activate it and then choose a user-defined phase.

GAS PHASE

Choose a **Gas phase** from the list.

PRINT RESULTS IN EVENT LOG

Select the **Print results in Event Log** checkbox to display/include all results in the Event Log window. This includes the **First solidified phase**, **Liquidus (K)**, **Solidus (K)**, and **Composition** information. Choose the **Output type**: **Single row** or **Full list for each iteration**.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

When selecting quantities on the Plot Renderer or Table Renderer, the quantity names include an abbreviated name for the Property Model it is associated to. This is useful in particular when you are calculating two or more Property Models that share names for the quantities. The short name identifying the specific Property Model is included in parentheses after the name of the quantity. Below are the full and abbreviated names for each Property Model.

For a list of the abbreviations associated to a Property Model, see Result Quantities: Property Model Abbreviations.

Select from these plot quantities:

- **Composition**
- **Temperature**
- **Liquidus temperature**
- **Solidus temperature**

Phase Transition Property Model Settings

The **Phase Transition** Property Model is available when using the Property Model Calculator in Thermo-Calc. By varying which condition to relax, it calculates the point when a new phase may form. It is useful to determine melting temperature, boiling temperature or solubility limits. It returns the phase transformation temperature, or composition, depending on the relaxed condition.

For an example, see PM_G_01: Phase Transition.

Configuration Settings

The settings are found on the Property Model Calculator when **Phase transition** is selected under **General Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

MATRIX PHASE

Choose a **Matrix phase**, the single phase region to start in. Select **Any phase** to use the phases that take part of the initial equilibrium or choose a specific phase.

PHASE TO FORM

For the new **Phase to form**, select **Any phase** or choose a specific phase.

CONDITION TO VARY

Choose a composition or temperature **Condition to vary** when calculating the phase transition.

SUSPEND ALL OTHER PHASES

Select the **Suspend all other phases** checkbox to suspend the phases that are not of interest, which allows for a faster calculation. However, this could mean that metastable equilibria are in fact calculated.

> It is best practice to suspend phases on the **System Definer** by selecting the applicable phases on the **Phases and Phase Constitution** tab.

SEARCH DIRECTION

For the composition or temperature condition being varied, choose the **Search direction** to be in a **Positive**, **Negative**, or **Positive and Negative** direction.

> The start value is taken from *Condition Definitions*. The closer the start value is to the actual transition point, the more likely it is that the model will find the transition. Note that the phase transition for a given phase may actually occur in the opposite direction from the selected one.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

When selecting quantities on the Plot Renderer or Table Renderer, the quantity names include an abbreviated name for the Property Model it is associated to. This is useful in particular when you are calculating two or more Property Models that share names for the quantities. The short name identifying the specific Property Model is included in parentheses after the name of the quantity. Below are the full and abbreviated names for each Property Model.

For a list of the abbreviations associated to a Property Model, see Result Quantities: Property Model Abbreviations.

Select from these plot quantities:

- **Composition**
- **Temperature**
- **Relaxed condition: Composition (fraction)**
- **Relaxed condition: Temperature**

> Since only one variable can serve as a **Relaxed condition** per calculation, the quantity that is not relaxed has a NaN result in its corresponding result quantity. The **Temperature** result quantity inherits the unit set in the conditions while the **Composition** result quantity inherits the normalization (mole or mass) but always returns a fraction.

Scheil Property Model Settings

Scheil is a Property Model available when using the Property Model Calculator in Thermo-Calc. It is used to calculate solidification under the Scheil assumption. The majority of the Model input parameters are taken from the Scheil Calculator to offer the outputs of the liquidus/solidus/solidification range so you can explore these in the calculation types of the Property Models.

For theory or background details about Scheil, start by reviewing Scheil-Gulliver Solidification Calculations.

Configuration Settings

The settings are found on the Property Model Calculator when **Scheil** is selected under **General Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

The advanced Scheil settings are described with Scheil Advanced Options: Property Models.

These parameters are the same as those used for the Scheil Calculator although some setting names are slightly different.

SCHEIL START TEMPERATURE

Enter a **Scheil start temperature** for the Scheil simulation that is higher than the liquidus temperature of the alloy. Is given in the same unit as the temperature in the **Condition Definitions**.

CALCULATION TYPE

Click to select a **Calculation type**: **Classic Scheil**, **Scheil with back diffusion in primary phase**, or **Scheil with solute trapping**. Then based on this selection, additional settings are made available as indicated.

> The back diffusion and solute trapping options require the selection of a mobility database on the System Definer.

FAST DIFFUSERS

Enter the element/component to make as **Fast diffusers**. Include a space between each entry, `C N`, for example, is the default entered for Carbon and Nitrogen to be fast diffusers.

CALCULATE TO

Use the **Calculate to** setting to choose from where the calculation should end, **End of Scheil** or **Temperature below solidus**.

- **End of Scheil** stops the calculation when the Scheil calculation is finished.
- **Temperature below solidus** is where a frozen structure is assumed below solidus. When this is selected also enter a **Temperature below solidus** in the field. The default is `298.15`.

ALLOW DELTA FERRITE TO AUSTENITE TRANSITION IN STEEL

This is available when **Classic Scheil** or **Scheil with back diffusion in primary phase** is selected.

Select the **Allow delta ferrite to austenite transition in steel** checkbox to enable BCC to FCC transition.

> ❗ This feature should only be used for such steels for which it is reasonable to assume infinitely fast diffusion (equilibrium conditions) when delta ferrite is present. When the **Allow delta ferrite to austenite transition in steel** checkbox is selected in Graphical Mode or the DELTA_FERRITE_AUSTENITE_TRANSITION command used in Console Mode, this essentially assumes that diffusion can be considered (infinitely) fast when delta ferrite is present as a solid phase, i.e assumes an equilibrium condition. After delta ferrite is no longer stable, the usual Scheil assumptions for the selected calculation type are in effect. This setting is therefore not suitable for steels where you DO NOT have a complete BCC to FCC transition during solidification. This setting is also NOT available in combination with solute trapping.

SHOW ADVANCED SCHEIL OPTIONS

Click the **Show advanced Scheil options** checkbox to enter several settings related to Scheil calculations. See Scheil Advanced Options: Property Models.

COOLING RATE (BACK DIFFUSION)

This field is available when **Scheil with back diffusion in primary phase** is selected.

Specify the **Cooling rate** in Kelvin per second (K/s). An increased value moves the result from equilibrium toward a Scheil-Gulliver calculation.

SECONDARY DENDRITE ARM SPACING (BACK DIFFUSION)

This field is available when **Scheil with back diffusion in primary phase** is selected.

The **Secondary dendrite arm spacing** is the distance in meters between two secondary dendrite arms. It is calculated from the cooling rate as $c*(\text{cooling rate})^{-n}$ where c and n are entered in these fields.

Enter values for **Secondary dendrite arm spacing c** and **Secondary dendrite arm spacing n**.

PRIMARY PHASE (BACK DIFFUSION AND SOLUTE TRAPPING)

This field is available when **Scheil with back diffusion in primary phase** or **Scheil with solute trapping** is selected.

The primary solidified phase is the phase where the back diffusion or solute trapping takes place.

If **Automatic** (Scheil Calculator) or **Any phase** (Property Models) is selected (or kept as the default), the program tries to find the phase which gives the most back diffusion or solute trapping.

To override this setting, choose a specific primary phase from the list:

- For back diffusion, only phases with diffusion data can be used as primary phases.
- For solute trapping, only phases that dissolve all elements in the system can be used as primary phases.

SCANNING SPEED AND A (SOLUTE TRAPPING)

These fields are available when **Scheil with solute trapping** is selected.

As needed, enter **Scanning speed** and **α**to define the **Calculated solidification speed**.

> On the Scheil Calculator, the **Calculated solidification speed** is shown. For Property Models, below is how the values are calculated from the **Scanning speed** and **α** values entered.

The **Calculated Solidification Speed** is Vs = $V_{scanning}$ * cos(α) m/s, where $V_{scanning}$ is the user specified **Scanning speed** in m/s and **α** is the alpha angle, α, between the solid/liquid boundary and scanning direction.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

When selecting quantities on the Plot Renderer or Table Renderer, the quantity names include an abbreviated name for the Property Model it is associated to. This is useful in particular when you are calculating two or more Property Models that share names for the quantities. The short name identifying the specific Property Model is included in parentheses after the name of the quantity. Below are the full and abbreviated names for each Property Model.

For a list of the abbreviations associated to a Property Model, see Result Quantities: Property Model Abbreviations.

Select from these plot quantities:

- **Temperature**
- **Liquidus temperature**
- **Solidus temperature**
- **Freezing range [K]**. The solidification freezing range (Liquidus - Solidus) given in Kelvin.
- **Volume fraction of solid phases**: The volume fraction of solid phases (evaluated at the lowest temperature from the simulation)
- **Mole fraction of solid phases**: The mole fraction of solid phases (evaluated at the lowest temperature from the simulation)
- **Total fraction of solid phases**: The total mole fraction of solid phases (evaluated at the lowest temperature from the simulation)
- **Eutectic fraction**: Eutectic fraction at eutectic point (evaluated using Gibbs phase rule).
- **Electric resistivity (ohm m)**
- **Electric conductivity (S/m)**
- **Thermal conductivity (W/mK))**
- **Thermal resistivity (MK/W)**
- **Thermal diffusivity (m2/s)**
- **Volumetric shrinkage (vol-%)**

About the Spinodal Property Model

Spinodal is a Property Model available when using the Property Model Calculator in Thermo-Calc and it calculates the spinodal line.

The spinodal is defined by the condition where the second derivative of Gibbs free energy is zero (`d2G/dx2 = 0`). The locus of these points is known as the *spinodal curve*.

With this Model up to two spinodal solutions can be found. When searching for the spinodal you can vary the temperature or a composition in mass percent, mole percent, mass fraction, or mole fraction (e.g. mass percent Fe, mole percent Fe, and so forth).

When within the miscibility gap, but above the spinodal curve, phase transformation occur by classical nucleation and growth of the spinodal phase. When within the miscibility gap, but below the spinodal curve, the phase transformation occur by spinodal decomposition of the spinodal phase.

The microstructure evolution of spinodal decomposition can be calculated with the phase field method. For some background information see [2018Bar].

Configuration Settings

The settings are entered on the **Configuration** window for the Property Model Calculator and described in Spinodal Property Model Settings.

Example

For an example, see PM_G_08: Spinodal.

Reference

[2018Bar] T. Barkar, PhD thesis, Modelling phase separation in Fe-Cr alloys: A continuum approach, KTH Royal Institute of Technology, Sweden (2018).

Spinodal Property Model Settings

Spinodal is a General Property Model available when using the Property Model Calculator in Thermo-Calc and it calculates the spinodal line.

Theory and Example

For theory, see About the Spinodal Property Model. For an example, see PM_G_08: Spinodal.

Configuration Settings

These settings are found on the Property Model Calculator when **Spinodal** is selected under **General Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

SPINODAL PHASE

From the **Spinodal phase** list select the applicable phase you want to search for the spinodal.

CONDITION TO VARY

From the **Condition to vary** list select an option to vary when searching for the spinodal. Up to two spinodals can be found. These options are **Temperature** or those based on the **Composition** (e.g. Fe, Cr, and so forth) and **Composition unit** (i.e. Mass percent, Mole percent, Mass fraction, or Mole fraction).

MANUAL SEARCH LIMITS

The **Manual search limits** checkbox is not selected by default and this sets automatic search limits.

Select the checkbox to enter user-defined search limits in the fields. Enter the **Lower condition limit** and **Upper condition limit**. Then enter the number of steps when estimating the position(s) of the spinodal(s)in the **Steps when estimating spinodal** field.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

When selecting quantities on the Plot Renderer or Table Renderer, the quantity names include an abbreviated name for the Property Model it is associated to. This is useful in particular when you are calculating two or more Property Models that share names for the quantities. The short name identifying the specific Property Model is included in parentheses after the name of the quantity. Below are the full and abbreviated names for each Property Model.

For a list of the abbreviations associated to a Property Model, see Result Quantities: Property Model Abbreviations.

Select from these plot quantities:

- **Composition**
- **Spinodal temperature**: The first spinodal when the search condition is temperature.
- **Spinodal temperature - 2nd solution**: The second spinodal when the search condition is temperature.
- **Spinodal**: The first spinodal regardless of search condition type.
- **Spinodal - 2nd solution**: The second spinodal regardless of search condition type.

About the T_0 Temperature Property Model

T-Zero Temperature is a Property Model available when using the Property Model Calculator in Thermo-Calc and it calculates the so-called T_0 line.

The T_0 temperature is defined as the temperature where two phases of identical chemical composition have the same molar Gibbs free energy. This temperature is an important quantity in the field of diffusionless phase transformations, e.g. martensitic transformation, since it is the upper limit where diffusionless phase transformations can occur.

Vary Temperature or Conditions

With this Model up to two solutions can be found. When searching for T_0 you can vary the condition of temperature or element composition in units of mass percent (e.g. mass percent Fe). This is managed using the settings **Condition to vary** and in some cases, **Manual search limits**.

When **Temperature** is the varied condition, T_0 is obtained as a solution. When a specific composition is selected as the condition to vary, then the temperature(s) is calculated when the T_0 condition is fulfilled. So the resulting temperature is equal to T_0.

In most cases the curvature of the Gibbs energies of the two phases is different and results in multiple solutions for T_0. If you keep the default settings (*Condition to vary* → *Temperature* and with no manual search limits) the Property Model Calculator can store up to two solutions. If the solution of interest is not calculated, including **Manual search limits** and/or changing the condition to vary to one of the listed compositions, allows you to find the solution of interest.

Gibbs Energy Addition

There is also an option to include a Gibbs energy addition to the second phase, which allows for inclusion of an energy barrier for martensitic phase transformations. This is done using the **Energy addition second phase [J/mol]** setting.

The energy addition field in Graphical Mode corresponds to the Console Mode command ADVANCED_OPTIONS PHASE_ADDITION (see EQUILIBRIUM_CALCUL for information). However, the energy addition can also be composition- and/or temperature-dependent, which is not possible in Console Mode. In addition, Property Models are not available in Console Mode. However, You can access the functionality using methods available with an applicable API such as TC-Python or TC-Toolbox for MATLAB®

Configuration Settings

The settings are entered on the **Configuration** window for the Property Model Calculator and described in T0 Temperature Property Model Settings.

Examples

For examples, see PM_G_09: T-Zero Temperature and PM_G_14: Ti-Fe T-Zero Martensite

T_0 Temperature Property Model Settings

T-Zero Temperature is a Property Model available when using the Property Model Calculator in Thermo-Calc and it calculates the so-called T_0 line.

Theory and Examples

For theory see About the T0 Temperature Property Model.

For examples, see:

- PM_G_09: T-Zero Temperature
- PM_G_14: Ti-Fe T-Zero Martensite

Configuration Settings

These settings are found on the Property Model Calculator when **T-Zero Temperature** is selected under **General Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

FIRST PHASE

From the **First phase** list select the applicable phase you want to search for the evaluation of Gibbs energy.

SECOND PHASE

From the **Second phase** list select the applicable phase you want to search for the evaluation of Gibbs energy.

ENERGY ADDITION SECOND PHASE

Use the **Energy addition second phase [J/mol]** field to include a Gibbs energy addition to the second phase. This allows for inclusion of an energy barrier for martensitic phase transformations.

For an example of this see PM_G_14: Ti-Fe T-Zero Martensite.

CONDITION TO VARY

From the **Condition to vary** list select an option to vary when searching for the solution (or root). Up to two solutions can be found. These options are **Temperature** or those based on the *Composition* + *Composition unit* for example **Mass percent Fe**, **Mass percent Cr**, **Mass percent Ni**, and so forth.

When **Temperature** is the varied condition, T_0 is obtained as a solution. When a specific composition is selected as the condition to vary, then the temperature(s) is calculated when the T_0 condition is fulfilled. So the resulting temperature is equal to T_0.

In most cases the curvature of the Gibbs energies of the two phases is different and results in multiple solutions for T_0. If you keep the default settings (*Condition to vary* → *Temperature* and with no manual search limits) the Property Model Calculator can store up to two solutions. If the solution of interest is not calculated, including **Manual search limits** and/or changing the condition to vary to one of the listed compositions, allows you to find the solution of interest.

MANUAL SEARCH LIMITS

The **Manual search limits** checkbox is not selected by default and this sets automatic search limits.

Select the checkbox to enter user-defined search limits in the fields. Enter the **Lower condition limit** and **Upper condition limit**. Then in the **Steps when estimating root(s)** field, enter the number of steps in a linear grid when estimating the position(s) of the conditions.

Root means a solution of T_0, so a composition and temperature where the Gibbs energies are the same. In other words, it finds the "root(s)" where the two selected phases have equal Gibbs energy. Think of the "root" as the conditions (temperature, composition) where the Gibbs energy of the two selected phases intersect, i.e. have equal Gibbs energies.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

When selecting quantities on the Plot Renderer or Table Renderer, the quantity names include an abbreviated name for the Property Model it is associated to. This is useful in particular when you are calculating two or more Property Models that share names for the quantities. The short name identifying the specific Property Model is included in parentheses after the name of the quantity. Below are the full and abbreviated names for each Property Model.

For a list of the abbreviations associated to a Property Model, see Result Quantities: Property Model Abbreviations.

Select from these plot quantities:

- **Composition**, when the search condition is temperature
- **Temperature**, when the search condition is composition (in this case temperature is equal to T-Zero.
- **T-Zero**: The first root (solution) when the search condition is temperature.
- **T-Zero - 2nd solution**: The second root (solution) when the search condition is temperature.
- **Varied condition**: The first varied condition regardless of search condition type.
- **Varied condition - 2nd solution**: The second varied condition regardless of search condition type.

About the Yield Strength Property Model

The **Yield Strength** Model is a general model to estimate the yield stress of a material that considers these contributions to the overall yield stress of the material:

- Intrinsic strength (σ_i) for the pure elements,
- Grain boundary strengthening (σ_{gb}),
- Solid solution strengthening (σ_{ss}),
- Precipitation strengthening (σ_p), and
- A user set, constant strength contribution (σ_c).

The temperature (T) is used to evaluate the equilibrium state of the system, and the resulting compositions and phase fractions are subsequently used in the evaluation of mechanical properties.

It returns the calculated yield strength at room temperature for the specified material using the equilibrium values calculated at temperature T (i.e. T is the freeze-in temperature).

Below follows a short summary for each of the contributions.

Intrinsic Strength

The *intrinsic strength* model formulation for this Property Model corresponds to a surface of reference with end-members. For example, for FCC_A1 modeled as (Fe,Ti)(C,Va), the intrinsic strength is a linear combination (as given by the composition) of Fe:Va (i.e. pure FCC Fe), Ti:Va (i.e. pure FCC Ti), Fe:C (i.e., FCC FeC) and Ti:C (i.e., FCC TiC). With such an implementation, it is possible to calculate yield strength for materials with a significant fraction of hard phases, such as carbides, embedded in a soft matrix and the intrinsic strengthening effect of interstitial elements.

The general form of the intrinsic strength model follows in the spirit of the Compound Energy Formalism (CEF) surface of reference term, where the intrinsic strength for, e.g., a two-sublattice phase model would correspond to:

$$\sigma_{\text{intrinsic}} = \Sigma_{i,j}\sigma_{i:j}y'_i y''_j$$

Such a formulation means that the intrinsic strength depends on the calculated site fractions from, e.g., an equilibrium calculation.

Phases with Assessed Intrinsic Strength

Not all compound phases are yet assessed in terms of intrinsic strength. The following phases are assessed: BCC_A2, CEMENTITE_D011, FCC_A1, FCC_L12, HCP_A3, M23C6_D84, M3C2_D510, M6C_E93, M7C3_D101, MC_SHP, MB2_C32, MOB2_C32, M3B2_D5A, M2B_CB, and MB_B33.

Temperature Dependence for Pure Elements

The following pure elements can be used to evaluate yield strength at non-room temperature conditions:

- Ag, Al, Au, Be, Ce, Co, Cr, Cu, Dy, Er, Fe, Gd, Hf, Ho, Ir, La, Mg, Mo, Nb, Nd, Ni, Pd, Pt, Rh, Sm, Ta, Ti, U, V, W, Y, Zn, and Zr

The temperature dependence is of the form:

$$ys_{pure} = A * exp(-B/T)$$

and is available for the listed pure elements where A and B are fitted to data from [1968Sam; 2017Wu]. This improves the results for evaluated yield strength at non-room temperature conditions.

The calculated solid solution strength can differ from versions of Thermo-Calc prior to 2022b where the pure element strength from Cordero et al. was used [2016Cor]. This is especially noticeable for pure element or dilute solution calculations. The pure element strength is only evaluated for FCC, BCC, and HCP.

Compound end-members of the intrinsic model are not modeled as temperature dependent, however, this should have only a small effect on most alloys.

Constant Addition of Strength

The *constant strength contribution* parameter, σ_c, is set by the user as a constant strength addition to the material.

Grain Boundary Strengthening

The *grain boundary strengthening*, σ_{gb}, is the contribution to the total strength stemming from the grain boundary's ability to hinder dislocation movement described by the Hall-Petch relation [2004Han].

The parameters entered are the Hall-Petch constant, k_{h-p}, in MPa µm$^{1/2}$, and the average grain diameter in µm.

Solid Solution Strengthening

The *solution strengthening*, σ_{ss}, is the contribution to total strength due to the elastic strains in the crystal lattice caused by alloying elements of a lattice parameter differing from the main constituent. For the solid solution strengthening the option of evaluating the strength at any temperature is available. The result is normalized with respect to the sum of all mole fractions for FCC, BCC, and HCP. This option uses the phase fractions and compositions calculated at the overall equilibrium temperature. The model by Walbrühl et al. [2017Wal] is implemented.

PM_G_06: Yield Strength HEA shows how this model is applied.

Precipitation Strengthening

The *precipitation strengthening*, σ_p, is the contribution to total strength due to precipitation of a secondary phase, e.g. gamma prime (γ') in Ni-base alloys or Al_3Sc precipitates in Al-base alloys. This model is available for any number of precipitating phases. The total particle strength is calculated by the square mean of the individual particle strength contributions:

$$\sigma_p = \sqrt{\sigma_{p1}^2 + \sigma_{p2}^2 + \ldots + \sigma_{pn}^2}$$

The **Simplified model (general)**, **Seidman model (Al-base)**, **Reppich model (Ni-based)**, and **Deschamps model (Al-base)** are available as settings on the **Configuration** window to estimate the precipitation strengthening contribution. These are briefly described next.

Simplified Model (General)

The **Simplified model (general)** is based on the work by Zander et al. [2008Zan] and considers the general mechanisms of cutting and looping without regard to any detailed dislocation mechanisms. The default parameters are, however, optimized against experimental data for the Al-0.3wt%Sc alloy described by Seidman et al. [2002Sei]. Also see Mean Precipitate Radius and Particle Size Distribution (PSD) below.

PM_G_04: Yield Strength compares the **Simplified model (general)**, **Seidman model (Al-base)**, and **Deschamps model (Al-base)** yield strength versus precipitate radius to experimental data for an Al-0.3wt%Sc alloy homogenized at 648 °C for 24 hours and subsequently aged at 350 °C.

Seidman Model (Al-base)

The **Seidman model (Al-base)** by Seidman et al. [2002Sei] considers several contributions to the overall precipitation strengthening - ordering, coherency stresses, shear modulus mismatch, and Orowan looping. The Seidman model is suitable for Al-base alloys with a low volume fraction of spherical precipitates. Also see Mean Precipitate Radius and Particle Size Distribution (PSD) below.

PM_G_04: Yield Strength compares the **Simplified model (general)**, **Seidman model (Al-base)**, and **Deschamps model (Al-base)** yield strength versus precipitate radius to experimental data for an Al-0.3wt%Sc alloy homogenized at 648 °C for 24 hours and subsequently aged at 350 °C.

Reppich Model (Ni-base)

The **Reppich model (Ni-base)** by Reppich et al. [1982aRep] considers both weak and strong coupling of dislocation as they propagate through an ordered secondary phase and is thus suitable for Ni-base alloys with relatively high volume fractions of gamma prime or gamma double prime. Also see Mean Precipitate Radius and Particle Size Distribution (PSD) below.

> The Reppich model is not valid for very small values of volume fraction precipitate and precipitate radius.

PM_G_05: Yield Strength NiAlCr is an example of this model.

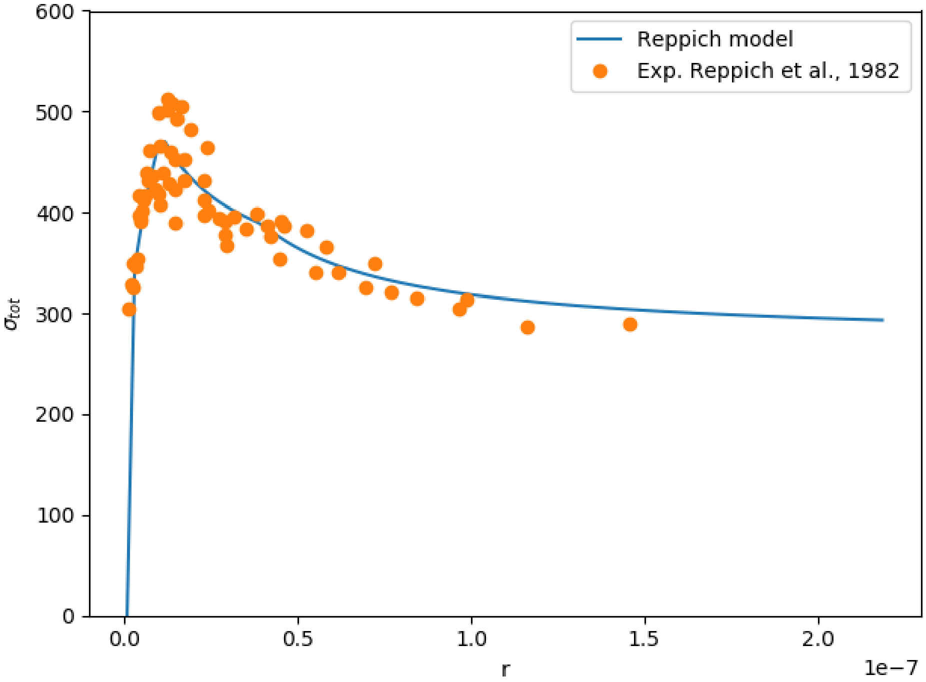


Figure 14: Reppich model plotted with results and experimental data for PE16 [1982bRep], all data is normalized with the square root of the volume fraction of precipitate.

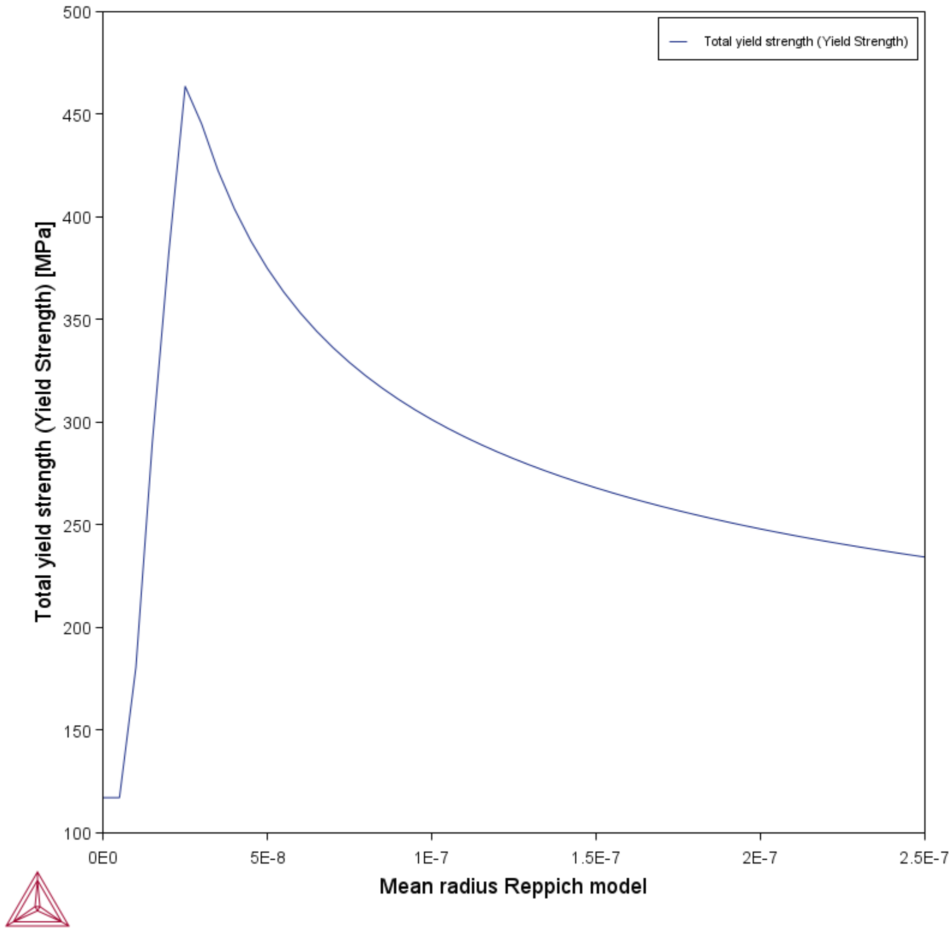


Figure 15: Reppich model yield strength vs mean precipitate radius for Ni-10Cr-10Al.

Deschamps Model (Al-base)

The **Deschamps model (Al-base)** by Deschamps and Brechet [1998Des] considers contributions to the overall precipitation strengthening precipitate from particle cutting and Orowan looping. The Deschamps model is suitable for Al-base alloys with a low volume fraction of spherical precipitates. However, it has been successfully validated against other alloy types, such as Fe-based ferritic materials with TiC precipitates. Also see Mean Precipitate Radius and Particle Size Distribution (PSD) below.

The Deschamps model considers Friedel statistics as a default setting, with the option to instead apply Kock's statistics, as shown in the PM_G_04 example.

PM_G_04: Yield Strength compares the **Simplified model (general)**, **Seidman model (Al-base)**, and **Deschamps model (Al-base)** yield strength versus precipitate radius to experimental data for an Al-0.3wt%Sc alloy homogenized at 648 °C for 24 hours and subsequently aged at 350 °C.

Mean Precipitate Radius and Particle Size Distribution (PSD)

The mean precipitate radius entered on the **Configuration** window for all precipitation strengthening models is transformed to a Lifshitz-Slyozov-Wagner (LSW) particle size distribution [2010Tir]. The distribution is stepwise integrated and the mean radius for all sections are used to calculate a partial precipitate strengthening contribution. The partial contributions are added as

$$\sigma_{tot}^2 = \sum(\sigma_p^2)$$

The use of a PSD smooths the transition between the cutting and Orowan regions. This change is implemented for the Simplified model (general) and Seidman model (Al-base).

When using the Yield Strength Model with the Precipitation Module (TC-PRISMA) the PSD as calculated by Precipitation Module (TC-PRISMA) is used for each time step. Also see Precipitation Calculator Plot Renderer for the settings input related to this.

Configuration Settings and References

Configuration Settings

The settings are entered on the **Configuration** window for the Property Model Calculator and described in Yield Strength Property Model: Simplified Mode Settings and Yield Strength Property Model: Advanced Mode Settings.

Yield strength is also available as a variable when working with Plots and Tables that are successors to the **Precipitation Calculator**.

References

[1968Sam] G. V. Samsonov, Handbook of the Physicochemical Properties of the Elements (Springer US, Boston, MA, 1968; 2012 American Edition).

[1982aRep] B. Reppich, Some new aspects concerning particle hardening mechanisms in γ’ precipitating Ni-base alloys—I. Theoretical concept. Acta Metall. 30, 87–94 (1982).

[1982bRep] B. Reppich, P. Schepp, G. Wehner, Some new aspects concerning particle hardening mechanisms in γ’ precipitating nickel-base alloys—II. Experiments. Acta Metall. 30, 95–104 (1982).

[1998Des] A. Deschamps, Y. Brechet, Influence of predeformation and ageing of an Al–Zn–Mg alloy—II. Modeling of precipitation kinetics and yield stress. Acta Mater. 47, 293–305 (1998).

[2002Sei] D. N. Seidman, E. A. Marquis, D. C. Dunand, Precipitation strengthening at ambient and elevated temperatures of heat-treatable Al(Sc) alloys. Acta Mater. 50, 4021–4035 (2002).

[2004Han] N. Hansen, Hall–Petch relation and boundary strengthening. Scr. Mater. 51, 801–806 (2004).

[2008Zan] J. Zander, R. Sandström, One parameter model for strength properties of hardenable aluminium alloys. Mater. Des. 29, 1540–1548 (2008).

[2010Tir] M. Tiryakioğlu, G. Ökten, D. Hudak, R. T. Shuey, J. P. Suni, On evaluating fit of the Lifshitz–Slyozov–Wagner (LSW) distribution to particle size data. Mater. Sci. Eng. A. 527, 1636–1639 (2010).

[2016Cor] Z. C. Cordero, B. E. Knight, C. A. Schuh, Six decades of the Hall–Petch effect – a survey of grain-size strengthening studies on pure metals. Int. Mater. Rev. 61, 495–512 (2016).

[2017Wal] M. Walbruhl, D. Linder, J. Ågren, A. Borgenstam, Modelling of solid solution strengthening in multicomponent alloys. Mater. Sci. Eng. A. 700, 301–311 (2017).

[2017Wu] Z. Wu, M. C. Troparevsky, Y. F. Gao, J. R. Morris, G. M. Stocks, H. Bei, Phase stability, physical properties and strengthening mechanisms of concentrated solid solution alloys. Curr. Opin. Solid State Mater. Sci. 21, 267–284 (2017).

Yield Strength Property Model: Simplified Mode Settings

This section has information about the **Simplified** mode configuration settings available for the **Yield Strength** Property Model.

The **Yield Strength** Model is available with the Property Model Calculator and calculates yield stress.

Yield strength is also available as a quantity when working with Plots and Tables that are successors to the **Precipitation Calculator**.

The Yield Strength Model returns the calculated yield strength at room temperature (per default) for the specified material using the equilibrium values calculated at temperature T (i.e. T is the freeze-in temperature). The Model is defined by further setting these contributions:

- Intrinsic strength (σ_i)
- Solid solution strengthening (σ_{ss})
- Grain boundary strengthening (σ_{gb})
- Precipitation strengthening (σ_p)
- Constant strength addition (σ_c)

These contributions are defined in About the Yield Strength Property Model.

For examples using the Property Model Calculator, see PM_G_04: Yield Strength, PM_G_05: Yield Strength NiAlCr, and PM_G_06: Yield Strength HEA.

For an example when it is available as an axis variable with the Precipitation Calculator, see P_01: Isothermal Precipitation of Al3Sc.

General Configuration Settings

The settings for these contributions are found on the Property Model Calculator when the **Yield Strength** Model is selected under **General Models**.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

There are settings described elsewhere when **Yield Strength** is selected as an axis variable for a Plot Renderer or Table Renderer that are successors to the **Precipitation Calculator**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

Simplified Mode Settings

Select **Simplified** as the **Mode**.

If the following set up is not sufficient for your simulation, see the Yield Strength Property Model: Advanced Mode Settings for more detailed options.

For all calculations in Simplified Mode, the automatically applied settings are as follows:

- Equilibrium minimization strategy is Global test preferred.
- The matrix phase is automatically identified.
- Burgers vector is calculated.
- Shear modulus for the matrix is calculated.

SOLID SOLUTION STRENGTHENING (SIMPLIFIED MODE)

Select the **Solid solution strengthening** checkbox to include solid solution strengthening in the calculation.

GRAIN BOUNDARY STRENGTHENING AND GRAIN SIZE (SIMPLIFIED MODE)

Click to select the **Grain boundary strengthening** checkbox to include calculated grain boundary strengthening (σ_{gb}). Then enter the **Grain size [um]**, which is the grain diameter in µm.

PRECIPITATION STRENGTHENING (SIMPLIFIED MODE)

Click to select the **Precipitation strengthening** checkbox to include calculated precipitation strengthening (σ_p).

> In Simplified Mode, the default **Precipitation strength model** is automatically the **Deschamps model (Al-base)**. However, if the major element is Ni and gamma prime is present in the system, the **Reppich model (Ni-base)** is used instead.

Then enter the following settings.

- Select a **Precipitate** from the list.
- Enter a **Mean precipitate radius**. The unit is meter (m).
- Enter a **Critical radius** (r_c), which determines the mean precipitate radius where transition between cutting and looping occurs. The unit is meter (m).

CONSTANT STRENGTH ADDITION (SIMPLIFIED MODE)

Enter a value for the **Constant strength addition**, σ_c. The unit is MPa.

Additional Settings

- Yield Strength Property Model: Calculation Type and Grid Definitions
- Yield Strength Property Model: Calculation Type and Grid Definitions
- Yield Strength Property Model: Plot and Table Settings

Yield Strength Property Model: Advanced Mode Settings

This section has information about the **Advanced** mode configuration settings available for the **Yield Strength** Property Model.

The **Yield Strength** Model is available with the Property Model Calculator and calculates yield stress.

Yield strength is also available as a quantity when working with Plots and Tables that are successors to the **Precipitation Calculator**.

The Yield Strength Model returns the calculated yield strength at room temperature (per default) for the specified material using the equilibrium values calculated at temperature T (i.e. T is the freeze-in temperature). The Model is defined by further setting these contributions:

- Intrinsic strength (σ_i)
- Solid solution strengthening (σ_{ss})
- Grain boundary strengthening (σ_{gb})
- Precipitation strengthening (σ_p)
- Constant strength addition (σ_c)

These contributions are defined in About the Yield Strength Property Model.

For examples using the Property Model Calculator, see PM_G_04: Yield Strength, PM_G_05: Yield Strength NiAlCr, and PM_G_06: Yield Strength HEA.

For an example when it is available as an axis variable with the Precipitation Calculator, see P_01: Isothermal Precipitation of Al3Sc.

General Configuration Settings

The settings for these contributions are found on the Property Model Calculator when the **Yield Strength** Model is selected under **General Models**.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

There are settings described elsewhere when **Yield Strength** is selected as an axis variable for a Plot Renderer or Table Renderer that are successors to the **Precipitation Calculator**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

Advanced Mode Settings

Select **Advanced** as the **Mode**. Available settings are displayed based on the choice.

For the specific **Simplified** settings, go to Yield Strength Property Model: Simplified Mode Settings.

SET MATRIX PHASE EXPLICITLY

Select the **Set matrix phase explicitly** checkbox and choose a **Matrix** phase from the list. This allows forcing a specific phase to be considered as the matrix phase.

This is an important parameter as it impacts the evaluation of the shear modulus and affects the result for the precipitation strengthening contribution.

The solid solution strengthening contribution is not affected by choice of matrix phase, since all stable FCC, BCC, and HCP phases always are evaluated for solid solution strength contributions. If this option is not selected, the matrix phase is automatically determined by the model.

SOLID SOLUTION STRENGTHENING (ADVANCED MODE)

Select the **Solid solution strengthening** checkbox to include solid solution strengthening in the calculation.

EVALUATE AT HIGHER TEMPERATURE

This checkbox is available when the **Solid solution strengthening** checkbox is selected. By default the checkbox is not and the simulation is evaluated at room temperature.

Select the **Evaluate at higher temperature** checkbox to evaluate the contribution σ_{ss} at temperatures higher than room temperature.

When selected, enter a **Solid solution strengthening temperature** in the field in numeric format (no expressions/functions are accepted). The unit of temperature is the same as that selected above under *Condition Definitions*.

> If no temperature is entered, the default, room temperature, is used.

GRAIN BOUNDARY STRENGTHENING AND GRAIN SIZE (ADVANCED MODE)

Click to select the **Grain boundary strengthening** checkbox to include calculated grain boundary strengthening (σ_{gb}). Then enter the **Grain size [um]**, which is the grain diameter in micrometers (µm).

USER-DEFINED HALL-PETCH COEFFICIENT

By default, a suitable default **Hall-Petch coefficient** is automatically calculated by the model. Select the **User defined Hall-Petch coefficient** checkbox to enter a different **Hall-Petch coefficient**: k_{h-p} in MPa µm$^{1/2}$.

PRECIPITATION STRENGTHENING (ADVANCED MODE)

Click to select the **Precipitation strengthening** checkbox to include calculated precipitation strengthening (σ_p). Then enter the settings that follow under the **Precipitation Strengthening Model** section.

The **Precipitate** list defaults to **Any phase**.

- If **Any phase** is selected as a Precipitate phase, the non-matrix-like phase with the highest volume fraction is selected. If more than one precipitate is defined and set to **Any phase**, non-matrix-like phases are selected in order of descending volume fraction.

- If more precipitates with **Any phase** are defined than there are stable non-matrix-like phases in the system, the redundant precipitates are ignored.
- Graphite is prohibited to be set as a precipitate phase.

Otherwise, select another phase from the list. Click the ⊕ and ⊖ buttons to add and remove additional Precipitates that can have different settings.

Precipitation Strengthening Model

The precipitation strengthening contribution (σ_p) is calculated by one of these models, which are further described below.

Select a **Precipitation strengthening model** from the list:

- **Simplified model (general)**
- **Seidman model (Al-base)**: Preferentially used for Al-based alloys.
- **Reppich model (Ni-base)**: Preferentially used for Ni-based alloys.

> The Reppich model is not valid for very small values of volume fraction precipitate and precipitate radius.

- **Deschamps model (Al-base)**: Preferentially used for Al-based alloys.

SIMPLIFIED MODEL (GENERAL) SETTINGS

For the **Simplified model (general)**, enter values in the fields for the following. The default values of k_p and r_c are optimized against experiments for Al-Sc.

- **Mean radius Simplified model**: The precipitate mean radius. The unit is meter (m). Also see Mean Precipitate Radius and Particle Size Distribution (PSD)
- **Critical radius** (r_c), which determines the mean precipitate radius where transition between cutting and looping occurs. The unit is meter (m).
- **k_p**: The prefactor for the **Simplified model**, which adjusts the overall height of the yield precipitation strength curve.

SEIDMAN MODEL (AL-BASE) SETTINGS

For the **Seidman model (Al-base)**, enter values in the fields for the following. The default parameters are optimized against experiments.

- **Mean radius Seidman model**: The precipitate mean radius. The unit is meter (m). Also see Mean Precipitate Radius and Particle Size Distribution (PSD)
- **Anti-phase boundary energy**: γ_{apb}, which is the average anti-phase boundary energy for the precipitate phase. The unit is Jm^{-2}.
- **m**: A Seidman exponent, it is a constant in the expression for strengthening by modulus mismatch. See [1985Ard] for details.
- α: A Seidman prefactor. It is a fitting constant in the expression for coherency strengthening. See [1985Ard] for details.

REPPICH MODEL (NI-BASE) SETTINGS

For the **Reppich model (Ni-base)**, enter values in the fields for the following. The default parameters are optimized against experiments.

- **Mean radius Reppich model**: The precipitate mean radius. The unit is meter (m).
- **Anti-phase boundary energy**: γ_{apb}, which is the average anti-phase boundary energy for an L12 ordered precipitate phase. The unit is Jm^{-2}.
- **Calculate anti-phase boundary energy**: Select the checkbox to use calculated anti-phase boundary energy in the yield strength calculation. The software uses the standalone APBE model in the Ni-library from within the Yield Strength Model for the calculation.

> The APBE can only be calculated for gamma prime (γ'). If the selected precipitate phase is not γ', the user-defined value in the configuration window is used.

- **w**: A parameter that accounts for elastic repulsion between strongly coupled dislocations.
- **A**: Numerical factor reflecting particle morphology (0.72 for spherical). See [1982Rep] for details.

- **C**: Correction factor in the Labusch hardening regime, i.e. for gamma prime hardended Ni-base alloys. Should be larger than or equal to unity. Set to `0` in order to disable correction.

DECHAMPS MODEL (AL-BASE) SETTINGS

For the **Dechamps model (Al-base)** enter values in the fields for the following. The default parameters are optimized against experiments.

- **Mean radius Dechamps model**: Precipitate mean radius. The unit is meter (m).
- **Critical radius** (r_c), which determines the mean precipitate radius where transition between cutting and looping occurs. The unit is meter (m).
- β: A parameter used to evaluate the dislocation line tension. Usually close to 1/2 but can deviate from this value.
- **Use Kock's statistics**: By default, Friedel statistics are used. Select the checkbox to use Kock's statistics instead. See [1998Des].

Additional Precipitation Parameters (Advanced Mode)

The following are available for all models and when the **Additional precipitation parameters** checkbox is selected.

TAYLOR FACTOR

Enter a value for the **Taylor factor**.

The value of the Taylor factor accounts for texture in the material. Normally the value is between 2.24 and 3.06 for random orientations.

SHEAR MODULUS

Enter a value for the **Shear modulus** of the matrix phase in Pa.

BURGERS VECTOR

Enter a value for the **Burgers vector**. The unit is meter (m).

CONSTANT STRENGTH ADDITION (ADVANCED MODE)

Select the **Constant strength addition** checkbox and enter a value for the **Constant strength addition**, σ_c. The unit is MPa This accounts for any contributions not accounted for in the Yield Strength model, e.g. martensite strengthening.

EQUILIBRIUM MINIMIZATION STRATEGY

Select an **Equilibrium minimization strategy**. The default uses the **Global test preferred** option.

The **Minimization Strategy** setting is used to ensure that the most stable minimum under the specified conditions is computed.

With either the *Global test preferred* or *Local minimization preferred* setting, the program cycles through options before it gives up:

- For **Global test preferred** the minimization starts with a global test and if that fails it runs full global minimization.
- For **Local minimization preferred**the minimization starts with a local minimization, in case of failure it tries a global test and finally a full global minimization.

If you choose **Local minimization only** or **Global minimization only**, the program just tries the one setting and gives up if it fails.

For general information about global minimization, see the topic related to the Console Mode command, GLOBAL_MINIMIZATION.

Precipitation Calculator Setting - Density of Points

This setting is only available for a precipitation calculation using the Precipitation Module (TC-PRISMA).

Select the **Density of points: Low** (the default), **Medium**, or **High**. This is a measure of how many time steps yield strength is calculated.

References

[1982Rep] B. Reppich, Some new aspects concerning particle hardening mechanisms in γ' precipitating Ni-base alloys—I. Theoretical concept. Acta Metall. 30, 87–94 (1982).

[1998Des] A. Deschamps, Y. Brechet, Influence of predeformation and ageing of an Al–Zn–Mg alloy—II. Modeling of precipitation kinetics and yield stress. Acta Mater. 47, 293–305 (1998).

Additional Settings

- Yield Strength Property Model: Calculation Type and Grid Definitions
- Yield Strength Property Model: Plot and Table Settings

Yield Strength Property Model: Calculation Type and Grid Definitions

This section has information about the *Calculation Type* and *Grid Definitions* **Configuration** settings available for the **Yield Strength** Property Model. It is a continuation from **Simplified** or **Advanced Mode** setting entries:

- Yield Strength Property Model: Simplified Mode Settings
- Yield Strength Property Model: Advanced Mode Settings

Calculation Type Settings

CALCULATION TYPE

- **Single** to calculate a single point. Any model can use this calculation type and no additional settings are required. The results from this calculation are displayed in the **Event Log** or if a **Table Renderer** is used, in the **Visualizations** window.
- **One Axis**: To vary a quantity on the *X*-axis.
- **Grid**: Evaluates two axis variables of the selected quantities in the specified range and number of steps.
- **Min/Max**: Evaluates the Property Model(s) for all variations of the selected quantities at the given limits. The **Mean** field is as defined under *Condition Definitions* for the respective quantity. The total minimum and maximum of the model(s) results are shown in the **Event** log.
- **Uncertainty**: Evaluates the Property Model(s) where the values of the quantities are sampled from Gaussian distributions. The **Mean** field is as defined under *Condition Definitions* for the respective quantity. The result is visualized as a histogram or normal probability plot by adding a Plot Renderer activity.
- **Batch**: Use this to allow for high throughput calculations and read data from a file, such as a spreadsheet, rather than, for example, having a fixed grid or random values. Results from these batch calculations can then be compared to experimental values (as long as this data is included), using a **Cross plot** on the Plot Renderer.

AXIS DEFINITION

For **One Axis**, select a **Quantity** to vary along the X-axis, for example, **Temperature** then enter a **Min**, **Max** and **Number of steps**.

Grid Definition Settings

GRID DEFINITIONS

For the **Grid** calculation type, define the two axes variables using the fields and menus: **Quantity**, **Min**, **Max**, and **Number of steps**. The number of steps along with the minimum and maximum values for the axes define a grid. For each grid point the selected models are evaluated.

> For a **Grid**, on the Plot Renderer, you can choose to plot a *Heat map*, *Contour*, or *3D* diagram.

Plot Type: Heat Map, Contour, and 3D

MIN/MAX DEFINITIONS

For the **Min/Max** calculation type, click to select the applicable checkboxes under **Quantity to enable or disable an axis**. The **Mean** field is as defined under *Condition Definitions* for the respective quantity.

Enter numerical values in the Δ **Min/Max** fields to evaluate the change to the quantity. The highest and lowest value of each selected model results are shown in the **Event Log**.

SAMPLING OF DATA FROM GAUSSIAN DISTRIBUTIONS

For the **Uncertainty** calculation type, click to select the applicable checkboxes under **Quantity to vary this quantity**. The **Mean** field is for the distribution function as defined under *Condition Definitions* for the respective quantity. The default ΔMin/Max is a 95% confidence interval.

About the Uncertainty Calculations

SAMPLING PARAMETERS

For the **Uncertainty** calculation type, choose a number of **Standard deviations** where you want to **Truncate the distribution**. Choose the **Total number of samples**.

About the Uncertainty Calculations

Additional Settings

🔍 Yield Strength Property Model: Plot and Table Settings

Yield Strength Property Model: Plot and Table Settings

This section has information about the Plot Renderer and Table Renderer Configuration settings available for the **Yield Strength** Property Model. It is a continuation from **Simplified** or **Advanced Mode** setting entries:

- Yield Strength Property Model: Simplified Mode Settings
- Yield Strength Property Model: Advanced Mode Settings
- Yield Strength Property Model: Calculation Type and Grid Definitions

For more information see:

Plot Renderer and Configuration Settings

Table Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

When selecting quantities on the Plot Renderer or Table Renderer, the quantity names include an abbreviated name for the Property Model it is associated to. This is useful in particular when you are calculating two or more Property Models that share names for the quantities. The short name identifying the specific Property Model is included in parentheses after the name of the quantity. Below are the full and abbreviated names for each Property Model.

For a list of the abbreviations associated to a Property Model, see Result Quantities: Property Model Abbreviations.

Calculations can be performed over a range for the model parameters available in each sub-model. If, for example, the mean precipitate radius in a precipitation strengthening model is set as the variable to step over, it becomes available as a plot quantity in the Plot Renderer.

Plot Quantities

The various *hardness* or *hardening* quantities are treated separately from the various *strength* or *strengthening* quantities and each (hardness and strength) are plotted on the respective axes. When setting up the simulation, the **Configuration** window (when in *Grouped Mode*) shows either *Vickers Hardness* or *Strength*. This corresponds to the labeling of axes in the **Visualizations** window when plotting two or more quantities of the same type. The legend then lists the specific quantity names selected on the **Configuration** window.

These plot quantities are available:

- **Total yield strength**
- **Intrinsic strength**
- **Solid solution strengthening**
- **Solid solution strengthening FCC**
- **Solid solution strengthening BCC**
- **Solid solution strengthening HCP**
- **Grain boundary strengthening**
- **Total precipitation strengthening**
- **Precipitation strengthening per phase**
- **Constant strength addition**
- **Volume fraction of precipitate phase**
- **Volume fraction of stable phase(s)**

For all strength quantities, there is a corresponding hardness quantity:

- **Total hardness**
- **Intrinsic hardness**
- **Total solid solution hardening**
- **Solid solution hardening FCC**
- **Solid solution hardening BCC**
- **Solid solution hardening HCP**

- **Grain boundary hardening**
- **Total precipitation hardening**
- **Precipitation hardening per phase**
- **Constant hardness addition**

Scheduler and Event Log Windows

In this section:

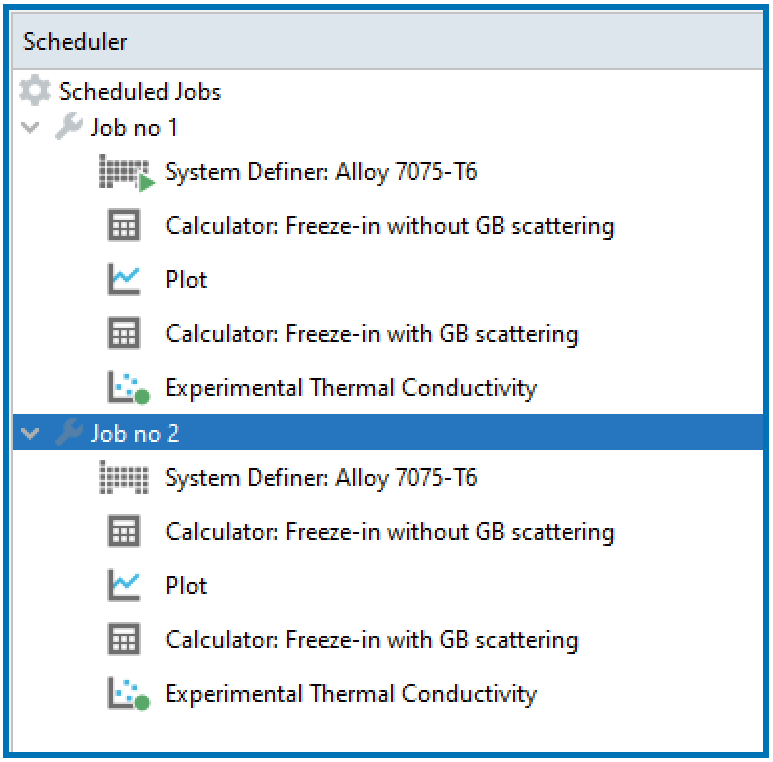
Using the Scheduler

The **Scheduler** window has activity information about current or scheduled jobs. A *job* is any activity you have selected to be performed. The Scheduler also indicates if there is an error during a job and when a job has stopped. If you have set an activity, tree or project to be performed at a later time then this is also listed.

About the Scheduler Jobs

- Whenever you trigger the performance of a whole project, tree or individual activity, all the activities to be performed are shown under a job heading.
- When all the activities belonging to a job are completed the job and its activities disappear from the Scheduler window.
- If there is an error during the performance of an activity, icons for that job and activity remain in the Scheduler window until removed.

Node or Window Status Markers



Scheduler
Scheduled Jobs
Job no 1
System Definer: Alloy 7075-T6
Calculator: Freeze-in without GB scattering
Plot
Calculator: Freeze-in with GB scattering
Experimental Thermal Conductivity
Job no 2
System Definer: Alloy 7075-T6
Calculator: Freeze-in without GB scattering
Plot
Calculator: Freeze-in with GB scattering
Experimental Thermal Conductivity

Managing the Schedule

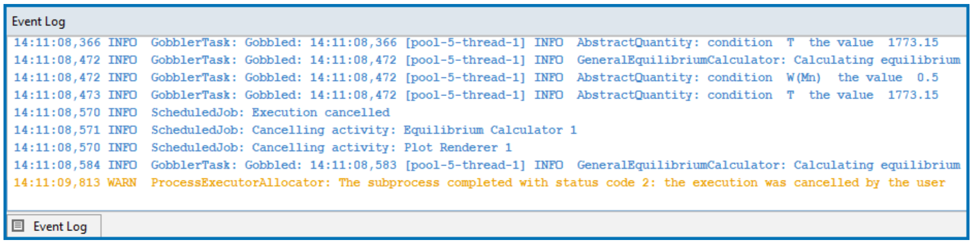
In the Scheduler window, you can cancel scheduled jobs, remove errors and show information about errors.

- To cancel all jobs: Right-click the **Scheduled Jobs** label or the cogwheel icon, and select **Cancel All Jobs**
- To remove (clear) all failed activities and jobs: Right-click the **Scheduled Jobs** label or the cogwheel icon, and select **Clear All Errors**
- To cancel a specific job: Right-click the job label (for example, **Job no 1**) and select **Cancel Job**
- To remove (clear) a specific failed job: Right-click the job label (for example, **Job no 1**) and select **Cancel Job**
- To open a window with error details: Right-click the label for the failed job (for example, **Job no 1**), and select **Show Error Log**

Event Log Window

The **Event Log** window is closed by default. Information about what Thermo-Calc is processing or doing is in blue text, an error message is in red text, and caution/warning information is in yellow text.

Global Settings



```
14:11:08,366 INFO  GobblerTask: Gobbled: 14:11:08,366 [pool-5-thread-1] INFO  AbstractQuantity: condition  T  the value  1773.15
14:11:08,472 INFO  GobblerTask: Gobbled: 14:11:08,472 [pool-5-thread-1] INFO  GeneralEquilibriumCalculator: Calculating equilibrium
14:11:08,472 INFO  GobblerTask: Gobbled: 14:11:08,472 [pool-5-thread-1] INFO  AbstractQuantity: condition  W(Mn)  the value  0.5
14:11:08,473 INFO  GobblerTask: Gobbled: 14:11:08,472 [pool-5-thread-1] INFO  AbstractQuantity: condition  T  the value  1773.15
14:11:08,570 INFO  ScheduledJob: Execution cancelled
14:11:08,571 INFO  ScheduledJob: Cancelling activity: Equilibrium Calculator 1
14:11:08,570 INFO  ScheduledJob: Cancelling activity: Plot Renderer 1
14:11:08,584 INFO  GobblerTask: Gobbled: 14:11:08,583 [pool-5-thread-1] INFO  GeneralEquilibriumCalculator: Calculating equilibrium
14:11:09,813 WARN  ProcessExecutorAllocator: The subprocess completed with status code 2: the execution was cancelled by the user
```

- To open the Event Log window: Click the **Event Log** window once to expand it or select it from the **Window → Event Log**menu. Double-clicking the window maximizes it.
- To clear all messages in the window, right-click in the text area and select **Clear**.
- To specify the level of detail in the Event Log, open the **Options** window:
  - Windows: Select **Tools →** ☰ **Options**.
  - Mac: Select **Thermo-Calc** *<version>* **→ Preferences** or **Settings** or press <⌘> on the keyboard.

  then click the **General** tab and set the **Log level** slide bar to anything between **Debug** (most detailed) and **Error** (least detailed).

Working with Plots and Tables

In this section:

Performing Projects, Trees, and Activities

You can trigger the performance of an activity (also called a *job*) and all the activities below it in the same tree in either the **Project** or **Configuration** window. In the Project window you can also perform a single activity without performing its successors or perform the whole project (all the activity trees).

In the **Configuration** window, click **Perform Tree** to perform the currently selected activity and all the activities below it. If there are no activities below the selected activity, then the button says **Perform** instead.

All activities that must be completed as prerequisites are automatically performed first. For example, if you Perform Tree for a Plot Renderer, then the predecessors, Equilibrium Calculator and System Definer, are automatically performed before the Plot Renderer.

In the **Project** window, you can do any of the following:

- Perform an activity: Right-click the activity and select **Perform Now**, or **Perform Later** and schedule a time to perform the activity
- Perform an activity and all activities below it in the tree: Right-click any node in the tree and select **Perform Tree Now**. Or select **Perform Tree Later** and schedule a time for all activities in the tree to be performed
- Perform a project: Right-click **My Project** and select **Perform Now** or **Perform Later** and schedule a time to perform all project activities in the tree

If there is an error during the performance of an activity, icons display status markers, which are described in Node or Window Status Markers.

Saving and Printing the Output in Graphical Mode

Global Settings: Graphical and Console Mode Plotting

Output can refer to results in the form of tabulated data in a table or a diagram.

The terms *diagram* and *plot* are interchangeable. The commands in Console Mode generally use the term diagram and in Graphical Mode it is also called a plot (e.g. the Plot Renderer).

In Graphical Mode the output is displayed in the **Visualizations** window. The output can be in the form of a table or a diagram (plot). In both cases you can save from the **Configuration** or **Visualizations** windows. You can print the table or diagram from the **Visualizations** window.

Saving a Parallel coordinates plot from the Visualizations window has less file type options. See Plot Type: Parallel Coordinates.

Saving Diagrams

You can save the output in a variety of file formats. For JPG and PNG images you can also adjust the image quality.

In Console Mode, the diagram is output to the **Console Results** window after using the PLOT_DIAGRAM command.

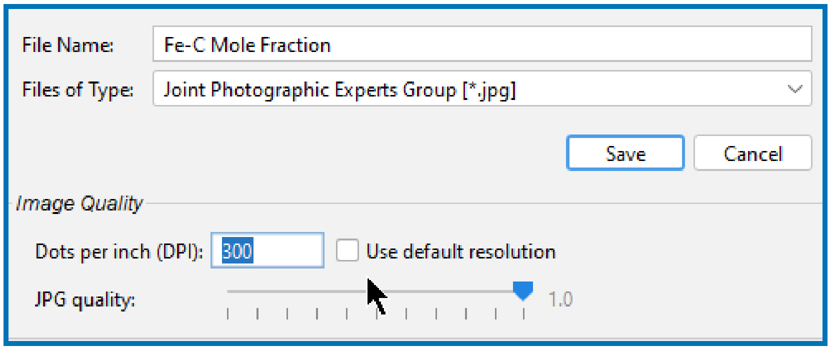
In Graphical Mode, the diagram is output to the **Visualizations** window after performing a tree that includes a Plot Renderer.

In the **Visualizations** window, right-click the diagram and select **Save as**.

In the Graphical Mode **Configuration** window you can also click the **Save Diagram** (or **Save table**) buttons to open the **Save** window.

Then in the **Save** window:

1. Navigate to where you want to save the diagram.
2. Enter a **File name**.
3. From the **Files of type** list choose **png** (the default), **jpg**, **ps**, **pdf**, **gif**, **svg**, or **emf**.
4. For PNG and JPG files only, under the **Image Quality** section, choose to improve the resolution of the image. For JPG files you can also adjust the file size.
    - To change the resolution of a PNG or JPG image, click to clear the **Use screen resolution** checkbox. Then enter a numerical value in the **Dots per inch (DPI)** field.
    - For JPEG files, you can also use the slider to choose a number between 0 and 1 for the **JPG quality**. The default is 0.9. The lower the number, the smaller the file.


File Name: Fe-C Mole Fraction

Files of Type: Joint Photographic Experts Group [*.jpg]

Image Quality

Dots per inch (DPI): 300 ☐ Use default resolution

JPG quality: 1.0

5. When you are ready, click **Save**.

Saving (Exporting) Tables

You can save the table output in different file formats from the Table Renderer and Plot Renderer **Configuration** and **Visualizations** windows.

In Graphical Mode, a table is output to the **Visualizations** window after performing a tree that includes a Table Renderer. It is also output using the **Table View** button located on the Plot Renderer **Configuration** window.

Generate a table. Then depending on which window you are in:

- In the **Visualizations** window, right-click the table and select **Save as**, or
- In the **Configuration** window click the **Save table** button.

Then in the **Save As** window:

1. Navigate to where you want to save the table.
2. Enter a **File Name**.
3. From the **Files of Type** list choose **Text [*.txt]**(the default), **Hyper Text Markup [*.html]**, or **Excel [*.xls]**.
4. When you are ready, click **Save**.

Printing Output

In the **Visualizations** window, right-click the table or diagram and choose **Print**. Select additional settings as required on the **Print** window.

Plotting Options

The Plot Renderer is a dynamic activity node with options such as being able to:

- add more than one Plot Renderer to its predecessor node (i.e. one of the calculator activities),
- add axes to the plots,
- merge results in one plot,
- filter quantities (only for a Parallel coordinates plot), and
- choose from a variety of plot types based on the selected combination of Calculator and Calculation Type.

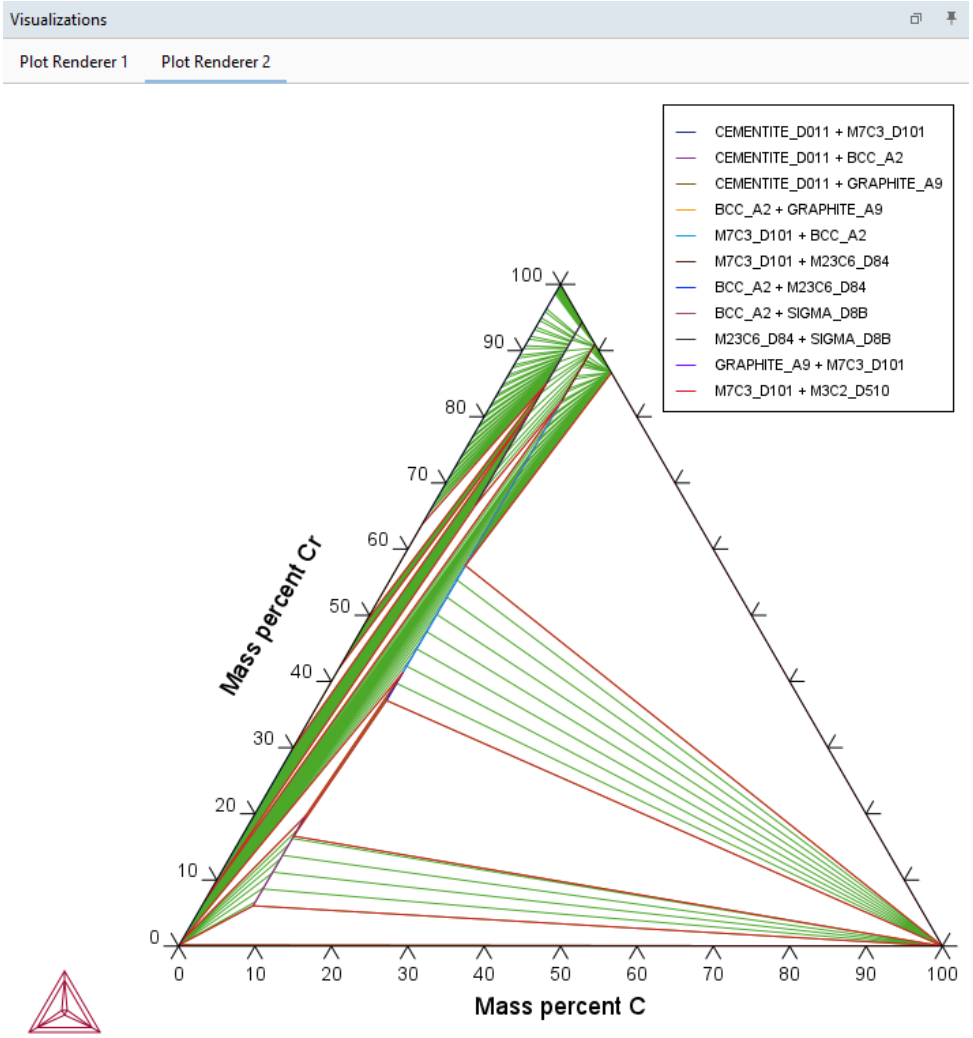
Additional settings are also described in Configuration Settings.

The specialized Add-on Additive Manufacturing (AM) Module has additional functionality. The information is described separately and included with the Module's documentation.

Plots Can Have More Than One Predecessor

A Plot Renderer can have several predecessors (if you want to plot several calculations in the same diagram), in which case there are several tabs in the Configuration window, one for each predecessor.

Plotting Several Calculations in One Diagram



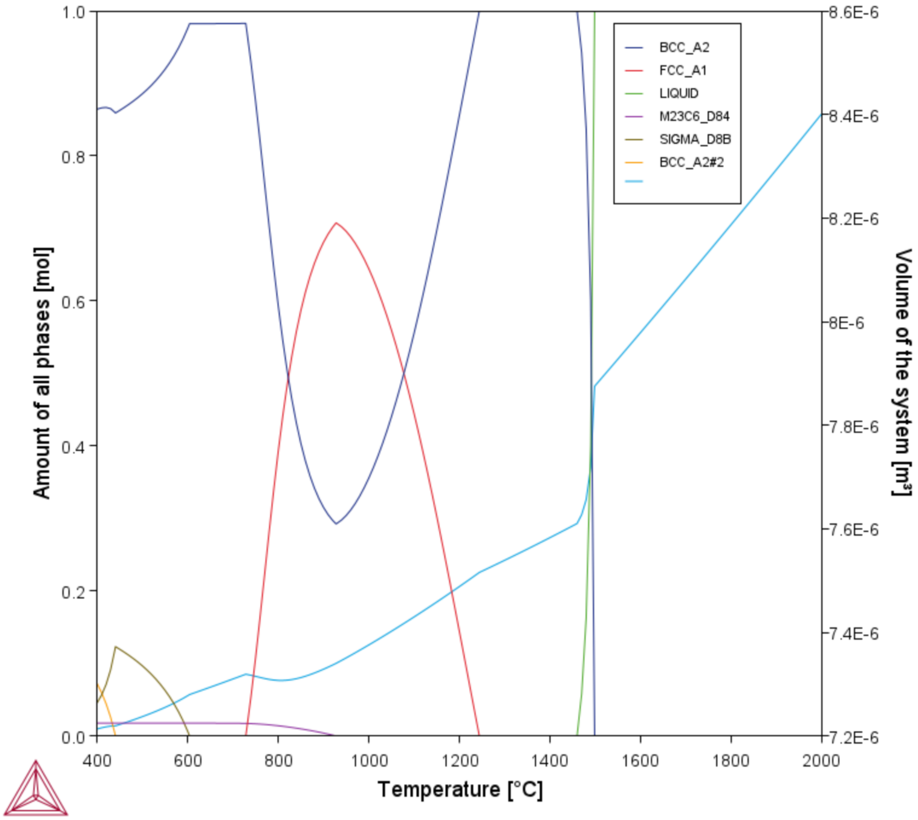
Several Plot Renderer activities (as well as Table Renderer activities) can be shown in the Visualizations window as different tabs. This is an example from Thermo-Calc Graphical Mode T_ 04_Fe-Cr-C_ternary_phase_diagram.

Add Axes to Plots

You can add additional axes (*X*, *Y*, and *Z* for **Grid** calculations) to a plot to compare two or more variables at the same time.

- To add an axis setting section, click the ⊕ **Add an axis** button.
- Once a new axis settings section is added, click ⊖ **Remove this axis** button to delete it.
- Wherever you see these plus or minus buttons, click to add or remove a section then define the axis as needed.

? [Adding Axes to a Diagram]



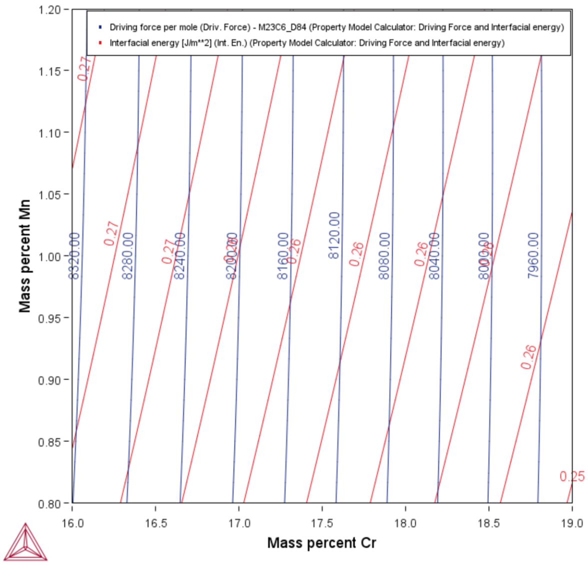
Two variables plotted on the Y-axis.

Merge Results in One Plot

You can merge (or overlay) calculated results for several variables into one plot. This is similar to adding an axis, but instead of displaying different variables along the *X*- and/or *Y*-axes, the same X and Y variables are used to compare the third variable (defined in the Plot Renderer as the *Z*-axis).

As in the figure (from example *PM_G_03* in Graphical Mode), the driving force and interfacial energy results are combined into one diagram. The *X*- and *Y*-axis is the same for both (Mass percent Cr/Mass percent Mn).

[Merging Plots into One Diagram](#)



A contour plot showing both the driving force and interfacial energy calculation results comparing Mass percent Cr to Mass percent Mn. From example PM_G_03.

Choose a Plot Type

When you set up most Calculators, there are calculation types to choose from on the **Configuration** window. The selection of the *Calculation Type* also provides options to choose from the *Plot type* menu for some of the associated **Plot Renderer** windows.

For a list of calculations for each Calculator, see [Calculation Types in Graphical Mode](#).

There are a variety of combinations of Calculator and *Calculation Type* that offer different [Plot Types](#). These are described in separate topics:

- Plot Type: Cross Plot and Statistical
- Plot Type: Heat Map, Contour, and 3D
- Plot Type: Parallel Coordinates
- Plot Type: Flexible Mode and Grouped Mode
- Plot Type: CCT Mode
- Plot Type: TTT Mode
- Plot Type: Simple Mode and Advanced Mode

If you also have a license for the Additive Manufacturing Module, there are additional plots available and described in the documentation, i.e. see About the AM Plot Types.

Filter Quantities on a Parallel Coordinates Plot

Use the **Filter** checkbox on a Plot Renderer to add various filters to the **Parallel coordinates** plot or table and based on the set up of the calculation.

When selected, click the ⊕ **Add quantity** and ⊖ **Remove quantity** buttons to add filters. For example, enter a **Min** and **Max** and choose an axis variable such as **Composition Cr** and the unit **Mass percent** to adjust the output in the **Visualizations** window. Click **Perform** each time you add or remove a filter for the results to update.

Quantities Groups Available for Plots and Tables

The following table lists the common quantities available as axis variables (plots) or columns (tables) when working in Graphical Mode. All the quantities are listed alphabetically in conditions, quantity function definitions, and table and plot results.

About Quantity Groups

The quantities are sometimes grouped into categories on the Plot Renderer or Table Renderer. Availability of the list and the variables themselves, is based on several factors, including the database selected, the Calculator used, and the type of calculation being performed. Other differences are based on the *Plot type* selected, e.g. what you see on the **Configuration** window changes if you use **Flexible Mode** or **Grouped Mode**. Other plot types do not group the quantities and each Calculator handles the information differently.

When working on a Plot Renderer (e.g. associated to the *Axes* X, Y, and Z) or Table Renderer (associated to *Columns*), there is sometimes the option to choose a quantity group from a list. When applicable, these are the categories:

- All variables
- System variables
- Phase equilibria
- Physical properties
- Kinetic properties
- Elastic properties

After selecting the group, you next choose from the available variables and continue to define each based on the additional settings specifically available, i.e. select a unit or a phase, and many other options that are only displayed when relevant.

> These quantities are also available in Console Mode but are entered manually.

Each quantity is selected on the **Configuration** window as required either as **Axis variables** for the Plot Renderer or when choosing the **Columns** for a Table Renderer.

Quantity	***Group (when available)***	***Units***	***Additional Settings or Link to More Information***
Activity of	Phase	dimensionless	Click to deselect the SER checkbox to use the

Quantity	***Group (when available)***	***Units***	***Additional Settings or Link to More Information***
component	equilibria		reference state you have selected. Choose an element from the list or choose All.
Activity referred to a phase	Phase equilibria	dimensionless	Choose a phase and an element.
Amount of component	Phase equilibria	Mole, Gram, Kilogram, Tonne, Pound	Select the Normalization variable or No normalization if you do not want to normalize the quantity. Choose a specific element or All and a unit.
Amount of component in phase	Phase equilibria	Mole, Gram, Kilogram, Tonne, Pound	Select the Normalization variable or No normalization if you do not want to normalize the quantity. Choose a specific element or All, then a specific phase or All phases, and a unit.
Amount of phase	Phase equilibria	Mole, Gram, Kilogram, Tonne, Pound	Select the Normalization variable or No normalization if you do not want to normalize the quantity. Choose a specific phase or All phases and a unit.
Bohr magneton number	Phase equilibria	dimensionless	Choose a specific phase or All phases
Bulk modulus	Elastic properties	Pascal, Gigapascal, Atmospheres, Bar	Choose All phases or a specific phase. Select a unit.
Chemical diffusion coefficient	Kinetic properties	m^2/s	Choose the diffusing element, Gradient element, and Reference element.
Chemical potential of component	Phase equilibria	Joule, Calorie, Electron volt, Gigajoule, Watt hour, Kilowatt hour	Click to deselect the SER checkbox to use the reference state you have selected.
Chemical potential referred to a phase	Phase equilibria	Joule, Calorie, Electron volt, Gigajoule, Watt hour, Kilowatt hour	Choose a phase, an element, and a unit.
Composition	System variables	Mass percent, Mole percent, Mass fraction,	Choose All or a specific element and a unit.

Quantity	***Group (when available)***	***Units***	***Additional Settings or Link to More Information***
		Mole fraction	
Composition of a phase	Phase equilibria	Mass percent, Mole percent, Mass fraction, Mole fraction	Choose a specific element or All, then a specific phase or All phases, and a unit.
Curie temperature	Phase equilibria	Kelvin, Celsius, Fahrenheit	Choose a specific phase or All phases, and a unit.
Density	Physical properties	Gram per cubic meter, Kilogram per cubic meter, Gram per cubic centimeter, Pound per cubic inch	Choose All phases, an individual phase, or System. Choose a unit.
Dynamic viscosity	Physical properties	Pascal-second, milliPascal-second, Poise, centiPoise	This defaults to the LIQUID phase. Choose a unit. ? About Thermophysical Properties Data Parameters
Electric conductivity	Physical properties	S/m	Choose All phases, an individual phase, or System. ? About Thermophysical Properties Data Parameters
Elastic constant	Elastic properties	Pascal, Gigapascal, Atmospheres, Bar	Choose the elastic constant C11, C12, C13, C33, or C44. Choose All phases or an individual phase. Select a unit. ? Elastic Properties Variables
Electric resistivity	Physical properties	Ωm	Choose All phases, an individual phase, or System. ? About Thermophysical Properties Data Parameters
Enthalpy	Physical properties	Joule, Calorie, Electron volt, Gigajoule, Watt hour, Kilowatt hour	Select the Normalization variable or No normalization if you do not want to normalize the quantity. Click to deselect the SER checkbox to use the reference state you have selected. Choose All phases, an individual phase, or System. Select a unit.

Quantity	*Group (when available)*	*Units*	*Additional Settings or Link to More Information*
Entropy	Physical properties	Joule per Kelvin, Calorie per Kelvin, Electron volt per Kelvin	Select the Normalization variable or No normalization if you do not want to normalize the quantity. Click to deselect the SER checkbox to use the reference state you have selected. Choose All phases, an individual phase, or System. Select a unit.
Function	All variables	No units.	This option is only available when you choose the group **All variables**. Select **Function** when you want to choose a user-defined function. For example, if `fraction_solid` is predefined defined on the **Functions** tab for an Equilibrium Calculator and you want to plot this, choose **Function**.
Gibbs energy	Physical properties	Joule, Calorie, Electron volt, Gigajoule, Watt hour, Kilowatt hour	Select the Normalization variable or No normalization if you do not want to normalize the quantity. Click to deselect the SER checkbox to use the reference state you have selected. Choose All phases, an individual phase, or System. Select a unit.
Heat capacity	Physical properties	Joule per mole Kelvin, Calorie per mole Kelvin, Joule per kilogram Kelvin, BTU per pound Fahrenheit	Choose All phases, an individual phase, or System. Select a unit.
Helmholtz energy	Physical properties	Joule, Calorie, Electron volt, Gigajoule, Watt hour, Kilowatt hour	Select the Normalization variable or No normalization if you do not want to normalize the quantity. Click to deselect the SER checkbox to use the reference state you have selected. Choose All phases, an individual phase, or System. Select a unit.
In(activity of component)	Phase equilibria	dimensionless	Click to deselect the SER checkbox to use the reference state you have selected. Choose an element from the list or choose All.
In(activity referred to a phase)	Phase equilibria	dimensionless	Choose a phase and an element.

Quantity	***Group (when available)***	***Units***	***Additional Settings or Link to More Information***
Internal energy	Physical properties	Joule, Calorie, Electron volt, Gigajoule, Watt hour, Kilowatt hour	Select the Normalization variable or No normalization if you do not want to normalize the quantity. Click to deselect the SER checkbox to use the reference state you have selected. Choose All phases, an individual phase, or System. Select a unit.
Intrinsic diffusion coefficient	Kinetic properties	m^2/s	Choose the diffusing element, Gradient element, and Reference element.
Isothermal compression	Physical properties	1/Pa	Choose All phases, an individual phase, or System.
Kinematic viscosity	Physical properties	Square meter per second, Stokes, Centistokes	This defaults to the LIQUID phase. Choose a unit. ? [About Thermophysical Properties Data Parameters]
L''	Kinetic properties	m^2/Js	Choose the diffusing element, Gradient element, and Reference element.
log10(Chemical diffusion coefficient)	Kinetic properties	m^2/s	Choose the diffusing element, Gradient element, and Reference element.
log10(Intrinsic diffusion coefficient)	Kinetic properties	m^2/s	Choose the diffusing element, Gradient element, and Reference element.
log10(Mobility)	Kinetic properties	m^2/s	
log10(Tracer diffusion coefficient)	Kinetic properties	m^2/s	
Mobility	Kinetic properties	m^2/s	
Normalized driving force	Phase equilibria	dimensionless	Select the Normalization variable - Per mole, Per mass in gram, Per volume in cubic meter, or Per mole formula unit. Then choose All phases or a specific phase.
Phase stability function	Phase equilibria	dimensionless	Choose All phases or a specific phase.
Pressure	System	Pascal,	Choose a unit.

Quantity	***Group (when available)***	***Units***	***Additional Settings or Link to More Information***
	variables	Atmospheres, Bar	
Shear modulus	Elastic properties	Pascal, Gigapascal, Atmospheres, Bar	Choose All phases or an individual phase. Select a unit. ? [Elastic Properties Variables]()
Site fraction	Phase equilibria	dimensionless	Choose All phases or a specific phase. Where applicable for individual phases also select a sublattice and then a specific element for the sublattice.
Surface tension	Physical properties	Joule per m^2, Millijoule per m^2	This defaults to the LIQUID phase. Choose a unit. ? [About Thermophysical Properties Data Parameters]()
System size	System variables	Mole, Gram, Kilogram, Tonne, Pound	Choose a unit.
Temperature	System variables	Kelvin, Celsius, Fahrenheit	Choose a unit.
Thermal conductivity	Physical properties	W/mK	Choose All phases, an individual phase, or System. ? [About Thermophysical Properties Data Parameters]()
Thermal diffusivity	Physical properties	m^2/s	Choose All phases, an individual phase, or System. ? [About Thermophysical Properties Data Parameters]()
Thermal expansivity	Physical properties	per Kelvin, per Fahrenheit	Choose Linear or Volumetric. Choose All phases, an individual phase, or System. Select a unit.
Thermal resistivity	Physical properties	mK/W	Choose All phases, an individual phase, or System. ? [About Thermophysical Properties Data Parameters]()
Thermodynamic	Kinetic	m^2/s	Choose the diffusing element, Gradient element,

Quantity	***Group (when available)***	***Units***	***Additional Settings or Link to More Information***
factor	properties		and Reference element.
Tracer diffusion coefficient	Kinetic properties	m^2/s	
u-fraction	Phase equilibria	dimensionless	Choose an element and then from the Components in denominator list, you can select or deselect specific elements using the checkboxes. ? The u-Fraction Variable
User-defined	System variables		Enter another axis variable.
Volume	Phase equilibria	Cubic meter, Cubic decimeter, Cubic centimeter, Normal cubic meter	Select the Normalization variable or No normalization if you do not want to normalize the quantity. Click to deselect the SER checkbox to use the reference state you have selected. Choose All phases, an individual phase, or System. Choose a unit.
Volume fraction of phase	Phase equilibria	dimensionless	Choose All phases or an individual phase.
Young's modulus	Elastic properties	Pascal, Gigapascal, Atmospheres, Bar	Choose All phases or an individual phase. Select a unit. ? Elastic Properties Variables

Plot Types

The Plot Renderer is a dynamic activity node with options such as being able to choose from a variety of *Plot types* based on the Calculator and, in most cases, *Calculation Type* selected.

The *Mode* plot types are related to groups of settings made available (or hidden) on the Plot Renderer, rather than a particular plot output type such as contour, cross plot, or heat map, for example.

The tables below list the *Plot types* available with the various Calculator and *Calculation Type* combinations, either By Calculator, By Plot Type, or By Calculation Type.

Calculation Types in Graphical Mode

There are a variety of combinations of Calculator and *Calculation Type* that offer different Plot Types. These are described in separate topics:

- Plot Type: Cross Plot and Statistical
- Plot Type: Heat Map, Contour, and 3D
- Plot Type: Parallel Coordinates
- Plot Type: Flexible Mode and Grouped Mode
- Plot Type: CCT Mode
- Plot Type: TTT Mode
- Plot Type: Simple Mode and Advanced Mode

If you also have a license for the Additive Manufacturing Module, there are additional plots available and described in the documentation, i.e. see About the AM Plot Types.

The following require additional licenses: Diffusion Calculator, Process Metallurgy Calculator, CCT Mode, and TTT Mode.

By Calculator

Calculator	*Calculation Type*	*Plot Types*	*Notes*
Diffusion Calculator	n/a	Simple Mode; Advanced Mode	There are no *Calculation Types* to choose when setting up a Diffusion Calculator.
Equilibrium Calculator	One Axis Phase diagram	Flexible Mode Grouped Mode	
	Grid	Heat Map Contour 3D	
Material to Material Calculator	One Axis Phase diagram	Flexible Mode Grouped Mode	
Process Metallurgy Calculator (Equilibrium calculations)	One Axis	Flexible Mode	

Calculator	***Calculation Type***	***Plot Types***	***Notes***
		Grouped Mode	
	Grid	Heat Map Contour 3D	
Process Metallurgy Calculator (Process simulation)	n/a	Flexible Mode Grouped Mode	There are no *Calculation Types* to choose when setting up a Process Metallurgy Calculator as a *Process simulation*.
Property Model Calculator	One Axis	Flexible Mode Grouped Mode	
		CCT Mode	Also select **Log10(cooling rate [K/s])** as the axis *Quantity*.
		TTT Mode	Also select **Temperature** as the axis *Quantity*.
	Grid	Heat Map Contour 3D	
		Parallel coordinates	At least three quantities under *Grid Definitions* must be selected on the Property Model Calculator; then this plot is available on the Plot Renderer.
	Uncertainty	Cross Plot Parallel coordinates	

Calculator	*Calculation Type*	*Plot Types*	*Notes*
		Statistical	
		Statistical - Histogram	Choose **Frequency** as the *Axis variable* and **Histogram** as the *Axis type*
		Statistical - Probability	Choose **Normal probability** as the *Axis variable* and **Probability** as the *Axis type*
	Batch	Statistical Cross Plot Parallel coordinates	
Ternary Calculator	Isothermal section Monovariant lines Liquidus projection	Flexible Mode Grouped Mode	

By Plot Type

Plot Type	*Calculation Type*	*Calculator(s)*	*Notes*
3D	Grid	Equilibrium Calculator Property Model Calculator Process Metallurgy Calculator	3D Plots with additional functionality are also available with the Add-on Additive Manufacturing (AM) Module. The information is described separately and included with the Module's documentation.
Advanced Mode	n/a	Diffusion Calculator	There are no *Calculation Types* to choose when setting up a Diffusion Calculator.
CCT Mode	One Axis	Property Model Calculator	Also select **Log10(cooling rate [K/s])** as the axis *Quantity*.
Contour	Grid	Equilibrium Calculator Property Model Calculator Process Metallurgy Calculator	
Cross Plot	Batch Uncertainty	Property Model Calculator	
Flexible Mode or Grouped Mode	One Axis	Equilibrium Calculator Material to Material Calculator Process Metallurgy Calculator (Equilibrium calculation)	

Plot Type	*Calculation Type*	*Calculator(s)*	*Notes*
		Property Model Calculator	
	Isothermal section Monovariant lines Liquidus projection	Ternary Calculator	
	n/a	Process Metallurgy (Process simulation)	There are no *Calculation Types* to choose when setting up a Process Metallurgy Calculator as a *Process simulation*.
	Phase diagram	Equilibrium Calculator Material to Material Calculator	
Heat Map	Grid	Equilibrium Calculator Property Model Calculator Process Metallurgy Calculator	
Parallel coordinates	Batch Grid Uncertainty	Property Model Calculator	For the **Grid** calculation at least three quantities under *Grid Definitions* must be selected on the Property Model Calculator, then this plot type is available on the Plot Renderer.
Simple Mode	n/a	Diffusion Calculator	There are no *Calculation Types* to choose when setting up a Diffusion Calculator.
Statistical	Batch Uncertainty	Property Model Calculator	

Plot Type	*Calculation Type*	*Calculator(s)*	*Notes*
Statistical - Histogram	Batch Uncertainty	Property Model Calculator	Choose **Frequency** as the *Axis variable* and **Histogram** as the *Axis type* Batch is only available with the Property Model Calculator
Statistical - Probability	Batch Uncertainty	Property Model Calculator	Choose **Normal probability** as the *Axis variable* and **Probability** as the *Axis type* Batch is only available with the Property Model Calculator
TTT Mode	One Axis	Property Model Calculator	Also select **Temperature** as the axis *Quantity*.

By Calculation Type

Calculation Type	*Plot Types*	*Calculator (s)*	*Notes*
Batch	Statistical Parallel coordinates	Property Model Calculator	
Grid	Heat Map Contour 3D	Equilibrium Calculator Property Model Calculator Process Metallurgy Calculator	
	Parallel coordinates	Property Model Calculator	At least three quantities under *Grid Definitions* must be selected on the Property Model Calculator, then the plot is available on the Plot Renderer.

Calculation Type	*Plot Types*	*Calculator (s)*	*Notes*
Isothermal section Liquidus projection Monovariant lines	Flexible Mode Grouped Mode	Ternary Calculator	
Min/Max	Flexible Mode Grouped Mode	Property Model Calculator	
One Axis	Flexible Mode Grouped Mode	Equilibrium Calculator Material to Material Calculator Process Metallurgy Calculator Property Model Calculator	
	CCT Mode TTT Mode	Property Model Calculator	CCT Mode: Also select **Log10(cooling rate [K/s])** as the axis *Quantity*. TTT Mode: Also select **Temperature** as the axis *Quantity*.
Phase diagram	Flexible Mode Grouped Mode	Equilibrium Calculator Material to Material Calculator	
Uncertainty	Parallel coordinates	Property Model Calculator	

Calculation Type	***Plot Types***	***Calculator (s)***	***Notes***
	Statistical		
	Statistical - Histogram		Choose **Frequency** as the *Axis variable* and **Histogram** as the *Axis type*
	Statistical - Probability		Choose **Normal probability** as the *Axis variable* and **Probability** as the *Axis type*

Plot Type: Cross Plot and Statistical

The Plot Renderer is a dynamic activity node with options such as being able to choose from a variety of *Plot types* based on the Calculator and Calculation Type selected.

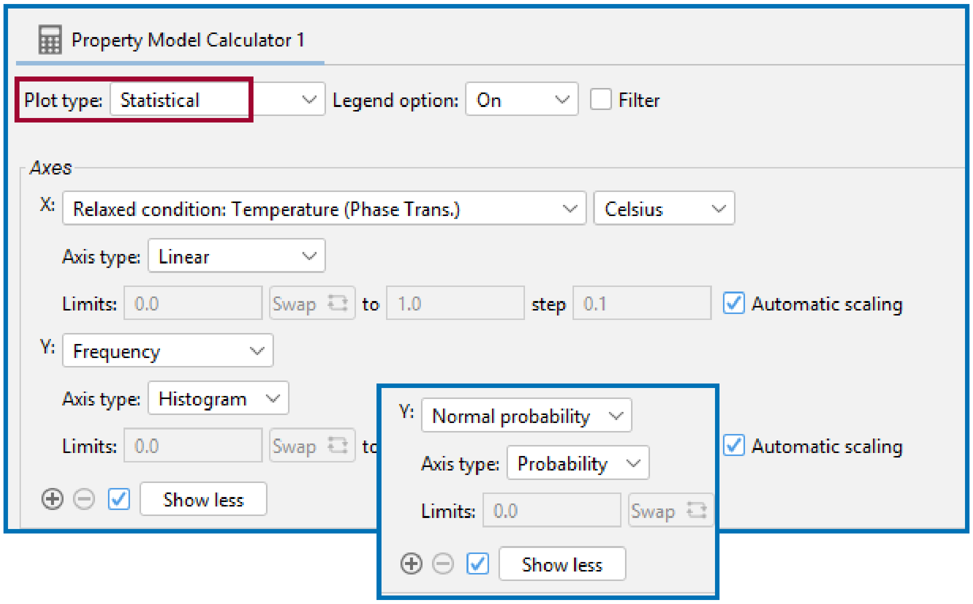
Calculation Types in Graphical Mode

See Plot Types detailing availability *By Calculator*, *By Plot Type*, or *By Calculation Type*.

Statistical (with a Histogram or Probability Axis Type)

Use a **Statistical** *Plot type* to select **Frequency** or **Normal probability** as the *Axis variable*. The *Axis type* is then set to **Histogram** or **Probability**, respectively.

The following uses a General Property Model example: PM_G_01: Phase Transition.



Property Model Calculator 1

Plot type: Statistical

Legend option: On

☐ Filter

Axes

X: Relaxed condition: Temperature (Phase Trans.) Celsius

Axis type: Linear

Limits: 0.0 to 1.0 step 0.1 ☑ Automatic scaling

Y: Frequency

Axis type: Histogram

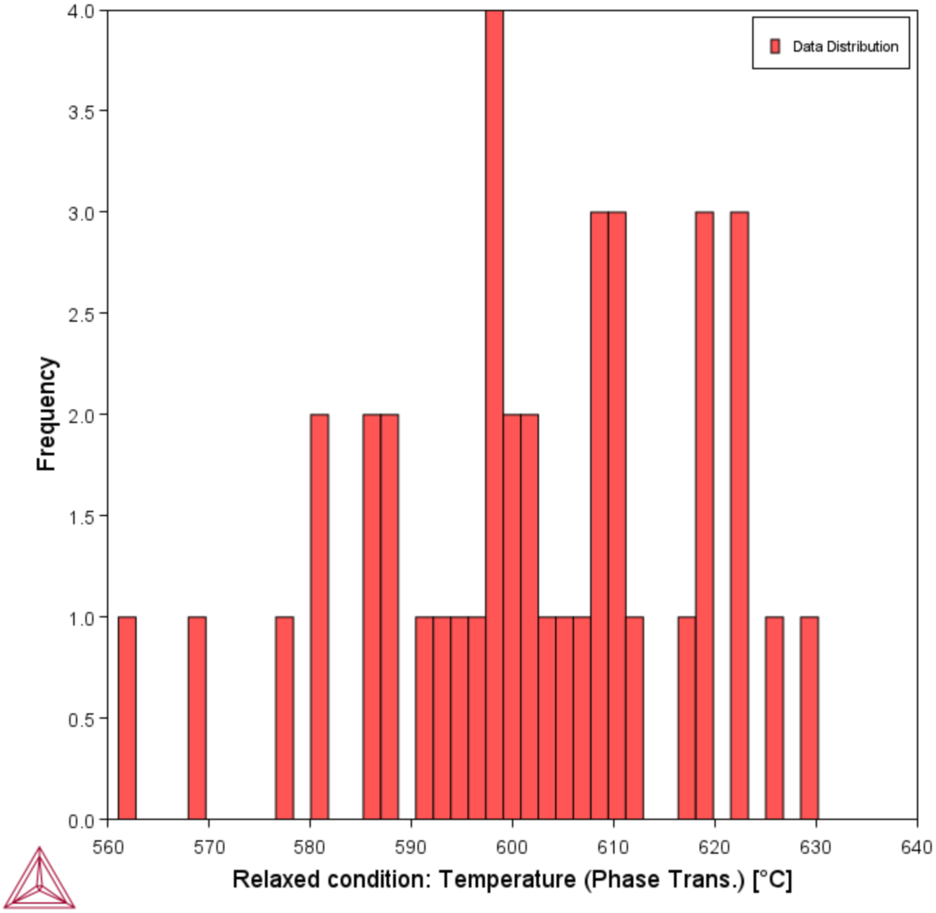
Limits: 0.0 ☑ Automatic scaling

Y: Normal probability

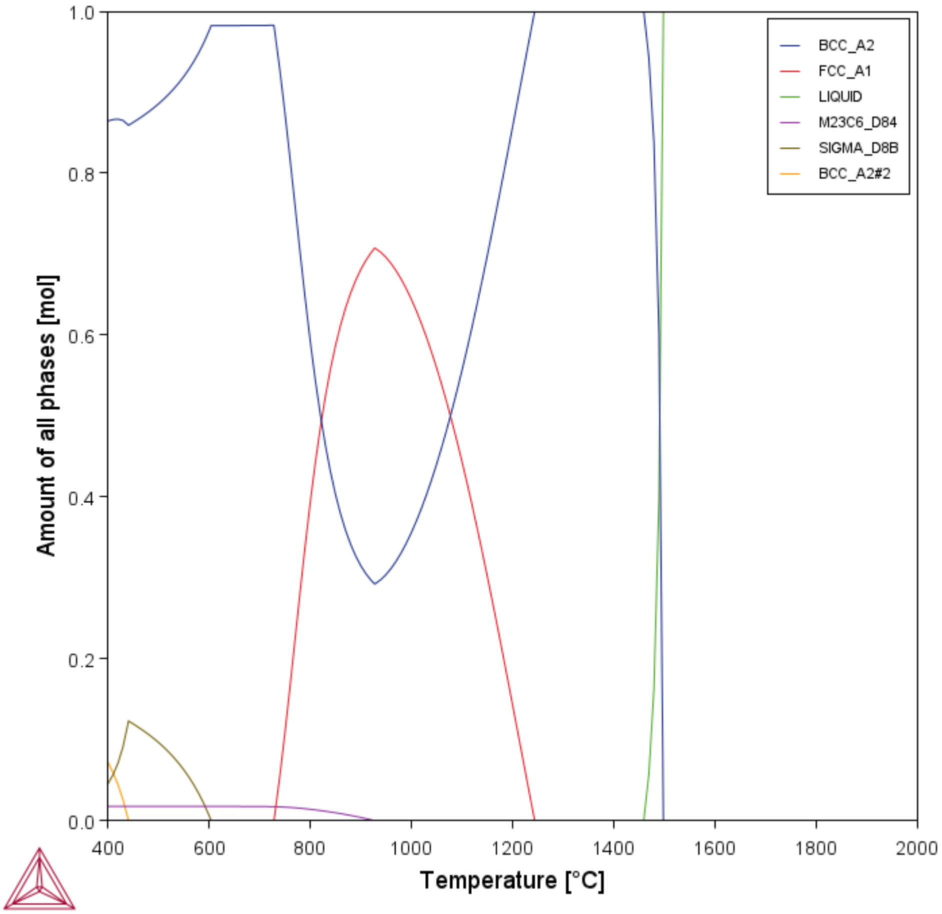
Axis type: Probability

Limits: 0.0

The two combination options, Frequency → Histogram or Normal probability → Probability, selected with Statistical on a Plot Renderer as a successor to a Property Model Calculator.


4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Frequency
560
570
580
590
600
610
620
630
640
Relaxed condition: Temperature (Phase Trans.) [°C]
Data Distribution

A Statistical Plot type, with the Frequency Axis variable and Histogram Axis type selected.

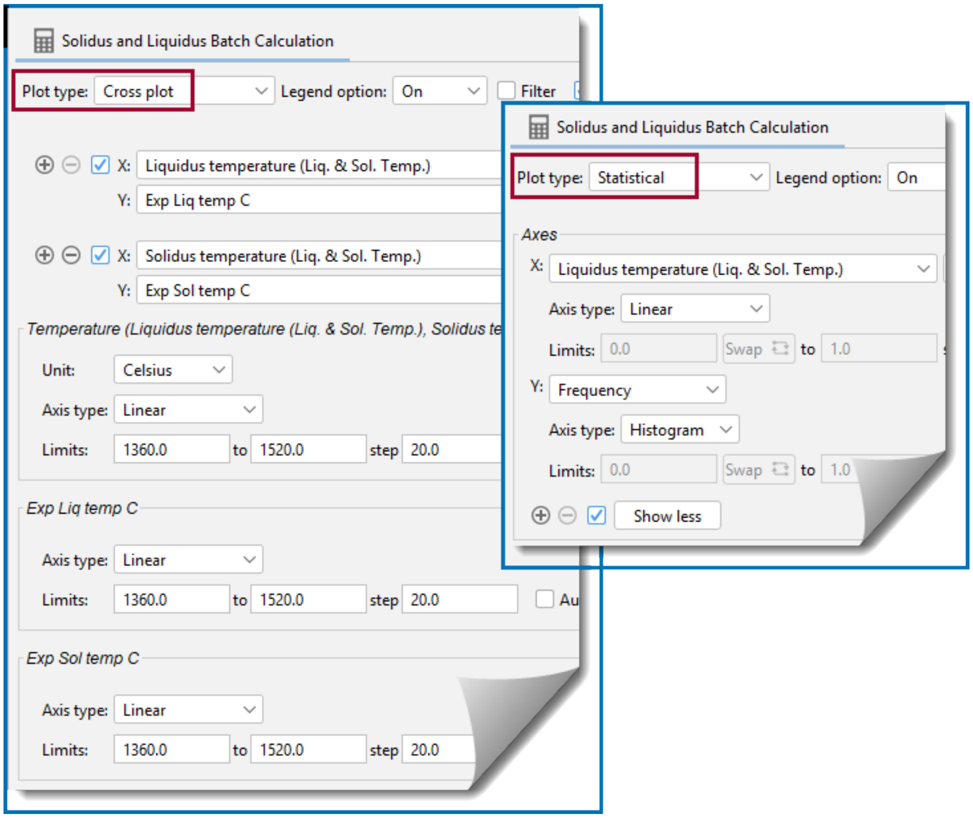


A Statistical Plot type, with the Normal probability Axis variable and Probability Axis type selected.

Cross Plot (Parity Plot)

Use **Cross plot** to plot the experimental data from a Batch calculation with the calculated result, e.g. you might be looking at liquidus temperature and now can plot both to compare the experimental data against the Thermo-Calc calculated results. You choose the experimental data value (which is read from the data file) as an *X*- or *Y*-axis variable and then the calculated result as the other *X*- or *Y*-axis variable. This is also known as a *parity* plot.

The following uses a General Property Model example: PM_G_12: Solidus and Liquidus Batch Calculation.



Solidus and Liquidus Batch Calculation

Plot type: Cross plot
Legend option: On
☐ Filter

☑ X: Liquidus temperature (Liq. & Sol. Temp.)
Y: Exp Liq temp C

☑ X: Solidus temperature (Liq. & Sol. Temp.)
Y: Exp Sol temp C

Temperature (Liquidus temperature (Liq. & Sol. Temp.), Solidus te

Unit: Celsius
Axis type: Linear
Limits: 1360.0 to 1520.0 step 20.0

Exp Liq temp C

Axis type: Linear
Limits: 1360.0 to 1520.0 step 20.0 ☐ Au

Exp Sol temp C

Axis type: Linear
Limits: 1360.0 to 1520.0 step 20.0

Solidus and Liquidus Batch Calculation

Plot type: Statistical
Legend option: On

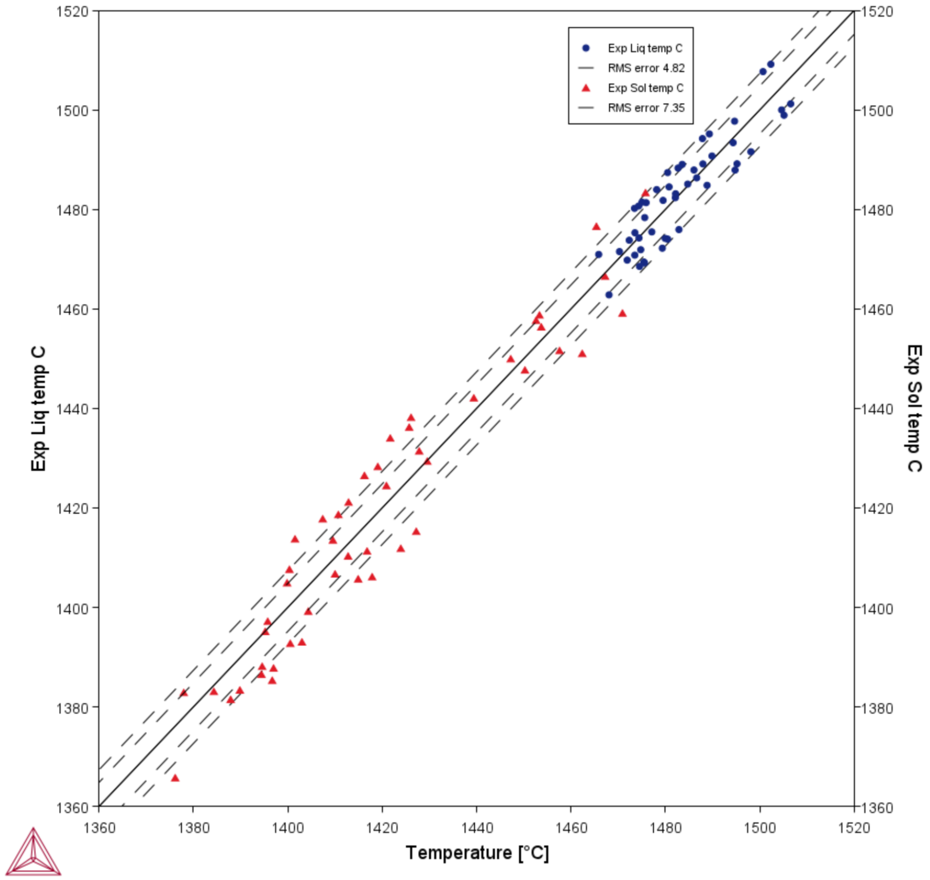
Axes

X: Liquidus temperature (Liq. & Sol. Temp.)
Axis type: Linear
Limits: 0.0 Swap to 1.0

Y: Frequency
Axis type: Histogram
Limits: 0.0 Swap to 1.0

☑ Show less

For a Batch calculation, and when the data file contains experimental (Exp) data, you can use Cross plot on a Plot Renderer to compare it to the simulated results.



A comparison of experimental liquidus and solidus data using a Cross plot with a Batch calculation. A root mean square (RMS) setting shows the distribution of the data points.

There is a blog post related to ICME Workflows that provides an additional example about the use of cross plots.

Another example showing the use of cross plots is PM_G_03: Driving Force and Interfacial Energy, which also has a video to accompany it.

Plot Type: Parallel Coordinates

The Plot Renderer is a dynamic activity node with options such as being able to choose from a variety of *Plot types* based on the Calculator and Calculation Type selected.

Calculation Types in Graphical Mode

See Plot Types detailing availability *By Calculator*, *By Plot Type*, or *By Calculation Type*.

The **Parallel coordinates** plot type is available when using the Property Model Calculator with a **Grid**, **Batch**, or **Uncertainty** *Calculation Type*.

The **Parallel coordinates** plot is useful when interpreting multidimensional data and to compare how different parameters affect each other. This is especially useful in materials design after performing a batch or uncertainty set of evaluations when multiple inputs are varied at the same time and multiple model outputs are given as a result.

It is recommended that you detach the **Visualizations** window and then drag the edges of it to fully display (i.e. stretch out) the results for this detailed plot.

For this plot type, there are some differences compared to other plots as to what can be done on the **Visualizations** window and the **Plot Renderer Configuration** window.

- **Visualizations** window: After a plot is generated, the options available when you right-click are slightly different. You can choose to **Select/Deselect a line** (to display additional information), and to **Save As** and **Copy** plot images. See Visualization Window Plot Options.

  Other options such as Plot Themes and plot formatting options are not available.

- **Plot Renderer Configuration** window: You can select the **Filter** checkbox and then filter one or more quantities. For some parameterized plot quantities, there is a filter list made available after the first time the quantity is plotted. See Plot Renderer Configuration Window Options.

To access this plot type on the Plot Renderer for a **Grid** calculation, at least three quantities under *Grid Definitions* must be selected on the Property Model Calculator.

Tips to Interpret the Plot Data

- When most lines between two parallel axes are somewhat parallel to each other, there is a positive relationship between these two dimensions.
- When lines cross in a kind of superposition of X-shapes, that is a negative relationship.
- When lines cross randomly it means that there is no particular relationship.

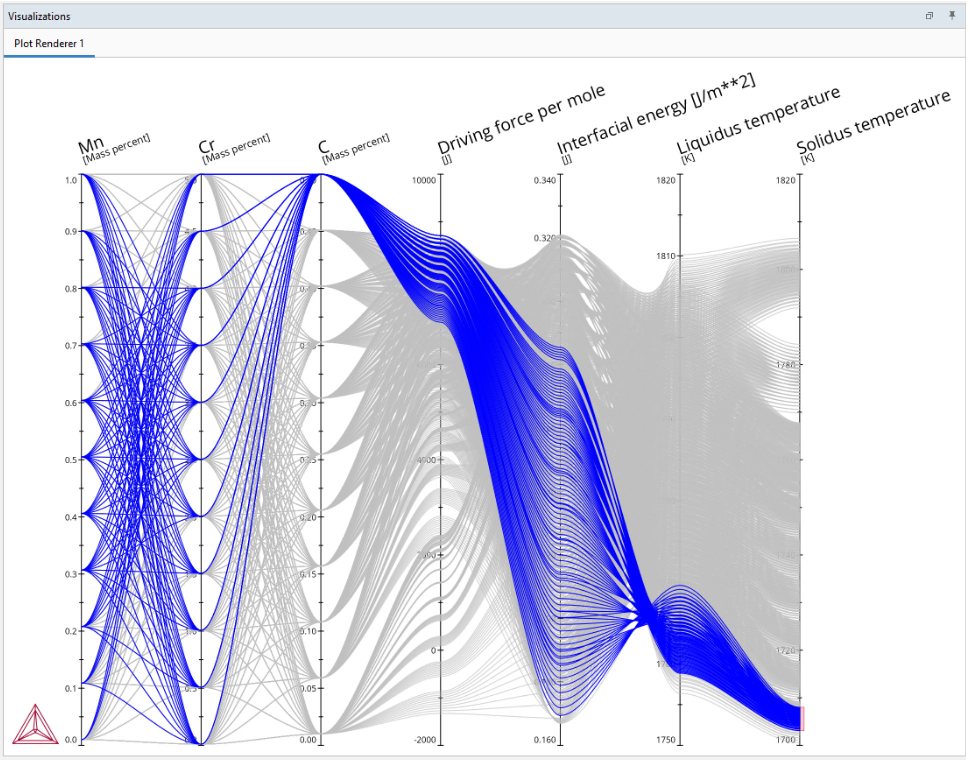


Figure 1: Parallel coordinates plot showing multidimensional data.

Overlay Compositions on the Same Plot

For this plot, you can combine and overlay calculated results from two or more Property Model Calculators and show it on one plot in the Visualizations window, even if they have been set up for different grids. This is available for a Grid calculation and when you are including three or more axis quantities for two Property Model Calculators. Each composition has its own line and it is color coded so you can identify which Property Model Calculator a given result is from.

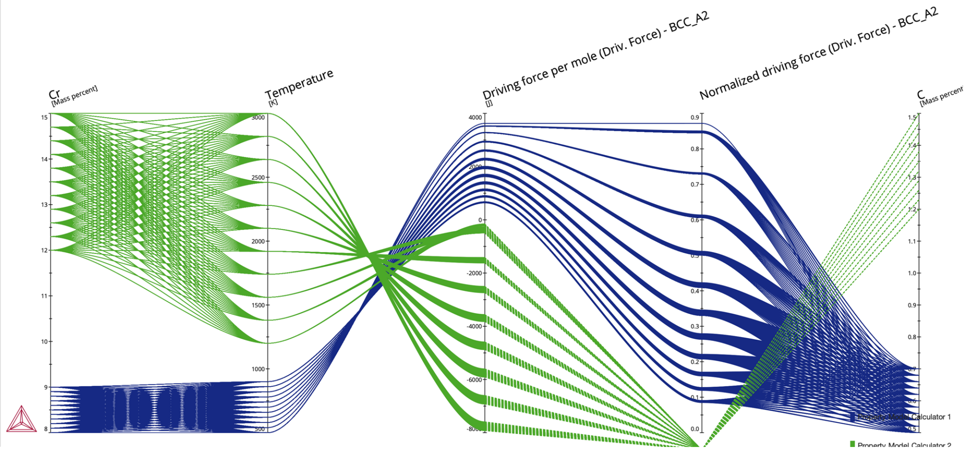


Figure 2: Parallel coordinates plot with two sets of composition data overlaid and color coded for each Property Model Calculator.

Visualization Window Plot Options

Once the plot is generated in the Visualizations window, you can right-click and choose one of these options:

- **Select/Deselect a line** (or Ctrl + right-click). For this option, you must right-click directly on an axis line to view the details and highlight the relevant information.
- **Save As** to save the plot (in its current state) as a **jpg**, **png**, or **gif** file.
- **Copy** to copy the plot (in its current state) to a clipboard. Then you can paste it into any supported application. The pasted image defaults to a **png** format.

For both **Save As** and **Copy** actions, the image is saved in the current state that the both the plot and Visualizations window is in, i.e. if you have selected one or more lines to display information, then this is what is included in the saved file. It is also saved based on the current size of the Visualizations window, i.e. to ensure that the entire plot is saved, you may need to expand the window to the full view you want to capture. Sometimes it is also useful to detach the window and drag it to full size before saving the image.

There are examples using this plot type available:

A Nickel Model Library example PM_Ni_04: Strain Age Cracking (SAC).

A Steel Model Library example PM_Fe_11: Steel Design Using the Parallel Coordinates Plot.

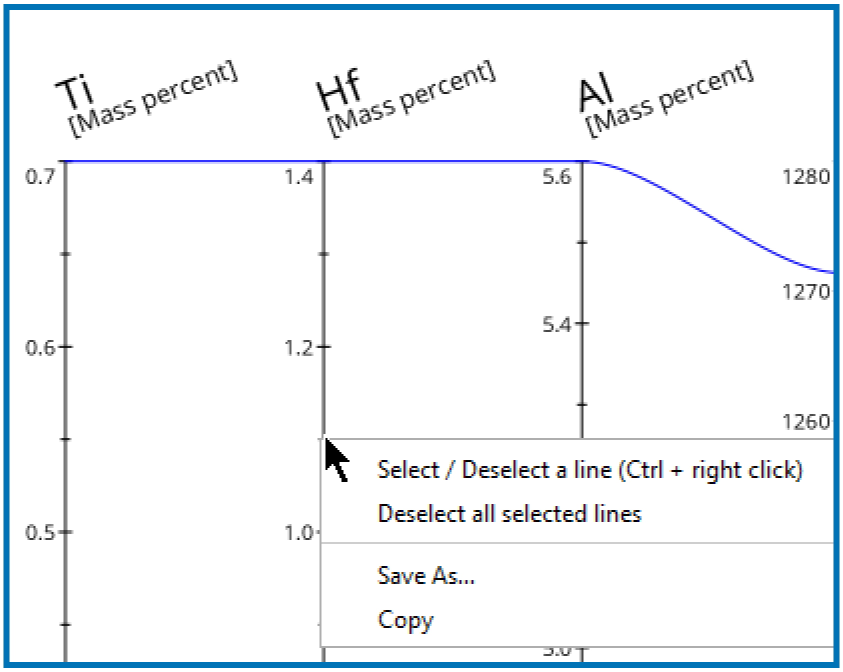
Select and Deselect Lines

In the **Visualizations** window, you can highlight and display details about any plot axis, which is useful particularly with complex plots.

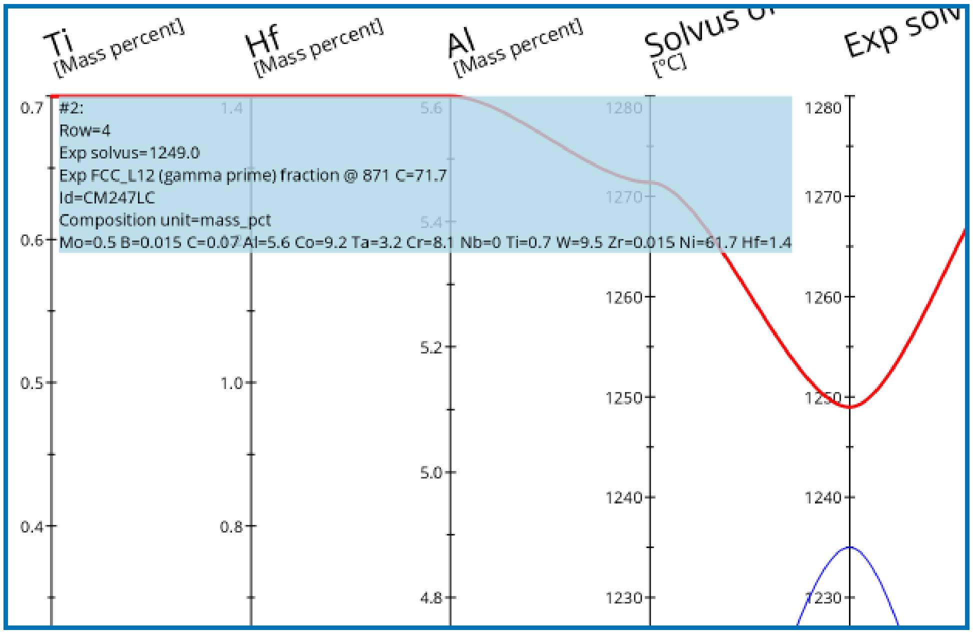
You must directly right-click the axis line to turn it on (select) or off (deselect); it does not work to just right-click anywhere in the Visualizations window for this action.

To toggle the **Select/Deselect a line** option on (select a line) and off (deselect a line), hover over an axis line then:

- Ctrl + right-click or
- Right-click and choose **Select/Deselect a line**.



To deselect all lines, either do this one at a time or when several lines are selected, you can right-click to choose **Deselect all selected lines**.



#2:
Row=4
Exp solvus=1249.0
Exp FCC_L12 (gamma prime) fraction @ 871 C=71.7
Id=CM247LC
Composition unit=mass_pct
Mo=0.5 B=0.015 C=0.07 Al=5.6 Co=9.2 Ta=3.2 Cr=8.1 Nb=0 Ti=0.7 W=9.5 Zr=0.015 Ni=61.7 Hf=1.4

Figure 3: Choosing to display specific axes lines and the associated information on the Visualizations window for a Parallel coordinates plot type.

Save As

1. Once the plot is generated in the **Visualizations** window, right-click anywhere in the window and choose **Save As**.
2. In the **Save** window:
    a. Navigate to where you want to save the plot.
    b. Enter a **File Name**.
    c. From the **Files of Type** list choose **png** (the default), **jpg**, or **gif**.
    d. When you are ready, click **Save**.

Copy

1. Once the plot is generated in the **Visualizations** window, right-click anywhere in the window and choose **Copy**.
2. Navigate to where you want to paste the image (i.e. Word, Slack, email, and so forth) and Ctrl + V to paste it. The pasted image defaults to a **png** format.

Plot Renderer Configuration Window Options

Filter Quantities

Use the **Filter** checkbox on a Plot Renderer to add various filters to the **Parallel coordinates** plot or table and based on the set up of the calculation.

When selected, click the ⊕ **Add quantity** and ⊖ **Remove quantity** buttons to add filters. For example, enter a **Min** and **Max** and choose an axis variable such as **Composition Cr** and the unit **Mass percent** to adjust the output in the **Visualizations** window. Click **Perform** each time you add or remove a filter for the results to update.

Filter Parameterized Quantities

For a **Parallel coordinates** *Plot type*, and only for parameterized result quantities, you can choose to show all or one specific quantity on the plot. By default, and when you first choose these types of results quantities, **All** quantities are plotted in the **Visualizations** window output after performing the first calculation. Once the secondary list is available you can then choose to plot only one of the quantities at a time. The availability of the filter list is dependent on the result of the initial calculation.

> This filter option does NOT use the **Filter** checkbox. The filter list displays AFTER clicking **Perform** for the chosen quantity. Once the quantity is plotted you can choose to filter by the individual quantities included in the list. Initially, **All** quantities are plotted.

1. From the **Axis variable** list, choose a quantity. For example, for the Martensitic Steel Strength Property Model, you can choose **Precipitate fraction (Tempering)**.
2. Continue adding and selecting any quantity you want to include in the **Parallel coordinates** plot.
3. Click **Perform**. Go to the **Visualizations** window to view your results.
4. If the type of quantity you selected has additional filtering options, on the **Plot Renderer Configuration** window, next to the original quantity chosen, there is now a secondary filter list available. It defaults to include **All** quantities or from the list you can choose to plot a specific quantity. When you use this list to filter, it includes **All** or one quantity, i.e. you cannot choose more than one option.
5. Click **Perform** each time you change the selection in order to regenerate the plot.

To plot more than one specific parameterized quantity at a time, click the ⊕ **Add quantity** button, select the same quantity again (e.g. **Precipitate fraction (Tempering)**) and then after performing the calculation, from the secondary filter list choose the second quantity you want to include. That is, add the parameterized quantity twice, perform to access the secondary filter list, then individually choose the two quantities you want to plot. Remember to click **Perform** to regenerate the plot.

Plot Type: Heat Map, Contour, and 3D

The Plot Renderer is a dynamic activity node with options such as being able to choose from a variety of *Plot types* based on the Calculator and Calculation Type selected.

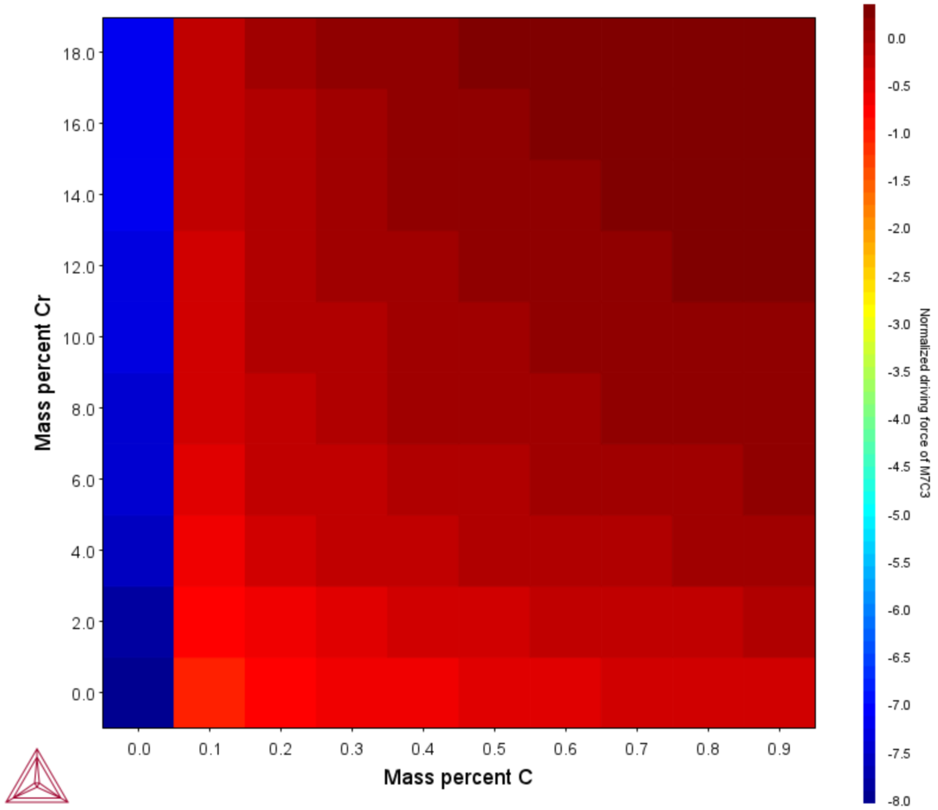
Calculation Types in Graphical Mode

See Plot Types detailing availability *By Calculator*, *By Plot Type*, or *By Calculation Type*.

Visit the website Application Examples → Process Metallurgy for examples of these Plot types using the Process Metallurgy Calculator.

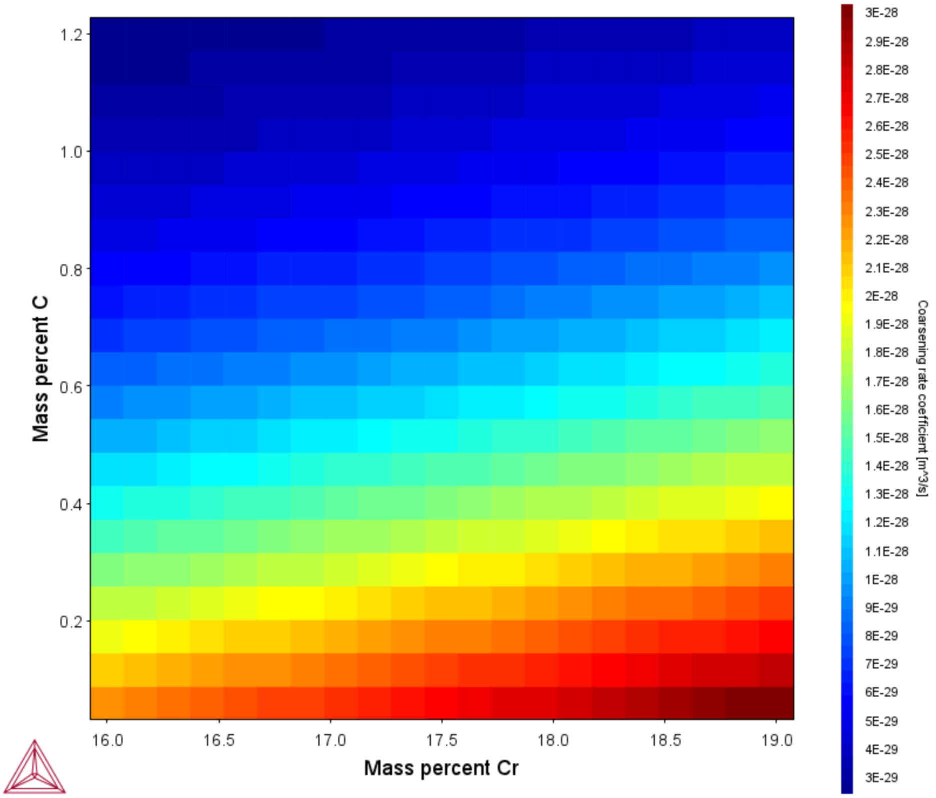
Heat Map

For a **Heat map** plot, each *Z*-axis variable value in the grid is represented by a color-coded area, where dark red represents the highest *Z*-axis variable value and dark blue represents the lowest *Z*-axis variable value.



Thermo-Calc example T_09 uses an Equilibrium Calculator with a Grid Calculation Type to generate a Heat map plot.

[T_09: Carbide Driving Force Heat Map](#)

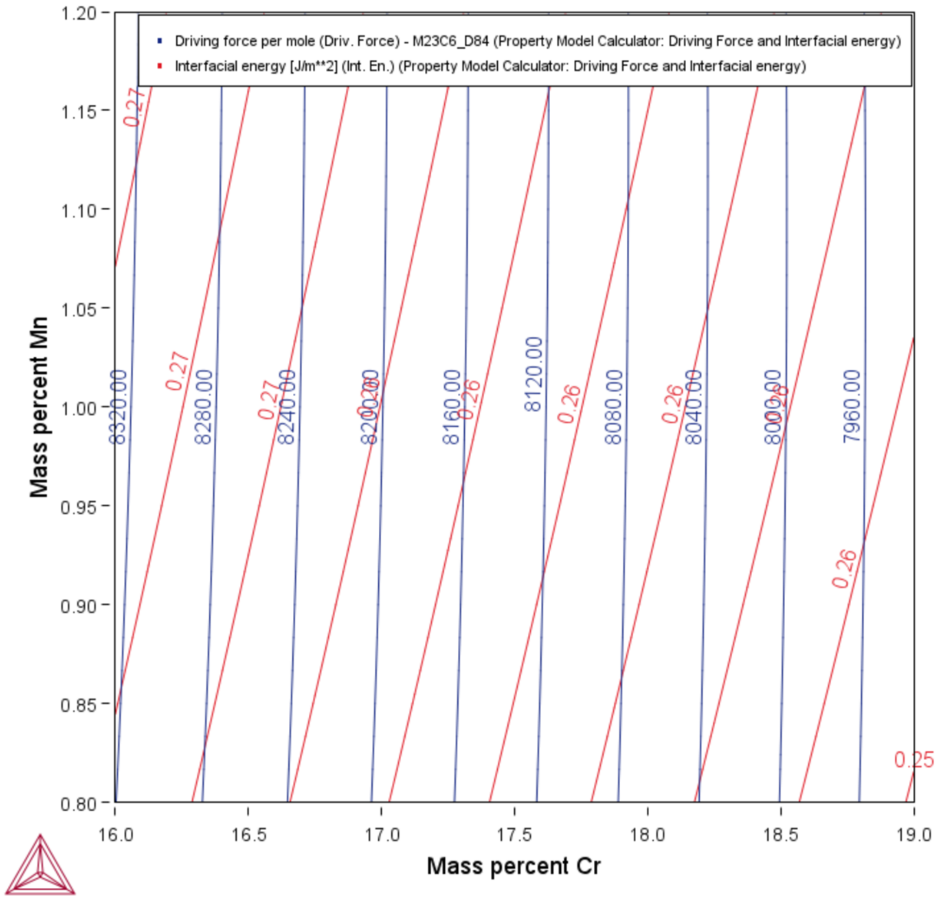


Thermo-Calc General Property Model example PM_G_02 uses a Property Model Calculator with a Grid Calculation type to plot the coarsening rate coefficient as a Heat map.

PM_G_02: Coarsening and Interfacial Energy

Contour

For a **Contour** plot, *Z*-axis variable values are traced with curves in the same way that height values are traced with curves on a topographical map. The colors used originate from the different data series.

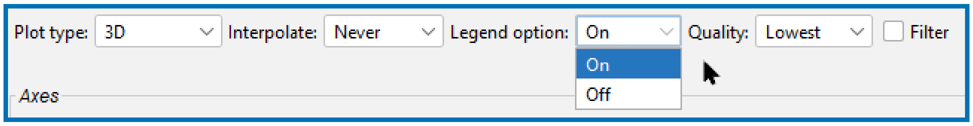


Thermo-Calc General Property Model example PM_G_03 uses a Property Model Calculator with a Grid Calculation type to compare the driving force and interfacial energy on an overlaid contour plot.

[PM_G_03: Driving Force and Interfacial Energy]

3D

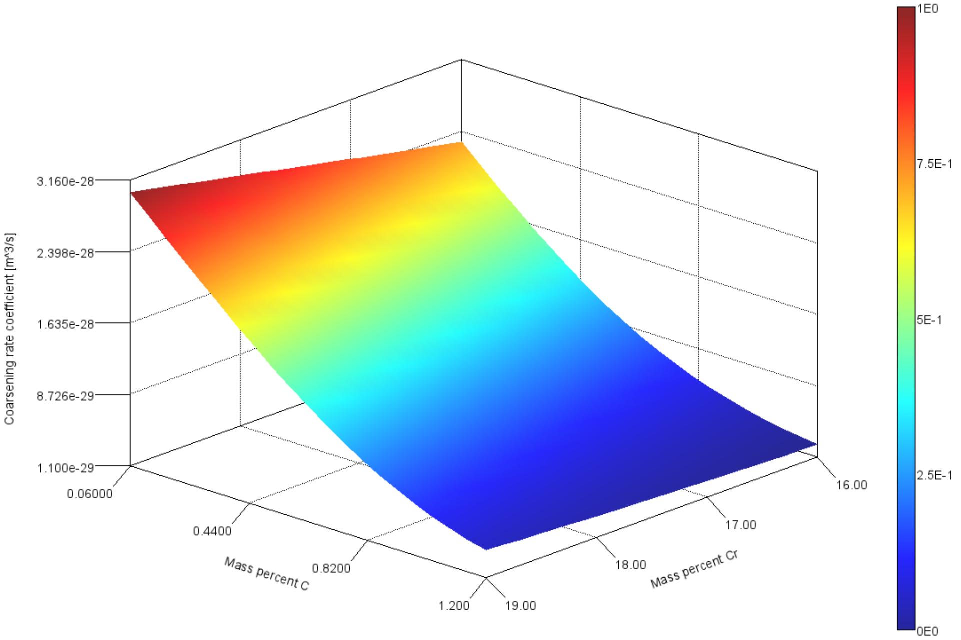
For a **3D** plot, the 3D surface is created by Delaunay tesselation of the calculated data. The surface uses a cold to warm color map where red represents the highest *Z*-axis variable value and blue represents the lowest *Z*-axis variable value. The color map color legend can be turned on or off with the legend option.



Plot type: 3D Interpolate: Never Legend option: On Quality: Lowest ☐ Filter

3D Plots with additional functionality are also available with the Add-on Additive Manufacturing (AM) Module. The information is described separately and included with the Module's documentation.

When in the Thermo-Calc help (press F1), go to Rotating 3D Plots to watch a short video showing you how to rotate this plot in the Visualizations window.



Thermo-Calc General Property Model example PM_G_02 uses a Property Model Calculator with a Grid Calculation type to plot the coarsening rate coefficient as a 3D plot.

PM_G_02: Coarsening and Interfacial Energy

Plot Type: Flexible Mode and Grouped Mode

The Plot Renderer is a dynamic activity node with options such as being able to choose from a variety of *Plot types* based on the Calculator and Calculation Type selected.

? Calculation Types in Graphical Mode

? See Plot Types detailing availability *By Calculator*, *By Plot Type*, or *By Calculation Type*.

Flexible Mode

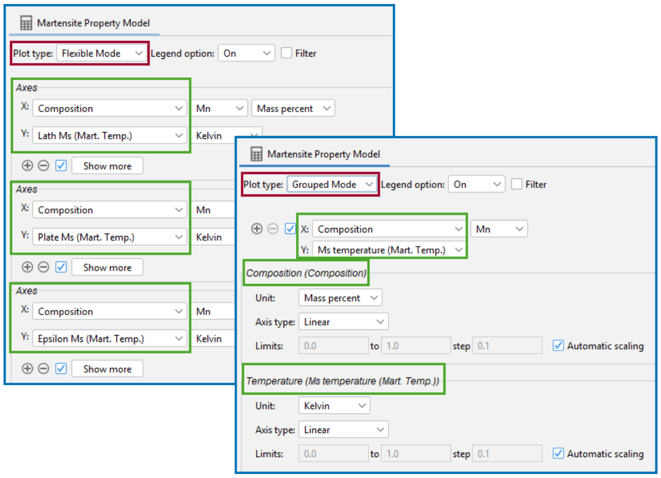
Use **Flexible Mode** to individually add and configure axes quantities and change the units or other associated settings one at a time.

Grouped Mode

Use **Grouped Mode** to add and configure groups of axis quantities at the same time and of the same type. For example, change units or settings in groups with similar settings like temperature units or axis types.

Switching Between Modes

If you have a license for the Steel Model Library, you can try yourself to switch between Flexible Mode and Group Mode and then change the settings to how you want it using the **Steels** example PM_Fe_02: Fe-Mn Martensite Morphologies.



Martensite Property Model

Plot type: Flexible Mode
Legend option: On
☐ Filter

Axes
X: Composition, Mn, Mass percent
Y: Lath Ms (Mart. Temp.), Kelvin

Axes
X: Composition, Mn
Y: Plate Ms (Mart. Temp.), Kelvin

Axes
X: Composition, Mn
Y: Epsilon Ms (Mart. Temp.), Kelvin

Martensite Property Model

Plot type: Grouped Mode
Legend option: On
☐ Filter

☑ X: Composition, Mn
Y: Ms temperature (Mart. Temp.)

Composition (Composition)
Unit: Mass percent
Axis type: Linear
Limits: 0.0 to 1.0 step 0.1
☑ Automatic scaling

Temperature (Ms temperature (Mart. Temp.))
Unit: Kelvin
Axis type: Linear
Limits: 0.0 to 1.0 step 0.1
☑ Automatic scaling

Comparing Flexible Mode (left) to Grouped Mode (right) on a Plot Renderer as a successor to a Property Model Calculator. The advantage of Grouped Mode is that you can, for example, configure or edit settings in one place, making it easier to manage and work with the plot quantities.

To experiment using the **Equilibrium Calculator**, see Thermo-Calc example T_02: Stepping in Temperature in the Fe-C System.

To experiment using the **Material to Material Calculator**, see Thermo-Calc example T_14: Fe-Cr-Ni Transition Comparison Using the Material to Material Calculator.

Plot Type: CCT Mode

The Plot Renderer is a dynamic activity node with options such as being able to choose from a variety of *Plot types* based on the Calculator and Calculation Type selected.

Calculation Types in Graphical Mode

See Plot Types detailing availability *By Calculator*, *By Plot Type*, or *By Calculation Type*.

Use **CCT Mode** to make a CCT diagram from a **One Axis** calculation with a *Quantity* of **Log10 (cooling rate [K/s])** selected for the CCT Diagram Property Model. The *X*- and *Y*-axes are *Time* and *Temperature*, respectively. Result quantities defined as time-temperature pairs are identified and plotted. Cooling curves are also automatically added in the plot.

This plot type is available with the Steel Model Library, which requires specific maintenance and database licenses. See About the Steel Model Library Property Models.

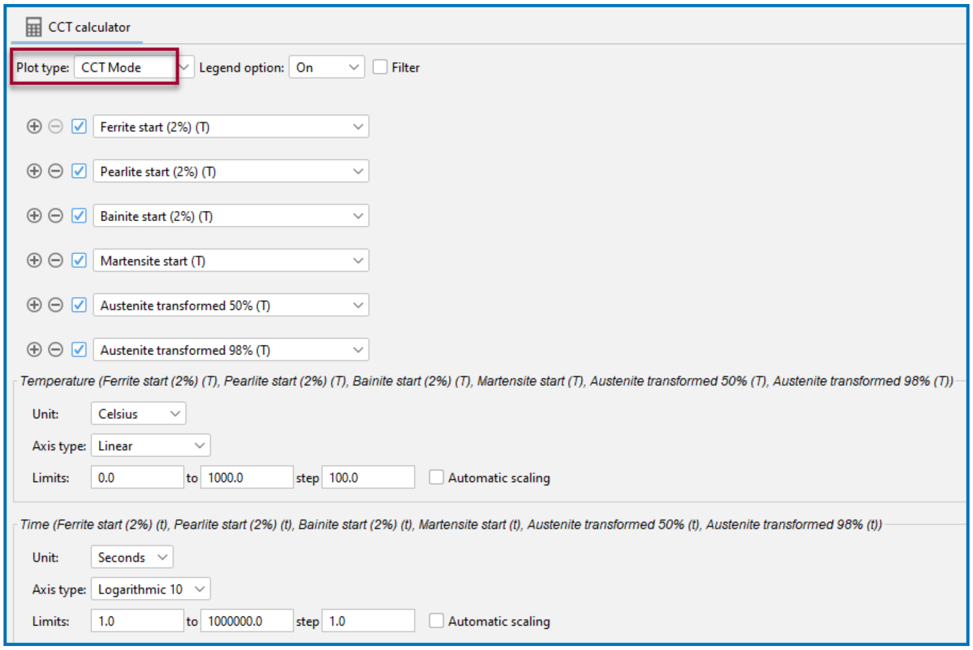
In general, this plot type is available from the drop-down list in these situations:

- When you add the **Steel - CCT** template (on the **My Projects Configuration** window under **Property Models**), it is the default type on the Plot Renderer (renamed CCT in the template).
- If a user-defined Property Model has both **Time** and **Temperature** quantities defined in a coupled manner, for example if you create your own Property Model with TC-Python. That is, if you select or create any model where the resulting combination of stepping-quantity and result-quantities has both time and temperature definitions.

Configuration Window Settings and Configuration Settings

Steel Library CCT Diagram Template

The settings example below uses Property Model example PM_Fe_08: CCT Diagram for Fe-C-Mn-Si-Cr-V.



Plot type: CCT Mode
Legend option: On
☐ Filter

☑ Ferrite start (2%) (T)
☑ Pearlite start (2%) (T)
☑ Bainite start (2%) (T)
☑ Martensite start (T)
☑ Austenite transformed 50% (T)
☑ Austenite transformed 98% (T)

Temperature (Ferrite start (2%) (T), Pearlite start (2%) (T), Bainite start (2%) (T), Martensite start (T), Austenite transformed 50% (T), Austenite transformed 98% (T))

Unit: Celsius
Axis type: Linear
Limits: 0.0 to 1000.0 step 100.0 ☐ Automatic scaling

Time (Ferrite start (2%) (t), Pearlite start (2%) (t), Bainite start (2%) (t), Martensite start (t), Austenite transformed 50% (t), Austenite transformed 98% (t))

Unit: Seconds
Axis type: Logarithmic 10
Limits: 1.0 to 1000000.0 step 1.0 ☐ Automatic scaling

CCT Mode on a Plot Renderer as a successor to a Property Model Calculator.

Plot Type: TTT Mode

The Plot Renderer is a dynamic activity node with options such as being able to choose from a variety of *Plot types* based on the Calculator and Calculation Type selected.

Calculation Types in Graphical Mode

See Plot Types detailing availability *By Calculator*, *By Plot Type*, or *By Calculation Type*.

Use **TTT Mode** to make a TTT diagram from a **One Axis** calculation with temperature. The *X*- and *Y*-axes are *Time* and *Temperature*, respectively. Time quantities (such as *Pearlite start*, *Bainite start*) are plotted as functions of temperature. Temperature quantities (such as *Martensite start*, *Martensite 50%*) are independent of time and plotted as horizontal lines.

This plot type is available with the Steel Model Library, which requires specific maintenance and database licenses. See About the Steel Model Library Property Models.

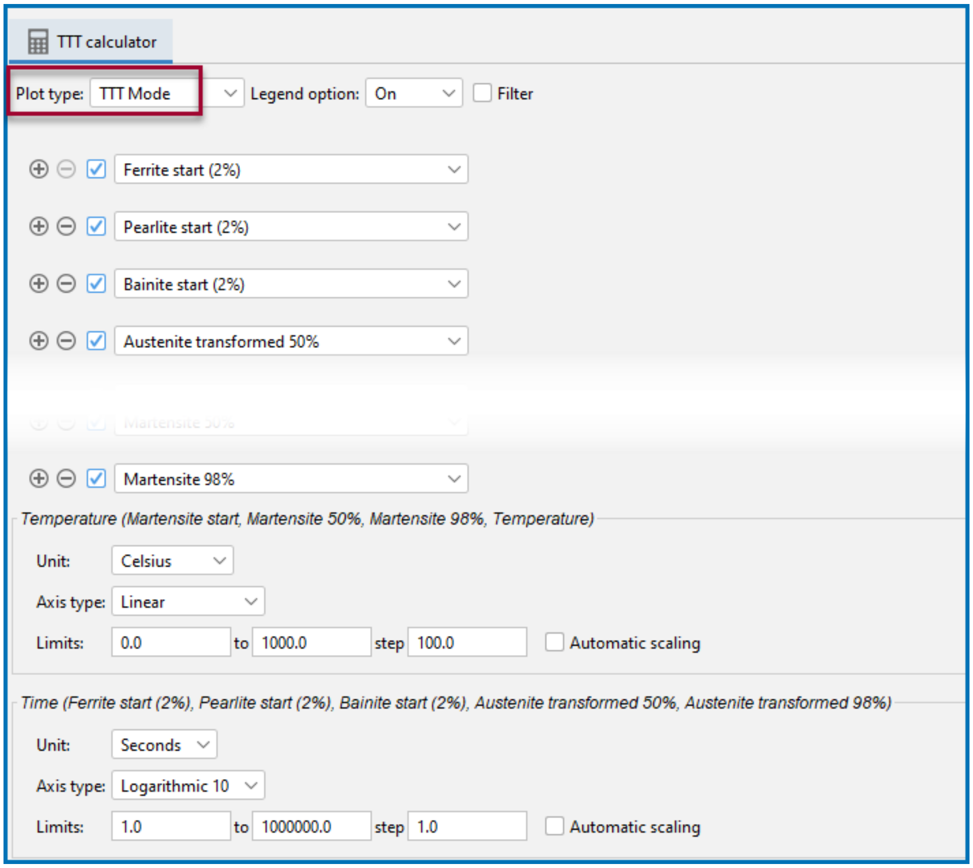
In general, this plot type is available from the drop-down list in these situations:

- When you add the **Steel - TTT** template (on the **My Projects Configuration** window under **Property Models**), it is the default type on the Plot Renderer (renamed TTT in the template).
- When you are using at least one of these Steel Property Models—**Martensite Temperatures**, **Pearlite**, or **Bainite** with a **One Axis** calculation and when both time and temperature quantities are selected on the Plot Renderer—the TTT Mode is available.
- If a user-defined Property Model has both time and temperature quantities defined in a coupled manner, for example if you create your own Property Model with TC-Python. That is, if you select or create any model where the resulting combination of stepping-quantity and result-quantities has both time and temperature definitions.

Configuration Window Settings and Configuration Settings

Steel Library TTT Diagram Template

The settings example below uses Property Model example PM_Fe_06: TTT Diagram for Fe-C-Mn-Si-Cr-V.


TTT calculator

Plot type: TTT Mode

Legend option: On

☐ Filter

☑ Ferrite start (2%)

☑ Pearlite start (2%)

☑ Bainite start (2%)

☑ Austenite transformed 50%

☑ Martensite 50%

☑ Martensite 98%

Temperature (Martensite start, Martensite 50%, Martensite 98%, Temperature)

Unit: Celsius

Axis type: Linear

Limits: 0.0 to 1000.0 step 100.0 ☐ Automatic scaling

Time (Ferrite start (2%), Pearlite start (2%), Bainite start (2%), Austenite transformed 50%, Austenite transformed 98%)

Unit: Seconds

Axis type: Logarithmic 10

Limits: 1.0 to 1000000.0 step 1.0 ☐ Automatic scaling

TTT Mode on a Plot Renderer as a successor to a Property Model Calculator.

Plot Type: Simple Mode and Advanced Mode

The Plot Renderer is a dynamic activity node with options such as being able to choose from a variety of *Plot types* based on the Calculator and Calculation Type selected.

Calculation Types in Graphical Mode and Plot Types

Simple Mode and **Advanced Mode** as a *Plot type* are only available for the Diffusion Module (DICTRA) in Graphical Mode. Unlike many other Calculators, the Diffusion Calculator does not require the selection of a *Calculation Type* before a Plot Type is available on the Diffusion Calculator Plot Renderer.

Simple Mode

Use **Simple Mode** to define the most common axis variables. The software automatically sets the correct **Plot condition** and **Independent variable**.

For one example using **Simple Mode**, see D_04: Fe-C Moving Boundary - Austenite to Ferrite.

Advanced Mode

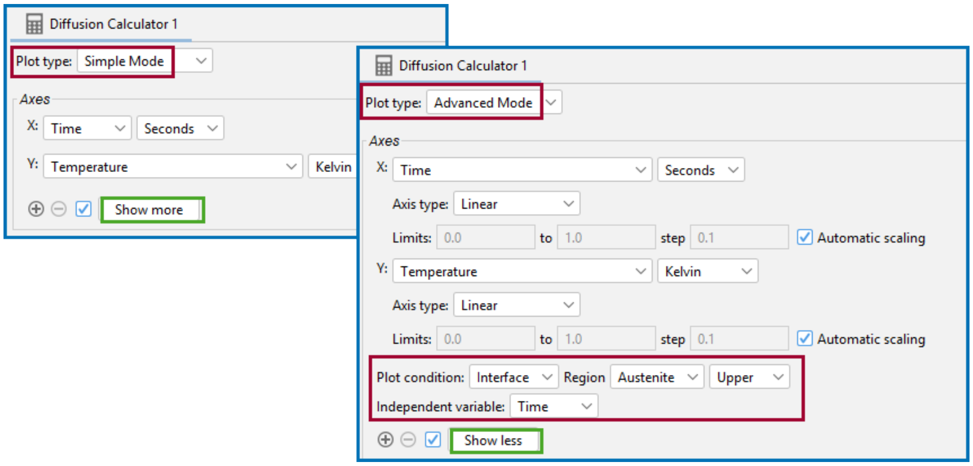
Use **Advanced Mode** to select any combination of axis variables, and then access further settings such as the **Plot condition**, **Region**, and **Independent variable**. Examples of advanced plot options are activity of a component at an interface, diffusivities, and diffusion paths. Also user-defined functions can be used as plot variables where Console Mode syntax is used to define functions. In some cases, sensible default values are selected, but they can be changed according to your needs.

For one example using **Advanced Mode**, see D_10: Iron (Fe) Homogenization in Scheil.

Switching Between Modes

You can try yourself to switch between **Simple Mode** and **Advanced Mode** and then change the settings to how you want it using example D_04: Fe-C Moving Boundary - Austenite to Ferrite.

In the **Plot Renderer** settings window, click **Show more** and **Show less** to toggle between viewing all or some of the available settings.



Diffusion Calculator 1

Plot type: Simple Mode

Axes

X: Time Seconds

Y: Temperature Kelvin

Diffusion Calculator 1

Plot type: Advanced Mode

Axes

X: Time Seconds

Axis type: Linear

Limits: 0.0 to 1.0 step 0.1 ☑ Automatic scaling

Y: Temperature Kelvin

Axis type: Linear

Limits: 0.0 to 1.0 step 0.1 ☑ Automatic scaling

Plot condition: Interface Region Austenite Upper

Independent variable: Time

Comparing Simple Mode (left) to Advanced Mode (right) on a Plot Renderer as a successor to a Diffusion Calculator. For Advanced Mode, there are additional settings made available based on the combination of axis variables.

Zooming In and Out

In the **Visualizations** window (where the plots are):

- Use the mouse scroll wheel to zoom in and out.
- Click and drag the mouse from left to right to highlight an area of the plot to zoom into a specific point. Use the scroll wheel to continue zooming in or out.

Resetting a Plot to the Default View

- For 2D plots, click and drag the mouse from right to left.
- For 2D and 3D plots, click **Perform Tree** to regenerate the plot in the **Visualizations** window.

Rotating 3D Plots

In the **Project** window (where the activity nodes are):

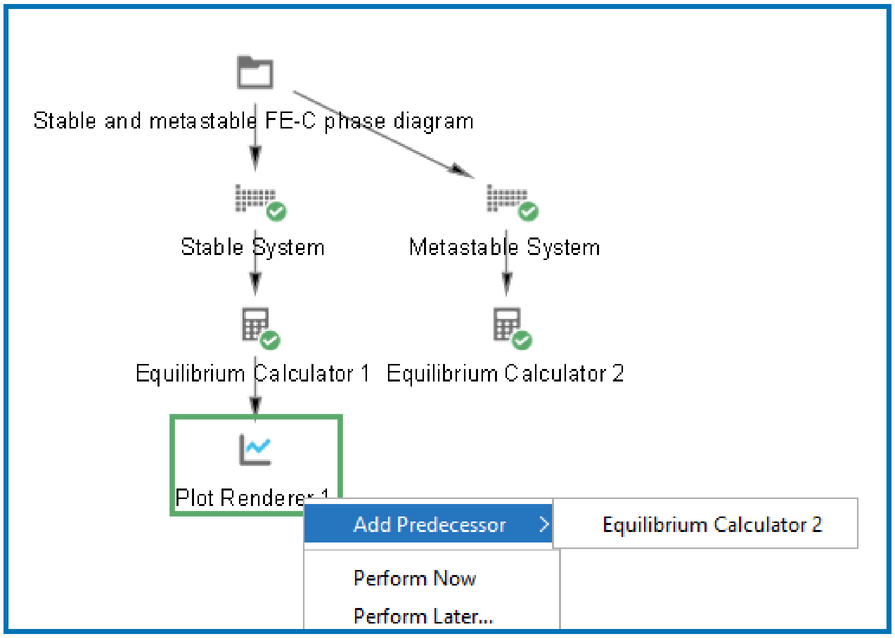
- Right-click and select **Zoom In** or **Zoom Out**.
- To go back to the default zoom, select **Reset Zoom**.

Plotting Several Calculations in One Diagram

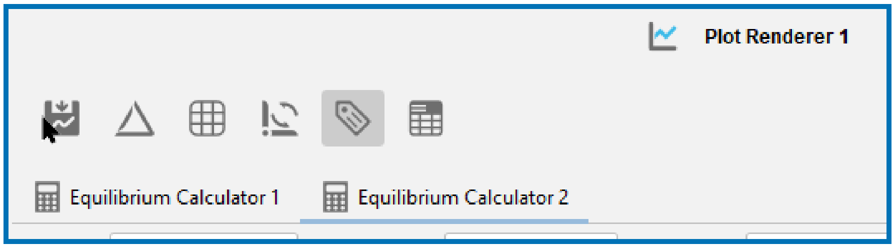
To plot several calculations in one diagram, you must have, in addition to the Plot Renderer's original predecessor, at least one available Plot Renderer predecessor in your project, for example, the additional predecessor can be an Equilibrium Calculator, Binary Calculator, Ternary Calculator, Scheil Calculator, or Experimental File Reader.

This example is based on Thermo-Calc example T_05: Stable and the Metastable Fe-C Phase Diagrams.

1. In the **Project** window click the **Plot Renderer** node.
2. In the **Configuration** window click **Add Predecessor**. Or right-click the **Plot Renderer** and choose **Add Predecessor**.

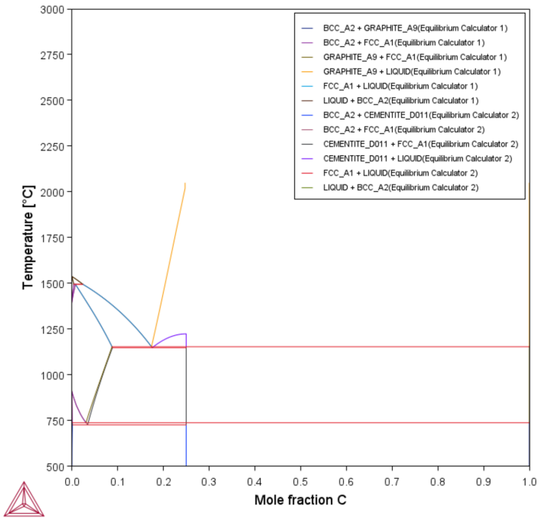


3. Select a predecessor. When added, the extra predecessor is linked to the Plot Renderer. On the **Plot Renderer Configuration** window, the predecessors are shown as two tabs:



4. Configure how you want each calculation plotted on the tabs in the **Configuration** window, then click to **Perform** the Plot Renderer activity.

   The calculations are plotted in the same diagram in a tab in the **Visualizations** window. If any of the axis variables of the plots differ, then the label and scale of all calculations are shown parallel to each other.



Plot Renderer: Convert a Plot to a Table and Export the Data

For all calculation types and calculators, the associated Plot Renderer has a **Table View** button you can use to convert a plot to table data. Once the plot data is converted, you can toggle between displaying the plot or table in the **Visualizations** window as well as save the table and export to file.

> For the Table Renderer only single equilibrium and property diagram (stepping) calculations are available.

Converting a Plot to a Table on the Plot Renderer

1. Set up the Plot Renderer for your particular calculation and click **Perform** to display the plot in the **Visualizations** window.
2. On the Plot Renderer **Configuration** window, click the **Table View** button (toggled ON).
3. Choose the **Decimal digits** and **Number format** (**Auto**, **Decimal**, or **Scientific**) to display in the table.
4. Click **Perform**. This converts the plot data to display table data in the **Visualizations** window.

Switching Between a Plot and a Table in the Visualizations Window

Once the plot data is converted, you can toggle between displaying the plot or table in the **Visualizations** window.

- To display the Table: On the Plot Renderer **Configuration** window, click the **Table View** button to toggle it ON and then click **Perform** to generate the table.
- To display the Plot: On the Plot Renderer **Configuration** window, click the **Table View**button to toggle it OFF and then click **Perform** to generate the plot.

Saving the Table (Exporting the Data)

Once the plot data is converted to a table, you can save/export this to file.

1. Convert the plot to a table (the **Table View** button is toggled ON).
2. Click **Save table** to export the table data.
3. In the **Save As** window navigate to where you want to save the table.
4. Enter a **File Name**.
5. From the **Files of Type** list choose **Text [*.txt]**(the default), **Hyper Text Markup [*.html]**, or **Excel [*.xls]**.
6. Click **Save**.

Saving and Printing the Output in Graphical Mode for more options.

Merging Plots into One Diagram

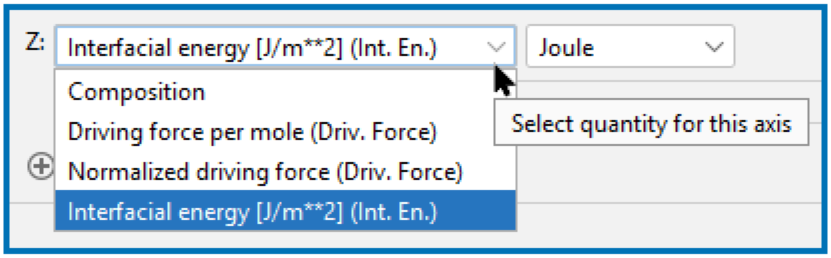
You can merge (or overlay) calculated results for several variables into one diagram. The same X and Y variables are used to compare the third variable (defined in the Plot Renderer as the *Z*-axis).

You cannot overlay heat map or frequency plots.

The following uses example PM_G_03: Driving Force and Interfacial Energy to describe the steps to overlay two plots: the driving force and interfacial energy results are combined into one diagram. The *X*- and *Y*-axis is the same for both (Mass percent Cr/Mass percent Mn).

In the **Plot Renderer** settings window, click **Show more** and **Show less** to toggle between viewing all or some of the available settings.

1. In the **Project** window right-click the calculator node (e.g. Property Model Calculator) and add a **Plot Renderer** node from the **Create New Successor** menu.
2. Click the **Plot Renderer** node.
3. In the **Configuration** window, define the plot. Choose **On** for the *Legend option* and **Contour** as the *Plot type*.
4. Click the ⊕ **Add an axis** button. A new axes settings section is added underneath.
5. For the *Z* axis, choose the variable. In this example, **Interfacial energy**. Select a unit or keep the default.

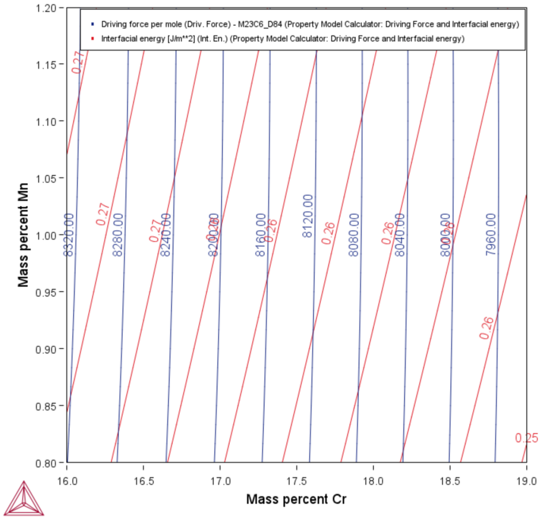


Z: Interfacial energy [J/m**2] (Int. En.)

Joule

6. Click **Perform** to plot both on the same diagram.

   In this case, a contour plot showing both the driving force and interfacial energy calculation results comparing Mass percent Cr to Mass percent Mn.


Driving force per mole (Driv. Force) - M23C6_D84 (Property Model Calculator: Driving Force and Interfacial energy)
Interfacial energy [J/m**2] (Int. En.) (Property Model Calculator: Driving Force and Interfacial energy)
Mass percent Mn
Mass percent Cr
1.20
1.15
1.10
1.05
1.00
0.95
0.90
0.85
0.80
16.0
16.5
17.0
17.5
18.0
18.5
19.0
8320.00
8280.00
8240.00
8200.00
8160.00
8120.00
8080.00
8040.00
8000.00
7960.00
0.27
0.27
0.27
0.26
0.26
0.26
0.26
0.25

Adding Axes to a Diagram

You can add additional axes (*X*, *Y*, and *Z* for **Grid** calculations) to a plot to compare two or more variables at the same time.

- To add an axis setting section, click the ⊕ **Add an axis** button.
- Once a new axis settings section is added, click ⊖ **Remove this axis** button to delete it.
- Wherever you see these plus or minus buttons, click to add or remove a section then define the axis as needed.

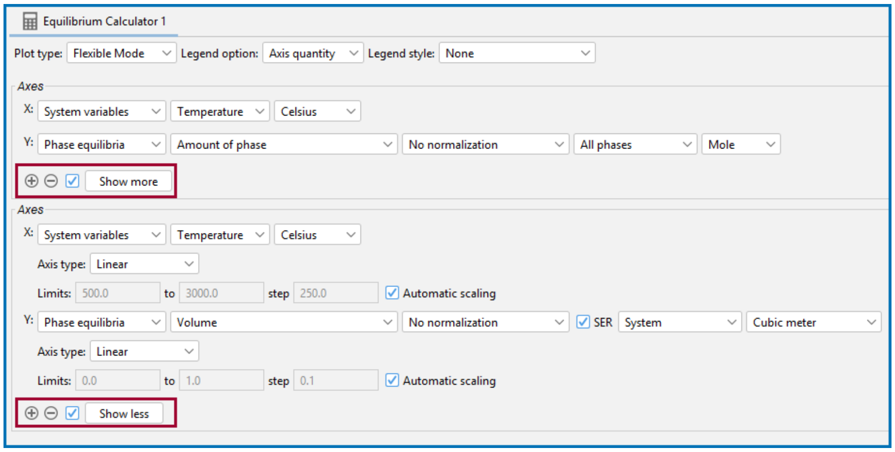
The following is based on example *PM_G_03_Driving_force_and_Interfacial_energy.tcu*.

How to Add and Define an Axis Settings Section

1. Open example PM_G_03. The example is the **Property Models → General** folder.
2. In the **Project** window right-click the **Equilibrium Calculator** node and add a **Plot Renderer** node from the **Create New Successor** menu. This is added to the existing tree so you can compare to the renamed **Equilibrium: Phase fractions vs T** node.
3. Click the new **Plot Renderer** node. The **Configuration** window is where you define the plot. Available settings are based on, for example, the database selected on the **System Definer** and calculation type selected on the Calculator node, in this example the **Equilibrium Calculator**.
4. For the purpose of this example, keep the default **Flexible Mode** as the *Plot type*. You can still switch between this and the **Grouped Mode** to see the differences.
5. In the *Axes* sections for each *X* and *Y* axis [and when relevant, *Z*], choose and define the variables:
    a. From the first list for each axis, select a variable group (i.e. **All variables**, **System variables**, **Physical properties**, etc.). In this example, **System variables** (X axis) and **Phase equilibria** (Y axis) are the defaults selected.
    b. From the second list, choose the axis variables, i.e. **Temperature** (X), and **Amount of phase** (Y).
    c. Based on the variable selected, from the additional lists displayed, choose the unit, i.e. for **Temperature** (X), select **Celsius**. For **Amount of phase** (Y), select **No normalization**, keep the default **All phases**, and select **Mole** as the unit. Any other relevant settings are associated specifically to the variable chosen.

6. To add additional axes, click the ⊕ **Add an axis** button. A new *Axes* settings group is added. Continue to add and define the variables to plot.
7. Keep the default X axis settings, which are the same as in the first group.
8. Define the Y axis. Choose the **Phase equilibria** group and then the variable **Volume**. Keep all the defaults.

> You can toggle between **Show more** and **Show less** to discover and define additional settings i.e. choose an **Axis type**, set **Limits**, adjust the scaling and much more. In this example, no changes are needed. You might also need to expand the **Configuration** window to the right if you cannot see all the settings.


Equilibrium Calculator 1

Plot type: Flexible Mode | Legend option: Axis quantity | Legend style: None

Axes

X: System variables | Temperature | Celsius

Y: Phase equilibria | Amount of phase | No normalization | All phases | Mole

⊕ ⊖ ☑ Show more

Axes

X: System variables | Temperature | Celsius

Axis type: Linear

Limits: 500.0 to 3000.0 step 250.0 ☑ Automatic scaling

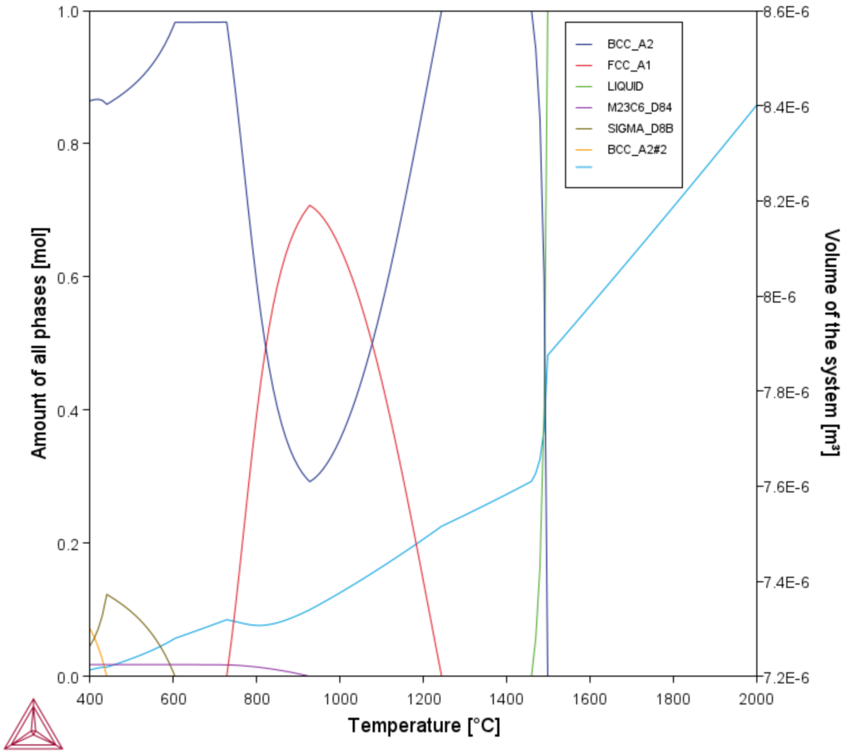
Y: Phase equilibria | Volume | No normalization | ☑ SER | System | Cubic meter

Axis type: Linear

Limits: 0.0 to 1.0 step 0.1 ☑ Automatic scaling

⊕ ⊖ ☑ Show less

9. Click **Perform** to plot both variables on the selected axis, in this example, the *Y*-axis.



Two variables plotted on the Y-axis.

Rotating 3D Plots

When you use a *Grid* calculation type you can plot the diagram in 3D.

Plot Type: Heat Map, Contour, and 3D and Calculation Types in Graphical Mode

3D Plots with additional functionality are also available with the Add-on Additive Manufacturing (AM) Module. The information is described separately and included with the Module's documentation.

In the **Visualizations** window after you create the 3D plot:

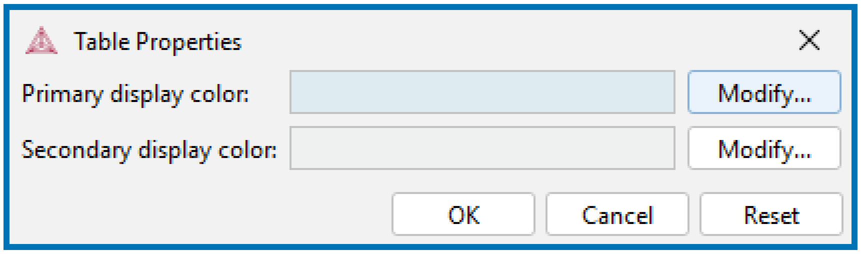
- Rotate the diagram automatically. Double-click in the **Visualizations** window and the diagram rotates clockwise. Left-click once to stop the automatic rotation.
- Rotate the diagram manually. Left-click and hold the mouse and move it around the **Visualizations** window.
- Scroll the mouse wheel/use your fingers on a trackpad to zoom on the Z-axis values.
- Right-click and move the mouse to shift the surface up or down without zooming.
- To reset the plot to its default view click **Perform Tree** to regenerate the plot.

Plot and Table Formatting

In this section:

Setting Background Colours

To change the background colours of the table, in the **Visualizations** window right-click a **Table Renderer** tab, and select **Properties**. Modify as required.



The defaults for these settings can be changed globally from the **Options** window.

To open the **Options** window:

- Windows: Select **Tools** → ☰ **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

then click the **Activities** tab and the **Tabulation** node in the tree.

Changing the Plot Properties

To make local changes to the appearance of a specific plot, in the **Visualizations** window right-click a plot and select **Properties**.

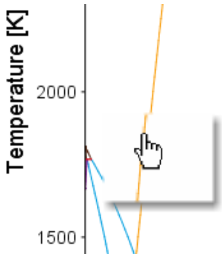
The available settings are the same as what you can globally set under the **Tools** → **Options** menus but are only applied to the specific plot. Below includes details about features that are unique to the local plot properties options.

To make global plot setting default changes, see the details in Global Settings: Graphical and Console Mode Plotting.

Edit Individual Plot Lines

You can also edit some properties for individual plot lines (the color, the line width and type, and whether data points are included).

In the **Visualizations** window, hover the mouse over a plot line. When it is over a line that can be clicked the crosshair cursor turns into a pointing finger. Click the line and then you can make changes for that specific line.



To prevent unintended edits, hold down <Ctrl> while moving the cursor around the plot to only display it as a crosshair.

Color Switching Plots Between Light and Dark Mode

Depending on whether you are using a **Light** or **Dark** look and feel for the user interface (see Global General Settings), you can also switch the default colors (lines, background, and more) of a plot using this local **Plot Properties** option. Alternatively, to set the global defaults for future project files (and plots), see Global Plot Settings: Design the Look and Feel.

Use the **Color switching** option to override the look and feel settings that may not be optimal. For example, when preparing a plot for publication, the **Dark** mode plot or line colors may not work well or do not follow a journal's guidelines. In other words, you can view and export the plot with **Light** mode color settings even though the interface is using Dark mode, and vice versa.

How to Use the Color Switching for Local Plots

Perform your calculation. Right-click in the **Visualizations** window and select **Plot Properties**. Select a **Color switching** option:

- **Switch automatically between Light mode and Dark mode**: The default, which matches the current look and feel for the GUI.
- **Always use Light mode colors**: If you are in **Dark** mode, this immediately switches the plot to **Light** default color settings.
- **Always use Dark mode colors**: If you are in **Light** mode, this immediately switches the plot to **Dark** default color settings.

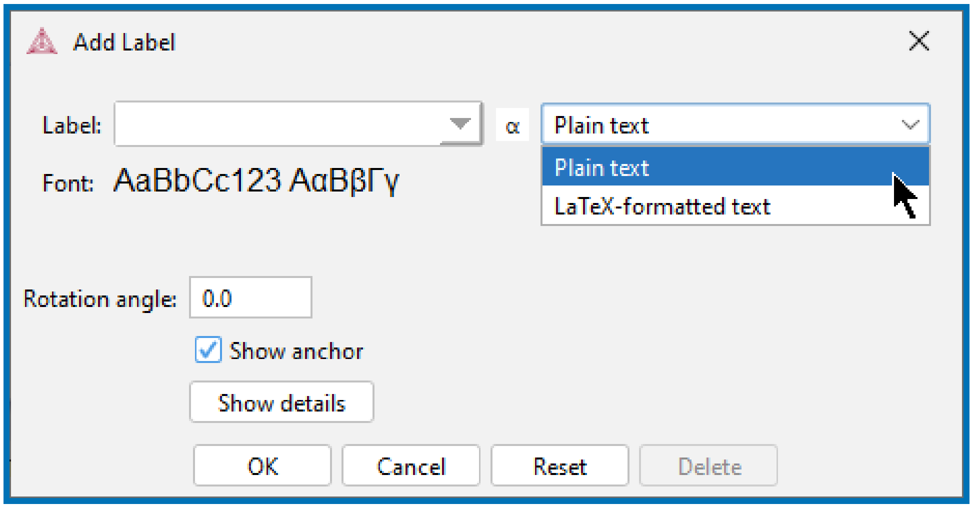
Tie lines and invariant lines are the same color for both Light and Dark modes, i.e. these colors do not change.

Additional Plot Color Changes are Locked to the Original Mode

When applying any of these settings, you can make further changes to the colors for the local plot but the change is locked to the mode. For example, you are in **Dark** mode and you change the plot background color to yellow. Then you switch to a **Light** look and feel mode. The background color for that plot is the default white background that is set for Light mode. Then if you change the background to blue, but now switch to a **Dark** look and feel, the background is yellow as this is the color applied in Dark mode to this particular plot. If you switch back to Light mode then the plot background is blue again.

Plot Labels

To add a label text at a certain point in a plot, right-click the point, and select **Add Label**. For phase diagrams, the program suggests a label that you can keep or edit. The suggested label specifies the names of the stable phases at the coordinate where you clicked. For all other plot types, you enter your own text, which can either be Plain text or LaTeX formatted text.



You can enter the label as **Plain text** or in **LaTeX-formatted text**. For **LaTeX-formatted text** enter or edit the text as required. For example, underscores (_) are added before the numbers to make subscripts in the label.

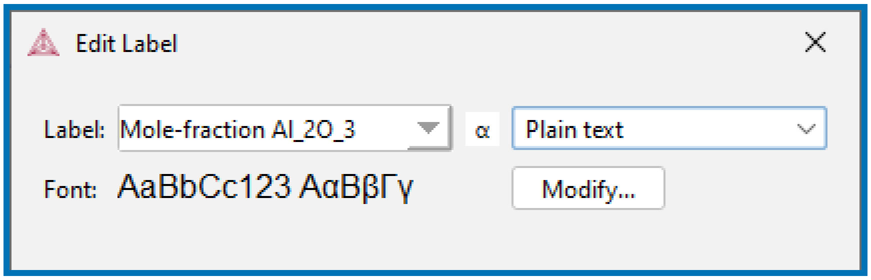
> By default when using the LaTeX command, you are in math mode and Thermo-Calc automatically interprets the entered text as math. The above link uses the dollar sign ($) in all the examples but this is NOT required. For example, if you enter `$E=mc^2$` this is displayed including the $ instead of the equation.

Plot Labels: Entering a Mixture of Plain Text and Equations

When you enter text using LaTeX formatted text it displays the text as an equation.

When using the **Plain text** format, the label does not display correctly because the label is a mixture of text (**Mole-Fraction**) and an equation needing subscripts (**Al_2O_3**).

Mole-fraction Al_2O_3



Edit Label

Label: Mole-fraction Al_2O_3

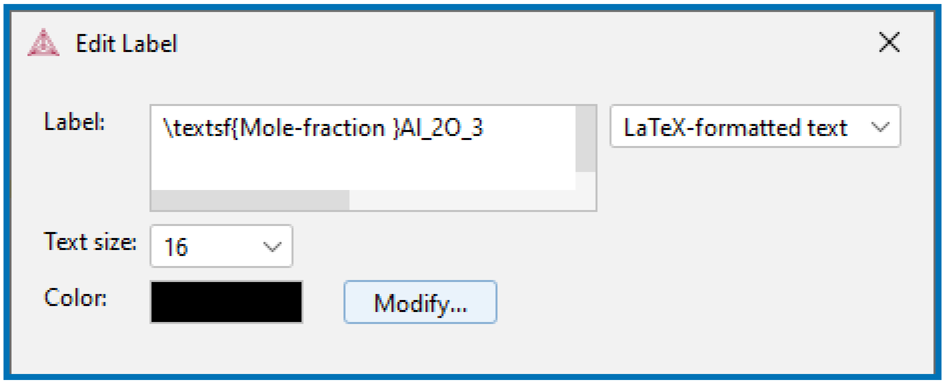
Plain text

Font: AaBbCc123 AαBβΓγ

To add a mixture of plain text and equation formatted text, exit math mode by using the string `\textsf` followed by the text to display enclosed in curly brackets `{}`.

For example `\textsf{Mole-fraction }Al_2O_3` results in this label. In this example, you need to add a space at the end of fraction in order to separate the text from the equation part of the label. You can also choose a color to apply to the label text.

Mole-fraction Al_2O_3



Edit Label

Label: \textsf{Mole-fraction }Al_2O_3

LaTeX-formatted text

Text size: 16

Color: ■

When working in Console Mode, you can also use the above windows on the Console Results window to add and edit labels. In addition, you can use the command.

It is possible to change the text style used in LaTeX labels, either for a section of the text or for the whole text (unless something else is specified).

Section of Text Within Curly Brackets	*All Text After the Command*	*Resulting Text Style*
`\textsf{}`	`\sf`	Sans serif (default)
`\textrm{}`	`\rm`	Roman
`\textbf{}`	`\bf`	Bold
`\textit{}`	`\it`	Italic
`\textem{}`	`\em`	Emphasis
`\texttt{}`	`\tt`	Monospace

Plot Labels: Rotation Angle and Show Anchor

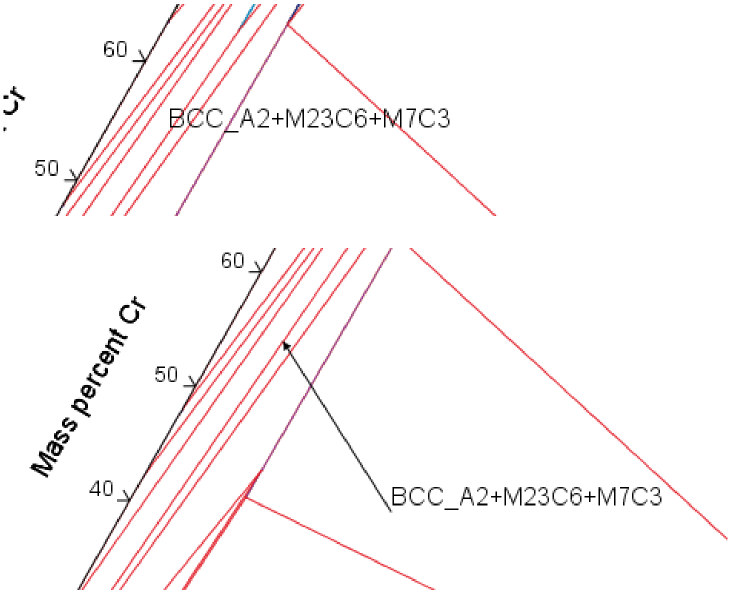
By default the **Show anchor** checkbox is selected, which includes an arrow from the label point to the coordinates.

If you do not want the label oriented horizontally in the Plot Renderer tab, then specify the number of degrees of rotation in the **Rotation angle** field.

Click **OK** to add the label to the plot. You can also move a label by clicking and dragging it. The default anchor arrow is added to indicate the point that belongs to the label.

Moving Plot Labels

Drag and drop labels anywhere on the plot. The anchor arrow points to the point of origin.



Close up of a plot label before being moved (top) and after being moved (bottom). The arrow in the lower image points to the label's original location on the plot.

About Legend Styles

There are a variety of legend styles you can use to display detail about the phases. The same legend styles are available for both Graphical Mode and Console Mode plots.

For Console Mode, use the command CHANGE_LEGEND.

In Graphical Mode the label styles are defined when using the Plot Renderer. You can select a **Legend style** for the **Stable phases** or **Axis quantity** selected for *Legend option*.

When there is a legend in the diagram you can append constitution and/or ordering descriptions to the phase name.

If constituent description is included in the legend, then for each equilibria along a line in the diagram, the largest constituent fractions are summed until they are equal or greater than 0.6. This is done separately for each sublattice. If the equilibria along the line gets different sets of constituents these are all appended to the list for that sublattice.

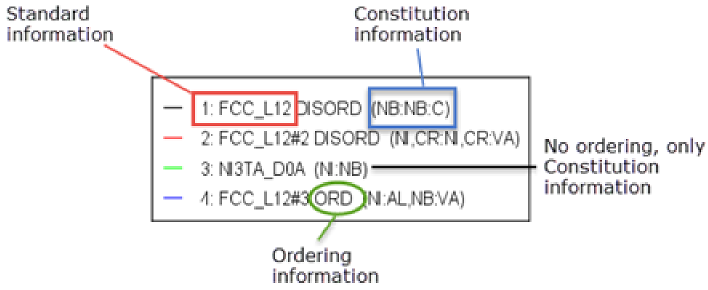
The ordering description is only printed for partitioned phases (phases that have a disordered contribution) that begins with at least two identical sublattices (sublattices where the set of constituents are identical). `DISORD` (disordered) is shown if site fractions are identical between identical constituents on all identical sub lattices (with an error margin) otherwise `ORD` (ordered) is shown in the legend.

If ordering between equilibria in a line are different, then `ORD + DISORD` is shown in the legend.

Legend and Label Styles

Legend Styles

When **All** is selected for this specific example the label includes the following:



Specifically:

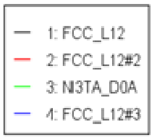
- There are two disordered FCC phases (matrix and carbide), one ordered FCC (gamma prime), plus a phase NI3TA_D0A (called Delta in Ni-alloys).
- ORDERING shows the different FCC phases.
- CONSTITUTION shows that FCC_L12#1 is NbC, FCC_L12#2 is matrix with Ni and Cr as major constituent, FCC_L12#3 is Ni3Al with Nb addition and NI3TA_D0A is Nb-rich (eg. Ni3Nb).

Label Styles

These examples are for each label style choice - **None**, **All**, **Constitution**, or **Ordering**. The instructions are for when you are setting the options using the Plot Renderer. In Console Mode, you choose the options (`ALL`, `NONE`, `CONSTITUTION`, or `ORDERING`) after the command CHANGE_LEGEND.

NONE

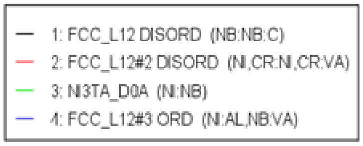
When **None** is selected the legend includes the standard information about the phases.



— 1: FCC_L12
— 2: FCC_L12#2
— 3: NI3TA_D0A
— 4: FCC_L12#3

ALL

When you select **All** the **Constitution description** and the **Ordering description** (when there is ordering) are included.



— 1: FCC_L12 DISORD (NB:NB:C)
— 2: FCC_L12#2 DISORD (NI,CR:NI,CR:VA)
— 3: NI3TA_D0A (NI:NB)
— 4: FCC_L12#3 ORD (NI:AL,NB:VA)

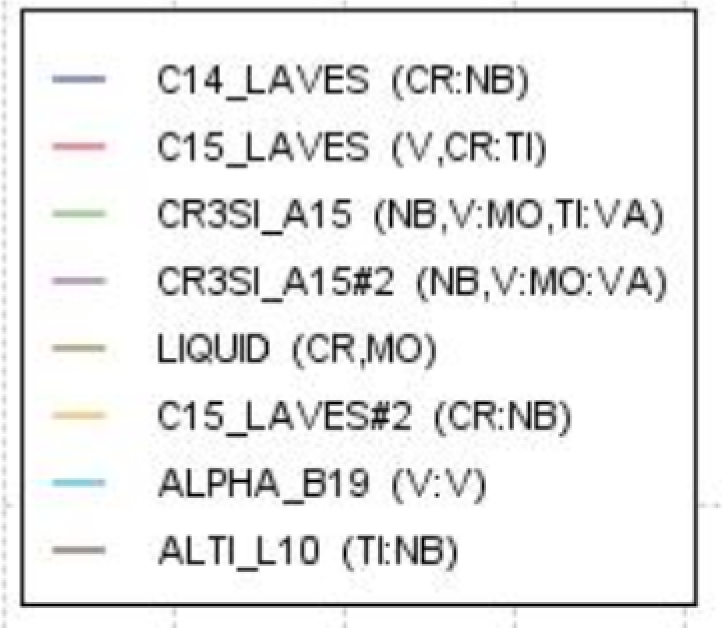
CONSTITUTION DESCRIPTION

When you select **Constitution description**, this is added to the standard description.

— 1: FCC_L12(NB:NB:C)
— 2: FCC_L12#2(NI,CR:NI,CR:VA)
— 3: NI3TA_D0A(NI:NB)
— 4: FCC_L12#3(NI:AL,NB:VA)

Here is an example with a brief explanation of what you might see when choosing this option.

> Only major constituents are listed.



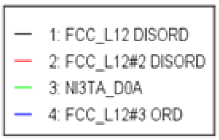
— C14_LAVES (CR:NB)
— C15_LAVES (V,CR:TI)
— CR3SI_A15 (NB,V:MO,TI:VA)
— CR3SI_A15#2 (NB,V:MO:VA)
— LIQUID (CR,MO)
— C15_LAVES#2 (CR:NB)
— ALPHA_B19 (V:V)
— ALTI_L10 (TI:NB)

First there is the phase name then (NB, V : MO, Ti : VA) meaning the first sub-lattice contains mostly NB and V. The second sub-lattice contains mostly Mo and TI, the third sub-lattice contains mostly VA= Vacancy= No atom/molecule at all.

Mostly" means Thermo-Calc sums the largest site fractions in a sub-lattice until it reaches 0.6. E.g. If sorted values are FE=0.5, AL=0.15, CR=0.15, NI=0.09 + smaller values then you will get "(Fe,AL,CR)" because FE+AL > 0.6 and then CR because it has same size as AL.

ORDERING DESCRIPTION

When you select **Ordering description** and when there is ordering, this is added to the standard description.



— 1: FCC_L12 DISORD
— 2: FCC_L12#2 DISORD
— 3: NI3TA_D0A
— 4: FCC_L12#3 ORD

Additive Manufacturing (AM) Module

In this section:

About the Additive Manufacturing (AM) Module

This guide is a supplement to the full Thermo-Calc documentation set. Access the help in Thermo-Calc by pressing F1, or choose **Help** → ⓘ **Online help**, or click **Online Help** on the main **My Project Configuration** window. See Additive Manufacturing (AM) Module Help Resources to learn other ways to access information.

The Additive Manufacturing (AM) Module (also referred to as the AM Module) is an Add-on Module to Thermo-Calc and it is available in Graphical Mode as the AM Calculator. The aim of the Additive Manufacturing Module is to better understand the laser powder bed fusion (LPBF) process by predicting the temperature distribution and melt pool geometry as a function of process parameters and using material properties from the Thermo-Calc thermodynamic and properties databases. Special focus is to have a unified treatment of alloy-dependent material properties and process parameters when solving the multiphysics problem of a moving heat source that melts and solidifies metal powder. The multiphysics simulation involves thermal conduction, fluid flow, evaporation-, radiation-, and convective-heat loss.

The Module can simulate the transition from conduction- to keyhole-mode. With experimental melt pool data you can calibrate the heat source. The calibrated heat source can be used to predict additional process conditions and/or to construct printability (aka process) maps.

Furthermore, once you have the temperature distribution, for instance as a function of time and space, you can also use this information for other Thermo-Calc Add-on-Module simulations such as with the Diffusion Module (DICTRA) or the Precipitation Module (TC-PRISMA), or for input to other external finite element programs.

Evaluation of the following is possible depending on the calculation type.

Steady-State

- Size of melt pool
- Peak temperature
- Velocity of fluid flow
- Property variations through the melt pool (temperature, viscosity, thermal conductivity, density) or any selected line

- 2D sectioning in any plane
- Heat source calibration
- Thermal gradient and solidification rate
- Keyhole mode (with Gaussian, Core-ring, or Top-hat heat sources) with or without fluid flow.

Transient and Transient with Heat Source from Steady-state

- Temperature vs. time response at selected points of the build and how this changes with process parameters
- Time-dependence of the properties listed above under steady-state
- Thermal gradient and solidification rate
- Connect the above temperature vs. time response with the Diffusion Module (DICTRA) and/or the Precipitation Module (TC-PRISMA)
- Keyhole mode (with a Transient from Steady-state calculation using a Gaussian, Core-ring, or Top-hat heat source) with or without fluid flow.

Overview of the Content

In This Guide

There are Additive Manufacturing (AM) Module Help Resources and Network License Restrictions to consider and access.

Theory is included in a variety of feature topics. Some basic equations pertaining to the logic behind the simulation and settings are discussed in Additive Manufacturing Module Theory, as well as particular details about other features are discussed in About Heat Source Calibration, About the Keyhole Model, and About the Absorptivity Model, and About the Heat Source Models for example.

Feature overviews are covered in a summary of the Additive Manufacturing Simulation Types as well as the Steady-state Calculation Types and associated About the AM Plot Types, which links you to feature-based topics for each calculation or plot type.

The workflow for the AM Module is outlined in Setting Up the Additive Manufacturing Simulation and there are two default Additive Manufacturing Templates you can use to start defining your project. You can also add nodes individually to build your own tree. There are two workflows, and in either workflow, defining the AM Calculator involves choosing one of the available simulation types: Steady-state, Transient, or Transient with heat source from Steady-state.

Then you can start building the simulation using the activity nodes and depending on which workflow you start with.

This involves the standard **System Definer** and **Scheil Calculator** settings, which are the same as what is used with a standard Thermo-Calc configuration. When you add an Additive Manufacturing Template (and need to generate some materials properties or do not have a material library to use), then some unique default settings for the Scheil Calculator and these particular types of simulations are already set by default. These are discussed in Setting Up the Additive Manufacturing Simulation.

This set of topics specifically includes details about the settings for the AM Calculator and the specialized AM Calculator: Plot Renderer Settings. There are many additional specialized sections related to working with, for example, probe data as well as experimental data files that are used in heat source calibrations and batch calculations.

There are many details related to visualizing the plots discussed in several sections, starting with Working with AM Visualizations and then extended with specialized sections Visualizing Heat Source Calibrations and Visualizing Batch Calculations in the AM Module. The power of the AM Module is that there are many ways visualize both the set up (i.e. you can preview a variety of settings) and then finally examine and work with your results using the AM Visualizations Window Plot Toolbar and many other settings.

There are also several examples included with the installation that are generally discussed and described in the examples section or as part of the *Graphical Mode Examples Guide*.

Databases

For compatibility with the Additive Manufacturing Module, a database needs the following properties added in addition to the thermodynamics: surface tension for liquid, viscosity for liquid, thermal conductivity, molar volume, and a complete gas description.

Available Databases

The Additive Manufacturing Module is currently available together with the following databases, starting with the version indicated:

- Aluminum-based Alloys Database (TCAL9 and newer)
- Copper-based Alloys Database (TCCU6)
- High Entropy Alloys Database (TCHEA6 and newer)
- Magnesium-based Alloys Database (TCMG6 and newer)
- Molybdenum-based Alloys Database (TCMO1)
- Nickel-based Superalloys Database (TCNI12)
- Niobium-based Alloys Database (TCNB1)
- Noble Metal Alloys Database (TCNOBL3)
- Solder Alloy Solutions Database (TCSLD5 and newer)
- Steel and Fe-alloys Database (TCFE13 and newer)
- Titanium and TiAl-based Alloys Database (TCTI5 and newer)

Read more about the Additive Manufacturing (AM) Module on our website including the details about database compatibility or to watch an introductory webinar. You can also use the Getting Started Guide to learn about the key features available.

Available Options

The Additive Manufacturing (AM) Module is an Add-on Module to the core Thermo-Calc software.

A separate license is required to perform calculations with the Additive Manufacturing (AM) Module. Without a license you are in *Demo Mode* where you can, for example, open and view example set ups, run some examples, add templates and nodes to the Project window, adjust some Configuration settings, and preview some functionality on the Visualizations window.

The Additive Manufacturing (AM) Module is not available with the free Educational version of Thermo-Calc.

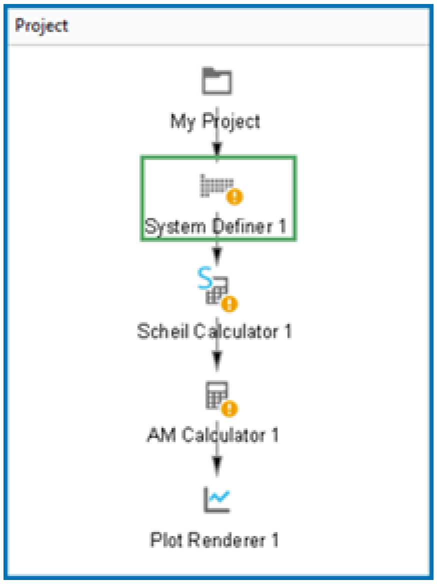
Additive Manufacturing Templates

Two types of **Additive Manufacturing** templates are under **Applications** and these are available to all Thermo-Calc users when in Graphical Mode. If you are in DEMO (demonstration) mode then this is indicated by the addition of **DEMO** text. See Figure 4.

Using the Templates

After opening Thermo-Calc in Graphical Mode, in the templates section under **Applications**, click the **Additive Manufacturing** button to add a *System Definer*, *Scheil Calculator*, *AM Calculator*, and *Plot Renderer* to the **Project** tree.

This template is used when you need to generate and use data from a Scheil calculation.



An alternate template is available when you already have data or can directly use or import a Material Library.

After opening Thermo-Calc in Graphical Mode, in the templates section under **Applications**, and to the right of **Additive Manufacturing**, click the **With Material Library** button to add an *AM Calculator* and *Plot Renderer* to the **Project** tree.

Demonstration (Demo) Mode

The Additive Manufacturing (AM) Module is available in a demonstration (DEMO) mode without an additional AM license. It includes access to the templates, some examples, and some access to the embedded predefined material properties libraries. You also have access to the fluid flow settings and a steady-state calculation can be done. However, there are limitations such as the ability to change settings and to fully run calculations.

What is Included?

- Some examples (i.e. AM_01, AM_02, AM_03, AM_06b, AM_13, and AM_14) use embedded and predefined Material Properties libraries that are included for all users. Although these examples can be run without a license, you cannot make any changes to the settings. If changes are made, the **Perform** button can still be clicked but the calculation will fail and a message displays above the **Perform Tree** button to inform you of the need for a license. In addition, the **Event Log** displays an error message, `ERROR AM Calculation: AM Calculation in Demo mode has limited functionality`. See Figure 5.

- Generally, when in DEMO mode and using the **With Materials Library** template, you can perform a calculation with default values. You cannot change any setting, including the calculation types (i.e. Steady-state, Transient, or Transient with heat source from Steady-state) as well as the Material Properties library i.e. meaning only Steady-state with the IN625 library is available with the default setup is possible.
- All plot configurations are possible to perform in the above cases.
- The following examples require a full license to the Additive Manufacturing (AM) Module to run, plus often additional licenses (i.e. for databases or other Add-on Modules):
    - AM_04, AM_05, AM_06a, and AM_07 to AM_12.
    - For those without the applicable licenses, you can still open the examples to review the settings and then refer to the documentation for discussions of what it is showing

You can also view the *Getting Started Guide* on the website, which uses AM_04 in the example.

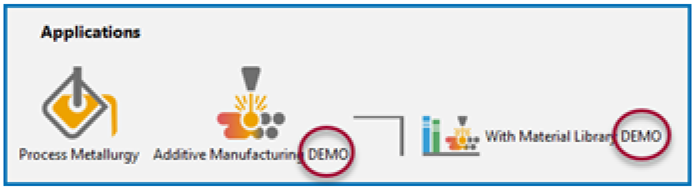
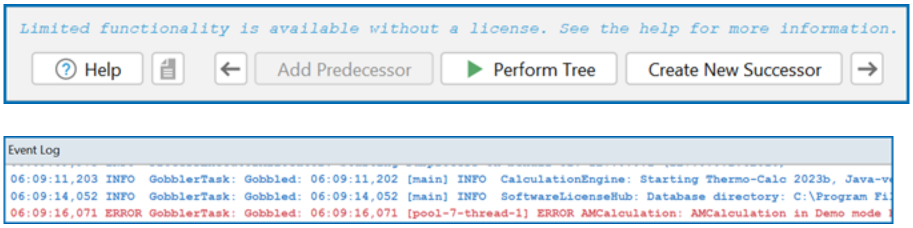


Figure 4: The templates indicate that you are in DEMO mode and would need an AM license to fully use the templates or run certain examples as listed in the text.



```
Limited functionality is available without a license. See the help for more information.
```

```
06:09:11,203 INFO  GobblerTask: Gobbled: 06:09:11,202 [main] INFO  CalculationEngine: Starting Thermo-Calc 2023b, Java-v
06:09:14,052 INFO  GobblerTask: Gobbled: 06:09:14,052 [main] INFO  SoftwareLicenseHub: Database directory: C:\Program Fi
06:09:16,071 ERROR GobblerTask: Gobbled: 06:09:16,071 [pool-7-thread-1] ERROR AMCalculation: AMCalculation in Demo mode
```

Figure 5: When in DEMO mode and you click on the AM Calculator node, the above note is included at the bottom of the Configuration window to remind you that a license is needed for full functionality. The Perform Tree button is not always available and sometimes even if it is available to click, the calculation itself cannot complete due to lack of a license. There will also be an error message in the Event Log to indicate the need for a license.

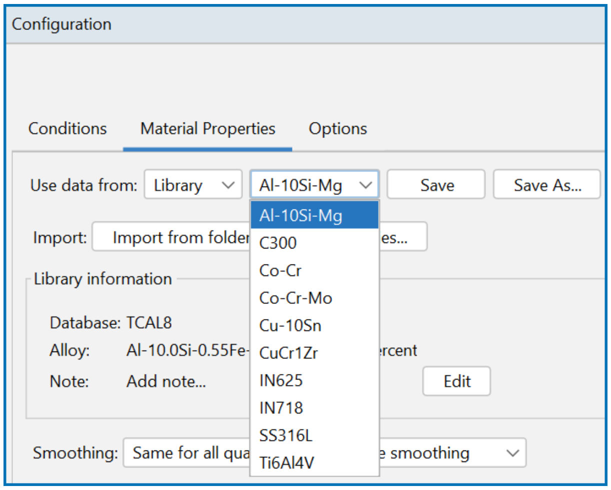
Material Properties and Libraries

> All predefined Material Properties libraries are available if you have a license for the Additive Manufacturing (AM) Module, even if you do not have the alloy database it is created with.

Create or Import Your Own Material Library

The use of the Scheil Calculator with an AM Calculator provides you with a way to generate the data you need to feed into any AM calculation. When this Scheil calculation is completed, and if you have a full license, you can save the results to the Material Properties Library for later use. From the AM Calculator there is an option to use either Scheil data (when it is connected to the Scheil Calculator) or predefined library data (as long as you have a license to the Additive Manufacturing (AM) Module the calculations can be run fully). With the applicable license, you can also import your own material library for a particular alloy of interest and then you can just use the AM Calculator (i.e. the **With Material Library** template setup) without needing the additional Scheil calculation step.

Users with a full Additive Manufacturing license can access all the predefined libraries for use in calculations (and also can create and import their own libraries and save these for reuse).


Use data from: Library
Al-10Si-Mg
Library information
Database: TCAL8
Alloy: Al-10.0Si-0.55Fe-
Note: Add note...
Smoothing: Same for all qua

Other Options

Using Data with other Add-on Modules

When you also have licenses either for the Diffusion Module (DICTRA) and/or the Precipitation Module (TC-PRISMA), for transient simulations you can additionally include probe data from the AM Calculator in the set up of the thermal profile for diffusion and precipitation calculations, respectively.

See AM Calculator: Working with Probe Data.

Additive Manufacturing (AM) Module and TC-Python

When you also have a license for the TC-Python Software Development Kit, you can use the Additive Manufacturing (AM) Module functionality. Some examples are available with just a TC-Python license. Learn more about TC-Python on our website.

Additive Manufacturing (AM) Module Help Resources

The technical content is available in HTML format as an Online Help system that you can access from two locations. Both versions are viewed in your browser.

- A local version that is available with each Thermo-Calc installation and does not require an Internet connection.
- A web version available online. The web help also matches the most recently released version of Thermo-Calc.

Between releases there may be minor updates to the web version compared to the installed version. All updates made to the web version are included in the next installed release version.

There are several resources available on our website to help you learn how to use Thermo-Calc and other Add-on Modules. Go to the Getting Started Guides page and choose one of the guides that provides new users an introduction to setting up simple calculations in Graphical Mode. The information there is also in this help documentation.

Opening the Web Version of the Help

- A web version **specific to each release version** is available at https://help.thermocalc.com/2025b/content/intro/help-home.htm
- The help at the link also matches the most recently released version of Thermo-Calc.

Opening the Installed Help: No Internet Required

There are several ways to access online help in a browser. The content opens in a browser but uses local content so you do not need an Internet connection except for links to external websites.

First open Thermo-Calc, then choose one of these options to go to the local browser version of the help:

- Press <F1> on the keyboard.
- Select **Help** → ⓘ **Online Help**.
- On the **My Project Configuration** window, click **Online Help**.
- At the bottom of any **Configuration** window, click ⓘ **Help**.

Additive Manufacturing (AM) Module Specific Information

Read more about the Additive Manufacturing (AM) Module on our website including the details about database compatibility or to watch an introductory webinar. You can also use the Getting Started Guide to learn about the key features available.

For more Additive Manufacturing (AM) Module learning resources, visit the video tutorials on our website or our YouTube playlist.

Network License Restrictions

The Additive Manufacturing (AM) Module requires a separate license. If you are using a network client installation of Thermo-Calc, then you may not be able to use it even if you have access to a license server with a valid network license file. The reason for this is because other clients who are part of your network installation may have checked out all instances of the network license allowed to run simultaneously.

For users with a network license, you must exit Thermo-Calc to release the license for other users. The license is checked out as soon as you add an AM Calculator and remains unavailable to other users until you exit the program.

With a network license, and if as per above you temporarily do not have access to a license, you are automatically put into *Demo Mode*. Then the AM Calculator is available.

Search the online help or see the *Thermo-Calc Installation Guide* for more about network licenses.

General Theory and Background

In this section:

Additive Manufacturing Module Theory

This section is an overview of the underlying fundamental theory used and applied to the calculations when you are setting up the AM Calculator using one of the Additive Manufacturing Simulation Types.

The settings related to the following are defined for the AM Calculator starting with the AM Calculator Conditions Settings section.

Energy Equation: The Enthalpy Formulation

The following formulation is based on a simple assumption that each volume element, which may contain several dendrites or a considerable part of a dendrite, is approximated as homogeneous, i.e., it is sufficient to characterize the whole volume with a single set of state variables. This assumption thus excludes the direct account of varying composition caused by microsegregation within the element.

The enthalpy formulation is based on the conservation of energy and is essentially equivalent with Fourier’s second law:

[*Eq. 1*] $$\dot{H}_V = -div(J_Q) + \dot{Q}$$

H_V is the enthalpy density and $\dot{H}_V$ is its time derivative.

The enthalpy density is related to the molar enthalpy H_m and molar volume V_m by:

[*Eq. 2*] $$H_V = \frac{H_m}{V_m}$$

div denotes the divergence operator and J_Q is the heat flux given by Fourier’s law:

[*Eq. 3*] $$J_Q = -\kappa\ grad(T)$$

where κ is the heat conductivity, $grad$ denotes the gradient operator and T is the temperature. $\dot{Q}$ is a source term and represents the heat added from the outside at a certain point. In modeling of a process like welding or additive manufacturing this is a key term and requires a lot of modeling.

As state functions the enthalpy and the molar volume depend on temperature, state of phase, and composition of the individual phases. In a volume element approximated as homogeneous, one thus has:

[*Eq. 4*] $$H_m = \sum_{\beta} f^{\beta} H_m^{\beta}\left(T, x_k^{\beta}\right)$$

[*Eq. 5*] $$V_m = \sum_\beta f^\beta V_m^\beta \left(T, x_k^\beta\right)$$

where f^β is the mole fraction of the phase β and x_k^β is the mole fraction of k in β. The time derivatives thus are:

[*Eq. 6*] $$\dot{H}_m = \sum_\beta \dot{f}^\beta H_m^\beta \left(T, x_k^\beta\right) + \sum_\beta f^\beta \left(c_P^\beta \left(T, x_k^\beta\right) + \sum_{k=1}^{n} \frac{\partial H_m^\beta}{\partial x_k^\beta} \frac{\partial x_k^\beta}{\partial T}\right) \dot{T}$$

[*Eq. 7*] $$\dot{V}_m = \sum_\beta \dot{f}^\beta V_m^\beta \left(T, x_k^\beta\right) + \sum_\beta f^\beta \left(V_m^\beta \alpha^\beta \left(T, x_k^\beta\right) + \sum_{k=1}^{n} \frac{\partial V_m^\beta}{\partial x_k^\beta} \frac{\partial x_k^\beta}{\partial T}\right) \dot{T}$$

Here c_P^β is the molar heat capacity of the β phase and α^β its volumetric thermal expansion. For a given volume element the rates can be calculated from Thermo-Calc for the temperature, fraction of phases and their composition with the input of the rates $\dot{f}^\beta$ and $\dot{T}$.

The rate of change of the enthalpy density, i.e., the left-hand side of Eq. 1 thus is obtained as:

[*Eq. 8*] $$\dot{H}_V = \frac{1}{V_m}\left(\dot{H}_m - H_m \frac{\dot{V}_m}{V_m}\right)$$

The first term inside the brackets represents the change for a constant number of atoms due to a change in temperature or phase. The second term represents a change in volume for a constant number of atoms. However, the second term is balanced by a corresponding contribution in the heat flux, which we do not usually account for, and we should thus leave it out.

[*Eq. 9*] $$\dot{H}_V = \frac{\dot{H}_m}{H_m}$$

The fraction of phases sums up to unity and in the case of only one solid phase:

$$\dot{f}^L = -\dot{f}^\beta$$

In most treatments the positive quantity

$$\Delta H_m = \left(H_m^L(T, x_k^L) - H_m^\beta(T, x_k^\beta)\right)$$

treated as constant and referred to as the latent heat. It is also common to neglect the difference in heat capacity between solid and liquid and the variation of ΔH_m with composition. Eq. 6 then is simplified into

[*Eq. 10*] $$\dot{H}_m = \dot{f}^L \Delta H_m + c_P \dot{T}$$

By the same token

$$\Delta V_m = \left(V_m^L(T, x_k^L) - V_m^\beta(T, x_k^\beta) \right)$$

is often approximated as constant and so Eq. 7 is simplified into

[*Eq. 11*] $$\dot{V}_m = \dot{f}^L \Delta V_m + V_m \alpha \dot{T}$$

where V_m is given by Eq. 5 and yields

$$V_m = f^L V_m^L + (1 - f^L) V_m^\beta = V_m^\beta + f^L \Delta V_m$$

Eq. 9 now becomes:

[*Eq. 12*] $$\dot{H}_V = \frac{1}{V_m} \left(\dot{f}^L \Delta H_m^L + c_P \dot{T} \right)$$

and Eq. 1 becomes:

[*Eq. 13*] $$\frac{1}{V_m} \left(\dot{f}^L \Delta H_m^L + c_P \dot{T} \right) = div(\kappa grad(T)) + \dot{Q}$$

The Equivalent Heat Capacity Method Using Thermo-Calc

If it is further assumed that the fraction liquid f^L is a unique function of temperature one has:

[*Eq. 14*] $$\dot{f}^L = \frac{df^L}{dT} \dot{T}$$

and Eq. 13 may be further simplified to:

[*Eq. 15*] $$\frac{c_p^{eff}}{V_m} \dot{T} = div(\kappa grad(T)) + \dot{Q}$$

where the effective heat capacity c_p^{eff} is given by:

[*Eq. 16*] $$c_P^{eff} = \left(\frac{df^L}{dT} \Delta H_m + c_P \right)$$

Eq. 15 is a normal heat-flow equation and the complication of the liquid/solid phase transformation is taken into account by means of an effective heat capacity. This method is referred to as the equivalent heat-capacity method by Rappaz [1989Rap].

It then remains to be discussed how to determine $f^L(T)$. It must be given by some extra information. Traditionally it was taken from experimental information but more recently it has been taken from the Scheil equation. The original equation was based on a number of approximations which are unnecessary today when thermodynamic and properties databases and efficient software such as Thermo-Calc are available. In fact, when using Scheil in Thermo-Calc one can directly calculate $c_p^{eff}(T)$, referred to as apparent heat capacity, for a given initial composition of the liquid. A possible approach thus is to calculate $c_p^{eff}(T)$ for the alloy under consideration and then store the result as a table and use that in the solution of Eq. 15. The molar volume may be extracted from the same calculation. An example for a 316L type of stainless steel is shown in the plots below.

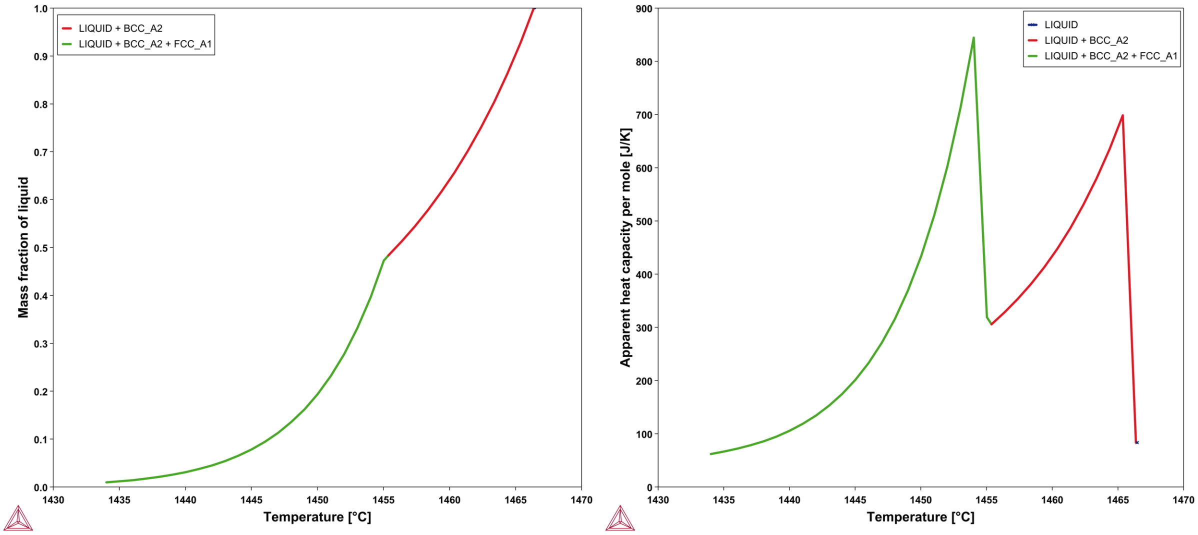


Figure 1: Results of a Scheil simulation of Fe-18Cr-10Ni alloy showing the mass fraction of the liquid (left) and the apparent heat capacity (right) both as a function of temperature.

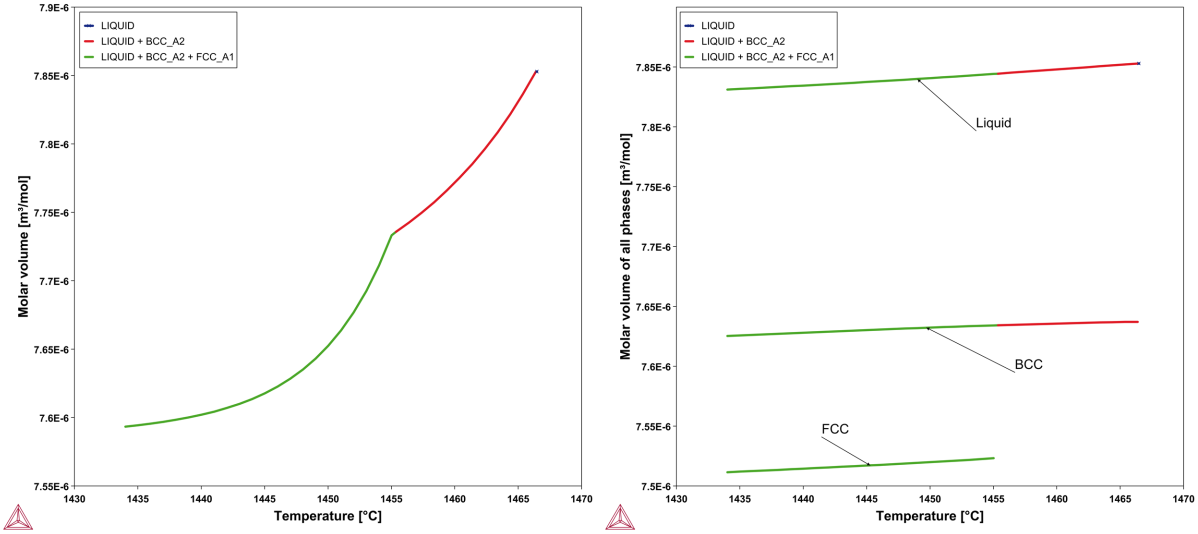


Figure 2: Molar volume from a Scheil simulation of Fe-18Cr-10Ni alloy. The right plot shows all phases as a function of temperature.

The Enthalpy Method Using Thermo-Calc

In the enthalpy method we keep Eq. 1 and use Eq. 9 to write

[*Eq. 17*]

$$\frac{\dot{H}_m}{V_m} = -div(J_Q) + \dot{Q}$$

As pointed out by Rappaz [1989Rap] there is no mathematical difference between the enthalpy method and the equivalent heat capacity method because the former is simply the integral of the heat capacity over T. For numerical reasons the cusps in the heat capacity may be disadvantageous and the enthalpy has a nicer behavior as shown in the plot below, where it gives temperature as a unique function of enthalpy.

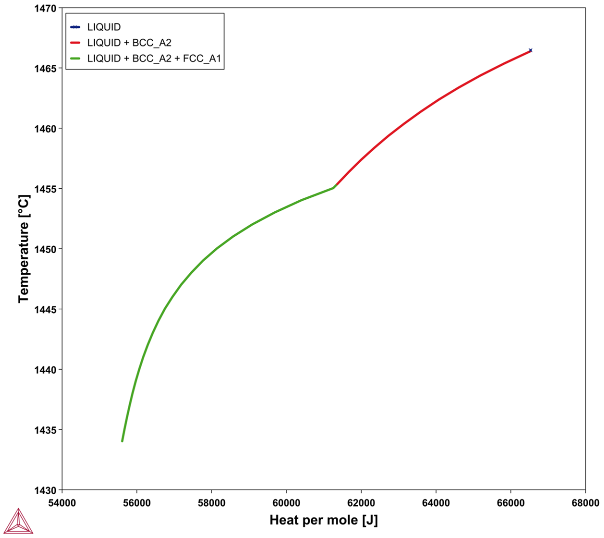


Figure 3: Enthalpy from a Scheil simulation of Fe-18Cr-10Ni alloy.

In the Additive Manufacturing Module, we therefore use Eq. 17 to predict the evolution of temperature during the laser powder bed fusion (LPBF) process for the given material properties and process parameters.

Steady-state Formulation

An important approximation is when one can solve the stationary heat-flow equation for a volume element moving with the heating source. In that case, we neglect the left-hand side of Eq. 17 and add a translation term as follows:

[*Eq. 18*]

$$div[\kappa grad(T)] - \frac{v_b}{V_m} grad(H_m) + \dot{Q} = 0$$

Where v_b is the velocity of the heat source. In case of additive manufacturing, v_b is the scanning speed.

Fluid Flow

When there is also fluid flow involved, a fluid transport term has to be added to the heat-flow equation and one obtains:

[*Eq. 19*] $$\frac{\dot{H}_m}{V_m} = div[\kappa grad(T)] - \frac{v}{V_m} grad(H_m) + \dot{Q}$$

where v is the velocity vector field and may be imposed or obtained from the solution of the Navier-Stokes equation:

[*Eq. 20*] $$\rho\dot{v} + \rho(vgrad)v - \mu(divgrad)v = F_V - gradP$$

where ρ is the density related to the molar volume by means of

[*Eq. 21*] $$\rho = \frac{1}{V_m}\sum_k x_k M_k$$

M_k is the molar weight in kg mol^{-1}. μ is the viscosity, F_V is a volume force, e.g., gravitational forces, and P is the internal pressure. The equation is often combined with approximating the liquid as incompressible.

[*Eq. 22*] $$div(v) = 0$$

LARGE EDDY SIMULATION USED FOR FLUID FLOW

The use of a subgrid model [1963Sma] relies on the eddy-viscosity assumption and this is applied to account for the unresolved turbulent motions that cannot be directly simulated due to computational limitations. The Smagorinsky model is the default for fluid flow, and it provides a simple way to estimate *Subgrid-scale (SGS)* viscosity in large eddy simulation as,

$$\nu_{SGS} = (C_S\,\Delta)2|\overline{S}|$$

where:

- C_S is the Smagorinsky constant (default value is 0.18).
- Δ represents the filter width (length scale).
- $|\overline{S}|$ is the magnitude of the resolved strain rate tensor.

Heat Source Models

See additional theory related to heat sources in About the Heat Source Models and About Heat Source Calibration. Settings information specific to heat sources is also found in AM Calculator Heat Source Settings.

Numerical Boundary Conditions

In order to obtain temperature distribution during the LPBF process in the Additive Manufacturing (AM) Module, incorporating fluid flow inside the melt pool, we couple energy equations with the Navier-Stokes equations, as explained earlier. In order to accurately reflect the physical process, both of these equations are subjected to a certain set of boundary conditions, which are given as follows.

BOUNDARY CONDITIONS FOR ENERGY EQUATION

The energy equation is subjected to four different boundary conditions. The first boundary condition is defined on the top surface (either the powder bed surface or the solid substrate) and represents the energy lost due to convection and radiation to the surrounding gas.

[*Eq. 23*] $$Q_L = h(T - T_{ambient}) + \varepsilon\sigma(T^4 - T^4_{ambient})$$

where h is the convective heat transfer coefficient, ϵ is the surface radiation emissivity and

$$\sigma = 5.669 \times 10^{-8} W/m^2K^4$$

is the Stefan-Boltzmann constant. $T_{ambient}$ is the ambient temperature or the temperature of the surrounding gas in the build chamber and can be set in the AM Calculator configuration.

The second boundary condition represents the heat lost through the vertical walls of the domain and for simplicity we have chosen adiabatic boundary conditions for these surfaces. The boundary condition for the vertical walls of the computational domain is thus given as:

[*Eq. 24*] $$Q_N = 0$$

The third boundary condition reflects the temperature of the base plate and is therefore applied to the bottom of the computational domain. Here we have assumed that the base plate of the build part is kept at a constant temperature and the boundary condition is therefore given as:

[*Eq. 25*] $$T = T_{baseplate}$$

$T_{baseplate}$ is the base plate temperature and can be set in the AM Calculator configuration.

The fourth and the most important boundary condition is the evaporation boundary condition that represents the heat lost due to evaporation of the material. Evaporation is implemented using a physics-based approach where the heat loss due to evaporation (Q_E) is given as:

[*Eq. 26*] $$Q_E = 0.82 J_E \Delta H_v$$

where J_E is the evaporation flux and ΔH_E is the evaporation enthalpy. For a multicomponent system, the evaporation flux is given as follows:

[*Eq. 27*] $$J_E = \frac{1}{\sqrt{2\pi MRT}}\left(P_o exp(-\frac{\Delta G_v}{RT}) - P\right)$$

where ΔG_v is the driving force for evaporation, M is the molar mass of the gas, P is the gas pressure inside the chamber, P_o is the atmospheric pressure, and R is the universal gas constant. The driving force for evaporation, the evaporation flux, and the molar mass of the gas are all temperature-dependent material properties which are obtained from Thermo-Calc databases and are included in the material library whereas the gas pressure inside the chamber can be set from the AM Calculator configuration.

BOUNDARY CONDITIONS FOR NAVIER-STOKES EQUATIONS

For the velocity, a no-slip boundary condition is used for the bottom surface of the computational domain. A no-slip boundary assumes that at a solid boundary, the fluid will have zero velocity relative to the boundary. For the pressure, a pinned boundary condition is used.

For the melted liquid at the top, the symmetry (front - in a steady-state simulation), and the keyhole surfaces, the free-slip boundary is used.

The most important boundary condition in Navier-Stokes setup is the Marangoni boundary condition that reflects the tangential force on the surface of the melt pool due to temperature variation of surface tension or the so-called Marangoni effect. In AM, large temperature gradients on the surface of the melt pool, leads to the Marangoni effect and is the primary cause of convective flow inside the melt pool. The Marangoni shear stress (τ) is modeled using the following equation:

[*Eq. 28*] $$\tau = \frac{\partial\gamma}{\partial T}\nabla_s T$$

where γ is the surface tension and ∇_s represents the tangential component of the spatial derivative.

Surface tension is also a temperature-dependent material property which is obtained from Thermo-Calc databases and is included in the material library.

Thermophysical Properties of Powder Material

When the option “Use separate material properties for powder” is selected, a different thermal conductivity, density and molar volume is used for the powder material as compared to the solid substrate. The above mentioned properties depend on the porosity (ϕ) of the powder. The density (ρ_{powder}) and molar volume (Vm_{powder}) of the powder are then simply given as follows:

$$\rho_{\text{powder}} = \rho_{\text{solid}}(1-\phi)$$

$$Vm_{\text{powder}} = Vm_{\text{solid}}\frac{1}{1-\phi}$$

For thermal conductivity of powder k_{powder}, an empirical expression is used which was suggested by Xue and Barlow [1991Xue]. The thermal conductivity of powder thus also depends on the conductivity of the surrounding gas. For simplicity, the surrounding gas is assumed to be air. The thermal conductivity of powder is given as follows:

[*Eq. 29*]
$$k_{\text{powder}} = \left(6.3 + 22\sqrt{0.09k_{\text{solid}} - 0.016}\right)\frac{k_{\text{solid}}\ (1-\phi)}{(k_{\text{solid}}\ /k_{\text{air}})(10^{0.523-0.594\phi})-1}$$

where $k_{\text{air}} = 0.05784$.

References

[1963Sma] J. Smagorinsky, General circulation experiments with the primitive equations: I. The basic experiment. Mon. Weather Rev. 91, 99–164 (1963).

[1989Rap] M. Rappaz, Modelling of microstructure formation in solidification processes. Int. Mater. Rev. 34, 93–124 (1989).

[1991Xue] S. Xue, J.W. Barlow, Models for the prediction of the thermal conductivities of powders, Solid Freeform Fabrication Symposium Proceedings, Center for Materials Science, University of Texas at Austin, Austin, TX (1991), pp. 62-69.

About the Heat Source Models

It is crucially important to correctly model the heat source in AM simulations since the heat source not only affects the size of the melt pool but also determines the temperature gradients around the melt pool. In the Additive Manufacturing (AM) Module, these heat source models are available: **Gaussian**, **Core-ring**, **Top-hat**, **Double-ellipsoidal**, and **Conical**.

The **Configuration** window settings for each of these heat sources are further described in both the AM Calculator Conditions Settings and AM Calculator Heat Source Settings topics.

There is a variety of additional background theory topics available.

- The main AM theory is in Additive Manufacturing Module Theory.
- **Keyhole model** for Gaussian, Core-ring, and Top-hat heat sources: About the Keyhole Model.
- **Absorptivity**: For Gaussian, Core-ring, and Top-hat heat sources: About the Absorptivity Model.
- **Heat source calibrations** for Gaussian, Double-ellipsoidal, and Conical heat sources: About Heat Source Calibration.

The **Double-ellipsoidal** and **Conical** heat sources are not available with the keyhole model.

The **Core-ring** and **Top-hat** heat sources are not available with **Heat Source Calibration** calculations.

Gaussian Heat Source

The **Gaussian** model is a surface heat source model which was initially proposed by Pavelic et al. [1969Pav]. By surface heat source model, it is meant that the power input from the heat source is only defined on the top surface of the workpiece, as a Neumann boundary condition on the computational domain, and the heat energy then diffuses into the workpiece depending on the thermal diffusivity of the selected material. As suggested by Pavelic et al., the heat flux (W/m^2) is defined as Gaussian distribution around the center of the heat source, deposited on the top surface of the domain, as given in the equation below. A schematic representation of the heat flux, as defined by Gaussian heat source is shown in Figure 4.

[Eq. 1]

$$Q = \frac{2\epsilon P}{\pi r^2} exp\left[-2\frac{(x-X_p)^2+(y-Y_p)^2}{r^2}\right]$$

Where Q is the power density deposited on the top surface (W/m^2),ϵ denotes absorptivity of the laser beam, P is the power of the heat source (W), r is the laser spot radius, and x and y denote coordinates of the computational domain while X_p and Y_p represent the location of the heat source.

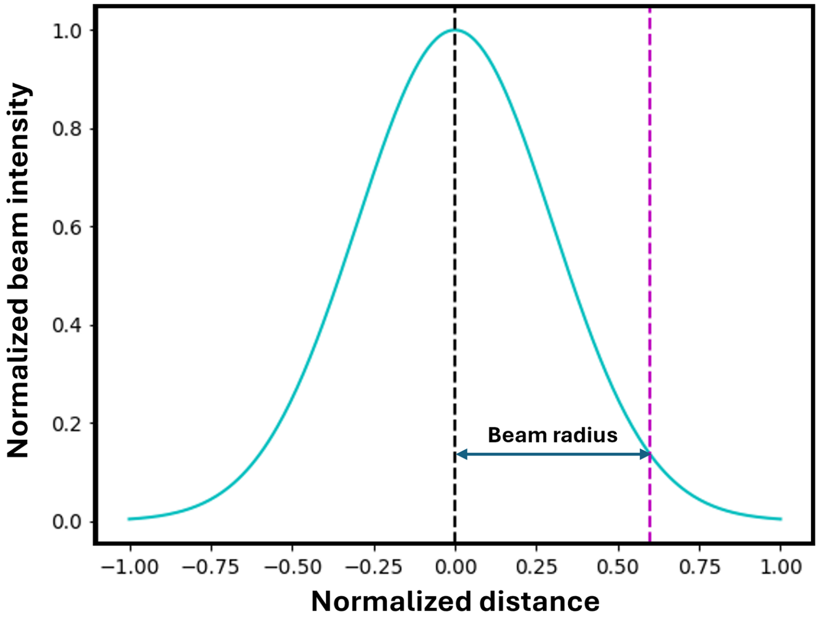


Figure 4: Schematic representation of energy distribution in Gaussian heat source model.

Also see additional theory related to using a Gaussian heat source with the keyhole option in About the Keyhole Model.

Core-ring Heat Source

Gaussian beam distribution in additive manufacturing often leads to high energy intensity peaks and strong thermal gradients causing manufacturing defects such as keyhole porosity and suboptimal material processing performance. To overcome these challenges, spatial beam shaping is available as an alternate method to customize energy distribution and control the resulting thermal field [2023Bi; 2025Bir]. One of the alternative beam shapes is the **Core-ring** profile where energy is distributed between a central core and an outer ring.

From a production point of view, the primary benefit of **Core-ring** and **Top-hat** beam shapes is that there is a much wider and more stable melt pool. This means that you can increase the productivity of the process so that it prints faster, consequently saving on printing costs [2021Grü].

The alternative beam shape, **Top-hat**, is described in the next section.

A **Core-ring** heat source, like a Gaussian heat source, is a surface heat source model, which means that the power input from the heat source is only defined on the top surface of the workpiece, as a Neumann boundary condition. The intensity of a core-ring heat source can be modeled as a combination of a central Gaussian core beam and an outer ring beam [2024Gal].

The intensity of the core beam, as shown in Eq. 1, is given as follows:

[Eq. 2]

$$Q_{\text{core}} = \frac{2\epsilon P}{\pi r_{\text{core}}^2} \exp\left[-2\frac{(x-X_p)^2+(y-Y_p)^2}{r_{\text{core}}^2}\right]$$

Where

- Q_{core} is the power density of the Gaussian core (W/m^2),
- ϵ denotes the absorptivity of the laser beam,
- P is the power of the heat source (W),
- r_{core} is the $1/e^2$ radius of the core beam,
- x and y denote coordinates of the computational domain, and
- X_p and Y_p represent the location of the heat source.

The intensity of the ring beam is derived by assuming the conservation of the total laser power, P, and is given as follows:

[Eq. 3]

$$Q_{ring} = \frac{\epsilon P}{2\pi\varpi} \exp\left[-2\frac{(r-w_{ring})^2}{r_{ring}^2}\right]$$

Where

- ϖ is the factor that ensures conservation of the total laser power,
- w_{ring} is the radial distance of the outer ring beam from the center of the heat source, and
- r_{ring} is the $1/e^2$ radius of the ring beam.

Assuming that the total power remains constant, ϖ takes the following form:

$$\varpi = -\frac{\sqrt{2}w_{ring}r_{ring}}{8}\left(-2\sqrt{\pi}\left(2-erfc\left(\frac{\sqrt{2}w_{ring}}{r_{ring}}\right)\right)-\frac{\sqrt{2}r_{ring}e^{-2\frac{w_{ring}^2}{r_{ring}^2}}}{w_{ring}}\right)$$

Finally, r is given as follow:

$$r = \sqrt{(x-X_p)^2+(y-Y_p)^2}$$

The total intensity of the core-ring beam is then given as:

$$Q = \alpha\ Q_{ring} + \ (1 - \alpha)\ Q_{core}$$

Where α denotes the fraction of power in the ring beam and $1 - \alpha$ consequently expresses the fraction of power in the core beam.

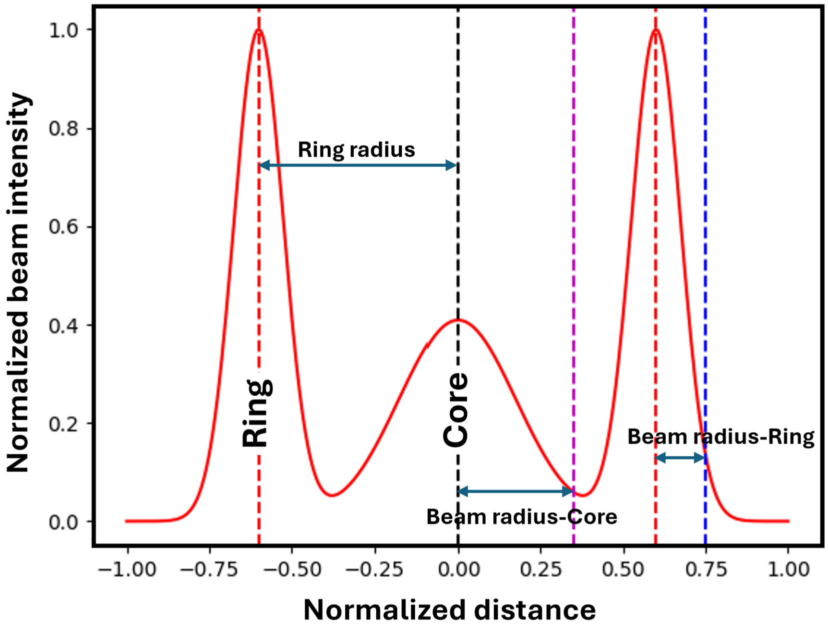


Figure 5: A schematic of the intensity profile of a core-ring heat source.

INDEX MODE (CORE-RING)

The intensity of the core-ring beam depends on different radii and the distribution of power between the core beam and the ring beam. For most users, these radii are not known since they are selected by the laser optics system of the additive manufacturing (AM) machine being used. The **Index Mode** is is available with the **Core-ring** heat source to guide the selection of settings for the **Beam radius-Ring**, **Ring radius**, and **Amount of power in ring**, based on the **Beam radius-Core** and **Index** number. The AM Module incorporates configurations commonly provided by AM machines and laser optics systems as described below.

The ratio between the **Beam radius-Core** and the outer radius i.e. **Beam radius-Ring** + **Ring radius** is assumed to be constant and is equal to 0.38. Furthermore, **Beam radius-Ring** is assumed to be a function of the **Beam radius-Core**. For instance, for a **Beam radius-Core** of 50 µm (i.e. diameter of 100 µm), the **Beam radius-Ring** would be 33 µm and the **Ring radius** would then be 98.58 µm. Similarly, for **Beam radius-Core** of 100 µm, the other Beam radii would also scale accordingly, such that the **Beam radius-Ring** would become 66 µm and the **Ring radius** would be 197.16 µm.

For the **Index Mode**, you provide the **Beam radius-Core** and select the **Index** number and the rest of the heat source parameters are set as described above.

The **Amount of power in ring** depends on the selected **Index** number and is set as follows:

Index	0	1	0	3	4	5	6
Amount of power in ring	7%	25%	35%	50%	70%	80%	90%

CUSTOM MODE (CORE-RING)

The **Custom Mode** for the **Core-ring** heat source allows you to manually enter all the parameters of the heat source. This requires an awareness of all the radii, either from the optics system of the AM machine in use, or from the calibration measurements of the laser beam.

> If you plan to use the beam radii from the **Index Mode** but perhaps require a different power distribution in the core/ring, you can first select the **Index Mode**, enter the **Beam radius-Core**, then change to **Custom Mode** and enter the user-defined **Amount of power in ring**.

Top-hat Heat Source

In addition to the Core-ring beam shape as an alternative to the Gaussian heat source, the **Top-hat** heat source is available with a flat and uniform energy distribution within a circular region and drops to zero outside the region. A **Top-hat** heat source is also called a *flat-top* and is considered a surface heat source model. In the AM Module, the top-hat heat source is approximated with a super-Gaussian beam, which means that the intensity drops to zero gradually within a given distance.

The intensity of such a beam is given as follows [1996Lu]:

[Eq. 4]

$$Q = Q_0 \exp\left(-2\left(\frac{r}{r_{tophat}}\right)^{2n}\right)$$

Where

- r_{tophat} is the $1/e^2$ radius of the top-hat beam and

$$r = \sqrt{(x - Xp)^2 + (y - Yp)^2}$$

- n is the order of the super Gaussian beam, which determines the steepness of the beam edges. To get a better approximation of the top-hat beam, Thermo-Calc uses $n = 5$.

- Q_0 is the peak intensity of the top-hat beam, and given the conservation of the total power, it takes the following form:

$$Q_0 = \left(\frac{\epsilon n P}{\pi r_{\text{tophat}}^2}\right) \cdot \frac{2^{1/n}}{\Gamma\left(\frac{1}{n}\right)}$$

where $\Gamma\left(\frac{1}{n}\right)$ represents the Gamma function evaluated at $\frac{1}{n}$, ϵ denotes the absorptivity of the laser beam, and P is the power of the heat source (W).

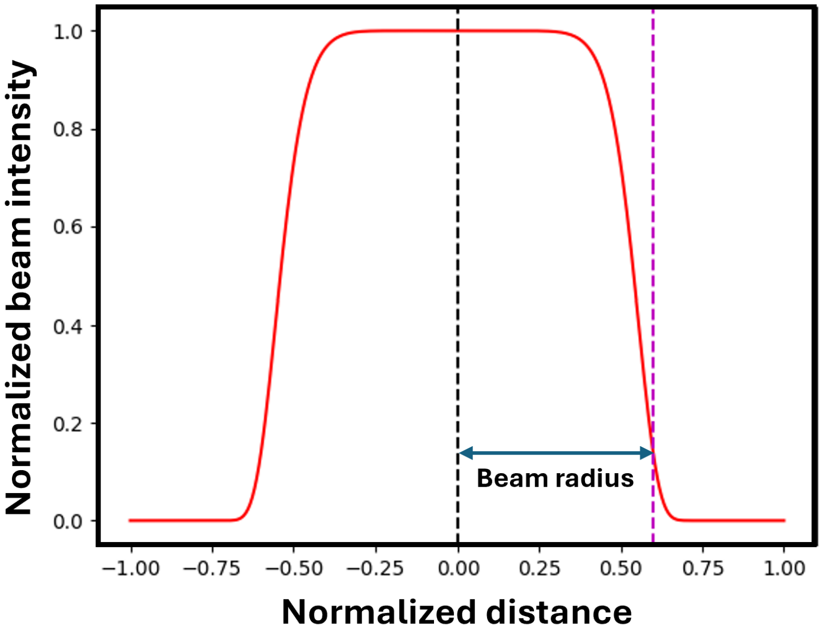


Figure 6: A schematic of the intensity profile of a top-hat heat source.

Double Ellipsoidal (Goldak) Heat Source

The **Double ellipsoidal** heat source model is a volumetric heat source model which was first proposed by Goldak et al. [1984Gol], and is now commonly used in LBPF simulations. In contrast to the surface heat source model, in the volumetric heat source model, the power input is defined not only on the surface of the workpiece but also inside the powder bed, along the depth of the powder bed. The heat distribution in the double-ellipsoidal heat source model is given by a combination of two ellipsoids; one in the front quadrant of the heat source and the other in the rear quadrant, as shown in the figure below. The power density is thus given by two different expressions, one for each quadrant of the heat source.

[*Eq. 5*]

$$Q_f = f_f \frac{6\sqrt{3}\varepsilon P}{\pi^{\frac{3}{2}} a_f bc} \exp\left[-2\frac{(x-X_p)^2}{a_f^2} + \frac{(y-Y_p)^2}{b^2} + \frac{(z-Z_p)^2}{c^2}\right]$$

$$Q_r = f_r \frac{6\sqrt{3}\varepsilon P}{\pi^{\frac{3}{2}} a_r bc} \exp\left[-2\frac{(x-X_p)^2}{a_r^2} + \frac{(y-Y_p)^2}{b^2} + \frac{(z-Z_p)^2}{c^2}\right]$$

Where Q_f and Q_r are the power densities (W/m^3) in the front and rear quadrant of the heat source, while a_f and a_r are the semi-axes of the front and rear ellipsoids, respectively. b and c are the semi-axes along the width and depth of the melt pool. f_f and f_r are the proportional coefficients for the front and rear ellipsoid of the heat source, with the condition $f_f + f_r = 2.f_f$ is then given as follows:

[*Eq. 6*] $f_f = \frac{2a_f}{a_f+a_r}$

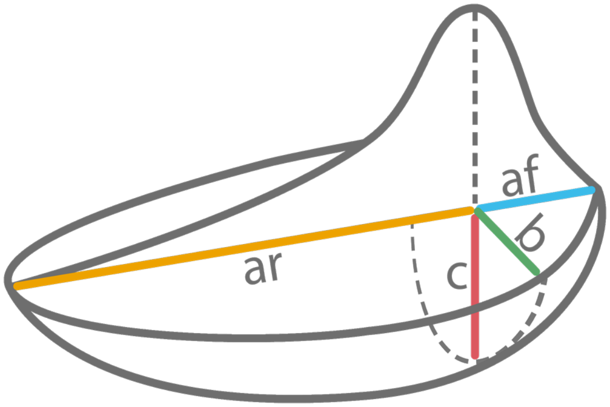


Figure 7: Schematic representation of energy distribution in double ellipsoidal heat source model.

Conical Heat Source

The **Conical** heat source model is also a volumetric heat source model, which was first employed for welding simulations but due to inherent similarities between welding and LPBF processes, this model is also commonly used for AM simulations. The conical heat source model is defined by a Gaussian heat distribution on the top surface of the workpiece and a conical distribution along the depth of the powder bed. A schematic representation of the energy distribution for conical heat source model is shown below.

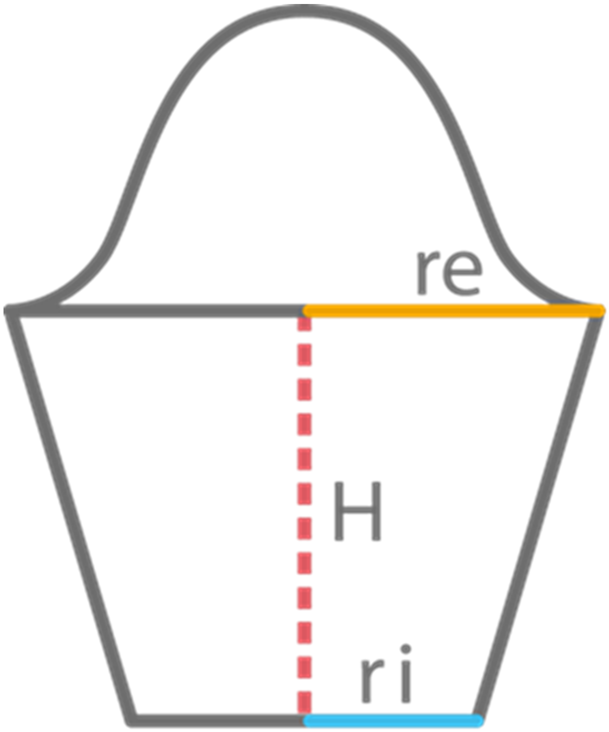


Figure 8: Schematic representation of energy distribution in conical heat source model.

The power density for the conical heat source is given as follows [2019Zha]:

[*Eq. 7*]
$$Q = \frac{6\varepsilon P}{\pi H\left(r_e^2 + r_e r_i + r_i^2\right)} \exp\left[-2\frac{\left(x - X_p\right)^2 + \left(y - Y_p\right)^2}{r_o^2}\right]$$

with

$$r_o = r_e + (z - ZP)\frac{(r_e - r_i)}{H}$$

where r_e and r_i are the cone radius at the top and bottom, respectively, while H is the height of the cone.

References

[1969Pav] V. Pavelic, Experimental and computed temperature histories in gas tungsten arc welding of thin plates. Weld. J. Res. Suppl. 48, 296–305 (1969).

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[2019Zha] Z. Zhang, Y. Huang, A. Rani Kasinathan, S. Imani Shahabad, U. Ali, Y. Mahmoodkhani, E. Toyserkani, 3-Dimensional heat transfer modeling for laser powder-bed fusion additive manufacturing with volumetric heat sources based on varied thermal conductivity and absorptivity. Opt. Laser Technol. 109, 297–312 (2019).

[2021Grü] J. Grünewald, F. Gehringer, M. Schmöller, K. Wudy, Influence of Ring-Shaped Beam Profiles on Process Stability and Productivity in Laser-Based Powder Bed Fusion of AISI 316L. Metals (Basel). 11, 1989 (2021).

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[2024Gal] F. Galbusera, L. Caprio, B. Previtali, A. G. Demir, Analytical modeling and characterization of ring beam profiles for high-power lasers used in industrial manufacturing. J. Manuf. Process. 117, 387–404 (2024).

[2025Bir] M. Birg, T. Novotny, F. Bayer, “Beam Shaping in Additive Manufacturing A Toolbox of New Possibilities (White paper)” (2025); https://www.eos.info/content/blog/entering-the-next-era-of-am-with-beam-shaping.

About Heat Source Calibration

There are models available to define the heat source in the AM process and that are also available with the **Heat Source Calibration** *Calculation Type*: **Gaussian**, **Double ellipsoidal**, or **Conical**. All these heat sources rely on different sets of parameters to fully define the heat input to the powder and solid substrate.

The standard Gaussian heat source model (a **Single Point** *Calculation Type*) requires defining the **Absorptivity** and the **Beam radius** on the **AM Calculator Configuration** window. The keyhole model takes into account the effect of evaporation recoil pressure that produces a keyhole, if present for the given processing conditions. Multiple reflections are also included in the keyhole model to improve the calculation of the keyhole shape. The absorptivity of the liquid can be calculated but often requires correction due to uncertainty in the model, surface oxides, and so forth. The beam radius of the heat source of the printer is, however, most often known but does not always match the definition of the beam size for the Gaussian heat source used in the simulation. Leveraging the experimental melt pool data and the relation between melt pool size and energy density can help to calibrate the absorptivity and beam radius for the Gaussian heat source model.

> The keyhole model is available for Gaussian, Core-ring, and Top-hat heat sources. See About the Keyhole Model for some additional information.

For information about using calculated or constant absorptivity with a Gaussian Heat Source Calibration, there is additional theory in About the Absorptivity Model. The associated settings for this type of calibration is in the subsection Heat Source Calibration.

Similarly, for volume heat sources, i.e. **Double ellipsoidal** and **Conical**, it is necessary to enter four and three parameters, respectively, along with the absorptivity. Since volume heat sources are a numerical way to correctly capture the shape of the melt pool, it is not always possible to know the values of these parameters for the processing conditions.

However, according to the literature [2021Gra] you can find a relationship between the size i.e., width and depth of the melt pool, and the energy density (defined as the ratio of power and scanning speed) and based on that, you can also find a relationship between the heat source parameters and the energy density.

See Additive Manufacturing Module Theory for a general overview including details about the heat sources.

This means that if a set of experimental data for an alloy can be provided in the form of power, scanning speed, width of the melt pool, and depth of the melt pool, then you can perform a heat source calibration to calibrate the heat source parameters for the given material. This is done by running an optimization algorithm for the selected experimental data and then choosing an appropriate function for each heat source parameter. As a result, the output includes expressions of the given parameters as a function of the energy density, which can be saved and is available later in heat source list as a **Users heat source**. This is for any given process parameter (i.e. the saved heat source can be used for any process parameter).

When a **Users heat source** option is available to choose in the heat source list, then only the **Power** of the heat source needs to be entered and the rest of the parameters, including the absorptivity, are automatically included in the simulation based on the selected expressions when originally saving the heat source calibration data.

In order to set up the calibration of the heat source, you select the **Steady-state** simulation type and then select **Heat Source Calibration** as the *Calculation Type*. The calibration is performed assuming steady-state conditions so most of the configurations are done in the same way as the **Single Point** Steady-state simulation. The difference is that you need to choose which heat source to use, i.e. **Gaussian**, **Core-ring**, **Top-hat**, **Double ellipsoidal**, or **Conical**.

> For more details about including the **Heat Source Calibration** *Calculation Type* during the simulation set up, go to AM Calculator Conditions Settings. Then go to Visualizing Heat Source Calibrations for details about navigating the various previews and results.

Heat Source Calibration with Experiment Data

When the **Heat Source Calibration** is selected in the **Steady-state** simulation type, there is an option to import a file with experimental data points that can be used in the simulation. Data can also be entered directly into the table on the AM Calculator Configuration window. However, if an **Experiment file** is imported it needs to be set up in a certain way so that the software can read the data.

AM Calculator Experiment File Requirements

Once the experiment data is entered, you can view the plot of melt pool dimensions vs. energy density (P/v) in the **Visualizations** window, and make a selection of the experiments to be used for calibration by checking the corresponding checkbox in the **Use** column. When this is done, click **Perform Tree** to perform the calibration.

> If you select **Depth** from the **Calibrate for** list, then the experimental values for only the melt pool depth is needed.

Examples Related to Heat Source Calibration

There are two examples included with the installation to help you understand how to calibrate a heat source and then use the calibration in simulations.

AM_06a: Calibrating a Heat Source for a 316L Steel: This example demonstrates the calibration of the heat source using the **Gaussian** and **Double ellipsoidal** heat sources.

AM_06b: Using the Calibrated Heat Source for a 316L Steel: The purpose of this example is to use the saved heat sources from AM_06a and then validate the results by comparing the melt pool size from the simulations with the experimental melt pool dimensions. It also uses the keyhole model.

Reference

[2021Gra] D. Grange, A. Queva, G. Guillemot, M. Bellet, J.-D. Bartout, C. Colin, Effect of processing parameters during the laser beam melting of Inconel 738: Comparison between simulated and experimental melt pool shape. J. Mater. Process. Technol. 289, 116897 (2021).

About the Keyhole Model

In additive manufacturing a laser beam melts the powder, and at high energy density of the laser also evaporation of the liquid metal occurs. The evaporation causes transfer of momentum from the metal to the vapour, i.e. a recoil. The conservation of total momentum then leads to a recoil pressure that pushes down the liquid/gas interface to form a cavity, also known as a keyhole. However, this free surface is computationally expensive to calculate due to the very dynamic movements of the keyhole. To reduce the complexity, the Additive Manufacturing (AM) Module has an analytic model based on [1994Kap] to pre-compute the keyhole shape and the corresponding mesh.

Example AM_06b: Using the Calibrated Heat Source for a 316L Steel includes the use of the keyhole model. The different processing conditions are selected to simulate both the conduction mode as well as the keyhole mode.

Also see examples AM_07, AM_08a, AM_08b, AM_09a, AM_09b, and AM_13 where the keyhole model is used with fluid flow, or AM_14 without fluid flow .

The analytical keyhole model approximates the heat conduction by a moving line source where the keyhole shape is obtained by heat balance at the keyhole wall using average material properties. A point-by-point scheme compares absorbed power and conduction losses to obtain the local inclination angle of the keyhole walls.

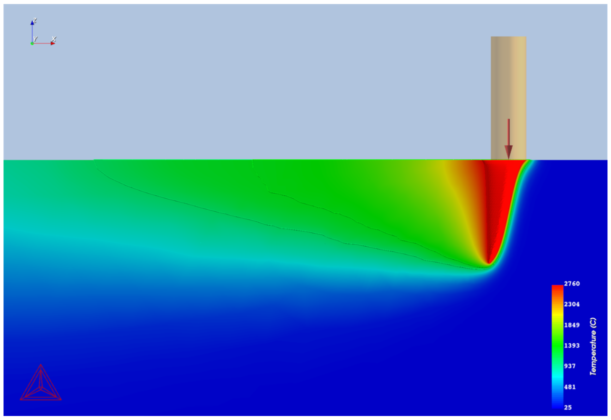


Figure 9: Side-view of a keyhole and melt pool for the material SS316L with Gaussian beam radius of 40 µm and the absorptivity set to 40%.

When a keyhole is formed, the energy is transmitted into the material through numerous reflections within the keyhole (see Figure 10).

For metals with an absorption factor of around 30% the reflections can increase the effective absorption to values around 90% or higher of the total laser beam energy. In the Additive Manufacturing (AM) Module, multiple reflections are implemented in the analytical keyhole mode according to the Coviello publication [2022Cov]. This strategy allows for computation of a keyhole shape, including multi reflections using ray tracing.

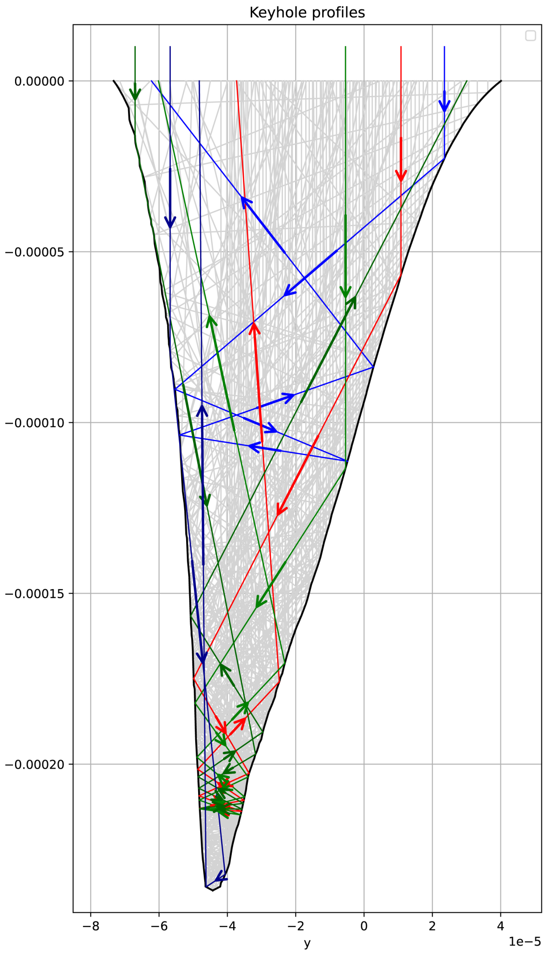


Figure 10: Ray tracking of the laser beam reflected at the wall of the keyhole. Blue, green and red lines highlight the path for three rays. Gray lines represent a fraction of all the reflected rays.

The keyhole model is limited to the surface heat sources (Gaussian, Core-ring and Top-hat) without separate material properties for powder. An additional input is the beam quality factor M^2 of the laser beam where the default value is 1.0. The beam quality factor is a measure of laser beam quality, it relates the beam divergence of a laser beam to the minimum focused spot size that can be achieved.

To include the keyhole feature, go to AM Calculator Heat Source Settings where you can enable this feature.

See About the Heat Source Models for background details about the heat sources.

References

[1994Kap] A. Kaplan, A model of deep penetration laser welding based on calculation of the keyhole profile. J. Phys. D. Appl. Phys. 27, 1805–1814 (1994).

[2022Cov] D. Coviello, A. D’Angola, D. Sorgente, Numerical Study on the Influence of the Plasma Properties on the Keyhole Geometry in Laser Beam Welding. Front. Phys. 9, 1–9 (2022).

About the Absorptivity Model

The absorptivity of a flat metal surface is a function of the alloy composition, temperature, the wavelength of the heat source, and the angle of incidence.

The absorptivity of a metallic powder is more complex. Most metallic powders are oxidized at the surface where a thin layer of oxide often increases absorptivity. Multiple reflections of the laser rays also increases the effective absorptivity, e.g. at surface roughness or between the particles within the powder layer. The additional complications of the metallic powder are neglected in this model, which focuses on an ideal flat surface of the liquid phase after the powder has melted. This simplification can be justified at steady-state conditions when a melt pool is established and most laser rays hit the liquid surface in the melt pool.

Additional related theory topics include: Additive Manufacturing Module Theory, About the Heat Source Models, and About the Keyhole Model.

Laser Beam Reflection

A fraction of the energy of a laser ray (E) is absorbed when it strikes a surface, the rest of the energy is reflected (R), i.e. the absorptivity is given by $A = (1 - R) * E$.

The Fresnel equation describes how the absorptivity depends on the angle of incidence α.

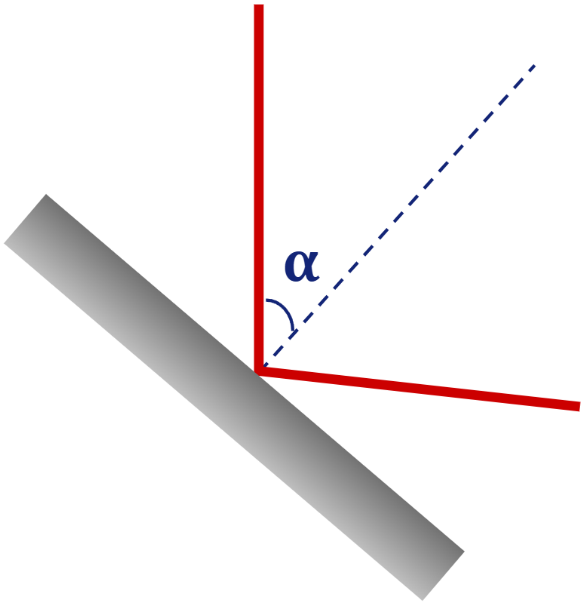


Figure 11: A laser ray strikes a surface at the incident angle α.

For an unpolarized laser beam, the reflection coefficient R is the average of the parallel and perpendicular component, denoted by R_s and R_p:

$$R = (R_s + R_p)/2$$

Both components of R are given by the Fresnel equations:

$$R_s = \left| \frac{cos\ \alpha - \sqrt{\widehat{n}^2 - sin^2\alpha}}{cos\ \alpha + \sqrt{\widehat{n}^2 - sin^2\alpha}} \right|^2$$

$$R_p = \left| \frac{\widehat{n}^2 cos\ \alpha - \sqrt{\widehat{n}^2 - sin^2\alpha}}{\widehat{n}^2 cos\ \alpha + \sqrt{\widehat{n}^2 - sin^2\alpha}} \right|^2$$

The refraction index $\widehat{n}$ is a complex number $\widehat{n} = n - ik$ where k corresponds to the extinction coefficient.

The refractive index is directly related to the electric permittivity, $\hat{\epsilon} = \varepsilon_r - i\varepsilon_i$:

$$n = \frac{1}{\sqrt{2}} \left[\left(\epsilon_r^2 + \epsilon_i^2 \right)^{1/2} + \epsilon_r \right]^{1/2}$$

$$k = \frac{1}{\sqrt{2}} \left[\left(\epsilon_r^2 + \epsilon_i^2 \right)^{1/2} - \epsilon_r \right]^{1/2}$$

About the Lorentz-Drude (LD) Model

The Lorentz-Drude model (LD) relates the electric permittivity with the electric resistivity [2021Yan].

> The electric resistivity thermophysical property is included in many Thermo-Calc databases. For a list of databases that include it, see the Properties that Can Be Calculated brochure on the website or refer to the specific database documentation.

The LD model only considers the intraband absorption and is neglecting the interband part. The interband part of absorption is, however, often less dominant for wavelengths larger than 1 µm; for smaller wavelengths the model shows larger deviations when compared to experimental data.

> For additive manufacturing lasers, the most common wavelength used is 1.06 µm.

The LD model is used as a first approximation of the dielectric constants of an alloy. The model is then further calibrated against the available experimental information of dielectric constants, refraction index, and absorptivity of liquid metal, i.e. the correction functions f^r and f^i are modeled:

$$\epsilon_r = \epsilon_r^{LD} \cdot \left[\sum_{i\in n} x_i \cdot f_i^r(\lambda, T) + \sum_{i\in n j\in n} \sum_i x_i \cdot x_j \cdot f_{i-j}^r(\lambda, T)\right]$$

$$\epsilon_i = \epsilon_i^{LD} \cdot \left[\sum_{i\in n} x_i \cdot f_i^i(\lambda, T) + \sum_{i\in n j\in n} \sum_j x_i \cdot x_j \cdot f_{i-j}^i(\lambda, T)\right]$$

where

- x_i is the mole-fraction of element i
- λ the laser wavelength, and
- T the temperature.

The correction improves the model accuracy for the entire wavelength spectrum.

Following the work by Yang [2021Yan], the LD model obtains the real and imaginary parts of the electric permittivity:

$$\epsilon_r^{LD} = 1 - \frac{\omega_p^2}{f_L^2 + \gamma^2}$$

$$\epsilon_i^{LD} = \frac{\gamma}{f_L} \cdot \frac{\omega_p^2}{f_L^2+\gamma^2}$$

where

- ω_p is the plasma frequency,
- f_L is the laser frequency, and
- γ is the damping frequency.

The plasma frequency is given by:

$$\omega_p = \sqrt{\frac{N_e q_e^2}{m_e \epsilon_0}}$$

where

- N_e is the number density of free electrons,
- q_e the absolute value of elementary charge, $q_e = 1.6 \times 10^{-19} C$,
- m_e is the electron mass, $m_e = 9.11 \times 10^{-31} kg$, and
- ϵ_0 is the vacuum permittivity, $\epsilon_0 = 8.85 \times 10^{-12} Fm^{-1}$.

The damping frequency can be expressed as:

$$\gamma = \omega_p^2 \cdot \epsilon_0 \cdot \rho(T, x)$$

where

- $\rho(T, x)$ is the temperature- and composition-dependent electrical resistivity.

The laser frequency can be expressed as:

$$f_l = 2\pi \cdot \frac{c}{\lambda}$$

where

- c is the speed of light in vacuum, and
- λ is the wavelength of the laser.

The free electron density N_e is assumed to be given directly by the atomic mass and mass density:

$$N_e = N_A \cdot \rho_m \sum_{i \in N} \frac{x_i Z_i}{m_i}$$

where

- N_A is the Avagadros constant,
- ρ_m is the mass density of the alloy,
- m_i is the atomic weight of element i, and
- Z is the number of valence electrons per atom of element i.

Heat Sources and Absorptivity

The LD model for liquid absorptivity describes a material property and is applicable to the **Gaussian**, **Core-ring**, and **Top-hat** heat sources where the energy is added to the surface of the material.

The LD model for absorptivity is not applicable to the volume heat sources **Double ellipsoidal** and **Conical**. Volume heat sources assume an effective absorptivity that indirectly can include the effect of keyholing by increasing the absorptivity as a function of energy density.

SURFACE HEAT SOURCES

The angle of incidence for a laser ray is zero when no keyhole forms. The angle of incidence varies greatly within the keyhole and the full angle dependent absorptivity model is used.

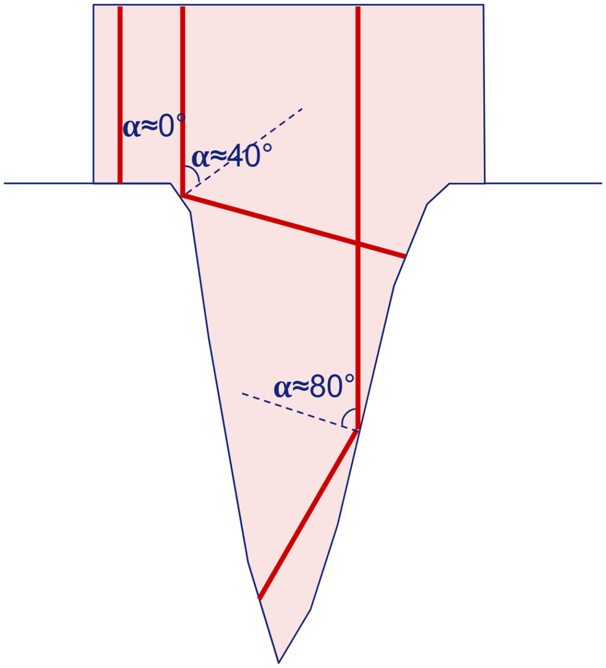
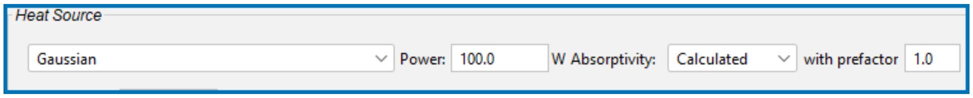


Figure 12: A schematic keyhole where three individual laser rays hit the surface at different incident angle α. The keyhole model in the AM Module accounts for multiple reflections, but only the first reflection for each ray is shown for clarity.

The absorptivity model takes the wavelength of the heat source as input together with a prefactor that can scale the calculated absorptivity up or down. The scaling can be required to calibrate the simulations against experiments.

The following absorptivity settings are described in the AM Calculator Heat Source Settings. The examples use Gaussian, but Core-ring and Top-hat area also available.



Heat Source

Gaussian Power: 100.0 W Absorptivity: Calculated with prefactor 1.0

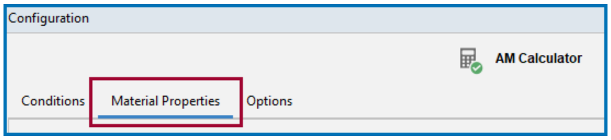
Figure 13: Gaussian Heat Source using the Calculated Absorptivity. The calculated value is scaled with the value of "prefactor" where the default is 1.0, i.e. to use the calculated value as-is.

Heat Source

Gaussian Power: 120.0 W Absorptivity: User-defined -1.6e-7*T*T+2.5e- %

Figure 14: Gaussian Heat Source with User-defined function of the absorptivity.

The resulting absorptivity (given the wavelength and prefactor) can be visualized from the **Material Properties** tab on the **AM Calculator Configuration** window.



The following absorptivity options are described in AM Calculator Heat Source Settings.

From the **Plot** list, select:

- **Absorptivity** to visualize the temperature dependent absorptivity for the liquid phase of the selected material (Figure 15).
- **Absorptivity vs angle** to visualize the angle dependent absorptivity at liquidus and the evaporation temperature (Figure 16).
- **Electric resistivity** to visualize it as a function of temperature (Figure 17).

The electric resistivity is not directly used in the AM simulations, only indirectly through the absorptivity model that uses the electric resistivity when modeling the composition, temperature, and angle dependent absorptivity.

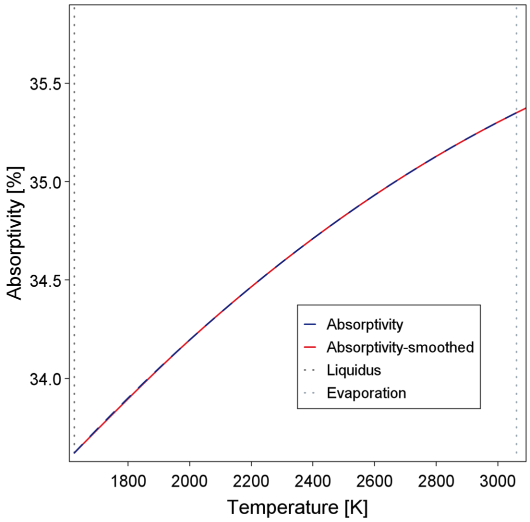


Figure 15: The calculated absorptivity as a function of temperature for the alloy IN738LC.

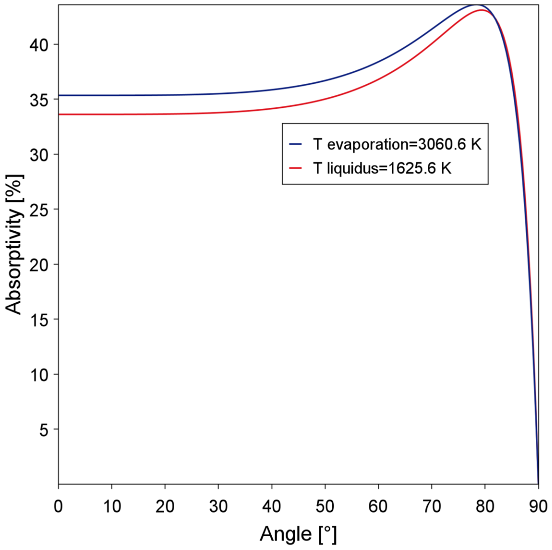


Figure 16: The calculated absorptivity as a function of angle of incidence for the alloy IN738LC. The red curve shows the absorptivity at the liquidus temperature and the blue curve the corresponding absorptivity at the evaporation temperature.

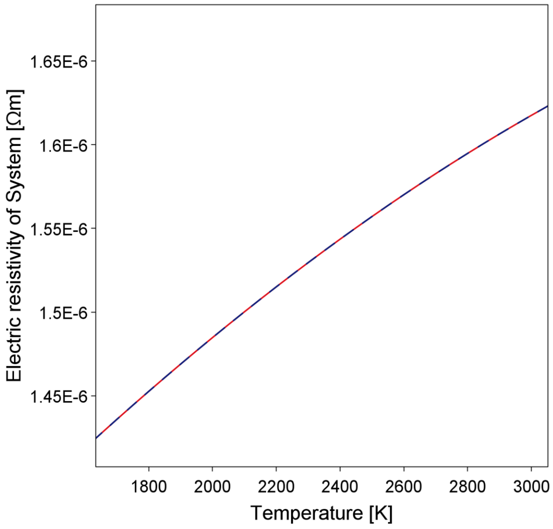


Figure 17: The electric resistivity of the liquid phase for the alloy IN738LC. The electric resistivity is used in the model for absorptivity for the liquid phase.

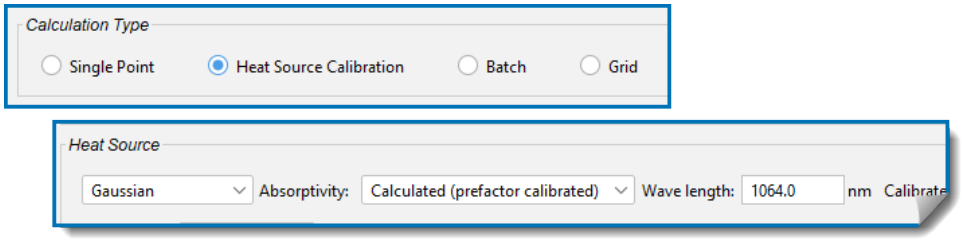
Heat Source Calibration

Additional settings are described in the AM Calculator Conditions Settings topic.

AM_06a: Calibrating a Heat Source for a 316L Steel

For **Gaussian** *Heat Source Calibration* calculations, you can use the temperature and angle dependent calculated absorptivity and calibrate the scaling prefactor to match the given experimental data. The settings are on the **AM Calculator Configuration** window.

For **Absorptivity** select **Calculated (prefactor calibrated)** then enter the **Wavelength** of the heat source or use the default value.

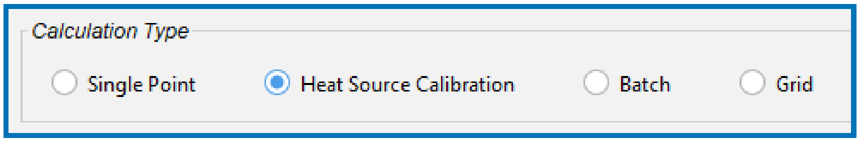

Calculation Type

○ Single Point ● Heat Source Calibration ○ Batch ○ Grid

Heat Source

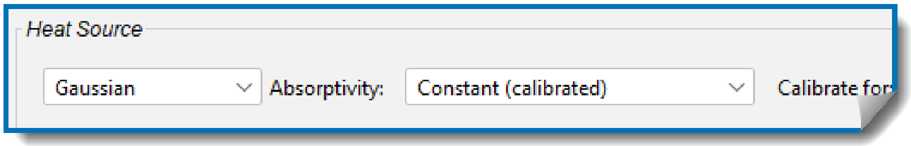
Gaussian Absorptivity: Calculated (prefactor calibrated) Wave length: 1064.0 nm Calibrate

In order to use a constant **Absorptivity**, you can instead select **Constant (calibrated)**, which uses a constant value of absorptivity i.e. it is not dependent on temperature or incidence angle. Then you can calibrate that value to match the given experimental data.



Calculation Type

○ Single Point ● Heat Source Calibration ○ Batch ○ Grid

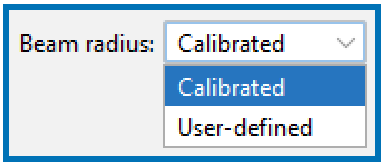


Heat Source

Gaussian Absorptivity: Constant (calibrated) Calibrate for:

For both **Absorptivity** options (**Calculated (prefactor calibrated)** or **Constant (calibrated)**) you can also either calibrate the **Beam radius** along with the absorptivity or the prefactor (choose **Calibrated**), or use a fixed value of **Beam radius** and calibrate only the absorptivity (choose **User-defined**).

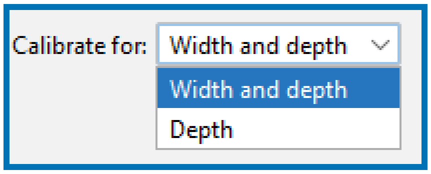
Another setting available with the Gaussian Heat Source Calibration, is to calibrate for both the **Width and depth** of the melt pool from the experimental data or use only the **Depth** of the melt pool for the calibration. If you choose **Width and depth**, the *Experiment Data* values in the table require both the width and depth of the melt pool whereas if you only calibrate the depth then the data file needs to only include the information for the depth of the melt pool.



Beam radius: Calibrated

Calibrated

User-defined



Calibrate for: Width and depth

Width and depth

Depth

Reference

[2021Yan] Z. Yang, A. Bauereiß, M. Markl, C. Körner, Modeling Laser Beam Absorption of Metal Alloys at High Temperatures for Selective Laser Melting. Adv. Eng. Mater. 23, 2100137 (2021).

Additive Manufacturing Simulation Types

Three simulation types are available on the AM Calculator – *Steady-state*, *Transient*, and *Transient with heat source from Steady-state*.

Additive Manufacturing Module Theory and About the Heat Source Models.

The **keyhole model** is available when **Gaussian**, **Core-ring**, or **Top-hat** heat sources are used for either the *Steady-state* or *Transient with heat source from Steady-state* types of simulation (see About the Keyhole Model. It is available with or without fluid flow.

Steady-state

For **Steady-state** simulations, you can also choose to run different Steady-state Calculation Types.

In the *Steady-state* mode it is assumed that the temperature distribution and the fluid flow around the heat source is in steady state and does not change with time. This is useful to get an estimation of the temperature distribution and size of the melt pool when you assume that the heat source is moving at a constant speed in a given path. In the single-track experiments, temperature distribution around the heat source and fluid flow inside the melt pool reach a steady state very quickly, and you should then perform steady-state simulations to predict melt pool geometry and cooling rates around the melt pool. In a sense, steady-state simulations give you an overall picture of the process but in order to get more precise details and predict temperature distribution in a multi-layer build, as a function of time, you should perform transient simulations. The benefit of the steady-state option is that these simulations are quick, and you get a solution typically within 1-5 minutes, depending on the process parameters and your computational resources. For the steady-state simulations, you can include or exclude fluid flow inside the melt pool due to the Marangoni effect. For the given processing conditions, if convection is the dominant mode of heat transfer, inclusion of fluid flow is crucial to enhance the accuracy of the model by correctly capturing the underlying physical behavior of melting and solidification of material. Furthermore, you can also perform simulations with a powder layer on the top of the substrate having different material properties than the bulk material. The steady-state simulations are performed on a symmetric domain where you specify only the height of the substrate and the thickness of the powder layer, if present. The length and width of the computational domain are determined automatically based on the process parameters. The temperature distribution is computed using the energy equation while the fluid flow is modeled using the Navier-Stokes equation.

Transient

In the *Transient* mode, you can perform full-scale transient simulations in a 3D rectangular build part and have the possibility to specify a scanning strategy comprising multiple tracks and multiple layers. Here you can enter the height, width, and length of the entire build part or a representative segment of the build part and configure a scanning strategy either for a single track or for multiple tracks (bidirectional or unidirectional). You can also add multiple layers of powder and rotate the scanning pattern between layers.

Similar to the *Steady-state* mode, here you can also choose to include fluid flow inside the melt pool to correctly capture the underlying physical phenomena of melting and solidification of the material and thereby increasing the accuracy of the model. The inclusion of fluid flow requires coupling the Navier-Stokes equations together with the energy equation which comes at the cost of increased numerical complexity resulting in longer simulation times.

Transient with Heat Source from Steady-state

In order to perform full scale 3D simulations in an efficient manner, with multitracks and multilayers, including fluid flow in the melt pool or with powder layer(s) having different properties than the solid material, you can use the *Transient with heat source from Steady-state* mode. This mode develops a novel approach where the effect of fluid flow due to Marangoni convection in the melt pool is incorporated without solving for Navier-Stokes equations in the full-scale 3D domain.

The concept involves the assumption that the temperature distribution and fluid flow inside the melt pool instantly reach steady state. First you solve for temperature distribution, using the energy equation and fluid flow due to Marangoni convection, using the Navier-Stokes equations for the given process parameters in the Steady-state mode. Once you have the steady state solution, use this solution inside the melt pool and map it as a “heat source” in the transient simulations. Using this approach, you do not have to solve for the complicated Navier-Stokes equations at each time step in the transient simulation, yet it still captures the effect of fluid flow on the shape of the melt pool. Furthermore, it also reduces the computational time by solving for the most non-linear region in the energy equation i.e., inside the melt pool, only once, and then reusing the solution as a boundary condition in the transient simulations. This approach considerably decreases the numerical complexity of the full-scale transient simulations, which consequently reduces the simulation time without making a significant compromise on the accuracy of the solution.

Steady-state Calculation Types

When setting up a **Steady-state** simulation on the **AM Calculator**, you can also select different *Calculation Types*.

Additive Manufacturing Simulation Types and for overall general theory, see Additive Manufacturing Module Theory.

For background theory related to Heat Sources, see About the Heat Source Models and About the Absorptivity Model. For *Gaussian*, *Double ellipsoidal*, and *Conical* heat sources, also see About Heat Source Calibration for additional details.

Single Point

The standard steady-state calculation for a single set of processing parameters. This is available with all heat sources.

See Calculation Type (Steady-state) for settings information on the AM Calculator.

Heat Source Calibration

To calibrate a heat source based on the imported or entered experimental data instead of performing a single point calculation. This is available with **Gaussian**, **Double ellipsoidal**, or **Conical** heat sources.

See Calculation Type (Steady-state) for settings information on the AM Calculator. For information about previewing configuration settings (on the AM Calculator) as well as plot results (on the Plot Renderer), see Visualizing Heat Source Calibrations.

Batch

To include power and scan speed data, which is read from a file such as a spreadsheet. You can optionally include experimental melt pool width and depth (if there is data), and compare this to the calculated results using a Parity plot on the Plot Renderer. This is available with all heat sources.

For settings information on the AM Calculator, see Calculation Type (Steady-state). For information about previewing configuration settings (on the AM Calculator) as well as plot results (on the Plot Renderer), see Visualizing Batch Calculations in the AM Module.

Grid

To evaluate two axis variables of power and scanning speeds in the specified range and number of steps. This is available with all heat sources.

For settings information on the AM Calculator, see Calculation Type (Steady-state). For Plot Renderer Configuration settings, see AM Calculator: Plot Renderer Settings.

AM Plots and Tables

In this section:

About the AM Plot Types

When working with an **AM Calculator** with the **Plot Renderer** as a successor, the visualization is different from the other calculators available in Thermo-Calc. When setting up the **AM Calculator**, there are many options available that impact what plot types are going to be available. Further, when defining the **Plot Renderer**, there are additional ways and axis variables or other setting requirements that enable you to display certain plot types, as well as preview a variety of settings on the **Visualizations** window.

In addition, when a **Plot Renderer** is added as a successor to the **AM Calculator**, the default layout of the **Configuration** window, with respect to the different tabs, relates to how the **AM Calculator** is set up. This is then further related to the tabs located on the **Visualizations** window.

See Working with AM Visualizations for information about how these tabs are connected between the windows. Also see Overlaying Plots in the AM Module.

See Plot Types for more information for the Scheil Calculator and Diffusion Calculator, which are also used with the Additive Manufacturing (AM) Module.

AM Plot Types

Simulation Type	*Calculation Type**	*Plot Type*	*Export Result Files*	*Display Type*	*Notes*	*Tab Name Configuration Window (Setting)*	*Tab Name Visualizations Window (Plot)*	*Link to More information*
Steady-state, Transient, or Transient with heat source from Steady-state	Steady-state → Single Point, Heat Source Calibration, Batch, and Grid	3D Plot	Yes	Surface colormap	From the **Display** list select **Surface colormap**. Available when Temperature, Surface tension,	3D Plot	3D Plot When overlaying certain plots, there is also a suffix in brackets that matches the	AM Plot Type: 3D Plot

Simulation Type	*Calculation Type**	*Plot Type*	*Export Result Files*	*Display Type*	*Notes*	*Tab Name Configuration Window (Setting)*	*Tab Name Visualizations Window (Plot)*	*Link to More information*
					Thermal conductivity, or Dynamic viscosity is selected as an Axis variable.		name of the AM Calculator it is connected to. e.g. **3D Plot (AM Calculator 1)**	
				Slice	From the **Display** list select **Surface colormap** or **Contour** and then click to select the **Slice** checkbox.			
				Contour	From the **Display** list select **Contour**. Available when Temperature, Surface tension, Thermal conductivity, or Dynamic viscosity is selected as an Axis variable.			
				Iso-surface	From the **Display** list select **Iso-**			

Simulation Type	*Calculation Type**	*Plot Type*	*Export Result Files*	*Display Type*	*Notes*	*Tab Name Configuration Window (Setting)*	*Tab Name Visualizations Window (Plot)*	*Link to More information*
					surface. Available when Temperature, Surface tension, Thermal conductivity, or Dynamic viscosity is selected as an Axis variable.			
				Arrow, 2D glyph, Cone, or Line	Available when **Flow velocity field** is selected as an Axis variable. Requires that the **Fluid flow including Marangoni effect** checkbox is selected on the AM Calculator.			
Steady-state, Transient, or Transient with heat source from Steady-state	Steady-state → Single Point, Heat Source Calibration, Batch, and Grid	Plot Over Line (2D)	No	not applicable	Once the plot is performed, switch between a plot and a table by clicking the **Table View** button on the **Visualizations**	Plot Over Line	Plot Over Line	AM Plot Type: Plot Over Line (2D) AM Plots: Table View Options

Simulation Type	***Calculation Type****	***Plot Type***	***Export Result Files***	***Display Type***	***Notes***	***Tab Name Configuration Window (Setting)***	***Tab Name Visualizations Window (Plot)***	***Link to More information***
					window.			
Steady-state	Heat Source Calibration	Heat Source Calibration (2D)	Yes	not applicable	This plot is available once the calibration is completed.	Heat Source Calibration	Heat Source Calibration Parameters	AM Plot Type: Heat Source Calibration Parameters
Steady-state	Heat Source Calibration	Melt Pool Dimensions (2D)	Yes	not applicable	This plot is available once the calibration is completed.	Heat Source Calibration	Melt Pool Dimensions	AM Plot Type: Melt Pool Dimensions
Steady-state	Batch and Grid	Printability Map (2D)	Yes	not applicable	Also toggle between **Show Table** and **Hide Table** on the **Configuration** window.	Batch or Grid	Printability Map	AM Plot Type: Printability Map AM Plots: Table View Options
Steady-state	Batch and Grid	Meltpool vs Energy Density (2D)	Yes	not applicable	Also toggle between **Show Table** and **Hide Table** on the **Configuration** window.	Batch or Grid	Meltpool vs Energy Density	AM Plot Type: Melt Pool vs Energy Density AM Plots: Table View Options
Steady-state	Batch	Parity Plot (2D)	Yes	not applicable	Also toggle between **Show Table** and **Hide Table** on the	Batch	Parity Plot	AM Plot Type: Parity Plot AM Plots: Table View

Simulation Type	*Calculation Type**	*Plot Type*	*Export Result Files*	*Display Type*	*Notes*	*Tab Name Configuration Window (Setting)*	*Tab Name Visualizations Window (Plot)*	*Link to More information*
					Configuration window.			Options
Steady-state, Transient, or Transient with heat source from Steady-state	Single Point, Heat Source Calibration, Batch, or Grid	Thermal Gradient vs Solidification Rate (2D)	No	not applicable	Once the plot is performed, switch between a plot and a table by clicking the **Table View** button on the **Visualizations** window. It is also possible to visualize this via the **3D Plot** tab when you define the Axis variables **Solidification rate** and **Thermal gradient**.	Thermal Gradient vs Solidification Rate	Thermal Gradient vs Solidification Rate	AM Plot Type: Thermal Gradient vs. Solidification Rate
Transient or Transient with heat source from Steady-state	not applicable	Probe (2D)	No	not applicable	Probe positions and time steps available. Defined and available from a specific a tab on the Plot Configuration window.	Probe	Probe	AM Plot Type: Probe (2D) AM Plots: Table View Options

Simulation Type	***Calculation Type****	***Plot Type***	***Export Result Files***	***Display Type***	***Notes***	***Tab Name Configuration Window (Setting)***	***Tab Name Visualizations Window (Plot)***	***Link to More information***
					Once the plot is performed, switch between a plot and a table by clicking the **Table View** button on the **Visualizations** window.			

* For **Transient** and **Transient with heat source from Steady-state** simulations there are no additional *Calculation Types* selected.

AM Plot Type: 3D Plot

The **3D Plot** is available with all simulation types (*Steady-state*, *Transient*, and *Transient with heat source from Steady-state*). It is also available with *Steady-state* calculation types **Heat Source Calibration**, **Batch**, and **Grid**.

The **3D Plot** type has its own tab on both the **Plot Renderer Configuration** window and the **Visualizations** window. This plot type is further visualized using additional **Display** options.

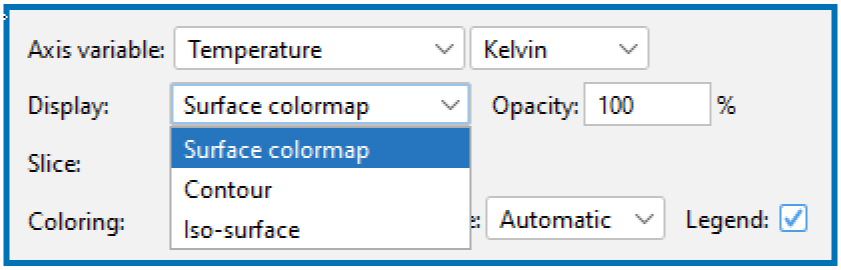
Further, when connecting two AM Calculators to plot combinations of axis variables, separate tabs are added to the **Visualizations** window that have a suffix of the name of the AM Calculator added in brackets, e.g. **3D Plot (AM Calculator 1)**. It is recommended that the AM Calculator is renamed to help you identify which tab belongs to which calculation.

See Overlaying Plots in the AM Module for more details and AM Plot Type: Thermal Gradient vs. Solidification Rate for an example.

3D Plot Display Options

The **Display** options available are also based on the **Axis variable** selected. The **Slice** plot, which is a unique type of plot, is also available when either **Surface colormap** or **Contour** is selected.

Surface colormap, Contour, and Iso-surface are available when **Temperature**, **Surface tension**, **Thermal conductivity**, or **Dynamic viscosity** is selected as an *Axis variable*.



Axis variable: Temperature Kelvin

Display: Surface colormap

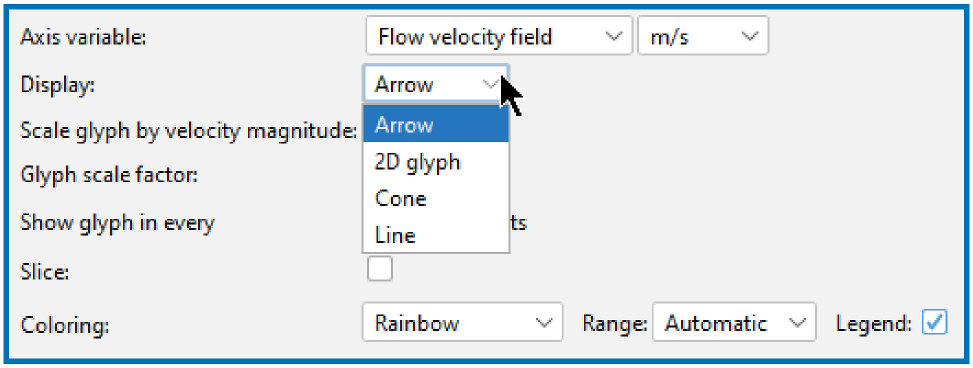
Opacity: 100 %

Slice:

Coloring: Automatic

Legend: ☑

Arrow, 2D Glyph, Cone, or Line are available when **Flow velocity field** is selected as an *Axis variable*. It also requires that the **Fluid flow including Marangoni effect** checkbox is also selected on the **AM Calculator**.



Axis variable: Flow velocity field m/s

Display: Arrow

Scale glyph by velocity magnitude:

Glyph scale factor:

Show glyph in every ts

Slice: ☐

Coloring: Rainbow Range: Automatic Legend: ☑

Examples

Surface Colormap

This is an example from AM_01: Transient Simulation of a Single Track.

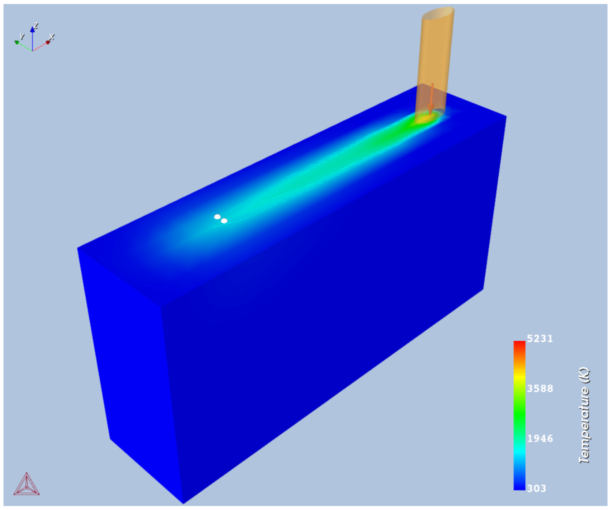


Figure 1: Surface plot of temperature distribution after the single track scan is completed. Probes P1 and P2 can also be seen on the top surface.

Slice Plot

This is an example from AM_01: Transient Simulation of a Single Track.

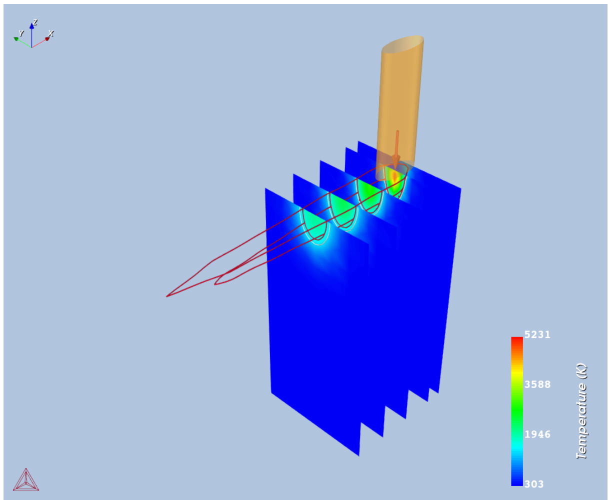
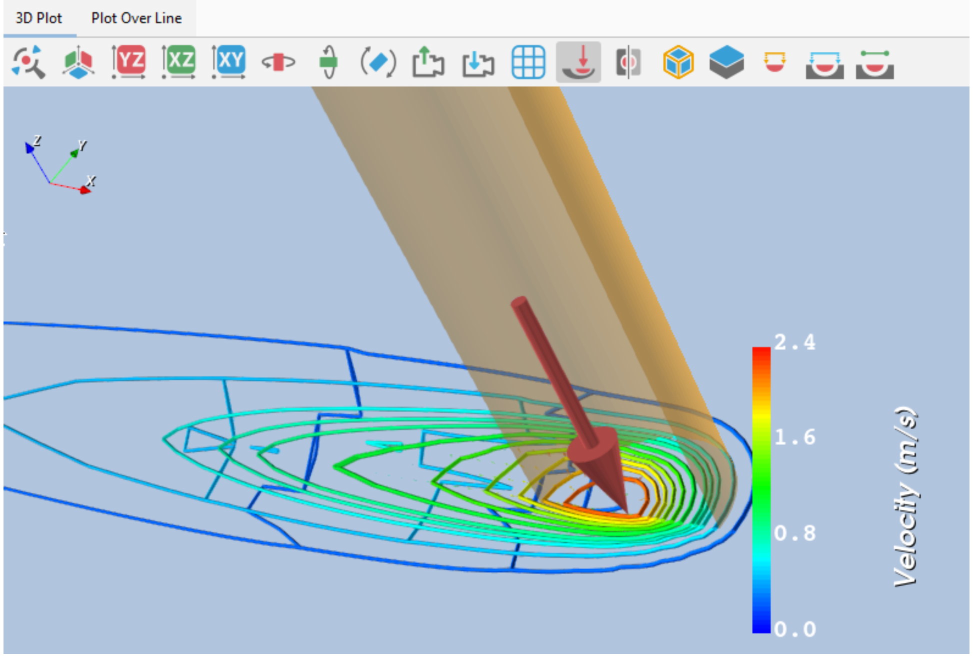


Figure 2: Slices of the computational domain, orthogonal to the scanning direction, showing temperature distribution at different cross-sections. Red tubes show the contour of the melt pool (at liquidus temperature).

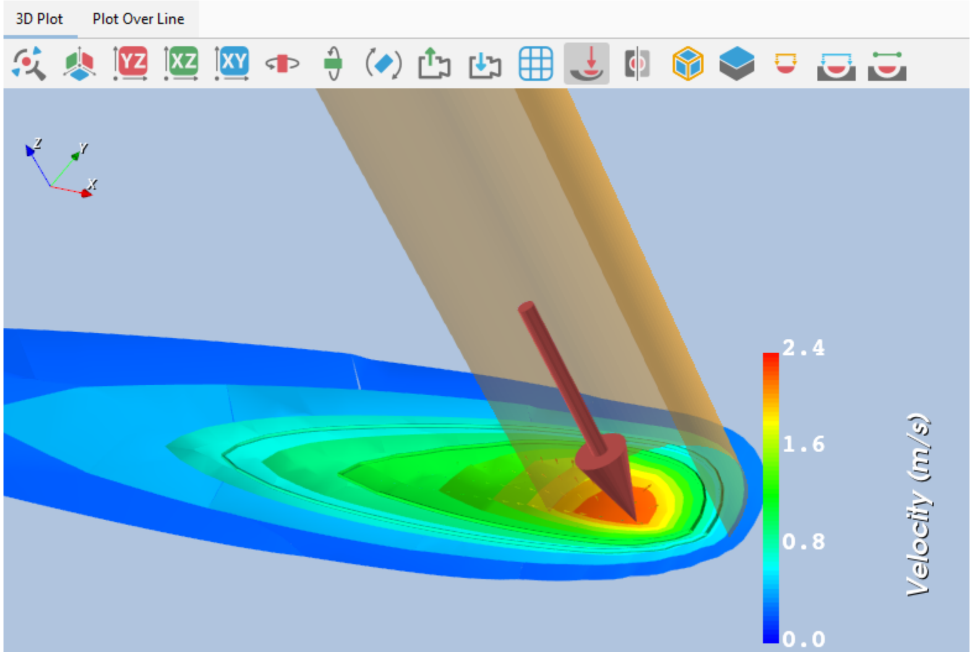
Contour

This is an example using AM_03: Steady-state Simulations to zoom into the **AM Calculator**, which in that example is renamed to **Gaussian HS, with Fluid**. On the **Plot Renderer**, the **Display** setting is changed from the default to **Contour**.



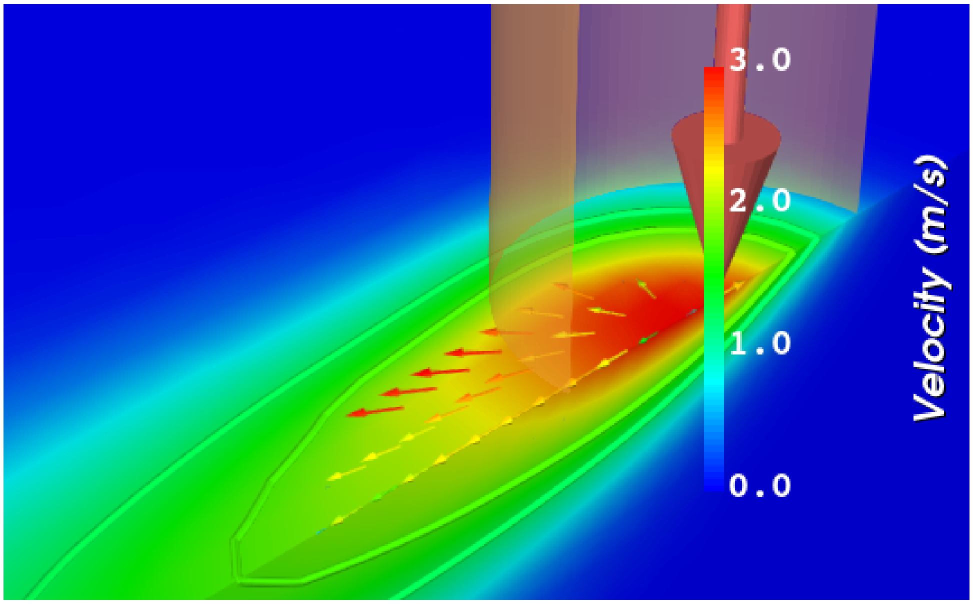
Isosurface

This is an example using AM_03: Steady-state Simulations to zoom into the **AM Calculator**, which in that example is renamed to **Gaussian HS, with Fluid**. On the **Plot Renderer**, the **Display** setting is changed from the default to **Iso-surface**.



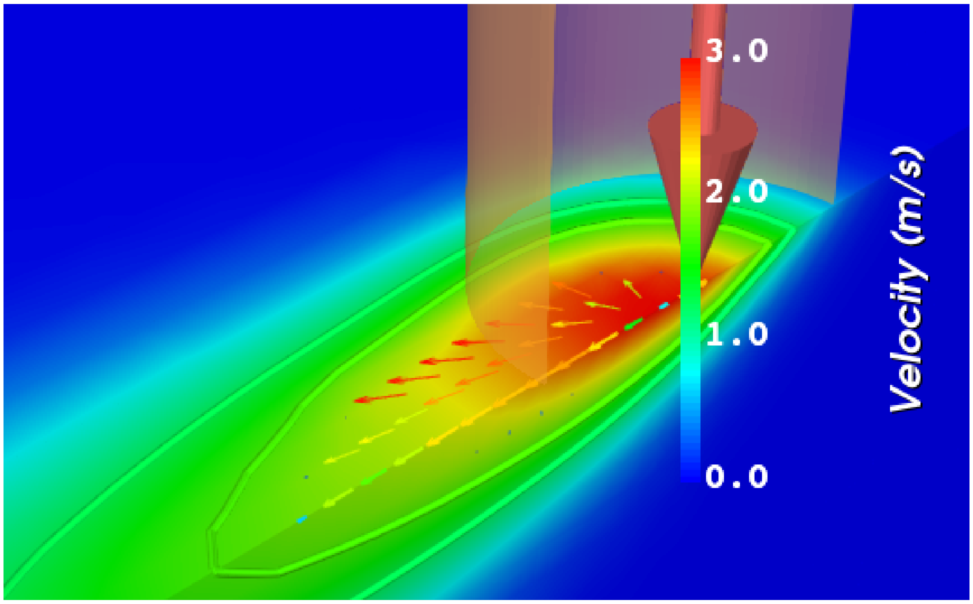
Arrow

This is an example using AM_04: Scheil Transient Steady-stateto zoom into one of the AM Calculators, which in this case is renamed to **Steady-state**. On the **Plot Renderer**, and when the *Axis variable* is set to **Flow velocity field**, the **Display** default setting is **Arrow**.



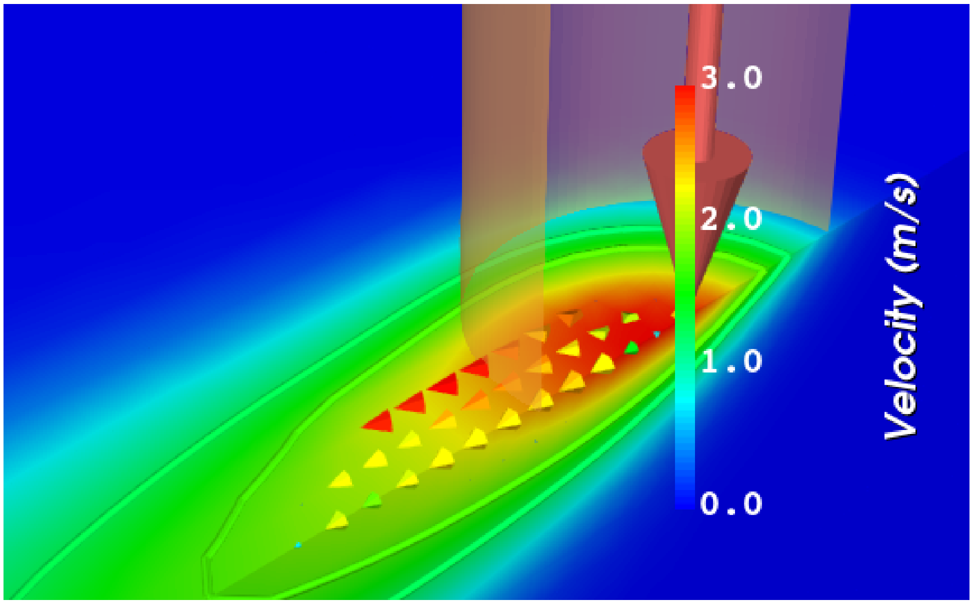
2D Glyph

This is an example using AM_04: Scheil Transient Steady-state to zoom into one of the AM Calculators, which in this case is renamed to **Steady-state**. On the **Plot Renderer**, and when the *Axis variable* is set to **Flow velocity field**, the **Display** setting is changed from the default to **2D Glyph**.



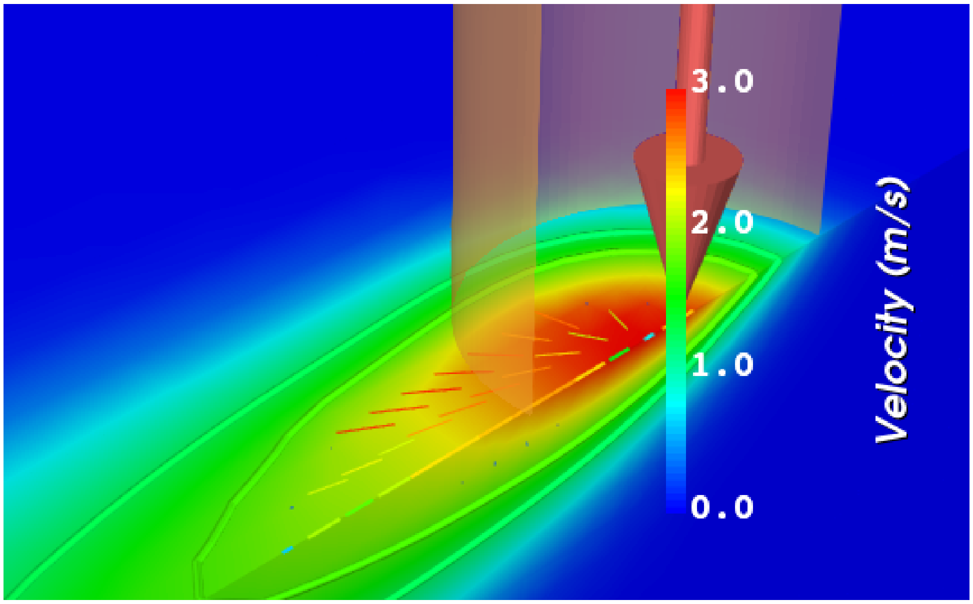
Cone

This is an example using AM_04: Scheil Transient Steady-state to zoom into one of the AM Calculators, which in this case is renamed to **Steady-state**. On the **Plot Renderer**, and when the *Axis variable* is set to **Flow velocity field**, the **Display** setting is changed from the default to **Cone**.



Line

This is an example using AM_04: Scheil Transient Steady-state to zoom into one of the AM Calculators, which in this case is renamed to **Steady-state**. On the **Plot Renderer**, and when the *Axis variable* is set to **Flow velocity field**, the **Display** setting is changed from the default to **Line**.



AM Plot Type: Plot Over Line (2D)

The **Plot Over Line** plot type is available with all simulation types (**Steady-state**, **Transient**, and **Transient with heat source from Steady-state**). For Steady-state simulations, it is also available with **Heat Source Calibration**, **Batch**, and **Grid** calculation types.

The **Plot Over Line** type is a 2D plot. On the **Visualizations** window it is available on the **Plot Over Line** tab and on the **Configuration** window on the tab of the same name.

Once the plot is performed, you can also switch between a plot and a **Table View** using the button available on the **Visualizations** window.

> The coordinates for the **Plot Over LineTransient with heat source from Steady-state** and its **Steady-state** model are synchronized. This means that if you switch between these computational models, the **Plot Over Line** coordinates show the same result.

Example

This is an example from AM_01: Transient Simulation of a Single Track.

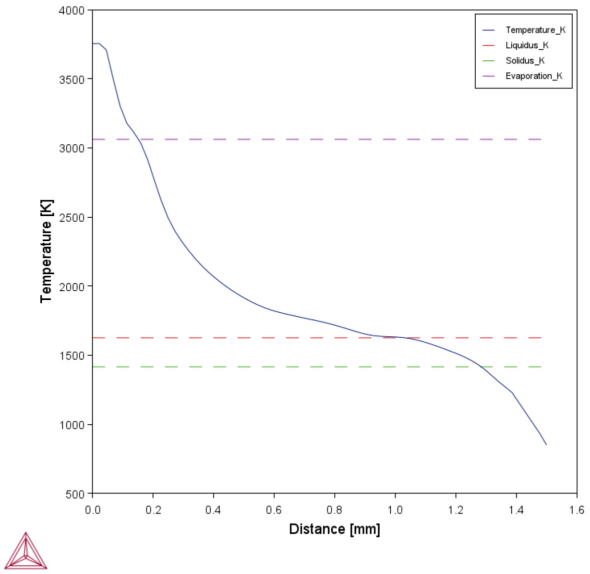


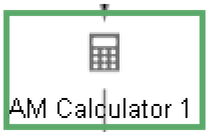
Figure 3: 2D plot over line showing temperature in the tail of the melt pool as a function of distance plotted along the scanning track.

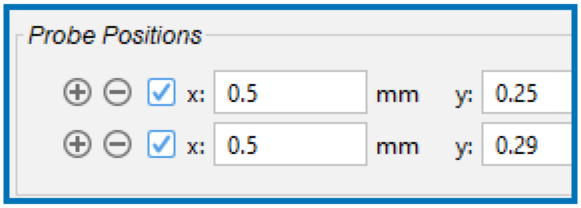
AM Plot Type: Probe (2D)

The **Probe** plot type is available with the **Transient** and **Transient with heat source from Steady-state** simulation types.

The **Probe** plot type is a 2D plot. On the **Visualizations** window it is available on the **Probe** tab and on the **Configuration** window on the tab of the same name.

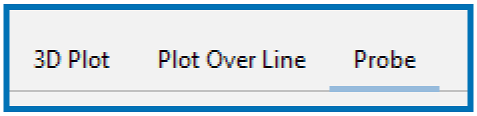
To define a Probe plot requires that *Probe Positions* are selected on the **AM Calculator**. Then when a **Plot Renderer** is added as a successor, a **Probe** tab is available on the **Configuration** window where you can further define the plot.




Probe Positions

⊕ ⊖ ☑ x: 0.5 mm y: 0.25

⊕ ⊖ ☑ x: 0.5 mm y: 0.29



Once the plot is performed, you can also switch between a plot and a **Table View** using the button available on the **Visualizations** window.

Probe data can also be used with the Diffusion Calculator and Precipitation Calculator when these Calculators are added as successors to the AM Calculator.

Example

The example below is taken from AM_01: Transient Simulation of a Single Track.

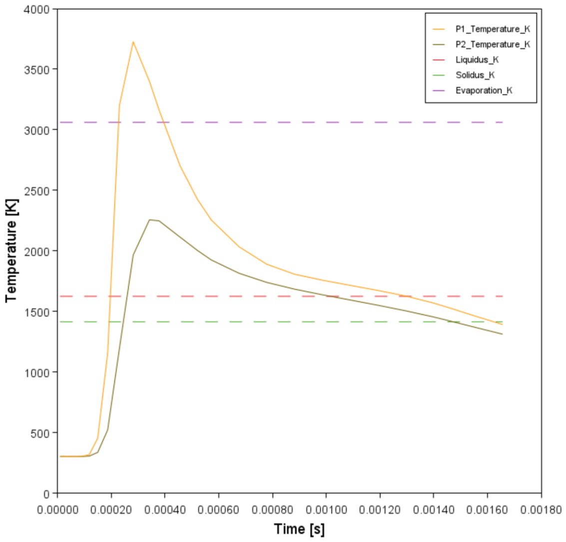


Figure 4: 2D probe plot showing temperature evolution as a function of time at probes P1 and P2.

For use of probe data with the Diffusion Module (DICTRA) see AM_05: Using AM Calculator Probe Data with the Diffusion Module (DICTRA).

For use of probe data with the Precipitation Module (TC-PRISMA) see AM_12: Using AM Calculator Probe Data with the Precipitation Module (TC-PRISMA).

AM Plot Type: Heat Source Calibration Parameters

The **Heat Source Calibration Parameters** plot type is available with a **Steady-state** simulation and when **Heat Source Calibration** is selected as the *Calculation Type*.

During the set up, the **Heat Source Calibration Parameters** type also has its own tab called **Heat Source Calibration** on the **Plot Renderer Configuration** window. For more information see Visualizing Heat Source Calibrations.

About Heat Source Calibration

Example

The following is from AM_06a: Calibrating a Heat Source for a 316L Steel.

Also see the companion example, AM_06b: Using the Calibrated Heat Source for a 316L Steel.

A **Heat Source Calibration Parameters** plot shows the calibrated heat source parameters as a function of energy density (P/v) (unit J/mm). From the **Plot Renderer Configuration** window, you can also continue to select which experiments to be used to fit the calibration.

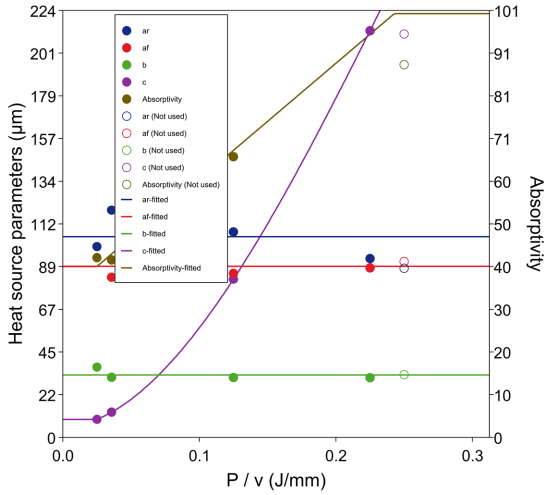


Figure 5: From example AM_06a, the Heat Source Calibration Parameters plot for the double ellipsoidal calibration.

For instance, you can deselect the points that seem to be outliers or where the error bar in experimental data is large.

AM Plot Type: Melt Pool Dimensions

The **Melt Pool Dimensions** plot type is available with a **Steady-state** simulation and when **Heat Source Calibration** is selected as the *Calculation Type*. For more information see Visualizing Heat Source Calibrations.

About Heat Source Calibration

Example

The following is from AM_06a: Calibrating a Heat Source for a 316L Steel.

Also see the companion example, AM_06b: Using the Calibrated Heat Source for a 316L Steel.

A **Melt Pool Dimensions** plot shows melt pool size, both from experiments and simulations, as a function of energy density (P/v). This plot can be used to compare the results from the experiments and optimization simulations.

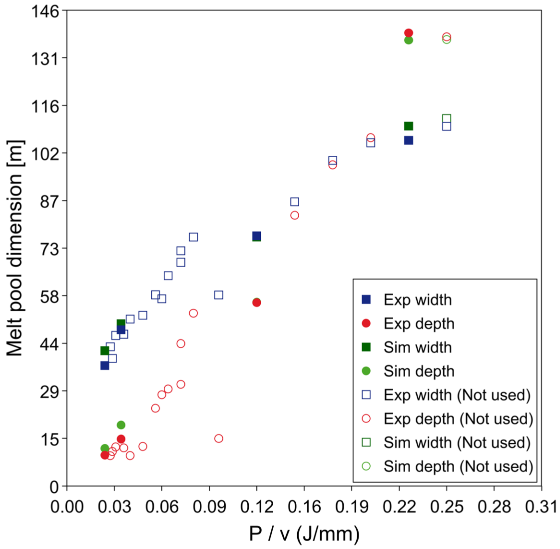


Figure 6: From example AM_06a, the Melt Pool Dimensions plot for the double ellipsoidal calibration.

AM Plot Type: Printability Map

This topic describes the plot type **Printability Map**, which is available with **Batch** or **Grid** calculations for a *Steady-state* simulation. A printability map is also known as a process map.

This plot is available with **Batch** and **Grid** calculations. However, using it with the **Grid** calculation is the preferred method as it provides full coverage of the plot area. Otherwise, if you are doing a **Batch** calculation and only base it on experimental conditions, it often leaves out the most extreme cases so you get areas in the Printability Map that are blank.

Printability maps allow you to plot the likelihood of three possible defects that occur during additive manufacturing: *Keyholing*, *lack of fusion*, and *balling*.

There is a video tutorial about the **Printability Map** on our website and on our YouTube channel. It is also included in the Additive Manufacturing Module YouTube playlist.

These examples highlight the use of the printability map: AM_08a: Grid Calculation for a Ti64 Alloy and AM_09a: Grid Calculation for an SS316L Alloy.

These defects occur based on the speed and power used during the AM process. Printability maps allow you to reduce the risks of these defects by showing the speed and power settings that are optimal, which in turn allows you to calibrate your system to avoid these issues.

- *Keyholing* occurs with low scanning speed and high power.
- *Lack of fusion* occurs with high scanning speed and low power.
- *Balling* occurs if you increase the scanning speed.

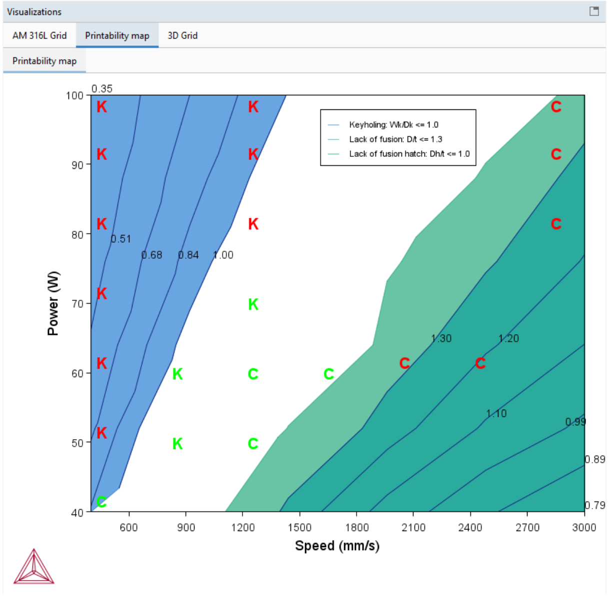


*Figure 7: Printability map for 316L showing regions of keyholing and lack-of-fusion. Experimental information from Hu et. al. [2019Hu] overlaid as coloured labels showing keyhole porosity (**K**), conduction mode with lack-of-fusion porosity (**C**). Green labels showing experiments without defects for conduction mode (**C**) and keyhole mode (**K**).*

The defect regions in the printability maps are defined by functions of the keyhole dimension (Wk, Dk), melt pool dimensions (W, D, L), hatch distance (h), and powder thickness (t) [2019Joh].

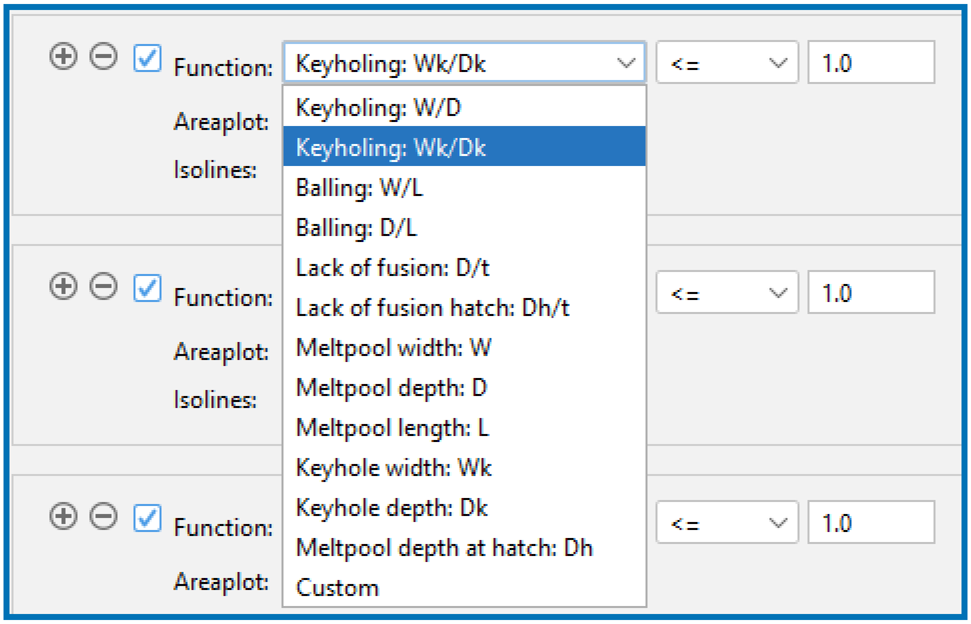


Figure 8: When defining the Printability map on the Plot Renderer for an AM Calculator, you can select from a variety of Functions.

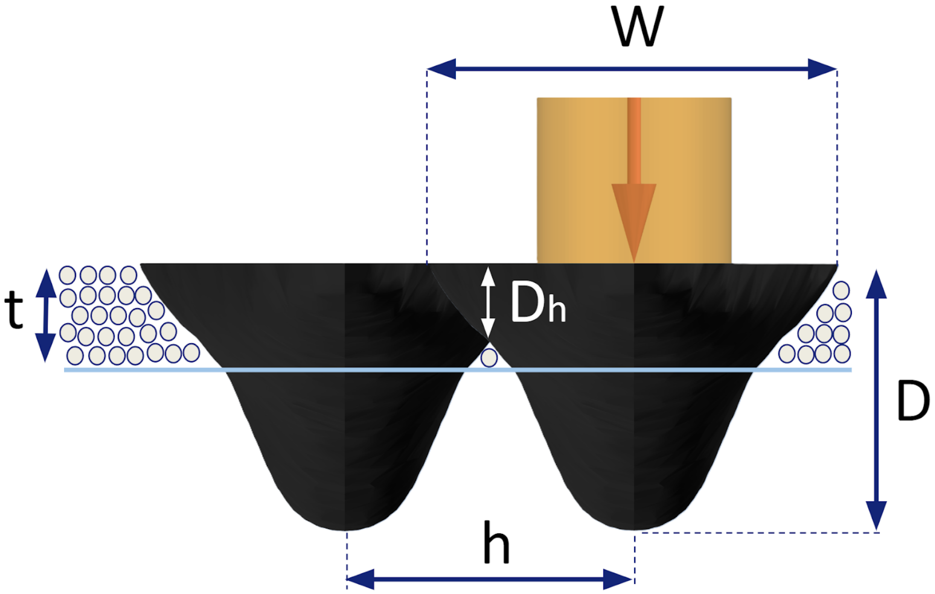


Figure 9: Two single tracks with the melt pool width (W) and depth (D). The hatch distance (h), powder thickness (t), and the melt pool depth at half of the hatch distance (Dh).

Keyholing Porosity

Keyholing is a critical feature in additive manufacturing that occurs at high energy densities (P/v). Keyholing is not only negative, the increased depth of the melt pool can increase productivity. However, deep and narrow keyholes are unstable and can collapse, and lead to keyholing porosity. Keyhole porosity appears close to spherical in shape.

Keyholing porosity can be defined to occur if the width/depth ratio of the keyhole is less than or equal to 1 (i.e. $W_k/D_k \leq 1$). Similarly if a volume heat source is used (that lacks information of the keyhole geometry) the ratio of the melt pool (W/D) can be used instead, where $W/D \leq 1$.

Lack of Fusion

Lack of fusion porosity occurs if the melt pool, due to low energy density (P/v), fails to penetrate the powder thickness. Lack of fusion gives porosity uneven in shape, compared to keyhole porosity that is close to spherical in shape.

Lack of fusion for a single track can be defined to occur if the melt pool depth is smaller than the powder thickness, i.e. $D/t < 1.0$. Additionally the lack of fusion between two tracks, at half of the hatch distance, can be defined to occur if $D_h/t < 1.0$.

Balling

The scan tracks can break up and produce agglomerated particles in spherical shape instead of a single bead. Balling has been defined to occur if ratios W/L [2019Joh] or D/L [2023Kat] are small .

Additional user-defined defect criteria can be defined with the Custom function using any combination of the keyhole dimension (Wk, Dk), melt pool dimensions (W, D, L), hatch distance (h) and powder thickness (t).

References

[2019Hu] Z. Hu, B. Nagarajan, X. Song, R. Huang, W. Zhai, J. Wei, Formation of SS316L Single Tracks in Micro Selective Laser Melting: Surface, Geometry, and Defects. Adv. Mater. Sci. Eng. 2019, 1–9 (2019).

[2019Joh] L. Johnson, M. Mahmoudi, B. Zhang, R. Seede, X. Huang, J. T. Maier, H. J. Maier, I. Karaman, A. Elwany, R. Arróyave, Assessing printability maps in additive manufacturing of metal alloys. Acta Mater. 176, 199–210 (2019).

[2023Kat] J. Katagiri, M. Kusano, S. Minamoto, H. Kitano, K. Daimaru, M. Tsujii, M. Watanabe, Melt Pool Shape Evaluation by Single-Track Experiments and Finite-Element Thermal Analysis: Balling and Lack of Fusion Criteria for Generating Process Window of Inconel738LC. Materials (Basel). 16, 1729 (2023).

AM Plot Type: Parity Plot

This topic describes the plot type **Parity Plot** which is available with Batch calculations for a Steady-state simulation. This plot type is only to select on the Plot Renderer when the simulation uses the **Batch** *Calculation Type* with an **AM Calculator**.

These examples highlight the use of this plot: AM_07: Batch Calculations for an IN718 Alloy, AM_08b: Batch Calculations for a Ti64 Alloy and AM_09b: Batch Calculations for an SS316L Alloy.

Parity plots are used when validating the Steady-state Batch calculation against experimentally measured melt pool width and depth. The plot shows the experimental width/depth on the X-axis and the calculated width/depth on the Y-axis. The data should follow the diagonal line for a perfect match between the calculated and experimental values.

The following are from example AM_07.

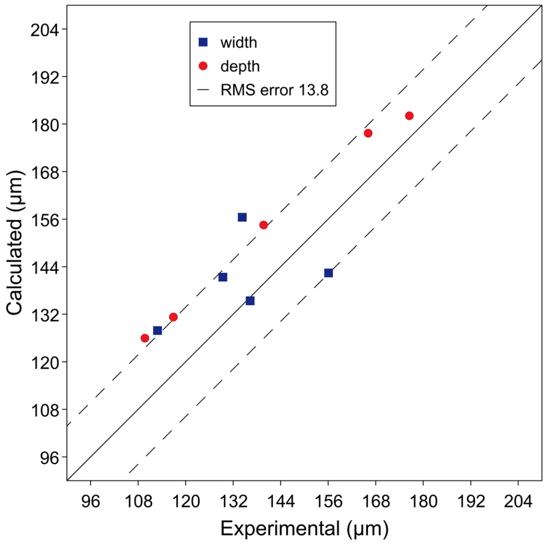
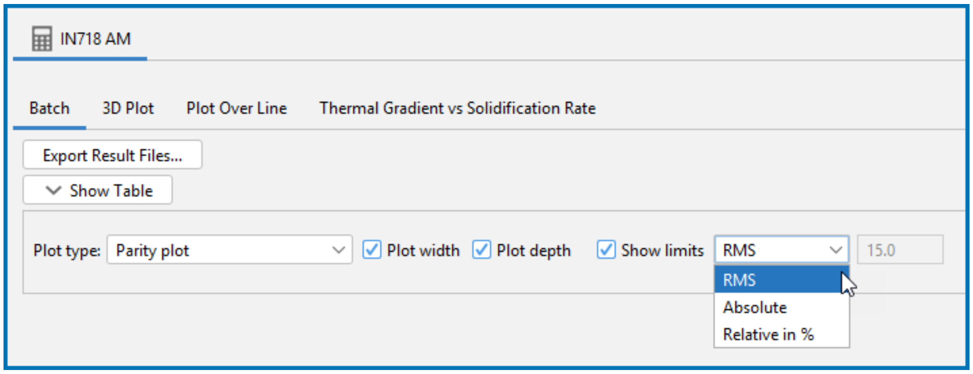


Figure 10: Parity plot comparing experimental versus calculated melt pool width and depth for all the experiments. The experiments are single tracks on bare plate IN718 with varied power and scan speed. The Root Mean Square (RMS) error can also be shown as a dashed line.



IN718 AM

Batch | 3D Plot | Plot Over Line | Thermal Gradient vs Solidification Rate

Export Result Files...

Show Table

Plot type: Parity plot ☑ Plot width ☑ Plot depth ☑ Show limits RMS 15.0

Figure 11: Alternatively, lines for user-defined Absolute or Relative in % error can be shown instead by selecting these options on the Configuration window.

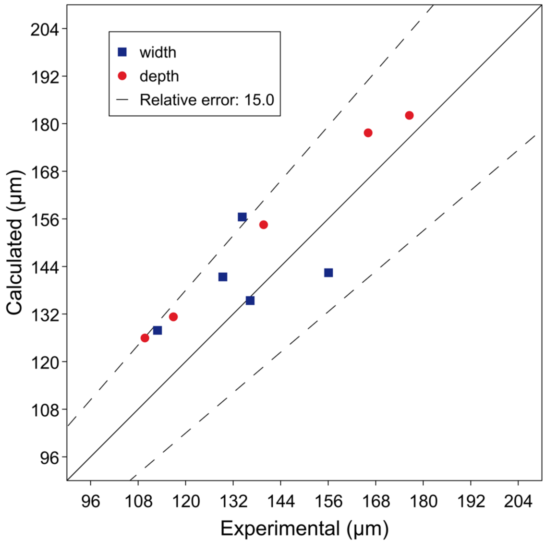


Figure 12: Parity plot comparing experimental versus calculated melt pool width and depth for all the experiments. The experiments are single tracks on bare plate IN718 with varied power and scan speed. In this plot, it is configured to show a Relative in % error of 5 instead of the RMS error.

Keyhole Model with Fluid Flow

This is an example application of using the parity plot when the keyhole model includes fluid flow, which can provide a better prediction of the melt pool size.

About the Keyhole Model

Keyholing can occur with low scanning speed and high power. Including fluid flow in the simulation makes the predictions of the entire melt pool size more accurate, which is especially important at higher energy densities when Marangoni forces are strong.

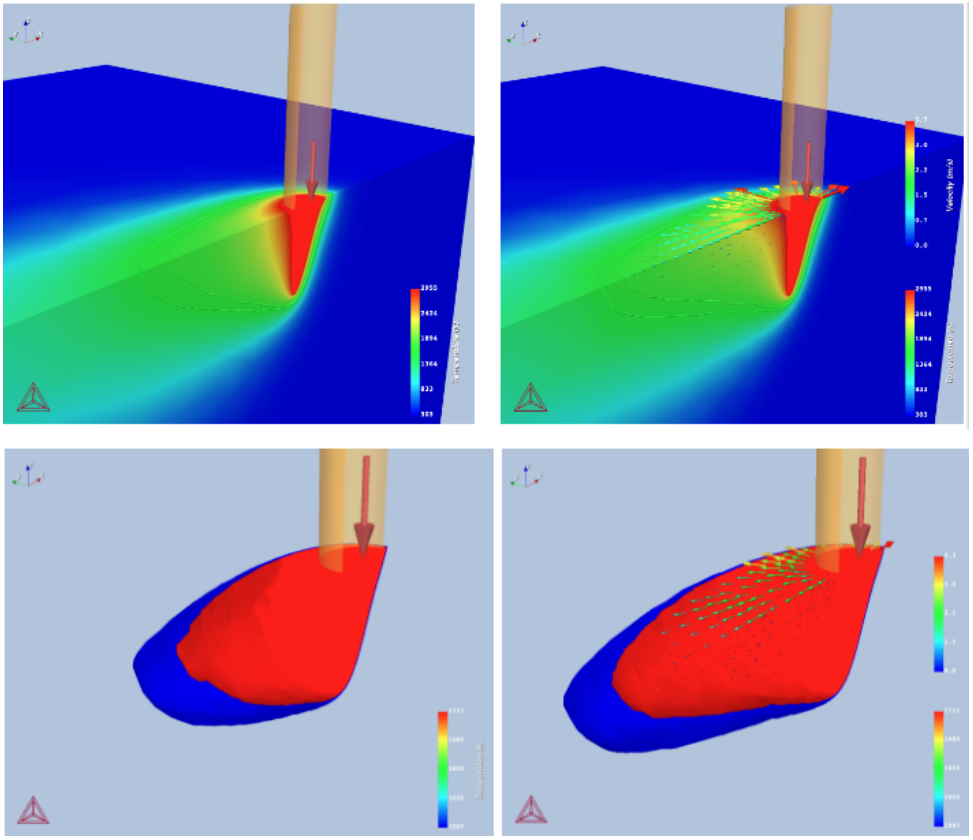


Figure 13: Fluid flow can make the melt pool wider and longer. This example shows the effect when enabling fluid flow for 316L for power 50 W and scan speed 400 mm/s. Left images show without fluid flow and right images with fluid flow enabled. Top row shows the temperature color map. Bottom row shows the isosurfaces for liquidus and solidus, i.e. the size of the melt pool and mushy zone.

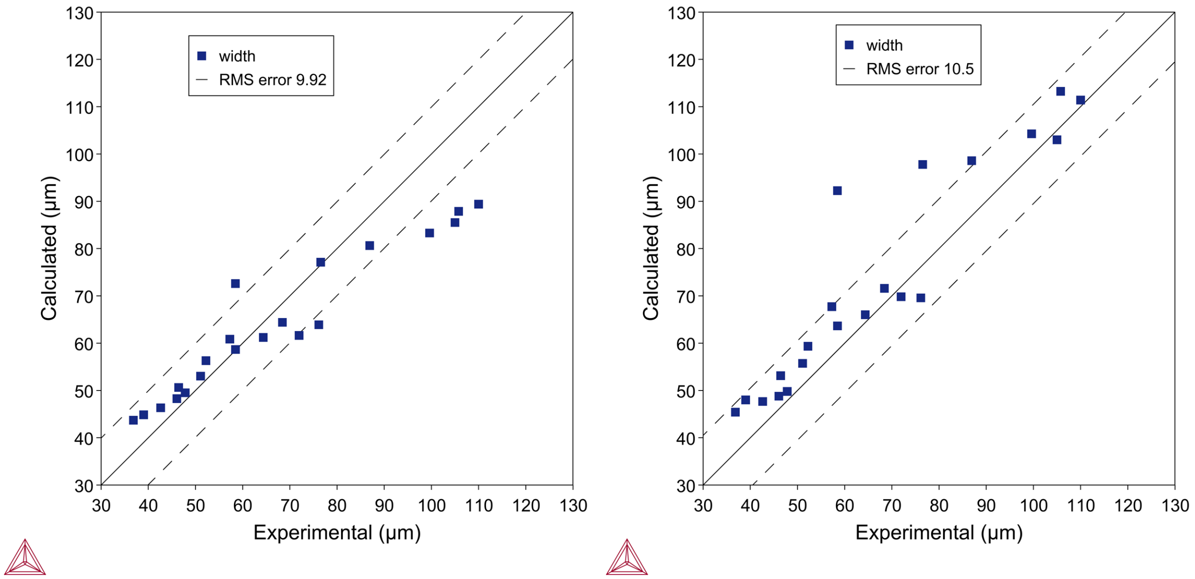


Figure 14: Parity plot for 316L showing how the RMS is reduced for the melt pool width when excluding fluid flow (left) compared to when it is included (right). Experiments from Hu et. al [2019Hu].

Reference

[2019Hu] Z. Hu, B. Nagarajan, X. Song, R. Huang, W. Zhai, J. Wei, Formation of SS316L Single Tracks in Micro Selective Laser Melting: Surface, Geometry, and Defects. Adv. Mater. Sci. Eng. 2019, 1–9 (2019).

AM Plot Type: Melt Pool vs Energy Density

This topic describes the plot type **Melt Pool vs Energy Density** which is available with **Batch** or **Grid** calculations for a *Steady-state* simulation.

These examples highlight the use of this plot: AM_08b: Batch Calculations for a Ti64 Alloy and AM_09b: Batch Calculations for an SS316L Alloy.

This plot type is used when validating the Steady state Batch calculation against experimentally measured melt pool width and depth. The plot shows the experimental and simulated melt pool dimensions as a function of the energy density (P/v). The plot type can also be used when experimental melt pool dimension are lacking, e.g. after the Grid calculation, but then naturally only shows the simulated melt pool dimensions as a function of the energy density (P/v).

This uses example AM_09b.

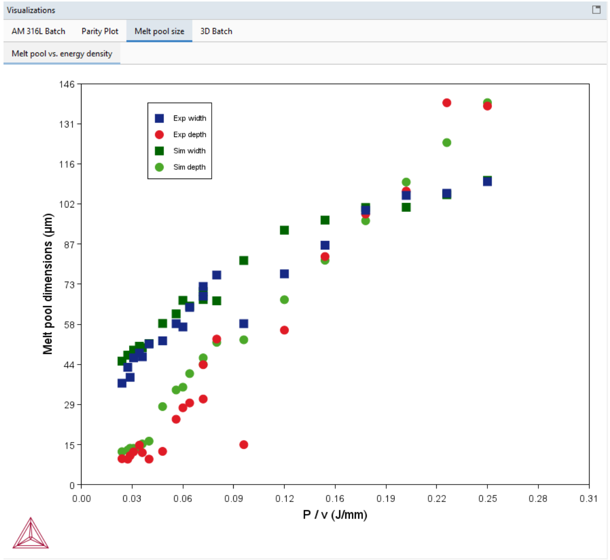
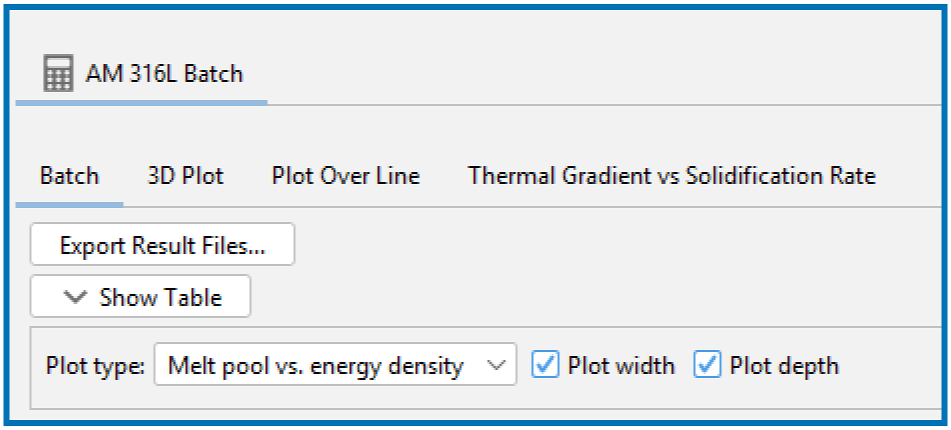


Figure 15: Plot comparing experimental versus calculated melt pool dimensions for all the Batch calculations. The experiments are single tracks with SS316L with varied power and scan speed. The melt pool width and depth are shown on the Y-axis and the energy density (P/v) on the X-axis.



Plot type: Melt pool vs. energy density ☑ Plot width ☑ Plot depth

Figure 16: For the plot, you can choose what to include on the plot, to show width and/or depth by selecting the relevant checkboxes on the Configuration window.

AM Plot Type: Thermal Gradient vs. Solidification Rate

This topic describes 2D and 3D versions of plots comparing *thermal gradient* to *solidification rate* along the liquid isotherm. Both the 2D and 3D versions are available for steady-state and transient simulations.

- The 2D version is accessed on the **Plot Renderer Configuration** window as a tab named **Thermal Gradient vs Solidification Rate**. It is visualized on a tab of the same name on the **Visualizations** window.
- The 3D version is available on the **3D Plot** tab on the **Configuration** (settings) window. It is further visualized on two **3D Plot** tabs on the **Visualizations** window.

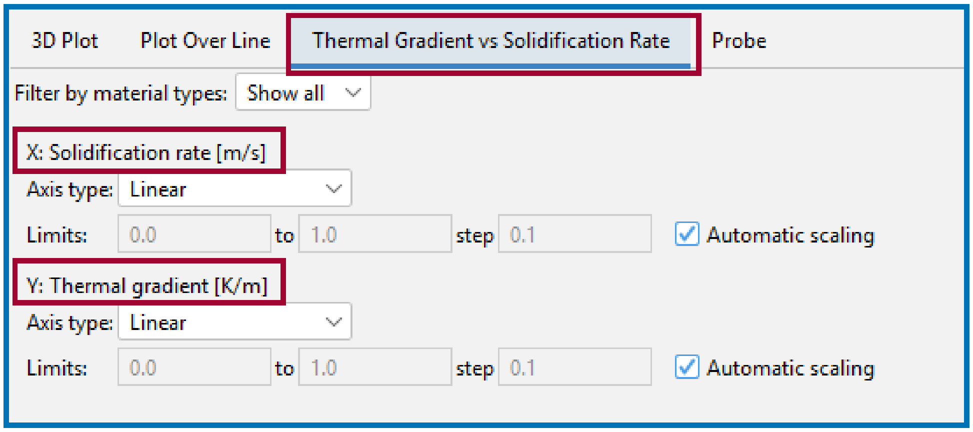
AM_10: CET Transition in an IN718 Alloy includes an example of this plot in both 2D and 3D.

2D Plot

The 2D version of this plot is available on the **Thermal Gradient vs Solidification Rate** tabs on both the **Configuration** (settings) and **Visualizations** window.

You do not need to configure anything on the **AM Calculator** to access the 2D plot.

On the **Thermal Gradient vs Solidification Rate** tab on **Plot Renderer Configuration** window you can adjust the settings for the **Solidification rate** (X-axis) and **Thermal gradient** (Y-axis).



Filter by material types: Show all

X: Solidification rate [m/s]

Axis type: Linear

Limits: 0.0 to 1.0 step 0.1 ☑ Automatic scaling

Y: Thermal gradient [K/m]

Axis type: Linear

Limits: 0.0 to 1.0 step 0.1 ☑ Automatic scaling

As you adjust settings, watch it dynamically change on the **Visualizations** window. The plot is on the tab of the same name (**Thermal Gradient vs Solidification Rate**). You can switch between the plot and a table format using the **Table View** button.

AM Plots: Table View Options

This uses example AM_10.

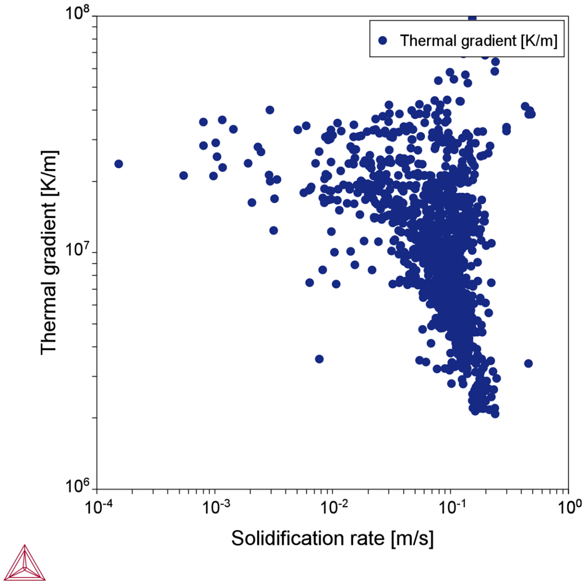
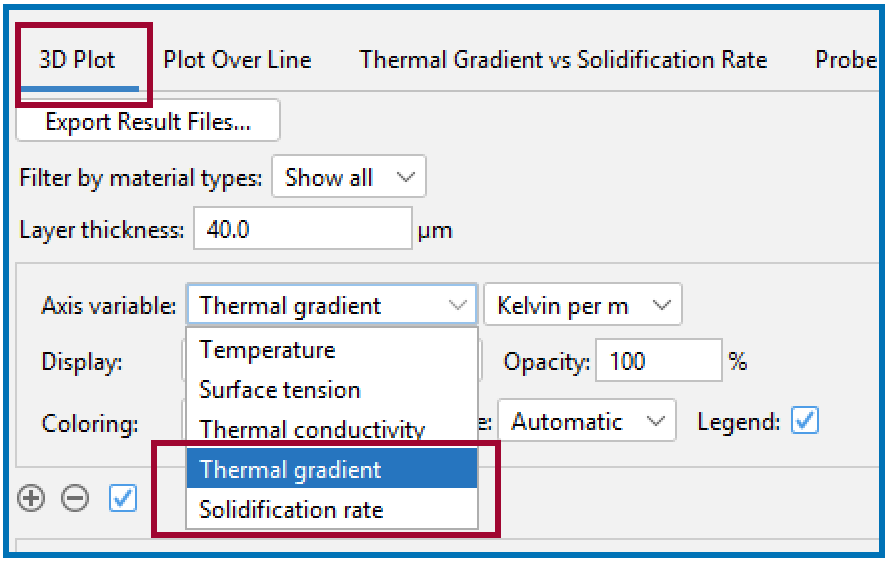


Figure 17: The solidification rate vs thermal gradient is shown on the AM Thermal Gradient & Solidification Rate Plot Renderer.

3D Plot

The 3D version of this plot is available on the **3D Plot** tab on the **Configuration** (settings) window. You choose **Solidification rate**and **Thermal gradient** as the **Axis variable**. Use the ⊕ and ⊖ buttons as usual to add and remove quantities.



Filter by material types: Show all

Layer thickness: 40.0 µm

Axis variable: Thermal gradient Kelvin per m

Opacity: 100 %

Automatic

Legend: ☑

On the **Visualizations** window the comparisons for the different calculation types and variable combinations are plotted on two **3D Plot** tabs.

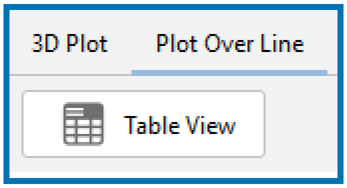
AM Plots: Table View Options

There are ways to view AM plot results as a table on either the **Configuration** or **Visualization** windows for various plots and calculation types.

2D Plots

For 2D plots (**Plot Over Line**, **Probe**, and **Thermal Gradient vs Solidification Rate**), and once the plot is performed, you can switch between a plot and a table by clicking the **Table View** button on the **Visualizations** window.

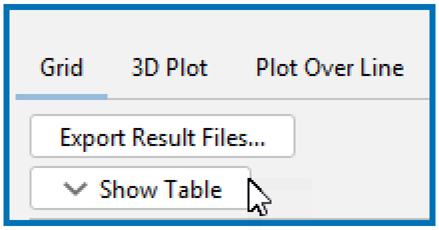
These plots are available with all calculation types (*Steady-state*, *Transient*, and *Transient with heat source from Steady-state*) simulations.

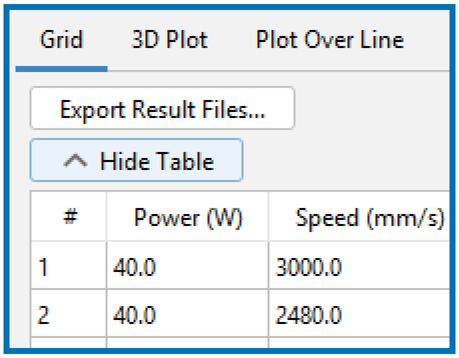


Batch and Grid Plots

For *Steady-state* **Batch** and **Grid** calculations, the available plots **Printability map**, **Meltpool vs energy density**, and **Parity plot**, can also be viewed as a table.

Once the plot is performed, you can toggle to between **Show Table** and **Hide Table** on the **Configuration** window.





#	Power (W)	Speed (mm/s)
1	40.0	3000.0
2	40.0	2480.0

Additive Manufacturing Workflow

In this section:

Setting Up the Additive Manufacturing Simulation

Setting up an Additive Manufacturing (AM) Module simulation can be done in one of two workflows.

General Overview

The general procedure of a simulation using the Additive Manufacturing Module is the following:

1. Define the system (Workflow 1 only):
    a. Choose a database.
    b. Select elements and composition.
2. Retrieve the materials data (Workflow 1 or 2):
    a. Either with a Scheil calculation (Workflow 1) or using the materials property data library (Workflow 2).
    b. Apply data smoothing.
3. Set up the AM Calculator (Workflow 1 or 2):
    a. Choose a simulation mode *Steady-state*, *Transient*, or *Transient with heat source from Steady-state*.
    b. For *Steady-state* you can also choose different *Calculation Type* options such as a *Heat Source Calibration* to calibrate a heat source based on the provided experimental data instead of using just a *Single point* calculation. *Batch* and *Grid* types are also available.
    c. For *Steady-state* or *Transient with heat source from Steady-state* simulations plus a Gaussian, Core-ring, or Top-hat heat source, choose to include a *keyhole model* with or without *fluid flow*.
    d. Set the simulation conditions.
4. Run the simulation and visualize the results (Workflow 1 or 2) based on the settings, for example:
    a. *3D Plot*
    b. *Plot Over Line* or *Thermal Gradient vs Solidification Rate* (2D). Once the plot is performed you can also switch to view it in a table.
    c. *Probe* 2D plot at a probe position (only available for transient calculations). You can also use and plot probe data with the Add-on Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA). Once the plot is performed you can also switch to view it in a table.

d. *Heat Source Calibration Parameters* and *Melt Pool Dimensions*: These plots are available for Heat Source Calibration calculations.

e. *Printability Map*, *Parity Plot*, and *Melt Pool vs Energy Density*: These plots are available for Batch and Grid calculations. This can also be viewed as a table.

Workflow 1: When You Need to Obtain the Material Properties Data for the Calculation

Use a System Definer and Scheil Calculator to extract some Scheil data, then feed the data into the AM Calculator. Then add the Plot Renderer to define the specific AM Calculator Plot Renderer features and visualize the results. In this workflow, you can also save the results from the Scheil Calculator into the Material Library and reuse this data in the future.

When you also have licenses either for the Diffusion Module (DICTRA) and/or the Precipitation Module (TC-PRISMA), for transient simulations you can additionally include probe data from the AM Calculator in the set up of the thermal profile for diffusion and precipitation calculations, respectively.

Workflow 2: When You Already Have the Material Properties Data Available - Material Library

When you know you have the available material library data available, either by using the provided libraries, importing your own external data, or by saving your own material library after running a Scheil calculation, then you can directly start defining the AM Calculator and add and define one or more plots to visualize the results.

The Scheil Calculator and System Definer function the same as with a regular Thermo-Calc simulation. There are features available on the Scheil Calculator that are particularly useful to these types of calculations. The Plot Renderer is also unique to this calculator but is still based on the standard activity node.

The various activity nodes for each workflow are briefly described below.

System Definer (Workflow 1)

The first step of the set-up is to select which database to use and define the material for the simulation. This is done in the System Definer.

In a **System Definer** activity, you select the database to use to retrieve thermodynamic data and define which elements the system has as components. You can also select the species to include as well as change the reference temperature and pressure for your components.

A **System Definer** node can be added either directly to the **My Project** node or by default when the **Additive Manufacturing** template is added.

See System Definer and then to learn more about the many settings go to Configuration Window Settings.

Scheil Calculator (Workflow 1)

Once you have defined your system, you need to retrieve the materials data necessary for the AM calculations. This is done using the Scheil Calculator when you are working in Workflow 1.

A **Scheil Calculator** node can be added either directly to the **System Definer** node or by default when the **Additive Manufacturing** template is added.

ABOUT THE SCHEIL CALCULATOR SETTINGS

The Scheil Calculator in the Additive Manufacturing Module template is configured to generate the data necessary for the AM calculation. It is configured to start the simulation at a temperature of 5000 degrees and capture the evaporation and calculate the material properties down to room temperature. If you add a Scheil Calculator manually from the System Definer, you need to change these settings yourself. If you are working with different materials, different settings might be more suitable to your material.

Materials Properties Library (Workflow 1 or 2)

A Scheil calculation using the Scheil Calculator (Workflow 1) can be saved for reuse in the Materials Libraries. Alternatively, if there is external data available to use, you can skip the Scheil Calculator and just use a library (Workflow 2). There are also some predefined materials libraries included with the installation that can be used, and are used, in the examples (e.g. AM_01, AM_02, and AM_03 and others) so that users without an AM license and necessary databases can see how this works.

Available Options

AM Calculator (Workflow 1 or 2)

Add an **AM Calculator** node to the Scheil Calculator. If you used the **Additive Manufacturing** template (on the **My Projects Configuration** window under **Applications**), click the node to display the **Configuration** settings window.

Transient simulations currently support only cuboid geometries. Both Steady-state and Transient models use adaptive mesh refinement to decrease computational cost. You have the option to either choose from the predefined mesh settings that defines the maximum and minimum element size based on the process parameters, or specify the maximum and minimum element size yourself.

You can use this either with or without the Scheil and System Definer if you already have the materials properties calculation you want.

AM Calculator, AM Calculator Conditions Settings, and AM Calculator Heat Source Settings

CHOOSE MATERIALS DATA SOURCE

Once the Scheil simulation is complete, click on the AM Calculator 1 node and then the Materials Properties tab to see the material property data obtained from the Scheil calculation. In the Material Properties tab, you can plot the properties required for the AM simulation. This is also where you select the data source that will be used in the simulation. In the Use data from: drop-down list you can choose either Scheil Calculator or Library. The Scheil Calculator option uses the Scheil results that you just calculated, while the Library option uses the data that was shipped with the software or previously calculated data that you have saved to the Library.

Visualizations Window

Working with AM Visualizations

Apply Data Smoothing

Before you run the AM Calculator, it is important that the data you will base the AM calculation on does not have any sharp peaks or curves to be able to solve the numerical problem. To avoid this, you can apply smoothing to your data. The default setting is **Little smoothing** but this can be changed depending on your simulation.

To determine how much smoothing to apply, you can plot the different properties. In the plot drop-down list you can select which property you want to plot to check the data and if there are any sharp peaks or curves in the plot. The plot appears immediately when you select a property. It is recommended to try running the simulations with only applying **Little smoothing**. If the calculation fails, you can increase the smoothing and try again. It is also possible to apply different levels of smoothing on different properties.

Additive Manufacturing Templates

There are two templates you can use to access the Additive Manufacturing Module settings and features in Thermo-Calc.

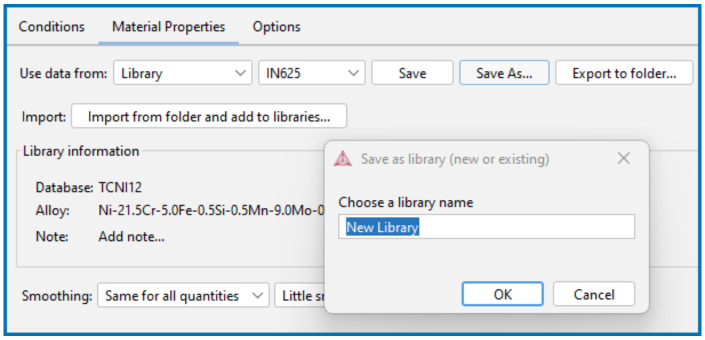
You can also add nodes individually to build your own tree.

When you also have licenses either for the Diffusion Module (DICTRA) and/or the Precipitation Module (TC-PRISMA), for transient simulations you can additionally include probe data from the AM Calculator in the set up of the thermal profile for diffusion and precipitation calculations, respectively.

Additive Manufacturing Template

On the main **Project Configuration** window, under **Applications**, click the **Additive Manufacturing** icon. This adds the following activity nodes as a tree in the Project window – **System Definer**, **Scheil Calculator**, **AM Calculator**, and **Plot Renderer**. When you add this Additive Manufacturing template (and need to generate some materials properties or do not have a material library to use), then some unique default settings for the Scheil Calculator and these particular types of simulations are already set by default. Then you continue defining the AM Calculator by choosing one of the available simulation types: Steady-state, Transient, or Transient with heat source from Steady-state.

There is also an option on the AM Calculator to save the material properties in a material library, and use these later for a new AM Calculator where you want to make calculations related to the same alloy.



Use data from: Library IN625

Import: Import from folder and add to libraries...

Library information

Database: TCNI12

Alloy: Ni-21.5Cr-5.0Fe-0.5Si-0.5Mn-9.0Mo-0

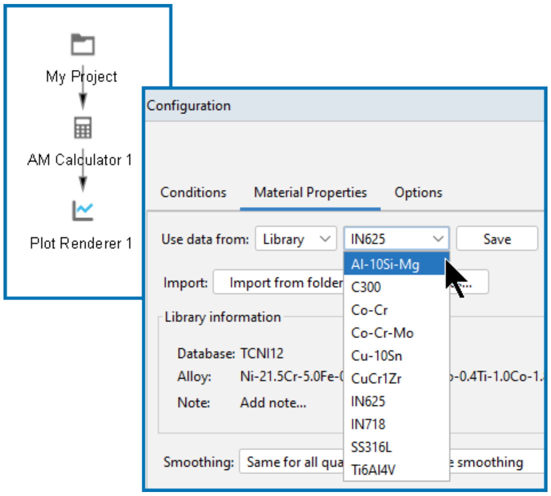
Note: Add note...

Smoothing: Same for all quantities Little s

Choose a library name: New Library

With Material Library Template

Click **With Material Library** to create an activity tree that only includes the AM Calculator and Plot Renderer nodes. The tree setup does not need the System Definer or Scheil Calculator. Instead you can select (or import) pre-saved Materials Properties data from a library and use these for your AM calculations. For example, if you have already run calculations for the Scheil Calculator for your alloy, and you want to perform a different AM calculation for the same alloy, this data can now be reused where you start the AM Calculator using the second option and use the material property data from the material library.



Use data from: Library IN625

Library information

Database: TCNI12

Alloy: Ni-21.5Cr-5.0Fe-(-0.4Ti-1.0Co-1.

Note: Add note...

Smoothing: Same for all qua smoothing

Working with the Activity Nodes for an AM Simulation

In this section:

AM Calculator

Depending how you set up your simulation, the **AM Calculator** can either be part of the workflow after a **Scheil Calculator** or directly at the root below the **My Project** node.

> There is an **Additive Manufacturing** template available under **Applications** that you can use to quickly set up either one of these workflow options for the AM simulation. See Additive Manufacturing Templates and Setting Up the Additive Manufacturing Simulation.

Configuration Window

Once you have added an AM Calculator, the **Configuration** window has these tabs where there are many available features to set on the **Conditions**, **Materials Properties**, and **Options** sections and with the specialized **Plot Renderer** and toolbar on the **Visualizations** window.

There are these simulation type pathways to choose: **Steady-state**, **Transient**, or **Transient with heat source from Steady-state**.

> In cases where convection is the dominant mode of heat transfer, fluid flow inside the melt pool plays a significant role in determining the correct shape of the melt pool.

> For more details about these see Additive Manufacturing Simulation Types. Also review the Additive Manufacturing Module Theory as needed.

- **Steady-state**: Compute temperature distribution in a steady-state environment, either on a bare metal substrate or with a powder layer on the top, with the possibility to add fluid flow inside the melt pool. For this simulation type, you can also choose the following *Calculation Types*:

  - **Single Point**, which is the standard steady-state calculation for a single set of processing parameters.
  - **Heat Source Calibration** to calibrate a heat source based on the imported or entered experimental data instead of performing a single point calculation. This is available with **Gaussian**, **Double ellipsoidal**, or **Conical** heat sources.
  - **Batch** to include power and scan speed data, which is read from a file such as a spreadsheet. You can optionally include experimental melt pool width and depth (if there is data), and compare this to the calculated results.
  - **Grid** to evaluate two axis variables of power and scanning speeds in the specified range and number of steps.

- **Transient**: Compute temperature distribution in a transient case with the given scanning strategy including multiple paths and layers and the possibility to add fluid flow inside the melt pool.
- **Transient with heat source from Steady-state**: Compute temperature distribution in a transient case with the given scanning strategy including multiple paths and layers.
  - A volume heat source is used in the transient simulations. This is based on the solution of a steady-state calculation.
- For a Gaussian, Core-ring, or Top-hat heat sources (*Steady-state* or *Transient with heat source from Steady-state*) you can also include a **Keyhole model**. This is available with or without fluid flow, or if you use separate material properties for powder.

There are several settings and these are described separately.

- AM Calculator Conditions Settings
- AM Calculator Heat Source Settings
- AM Calculator Materials Properties Settings
- AM Calculator Options Settings

Plot Renderer as a Successor

Also as a successor to the **AM Calculator**, you can right-click the node to add one or more **Plot Renderer** nodes to visualize your results. Although the node works the same as with the other calculators in Thermo-Calc, there are additional features and settings unique to this Module. Useful information is included throughout the documentation. See About the AM Plot Types and AM Calculator: Plot Renderer Settings as starting points.

When setting up an AM simulation, the **Visualizations** window shows both active configuration changes and other design states as set up on the **AM Calculator** as well as the results generated by the **Plot Renderer** calculations. There are several related topics to visualize results as well as when you are setting up the simulations. See Working with AM Visualizations as a starting point to learn more.

AM Calculator Conditions Settings

Once you have added an AM Calculator, the **Configuration** window has these settings tabs where there are many available conditions to set on the **Conditions**, **Materials Properties**, and **Options** tabs and with the specialized **Plot Renderer**.

This topic describes the available main settings on the **Conditions** tab.

AM Calculator Materials Properties Settings, and AM Calculator Options Settings

Additive Manufacturing Module Theory

Global Settings

Gas Pressure

Pressure is used to calculate the heat loss due to evaporation from the top surface of the given material.

Gas pressure: The pressure of the gas inside the build chamber. The default is 100000 **Pascal**. Select **Atmospheres** or **Bar**.

When you select a different unit the default value does not change.

Enter a different value in the field.

Temperature Unit

Temperature unit: Select a unit **Kelvin**, **Celsius**, or **Fahrenheit**.

Base Plate Temperature

If you change the **Temperature unit** then double check that the value in this field is also updated or correct as expected if you are keeping the default. This field does not update automatically when the unit changes.

Base plate temperature: The base plate of the build part is assumed to have a constant temperature. This temperature is used as a boundary condition for the base of the computational domain.

The default is 303.15 K.

Ambient Temperature

The **Ambient temperature** is used to calculate the heat loss from the top surface due to radiation, convection, and evaporation.

This setting is the temperature of the air in the immediate surrounding environment.

If you change the **Temperature unit** then double check that the value in this field is also updated or correct as expected if you are keeping the default. This field does not update automatically when the unit changes.

Fluid Flow Including Marangoni Effect

Also see the theory section, Fluid Flow and if also using the keyhole model, see About the Keyhole Model.

Choose to use **Fluid flow including Marangoni effect** if you want to calculate and include for the effect of fluid flow due to gradient of surface tension in the melt pool. The checkbox is selected by default. This solves the Navier-Stokes equation to include fluid flow inside the melt pool due to the Marangoni effect.

If you want to use separate properties for the powder layer, click to clear the checkbox to enable **Use separate material properties for powder** fields and then continue with the settings below.

Use Separate Material Properties for Powder

This option is available when the **Fluid flow including Marangoni effect** checkbox is NOT selected.

> If you want to use the keyhole model, then do not select this checkbox.

Use separate material properties for powder: Select to use different density and thermal conductivity for the powder layer; otherwise by default the same properties as for the solid are used. Then enter a **Powder density** as a percentage (0-100%) of the solid material. The default is 80 % of the solid material.

Geometry

For a **Steady-state** simulation you only need to enter the height. For **Transient** or **Transient with heat source from Steady-state** these are volumetric and you also define the width and length. For all simulation types you define the coarseness of the mesh.

Height for Steady-state Simulation

Height: Enter the build height (mm). Length and width of the computational domain is automatically chosen as a function of the heat source parameters and the scanning speed.

Height, Width, and Length for Transient Simulations

- **Height**: Enter the initial build height (mm). Powder layer(s) with the given layer thickness will be added on the top. In mm.
- **Width**: Enter the build width (along y direction). In mm.
- **Length**: Enter the build length (along x direction). In mm.

Mesh

Mesh: The initial mesh size —**Coarse**, **Medium**, **Fine**, or **Custom**. It is adaptive and refined as required.

If **Custom** is selected, enter the maximum and minimum element sizes:

- **Maximum element size:** The initial element size (in µm) in the mesh.
- **Minimum element size**: The minimum element size (in µm) that the adaptive mesh can refine to.

Heat Source

The heat source settings are described in a separate topic: AM Calculator Heat Source Settings. The theory is also described in About the Heat Source Models.

Scanning Strategy

The scanning strategy determines the build geometry for one or multiple layers. Green layer on the top of the geometry is the powder and the grey part is the solid substrate.

For **Steady-state** simulations, you only need to define the **Scanning speed** and **Layer thickness**.

Scanning Speed

Enter a **Scanning speed**, which is the velocity of the moving heat source. The default is 500 mm/s.

Layer Thickness

Enter a **Layer thickness**, which is the thickness of the powder layer. The default is 40 mm. When you change the layer thickness, the meshing size changes too.

Pattern

Select the scanning **Pattern**—**Single track**, **Bidirectional**, or **Unidirectional**.

- Select **Unidirectional** to use same scanning direction of the heat source for all tracks.
- Select **Bidirectional** to flip scanning direction of the heat source between alternate tracks.

SINGLE TRACK

- **Margin**: Offset of the laser scanning path from the sides of the computational domain. In case of Single track, offset is placed from the sides transverse to the scanning direction, whereas the scanning path is always in the middle of the domain going along the length of the workpiece.
- **Number of layers**: Enter the number of layers or scroll using the arrows.
- **Powder fill time**: Powder recoating time (unit = s) between two consecutive layers. This does not include lift time. This field is available when more than 1 is entered in the **Number of layers** field.
- **Cooling time**: Enter a cooling time (unit = s) This is the time for which the material is left to cool down after the scanning is completed. During cooling time, the heat source is completely turned off.

BIDIRECTIONAL AND UNIDIRECTIONAL

- **Margin**: Offset of the laser scanning path from the sides of the computational domain.
- **Hatch spacing**: Separation (unit = mm) between two consecutive tracks.
- **Lift time**: Time (unit = s) between two tracks where the heat source is inactive.
- **Number of layers**: Enter the number of layers or scroll using the arrows.
- **Powder fill time**: Powder recoating time (unit = s) between two consecutive layers. This does not include lift time.
- **Rotation between layers**: Rotation (unit = degrees) of the scanning direction between two consecutive layers. The scanning pattern of the first layer is always aligned to the X axis then the second layer will be rotated (if you choose this setting) with the specified angle then the next layer will be rotated at the same angle as compared to the previous layer and so on. This way you can change the rotation of the layers.
- **Cooling time**: Enter a cooling time (unit = s) This is the time for which the material is left to cool down after the scanning is completed. During cooling time, the heat source is completely turned off.

Top Boundary Conditions

Numerical Boundary Conditions in the theory section.

Radiation Emissivity

Enter a **Radiation emissivity** to include the effect of radiation from the top surface to the surrounding gas. Enter a value between 0 and 1. If you want to neglect the heat loss, then enter 0 to disable radiation.

Convective Heat Transfer Coefficient

Enter a **Convective heat transfer coefficient** for the top surface to the surrounding gas. If you want to ignore this then enter 0 to disable convective heat transfer. The default is 20 W/m^2.

Evaporation

Select the **Evaporation** checkbox to include the effect of evaporation heat loss due to heating of the powder layer or the metallic surface close to the evaporation temperature.

The **Evaporation** heat loss is calculated based on the settings on the **Materials Properties** tab, i.e. evaporation enthalpy per mole, the driving force for evaporation per mole quantity and the molar mass of gas. These are also calculated by the databases.

Calculation Type (Steady-state)

Single Point

By default for **Steady-state** calculations, **Single point** is selected, which by default uses the **Gaussian** *Heat Source*. In addition to settings described in this topic, you can also find more details in AM Calculator Heat Source Settings. This is available with all heat sources.

Heat Source Calibration

For some background, see About Heat Source Calibration. Also see Visualizing Heat Source Calibrations for various options related to visualizing the calibration settings.

Select **Heat Source Calibration**to calibrate a heat source based on the imported or entered experimental data instead of performing a single point calculation. All types of heat sources can be used. See below for additional information to enter the *Experiment Data*. This is available with **Gaussian**, **Double ellipsoidal**, or **Conical** heat sources.

Experiment Data (Heat Source Calibration)

> It is important to prepare the experiment data file correctly so the simulation performs smoothly. See AM Calculator Experiment File Requirements.

This section is available when **Heat Source Calibration** is selected as the *Calculation Type*.

In the **Experiment file** field, either enter a file path or click the file button (📁) to navigate to a data file such as an Excel spreadsheet (with *.xls or *.xlsx extensions) or a *.csv file. You can also use other programs (e.g. Google Sheets) to enter data and export to a CSV format that can be read by the software.

Click **Open** to import the data. In the **Experiment file** field you can see the file path to the selected file. The next time you click the file button (📁) the program remembers the last location from where the file is opened.

Choose the delimiter—**Comma** (,), **Colon** (:), **Equals sign** (=), **Semicolon** (;), or **Tab**—that matches the delimiter in the experiment file and click the **Reload** (🔄) button.

Batch

Select **Batch** to include power and scan speed data, which is read from a file such as a spreadsheet and entered or imported to the *Batch Experiment Data* table. You can optionally include experimental melt pool width and depth (if there is data), and compare this to the calculated results using a **Parity plot** on the Plot Renderer.

This is available with all heat sources.

> In addition to settings described in this topic, you can also find more details in AM Calculator Heat Source Settings and Visualizing Batch Calculations in the AM Module.

Batch Experiment Data

It is important to prepare the experiment data file correctly so the simulation performs smoothly. See AM Calculator Experiment File Requirements.

This section is available when **Batch** is selected as the *Calculation Type*.

In the **Experiment file** field, either enter a file path or click the file button (📁) to navigate to a data file such as an Excel spreadsheet (with *.xls or *.xlsx extensions) or a *.csv file. You can also use other programs (e.g. Google Sheets) to enter data and export to a CSV format that can be read by the software.

Click **Open** to import the data. In the **Experiment file** field you can see the file path to the selected file. The next time you click the file button (📁) the program remembers the last location from where the file is opened.

Choose the delimiter—**Comma** (,), **Colon** (:), **Equals sign** (=), **Semicolon** (;), or **Tab**—that matches the delimiter in the experiment file and click the **Reload** (🔄) button.

Grid

Select **Grid** to evaluate two axis variables of power and scanning speeds in the specified range and number of steps. Then continue with the *Grid Definitions*. In addition to settings described in this topic, you can also find more details in AM Calculator Heat Source Settings.

This is available with all heat sources.

Grid Definitions

This section is available when **Grid** is selected as the *Calculation Type*.

For the **Grid** calculation type, define the two axes variables using the fields and menus: **Quantity**, **Min**, **Max**, and **Number of steps**. The number of steps along with the minimum and maximum values for the axes define a grid. For each grid point the selected models are evaluated.

Enter a **Min**, **Max**, and **Number of steps** for:

- **Power (W)** for the selected *Heat Source* model.
- **Scanning speed (mm/s)** for the velocity of the moving heat source.

Probe Positions (Transient Simulations Only)

It is important to add the probes locations before the simulation is run or the action is not recorded.

You can add probes in the domain that record temperature and all other temperature related properties when the simulation is being run.

Click the **Add** ⊕ and **Remove** ⊖ buttons to add each probe and then you can either manually enter the probe coordinates (enter the **x**, **y**, and **z** coordinates in the fields) or click **Pick coordinate** to choose each of the points specifically on the **Geometry** tab in the **Visualizations** window.

Some advance options can be selected from a popup menu;

- Double-click on the geometry to pick a coordinate
- Hold Ctrl key to pick a probe in the middle of a layer
- Hold Shift key to map the picking position with a scanning path, i.e. you can pick a probe that snaps to a nearest scanning path
- Hold Shift+Alt keys to map the picking position to the middle of two scanning paths, i.e. pick a probe in the middle of the two nearest scanning paths.

AM Calculator: Working with Probe Data

Using Probe Data in Diffusion and Precipitation Calculations

When you also have licenses either for the Diffusion Module (DICTRA) and/or the Precipitation Module (TC-PRISMA), for transient simulations you can additionally include probe data from the AM Calculator in the set up of the thermal profile for diffusion and precipitation calculations, respectively.

AM Calculator Heat Source Settings

These settings are found on the AM Calculator Conditions tab. The other settings are described in AM Calculator Conditions Settings.

Choose the heat source model: **Gaussian**, **Core-ring**, **Top-hat**, **Double ellipsoidal**, or **Conical**. When available you can also choose predefined *Users heat sources* from the list.

For background theory related to Heat Sources, see About the Heat Source Models and About the Absorptivity Model. For *Gaussian*, *Double ellipsoidal*, and *Conical* heat sources, also see About Heat Source Calibration for additional details.

When a **Users heat source** option is available to choose in the heat source list, then only the **Power** of the heat source needs to be entered and the rest of the parameters, including the absorptivity, are automatically included in the simulation based on the selected expressions when originally saving the heat source calibration data.

The **Core-ring** and **Top-hat** heat sources are not available with **Heat Source Calibration** calculations.

Gaussian Heat Source

Gaussian is a surface heat source, and it is applied to the top surface of the domain. Then the heat is diffused based on the diffusivity of the material. This is most commonly used heat source in the industry.

- Settings below: Power, Absorptivity (incl prefactor, Wave length), Beam radius, Use keyhole model, Beam quality factor M^2.

Core-ring Heat Source

A **Core-ring** heat source, like a Gaussian heat source, is a surface heat source model which means that the power input from the heat source is only defined on the top surface of the workpiece, as a Neumann boundary condition. The intensity of a core-ring heat source can be modeled as a combination of a central Gaussian core beam and an outer ring beam.

- Settings below: Power, Absorptivity (incl prefactor, Wave length), Beam radius-Core, Beam radius-ring, Ring radius, Amount of power in ring, Use keyhole model, Beam quality factor M^2, Mode (Index or Custom).

Top-hat Heat Source

A **Top-hat** heat source is also called a *flat-top* and is considered a surface heat source model. In the AM Module, the top-hat heat source is approximated with a super-Gaussian beam, which means that the intensity drops to zero gradually within a given distance.

- Settings below: Power, Absorptivity (incl prefactor, Wave length), Beam radius, Use keyhole model, Beam quality factor M^2, Mode (Index or Custom).

Double Ellipsoidal Heat Source

The **Double ellipsoidal** heat source, also referred to as Goldak, is a volume model where the heat intensity is in the front and the back of the heat source is defined with the help of two different ellipsoids. The axis of the each ellipsoid is needed.

- Settings below: Power, Absorptivity (% only), ar, af, b, c.

Conical Heat Source

The **Conical** option is also a volumetric heat source where heat intensity is described as Gaussian distribution at the top surface, defined by a top radius, that varies linearly in the depth of the workpiece until it reaches a bottom radius within the prescribed depth.

- Settings below: Power, Absorptivity (% only), re, ri, H.

Settings

POWER

For a **Single Point** calculation enter the **Power**.

ABSORPTIVITY (GAUSSIAN, CORE-RING, TOP-HAT)

The **Absorptivity** settings are based on the *Heat Source* and *Calculation Type* selected.

For a **Single Point**, **Batch**, or **Grid** *Calculation Type*:

- Select **Calculated** (the default) to use the alloy's liquid resistivity to calculate the absorptivity as a function of temperature. To adjust this calculation, enter a different prefactor than the default (`1.0`) in the **with prefactor** field.
- Choose **User-defined** to enter absorptivity in **%** where you also can enter this as a function of temperature (T) i.e. `-1.6e-7*T*T+2.5e-3*T+31`.

For a **Heat Source Calibration** *Calculation Type* the absorptivity is calibrated separately for each row in the **Experiment Data** table. Select an option to calibrate absorptivity:

- **Calculated (prefactor calibrated)** (the default) to use the calculated absorptivity and calibrate the prefactor.
- **Constant (calibrated)** to calibrate the absolute value of absorptivity.

About the Absorptivity Model and the section Heat Source Calibration for more.

ABSORPTIVITY (DOUBLE ELLIPSOIDAL, CONICAL)

The **Absorptivity** settings are based on the *Heat Source* and *Calculation Type* selected.

For this heat source and with a **Single Point**, **Batch**, or **Grid** *Calculation Type* enter the absorptivity **%** for the selected heat source model. The default is 60 %. For **Heat Source Calibration** calculations there are no further settings.

WAVE LENGTH (GAUSSIAN, CORE-RING, TOP-HAT)

This field is available:

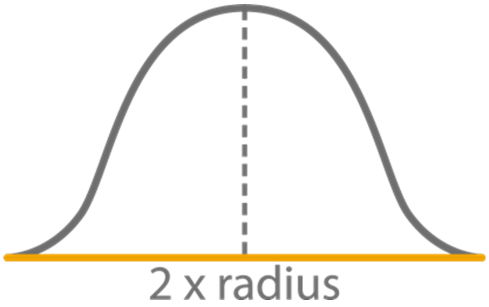
- For a **Single Point**, **Batch**, or **Grid** *Calculation Type* and when **Calculated** is selected as the **Absorptivity**.
- For a **Heat Source Calibration** *Calculation Type* and when **Calculated (prefactor calibrated** is selected as the **Absorptivity**.

About the Absorptivity Model and the section Heat Source Calibration for more.

Enter the **Wave length** in nm.

BEAM RADIUS (GAUSSIAN)

The beam radius is where the power reduces to $1/e^2$ as compared to its peak value. This is only applied on the top surface and then heat is diffused into the material based on the diffusivity of the material.



For a **Single Point**, **Batch**, or **Grid** *Calculation Type* enter the **Beam radius** size for the **Gaussian** heat source model. The default is 110 µm. Hover over the field in the GUI to view the example of it as below.

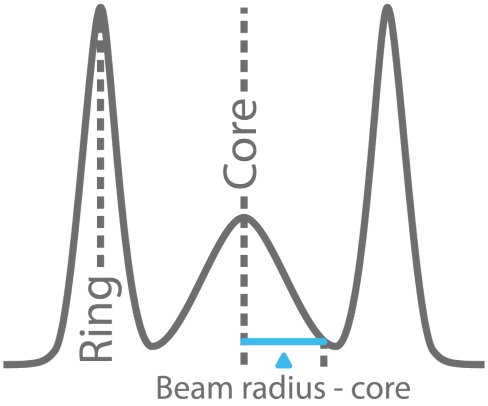
For a **Heat Source Calibration** *Calculation Type* and when **Calculated (prefactor calibrated** is selected as the **Absorptivity**.

- Select **Calibrated** to calibrate the beam radius and the absorptivity or **User-defined** to enter a specific beam radius in the field (unit = µm) and only calibrate the absorptivity.
- Then choose what to **Calibrate for**. Select **Width and depth** of the melt pool, or **Depth**to calibrate using only the depth of the melt pool.

? About the Absorptivity Model and the section Heat Source Calibration for more.

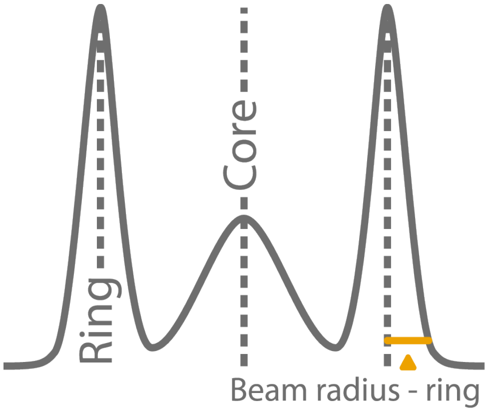
BEAM RADIUS-CORE (CORE-RING)

The **Beam radius-Core** for a **Core-ring** heat source is the $1/e^2$ radius of the core beam where the power reduces to $1/e^2$ as compared to its peak value. Also see the equations in Core-ring Heat Source.



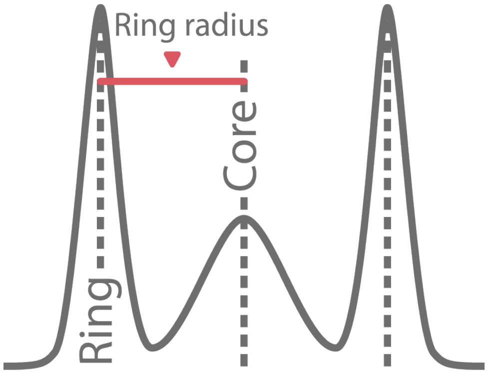
BEAM RADIUS-RING (CORE-RING)

The **Beam radius-Ring** for a **Core-ring** heat source is the $1/e^2$ radius of the ring beam. Also see the equations in Core-ring Heat Source.



RING RADIUS (CORE-RING)

The **Ring radius** for a **Core-ring** heat source is the ring radius i.e. the distance between the center of the core beam to the center of the ring beam. Also see the equations in Core-ring Heat Source.



AMOUNT OF POWER IN RING (CORE-RING)

Enter a value for the percent (%) of **Amount of power in ring**. This is the % of power for the ring beam. When using the **Index Mode**, the amount of power in the ring is set based on the selected index value (0-6).

? Index Mode (Core-ring)

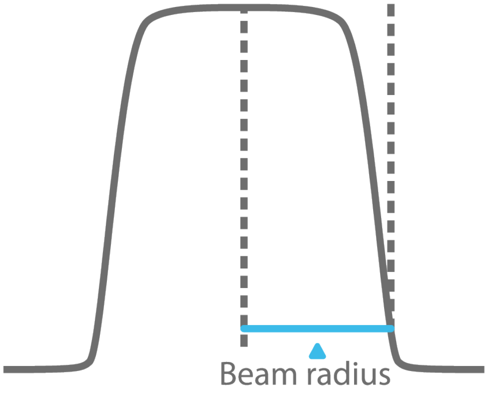
MODE (CORE-RING)

Select a **Mode**:

- **Custom** to manually enter all parameters (the Beam radius-Core, Beam radius-Ring, Ring radius, and Amount of power in ring). See Custom Mode (Core-ring) in the theory section for more details.
- **Index** to select the index value (0, 1, 2, 3, 4, 5, or 6). Enter a value for **Beam radius-Core** and then preset values for Beam radius-Ring, Ring radius, and Amount of power in ring are based on this selection. See Index Mode (Core-ring) in the theory section for more details.

BEAM RADIUS (TOP-HAT)

The **Beam radius** for a **Top-hat** heat source is the $1/e^2$ radius of the top-hat beam i.e. where the power reduces to $1/e^2$ as compared to its peak value. Also see the equations in detailed in Top-hat Heat Source.



KEYHOLE MODEL

About the Keyhole Model

The **Use keyhole model** checkbox is available for a **Gaussian** , **Core-ring**, or **Top-hat** *Heat Source* and when the **Use separate material properties for powder** checkbox is NOT selected.

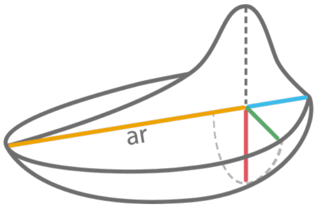
BEAM QUALITY FACTOR M^2

Enter the **Beam quality factor M^2** of the laser beam.

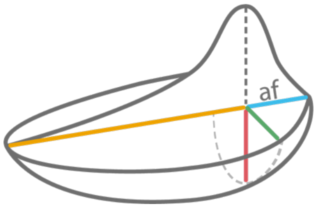
AR, AF, B, AND C (DOUBLE ELLIPSOIDAL)

For **Double ellipsoidal**, also enter the following. For each field you can hover over it in the GUI to see these images that show you the location.

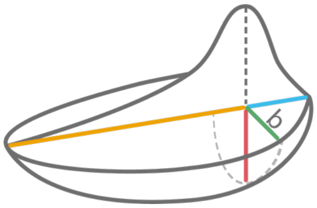
- **ar** (default is 70 µm).



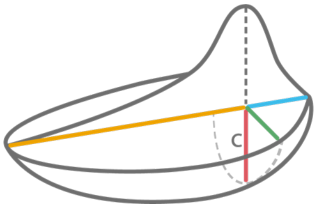
- **af** (default is 70 µm).



- **b** (default is 85 µm).



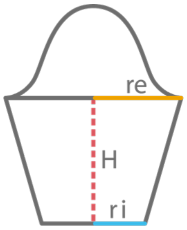
- **c** (default is 200 µm).



RE, RI, H (CONICAL)

For **Conical**, also enter the following. For each field you can hover over it in the GUI to see these images that show you the location.

- **re** (default is 100 µm).
- **ri** (default is 60 µm).
- **H** (default is 100 µm).



AM Calculator Experiment File Requirements

The following describes the requirements for importing experimental file data to be used with an **AM Calculator** either for a **Heat Source** or **Batch** *Calculation Type* and when setting it up on the **Configuration** window.

? AM Calculator Conditions Settings

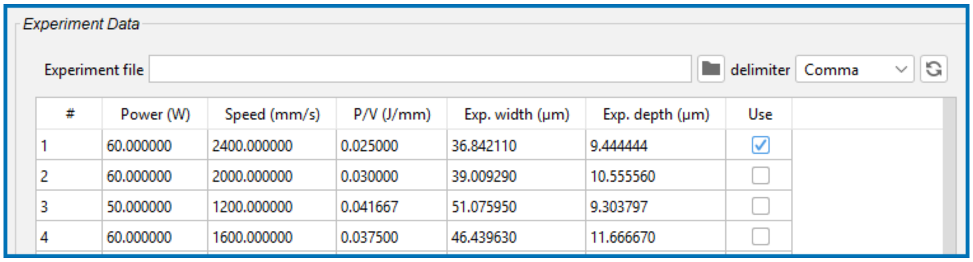
> ! It is important that the experiment data file contents are correctly entered in order for the calculation to perform smoothly.

Heat Source Calibration Calculations

When the **Heat Source Calibration** *Calculation Type* is selected in the **Steady-state** mode, there is an option to import a file with experimental data points that are used to calibrate the heat source.

Data can also be entered directly into the table on the **AM Calculator Configuration** window. However, if an **Experiment file** is imported it needs to be set up in a certain way so that the software can read the data.

These examples use experiment data, key holing, and heat source calibration: AM_06a: Calibrating a Heat Source for a 316L Steel and AM_06b: Using the Calibrated Heat Source for a 316L Steel.



Experiment file

delimiter Comma

#	Power (W)	Speed (mm/s)	P/V (J/mm)	Exp. width (µm)	Exp. depth (µm)	Use
1	60.000000	2400.000000	0.025000	36.842110	9.444444	☑
2	60.000000	2000.000000	0.030000	39.009290	10.555560	☐
3	50.000000	1200.000000	0.041667	51.075950	9.303797	☐
4	60.000000	1600.000000	0.037500	46.439630	11.666670	☐

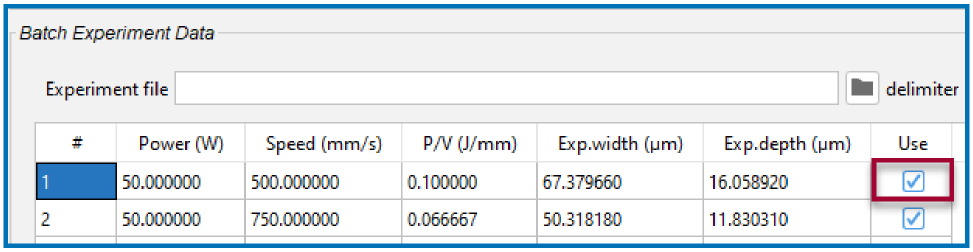
Figure 1: From example AM_06a, this shows the data imported from an experiment file into the table. The "Use" column allows you to choose the points to include or exclude for the simulation. Here row (experiment) #1 is selected to show the data point. Further down in this list, rows 9, 14, 20, and 21 are also selected to be included.

Batch Calculations

When the **Batch** *Calculation Type* is selected in the **Steady-state** mode, there is an option to import a file with experimental data points.

Data can also be entered directly into the table on the **AM Calculator Configuration** window. However, if an **Experiment file** is imported it needs to be set up in a certain way so that the software can read the data.

These examples use Batch calculations AM_07: Batch Calculations for an IN718 Alloy, AM_08b: Batch Calculations for a Ti64 Alloy, and AM_09b: Batch Calculations for an SS316L Alloy.



Experiment file

delimiter

#	Power (W)	Speed (mm/s)	P/V (J/mm)	Exp.width (µm)	Exp.depth (µm)	Use
1	50.000000	500.000000	0.100000	67.379660	16.058920	☑
2	50.000000	750.000000	0.066667	50.318180	11.830310	☑

Figure 2: From example AM_08b, this shows the data imported from an experiment file into the table. Here the "Use" checkbox for Experiment 1 is about to be deselected to exclude the data point after previewing it on the Visualizations window.

Experiment File Requirements

Only the columns described here are read / used in the calculation. It is important to enter the information exactly as described. All header text (the first line in the file) must also be written in English, i.e. no translations into other languages will be read correctly by the experiment file.

The experiment file is set up as follows.

- The first row in the file is the header.
- Include only four columns in the file and these must be in the following order and must use the indicated units.

  Default Global units (i.e. set via the **Tools → Options** menu) are not applicable. The data must be in the indicated units.

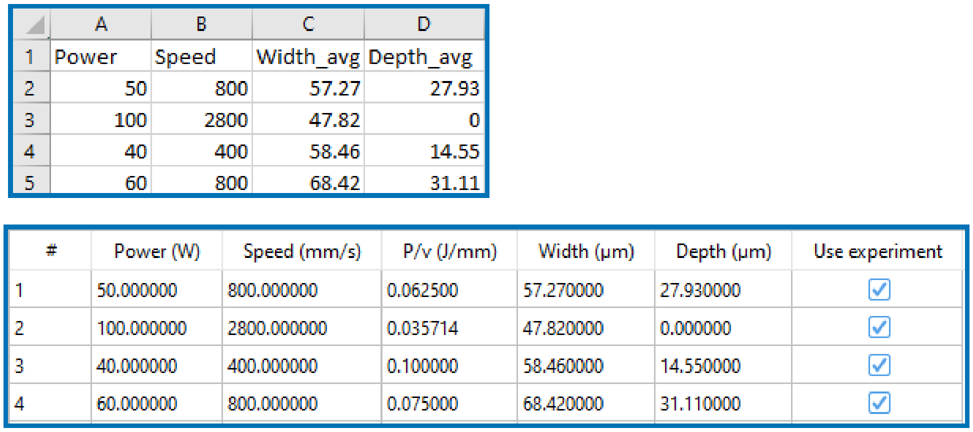
  - **Power** (unit = W)
  - Scanning **Speed** (unit = mm/s)
  - **Width** of the melt pool (unit = µm)
  - **Depth** of the melt pool (unit = µm)
- All of the values entered or imported to the table must be positive and greater than zero.

If you select **Depth** from the **Calibrate for** list, then the experimental values for only the melt pool depth is needed.

Do not include the following in the file:

- **#** this is the experiment number that is automatically associated to each imported or entered set of data. It is used to identify the applicable rows by a unique number so that you can easily identify these points (i.e. points are identified by labels on the plots), or when choosing to include or exclude the experiment point from the simulation or later from a plot.

- **P/v (J/mm)**. This is the energy density and is defined as the ratio of power and scanning speed. This is not included in any data file. This is automatically calculated based on the **Power** and **Speed** entered or included in the file (i.e it is defined as the ratio of power and scanning speed).
- **Use**. This column is not part of the text file, it is available once the data is imported or entered in the table. Then you can choose to include or exclude specific data points as you examine this output in the **Visualizations** window.

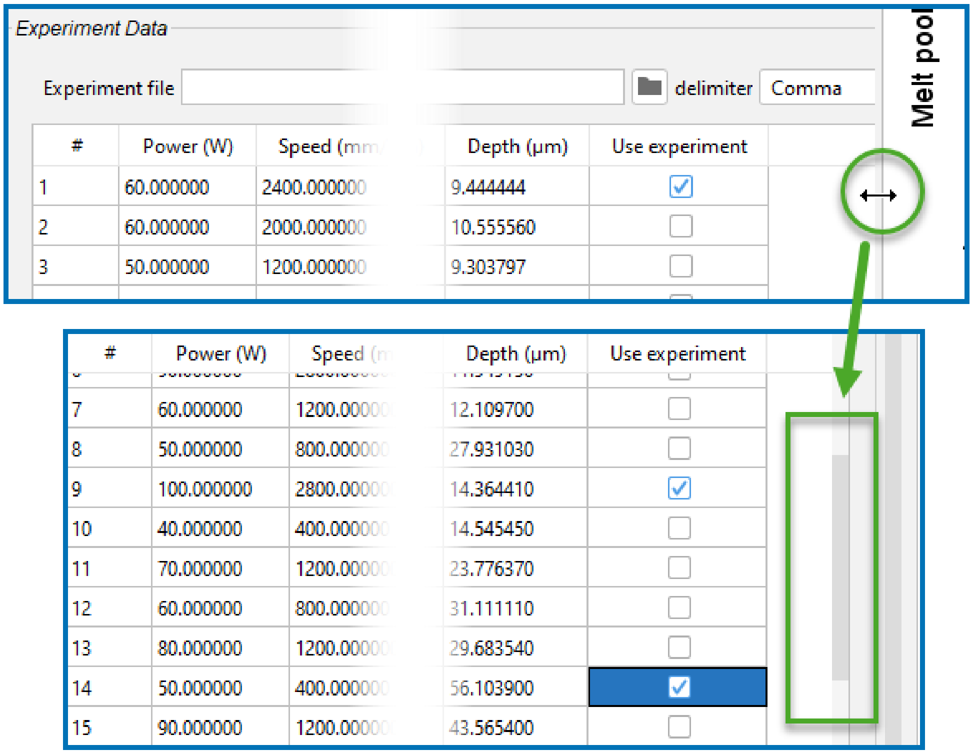


	A	B	C	D
1	Power	Speed	Width_avg	Depth_avg
2	50	800	57.27	27.93
3	100	2800	47.82	0
4	40	400	58.46	14.55
5	60	800	68.42	31.11

#	Power (W)	Speed (mm/s)	P/v (J/mm)	Width (µm)	Depth (µm)	Use experiment
1	50.000000	800.000000	0.062500	57.270000	27.930000	☑
2	100.000000	2800.000000	0.035714	47.820000	0.000000	☑
3	40.000000	400.000000	0.100000	58.460000	14.550000	☑
4	60.000000	800.000000	0.075000	68.420000	31.110000	☑

Figure 3: An example of the original experiment data file, with the four headings in the correct order and these do not need the units included here. When the file is imported, there is a standard header that is kept, plus the additional columns (i.e. #, P/V, and Use experiment), which are automatically available and updated as needed.

Once a set of data is imported to the table (or entered manually), expand the **Configuration** window to reveal the scroll bars. Then you can scroll up or down, left or right, within the table to select checkboxes for the relevant data points you want to include or exclude. This is applicable to the tables found on the AM Calculator as well as those on the Plot Renderer for the data.



Experiment Data

Experiment file delimiter Comma

#	Power (W)	Speed (mm	Depth (µm)	Use experiment
1	60.000000	2400.000000	9.444444	☑
2	60.000000	2000.000000	10.555560	☐
3	50.000000	1200.000000	9.303797	☐

#	Power (W)	Speed (	Depth (µm)	Use experiment
7	60.000000	1200.0000	12.109700	☐
8	50.000000	800.00000	27.931030	☐
9	100.000000	2800.0000	14.364410	☑
10	40.000000	400.00000	14.545450	☐
11	70.000000	1200.0000	23.776370	☐
12	60.000000	800.00000	31.111110	☐
13	80.000000	1200.0000	29.683540	☐
14	50.000000	400.00000	56.103900	☑
15	90.000000	1200.0000	43.565400	☐

You can edit the table after importing data, or manually enter information. To add a row, scroll to the bottom of the table and press <Enter>.

AM Calculator Materials Properties Settings

Once you have added an AM Calculator, the **Configuration** window has these settings tabs where there are many available conditions to set on the **Conditions**, **Materials Properties**, and **Options** tabs and with the specialized **Plot Renderer**.

This section describes the settings for the **Materials Properties** tab.

AM Calculator Conditions Settings and AM Calculator Options Settings

Use Data From

If there is a Scheil Calculator predecessor to the AM Calculator, you can import the material properties from a **Library** or **Scheil Calculator**. When the AM template is added, the default is to import material properties from Scheil calculations.

When the **with Material Library** template is used, then the AM Calculator > Materials properties are available to import from a **Library** only.

In this case you also can **Save**, **Save as**, **Export to Folder**, **Delete**, and **Rename** the material data both from Scheil and from material library. With **Save** or **Save as**, original data is saved i.e. without any smoothing. With **Export to Folder**, the data is saved with **Smoothing**. the material data both from Scheil and from material library.

Export to folder is intended for using the data in an external simulation software, where using smoothed data is expected to result in fewer numerical issues. **Save** and **Save as** are intended for when the data is to be used in the AM Module. The data will be smoothed according to the smoothing setting before use in the FEM simulation.

Account for Interface Scattering

When **Use data from Scheil Calculator** is selected, you can also select the **Account for interface scattering** checkbox.

The electrical resistivity due to phase interface scattering is evaluated as the scattering constant times sum of the interaction between the volume fraction of all the phases. The default value for the **Phase interface scattering constant** is found to be `4.0e-8` Ωm for aluminum alloys produced with conventional methods. A higher value could be required for the AM process where the rapid solidification results in a very fine microstructure with a large amount of phase interfaces.The contribution to thermal conductivity is assumed to be related to that to electrical resistivity, following the Wiedemann-Franz law.

Either keep the default **Phase interface scattering constant**, which is a constant for evaluating thermal conductivity due to scattering at phase interfaces, or enter another value.

Import

You can import material properties contained in a folder.

Click the **Import from folder and add to libraries** button and navigate to the folder location where the material properties are located.

Smoothing

From the **Smoothing** list, select **Same for all quantities** (where **Little smoothing** is the default) or **Per quantity**. Then either define the smoothing once (**Same for all quantities**) or individually for each quantity. Options are **No smoothing**, **Little smoothing**, **Medium smoothing**, **Large smoothing**, or **Linear**.

Available quantities to define smoothing:

- Heat
- Apparent heat capacity per kg
- Density
- Thermal conductivity
- Dynamic viscosity
- Surface tension
- Molar volume
- Molar mass of gas
- Driving force for evaporation per mole
- Evaporation enthalpy per mole
- Electric resistivity
- Absorptivity
- Absorptivity vs angle

Plot

From the **Plot** list, choose what quantity to plot:

- Heat
- Apparent heat capacity per kg
- Density
- Thermal conductivity
- Dynamic viscosity
- Surface tension
- Molar volume
- Molar mass of gas

- Driving force for evaporation per mole
- Evaporation enthalpy per mole
- Electric resistivity

Plot: Absorptivity Options

The following absorptivity options depend on what combination of heat source and calculation type is selected on the **Conditions** tab. See AM Calculator Heat Source Settings.

Absorptivity and **Absorptivity vs angle** plot options are available when the conditions below are met:

- When a **Gaussian**, **Core-ring**, or **Top-hat** heat source is selected, plus any one of the **Single Point**, **Batch**, or **Grid** calculation types AND when **Calculated** or **User-defined** is selected.
- When a **Gaussian** heat source is selected, plus a **Heat Source Calibration** calculation type AND when **User-defined** is selected.

Also, for a **Gaussian** heat source, **Heat Source Calibration** calculation type, AND when **Calculated** is selected, then the options are:

- **Absorptivity (wavelength is** *<value from Heat Source settings>* **with prefactor 1.0)**.
- **Absorptivity vs angle (wavelength is** *<value from Heat Source settings>* **with prefactor 1.0)**.

> The wavelength *<value from Heat Source settings >* for the **Absorptivity** and **Absorptivity vs angle** is the same as what is entered on the **Conditions** tab. For example, if 1064 nm is entered, it displays on the **Material Properties** tab as **Absorptivity (wavelength is 1064 nm with prefactor 1.0)**.

Show Transition Temperatures

You can also choose to **Show transition temperatures**:

- Solidus, Liquidus, Evaporation
- Solidus
- Liquidus

- Evaporation
- Custom: If selected, also enter a value in the field. The default unit is the same as what is selected globally on the **Tools → Options → Graphical Mode → Default Units** tab.
- None

AM Calculator Options Settings

Once you have added an AM Calculator, the **Configuration** window has these settings tabs where there are many available conditions to set on the **Conditions**, **Materials Properties**, and **Options** tabs, as well as with the specialized **Plot Renderer**.

This section describes the settings for the **Options** tab.

AM Calculator Conditions Settings, AM Calculator Heat Source Settings, and AM Calculator Materials Properties Settings

Streamline Upwind Petrov-Galerkin (SUPG)

Select the **Streamline upwind Petrov-Galerkin (SUPG)** checkbox to enable SUPG stabilization scheme for the energy and Navier-Stokes equations.

Damping Factor for the Damped Newton Iteration

Select the **Damping factor for the damped Newton iteration** checkbox to add a damping factor for the damped Newton iteration and enter a value between 0 and 1. The default is 0.7.

It may improve stability but it slows down convergence of the simulation.

Smagorinsky Constant

Enter a **Smagorinsky constant** in the field. This is the value of the constant to use in the fluid flow model. The default is 0.18.

For more information see Fluid Flow in the theory section.

Save Interval for Transient Simulation

Select the interval to save results from transient simulations. If the number of files saved are specified, choose if the step size should increase linearly or exponentially.

From the **Save interval for transient simulation** list choose **Automatic**, **Every Nth time step**, or **Time in seconds**. Then for each also enter as indicated:

- **Automatic**
  - **Max number of files**: The default is`100`**Linear**.
  - Then choose **Linear** or **Exponentially increasing**. Enter another number of files in the field as needed.
- **Every Nth time step**: The default is 1 or enter or use the up and down arrows to choose another number.
- **Time in seconds**: The default is 0.01 or enter another number in the field.

Number of Cores

Select or enter the **Number of cores** available for the simulations. The default value is the total number of physical cores available in the system.

AM Calculator: Working with Probe Data

When you also have licenses either for the Diffusion Module (DICTRA) and/or the Precipitation Module (TC-PRISMA), for transient simulations you can additionally include probe data from the AM Calculator in the set up of the thermal profile for diffusion and precipitation calculations, respectively.

Workflow to Include Probe Data from Diffusion or Precipitation Simulations

You can use installed examples to visualize how the probes are set up for a Diffusion Calculator (see AM_05: Using AM Calculator Probe Data with the Diffusion Module (DICTRA)) and for the Precipitation Calculator (see AM_12: Using AM Calculator Probe Data with the Precipitation Module (TC-PRISMA)).

1. Set up the probes on the **AM Calculator**. Probes are available for transient calculations only. See AM Calculator Conditions Settings. This must be done before you can use the probe data in the calculations connected to a Diffusion Calculator or Precipitation Calculator.
2. If not already done, add a **Diffusion Calculator** or **Precipitation Calculator** as a successor to the **AM Calculator**.
3. Set up your Diffusion or Precipitation Calculator as needed. Follow the basic settings details for the **Thermal Profile** section as described in Diffusion Calculator Thermal Profile and Precipitation Calculator Thermal Profile.
4. Once the standard settings are completed, and as long as probes are set up, on the **Configuration** window, the section **Probes** is available. Until the AM Calculator is run, the list is empty. After the AM simulation is completed, the data is imported into the table you can choose how to **Condense time-temperature data**. These settings are described below.

Probes

The list of **Probes** is available as long as *Probe Positions* are set up on the AM Calculator and the AM Calculator is performed to generate the data, which is fed into the applicable Calculator (Diffusion or Precipitation). Select the probe you want to plot, for example as a Segregation Profile as shown in example AM_05.

Condense Time-Temperature Data

Use the **Condense time-temperature data** setting to adjust how many time-temperature points are included in the **Thermal Profile** displayed in the **Visualizations** window. For example, for a complex calculation you can choose a **Medium** or **Large** setting to save fewer time steps at this stage of design, which in turn can ensure that a complex diffusion or precipitation calculation is able to finish.

Choose **None**, **Small**, **Medium**, **Large**, or **Custom**.

- **None** (the default) includes all points, i.e. no points are condensed together and all point data are included in the **Thermal Profile** preview. When using the **Custom** setting, this is equivalent to entering a value greater than 1 in the field.
- **Small** condenses a minimum number of points, which means that a *large* number of time steps are used in the calculation and thus lots of time steps are shown.
- **Medium** is when that a medium number of points are condensed together, which means that a *medium* number of time steps are used in the calculation.
- **Large** is when a large number of points are condensed together, which means that there are few, or a *small* number of time steps used in the calculation.

- When **Custom** is selected you can fine-tune the number of points to include. Enter a value between 0 and 1, where 0 maximizes condensing the points (the same as choosing **Large**), 1 minimizes condensing the points (the same as choosing **Small**), and 0.5 is a medium number of points being condensed (the same as choosing **Medium**). If you enter a value greater than 1, it is the same as choosing **None**, i.e. all data points are included. The larger the value, the more points are condenses, until only two points are shown.

AM Calculator: Plot Renderer Settings

Once you have added an AM Calculator, you can add the specialized **Plot Renderer**. The following is information about the settings available for a **Plot Renderer** when it is a successor to an **AM Calculator**.

The settings listed below are made available based on a variety of combinations, e.g. the type of *simulation* (**Steady-state**, **Transient**, or **Transient with heat source from Steady-state**), whether *fluid flow* or the *keyhole* checkboxes are selected, whether *probes* are used, and so on. There are also *Calculation Types* (**Single Point**, **Heat Source Calibration**, **Batch**, and **Grid**), that impact the settings shown, and these options are further included on separate tabs (i.e. **Batch**, **Grid**, **Heat Source Calibration**, **3D Plot**, **Plot Over Line**, **Thermal Gradient vs Solidification Rate**, etc.), which are further fine-tuned based on the *plot types* or *display types* selected on the **Plot Renderer**.

The software guides you by only providing the relevant settings to define. Due to the number of settings available, these are not in order as to what you see on the **Configuration** window. Where relevant or logical, settings are grouped together and some detail of when or how you would access the setting is included. Scroll or search for the setting or field name as there are many simulation, calculation, display options, and plot type combinations that are available on the relevant tab on the **Plot Renderer Configuration** window.

About the AM Plot Types and Working with AM Visualizations

General

Add a Quantity and Remove a Quantity or Function Buttons

Use the **Add quantity** or **Add function** ⊕ and **Remove quantity** or **Remove function** ⊖ buttons to add additional setting groups that include all of the available settings. Click the checkbox next to these buttons to enable or disable any particular settings group.

Show Table or Hide Table

These buttons are available on the **Batch** or **Grid** tabs after running either a **Batch** or **Grid** calculation, respectively.

Use the **Show Table** or **Hide Table** buttons to view the simulation data and using the table you can fine tune the plot. Also see Visualizing Batch Calculations in the AM Module for more information about the columns in the table.

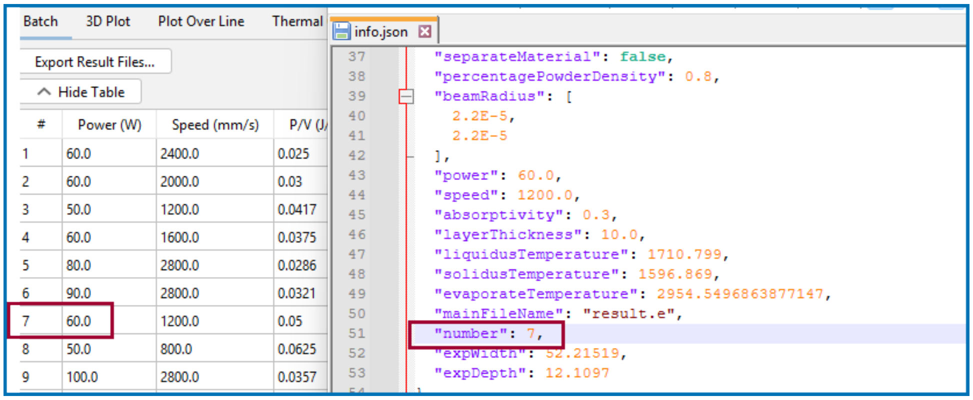
Export Result Files

This option is available on the **Plot Renderer Configuration** window for the following tabs (and the associated plots that are available for each): **3D Plot**, **Grid**, **Batch**, or **Heat Source Calibration**. The button is available after the simulation is run.

Click **Export Result Files** to export the files and visualize the results in external software. The result file(s) in Exodus format (`*.e`) and the json file info `.json` are copied to the folder selected. The json info file contains the settings and results from each data point. You can open the json info file in a text reader (i.e. Notepad) to review it before using the Exodus file in the external software.

When exporting from the **Grid**, **Batch**, and **Heat Source Calibration** tabs, the results are saved in separate subfolders, each containing the `.e` and `.json` files. The Exodus file format is used for finite element analysis.

> The folders containing the sets of results files are exported in random order. To match the folder to the original datapoint, open the json file in a text editor. In this file there is a `number` field that matches the row (experiment) number in the table found on the **Plot Renderer Configuration** window for the applicable tab (click **Show Table**). You can use this to match the folder contents back to the datapoint as needed.



#	Power (W)	Speed (mm/s)	P/V (J/
1	60.0	2400.0	0.025
2	60.0	2000.0	0.03
3	50.0	1200.0	0.0417
4	60.0	1600.0	0.0375
5	80.0	2800.0	0.0286
6	90.0	2800.0	0.0321
7	60.0	1200.0	0.05
8	50.0	800.0	0.0625
9	100.0	2800.0	0.0357

```
  "separateMaterial": false,
  "percentagePowderDensity": 0.8,
  "beamRadius": [
    2.2E-5,
    2.2E-5
  ],
  "power": 60.0,
  "speed": 1200.0,
  "absorptivity": 0.3,
  "layerThickness": 10.0,
  "liquidusTemperature": 1710.799,
  "solidusTemperature": 1596.869,
  "evaporateTemperature": 2954.5496863877147,
  "mainFileName": "result.e",
  "number": 7,
  "expWidth": 52.21519,
  "expDepth": 12.1097
```

In the **Export Result Files** window, in the **Folder Name** field, navigate to the location or enter a file path to where you want to save the files. Create a new folder as needed. Click **Save**. The individual exported files in each folder are named `info.json` and `result.e` and can be used in external software. When there are multiple subfolders (i.e. for Grid, Batch and Heat Source Calibration) the number of folders exported is the same as the number of rows of data selected to be used. If the **Use** checkbox is not selected, the result folder (and files) for that data point is not exported. Click the **Show Table** button to review the rows of data and choose to include or exclude data points from the **Use** column.

Filter by Material Types

This option is available when **Use separate material properties for powder** is selected on the **AM Calculator**.

Select **Filter by material types** to visualize specific material types from the list.

Layer Thickness

Enter a **Layer thickness** in µm. The printed layer thickness is equal to the powder thickness first after multiple layers have been printed. For a single track, or a few layers, the printed layer is often much less than the powder thickness.

Table View

Click the **Table View** button to toggle it ON and OFF between a plot and a table.

[AM Plots: Table View Options]

Transient-related Simulations

Time

Once a **Transient** simulation plot is calculated, the **Time** step results are listed in a drop-down list. You can choose to look at a specific time point, or click the buttons to the right of the drop-down to navigate the time steps. Hover over the buttons to see the tooltips or see Time Step Navigation Buttons.

Time Step Navigation Buttons

Button	Action
|<	Move to the first time step
<	Move to the previous time step
▶	Play from the current time step to the last one
>	Move to the next time step
>|	Move to the last time step

Rescale Plotting Data Range Over All Time Steps

This is available for **Transient** simulations.

Select the **Rescale plotting data range over all time steps** checkbox to scale min and max values of legends and plots over all time steps.

Axis Variables and Display Options

Axis Variable

Set the state variable you want plotted along the X-axis and the Y-axis. The available variables in the list are based on how your system is set up and options vary.

Choose an **Axis variable** and an applicable unit (indicated in the brackets) from each of the drop-down lists.

- **Temperature** (Kelvin, Celsius, or Fahrenheit)
- **Surface tension** (Joule per m^2 or Millijoule per m^2)
- **Thermal conductivity** (unitless)
- Available when the **Fluid flow including Marangoni effect** checkbox is selected:
    - **Dynamic viscosity** (Pascal-second, milliPascal-second, Poise, or centiPoise)
    - **Flow velocity field** (m/s, mm/s, µm/s, or nm/s)
    - **Solidification rate**(m/s, mm/s, µm/s, or nm/s)
- **Thermal gradient** (Kelvin per m)

Display

Based on the **Axis variable** selected, choose the way to **Display** it.

- For **Temperature**, **Surface tension**, **Thermal conductivity**, or **Dynamic viscosity**, choose **Surface colormap**, **Contour**, or **Iso-surface**. For Surface colormap and Contour, you can also click to select the **Slice** checkbox.
- For **Flow velocity field**, choose the object shape to display velocity vectors: **Arrow**, **2D glyph**, **Cone**, or **Line**.

The settings are further described below.

Tubes

Available for display type **Contour**.

The **Tubes** checkbox is selected by default and this displays contour plots as 3D tubes. Click to clear the checkbox and instead display the contours as 2D lines.

Values

Available for display types **Contour** and **Iso-surface**. For Iso-surface you can also specify the opacity of surface plot in %.

Choose the **Values**: **Automatic** (the default), **Custom values**, **Custom range**, **Solidus**, **Liquidus**, or **Solidus and Liquidus**.

- For **Automatic**, enter the **Number of steps**.
- For **Custom values** enter a number in the field.
- For **Custom range** enter the **Min** and **Max** number of lines, then **Number of steps**.
- Select **Solidus** to plot contour/iso-surface at solidus temperature.
- Select **Liquidus** and **Solidus and Liquidus** to plot contour/iso-surface at both solidus and liquidus temperatures.

Some settings are further described in separate sections below.

Number of Steps

Available for **Contour** and **Iso-surface** Display types, and when **Automatic** or **Custom range** Values are selected.

Enter or choose the **Number of steps**.

> In some cases for a **Custom range** selection, you need to expand the Configuration window to the right to access this setting.

Opacity

Available for **Surface colormap** and **Iso-surface** (available for all **Values** options).

Enter a value between 0-100 as the percent (%) of **Opacity**.

Slice

This is available for display types **Surface colormap** or **Contour**.

Select the **Slice** checkbox to visualize the **Axis variable** on a cross-sectional plane. You can choose the normal of the cross-sectional plane and the distance of the plane from the center of the heat source.

Then choose **X-direction**, **Y-direction**, or **Z-direction**, for the **Distance from center of heat source** and for the **beam radius**.

Coloring and Range

Choose **Rainbow**, **Cool to warm**, **Purple Orange**, **Green Purple**, **Blue Brown**, **Green Red**, **Solid color**.

For all but **Solid color**, choose a **Range**—**Automatic** or **Custom**. Then for **Custom** enter a **Min** and **Max** number.

Legend

Click the **Legend** checkbox to include or click to clear to exclude a legend.

Scale Glyph by Velocity Magnitude

This setting is for a **Flow velocity field Axis variable**. It is available for all **Display** types.

Select the **Scale glyph by velocity magnitude** checkbox to scale the velocity display object (glyph) according to the velocity magnitude. Otherwise the glyphs are scaled uniformly.

Glyph Scale Factor

This setting is for a **Flow velocity field Axis variable**.

Enter a numerical value for the **Glyph scale factor**.

Show Glyph in Every

This setting is for a **Flow velocity field Axis variable**.

For the **Show glyph in every setting**, enter or select the number of grid **points** where velocity glyphs are displayed.

2D Plot Types

You can plot the material properties (2D) so you can specify the quantities and add as many lines as you want directly to the plot in the **Visualizations** window. What you see is **Distance vs Temperature**, first is first layer, second is second layer, and so forth on the 2D plots. You can select the different times from the list at the top at different points and see it on the plot, for example it might be at 26 minutes where you can see it is as the peak of the melt pool max temperature.

Show Transition Temperatures

Available with 2D plot types, such as **Probe** or **Plot Over Line**. It is a dynamic list that updates the plot in the **Visualizations** window after the 2D plot is performed.

Select the different options to better visualize the transition temperature results. From the **Show transition temperatures** list, choose **Solidus, Liquidus, Evaporation**, **Solidus**, **Liquidus**, **Evaporation**, **Custom**, or **None**. For **Custom**, also enter a specific temperature value in the field. Then observe the changes on the plot, where the legend updates and the lines for each option are added or removed based on the selection.

Grid Calculations (Grid, 3D Plot, and Plot Over Line Tabs)

These settings are specific to **Grid** calculations and are on the **Grid** tab. Also see plot related settings: Melt Pool vs Energy Density Plot Type (Batch and Grid Tabs) and Printability Map Plot Type (Batch and Grid Tabs).

Grid Data

This is available on the **3D Plot** and **Plot Over Line** tabs after running a **Grid** *Calculation Type*.

The data in the **Grid data** list shows all the power and scan speed combinations and it is sorted in order of energy density.

Grid Calculation Table

The following is on the **Grid** tab after a **Grid** calculation.

Use the **Show Table** or **Hide Table** buttons to view the simulation data and using the table you can fine tune the plot. The table includes these columns:

- The **Power (W)** and **Speed (mm/s)** columns are the from what was entered under *Grid Definitions*, on the **AM Calculator** i.e. the **Min**, **Max**, and **Number of steps**.
- The **P/v (J/mm)** column is the automatically calculated energy density, defined as the ratio of power and scanning speed.
- The calculated width and depth points, with the prefix **Sim.**, i.e. **Sim.width (µm)** and **Sim.depth (µm)**, to indicate it is the result of the simulation.
- The **Use** column has a checkbox available to include or exclude these points on the plots. When a **Use** checkbox is not selected, the results are also not included if you choose to export the result files. See Export Result Files.

Batch Calculations

These settings are specific to **Batch** calculations. Also see plot related settings: Parity Plot (Batch Tab), Melt Pool vs Energy Density Plot Type (Batch and Grid Tabs), and Printability Map Plot Type (Batch and Grid Tabs).

After the **Batch Experiment Data** set up is completed on the **AM Calculator** and the simulation run, then on the **Plot Renderer** you can start to work with the data you want to plot. Also see Including or Excluding Data Points to understand the interaction between these two tables.

Batch Experiments

Plot Renderer → 3D Plot, **Plot Over Line**, and **Thermal Gradient vs Solidification Rate** tabs after running a **Batch** *Calculation Type*.

The data in the **Batch Experiments** list shows all the power and scan speed combinations and it is sorted in order of energy density.

Batch Calculation Table

Plot Renderer → Batch tab.

You may have already included or excluded data points earlier when previewing the data. Use the **Show Table** or **Hide Table** buttons to view the included or excluded data and continue to fine tune the plot.

On the **Batch** tab the table includes these columns:

- The original experiment data for **Power (W)** and **Speed (mm/s)**, plus the **P/v (J/mm)**.
- The original experiment data for **Width** and **Depth**, now with a prefix **Exp.** e.g. **Exp.width (µm)**, to indicate this is the experimental data.
- The calculated **Width** and **Depth** points, with the prefix **Sim.**, e.g. **Sim.width (µm)**, to indicate it is the result of the simulation.

Only the experiment data points selected for inclusion when setting up the AM Calculator have data in these two **Sim.** columns.

- The **Use** column has a checkbox available to continue to include or exclude those points on the plots. When a checkbox is not selected, the results are also not included if you choose to export the result files.

> Only points that were originally included in the simulation can be selected or deselected from the **Use** column. If an experiment data point needs to be added, return to the AM Calculator, choose the point (s) to include there, and run the simulation again. Once the simulation is complete, the points are included in this table.

Parity Plot (Batch Tab)

The following settings are available on the **Batch** tab when a **Parity plot** is selected as the plot type.

Plot Width and Plot Depth

Click the **Plot width** and **Plot depth** checkboxes to toggle between displaying these points on the associated tab on the **Visualizations** window for the plot.

Show Limits

Select the **Show limits** checkbox to include additional visual cues on the plot. Choose **RMS**, **Absolute**, or **Relative in %**. For **Absolute** or **Relative in %** enter a number in the field. The plot dynamically updates as you toggle between these options.

Melt Pool vs Energy Density Plot Type (Batch and Grid Tabs)

The following settings are available on the **Batch** or **Grid** tab when a **Melt pool vs energy density** is selected as the plot type.

Plot Width and Plot Depth

Click the **Plot width** and **Plot depth** checkboxes to toggle between displaying these points on the associated tab on the **Visualizations** window for the plot.

Printability Map Plot Type (Batch and Grid Tabs)

The following settings are available on the **Batch** or **Grid** tab when a **Printability map** is selected as the plot type and after running a **Batch** or **Grid** calculation, respectively. The example used in the images is AM_08a.

Show Result Points

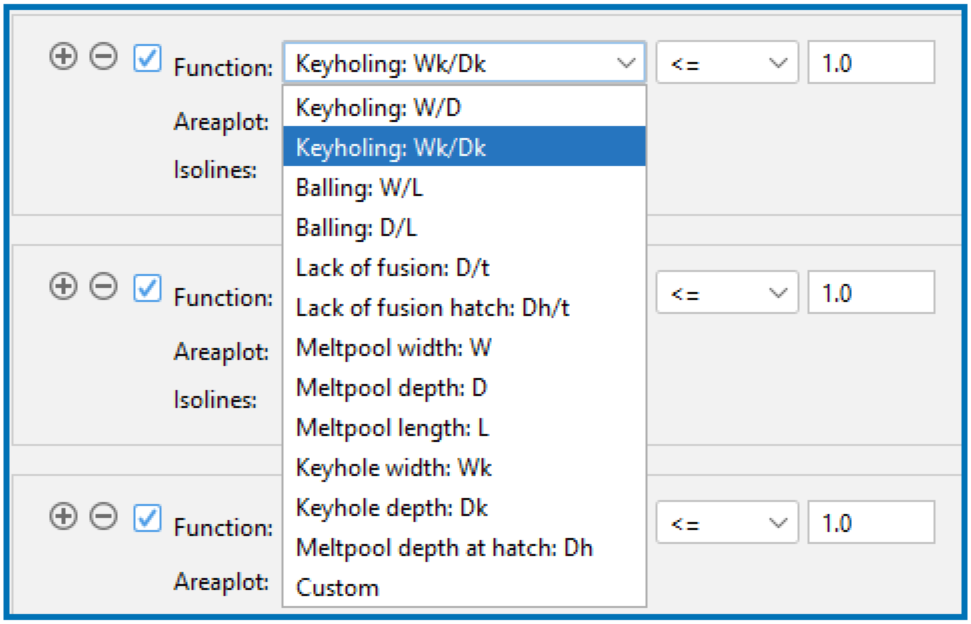
Select or deselect the **Show result points** checkbox to toggle these on and off on the **Visualizations** window. The plot updates dynamically.

Hatch Distance

Enter a **Hatch distance** in µm.

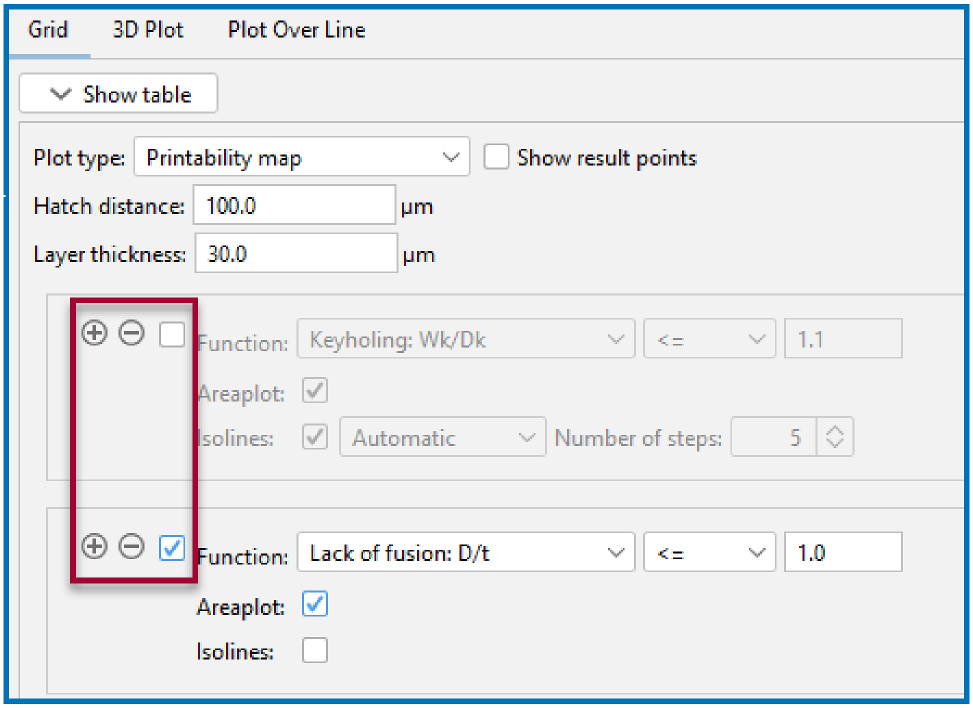
Function

Printability maps with varied power and scanning speeds can be simulated showing regions where the defects keyholing porosity, lack of fusion, and balling occur. The defect regions are defined by functions of the keyhole dimension (**Wk**, **Dk**), melt pool dimensions (**W**, **D**, **L**), hatch distance (**h**), and powder thickness (**t**). Use the ⊕ plus and ⊖ minus buttons to add and remove sections to define each **Function**.



⊕ ⊖ ☑ Function: Keyholing: Wk/Dk <= 1.0

Click to toggle the **Function** checkbox to show and hide the selected functions as needed on the **Visualizations** window.



Plot type: Printability map ☐ Show result points

Hatch distance: 100.0 µm

Layer thickness: 30.0 µm

☐ Function: Keyholing: Wk/Dk <= 1.1

Areaplot: ☑

Isolines: ☑ Automatic Number of steps: 5

☑ Function: Lack of fusion: D/t <= 1.0

Areaplot: ☑

Isolines: ☐

From the list select one of the following for each section added then for each choose **All**, **<=** (less than or equal to), or **>=** (greater than or equal to) and enter a number in the field associated field. On the **Visualizations** window, there are numbered labels to indicate experiments with defects, in **red** , or without defects, in **green**.

- **Keyholing: W/D**
- **Keyholing: Wk/Dk**
- **Balling: W/L**
- **Balling: D/L**
- **Lack of fusion: D/t**
- **Lack of fusion hatch: Dh/t**
- **Meltpool width: W**
- **Meltpool depth: D**
- **Meltpool length: L**
- **Keyhole width: Wk**

- **Keyhole depth: Dk**
- **Meltpool depth at hatch: Dh**
- **Custom**. Then enter a **Name** in the field.

Areaplot

Click the **Areaplot** checkbox to toggle between including the colored sections on the plot.

Isolines

Click the **Isolines** checkbox to include or exclude isolines.

Choose **Automatic**, **Custom**, or **Custom values**.

- For **Automatic**, enter the **Number of steps**.
- For **Custom**, enter the distance between lines i.e. `1.0 1.25 1.5`.
- For **Custom values**, enter a **Min**, **Max**, and **Number of steps**.

Heat Source Calibration Calculations

See AM Calculator Conditions Settings and Visualizing Heat Source Calibrations for more detailed information.

Heat Source Calibration Experiments

Plot Renderer → 3D Plot and **Plot Over Line** tabs after running a **Heat Source Calibration** *Calculation Type*.

The data in the **Heat Source Calibration Experiments** list shows all the power and scan speed combinations and it is sorted in order of energy density.

Heat Source Calibration Table

Plot Renderer → Heat Source Calibration tab.

Click the **Show Table** or **Hide Table** buttons to view or hide the experimental and simulation data. To fine-tune the choice of data points, click the checkbox for the **Use** column for each row (experiment #) to observe the dynamic changes on the **Heat Source Calibration Parameters** and/or **Melt Pool Dimensions** tabs on the **Visualizations** window.

> Experiment data and other settings must be configured for this to be available. The data points available in the table are selected on the **AM Calculator** under *Experiment Data* and then you can include or exclude points by selecting or deselecting the relevant checkboxes in the **Use** column.

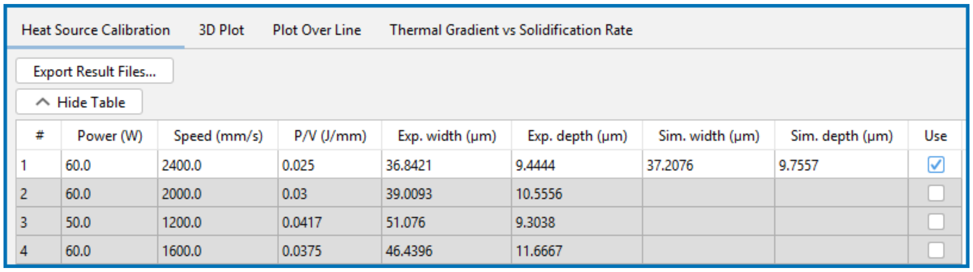
On the **Heat Source Calibration** tab (Plot Renderer) the table includes these columns:

- The original experiment data for **Power (W)** and **Speed (mm/s)**, plus the energy density **P/v (J/mm)**.
- The original experiment data for **Width** and **Depth**, now with a prefix **Exp.** to indicate this is the experimental data, e.g. **Exp. width (µm)**.
- The calculated **Width** and **Depth** points, with the prefix **Sim.** to indicate it is the result of the simulation, , e.g. **Sim. width (µm)**.

  > Only the experiment data points selected for inclusion when setting up the AM Calculator have data in these two **Sim.** columns.

- The **Use** column has a checkbox available to include or exclude those points on the *Heat Source Calibration Parameters* and *Melt Pool Dimensions* tabs on the **Visualizations** window. Furthermore, if a simulation is not used in a fit, the results from that simulation are not included to generate functions for **Heat Source Calibration** parameters.

> Only points that were originally included in the simulation can be selected or deselected from the **Use** column. If an experiment data point needs to be added, return to the AM Calculator, choose the point (s) to include there, and run the simulation again. Once the simulation is complete, the points are included in this table.



#	Power (W)	Speed (mm/s)	P/V (J/mm)	Exp. width (µm)	Exp. depth (µm)	Sim. width (µm)	Sim. depth (µm)	Use
1	60.0	2400.0	0.025	36.8421	9.4444	37.2076	9.7557	☑
2	60.0	2000.0	0.03	39.0093	10.5556			☐
3	50.0	1200.0	0.0417	51.076	9.3038			☐
4	60.0	1600.0	0.0375	46.4396	11.6667			☐

Figure 4: From example AM_06a, the Heat Source Calibration tab on the Plot Renderer for a double ellipsoidal heat source calibration for the double ellipsoidal heat source calculation. Here experiment from row #1 is included in the simulation as indicated by the white row and the check mark in the Use column. Rows 2-4 were not included in this simulation and are greyed out. When a checkbox is not selected, the results are also not included if you choose to export the result files.

Heat Source Parameters

Plot Renderer → Heat Source Calibration tab.

These are the parameters you choose on the **Plot Renderer Configuration** window. There is also a **Heat Source Calibration Parameters** tab on the **Visualizations** window that is used in combination with the table to choose data points.

The heat source parameters available to plot for each *Heat Source* type (i.e. *Gaussian*, *Double ellipsoidal*, or *Conical*) selected on the **AM Calculator**:

- *Gaussian*: **Beam radius**. Then based on the **Absorptivity** setting—**Calculated (prefactor calibrated)** or **Constant (calibrated)**—also **Absorptivity prefactor** plus additional options.
- *Double ellipsoidal*: **Absorptivity**, **ar**, **af**, **b**, and **c**
- *Conical*: **Absorptivity**, **re**, **ri**, and **H**.

There is more information about using these parameters in AM Calculator Heat Source Settings.

For all heat source parameters, you can also choose to select:

- A **Constant function** value i.e. the average value from all experiments or a function of energy density, which could also be a **Linear function**, **Cubic function**, or a **Sigmoid function**.

- A **2d cubic function P and v** of *Power* (P) and *Scanning speed* (v).
- For extrapolating outside the range of energy density as given from the experimental data, select a **Constant** value, **Extrapolate linear**, or choose **Extrapolate** for extrapolation using the same function as chosen for interpolation.
- Set the range of energy density to interpolate the heat source parameters by entering the appropriate values in the **Below P/v** and **Above P/v** fields.

There are **R2** values (the coefficient of determination) included that say how well the selected function fits the data. R2 ranges from zero to one, where `1` is a perfect match. E.g. A linear function between two points.

Once all the parameter adjustments are made, you can also retain this information for future reuse (click **Save As** or **Save**). You can also **Rename** or **Delete** these from the list as needed.

The name of the file defaults to using the *Heat Source type* + the *material type*. For example, Double ellipsoidal - 316L, or Gaussian - 316L.

Working with AM Visualizations

The AM Calculator visualization using the Plot Renderer is different from the other Calculators available in Thermo-Calc.

See Plot Types for more information for the Scheil Calculator and Diffusion Calculator, which are also used with the Additive Manufacturing (AM) Module.

About the AM Plot Types

How the Project Nodes are Connected to the Configuration and Visualizations Tabs

The following examples use a mix of adding an AM template and example AM_01 to provide an overview of how the nodes in the **Project** window are connected to the **Configuration** window settings tabs and to the different levels of tabs in the **Visualizations** window. Try this yourself either by adding an AM template or open any of the examples and click around to understand how the geometry, heat source calibration (when applicable), and various plots are connected between all the windows.

Window Connectivity

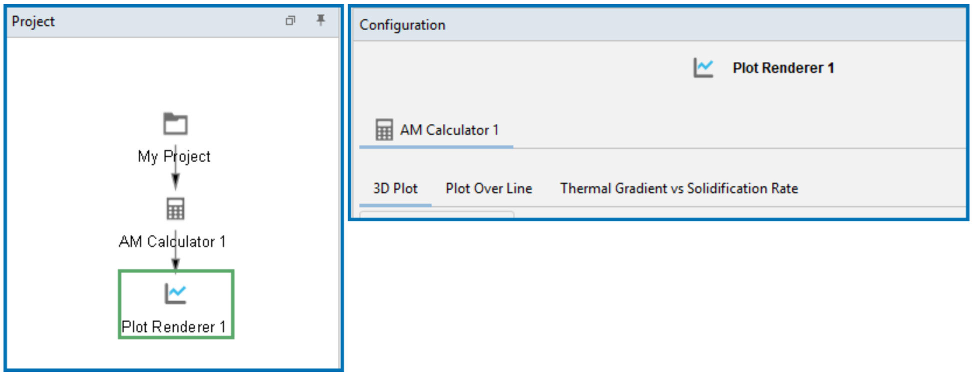
In general:

- In the **Project** window, the AM Calculator, Diffusion Calculator, and Precipitation Calculator nodes, plus all the associated successor Plot Renderer or Table Renderer nodes, are listed in the **Visualizations** window on the top level tabs using the same name as the node.
- It is recommended you rename the nodes in the Project window to meaningful names that make it easier to navigate the visualizations.
- In the **Visualizations** window, a **Geometry** tab is always associated to the **AM Calculator** node in the Project window. In addition, when a *Heat Source Calibration* calculation is chosen on the **AM Calculator**, there is also a **Heat Source Calibration** secondary level tab associated to this (at the same level as the **Geometry** tab).
- An AM Calculator and all its Plot Renderer successors are listed on the top level tab. The secondary level tab has visualizations related to geometry, heat source calibration, and the available plot types (3D Plot, Plot Over Line, Probe Plot, and the plots associated to heat source calibration).
- The Diffusion Calculator and any Plot Renderer or Table Renderer successors are all listed in the Visualizations window on the top level tab. The secondary level tab has visualizations related to the Composition Profile and Thermal Profile.
- The Precipitation Calculator and any Plot Renderer or Table Renderer successors are all listed in the **Visualizations** window on the top level tab. The secondary level tab has visualizations related to the Thermal Profile.
- The Scheil Calculator is not listed on the top level tab in the **Visualizations** window, but any Plot Renderer or Table Renderer successor for this Calculator is listed on the top level tab.
- Renaming any node in the **Project** window also renames the top level tabs in the Visualizations window.
- The second level tabs on the **Visualizations** window cannot be renamed as these represent the visualization type named by the system e.g. a geometry, plot type (3D Plot, Plot Over Line, Probe Plot, etc.), or a Composition Profile (diffusion simulations) or Thermal Profile (diffusion or precipitation simulations).

- For 2D plots (Plot Over Line 2D Plot, Probe 2D Plot), click the **Table View** button on the applicable tab in the **Visualizations** window to convert the values into a table format.

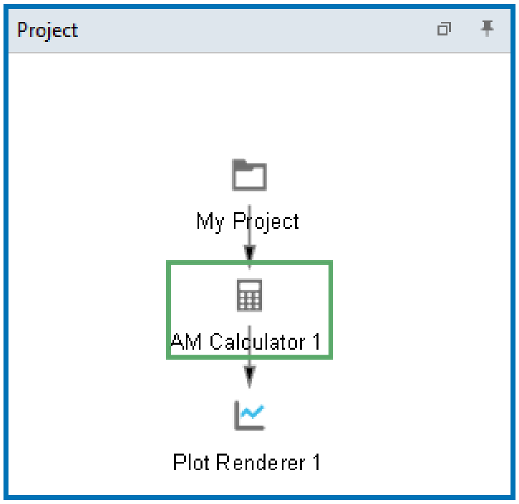
Configuration Window

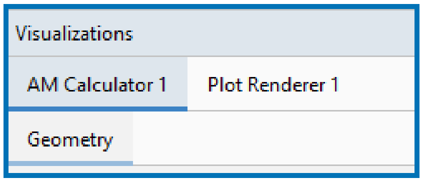
When a Plot Renderer is added to an AM Calculator in the **Project** window, there are default tabs added to the **Configuration** window where you can further set up the available plot types. In this example, two tabs, **3D Plot** and **Plot Over Line**, are provided for you to set up these plot types.



Visualizations Window

In the **Visualizations** window, the upper tab level is connected to a second level of tabs that represent the available visualizations. A **Geometry** tab is always associated to the **AM Calculator** node. Then for any **Plot Renderer** node, all of the plotting types such as a **3D Plot**, **Plot Over Line**, **Probe**, and **Thermal Gradient vs Solidification Rate** are listed in the secondary tab level.





There is not always something to visualize at the second tab level. Keep an eye on the underlined tabs on both levels, i.e. click the upper level tab and look for the underlined second level tab associated to it and that is what is displayed. Also note that clicking the upper level tabs in the Visualizations window does not change the focus of the node clicked in the Project window, although the opposite is true.

Each node in the **Project** window is represented across the top set of tabs in the **Visualizations** window. Then the associated tab on the **Visualizations** window displays below as a secondary level. For example, in the **Project** window, if you click the AM Calculator node (in AM_01 it is renamed to **Transient, DE HS**), then on the Visualizations window the **Transient, DE HS** tab is highlighted and has a blue underline. On the second tab level, the **Geometry** tab is also underlined to indicate it is associated to the **Transient, DE HS** tab. What is actually displayed in the Visualizations window is based on the second tab.

Then for each Plot Renderer added and defined, the secondary tab level is connected to what is visualized. For example, a Plot Renderer is added to the AM Calculator in the **Project** window. In this case, the node is renamed to **3D plot**. When this node is clicked in the Project window, the **3D plot** tab is highlighted and underlined in the **Visualizations** window.

You can also click each of the top level tabs in the **Visualizations** window at any time to navigate the visualizations, but the node focus in the **Project** window does not change to match.

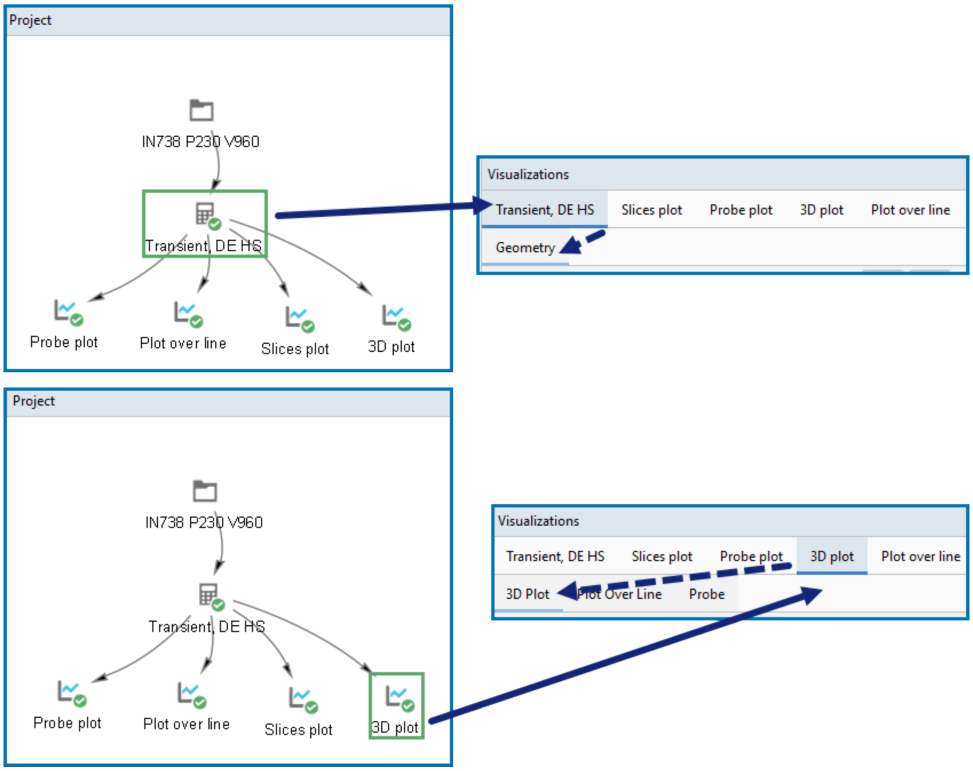
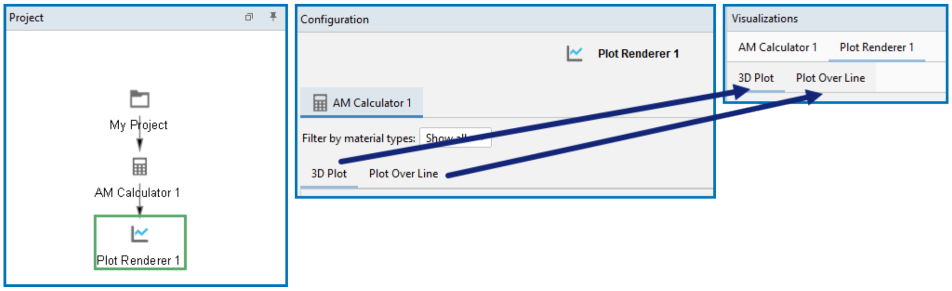


Figure 5: When you click a node in the Project window, the associated tab is highlighted and underlined in the Visualizations window. Then the second level of tabs are further underlined to indicate what is associated to the selected top level tab, and this is what actually displays in the Visualizations window.



In the **Visualizations** window, the top level tab for Plot Renderer is further connected to the **3D Plot** and **Plot Over Line** tabs. You can determine what you are actually viewing in the Visualizations window based on the upper level highlighted and underlined tab and then further by the second level underlined tab.

Visualizing Heat Source Calibrations

The following is available for a **Steady-state → Heat Source Calibration** *Calculation Type*.

About Heat Source Calibration

During the set up of the **Heat Source Calibration**, experiment data is either entered or imported to the AM Calculator. You can then view the *Heat Source Calibration* on a second level tab in the **Visualizations** window. This is associated to the AM Calculator.

Then once the experiment data is included and the heat source calibration is performed, you can further create plots on the Plot Renderer to examine the *Heat Calibration Parameters* and *Melt Pool Dimensions*.

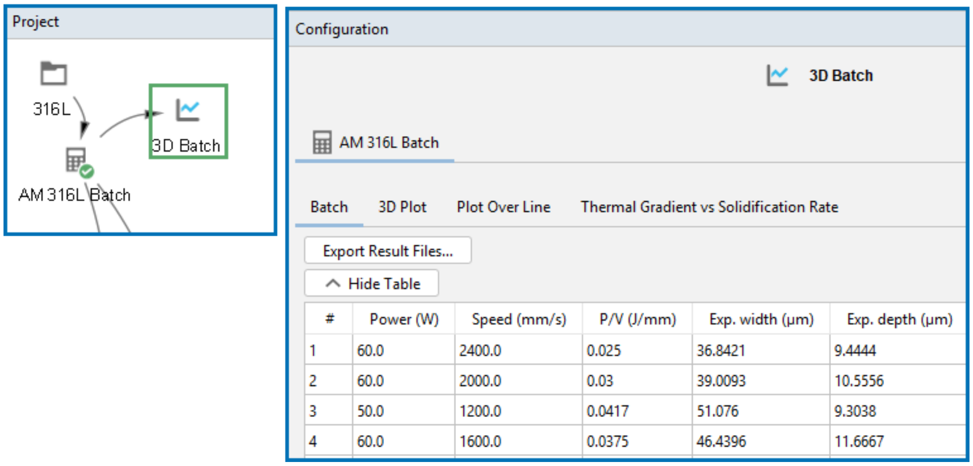
> More details about this are described in a separate topic. See Visualizing Heat Source Calibrations.

Visualizing Batch and Grid Calculations

The following is available for a **Steady-state → Batch** or **Grid** *Calculation Type*.

Results from **Steady-state** simulations using **Batch** or **Grid** calculations contain multiple steady-state results, one for each power and scan speed. The results can be visualized individually using a **3D Plot** and **Plot Over Line** (described above). The combined result from all steady-state simulations can additionally be visualized from the **Batch** tab (available on the **Plot Renderer Configuration** window after the **Batch** calculation), and similarly from the **Grid** tab after a **Grid** calculation. On these tabs you choose additional plot types **Printability map**, **Parity plot**, and **Melt pool vs energy density**.

A table of the experimental and calculated values can be viewed when you click to toggle between the **Show Table** or **Hide Table** buttons. The table is displayed in the **Plot Renderer Configuration** window for the relevant **Batch** or **Grid** tab.



#	Power (W)	Speed (mm/s)	P/V (J/mm)	Exp. width (µm)	Exp. depth (µm)
1	60.0	2400.0	0.025	36.8421	9.4444
2	60.0	2000.0	0.03	39.0093	10.5556
3	50.0	1200.0	0.0417	51.076	9.3038
4	60.0	1600.0	0.0375	46.4396	11.6667

Figure 6: The simulated and experimental melt pool dimension can also be tabulated for all data using the toggle button to Show Table or Hide Table. This is from example AM_09b.

More details about this are described in separate topics. See Visualizing Batch Calculations in the AM Module and for the various plot settings for a Grid, these are included with the general topic, AM Calculator: Plot Renderer Settings.

There is a video tutorial about the **Printability Map** on our website and on our YouTube channel. It is also included in the Additive Manufacturing Module YouTube playlist.

AM Visualizations Window Plot Toolbar

The **Visualizations** window by default has tabs included to help you visualize both the set up using the available Calculators (e.g. AM Calculator, Diffusion Calculator, and Precipitation Calculator) and the results that are calculated via a **Plot Renderer** or **Table Renderer**. For 2D plots, you can also view data by clicking the **Table View** button.

Rotate, Zoom, and Pan 3D Plots: AM Calculations

Working with AM Visualizations

Button	*Name*	*Action*
	Zoom to heat source position	Click to zoom to the heat source.

Button	*Name*	*Action*
	Set view to 3D	Click to reset the view where you zoom out to see the whole geometry.
YZ XZ XY	Set view direction to YZ, XZ, or XY	Click to orient to a side view in the • YZ-axes direction. • XZ-axes direction. • XY-axes direction.
	Azimuth rotation, Ctrl+ for invert rotation	Click to rotate around the free axis. Press and hold CTRL + click the mouse to control the direction turned.
	Elevation rotation, Ctrl+ for invert rotation	Click to rotate around the free axis. Press and hold CTRL + click the mouse to control the direction turned.
	Roll rotation, Ctrl+ for invert rotation	Rotate around the free axis Click Ctl+button to control the direction turned
	Save camera view angle and zoom level	There are two attributes that are saved when the **Save camera view angle and zoom level** button is clicked. The view angle of the camera and the zoom level. Then when you click the **Apply saved camera view and zoom level** , it mirrors the view angle of the camera and the zoom level. This is available for any 3D plot tab on the Visualizations window. Only one camera position can be saved/retained at any time for use.
	Apply saved camera view angle and zoom level	First use the **Save camera view angle and zoom level** to save the desired view. Then click the **Apply saved camera view and zoom level** button to mirror the view angle of the camera and the zoom level. This is available for any 3D plot tab on the Visualizations window. Only one camera position can be saved/retained at any time for use.
	Show grid	Click to turn on and off the mesh grid.
	Show heat source	Click to show and hide the heat source. This button also toggles displaying the **Heat Source Intensity (W/mm^2)** legend on and off in the plot area.

Button	Name	Action
	Mirror geometry	When in steady state you only see half the geometry. Click to show the whole geometry, click again to show half the geometry.
—	Hide layers	Enter a number of layers to hide
	Show Outer Box	Click to turn on and off the outer box geometry.
	Show line between powder and solid	Click to turn on and off a line and plane around the powder layer thickness.
	Show Size of the Melt Pool	Click to show or hide the melt pool. This is the same thing as showing the size of the liquidus iso-surface plot. When clicked you also see the measurements in the **Event Log** window and shows on the **Visualizations** window.
	Show Size of Melt Pool plus Mushy Zone	Click to show or hide the melt pool and mushy zone. This is the same thing as showing the size of the solidus iso-surface plot. When clicked you also see the measurements in the **Event Log** window and shows on the **Visualizations** window.
	Show Manual Ruler	Click to use the manual ruler to measure the melt flow. • Double click each time to add the start and end points. • To align a ruler on the x-, y-, or z- axis: Hold CTRL when adding or moving the end point. The ruler snaps to the closest point on the same axis. • To move a ruler: Click and hold a point, then drag to reposition. • Right-click a point to delete it.

Menu or Keyboard Options: Geometry and 3D Plots

When working with the AM Calculator (probes) and its associated Plot Renderer (for 3D Plots), there are menu options or tooltip guidelines available to access certain actions for probes, markers, or to save a snapshot image from the **Visualizations** window.

Plot- and Geometry-related Menus to Save Images

When available, right-click in the **Visualizations** window and choose **Save As** from the menu to save the current view in png, gif, or jpg format. This saves an image snapshot of the 3D Plot or Geometry at the zoom level and angle you are currently viewing.

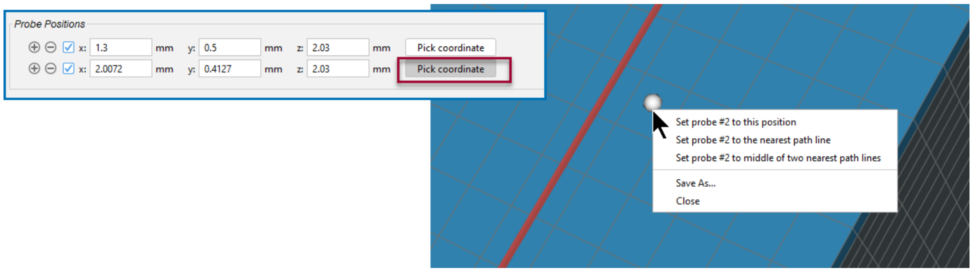
- Geometry: When setting up probes, you can right-click on the Geometry to save the current view.
- 3D Plot: When working with a 3D Plot, you can right-click anywhere on the 3D Plot to save the current view. This option is only available with AM Calculator 3D plots.

Probe-related Menus and Tooltips

AM Calculator: Working with Probe Data

When you are picking the coordinates for the probe location, there is a menu available when you right-click a point on the Geometry in the Visualizations window. There are also tooltips that can help guide you.

1. On the **Configuration** window for an **AM Calculator**, under *Probe Positions*, click **Pick coordinate**. Hover over the button to view the tooltips with options to:
    a. Double-click on the geometry to pick a coordinate.
    b. Hold the <Ctrl> key and double-click to pick the position at the middle of a layer.
    c. Hold the <Shift> key and double-click to map the picking position with a scanning path.
    d. Hold the <Shift+Alt> keys and double-click to map the picking position to the middle of the scanning path.
2. In the **Visualizations** window on the **Geometry** tab, use one of the methods to add a probe point to the geometry, for example double-click to add a probe.
3. In the **Visualizations** window, right-click to choose an option from the menu associated to the new **Pick coordinate** probe point:
    a. **Set probe to this position**: Sets to the location where the probe is located at the time of selecting.
    b. **Set probe to the nearest path line**: Moves the probe to the path line, which can be where other probes are already set up.
    c. **Set probe to the middle of the two nearest path lines**: This only works if there are two path lines, otherwise the probe does not move.
    d. **Save As...**: Select this to save an image of the current view of the probes (a snapshot at the zoom level chosen). You can save in png, gif, or jpg formats.
    e. **Close** : Closes this menu.



Probe Positions

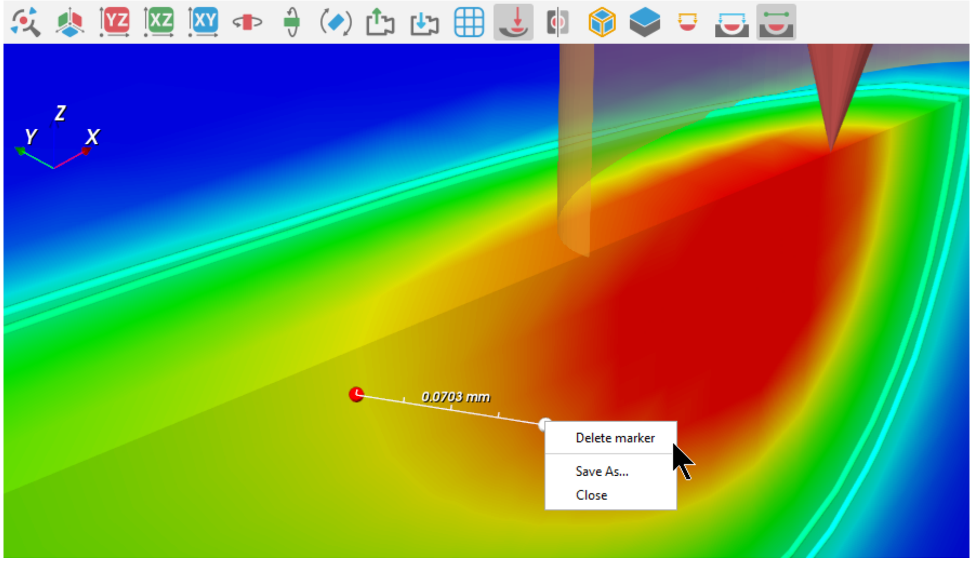
☑ x: 1.3 mm y: 0.5 mm z: 2.03 mm

☑ x: 2.0072 mm y: 0.4127 mm z: 2.03 mm

Marker-related Menus and Tooltips for 3D Plots (AM Module Only)

Markers are added to 3D plots in the **Visualizations** window. For example, you are measuring the distance between two points on a heat source.

1. On the **Visualizations** window for an AM Calculator **Plot Renderer** (and after running a **3D Plot**), click the **Show Manual Ruler** button on the toolbar. Hover over the button to view the tooltips with options to:
    a. Double-click each time to add the start and end points.
    b. To align a ruler on the x-, y-, or z-axis: Hold <Ctrl> when adding or moving the end point. The ruler snaps to the closest point on the same axis.
    c. To move a ruler: Click and hold a point, then drag to reposition.
    d. Right-click a point to delete the ruler.
2. Click in the plot area to add markers for the start and end points, for example. Once the marker is on the plot, you can delete it or save an image of the plot at the current view.
    - To delete a marker, zoom as close to it as possible and right-click the marker to bring up the menu. Select **Delete marker** from the list. You might have to move the mouse around the area of the marker or zoom further to access the menu options.
    - To save an image of the plot at the current view, click anywhere in the plot and select **Save as**. Select this to save an image in png. gif, or jpg format.



Rotate, Zoom, and Pan 3D Plots: AM Calculations

When working with the Additive Manufacturing (AM) Module and the results from an AM Calculator simulation, two general plot types are added to the **Visualizations** window: a *3D plot* and a *Plot over line 2D plot*. The 2D plot has the same functionality as for other calculations but the 3D plot is specific to this Module.

In addition to the **Visualizations** window for an AM 3D plot having its own set of buttons (see AM Visualizations Window Plot Toolbar) there are also different ways to work with the 3D plots with respect to rotating, zooming, and panning the geometry around the window.

- In combination with the following actions use these buttons on the toolbar:

  Set View to 3D

  Set View Direction YZ XZ XY .

- **Rotate the geometry** : Left-click and hold the mouse, then move it around the window to rotate in any direction. Hold CTRL + left mouse button to rotate on a specific axis.
- **Zoom in and out**: Scroll the mouse wheel or right-click and move the mouse up and down in the window.
- **Pan the geometry**: Hold Shift + left mouse button then move the mouse up or down, left or right, to move the geometry around the window without zooming.

Go to the Help (press F1 in Thermo-Calc) to view a short video showing the use of these actions.

Overlaying Plots in the AM Module

In general, it is now possible to overlay plots from any Calculator with plots from any other Calculator.

2D plots are overlaid pair-wise which means if you add two or more AM Calculators as a predecessor in one Plot Renderer, similar 2D plots (such as Probe with Probe and Plot Over Line with Plot Over Line, etc.) are grouped and overlaid in one tab on the Visualizations window.

The most important use case is that you can overlay Probe plots from different Transient and Transient with heat source from Steady-state Calculators and Plot Over Line plots from all AM Calculators. Similarly, you can also overlay Meltpool vs energy density and Parity plot from different Batch, Grid, and Heat Source Calibration calculators.

You need to click **Perform** to make plot overlaying work.

It is not possible to overlay two 3D plots. However, when you want to plot two or more variables in a comparable way to overlaying plots in 2D, you use one **Plot Renderer** connected to at least two AM Calculators. Then on the **3D Plot** tab on the **Configuration** (settings) window you choose different quantities from the **Axis variable** list. Use the ⊕ and ⊖ buttons as usual to add and remove quantities. The plots are then viewed on separate **3D Plot** tabs on the **Visualizations** window. After defining the axis variables, click **Perform** to update the plots on the respective **Visualization 3D Plot** tabs. It is also important to rename your AM Calculators in order to better work with these plots.

Visualizing Heat Source Calibrations

This topic describes both the **AM Calculator** and the **Plot Renderer** visualization outcomes related to the heat source calibration calculations for a **Steady-state** simulation.

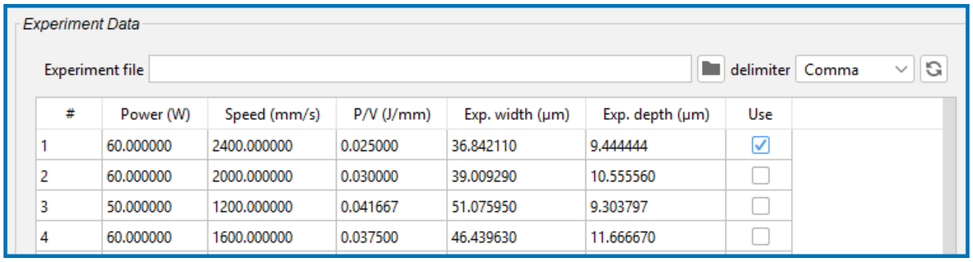
To import data for use in batch calculations, it is recommended you review AM Calculator Experiment File Requirements. Also review Working with AM Visualizations, which provides an overview of how most of the windows are connected.

It is recommended to open and run one of the examples to best understand the wide variety of visualization outcomes.

AM_06a: Calibrating a Heat Source for a 316L Steel and AM_06b: Using the Calibrated Heat Source for a 316L Steel

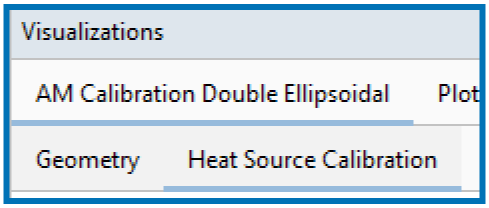
Working with AM Calculator Heat Source Calibration Experiment Data

During the set up of the **Heat Source Calibration**, experiment data is either entered or imported to the **AM Calculator** table where it is visible on its associated **Configuration** window.



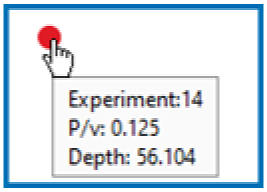
#	Power (W)	Speed (mm/s)	P/V (J/mm)	Exp. width (μm)	Exp. depth (μm)	Use
1	60.000000	2400.000000	0.025000	36.842110	9.444444	☑
2	60.000000	2000.000000	0.030000	39.009290	10.555560	☐
3	50.000000	1200.000000	0.041667	51.075950	9.303797	☐
4	60.000000	1600.000000	0.037500	46.439630	11.666670	☐

Click the relevant AM Calculator node in the **Project** window to preview the table data via a **Heat Source Calibration** tab on the **Visualizations** window.



Use the table's **Use** column on the AM Calculator Configuration window to select the relevant checkboxes for which **Width** and **Depth** points to include (i.e. *use*) or exclude (i.e. *not use*).

You can click or hover over any point on the **Heat Source Calibration** preview to display the label, which also includes the corresponding table row (i.e. *Experiment*) number for the point.



Experiment:14
P/v: 0.125
Depth: 56.104

On the **Heat Source Calibration** window :

- For this calibration view, **Width** uses blue squares (solid color means used, hollow with same color outline means not used)
- For this calibration view, **Depth** uses red circles (solid color means used, hollow with same color outline means not used)
- The preview shows the energy density (P/v) on the *X*-axis and melt pool dimensions on the *Y*-axis.

Click to select or deselect checkboxes in the table to dynamically watch the selection change on the **Visualizations** window. The points that are selected in this table are used in the simulation results and are later labeled **Exp.Width** and **Exp.Depth** in the Plot Renderer Configuration table (see Figure 9). Then the calculated results are added to new columns labeled **Sim.Width** and **Sim.Depth** in the data table on the Plot Renderer Configuration window (see below).

> Sometimes an experiment data point is selected in the table on the AM Calculator but after running the simulation it is not available in the corresponding Plot Renderer table (i.e. it is a greyed out row). This indicates that the calibration could not be calculated for that particular data point.

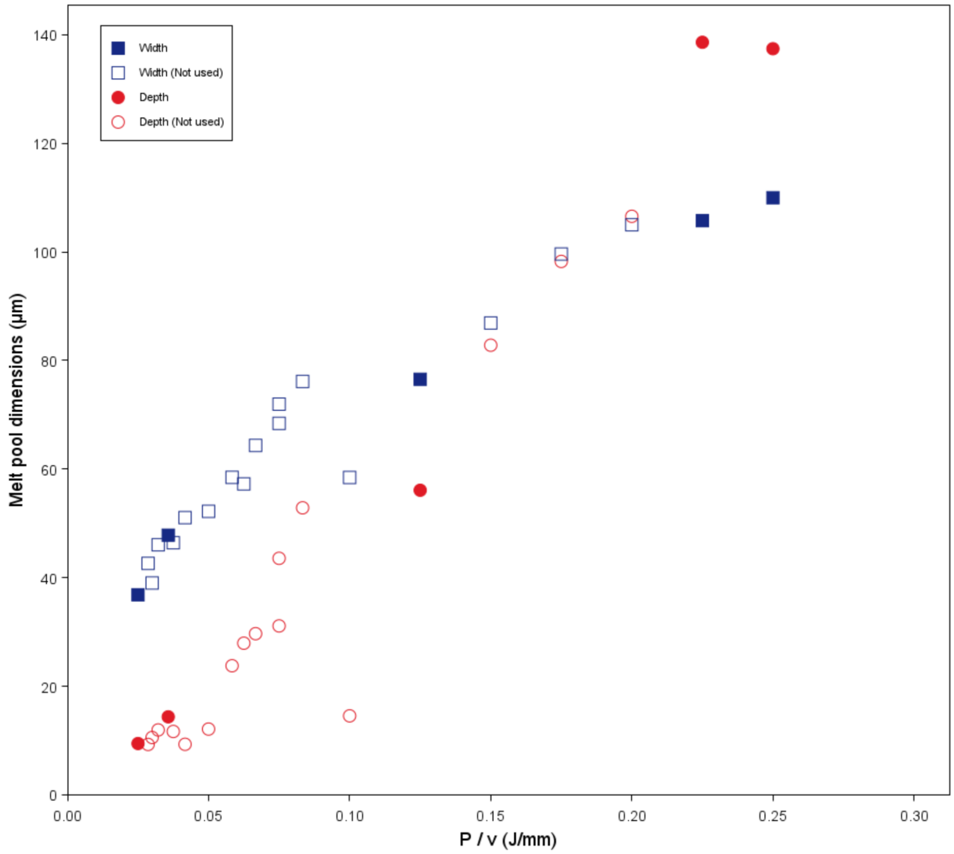
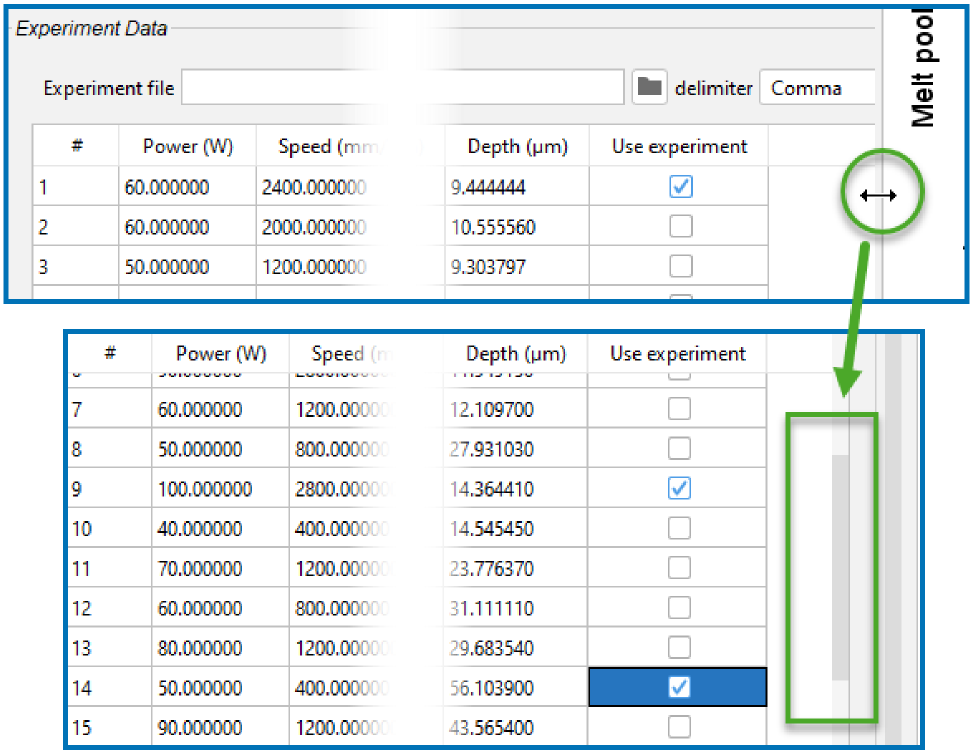


Figure 7: From example AM_06a, this is the heat source calibration preview for the data imported to the AM Calculator node (renamed to AM Calibration Double Ellipsoidal). As per the legend, both "used" (solid color) and "not used" (hollow with outline color) points are included in this preview.

Once a set of data is imported to the table (or entered manually), expand the **Configuration** window to reveal the scroll bars. Then you can scroll up or down, left or right, within the table to select checkboxes for the relevant data points you want to include or exclude. This is applicable to the tables found on the AM Calculator as well as those on the Plot Renderer for the data.



Experiment Data

Experiment file: delimiter Comma

#	Power (W)	Speed (mm	Depth (µm)	Use experiment
1	60.000000	2400.000000	9.444444	☑
2	60.000000	2000.000000	10.555560	☐
3	50.000000	1200.000000	9.303797	☐

#	Power (W)	Speed (m	Depth (µm)	Use experiment
7	60.000000	1200.00000	12.109700	☐
8	50.000000	800.000000	27.931030	☐
9	100.000000	2800.00000	14.364410	☑
10	40.000000	400.000000	14.545450	☐
11	70.000000	1200.00000	23.776370	☐
12	60.000000	800.000000	31.111110	☐
13	80.000000	1200.00000	29.683540	☐
14	50.000000	400.000000	56.103900	☑
15	90.000000	1200.00000	43.565400	☐

Working with the Plot Renderer for Heat Source Calibrations

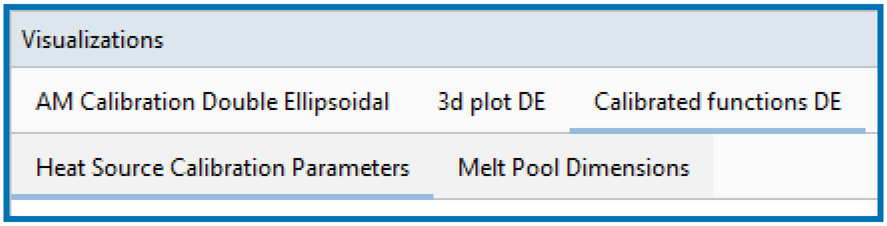
After the calibration is completed on the AM Calculator and the simulation run, then on the **Plot Renderer Configuration** window you can start to use the data.

For additional **Plot Renderer** settings (and other visualization options for plotting) go to AM Calculator: Plot Renderer Settings.

Adding the Heat Source Calibration Plots

1. Add a **Plot Renderer** to the **AM Calculator**.
2. Choose an experiment point from the **Heat Source Calibration** list. The points in this list match the points selected in the **Use** column on the **AM Calculator**.
3. Click **Perform**.
4. Click the **Heat Source Calibration** tab on the **Plot Renderer Configuration** window to (1) view the table of data and (2) view the *Heat Source Calibration Parameters* and *Melt Pool Dimensions* tabs in the **Visualizations** window on the secondary level of tabs. These tabs are where you fine-tune the choice of data points: Click the

checkbox for the **Use** column for each row (experiment #) to observe the dynamic changes on the **Heat Source Calibration Parameters** and **Melt Pool Dimensions** tabs on the **Visualizations** window.



Navigating the Heat Source Calibration Table

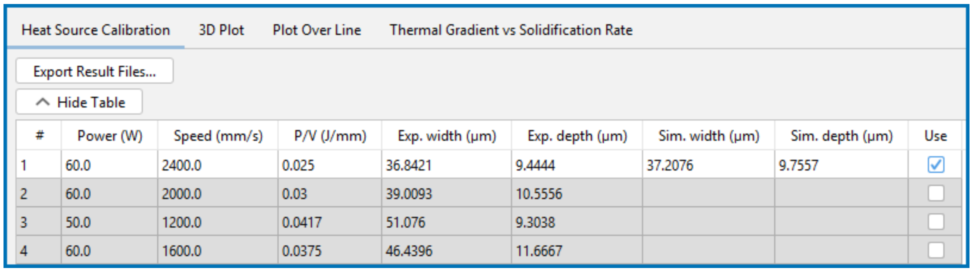
On the **Heat Source Calibration** tab (Plot Renderer) the table includes these columns:

- The original experiment data for **Power (W)** and **Speed (mm/s)**, plus the energy density **P/v (J/mm)**.
- The original experiment data for **Width** and **Depth**, now with a prefix **Exp.** to indicate this is the experimental data, e.g. **Exp. width (µm)**.
- The calculated **Width** and **Depth** points, with the prefix **Sim.** to indicate it is the result of the simulation, , e.g. **Sim. width (µm)**.

Only the experiment data points selected for inclusion when setting up the AM Calculator have data in these two **Sim.** columns.

- The **Use** column has a checkbox available to include or exclude those points on the *Heat Source Calibration Parameters* and *Melt Pool Dimensions* tabs on the **Visualizations** window. Furthermore, if a simulation is not used in a fit, the results from that simulation are not included to generate functions for **Heat Source Calibration** parameters.

Only points that were originally included in the simulation can be selected or deselected from the **Use** column. If an experiment data point needs to be added, return to the AM Calculator, choose the point (s) to include there, and run the simulation again. Once the simulation is complete, the points are included in this table.



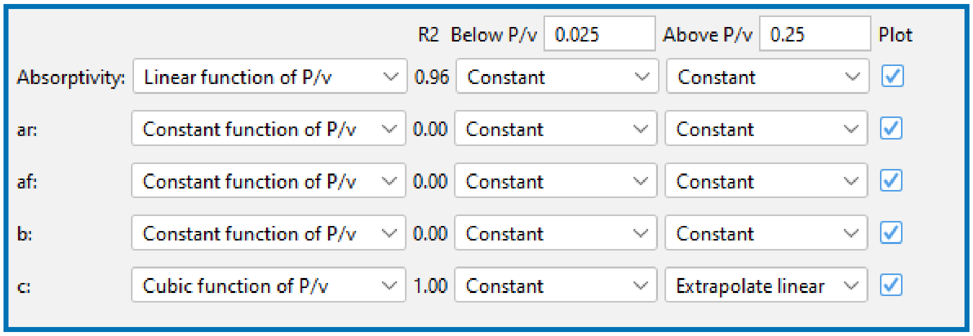
#	Power (W)	Speed (mm/s)	P/V (J/mm)	Exp. width (µm)	Exp. depth (µm)	Sim. width (µm)	Sim. depth (µm)	Use
1	60.0	2400.0	0.025	36.8421	9.4444	37.2076	9.7557	☑
2	60.0	2000.0	0.03	39.0093	10.5556			☐
3	50.0	1200.0	0.0417	51.076	9.3038			☐
4	60.0	1600.0	0.0375	46.4396	11.6667			☐

Figure 8: From example AM_06a, the Heat Source Calibration tab on the Plot Renderer for a double ellipsoidal heat source calibration for the double ellipsoidal heat source calculation. Here experiment from row #1 is included in the simulation as indicated by the white row and the check mark in the Use column. Rows 2-4 were not included in this simulation and are greyed out. When a checkbox is not selected, the results are also not included if you choose to export the result files.

Working with the Heat Source Calibration Parameters

Based on the type of heat source selected on the AM Calculator, below the *Heat Source Calibration* table there are additional parameters you can choose to include or exclude from the *Heat Source Calibration Parameters* and *Melt Pool Dimensions* plots.

Once the selection of experiments is made in the **Configuration** window for the **Heat Source Calibration**, you can choose appropriate functions for each heat source parameter including the absorptivity. See Figure 9 for an example of the available parameters for a **Double ellipsoidal** *Heat Source*.



		R2	Below P/v 0.025	Above P/v 0.25	Plot
Absorptivity:	Linear function of P/v	0.96	Constant	Constant	☑
ar:	Constant function of P/v	0.00	Constant	Constant	☑
af:	Constant function of P/v	0.00	Constant	Constant	☑
b:	Constant function of P/v	0.00	Constant	Constant	☑
c:	Cubic function of P/v	1.00	Constant	Extrapolate linear	☑

Figure 9: From example AM_06a, these are the available parameters for a double ellipsoidal heat source simulation. The available parameters are based on the heat source chosen on the AM Calculator during set up.

Click to select or deselect the **Plot** checkbox and watch the change on the **Visualizations** window for both the *Heat Source Calibration Parameters* and *Melt Pool Dimensions* plots. There are several options to choose from in this section that each change the plots dynamically.

The heat source parameters available to plot for each *Heat Source* type (i.e. *Gaussian*, *Double ellipsoidal*, or *Conical*) selected on the **AM Calculator**:

- *Gaussian*: **Beam radius**. Then based on the **Absorptivity** setting—**Calculated (prefactor calibrated)** or **Constant (calibrated)**—also **Absorptivity prefactor** plus additional options.
- *Double ellipsoidal*: **Absorptivity**, **ar**, **af**, **b**, and **c**
- *Conical*: **Absorptivity**, **re**, **ri**, and **H**.

There is more information about using these parameters in AM Calculator Heat Source Settings.

For all heat source parameters, you can also choose to select:

- A **Constant function** value i.e. the average value from all experiments or a function of energy density, which could also be a **Linear function**, **Cubic function**, or a **Sigmoid function**.
- A **2d cubic function P and v** of *Power* (P) and *Scanning speed* (v).

- For extrapolating outside the range of energy density as given from the experimental data, select a **Constant** value, **Extrapolate linear**, or choose **Extrapolate** for extrapolation using the same function as chosen for interpolation.
- Set the range of energy density to interpolate the heat source parameters by entering the appropriate values in the **Below P/v** and **Above P/v** fields.

There are **R2** values (the coefficient of determination) included that say how well the selected function fits the data. R2 ranges from zero to one, where `1` is a perfect match. E.g. A linear function between two points.

Once all the parameter adjustments are made, you can also retain this information for future reuse (click **Save As** or **Save**). You can also **Rename** or **Delete** these from the list as needed.

The name of the file defaults to using the *Heat Source type* + the *material type*. For example, Double ellipsoidal - 316L, or Gaussian - 316L.

Visualizations Window

Heat Source Calibration Parameters Plot

A **Heat Source Calibration Parameters** plot shows the calibrated heat source parameters as a function of energy density (P/v) (unit J/mm). From the **Plot Renderer Configuration** window, you can also continue to select which experiments to be used to fit the calibration.

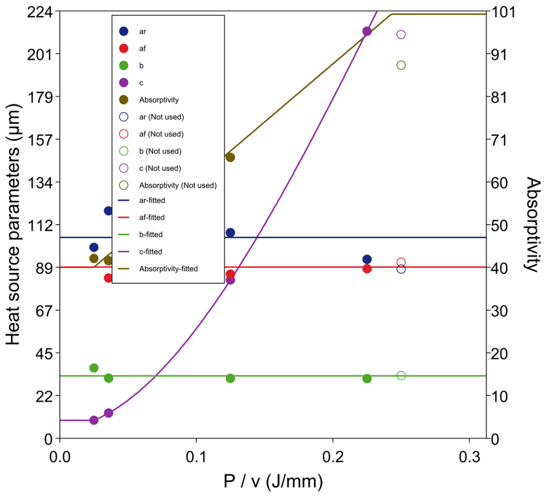


Figure 10: From example AM_06a, the Heat Source Calibration Parameters plot for the double ellipsoidal calibration.

For instance, you can deselect the points that seem to be outliers or where the error bar in experimental data is large.

The selection is done via the checkboxes available in the **Use** column.

Melt Pool Dimensions Plot

A **Melt Pool Dimensions** plot shows melt pool size, both from experiments and simulations, as a function of energy density (P/v). This plot can be used to compare the results from the experiments and optimization simulations.

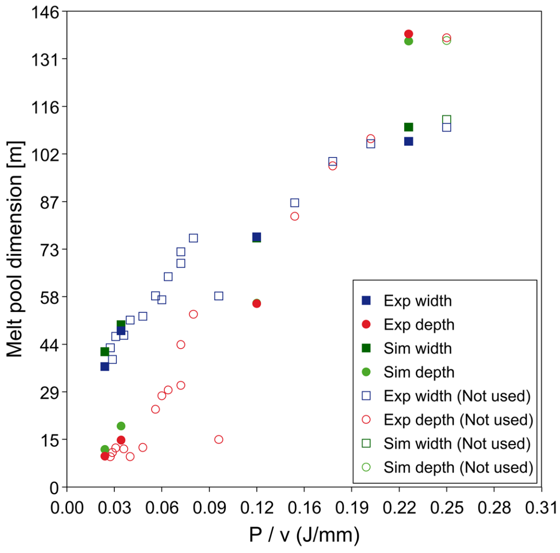


Figure 11: From example AM_06a, the Melt Pool Dimensions plot for the double ellipsoidal calibration.

3D Plot and Plot Over Line

Use a **3D Plot** to visualize all the experiments for which the calibration is performed. To show the 3D plot for a certain experiment, select the corresponding experiment from the **Heat Source Calibration Experiments** menu. The configuration in the **3D Plot** works in the same way as for a single point steady-state calculation.

For **Plot Over Line**, plot the data along a line for the selected experiment. To show the plot over line for a specific experiment, select the corresponding experiment from the **Heat Source Calibration Experiments** menu. The configuration in the **Plot Over Line** works in the same way as for a single point steady-state calculation.

? About the AM Plot Types

Visualizing Batch Calculations in the AM Module

This topic describes the **AM Calculator** visualizations related to the **Batch** calculations for a **Steady-state** simulation. There are further settings and visualization possibilities s that are available when you are working on the **Plot Renderer**.

To import data for use in batch calculations, it is recommended you review AM Calculator Experiment File Requirements. Also review Working with AM Visualizations, which provides an overview of how most of the windows are connected.

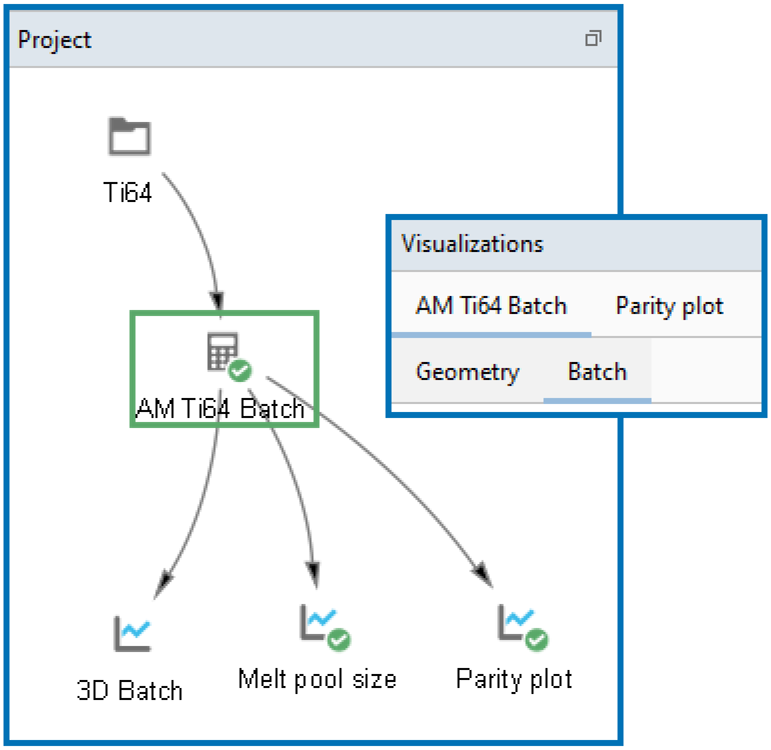
It is recommended to open and run one of the examples to best understand the wide variety of visualization outcomes.

AM_07: Batch Calculations for an IN718 Alloy, AM_08b: Batch Calculations for a Ti64 Alloy, and AM_09b: Batch Calculations for an SS316L Alloy.

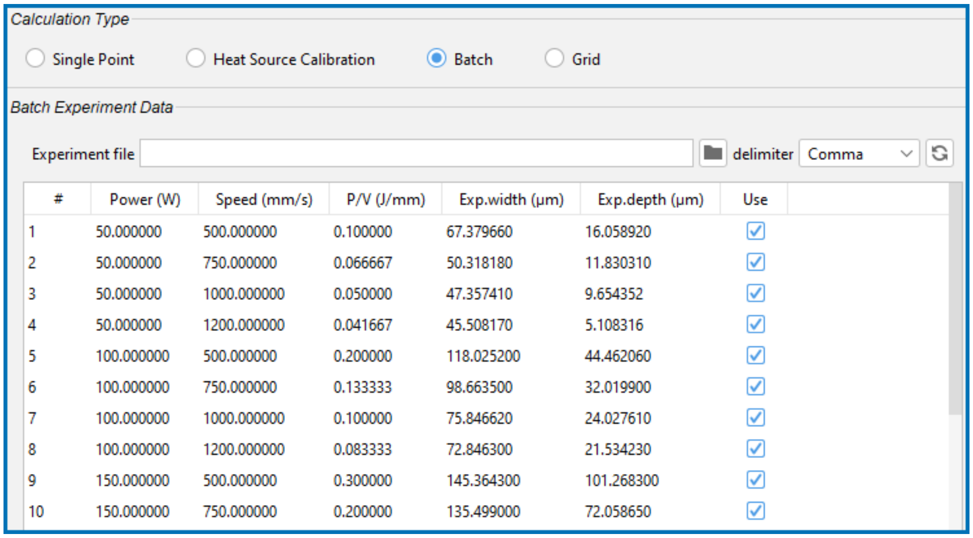
Working with AM Calculator Batch Experiment Data

From example AM_08b, where the general behavior related to importing data to the table is the same as other places in Thermo-Calc.

In the **Project** window, click the relevant **AM Calculator** node (in this example renamed to **AM Ti64 Batch**) to work on the **Configuration** window and preview the table data via a **Batch** tab on the **Visualizations** window.



During the set up of a calculation, the *Batch Experiment Data* is imported into the **AM Calculator Configuration** window, where you can review the data and choose to include or exclude data points by selecting and deselecting the checkboxes as needed in the **Use** column (see Figure 12). At the same time, you can observe the change as this is updated in the **Visualizations** window (see Figure 13). Data can also be entered directly into the table.



Calculation Type

○ Single Point ○ Heat Source Calibration ● Batch ○ Grid

Batch Experiment Data

Experiment file: delimiter: Comma

#	Power (W)	Speed (mm/s)	P/V (J/mm)	Exp.width (µm)	Exp.depth (µm)	Use
1	50.000000	500.000000	0.100000	67.379660	16.058920	☑
2	50.000000	750.000000	0.066667	50.318180	11.830310	☑
3	50.000000	1000.000000	0.050000	47.357410	9.654352	☑
4	50.000000	1200.000000	0.041667	45.508170	5.108316	☑
5	100.000000	500.000000	0.200000	118.025200	44.462060	☑
6	100.000000	750.000000	0.133333	98.663500	32.019900	☑
7	100.000000	1000.000000	0.100000	75.846620	24.027610	☑
8	100.000000	1200.000000	0.083333	72.846300	21.534230	☑
9	150.000000	500.000000	0.300000	145.364300	101.268300	☑
10	150.000000	750.000000	0.200000	135.499000	72.058650	☑

Figure 12: The experimental data used for the Batch calculation for the single track experiments of Ti64 is imported to the AM Calculator table where you can review the data points and include or exclude as needed using the checkboxes.

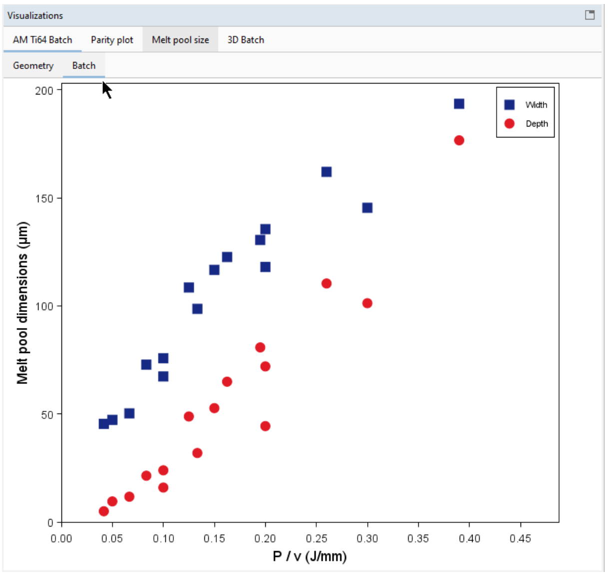
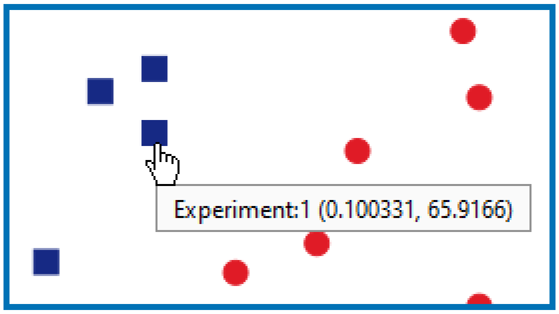


Figure 13: The visualization of the experimental melt pool dimensions are shown as a function of the energy density P/v. You can adjust the selected points in the Batch Experiment Data table and watch the updates dynamically in this window.

Including or Excluding Data Points

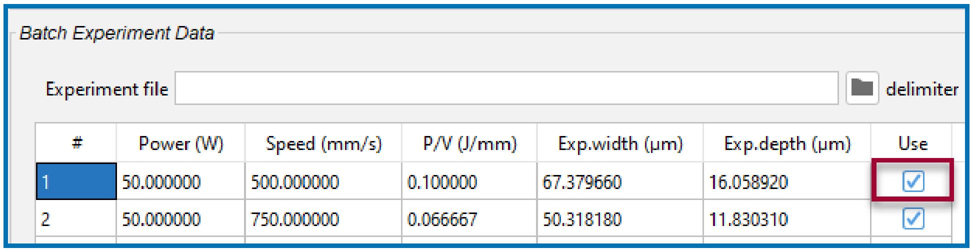
The following discusses visualization options available on the **Configuration** windows for both the **AM Calculator** and **Plot Renderer**.

You can click or hover over any point on the **Batch** preview to display the label, which also includes the corresponding table row (i.e. *Experiment*) number for the point.



Experiment:1 (0.100331, 65.9166)

Use the table's **Use** column on the **AM Calculator Configuration** window to select the relevant checkboxes for which **Width** and **Depth** points to include (i.e. *use*) or exclude (i.e. *not use*).



Batch Experiment Data

Experiment file

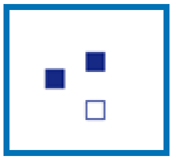
#	Power (W)	Speed (mm/s)	P/V (J/mm)	Exp.width (µm)	Exp.depth (µm)	Use
1	50.000000	500.000000	0.100000	67.379660	16.058920	☑
2	50.000000	750.000000	0.066667	50.318180	11.830310	☑

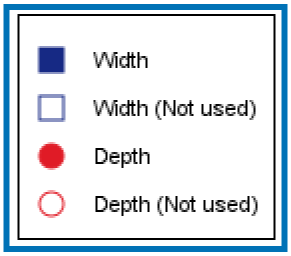
Figure 14: From example AM_08b, on the AM Calculator, the checkbox for row (experiment) #1 can be deselected to exclude the data point in the calculations.

On the **Batch** tab on the **Visualizations** window, the preview shows the **P/v** on the *X*-axis and **Melt pool dimensions** on the *Y*-axis:

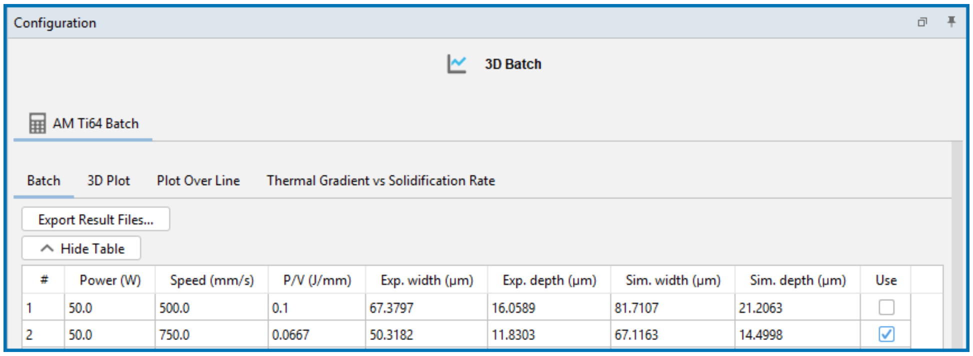
- **Width** uses blue squares (solid color means used, hollow with same color outline means not used)
- **Depth** uses red circles (solid color means used, hollow with same color outline means not used)

When you toggle the **Use** checkbox selection, the preview dynamically updates in the **Visualizations** window to indicate which data points are used (filled) or not used (hollow), both on the preview and in the legend.





The points that are selected in the *Batch Experiment Data* table are used in the simulation results and are later labeled **Exp.Width** and **Exp.Depth** in the **Plot Renderer Configuration** table (see Figure 15). Then the calculated results are added to new columns labeled **Sim.Width** and **Sim.Depth**.



#	Power (W)	Speed (mm/s)	P/V (J/mm)	Exp. width (µm)	Exp. depth (µm)	Sim. width (µm)	Sim. depth (µm)	Use
1	50.0	500.0	0.1	67.3797	16.0589	81.7107	21.2063	☐
2	50.0	750.0	0.0667	50.3182	11.8303	67.1163	14.4998	☑

Figure 15: From example AM_08b, this is the Batch tab on the Plot Renderer Configuration window where row (experiment) #1 data point is excluded from the results after selecting it on the AM Calculator. When a checkbox is not selected here, the results are also not included if you choose to export the result files. The details about Plot Renderer settings are in the topicAM Calculator: Plot Renderer Settings.

Working with the Batch Table on the Plot Renderer

After the **Batch Experiment Data** set up is completed on the **AM Calculator** and the simulation run, then on the **Plot Renderer Configuration** window you can start to work with the data you want to plot. Also see Including or Excluding Data Points to understand the interaction between these two tables.

For additional **Plot Renderer** settings (and other visualization options for plotting) go to Batch Calculations.

Navigating the Batch Table

You may have already included or excluded data points earlier when previewing the data. Use the **Show Table** or **Hide Table** buttons to view the included or excluded data and continue to fine tune the plot.

On the **Batch** tab the table includes these columns:

- The original experiment data for **Power (W)** and **Speed (mm/s)**, plus the **P/v (J/mm)**.
- The original experiment data for **Width** and **Depth**, now with a prefix **Exp.** e.g. **Exp.width (µm)**, to indicate this is the experimental data.
- The calculated **Width** and **Depth** points, with the prefix **Sim.**, e.g. **Sim.width (µm)**, to indicate it is the result of the simulation.

> Only the experiment data points selected for inclusion when setting up the AM Calculator have data in these two **Sim.** columns.

- The **Use** column has a checkbox available to continue to include or exclude those points on the plots. When a checkbox is not selected, the results are also not included if you choose to export the result files.

> Only points that were originally included in the simulation can be selected or deselected from the **Use** column. If an experiment data point needs to be added, return to the AM Calculator, choose the point (s) to include there, and run the simulation again. Once the simulation is complete, the points are included in this table.

The Process Metallurgy Module

In this section:

About the Process Metallurgy Module

The Process Metallurgy Module is an Add-on Module to Thermo-Calc and it is available in Graphical Mode as the *Process Metallurgy Calculator*. The Add-on Module is designed to model reactions that occur in metallurgical processes. Although primarily used in steelmaking and steel refining processes—such as basic oxygen furnaces, electric arc furnaces, ladle furnace metallurgy, and so forth—applications are not limited to steelmaking.

There are two main branches of calculations possible: **Equilibrium** and **Process simulation**. Equilibrium calculations do not consider any kinetics, the process simulation includes reaction kinetics.

In general, for both types, the main difference compared to using a standard Equilibrium Calculator is that it is easy to handle the different materials present in a metallurgical process. The materials used in the process can be pre-defined, saved and used for the equilibrium calculations. Metallic materials can be defined in element weight percent, oxide materials in weight percent of oxide components, the gas phase in volume percent of gas components and its amount can be defined in normal cubic meters, and so forth. In principle this can be done in a standard Equilibrium Calculator. However, it is much easier when using the Process Metallurgy Calculator as this is designed for this specific purpose.

When using the **Equilibrium** branch of calculations, both isothermal and adiabatic calculations are possible. Adiabatic calculations assume no heat and mass exchange with the environment during the equilibrium reaction, meaning that the temperature changes as a result of exothermal or endothermal reactions taking place.

For a **Process simulation** branch of calculation, the reaction kinetics of the process are considered. This is done by dividing the system into zones. Typically one would have one steel zone containing liquid metal and a slag zone containing liquid oxide (slag). The kinetic model assumes that only a fraction of the steel zone reacts with a fraction of the slag zone per time step. This reacting fraction of the whole system is termed the reaction zone (in literature it has become known as Effective Equilibrium Reaction Zone or EERZ).

You can use the Process Metallurgy Module to calculate the following:

- The equilibrium between custom-defined steels, slags, and gasses.
- The equilibrium between other metallic and non-metallic phases.
- Desulfurization, dephosphorization, and decarburization.
- Any partition coefficient, for example the partitioning of sulfur between the liquid steel and slag phase.
- Slag characteristics, such as slag basicity or sulfur capacity.
- The fraction of liquid and solid in the slag.

- The temperature change in an adiabatic process.
- Kinetics of the reaction between phases. Typically this is the reaction between a liquid metal and slag phase, but it could also be the reaction between a solid oxide and slag (simulation of refractory wear) or between a solid metal and liquid metal (simulation of dissolution of alloy), etc.

The Process Metallurgy Module requires both a valid Maintenance and Support Subscription (M&SS) and a license for the TCS Metal Oxide Solutions Database (TCOX8 or newer).

All users can test the Process Metallurgy Module with the included OXDEMO database, which is limited to these elements: Al, C, Ca, Fe, O, S, and Si. For more information about this and other products visit our website.

Available Options with the Process Metallurgy Module

The Process Metallurgy Module is an Add-on Module to the core Thermo-Calc software.

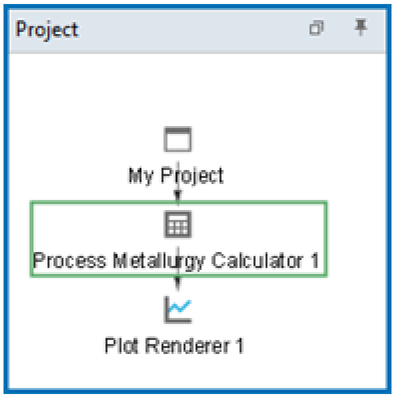
A separate license is required to perform calculations for more than three elements. Without it you are able to use the module in *Demo Mode*.

Process Metallurgy Template

A **Process Metallurgy** template under **Applications** is available to all Thermo-Calc users when in Graphical Mode. If you are in DEMO mode then this is indicated by the addition of **DEMO** text.

Using the Template

After opening Thermo-Calc in Graphical Mode, in the templates section under **Applications** click **Process Metallurgy** to add a *System Definer*, *Process Metallurgy Calculator*, and *Plot Renderer* to the **Project** tree.



Creating a Project from a Template

Process Metallurgy Calculator

A Process Metallurgy Calculator allows you to set the conditions for, and perform, a process metallurgy calculation.

Demonstration (Demo) Mode

The Process Metallurgy Module, and some examples, are available to all Thermo-Calc users but only for simulations of alloys with up to three elements. If you do not have a license for the Process Metallurgy Module then you are in *Demonstration Mode* when using the Process Metallurgy Calculator or its template.

Process Metallurgy Template

A **Process Metallurgy** template under **Applications** is available to all Thermo-Calc users when in Graphical Mode. If you are in DEMO mode then this is indicated by the addition of **DEMO** text.

Process Metallurgy Calculator

If you are experimenting with the Process Metallurgy Calculator in Demo Mode, you may have access to a variety of databases based on your license. However, you can only define up to three elements for a demo simulation.

If you define more than three elements and try to run the simulation the **Event Log** displays an error message.

Network License Restrictions

The Process Metallurgy Module requires a separate license. If you are using a network client installation of Thermo-Calc, then you may not be able to use it even if you have access to a license server with a valid network license file. The reason for this is because other clients who are part of your network installation may have checked out all instances of the network license allowed to run simultaneously.

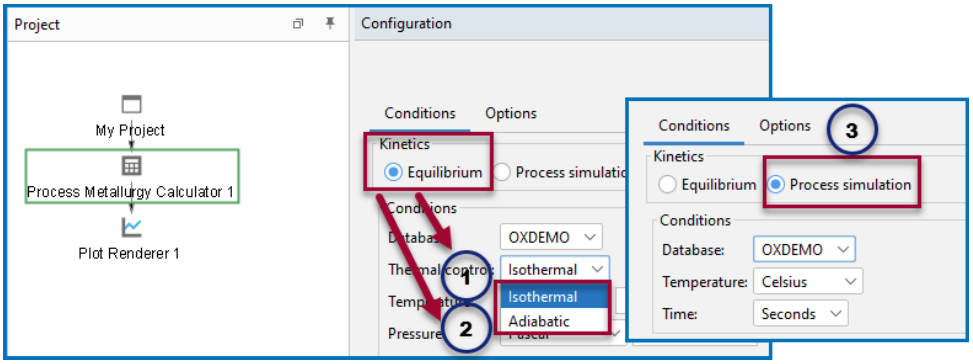
For users with a network license, you must exit Thermo-Calc to release the license for other users. The license is checked out as soon as you add a Process Metallurgy Calculator and remains unavailable to other users until you exit the program.

With a network license, and if as per above you temporarily do not have access to a license, you are automatically put into *Demo Mode*. Then the Process Metallurgy Calculator is available with three elements.

Search the online help or see the *Thermo-Calc Installation Guide* for more about network licenses.

Setting Up a Process Metallurgy Simulation

The following basic steps need to be carried out to set up calculations in the **Process Metallurgy Calculator**. There are three branches of simulation to choose from on the **Configuration** window when setting up the simulation an isothermal equilibrium calculation, an adiabatic equilibrium calculation, and a process simulation.



Database: OXDEMO

Thermal control: Isothermal

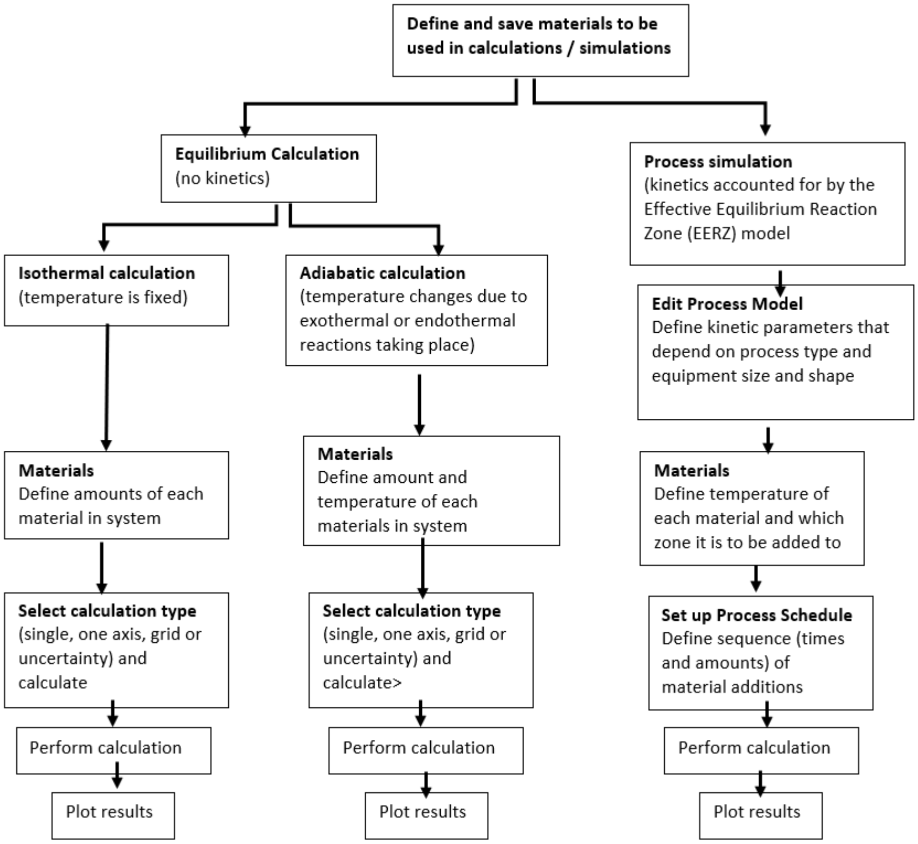
Temperature: Celsius

Time: Seconds

Examples of using the Process Metallurgy Calculator for Basic Oxygen Furnace (BOF) (with and without kinetics), a Ladle Furnace (LF) simulation, an Argon Oxygen Decarbarization (AOD), and a Vacuum Oxygen Decarborization (VOD) simulation are included with your installation. See the Process Metallurgy Module Examples Collection for links.

You can find several learning resources on the Process Metallurgy page of our website (or in Thermo-Calc, go to **Help → Thermo-Calc website**). You can also subscribe to the Thermo-Calc newsletter to be kept up-to-date about upcoming releases, training, examples, videos and much more.

Isothermal and Adiabatic Equilibrium Calculations and Process Simulation Options



The three branches of simulations available for the Process Metallurgy Calculator (1) an isothermal equilibrium calculation, (2) an adiabatic equilibrium calculation, and (3) a process simulation.

Equilibrium Simulations

Two **Equilibrium** simulation types are available: **Isothermal** and **Adiabatic**. In general for the equilibrium simulation, the three most common material groups—*Steel*, *Slag*, and *Gas*—are automatically included with the default composition input types that are relevant to each material group. You can add materials and save your material compositions directly from the Process Metallurgy Calculator and quickly access these for other simulations. For example, you might want to predefine compositions of steels, ferro-alloys, slags, and slag additions. The overall composition of the steel and slag is then obtained by adding amounts of these predefined materials.

Each group of materials is automatically added to the similar group where it is defined. You can manage these groups using the *Material Manager* (see Working with the Material Manager).

For adiabatic calculations, the selection of material type (steel, slag, gas) has an influence on the calculation. For isothermal calculations, the results are identical.

The reason the selection of materials for adiabatic calculations has an influence is because there are different strategies to calculate the enthalpy of the materials at the temperature at which these are added. Therefore, defining FeO as a *steel* containing 50 at% Fe and 50 at% O or as a *slag* with 50 at% Fe and 50 at% O or as *slag* with 100% FeO, all result in different enthalpies assigned to the component FeO, which in turn results in different equilibrium temperatures.

Defining the Equilibrium Simulation and Equilibrium Simulation: Conditions Tab

Adiabatic Calculations: Material Enthalpy

Process Simulations

When you choose to do a **Process simulation** it includes the reaction kinetics. Using the EERZ (Effective Equilibrium Reaction Zone) model, you can first define your materials as you do with an **Equilibrium** simulation. You also need to define the **Process model** where you define the kinetic parameters of the simulation by setting up reaction zones, reaction rates, heat transfer coefficients, and so forth. You also need to define the **Process schedule** where the sequence and amounts of added materials are defined.

Defining the Process Simulation and Process Simulation: Conditions Tab

Calculation Types

The calculations available for an **Equilibrium** simulation, for both isothermic and adiabatic calculations, are *Single* equilibrium, *One Axis*, *Grid*, and *Uncertainty*. After adding a **Plot Renderer** or **Table Renderer**, you can choose a variety of quantities, including slag properties such as Bells ratio and B2, to output results that provide useful visual representations of the steelmaking systems being analyzed.

Process Metallurgy Calculator and Defining the Equilibrium Simulation

Working with the Process Metallurgy Module

Working with the **Process Metallurgy Calculator** allows you to easily define complex metallurgical reactions. The calculator streamlines how you set up these steel and slag systems but there are details about various inputs and outputs that are different from other calculators. This topic is a general collection of information related to the Process Metallurgy Module and is intended to help you better understand how to interpret and make choices when you are setting up your steelmaking simulation.

Database Dependency

It is not possible to use custom user databases with the Process Metallurgy Module. This is because several internal calculations, such as determining the component compositions of ionic phases, are dependent on the database. Therefore, only TCS Metal Oxide Solutions Database (TCOX) versions 8 and newer, and to a limited extent, OXDEMO, can be used with this Module.

Material Manager

For information about saving and deleting materials used with the Process Metallurgy Calculator, see Working with the Material Manager. Also see the next section.

Working with Material Groups (Steel, Slag, and Gas)

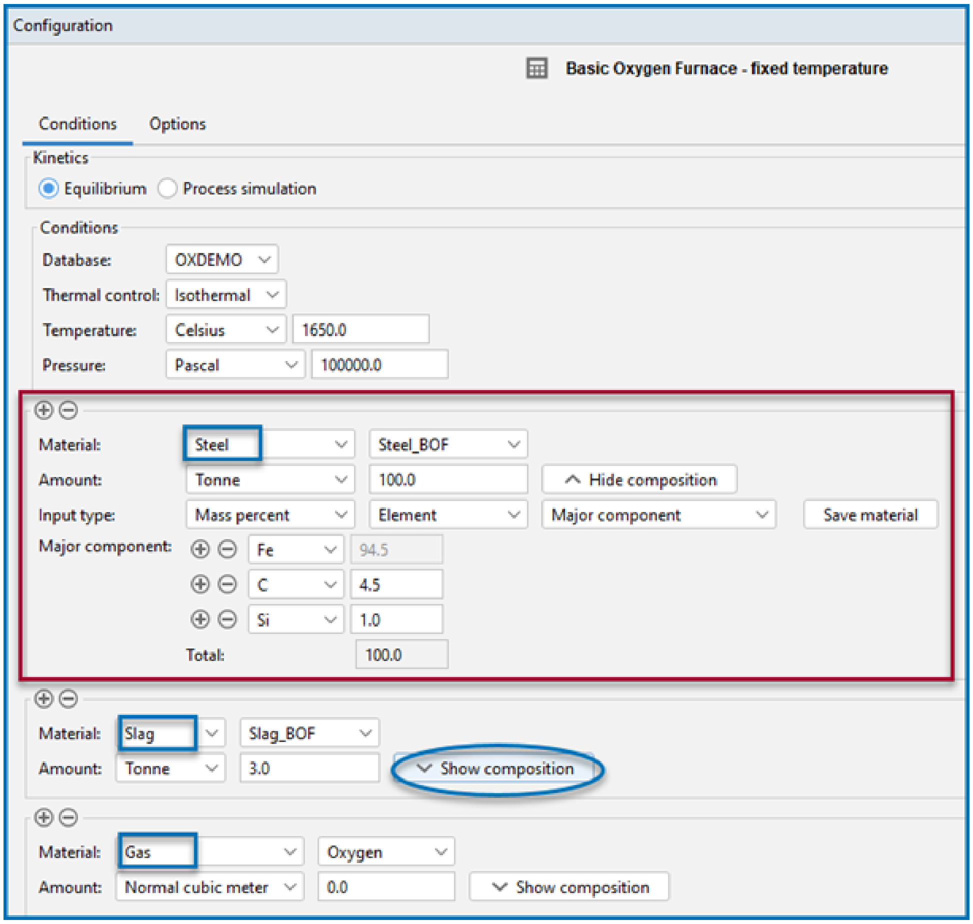
For more details about these fields, see Defining the Equilibrium Simulation. For information about saving and deleting materials, see Working with the Material Manager.

There are three groups to define: **Steel** (or another user-defined **Metal** group), **Slag**, and **Gas**.

It is recommended you open the PMET_01: Basic Oxygen Furnace (BOF) example to follow along with the descriptions. Version b is used in the screenshots.

Open the example project file(s) from Thermo-Calc **Help** → **Example Files** → **Process Metallurgy** → **PMET_01_Basic_Oxygen_Furnace.tcu**. Choose a, b, or c versions of the example based on whether you have a license for the TCOX database.

In the image below, the red-highlighted area is where the Steel material group is defined. The drop-down menu that displays *Steel_BOF* shows a user-defined material. This can be defined and then saved to the material library.



● Equilibrium ○ Process simulation

Database: OXDEMO
Thermal control: Isothermal
Temperature: Celsius 1650.0
Pressure: Pascal 100000.0

Material: Steel Steel_BOF
Amount: Tonne 100.0
Input type: Mass percent Element Major component
Major component: Fe 94.5
C 4.5
Si 1.0
Total: 100.0

Material: Slag Slag_BOF
Amount: Tonne 3.0

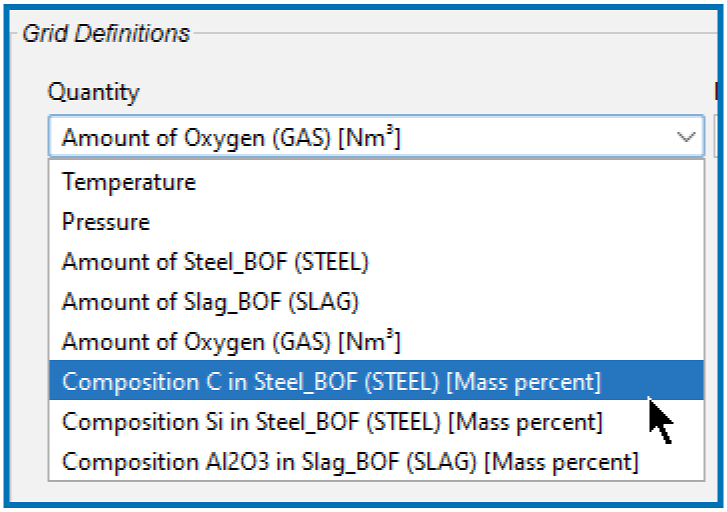
Material: Gas Oxygen
Amount: Normal cubic meter 0.0

The three material group areas on the Process Metallurgy Calculator where you can define components and save materials. You can create your own material groups using the Material Manager.

When you click **Show composition** next to any material group, additional fields display to give composition and input type where you can further define each material group. You can remove materials and add and remove material groups using the *Material Manager* (available on the **Configuration** window → **Options** tab).

In the example, click **Show composition** next to the **Slag** and **Gas** groups to see how the *Slag_BOF* and *Oxygen* materials are defined.

From this composition area you can click the **Save material** button to add the new material to the group's list. The newly named material composition is then available for use with that material group. In this example, the *Steel_BOF* material was defined first and then named at the end. It is now available in the lists wherever you select the **Steel** material or need to choose quantities to plot.



After defining and saving a material composition, the named material is available for selection in a variety of places such as when choosing quantities on the calculator and defining axis variables on the Plot Renderer.

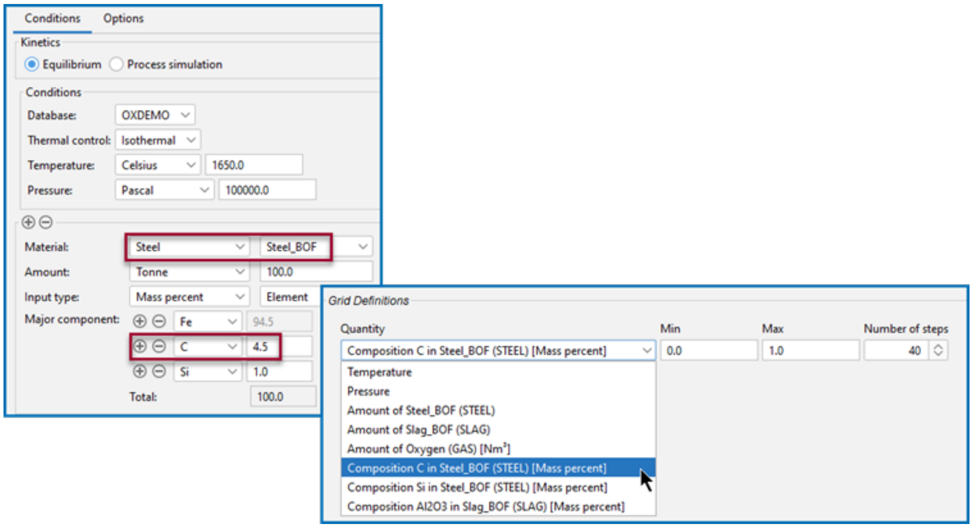
To add one or more material groups click the add ⊕ button. Click the minus ⊖ button to remove a material group. The new material inherits the default settings of that group.

Understanding the Grid Definitions Quantities and How These Relate to the Composition

When you choose a **One Axis** or **Grid** *Calculation Type*, you also choose a **Quantity** under the *Grid Definitions*. The relationship between these quantities and how the material group composition is defined as follows.

The following uses **Composition of C in Steel_LF (STEEL)** as an example quantity for a **One Axis** calculation.

Under *Grid Definitions*, the availability of the **Quantity** in the list is based on the material (**Steel_BOF**) that is defined and saved for the **Steel** group (or any user-defined metal, slag, or gas group).



● Equilibrium ○ Process simulation

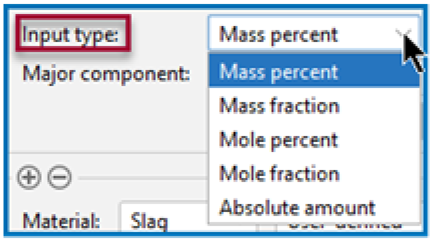
Database: OXDEMO
Thermal control: Isothermal
Temperature: Celsius 1650.0
Pressure: Pascal 100000.0
Material: Steel Steel_BOF
Amount: Tonne 100.0
Input type: Mass percent Element
Major component: Fe 94.5
C 4.5
Si 1.0
Total: 100.0

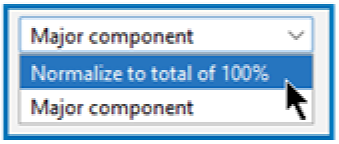
Quantity	Min	Max	Number of steps
Composition C in Steel_BOF (STEEL) [Mass percent]	0.0	1.0	40

Defining the Material Composition

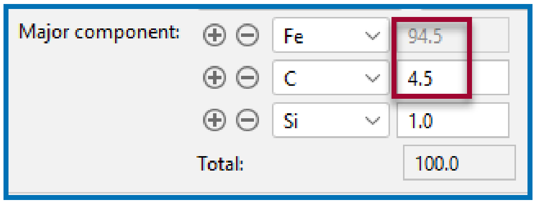
Click **Show composition** so that when you choose the **Input type** for a steel the composition of the elements can be set up using a combination of settings starting with **Mass**- or **Mole percent**, **Mass**- or **Mole fraction**, or for Equilibrium calculations, **Absolute amount**. Then you further choose to define the composition using either the **Major component**or **Normalize to total of 100%** options.

The *Amount of X in Y* quantities you can choose from the various drop-down lists (such as under *Grid Definitions*) are defined as Min-Max variation of the component X in Y. If a dependent element is present that is adapted as usual.

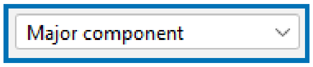




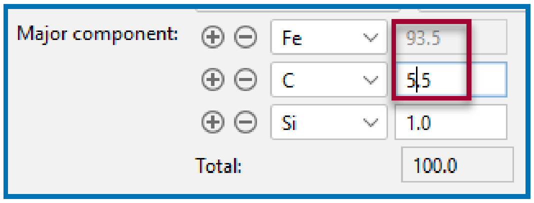
When you use **Major component**, as you add other components or adjust the composition, the major one is adjusted to be the rest of the composition.



Major component:
Fe 94.5
C 4.5
Si 1.0
Total: 100.0

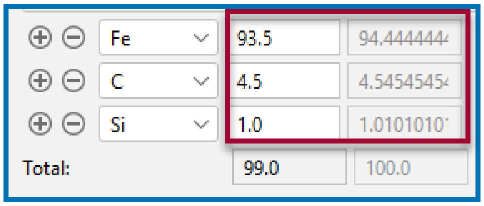


Major component

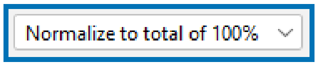


Major component:
Fe 93.5
C 5.5
Si 1.0
Total: 100.0

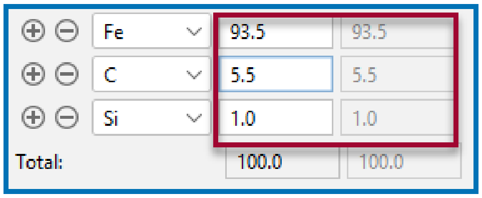
When you use **Normalize to total of 100%**, the sum is adapted to 100%. This is useful if you need to work with a given composition that does not sum up to 100%.



Fe 93.5 94.444444
C 4.5 4.5454545
Si 1.0 1.0101010
Total: 99.0 100.0

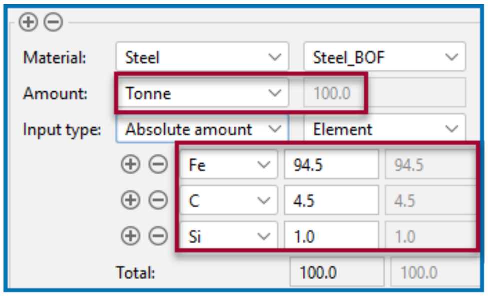


Normalize to total of 100%



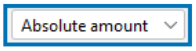
Fe 93.5 93.5
C 5.5 5.5
Si 1.0 1.0
Total: 100.0 100.0

Sometimes its preferable to use input of amount of each component **Amount** by weight (**Tonne**, **Kilogram**, **Gram**, or **Pound**), it can useful to choose **Absolute amount** as the **Input type**. In this case, the total amount of material automatically adjusts the total.

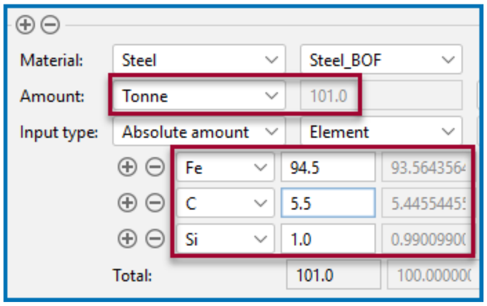


Material: Steel | Steel_BOF
Amount: Tonne | 100.0
Input type: Absolute amount | Element

Fe	94.5	94.5
C	4.5	4.5
Si	1.0	1.0
Total:	100.0	100.0



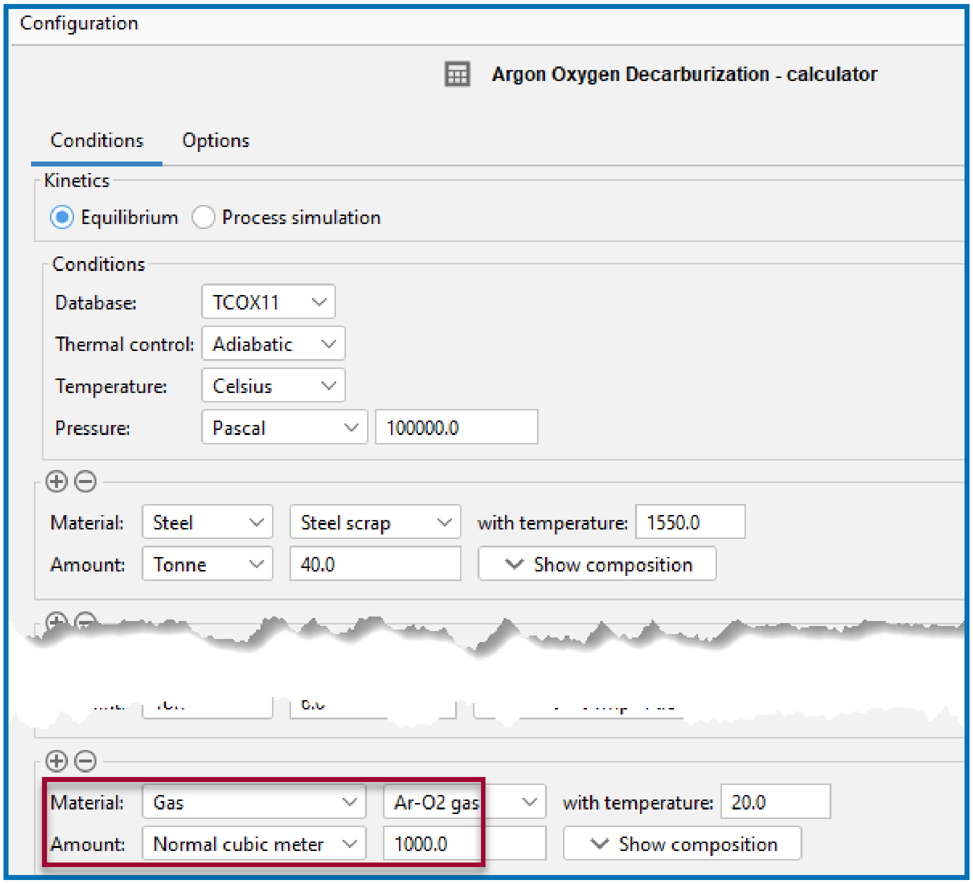
Absolute amount



Material: Steel | Steel_BOF
Amount: Tonne | 101.0
Input type: Absolute amount | Element

Fe	94.5	93.564356
C	5.5	5.4455445
Si	1.0	0.9900990
Total:	101.0	100.00000

For the **Gas** component, if you choose **Normal cubic meter** as the **Amount**, then beside regular mass units, the amount of gas can also be provided in Nm^3.



Database: TCOX11
Thermal control: Adiabatic
Temperature: Celsius
Pressure: Pascal 100000.0

Material: Steel | Steel scrap | with temperature: 1550.0
Amount: Tonne | 40.0 | Show composition

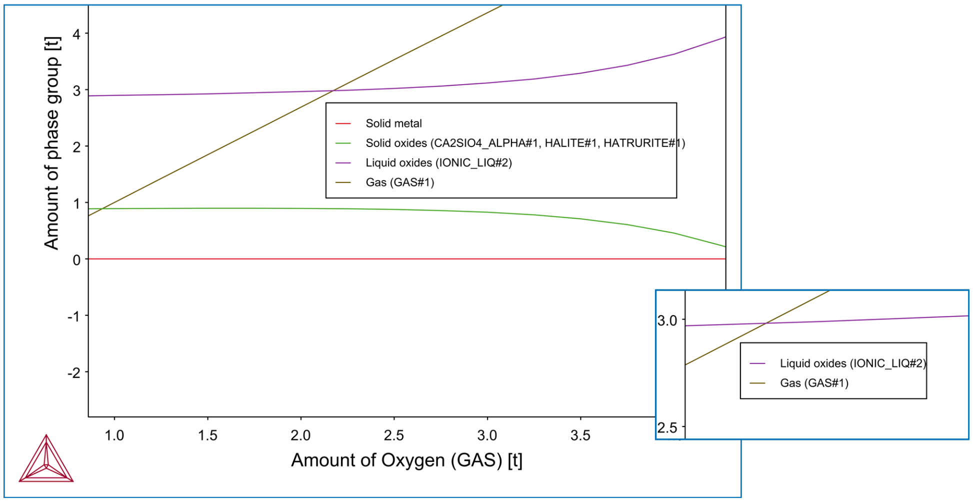
Material: Gas | Ar-O2 gas | with temperature: 20.0
Amount: Normal cubic meter | 1000.0 | Show composition

Phase Groups

The phases that are plotted after you run a simulation are grouped together on the plot to make the interpretation of the results easier.

Phases of similar type are bundled together in the groups *liquid metal*, *solid metal*, *solid oxides*, *liquid oxides*, and *gas*. Except for the gas phase, all the groups can have more than one phase. This grouping is particularly useful for liquid metal and liquid oxide because they are both described by the same phase, IONIQ_LIQUID, and because there is typically two or more compositions sets of IONIQ_LIQUID. This is also useful for solid oxides, because a large number of phases can be stable, making the interpretation of results difficult without this grouping.

The term *oxides* in the Process Metallurgy Module can also mean carbides, sulfides, and fluorides.



Example of the plot labels with the phases grouped together. As you zoom in, only the phases that you can see are listed in the label, making it easier to examine the results.

Slag Property Quantities

The slag properties describe the capability of a slag to take up sulfur from the metal melt. The Process Metallurgy Module defines so-called phase groups. These contain all phases of a certain kind, for example all solid slag or all slag phases. The component composition of such a phase group is calculated by weighting the component composition of each phase with their fraction in the group.

This allows to calculate slag properties for the phase groups, for example for the overall slag.

On the Plot Renderer (for axis quantities) and Table Renderer there is an option to choose or define the **Slag property**. The associated quantity that you select has these options: **All**, **B2**, **B3**, **B4**, **Bas2**, **Bells ratio**, **Ls**, or **Log10 (Sulphur capacity)**.

Details, including references and equations, are described in Process Metallurgy Slag Properties.

Adiabatic Calculations

When setting up the Process Metallurgy Calculator under the **Equilibrium Kinetics** branch, you choose the thermal control to be either **Isothermal** or **Adiabatic**. Adiabatic calculations assume no heat and mass exchange with the environment during the equilibrium reaction. The adiabatic process is implemented by an isenthalpic process with constant pressure (i.e. H=CONST), which is equivalent.

Adiabatic Calculations: Material Enthalpy

Gas Volume Units

Beside regular mass units, the amount of gas can also be provided in **Normal cubic meter** (Nm^3). The applied reference conditions are 1013.25 hPa and 15.0 °C (according to ISO 2533).

There are slightly deviating definitions present in the industry, which need to be converted for precise results. For most applications of the Process Metallurgy Module this difference has a minor influence.

Calculation of Component Compositions

The composition of all ionic phases is provided as elemental as well as component composition (i.e. Fe_2O_3, FeO, CaO, …). In order to provide a representation similar to that usually used in the industry, the content of S is provided as elemental content and the content of P is given as component content of P_2O_5. This is a simplification because P and S can also be present as sulphates and phosphates in the slag and can bind to different metal cations. This can cause deviations in the overall component composition if the content of S and P is high in the phases. In doubt, the elemental composition can be used, it will always be exactly correct.

For non-ionic phases such as ALABANDITE, always the elemental composition will be shown only. This is also true if the IONIC_LIQ composition cannot be described by components only due to constraints of the overall composition (for example if the material has been oxidized completely and forces a certain composition of the ionic liquid slag).

Definition of Partial Pressure of Oxygen

The oxygen partial pressure in the gas phase is calculated with the following formula:

$$p_{O_2} = p \cdot AC(O_2, GAS)$$

In the formula, *p* describes the total system pressure and *AC* the activity of oxygen in the gas phase.

Activities of Slag Components

The chemical activity of each component *AC(COMPONENT, REFERENCE_PHASE)* is available either with reference to the liquid or the solid slag phase. It can only be calculated for components being present in the thermodynamic database.

Process Schedule

When you are working with the **Process simulation** branch you set up a process schedule. There are some useful details about this described in Working with the Process Schedule.

Dynamic Time Stepping

The nature of a **Process simulation** requires a dynamic choice of the time step lengths. To understand this better, see About Dynamic Time Stepping. These settings are done on the Options Tab.

Pressure-Dependent Calculations

It is possible to apply variable pressure during process metallurgical calculations, which is relevant in various processes such as Vacuum Oxygen Decarburization (VOD) or Ruhrstahl-Heraeus (RH). See About Pressure-Dependent Calculations.

Working with the Process Schedule

Defining the Process Simulation

Process Simulation: Process Schedule Tab

About Dynamic Time Stepping

Materials and heat can be added at any time in any amount. They can be either added to a:

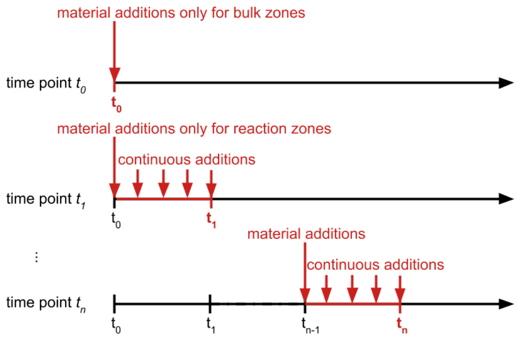
- bulk zone (such as steel, slag, etc.), or
- reaction zone (interface between two bulk zones).

These types of materials are used in the process schedule set up:

- Material addition (in tonne, kilogram, etc.)
- Continuous material addition (in kilogram per minute, etc.)
- Thermal / electrical power (i.e. a continuous heat addition in MW)

A material addition is typically used to model some event like emptying a bucket into the melt. A continuous material addition is instead used to model a continuous material feeding into the melt, such as wire feeding. Finally, heat can be added or removed during a time step and this is defined as power.

A Process Schedule Additions Scheme



Generally the addition of materials and heat is modeled in the process simulations for any time point t_n as follows:

- Material additions happen immediately after the previous time point t_{n-1}, i.e. at the beginning of the time step.
- Continuous material and heat additions (power) are conceptually happening during the complete time step between t_{n-1} and t_n.

The data presented in the results is always referring to the time point, i.e. to the end of the time step. This means that reactions and heat transfer have happened between adding materials and heat at the beginning of the time step and the end of the time step. If for example a strongly cooling material is added, a possibly quite large heating of the zone might have happened until the end of the time step.

The first two time points are different:

- The first time point t_0 at $t=0$ does not represent a time step, instead only a mixing and equilibrium reaction of the material additions in each bulk zone is taking place. There are no reaction zones existing at this time point.
- The second time point t_1 represents the first time step in the simulation where the different bulk zones react between each other via the reaction zones. Nevertheless it is conceptually identical to any other time point.

Working with the Material Manager

Use the *Material Manager* to create and delete groups of materials and delete materials you have saved directly from the **Process Metallurgy Calculator**. It is useful for frequently used materials.

The Material Manager is only available for the Process Metallurgy Calculator.

Material groups created in the Material Manager display in all of the Process Metallurgy Calculator drop down lists, and these are also globally removed. Deleted group data directories are moved to the computer's trash bin.

A material saved in any of the material configuration panels is directly accessible globally in the Process Metallurgy Calculator Configuration window. When a material is removed in the Material Manager panel it is globally removed from the Process Metallurgy Calculator.

The settings are available on the **Configuration** window Options Tab.

Saving a Material

This is done directly from the **Process Metallurgy Calculator** → **Configuration** window.

1. Add the Process Metallurgy Calculator to **My Project** directly (right-click and select it from the **Create New Activity** menu) or use the available Process Metallurgy template on the **My Projects Configuration** window under **Applications**.
2. On the **Configuration** window, next to the **Material** group you want to define, for example **Steel** (or another user-defined metal group), **Slag**, or **Gas**. Click **Show composition**.
3. Enter the composition and the **Major component** of the material you want to save for future use. You can alternatively select **Normalize to total of 100%** and enter the percentages for each element.
4. Click **Save material**.
5. In the window that opens, enter a **Material name**. Click **OK**.

   When you go to the *Material Manager*, you can select this saved material from the applicable list if you need to delete it.

> It is not possible to rename a saved material—you need to recreate/redefine the material and save it again with the new name.

Deleting a Material

This is done with the *Material Manager*, located on the **Configuration** window, **Options** tab.

1. After Saving a Material, go to the *Material Manager*.
2. Select the **Material** group associated to the material saved previously, for example, **Steel** (or another user-defined metal group), **Slag**, or **Gas**.
3. From the **Material** list, select the material you want to delete and click **Delete material**.
4. In the window that opens, click **Yes** to delete the material and **No** to cancel.

Creating a Material Group

This is done with the *Material Manager*, located on the **Configuration** window, **Options** tab.

1. Go to the *Material Manager*.
2. Click **Create group**.
3. In the window that opens, select the **Material group type** (**Metal**, **Slag**, or **Gas**) you want to create.
4. Enter a **Material group name**. The new group is now available to select from the **Material group** list.

Deleting a Material Group

This is done with the *Material Manager*, located on the **Configuration** window, **Options** tab.

1. Go to the *Material Manager*.
2. From the **Material group** list, select the group you want to delete and click **Delete group**.
3. In the window that opens, click **Yes** or **No**.

About Dynamic Time Stepping

? Defining the Process Simulation

? Working with the Process Schedule

? Options Tab

The nature of a process simulation requires a dynamic choice of the time step lengths. On the one hand the simulation needs to capture very fast changes of temperature and composition, for example after addition of cold material. On the other hand it should calculate processes that take several hours in reality within an appropriate calculation time.

The time step control algorithm is primarily controlling the change of the temperature in each zone (including the reaction zones) such that it stays below a specified limit but is always as large as possible.

The dynamic time stepping can be switched off by choosing a very large maximum allowed temperature change per step (such as 1.0e6 K). In this case the maximum time step is always used, however this is only recommended in special situations.

If a temperature change is too large, the algorithm reverts the time step and returns to the previous time point in order to try a smaller time step. Therefore you can see in the Event Log output that the time points can jump back. Except for larger additions this is a rare event.

The parameters of the time-step control algorithm are:

- initial time step a *t=0*,
- smallest allowed time step,
- largest allowed time step, and
- maximum allowed temperature change of a zone within a time step.

The initial time step as well as the largest allowed time step are defined in percent of the total duration of the process while the smallest allowed time step is given in seconds. This allows that these parameters normally need no change even if switching between processes with very short and very long duration.

Making the largest allowed time step bigger can reduce the number of steps and consequently the calculation time, but only if the time step is not limited by the maximum temperature change per time step. This means that both parameters need to be considered together.

Taking a too large smallest allowed time step can cause numerical difficulties, especially if large cold material additions are part of the process schedule.

The initial time step is usually of limited relevance for the overall calculation time, but should usually not be larger than the default value of 1.0%.

As different processes show very different temperature changes, it is probably most common to adapt the maximum temperature change per time step in order to have a good balance between accuracy of the results and calculation time. Usually it should be possible to change this parameter without adapting the other algorithm parameters.

The effects of the dynamic time step algorithm can be inspected by activating the data points in the plots.

> To show the data points, in the **Visualizations** window in Thermo-Calc, right-click in the plot area and choose **Properties**, then click **Show data points**.

About Pressure-Dependent Calculations

Defining the Process Simulation

It is possible to apply variable pressure during process metallurgical calculations, which is relevant in various processes such as Vacuum Oxygen Decarburization (VOD) or Ruhrstahl-Heraeus (RH).

The implementation includes all relevant features for a realistic modeling of the pressure-dependency:

- the set pressure at a time-step is valid for all bulk and reaction zones of the system
- the exhaust gas zone has always atmospheric pressure
- the added material (only relevant for gas) has initially always atmospheric pressure
- the material transferred to and from the zones (i.e. the added material and the exhaust gas from the zones) is undergoing an adiabatic expansion / compression because it is moved between different pressures

Generally there is no effect of pressure change on anything else than gas (due to physics and the implementation of the database).

PMET_07: Vacuum Oxygen Decarburization Kinetics

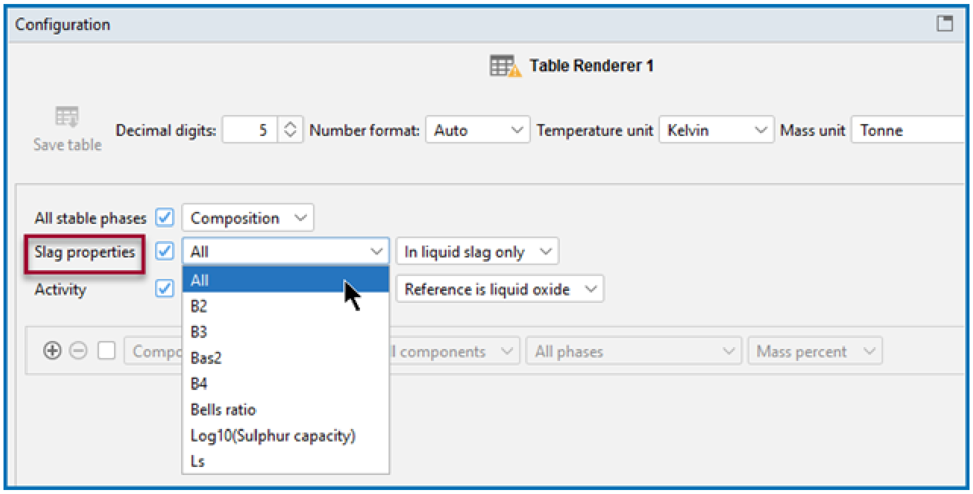
Process Metallurgy Slag Properties

The slag properties describe the capability of a slag to take up sulfur from the metal melt. The Process Metallurgy Module defines so-called phase groups. These contain all phases of a certain kind, for example all solid slag or all slag phases. The component composition of such a phase group is calculated by weighting the component composition of each phase with their fraction in the group.

This allows to calculate slag properties for the phase groups, for example for the overall slag.

Various predefined slag properties such as different definitions of slag basicity, sulfur capacity and so forth are available for plotting or tabulating. On the **Process Metallurgy Calculator** when selecting axis variables on the **Plot Renderer** or choosing the properties to list with the **Table Renderer**, there is an option to include these slag properties.

The associated quantity selected from the next drop-down list has these options: **All**, **B2**, **B3**, **B4**, **Bas2**, **Bells ratio**, **Ls**, or **Log10(Sulphur capacity)**. Also choose **In liquid slag only**, **In solid slag only**, or **In all slag**. Depending on this setting, the composition averaged over liquid, solid, or all slag is applied as a basis for the slag property calculation. Example PMET_01c is used for the figures below, where a table was added to one of the calculators.



Configuration

Table Renderer 1

Decimal digits: 5

Number format: Auto

Temperature unit: Kelvin

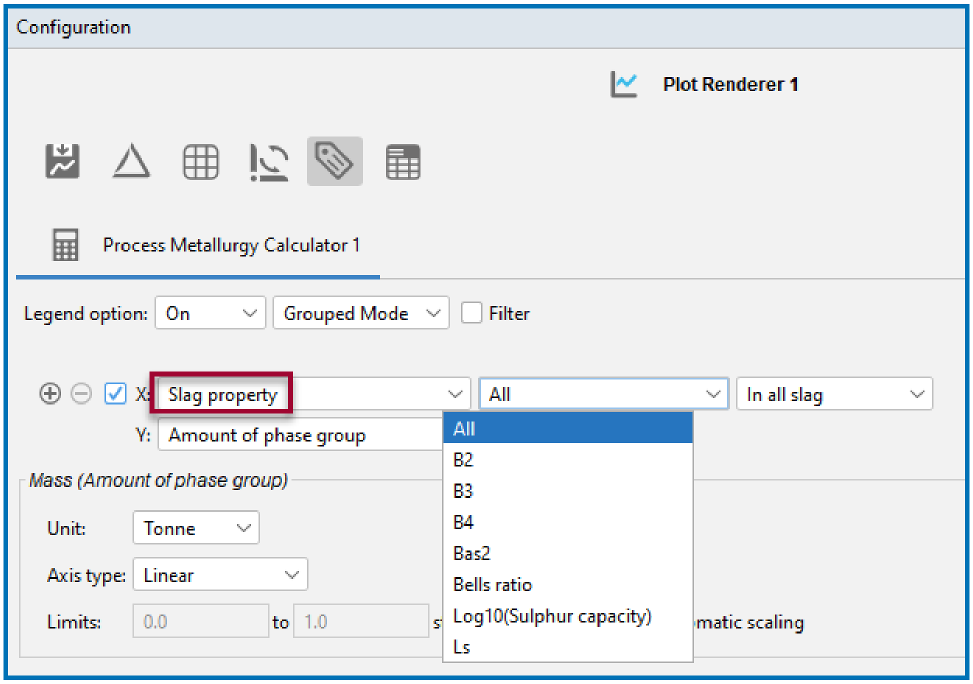
Mass unit: Tonne

All stable phases ☑ Composition

Slag properties ☑ All — In liquid slag only

Activity ☑ — Reference is liquid oxide

Slag properties for a Table Renderer.



Legend option: On | Grouped Mode | ☐ Filter

☑ X: Slag property | All | In all slag

Y: Amount of phase group

Mass (Amount of phase group)

Unit: Tonne

Axis type: Linear

Limits: 0.0 to 1.0

Slag properties for a Plot Renderer.

Equations and References

The equations and references for the slag properties are defined below. Composition can be given in mass (% or fraction).

The formulas are given in Thermo-Calc console-like syntax (B: mass, W: weight fraction, AC: activity). A slag property is available if all of its components are present in the phase group. Steel and slag are the actual phase groups chosen depending on the user request, i.e. the slag property can be calculated for the liquid slag only or for the overall slag (liquid and solid).

Basicity is defined as:

$$\mathrm{B2} = \frac{B(CaO)}{B(SiO_2)}$$

$$\mathrm{B3} = \frac{B(CaO)+B(MgO)}{B(SiO_2)}$$

$$\mathrm{B4} = \frac{B(CaO)+B(MgO)}{B(SiO_2)+B(Al_2O_3)}$$

$$\mathrm{Bas2} = \frac{B(CaO)+B(MgO)}{B(SiO_2)+B(Al_2O_3)+B(TiO_2)}$$

$$\text{Bells ratio} = \frac{B(CaO)+0.7\cdot B(MgO)}{0.94\cdot B(SiO_2)+0.18\cdot B(Al_2O_3)}$$

Sulfur capacity is defined as:

$$\text{Ls} = \frac{W_{(slag)}(S)}{W_{(steel)}(S)}$$

$$\text{Log10}(C_s) = log10(W_{(slag)}(S)\cdot 100\cdot (\frac{AC(O_2,GAS)}{AC(S_2,GAS)})^{(0.5)})$$

References

Basicity and MgO Saturation: For definitions of the basicity and MgO saturation properties B2, B3, B4, and Bells ratio see [2015Kes]. Also see the Slag Atlas [1995Ver].

Sulfur Distribution and Capacity: For definitions of the sulfur distribution properties L_S see [1999And]. For the sulfur capacity, see Slag Atlas [1995Ver].

[1995Ver] Verein Deutscher Eisenhuttenleute (VDEh), ed. 1995. Slag Atlas 2nd Edition. Dusseldorf, Germany: Verlag Stahleisen GmbH.

[1999And] Andersson, Margareta A. T., Par G. Jönsson, and Mselly M. Nzotta. 1999. “Application Ladle Slags of the Used Sulphide Capacity Concept on High-Basicity in Bearing-Steel Production.” ISIJ International 39 (11): 1140–49.

[2015Kes] Keskitalo, Björn. 2015. “Model Studies on the Effects of Composition Differences of Direct Reduction Pellets and an Adaptive Addition of Slag Formers for the EAF Process.” Master's thesis, KTH Royal Institute of Technology, http://urn.kb.se/resolve?urn=urn:nbn:se:kth:diva-168296.

Adiabatic Calculations: Material Enthalpy

An adiabatic calculation requires the enthalpy of the input materials as an initial condition. The Process Metallurgy Module uses different approaches for the different material types metal, gas, and slag. Any mechanical mixture is only applied for 1 bar / 1013 hPa.

Metal

Frozen-in global equilibrium calculation at T = 700 °C, taking the resulting enthalpy at the actual initial material temperature. This corresponds to a frozen-in microstructure. At initial material temperatures above 700 °C the equilibrium is instead calculated directly.

Gas

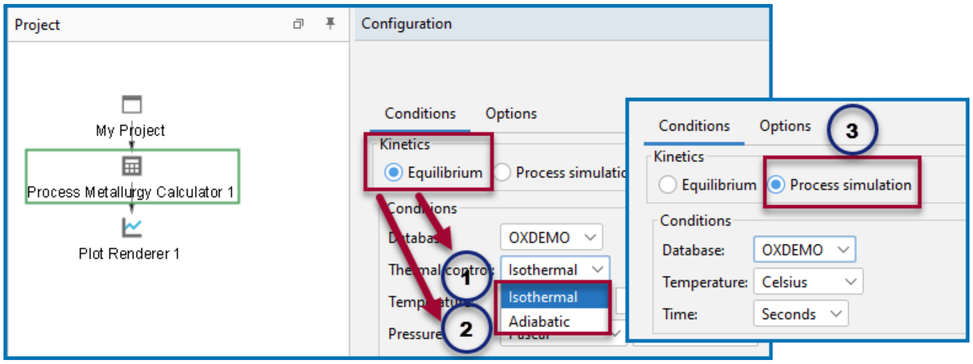
Mechanical mixture between the enthalpy of the gas components. This is no limitation because all gas components in the databases are assumed to be ideal gas.

Slag

- **Mechanical mixture**: If the temperature is below T=1000 °C and every single material component (such as MgO, CaO, …) is fully solid at the requested material temperature, mechanical mixture is assumed. This means that the enthalpy of every component is calculated separately and summed up (weighted by mass fraction). This corresponds to the assumption that different separate components have been added to the slag (such as burnt lime and magnesite). If any component forms gas or liquid at the initial material temperature, this mode is not used. Note that mechanical mixture is also applied if pure elements are added to the slag material, i.e. it is not the same in respect to the material enthalpy to define CaO and Ca + O.
- **Equilibrium**: If no mechanical mixture of the material components is possible or if the temperature is above T=1000 °C. This corresponds to the assumption of a fully homogenized slag material.

Setting Up a Process Metallurgy Simulation

The following basic steps need to be carried out to set up calculations in the **Process Metallurgy Calculator**. There are three branches of simulation to choose from on the **Configuration** window when setting up the simulation an isothermal equilibrium calculation, an adiabatic equilibrium calculation, and a process simulation.



Kinetics: ● Process simulation

Database: OXDEMO

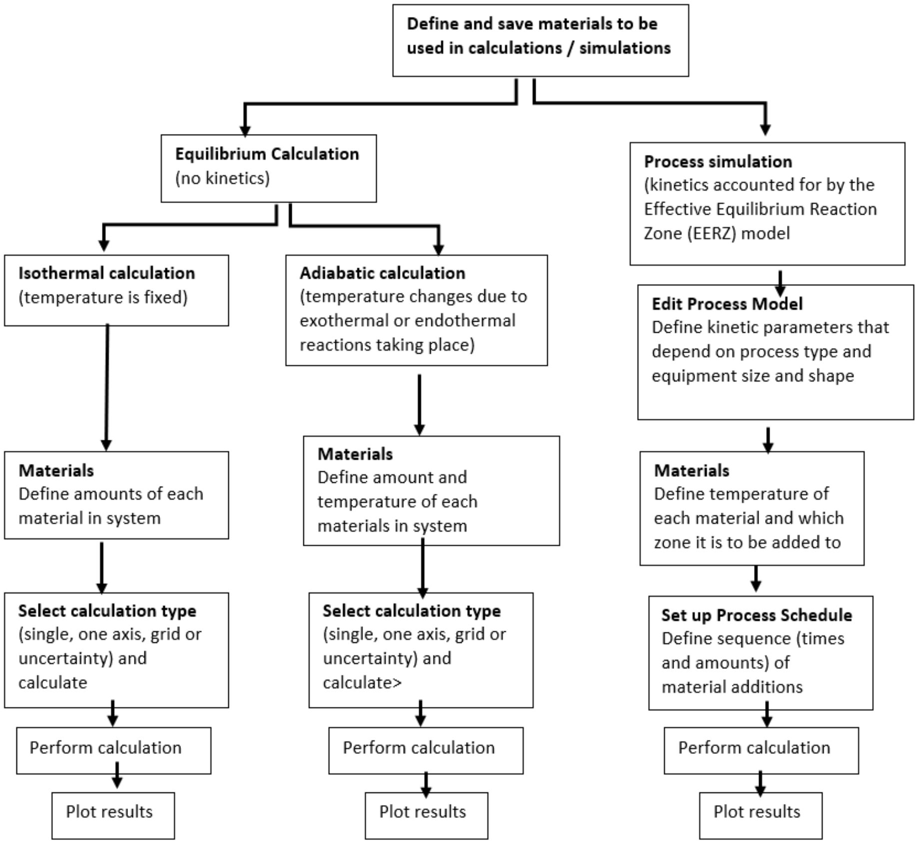
Temperature: Celsius

Time: Seconds

Examples of using the Process Metallurgy Calculator for Basic Oxygen Furnace (BOF) (with and without kinetics), a Ladle Furnace (LF) simulation, an Argon Oxygen Decarbarization (AOD), and a Vacuum Oxygen Decarborization (VOD) simulation are included with your installation. See the Process Metallurgy Module Examples Collection for links.

You can find several learning resources on the Process Metallurgy page of our website (or in Thermo-Calc, go to **Help → Thermo-Calc website**). You can also subscribe to the Thermo-Calc newsletter to be kept up-to-date about upcoming releases, training, examples, videos and much more.

Isothermal and Adiabatic Equilibrium Calculations and Process Simulation Options



The three branches of simulations available for the Process Metallurgy Calculator (1) an isothermal equilibrium calculation, (2) an adiabatic equilibrium calculation, and (3) a process simulation.

Equilibrium Simulations

Two **Equilibrium** simulation types are available: **Isothermal** and **Adiabatic**. In general for the equilibrium simulation, the three most common material groups—*Steel*, *Slag*, and *Gas*—are automatically included with the default composition input types that are relevant to each material group. You can add materials and save your material compositions directly from the Process Metallurgy Calculator and quickly access these for other simulations. For example, you might want to predefine compositions of steels, ferro-alloys, slags, and slag additions. The overall composition of the steel and slag is then obtained by adding amounts of these predefined materials.

Each group of materials is automatically added to the similar group where it is defined. You can manage these groups using the *Material Manager* (see Working with the Material Manager).

For adiabatic calculations, the selection of material type (steel, slag, gas) has an influence on the calculation. For isothermal calculations, the results are identical.

The reason the selection of materials for adiabatic calculations has an influence is because there are different strategies to calculate the enthalpy of the materials at the temperature at which these are added. Therefore, defining FeO as a *steel* containing 50 at% Fe and 50 at% O or as a *slag* with 50 at% Fe and 50 at% O or as *slag* with 100% FeO, all result in different enthalpies assigned to the component FeO, which in turn results in different equilibrium temperatures.

Defining the Equilibrium Simulation and Equilibrium Simulation: Conditions Tab

Adiabatic Calculations: Material Enthalpy

Process Simulations

When you choose to do a **Process simulation** it includes the reaction kinetics. Using the EERZ (Effective Equilibrium Reaction Zone) model, you can first define your materials as you do with an **Equilibrium** simulation. You also need to define the **Process model** where you define the kinetic parameters of the simulation by setting up reaction zones, reaction rates, heat transfer coefficients, and so forth. You also need to define the **Process schedule** where the sequence and amounts of added materials are defined.

Defining the Process Simulation and Process Simulation: Conditions Tab

Calculation Types

The calculations available for an **Equilibrium** simulation, for both isothermic and adiabatic calculations, are *Single* equilibrium, *One Axis*, *Grid*, and *Uncertainty*. After adding a **Plot Renderer** or **Table Renderer**, you can choose a variety of quantities, including slag properties such as Bells ratio and B2, to output results that provide useful visual representations of the steelmaking systems being analyzed.

Process Metallurgy Calculator and Defining the Equilibrium Simulation

Process Metallurgy Calculator

For information about licenses and availability, see About the Process Metallurgy Module.

Use a **Process Metallurgy Calculator**to set up calculations for steel and slag used in steelmaking. Define the composition of a steel (or other metal) and slag system using material groups: one each for steel, slag, and gas. You can save your material compositions directly from the calculator and quickly access and manage the materials and groups—it collects groups of saved materials according to type, thus making it easy to retrieve them.

You can add the calculator to **My Project** directly (right-click and select it from the **Create New Activity** menu) or use the Process Metallurgy Template.

Examples of using the Process Metallurgy Calculator for Basic Oxygen Furnace (BOF) (with and without kinetics), a Ladle Furnace (LF) simulation, an Argon Oxygen Decarbarization (AOD), and a Vacuum Oxygen Decarborization (VOD) simulation are included with your installation. See the Process Metallurgy Module Examples Collection for links.

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Kinetics - Equilibrium or Process Simulation

Once you have added a Process Metallurgy Calculator, the **Configuration** window is further branched based on the **Kinetics** option you choose, **Equilibrium**, where kinetics are not considered, or **Process simulation**, where kinetics are considered using the Effective Equilibrium Reaction Zone (EERZ) model.

All settings, no matter what kinetics branch, are defined on the **Configuration** window **Conditions** and **Options** tabs.

Conditions Tab

Equilibrium

For information about the individual settings on this tab, see Equilibrium Simulation: Conditions Tab.

Set the conditions for your calculation that define the slag, metal, and gas. The topic, Defining the Equilibrium Simulation, has instructions that walk you through the steps that represent a simplified steelmaking process.

Process Simulation

For information about the individual settings on this tab, see Process Simulation: Conditions Tab.

Set the conditions for your calculation that best describes the process you want to simulate. The topic, Defining the Process Simulation, has instructions that walk you through the steps. Also the description of the kinetics examples are useful to help you better understand the settings.

Options Tab

For information about the individual settings, see Options Tab.

Use the **Material Manager** to create and delete groups of materials and delete materials you have saved directly from the Process Metallurgy Calculator. It is useful for frequently used materials. Also see Working with the Material Manager.

The settings in **Process Material Equilibrium and Grid** define certain numerical settings used by the Thermo-Calc calculation engine for equilibrium calculations such as whether tests for global minimization should always be performed (this significantly slows down the calculations) or never be performed (this speeds up calculations but miscibility gaps might not be found), and so forth.

Calculations of oxide systems are numerically challenging, and they can often fail. The default values are chosen to give the best general performance and reliability and should only be changed by an expert user. Also, a large amount of logic is implemented in the Process Metallurgy Module to improve the convergence and calculation speed of equilibrium calculations. The timestep control is related to how finely the times defined in the **Process schedule** are resolved. See About Dynamic Time Stepping for more information.

Local versus Global Options Settings

The **Options** tab is where you can locally define specific Process Metallurgy Calculator settings. Settings can also be applied globally from the **Options** window.

To open the **Options** window: From the main menu select **Tools → Options → Graphical Mode** and click the **Activities** tab. Then click **Process Metallurgy**. See Global Settings: Process Metallurgy.

Plots and Tables

Right-click the node to add a Plot Renderer or Table Renderer to visualize your results. Although both nodes work the same as with the other calculators in Thermo-Calc, there are additional features and settings unique to the Process Metallurgy Module. Useful information is included throughout the documentation. You can also read more about the unique features in Working with the Process Metallurgy Module.

Defining the Equilibrium Simulation

After adding a **Process Metallurgy Calculator** to your project, you can choose to conduct an **Equilibrium** simulation, where you define the steel, slag, and gas groups of materials, or a **Process simulation**, where you set up a process using the EERZ (Effective Equilibrium Reaction Zone) model.

> The following steps are for **Equilibrium** simulations. If you choose to do a **Process simulation**, see Defining the Process Simulation.

This is a general overview of the setup based on the PMET_01: Basic Oxygen Furnace (BOF) example, which walks you through the steps that represent a simplified steelmaking process.

1: Add the Calculator and Choose the Simulation Type

1. Add a **Process Metallurgy Calculator** node to **My Projects** node. If you used the **Process Metallurgy** template on the **My Projects Configuration** window under **Applications**), click the node to display the **Configuration** settings window.
2. Under **Kinetics**, choose the simulation type, **Equilibrium** or **Process simulation**. For the following steps, choose **Equilibrium**.

2: Select a Database and Enter a Temperature

1. In the **Configuration** window, for the *Database* selection, the program automatically defaults to the highest available version of the TCOX database.

> The Process Metallurgy Module requires both a valid Maintenance and Support Subscription (M&SS) and a license for the TCS Metal Oxide Solutions Database (TCOX8 or newer).

It is not possible to use custom user databases with the Process Metallurgy Module. This is because several internal calculations, such as determining the component compositions of ionic phases, are dependent on the database. Therefore, only TCS Metal Oxide Solutions Database (TCOX) versions 8 and newer, and to a limited extent, OXDEMO, can be used with this Module.

All users can test the Process Metallurgy Module with the included OXDEMO database, which is limited to these elements: Al, C, Ca, Fe, O, S, and Si. For more information about this and other products visit our website.

2. Set the **Thermal Control** as being **Isothermal** or **Adiabatic**.
3. Select a **Temperature** unit (**Kelvin**, **Celsius**, or **Fahrenheit**) and enter a numerical value in the field.
4. Select a **Pressure** unit (**Pascal**, **Atmospheres**, or **Bar**) and then enter a numerical value in the field.

3: Define the Conditions for the Steel, Slag, and Gas Material Groups

Next define each material group—**Steel** (or any user-defined **Metal** group), **Slag**, and **Gas**.

See Equilibrium Simulation: Conditions Tab for an overview of the layout of this section. There is also an overview of these material groups in Working with the Process Metallurgy Module.

1. Choose a **Material** to set up first, **Steel** (or any user-defined metal), **Slag**, or **Gas**.
2. Select an **Amount** from the list—**Tonne**, **Kilogram**, **Gram**, or **Pound**. Enter a numerical value in the field.
3. If this is the first time you are defining a material, or at any time when **User-defined** is selected, click **Show composition** to set the composition for the material (steel, slag, or gas or another user-defined metal).

The composition for each material is hidden by default because the Module allows you to easily save materials and access these from the material menu. Once you save a collection of materials, you will rarely have to click **Show composition**. See Working with the Material Manager for details about saving and deleting materials.

4. To the right of the **Material** list (e.g. for the **Steel** group), choose the material composition you want to use for this simulation. Predefined **Example Steel** and **Example Slag** compositions are included with the installation.
    - If you chose **Adiabatic** as the **Thermal Control**, also enter a **temperature** in the field for each material. This is the initial temperature before the material is added to the process.
5. From the first **Input type** list select **Mass percent**, **Mass fraction**, **Mole percent**, **Mole fraction**, or **Absolute amount**. For **Absolute amount**, you can directly enter values in the fields in the unit selected above for **Amount** (**Tonne**, **Kilogram**, **Gram**, or **Pound**).
6. For the next list, the default is based on which group you are defining. For the Steel (Metal) group it is **Element**, for Slag it is **Component**, and for Gas it is **Gas component**.
7. Choose **Major component** so that as you add other components, the major one is adjusted to be the rest of the composition. Choose **Normalize to total of 100%** so that the sum is adapted to 100%. This is useful if you need to work with a given composition that does not sum up to 100% If you select **Absolute amount**, **Normalize to total of 100%** is not available.
8. Based on which material group you are working with, add the **Element**, **Component**, or **Gas component**.

To add one or more material groups click the add ⊕ button. Click the minus ⊖ button to remove a material group. The new material inherits the default settings of that group.

9. After you have added and defined the element, component, or gas component it is recommended you save and name the material. This makes it easier to work with because the name of the material is automatically updated in the lists (and available as part of your library) instead of being named *User-defined* everywhere.

The material is automatically saved in the relevant material group, so only steel materials are shown in the steel menu, only slag materials are shown in the slag menu, and only gas in the gas menu. You can also create additional material groups if there are groups you use regularly, such as scrap compositions, ferro-alloys or slag additions. See Working with the Material Manager for more details about creating and deleting material groups and deleting materials.

10. Continue adding and defining the material groups (e.g. Steel, Slag, and Gas). You could, for example, add another Steel group if you wanted to define a composition of a steel scrap to add to a basic oxygen furnace (BOF).

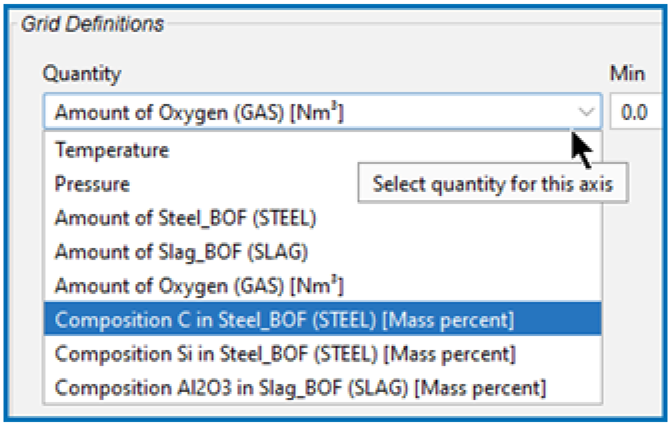
4: Select the Calculation Type and Associated Definitions

These settings are described more in Equilibrium Simulation: Conditions Tab.

1. Under *Calculation Type*, click to choose **Single** (no axes), **One Axis**, **Grid**, or **Uncertainty**.

For more complex calculations, it is good practice to start with a **Single** equilibrium calculation to make sure the calculation converges. Also see the settings described in Options Tab. These can be useful if your calculation fails.

2. Based on the calculation type, define either the *Grid Definitions* (for **One Axis** or **Grid** calculations) or the *Sampling of Data from Gaussian Distributions* (for **Uncertainty** calculations). The **Quantity** displays all the stepping options set up with the material groups for **Steel**, **Slag**, and **Gas**. The example shows the steel group quantities.



The *Amount of X in Y* quantities you can choose from the various drop-down lists (such as under *Grid Definitions*) are defined as Min-Max variation of the component X in Y. If a dependent element is present that is adapted as usual.

How these quantities relate to the material definition is described in Working with the Process Metallurgy Module.

5: Add and Define a Plot or Table and Run the Simulation

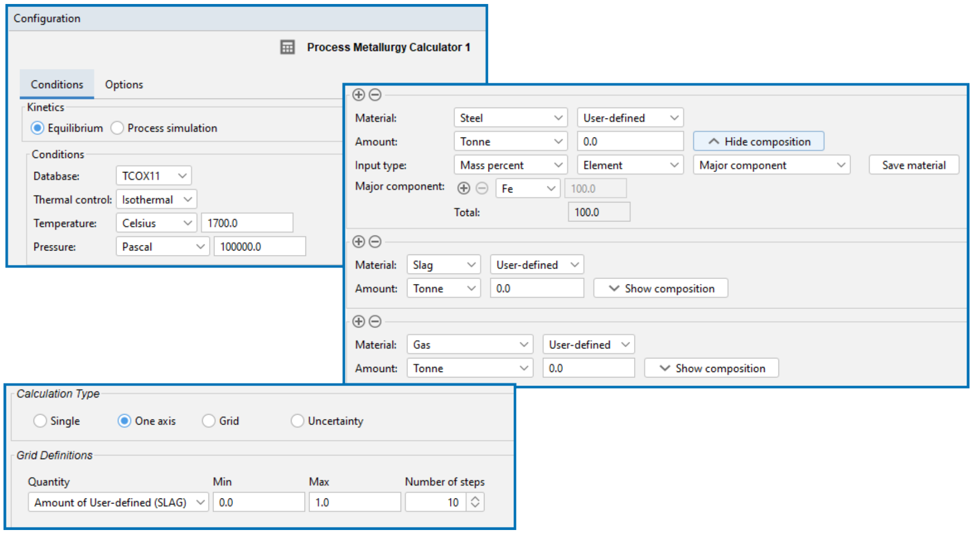
Once you have finished defining the Process Metallurgy Calculator, you also define the plot or table settings. To add a Plot Renderer or Table Renderer, right-click the calculator node and select an option from the **Create New Successor** menu.

The settings are generally described for the individual nodes. See Plot Renderer and Table Renderer. Some useful information about the plots is also described in Working with the Process Metallurgy Module.

Equilibrium Simulation: Conditions Tab

The following outlines what you can set on the **Configuration** window **Conditions** tab when working with the **Process Metallurgy Calculator** and an **Equilibrium** simulation.

Also see Defining the Equilibrium Simulation for instructions that walk you through the steps that represent a simplified steelmaking process. A more complex process is described in Defining the Process Simulation.



Kinetics: ● Equilibrium ○ Process simulation

Conditions

Database: TCOX11

Thermal control: Isothermal

Temperature: Celsius 1700.0

Pressure: Pascal 100000.0

Material: Steel User-defined

Amount: Tonne 0.0

Input type: Mass percent Element Major component

Major component: Fe 100.0

Total: 100.0

Material: Slag User-defined

Amount: Tonne 0.0

Material: Gas User-defined

Amount: Tonne 0.0

Calculation Type

○ Single ● One axis ○ Grid ○ Uncertainty

Grid Definitions

Quantity	Min	Max	Number of steps
Amount of User-defined (SLAG)	0.0	1.0	10

An example of the different settings areas for a default Configuration window for a Process Metallurgy Calculator when an Equilibrium simulation type is selected. There are many settings available depending on the parameters.

DATABASE

The most recent available version of TCS Metal Oxide Solutions Database (TCOX) is selected by default.

The Process Metallurgy Module requires both a valid Maintenance and Support Subscription (M&SS) and a license for the TCS Metal Oxide Solutions Database (TCOX8 or newer).

It is not possible to use custom user databases with the Process Metallurgy Module. This is because several internal calculations, such as determining the component compositions of ionic phases, are dependent on the database. Therefore, only TCS Metal Oxide Solutions Database (TCOX) versions 8 and newer, and to a limited extent, OXDEMO, can be used with this Module.

All users can test the Process Metallurgy Module with the included OXDEMO database, which is limited to these elements: Al, C, Ca, Fe, O, S, and Si. For more information about this and other products visit our website.

THERMAL CONTROL

Choose **Isothermal** or **Adiabatic**. When **Adiabatic** is selected, no global temperature is defined (as this changes during the process). Instead the initial temperature has to be defined separately for each material. Adiabatic calculations assume no heat and mass exchange with the environment during the equilibrium reaction. Certain types of processes run at almost constant temperatures. For such processes isothermal conditions are acceptable. But in most metallurgical processes the temperature will change sometimes dramatically in function of time due to heating or cooling of the system and due to exothermal or endothermal reactions taking place. For such processes adiabatic conditions are a better choice.

TEMPERATURE

Choose a **Temperature** unit (**Kelvin**, **Celsius**, or **Fahrenheit**) and then enter a numerical value in the field.

PRESSURE

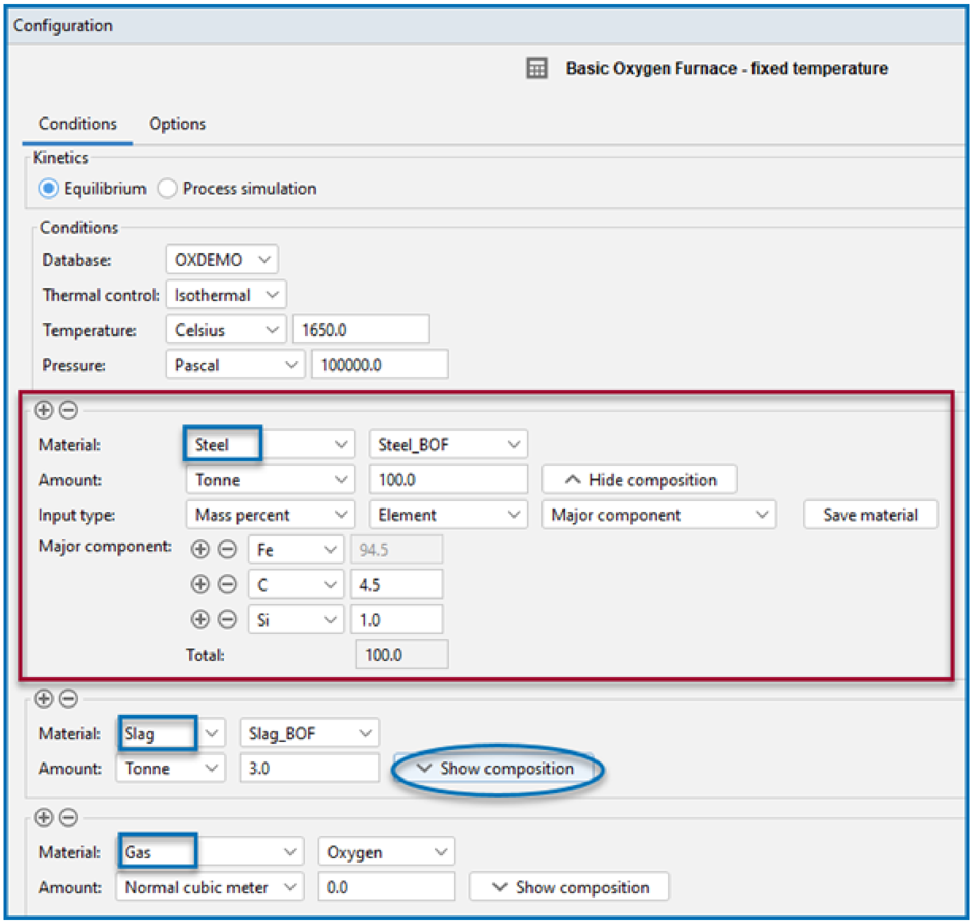
Choose a **Pressure** unit (**Pascal**, **Atmospheres**, or **Bar**) and then enter a numerical value in the field.

MATERIAL GROUPS (STEEL, SLAG, AND GAS)

For more details about these fields, see Defining the Equilibrium Simulation. See also Working with the Material Manager.

There are three groups to define: **Steel** (or another user-defined **Metal** group), **Slag**, and **Gas**.

In the image below, the red-highlighted area is where the **Steel** material group is defined. The drop-down menu that displays *Steel_BOF* is a user-defined material. This can be defined and then saved to the material library.



Configuration

Basic Oxygen Furnace - fixed temperature

Conditions | Options

Kinetics

● Equilibrium ○ Process simulation

Conditions

Database: OXDEMO

Thermal control: Isothermal

Temperature: Celsius 1650.0

Pressure: Pascal 100000.0

Material: Steel Steel_BOF

Amount: Tonne 100.0

Input type: Mass percent Element Major component

Major component: Fe 94.5

C 4.5

Si 1.0

Total: 100.0

Material: Slag Slag_BOF

Amount: Tonne 3.0

Material: Gas Oxygen

Amount: Normal cubic meter 0.0

The three material group areas on the Process Metallurgy Calculator where you can define components and save materials.

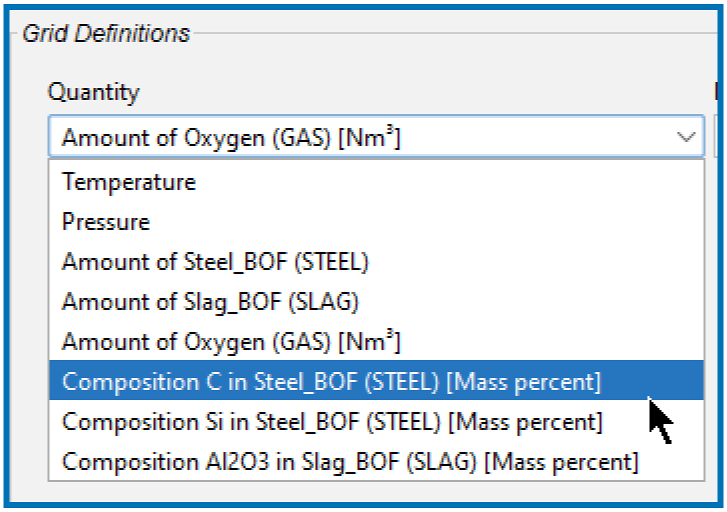
When you click **Show composition** next to any material group, additional fields display (e.g. **Input type**, **Major components**, and so forth) where you can further define each material group. You can add and remove materials using the *Material Manager* (available via the **Configuration** window → **Options** tab).

You can open the example project PMET_01: Basic Oxygen Furnace (BOF) from Thermo-Calc **(Help → Example Files → Process Metallurgy → PMET_01_Basic_Oxygen_Furnace.tcu)**. Then click **Show composition** next to the **Slag** and **Gas** groups to see how the *Slag_BOF* and *Oxygen* materials are defined.

From this composition area you can click the **Save material** button to add the new material to the group's list. The newly named material composition is then available for use with that material group. In this example, the *Steel_BOF* material was defined first and then named at the end. It is now automatically available wherever you select the Steel material or need to choose quantities to plot.

The *Amount of X in Y* quantities you can choose from the various drop-down lists (such as under *Grid Definitions*) are defined as Min-Max variation of the component X in Y. If a dependent element is present that is adapted as usual.

To add one or more material groups click the add ⊕ button. Click the minus ⊖ button to remove a material group. The new material inherits the default settings of that group.



Grid Definitions

Quantity

Amount of Oxygen (GAS) [Nm³]

- Temperature
- Pressure
- Amount of Steel_BOF (STEEL)
- Amount of Slag_BOF (SLAG)
- Amount of Oxygen (GAS) [Nm³]
- Composition C in Steel_BOF (STEEL) [Mass percent]
- Composition Si in Steel_BOF (STEEL) [Mass percent]
- Composition Al2O3 in Slag_BOF (SLAG) [Mass percent]

After defining and saving a material composition, the named material is available for selection in a variety of places such as when choosing quantities on the calculator and defining axis variables on the Plot Renderer.

CALCULATION TYPE

Click to select a *Calculation Type*.

- **Single**: To calculate a single point. The results from this calculation can be displayed in the **Visualizations** window using a **Table Renderer**.
- **One Axis**: To vary a quantity on the *X*-axis.
- **Grid**: Evaluates two axis variables of the selected quantities in the specified range and number of steps.
- **Uncertainty**: Evaluates calculations where the values of the quantities are sampled from Gaussian distributions. The **Mean** field is as defined under *Condition Definitions* for the respective quantity. The result is visualized as a histogram or normal probability plot by adding a Plot Render activity.

Plot Types

GRID DEFINITIONS (ONE AXIS OR GRID)

The **Quantity** menu displays all the stepping options set up with the material groups for **Steel** (or any user-defined metal group), **Slag**, and **Gas**.

For **One Axis**, select a **Quantity** to vary along the X-axis, for example, **Temperature** then enter a **Min**, **Max**, and **Number of steps**.

For the **Grid** calculation type, define the two axes variables using the fields and menus: **Quantity**, **Min**, **Max**, and **Number of steps**. The number of steps along with the minimum and maximum values for the axes define a grid. For each grid point the selected equilibrium is evaluated.

Depending on the calculation type selected, there are also a variety of Plot Types to choose from.

SAMPLING OF DATA FROM GAUSSIAN DISTRIBUTIONS (UNCERTAINTY)

For the **Uncertainty** calculation type, click to select the applicable checkboxes under **Quantity**. The **Mean** field is for the distribution function as defined under *Condition Definitions* for the respective quantity. The default ΔMin/Max is a 95% confidence interval.

About the Uncertainty Calculations

SAMPLING PARAMETERS (UNCERTAINTY)

For the **Uncertainty** calculation type, choose a number of **Standard deviations** where you want to **Truncate the distribution**. Choose the **Total number of samples**.

? About the Uncertainty Calculations

Defining the Process Simulation

After adding a **Process Metallurgy Calculator** to your project, you can choose to conduct an **Equilibrium** simulation, where you define the steel, slag and gas groups of materials, or a **Process simulation**, where you set up a process using the EERZ (Effective Equilibrium Reaction Zone) model.

Setting Up a Process Metallurgy Simulation

The following steps are for **Process simulation**. If you choose to do an **Equilibrium**, see Defining the Equilibrium Simulation.

1: Add the Calculator and Choose the Simulation Type

1. Add a **Process Metallurgy Calculator** node to **My Projects** node. If you used the **Process Metallurgy** template on the **My Projects Configuration** window under **Applications**), click the node to display the **Configuration** settings window.

2. Under **Kinetics**, choose the simulation type, **Equilibrium** or **Process simulation**. For the following steps, choose **Process simulation**.

   Only adiabatic conditions are available for process simulations as this corresponds best to most practical processes.

2: Select a Database and Enter a Temperature

Process Simulation: Conditions Tab

1. In the **Configuration** window, for the *Database* selection, the program automatically defaults to the highest available version of the TCOX database.

> The Process Metallurgy Module requires both a valid Maintenance and Support Subscription (M&SS) and a license for the TCS Metal Oxide Solutions Database (TCOX8 or newer).

> It is not possible to use custom user databases with the Process Metallurgy Module. This is because several internal calculations, such as determining the component compositions of ionic phases, are dependent on the database. Therefore, only TCS Metal Oxide Solutions Database (TCOX) versions 8 and newer, and to a limited extent, OXDEMO, can be used with this Module.

> All users can test the Process Metallurgy Module with the included OXDEMO database, which is limited to these elements: Al, C, Ca, Fe, O, S, and Si. For more information about this and other products visit our website.

2. Select a **Temperature** unit (**Kelvin**, **Celsius**, or **Fahrenheit**).
3. Select a **Time** unit (**Seconds**, **Minutes**, **Hours**, or **Days**).

3: Define the Process Model

Process Simulation: Process Model Settings

1. Enter a **Name** for the process and the total **Duration** of the process.
2. Choose a **Process model** from the list or click **Edit Process Model** to define a new model or edit an existing one.

3. In the **Process model** the following is defined:

a. **Pressure**. This is can be either **Constant** throughout the process (enter a constant via the Edit Process Model) or be changed during the process (select **Table input** via the Edit Process Model) and then enter pressure in the **Process schedule** table.

b. **Zones of the Effective Equilibrium Reaction Zone model**. Only two zones can be defined. The densities need to be given manually. They are used to calculate the volume of the reaction zones, which is in turn used for the calculation of the reaction kinetics. Choose to allow degassing or not.

c. **Area of the Reaction zone and mass transfer coefficients**. The area is typically the area of the interface between the two zones. The mass transfer coefficients state how fast material is moved into the reaction zone. Large values result in fast kinetics, small numbers in slower kinetics. These values strongly depend on the type of material (mass transfer in slags is slower than in liquid steel due to its higher viscosity) and type of process (the violent reactions in a basic oxygen furnace have higher mass transfer coefficients compared to the gentle stirring performed in a ladle furnace. These parameters are basically fitting parameters that need to be determined based on comparison with experimental data. Typical values can also be found in the literature. Choose to allow degassing or not.

d. **Transfer of phase group**. This defines how fast “foreign” phases are moved from one zone to the other. Foreign phases could be solid or liquid oxide inclusions in the liquid steel, or metallic droplets in the slag phase. A typical application is the simulation of the flotation of oxide inclusions out of the liquid steel into the slag phase during refining in a ladle furnace.

e. **The Heat entering or leaving the system and being transferred between the zones.** Constant cooling defines how much heat is lost from the system by radiation and convection. Separate values can be given to each zone if needed. Heat is used when the system is actively heated by an external heat source such as an electric arc or induction heater. Here only the heating efficiency is given, which is the percentage of for example electrical power that is transferred to the system as heat. The times and power are defined in the **Process schedule**. Different amounts of heat and material are added to the zones resulting in the zones having different temperatures. Heat transfer defines how heat flows from one zone to the other. A high value results in a quick equalization of temperature, a small value results in the zones keeping their different temperatures.

4: Define the Materials

Process Simulation: Materials Tab

The materials can be defined, saved and retrieved in the same way as for an equilibrium simulation. For a process simulation, it must be defined to which zone the material is added. Typically, oxide materials are added to the slag zone and metallic materials are added to the steel zone. Gas or other injected materials (such as carbon or lime powder) are typically added to the reaction zone. But this choice depends on the process to be simulated and must be carefully chosen. By defining the same material twice or even three times, it can be split, so that part of the material is added to one zone and part of it to another zone.

5: Define the Process Schedule

- ? Working with the Process Schedule
- ? Process Simulation: Process Schedule Tab

On the **Process schedule** tab, the sequence and amounts of additions during the duration of the process are defined. All the materials defined in the **Materials** tab automatically are included in the table. If a heat addition is defined in the Process Model this is also included in the table. If the units **Tonne**, **Kilogram**, or **Pound** are selected, then the additions are defined as one-time additions at a certain time. If a rate is chosen as unit of the addition (such as **Kilogram per minute** or **Kilogram per second**, for gas also **Normal cubic meter per minute** or per second can be given) then the rate of addition is entered into the table. The additions are visualized in a plot for clarity.

6: Run the Simulation and Add and Define a Plot or Table

When the simulation is set up, click **Perform Tree** to run it. Plots and tables can be added in the same way as for equilibrium calculations.

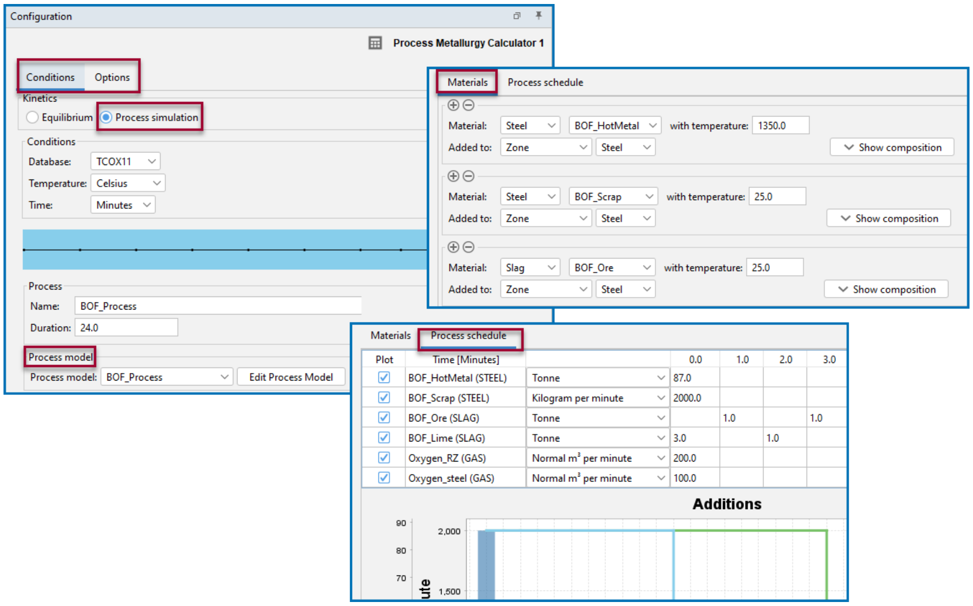
Process Simulation: Conditions Tab

See Defining the Equilibrium Simulation for instructions that walk you through the steps that represent a simplified steelmaking process. A more complex process is described in Defining the Process Simulation and where the settings in the following topics are described.

Examples of using the Process Metallurgy Calculator for Basic Oxygen Furnace (BOF) (with and without kinetics), a Ladle Furnace (LF) simulation, an Argon Oxygen Decarbarization (AOD), and a Vacuum Oxygen Decarborization (VOD) simulation are included with your installation. See the Process Metallurgy Module Examples Collection for links.

The following outlines what you can set on the **Configuration** window **Conditions** tab when working with the **Process Metallurgy Calculator**.

Below is based on selecting a **Process simulation** under **Kinetics**. The settings to complete are for the **Process Model**, the **Materials**, and the **Process Schedule**.



Kinetics: ○ Equilibrium ● Process simulation

Conditions
Database: TCOX11
Temperature: Celsius
Time: Minutes

Process
Name: BOF_Process
Duration: 24.0

Process model
Process model: BOF_Process

Material: Steel BOF_HotMetal with temperature: 1350.0
Added to: Zone Steel

Material: Steel BOF_Scrap with temperature: 25.0
Added to: Zone Steel

Material: Slag BOF_Ore with temperature: 25.0
Added to: Zone Steel

Plot	Time [Minutes]		0.0	1.0	2.0	3.0
☑	BOF_HotMetal (STEEL)	Tonne	87.0			
☑	BOF_Scrap (STEEL)	Kilogram per minute	2000.0			
☑	BOF_Ore (SLAG)	Tonne		1.0		1.0
☑	BOF_Lime (SLAG)	Tonne	3.0		1.0	
☑	Oxygen_RZ (GAS)	Normal m³ per minute	200.0			
☑	Oxygen_steel (GAS)	Normal m³ per minute	100.0			

An example of the different sections on the Configuration window for a Process Metallurgy Calculator when a Process simulation type is selected. This screen shot is from the example PMET_ 04c. There are many settings available depending on the parameters.

DATABASE

The most recent available version of TCS Metal Oxide Solutions Database (TCOX) is selected by default.

The Process Metallurgy Module requires both a valid Maintenance and Support Subscription (M&SS) and a license for the TCS Metal Oxide Solutions Database (TCOX8 or newer).

It is not possible to use custom user databases with the Process Metallurgy Module. This is because several internal calculations, such as determining the component compositions of ionic phases, are dependent on the database. Therefore, only TCS Metal Oxide Solutions Database (TCOX) versions 8 and newer, and to a limited extent, OXDEMO, can be used with this Module.

All users can test the Process Metallurgy Module with the included OXDEMO database, which is limited to these elements: Al, C, Ca, Fe, O, S, and Si. For more information about this and other products visit our website.

TEMPERATURE

Select a **Temperature** unit (**Kelvin**, **Celsius**, or **Fahrenheit**).

TIME

Select a **Time** unit (**Seconds**, **Minutes**, **Hours**, or **Days**).

Process Simulation: Process Model Settings

The following outlines what you can set on the **Configuration** window under Process and when you click **Edit Process Model**. The overall steps to set this up are described in Defining the Process Simulation.

PROCESS

Under *Process*, enter a **Name** and **Duration**.

For more complex processes, you could, for example, enter the process reference as its *Name* as is done for the EERZ example **PMET_06_Ladle_Furnace_Kinetics.tcu**.

PROCESS MODEL

Choose a *Process model*. Click **Edit Process Model** to enter details as below.

You can create your own **Process model** and name them so these are available to choose from the list in the future. This is done using the **Edit Process Model** window.

Edit Process Model

To open the **Edit Process Model** window, click **Edit Process Model** to access the following settings.

Pressure

For **Pressure**, this is can be either **Constant** throughout the process or be changed during the process (using **Table input** here and then entering values in the Process Schedule). Choose:

- **Constant** to choose a unit (**Pascal**, **Atmospheres**, or **Bar**) and then enter a numerical value in the field.

> Only constant pressure throughout the process can be used. Also, the pressure only influences reactions involving the gas phase.

- **Table input** to add or use the values entered in the **Process Schedule** table.

Zones

In this section define the material zone(s), which are added to a **Zone** or **Reaction zone** on the **Materials** tab.

Enter a **Name** and **density** (in kg/m^3) for the zones.

For example, enter `Steel` and `Slag`, which in the next section are available to define for **Zone 1** or **Zone 2** in the Reaction zone.

Select the **Allow degassing** checkbox to be able to simulate vacuum degassing, for example.

Click the ⊕ **Add** button to define additional items and the ⊖ **Remove** button to delete items.

Reactions

In this section you are defining either a **Reaction zone** and/or **Transfer of phase group**.

Select the **Allow degassing** checkbox to be able to simulate vacuum degassing, for example.

Click the ⊕ **Add** button to define additional items and the ⊖ **Remove** button to delete items.

REACTION ZONE

If you choose **Reaction zone** from the list then enter an *area* (in m^2).

Next choose from each **Zone 1** and **Zone 2** list the Zone as defined above, for example **Steel** or **Slag**.

For **mass transfer coefficient** choose:

- **Constant** to enter a numeric value in the field in m/s for each.
- **Table input** to add or use the values entered in the **Process Schedule** table.

Reaction zone area and mass transfer coefficient defines the kinetics of the reaction between the two zones. A large area and fast mass transfer results in fast kinetics.

TRANSFER OF PHASE GROUP

If you choose to define a **Transfer of phase group**, then choose the state as **Liquid metal**, **Solid metal**, **All metal**, **Solid oxides**, **Liquid oxides**, **All oxides**, or **Gas**.

Then choose the two zones (e.g. Steel or Slag) to define **from zone** and **to zone**. Then enter a value and choose a time from the list, **Percent per minute** or **Percent per second**.

This parameter defines how fast "foreign" phases are transferred from one zone to another. A typical example is the flotation of oxide inclusions in liquid steel up into the slag phase.

Heat

Choose the type of heat to apply to the process: **Constant cooling**, **Heat transfer**, and/or **Heat**.

Click the ⊕ **Add** button to define additional items and the ⊖ **Remove** button to delete items.

CONSTANT COOLING

If you choose **Constant cooling**, enter a **Name**, choose either **Zone** or **Reaction Zone** and enter a numerical value in the field in MW (megawatts).

If you choose **Zone**, you can further choose either Zone defined above (e.g. **Steel** or **Slag**). If you choose **Reaction Zone**, then heat is lost from the EERZ, the size of which is calculated at each timestep depending on the kinetic parameters defined in **Reaction Zone**.

This parameter defines how much heat is lost from a zone (or the reaction zone) by radiation or convection and results in an overall cooling of the system.

HEAT TRANSFER

If you choose **Heat transfer**, select two zones between where heat should flow and enter a **heat transfer coefficient** in Wm^2/K.

As different amounts of material and also different amounts of heat can be added to the different zones, these temperature are different. As the two zones are in contact heat flows from the hotter zone to the cooler zone thus equalizing the temperature. The amount of heat flowing from one zone to the other is defined by the **Heat transfer**. A high heat transfer coefficient leads to fast temperature equalization, a small heat transfer coefficient results in the zones keeping different temperatures.

HEAT

If you choose **Heat**, enter a *Name*, then select **Zone** or **Reaction zone**, choose a Zone (e.g. **Steel** or **Slag**) and enter a percentage of **MW efficiency** in the field.

Select **Heat** if the system is actively heated by an external heat source such as an electric arc or induction coil. Here only the efficiency is defined, which is the percentage of power (for example electrical power) that is transformed into heat that enters the system and heats it up. The profile of power versus time is defined in the **Process Schedule**.

Click **Save** when the Process Model is defined and enter a **Process model name**. Each time you save a process model it adds it to the list on the main **Configuration** window, which you can use in future set ups.

Process Simulation: Materials Tab

The following outlines what you can set on the **Configuration** window **Materials** tab. The overall steps to set this up are described in Defining the Process Simulation.

This section is similar to how you define the materials for the Equilibrium branch. Some information is explained in more detail for Equilibrium Simulation: Conditions Tab and not repeated here.

MATERIAL

Materials are grouped into **Steel** (or another user-defined **Metal** group), **Slag** (or another user-defined non-metallic group), and **Gas**.

Some of what you choose from lists in this section depend on what you have entered as the **Process Model** above. For example, the **Zone** or **Reaction zone** options are based on those entries (e.g **Steel** or **Slag**).

To add one or more material groups click the add ⊕ button. Click the minus ⊖ button to remove a material group. The new material inherits the default settings of that group.

After choosing the Material for the section being defined, also enter a value of the *temperature* in the field. Choose what **Zone** or **Reaction zone** it is to be **Added to**.

The times and amounts of additions are defined in the **Process schedule**.

SHOW COMPOSITION

When you click **Show composition** next to any material group, additional fields display where you can further define each material group.

From this composition area you can click the **Save material** button to add the new material to the group's list. The newly named material composition is then available for use with that material group.

From the first **Input type** list select **Mass percent**, **Mass fraction**, **Mole percent**, or **Mole fraction**.

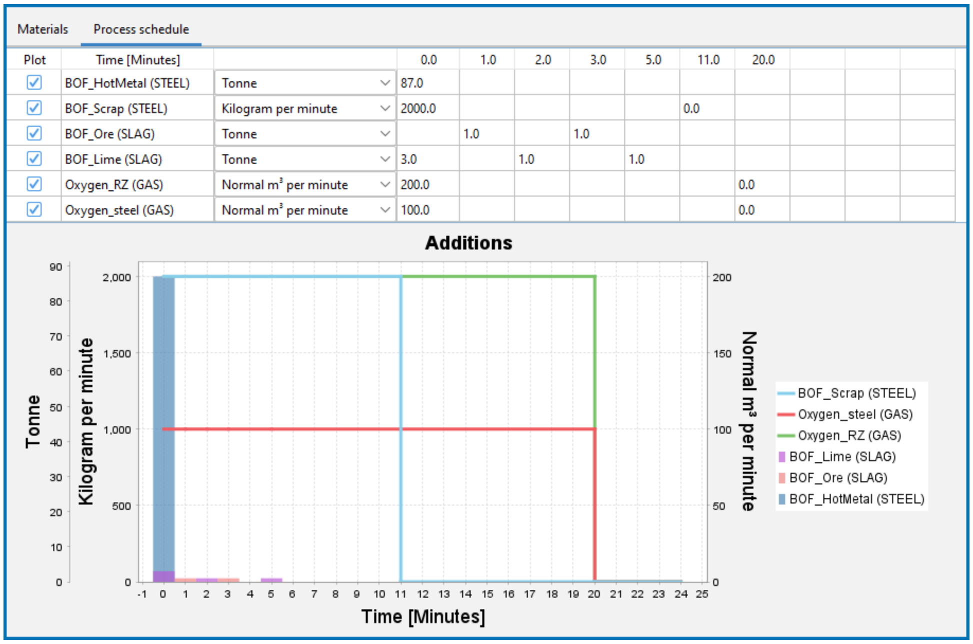
For the next list, the default is based on which group you are defining. For the Steel (Metal) group it is **Element**, for Slag it is **Component**, and for Gas it is **Gas component**.

Choose **Major component** so that as you add other components, the major one is adjusted to be the rest of the composition. Choose **Normalize to total of 100%** so that the sum is adapted to 100%. This is useful if you need to work with a given composition that does not sum up to 100%.

Process Simulation: Process Schedule Tab

The following outlines what you can set on the **Configuration** window **Process Schedule** tab. The overall steps to set this up are described in Defining the Process Simulation. Also see Working with the Process Schedule.

On the **Process schedule** tab, the sequence and amounts of additions during the duration of the process are defined. All the materials defined in the **Materials** tab automatically are included in the table. If a heat addition is defined in the *Process Model* this is also included in the table.



Plot	Time [Minutes]		0.0	1.0	2.0	3.0	5.0	11.0	20.0
☑	BOF_HotMetal (STEEL)	Tonne	87.0						
☑	BOF_Scrap (STEEL)	Kilogram per minute	2000.0					0.0	
☑	BOF_Ore (SLAG)	Tonne		1.0		1.0			
☑	BOF_Lime (SLAG)	Tonne	3.0		1.0		1.0		
☑	Oxygen_RZ (GAS)	Normal m³ per minute	200.0						0.0
☑	Oxygen_steel (GAS)	Normal m³ per minute	100.0						0.0

PLOT

Select the **Plot** checkbox to include or exclude the components in the process schedule plot area, for example, to help you examine the changes in the plot window, after defining the Steel, Scrap, Slag, or Gas rows, see what happens when you remove one or more items from the plot.

UNIT

Enter a value and choose a unit **Tonne**, **Kilogram**, **Pound**, **Kilogram per second**, or **Kilogram per minute**. For **Gas** you can also choose **Normal m3 per minute** as the unit.

If a unit **Tonne**, **Kilogram**, or **Pound** is selected, then the additions are defined as one-time additions at a certain time. If a rate is chosen as unit of the addition (such as Kilogram per minute or second, for gas Normal cubic meter per minute or second) then the rate of addition is entered into the table and it stays constant until a different value is entered.

Options Tab

These settings are for the **Process Metallurgy Calculator** and are located on the **Configuration** window → **Options** tab. Only unique settings are described below.

You can change these settings locally for a specific Calculator or globally for some defaults in the **Options** *window* (a different location than the tab).

To open the **Options** window:

- Windows: Select **Tools → Options**.
- Mac: Select **Thermo-Calc** *<version>* **→ Preferences** or **Settings** or press <⌘> on the keyboard.

then click the **Graphical Mode** tab and the **Process Metallurgy** node in the tree.

Equilibrium Simulation: Conditions Tab

Material Manager

Use the **Material group** and **Material** lists to create and delete material groups, as well as delete material compositions that are saved from the Process Metallurgy Calculator. It is useful for frequently used materials.

See Working with the Material Manager for details.

- **Material group**: To create or delete a group, choose it from this list, e.g. **Steel**, **Slag**, or **Gas**. The *Steel* group is simply a generic **Metal** group. You can create other user-defined metal groups and then these are listed. Click **Create group** or **Delete group** as required to manage the list.
- **Material**: To delete a material, choose the group type then select the material composition to delete. For example, select the **Slag** material group, then choose the **Example Slag** material and click **Delete material** to remove it from all lists.

Process Material Equilibrium and Grid

MINIMIZATION STRATEGY

Under *Process Material Equilibrium and Grid*, the default uses the **Global test preferred** option for **Equilibrium** simulations and the **Local minimization preferred** option for **Process simulations**.

The **Minimization Strategy** setting is used to ensure that the most stable minimum under the specified conditions is computed.

With either the *Global test preferred* or *Local minimization preferred* setting, the program cycles through options before it gives up:

- For **Global test preferred** the minimization starts with a global test and if that fails it runs full global minimization.
- For **Local minimization preferred**the minimization starts with a local minimization, in case of failure it tries a global test and finally a full global minimization.

If you choose **Local minimization only** or **Global minimization only**, the program just tries the one setting and gives up if it fails.

For general information about global minimization, see the topic related to the Console Mode command, GLOBAL_MINIMIZATION.

MAX NO. OF ITERATIONS

Under *Process Material Equilibrium and Grid*, the default for the **Max no. of iterations** is that the program tries 2000 iterations before it gives up.

REQUIRED ACCURACY

The default **Required accuracy** is `1.0E-6`. This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.

SMALLEST FRACTION

Under *Process Material Equilibrium and Grid*, the default **Smallest fraction** is `1.0E-16`. If this value fails, the program tries other values. This is the value assigned to constituents that are unstable.

> The default value is for all phases except for the IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) where the default value is always as 1E-30.

MAX GRID POINTS (IN GLOBAL MINIMIZATION)

Under *Process Material Equilibrium and Grid*, from the **Max grid points** list choose:

- **Coarse** for 2000 grid points, the default,
- **Medium** for 20,000 grid points,
- **Fine** for 200,000 grid points, or
- **Custom** to set your own number of grid points.

APPROXIMATE DRIVING FORCE FOR METASTABLE PHASES

Under *Process Material Equilibrium and Grid*, the **Approximate driving force for metastable phases** checkbox is selected by default, which means the metastable phases are included in all iterations. However, these may not have reached their most favorable composition and thus these driving forces may be only approximate.

FORCE POSITIVE DEFINITE PHASE HESSIAN

Under *Process Material Equilibrium and Grid*, the **Force positive definite phase Hessian** checkbox is selected by default and this setting determines how to reach the minimum of an equilibrium state.

CONTROL STEP SIZE

Under *Process Material Equilibrium and Grid*, the **Control step size** checkbox is selected by default and this setting determines how to reach the minimum of an equilibrium state.

Timestep Control

This section is used with the **Process simulation** calculations. Read About Dynamic Time Stepping to better understand these settings.

TIMESTEP

Under *Timestep control*, enter numerical values in the fields for the **Timestep**:

- **Initial %**
- **Smallest allowed** in seconds (s)
- **Max % of duration**

MAX TEMPERATURE CHANGE PER TIME STEP

Under *Timestep control*, in the field enter the **Max temperature change per time step** in Kelvin (K).

Nickel Model Library Property Models

? Property Model Calculator

In this section:

About the Nickel Model Library Property Models

These **Nickel Models** are available with the Property Model Calculator and as part of the Nickel Model Library.

To run calculations with the **Nickel Models** requires a valid maintenance license plus licenses for both the TCNI (version 11 and newer) and MOBNI (version 5 and newer) databases. For some Property Models, additional recommendations for the database version to use is indicated in its description. Also see our website to learn more about the Nickel Model Library.

Antiphase Boundary Energy - Ni

The **Antiphase Boundary Energy - Ni** Property Model, available with the Property Model Calculator and the Nickel Model Library, calculates the antiphase boundary energy for the gamma prime (γ') phase in Ni-base alloys.

See About the Antiphase Boundary Energy Property Model and Antiphase Boundary Energy Property Model Settings for background theory and input parameter details.

Coarsening - Ni

The **Coarsening - Ni** Property Model, available with the Property Model Calculator and the Nickel Model Library, calculates the coarsening rate coefficient *K* of one or several precipitate phases in a matrix phase, assuming spherical geometry of the precipitating phase (s).

See About the Coarsening Nickel Property Model and Coarsening Nickel Property Model Settings.

Equilibrium with Freeze-in Temperature - Ni

The **Equilibrium with Freeze-in Temperature - Ni** Property Model, available with the Property Model Calculator and the Nickel Model Library, calculates equilibrium at the freeze-in temperature and evaluates the properties at a different temperature.

See About the Equilibrium with Freeze-in Temperature Nickel Property Model and Equilibrium with Freeze-in Temperature Nickel Property Model Settings.

Solvus for Ordered Phase - Ni

The **Solvus for Ordered Phase - Ni** Property Model, available with the Property Model Calculator and the Nickel Model Library, calculates the solvus of ordered phases such as FCC_L12, BCC_B2, NI3TA_D0A, NI3TI_D024, TCP-phases (Sigma), and so forth.

See About the Solvus for Ordered Phase Property Model and Solvus for Ordered Phase Property Model Settings.

Strain-Age Cracking - Ni

The **Strain-Age Cracking - Ni** Property Model, available with the Property Model Calculator and the Nickel Model Library, is used in applications related to welding or additively manufactured components, where there are interface strains between γ' (gamma prime) and the matrix.

See About the Strain-Age Cracking Property Model and Strain-Age Cracking Property Model Settings.

About the Antiphase Boundary Energy Property Model

The **Antiphase Boundary Energy - Ni** Property Model, available with the Property Model Calculator and the Nickel Model Library, calculates the antiphase boundary energy for the gamma prime (γ') phase in Ni-base alloys.

Alloy strength can be assumed [2014Cru] to be proportional to the product of the antiphase boundary energy and the square root of the fraction of the strengthening gamma-prime phase.

Equilibrium is calculated with the selected phases and conditions. The antiphase boundary energy is then evaluated for the gamma prime phase given the equilibrium composition.

To run calculations with the **Nickel Models** requires a valid maintenance license plus licenses for both the TCNI (version 11 and newer) and MOBNI (version 5 and newer) databases. For some Property Models, additional recommendations for the database version to use is indicated in its description. Also see our website to learn more about the Nickel Model Library.

Configuration Settings

The input parameters are entered on the **Configuration** window for the Property Model Calculator. There are also settings on the Plot Renderer where you can choose from the available and relevant axis variables.

See Antiphase Boundary Energy Property Model Settings for details.

Example

For an example, see PM_Ni_02: Antiphase Boundary Energy of γ'.

References

[1995Mio] A. P. Miodownik, N. J. Saunders, “The calculation of APB Energies in Ll, Compounds Using a Thermodynamic Database,” in Applications of Thermodynamics in the Synthesis and Processing of Materials, P. Nash, B. Sundman, Eds. (TMS, Warrendale, PA, 1995), pp. 91–104.

[2000Sau] N. Saunders, M. G. Fahrmann, C. J. Small, in Superalloys 2000 (TMS, Warrendale, Pa., 2000; pp. 803–811.

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Antiphase Boundary Energy Property Model Settings

The **Antiphase Boundary Energy - Ni** Property Model, available with the Property Model Calculator and the Nickel Model Library, calculates the antiphase boundary energy for the gamma prime (γ') phase in Ni-base alloys.

About the Antiphase Boundary Energy Property Model

For an example, see PM_Ni_02: Antiphase Boundary Energy of γ'

Configuration Settings

These settings are found on the Property Model Calculator when **Antiphase Boundary Energy - Ni** is selected under **Nickel Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

FREEZE-IN TEMPERATURE

Enter a **Freeze-in temperature** value in the field. The unit matches those selected under *Condition Definitions*. This is the temperature where the equilibrium is calculated.

The default is 623.15 K (350 °C).

SUBSET OF PHASES

The **Subset of phases** setting allows you to select a subset of phases relevant to the material type under investigation. The purpose is to consider only phases relevant to typical commercial Ni-base alloys, for example it excludes the eta and delta phases that are normally thermodynamically stable at heat treatment temperatures but rarely form in practice due to their slow formation. Select one of these options to include the specified phases in the calculation:

- **All phases**: To include all phases in the current system.
- **Gamma and gamma prime only** (γ and γ' only): To include only disordered FCC (γ) and L12 ordered FCC (γ').

For the **Coarsening - Ni** Property Model, you select **Gamma and selected precipitate(s)** instead and it still includes only disordered FCC (γ) and L12 ordered FCC (γ').

For **Solvus for Ordered Phases - Ni** and **Strain-Age Cracking - Ni**, this option is **Gamma + Gamma Prime**.

- **Typical Ni-base superalloy**: To include phases typically present in Ni-base superalloys, i.e. liquid, gamma (γ), gamma prime (γ'), gamma double prime (γ") and carbides (FCC_L12#3, HCP_A3#1, HCP_A3#2, M23C6, M6C, M7C3) along with some additional phases (BCC_A2, BCC_A2#2, BCC_B2, BCC_B2#2, BCT_D022, NI3B_D011, M2B_TETR, D5A_M3B2, M3B2, MB_B33, MB2_C32, G_PHASE, NI5ZR, NI7ZR2, CR3NI5SI2, CR3NI5SI2, SPINEL, ALPHA_SPINEL, CORUNDUM).
- **Typical Ni-base superalloy plus eta and delta**: To include the phases listed above for a **Typical Ni-base superalloy** plus eta (η) (NI3TI_D024) and delta (δ) (NI3TA_D0A) phases.
- **Typical Ni-base superalloy plus TCP phases**: To include the phases listed above for a **Typical Ni-base superalloy** plus topologically close packed (TCP) phases. TCP phases are laves (C14_LAVES), sigma (σ) (SIGMA), mu (μ) (MU_PHASE), R (R_PHASE), P (P_PHASE), Z (Z_PHASE) and CR3SI (CR3SI_A15).

EQUILIBRIUM MINIMIZATION STRATEGY

This setting is not available if **Gamma and gamma-prime only** is selected as the **Subset of phases**.

Select an **Equilibrium minimization strategy**. The default uses the **Global test preferred** option. For this Property Model, and for either Global option, also enter the **Max number of global gridpoints**, where the default is 20000.

The **Minimization Strategy** setting is used to ensure that the most stable minimum under the specified conditions is computed.

With either the *Global test preferred* or *Local minimization preferred* setting, the program cycles through options before it gives up:

- For **Global test preferred** the minimization starts with a global test and if that fails it runs full global minimization.
- For **Local minimization preferred**the minimization starts with a local minimization, in case of failure it tries a global test and finally a full global minimization.

If you choose **Local minimization only** or **Global minimization only**, the program just tries the one setting and gives up if it fails.

For general information about global minimization, see the topic related to the Console Mode command, GLOBAL_MINIMIZATION.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

Select from these plot quantities and then choose the unit Joule per m^2 or Millijoule per m^2:

- **Composition**
- **APBE for 111 plane (1/2)**: The antiphase boundary energy for the 111-plane for the first γ' phase.
- **APBE for 100 plane (1/2)**: The antiphase boundary energy for the 100-plane for the first γ' phase.
- **APBE average (1/2)**: The average of the antiphase boundary energy for the 100- and 111-plane for the first γ' phase.
- **APBE for 111 plane (2/2)**: The antiphase boundary energy for the 111-plane for the second γ' phase in the case more than one FCC_L12 composition set is identified as γ'.
- **APBE for 100 plane (2/2)**: The antiphase boundary energy for the 100-plane for the second γ' phase in the case more than one FCC_L12 composition set is identified as γ'.

- **APBE average (2/2)**: The average of the antiphase boundary energy for the 100- and 111-plane for the first γ' phase in the case more than one FCC_L12 composition set is identified as γ'.
- **Delta APBE rel.pure Ni3Al**: w.r.t. Ni3Al - The antiphase boundary energy of the 111-plane for the current γ' relative to 'pure' Ni3Al γ'.

About the Coarsening Nickel Property Model

The **Coarsening - Ni** Property Model, available with the Property Model Calculator and the Nickel Model Library, calculates the coarsening rate coefficient *K* of one or several precipitate phases in a matrix phase, assuming spherical geometry of the precipitating phase (s).

This model is based on the **General Models → Coarsening** Property Model, the primary difference that with the **Nickel Models** version you are guided to the selection of phases during the set up.

See About the Coarsening Property Model for the background theory described for the **General Models** version.

Configuration Settings

The input parameters are entered on the **Configuration** window for the Property Model Calculator. There are also settings on the Plot Renderer where you can choose from the available and relevant axis variables.

See Coarsening Nickel Property Model Settings for details.

Coarsening Nickel Property Model Settings

The **Coarsening - Ni** Property Model, available with the Property Model Calculator and the Nickel Model Library, calculates the coarsening rate coefficient *K* of one or several precipitate phases in a matrix phase, assuming spherical geometry of the precipitating phase (s).

About the Coarsening Nickel Property Model

This Property Model requires a kinetic database with mobilities for the matrix phase.

Configuration Settings

The settings are found on the Property Model Calculator when **Coarsening - Ni** is selected under **Nickel Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

SUBSET OF PHASES

The **Subset of phases** setting allows you to select a subset of phases relevant to the material type under investigation. The purpose is to consider only phases relevant to typical commercial Ni-base alloys, for example it excludes the eta and delta phases that are normally thermodynamically stable at heat treatment temperatures but rarely form in practice due to their slow formation. Select one of these options to include the specified phases in the calculation:

- **All phases**: To include all phases in the current system.
- **Gamma and gamma prime only** (γ and γ' only): To include only disordered FCC (γ) and L12 ordered FCC (γ').

For the **Coarsening - Ni** Property Model, you select **Gamma and selected precipitate(s)** instead and it still includes only disordered FCC (γ) and L12 ordered FCC (γ').

For **Solvus for Ordered Phases - Ni** and **Strain-Age Cracking - Ni**, this option is **Gamma + Gamma Prime**.

- **Typical Ni-base superalloy**: To include phases typically present in Ni-base superalloys, i.e. liquid, gamma (γ), gamma prime (γ'), gamma double prime (γ'') and carbides (FCC_L12#3, HCP_A3#1, HCP_A3#2, M23C6, M6C, M7C3) along with some additional phases (BCC_A2, BCC_A2#2, BCC_B2, BCC_B2#2, BCT_D022, NI3B_D011, M2B_TETR, D5A_M3B2, M3B2, MB_B33, MB2_C32, G_PHASE, NI5ZR, NI7ZR2, CR3NI5SI2, CR3NI5SI2, SPINEL, ALPHA_SPINEL, CORUNDUM).
- **Typical Ni-base superalloy plus eta and delta**: To include the phases listed above for a **Typical Ni-base superalloy** plus eta (η) (NI3TI_D024) and delta (δ) (NI3TA_D0A) phases.
- **Typical Ni-base superalloy plus TCP phases**: To include the phases listed above for a **Typical Ni-base superalloy** plus topologically close packed (TCP) phases. TCP phases are laves (C14_LAVES), sigma (σ) (SIGMA), mu (μ) (MU_PHASE), R (R_PHASE), P (P_PHASE), Z (Z_PHASE) and CR3SI (CR3SI_A15).

EQUILIBRIUM MINIMIZATION STRATEGY

This setting is NOT available if **Gamma and selected precipitate(s)** is selected.

Select an **Equilibrium minimization strategy**. The default uses the **Global test preferred** option. For this Property Model, and for either Global option, also enter the **Max number of global gridpoints**, where the default is 20000.

The **Minimization Strategy** setting is used to ensure that the most stable minimum under the specified conditions is computed.

With either the *Global test preferred* or *Local minimization preferred* setting, the program cycles through options before it gives up:

- For **Global test preferred** the minimization starts with a global test and if that fails it runs full global minimization.
- For **Local minimization preferred**the minimization starts with a local minimization, in case of failure it tries a global test and finally a full global minimization.

If you choose **Local minimization only** or **Global minimization only**, the program just tries the one setting and gives up if it fails.

For general information about global minimization, see the topic related to the Console Mode command, GLOBAL_MINIMIZATION.

MATRIX PHASE

Choose a **Matrix phase**. The default is **Gamma** (γ).

PRECIPITATE PHASE

Choose a **Precipitate phase** to calculate its coarsening rate. Click the ⊕ **Add phase** button to add another Precipitate phase. Click the ⊖ **Remove phase** button to remove a phase.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

Select from these plot quantities:

- **Temperature**
- **Coarsening rate coefficient Ni [m^3/s]** for the precipitate phase.
- **Interfacial energy Ni [J/m^2]** for it to be between the matrix and precipitate phase.

About the Equilibrium with Freeze-in Temperature Nickel Property Model

The **Equilibrium with Freeze-in Temperature - Ni** Property Model, available with the Property Model Calculator and the Nickel Model Library, calculates equilibrium at the freeze-in temperature and evaluates the properties at a different temperature.

This Property Model is based on the **General Models** version but specifically implemented for use with nickel alloys.

The assumption is that diffusion and phase transformations are negligible when changing from the freeze-in-temperature and, therefore, that the phase amounts and compositions of phases are kept at the evaluation temperatures.

Typically, the freeze-in occurs during cooling where equilibrium can be assumed above the freeze-in temperature. This is the default setting and the **Equilibrium above freeze-in temperature** checkbox is automatically selected for this model. Change this default setting (i.e. click to clear the checkbox) when the frozen structure should be evaluated at a higher temperature than the freeze-in temperature.

The electrical resistivity due to phase interface scattering is evaluated as the scattering constant times sum of the interaction between the volume fraction of all the phases. The default value for the constant is 4.0e-8 Ωm. The contribution to thermal conductivity is assumed to be related to that of electrical resistivity, following the Wiedemann-Franz law.

A selection of homogenization functions is available for the evaluation of thermal- and electric-properties. Thermal and electric properties depend on the microstructure and the geometrical representation of phases in the microstructure can be linked to different homogenization functions. The homogenization function is applied on thermal- and electrical-resistivity. The electric conductivity, thermal conductivity, and thermal diffusivity are evaluated from the resistivities.

To run calculations with the **Nickel Models** requires a valid maintenance license plus licenses for both the TCNI (version 11 and newer) and MOBNI (version 5 and newer) databases. For some Property Models, additional recommendations for the database version to use is indicated in its description. Also see our website to learn more about the Nickel Model Library.

Configuration Settings

The input parameters are entered on the **Configuration** window for the Property Model Calculator. There are also settings on the Plot Renderer where you can choose from the available and relevant axis variables.

See Equilibrium with Freeze-in Temperature Nickel Property Model Settings.

Example

For an example see PM_Ni_01: Lattice Parameter of γ/γ'.

References

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Equilibrium with Freeze-in Temperature Nickel Property Model Settings

The **Equilibrium with Freeze-in Temperature - Ni** Property Model, available with the Property Model Calculator and the Nickel Model Library, calculates equilibrium at the freeze-in temperature and evaluates the properties at a different temperature.

About the Equilibrium with Freeze-in Temperature Nickel Property Model

For an example, see PM_Ni_01: Lattice Parameter of γ/γ'

Configuration Settings

The settings are found on the Property Model Calculator when the **Equilibrium with Freeze-in Temperature - Ni** Model is selected under **Nickel Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

FREEZE-IN TEMPERATURE

Enter a **Freeze-in temperature** value in the field. The unit matches those selected under *Condition Definitions*. This is the temperature where the equilibrium is calculated.

The default is 1273.15 K (1000 °C).

EQUILIBRIUM ABOVE FREEZE-IN TEMPERATURE

The **Equilibrium above freeze-in temperature** checkbox is selected by default and it calculates equilibrium above freeze-in temperature. Click to clear the checkbox when evaluating the frozen-in structure at higher temperatures than the freeze-in temperature.

SUBSET OF PHASES

The **Subset of phases** setting allows you to select a subset of phases relevant to the material type under investigation. The purpose is to consider only phases relevant to typical commercial Ni-base alloys, for example it excludes the eta and delta phases that are normally thermodynamically stable at heat treatment temperatures but rarely form in practice due to their slow formation. Select one of these options to include the specified phases in the calculation:

- **All phases**: To include all phases in the current system.
- **Gamma and gamma prime only** (γ and γ' only): To include only disordered FCC (γ) and L12 ordered FCC (γ').

> For the **Coarsening - Ni** Property Model, you select **Gamma and selected precipitate(s)** instead and it still includes only disordered FCC (γ) and L12 ordered FCC (γ').

> For **Solvus for Ordered Phases - Ni** and **Strain-Age Cracking - Ni**, this option is **Gamma + Gamma Prime**.

- **Typical Ni-base superalloy**: To include phases typically present in Ni-base superalloys, i.e. liquid, gamma (γ), gamma prime (γ'), gamma double prime (γ'') and carbides (FCC_L12#3, HCP_A3#1, HCP_A3#2, M23C6, M6C, M7C3) along with some additional phases (BCC_A2, BCC_A2#2, BCC_B2, BCC_B2#2, BCT_D022, NI3B_D011, M2B_TETR, D5A_M3B2, M3B2, MB_B33, MB2_C32, G_PHASE, NI5ZR, NI7ZR2, CR3NI5SI2, CR3NI5SI2, SPINEL, ALPHA_SPINEL, CORUNDUM).
- **Typical Ni-base superalloy plus eta and delta**: To include the phases listed above for a **Typical Ni-base superalloy** plus eta (η) (NI3TI_D024) and delta (δ) (NI3TA_D0A) phases.
- **Typical Ni-base superalloy plus TCP phases**: To include the phases listed above for a **Typical Ni-base superalloy** plus topologically close packed (TCP) phases. TCP phases are laves (C14_LAVES), sigma (σ) (SIGMA), mu (µ) (MU_PHASE), R (R_PHASE), P (P_PHASE), Z (Z_PHASE) and CR3SI (CR3SI_A15).

EVALUATE FOR A SINGLE PHASE ONLY

Select the **Evaluate for a single phase only** checkbox to evaluate the properties of a specific phase or deselect to evaluate the properties for the entire system.

PHASE FOR EVALUATION

This setting is available when the **Evaluate for a single phase only** checkbox is selected.

From the **Phase for evaluation** list, select any available phase or **None**.

EQUILIBRIUM MINIMIZATION STRATEGY

This setting is NOT available if **Gamma and selected precipitate(s)** is selected.

Select an **Equilibrium minimization strategy**. The default uses the **Global test preferred** option. For this Property Model, and for either Global option, also enter the **Max number of global gridpoints**, where the default is 20000.

The **Minimization Strategy** setting is used to ensure that the most stable minimum under the specified conditions is computed.

With either the *Global test preferred* or *Local minimization preferred* setting, the program cycles through options before it gives up:

- For **Global test preferred** the minimization starts with a global test and if that fails it runs full global minimization.
- For **Local minimization preferred**the minimization starts with a local minimization, in case of failure it tries a global test and finally a full global minimization.

If you choose **Local minimization only** or **Global minimization only**, the program just tries the one setting and gives up if it fails.

For general information about global minimization, see the topic related to the Console Mode command, GLOBAL_MINIMIZATION.

HOMOGENIZATION FUNCTION

The **Homogenization function** is used for the evaluation of the systems thermal and electric properties. The function is applied on thermal- and electrical-resistivity. The electric conductivity, thermal conductivity, and thermal diffusivity are evaluated from the resistivities.

The geometrical interpretation of the Hashin-Shtrikman bounds are concentric spherical shells of each phase.

- **Rule of mixtures (upper Wiener bound)**: the geometrical interpretation are continuous layers of each phase parallel with the direction of evaluation of the property.
- **Inverse rule of mixtures (lower Wiener bound)**: The geometrical interpretation are continuous layers of each phase orthogonal to the direction of evaluation of the property.
- **General lower Hashin-Shtrikman bound**: The outermost shell consists of the phase with the most sluggish property.
- **General upper Hashin-Shtrikman bound**: The innermost shell consists of the phase with the most sluggish property.
- **Hashin-Shtrikman bound with majority phase as matrix phase**: The outermost shell consists of the phase with the highest local volume fraction.

ACCOUNT FOR PHASE INTERFACE SCATTERING

The **Account for phase interface scattering** checkbox is selected by default.

The electrical resistivity due to phase interface scattering is evaluated as the scattering constant times sum of the interaction between the volume fraction of all the phases. The default value for the constant is 4.0e-8 Ωm. The contribution to thermal conductivity is assumed to be related to that of electrical resistivity, following the Wiedemann-Franz law.

PHASE INTERFACE SCATTERING CONSTANT

This setting is available when the **Account for phase interface scattering** checkbox is selected.

The **Phase interface scattering constant** default value is 4.0e-8 Ωm.

Set Reference Temperature for Technical CTE

This setting is available when the **Account for phase interface scattering** checkbox is selected.

In the field, enter the **Reference temperature for technical CTE**, where CTE is the coefficient of thermal expansion. Typically room temperature is used as the default 293.15 K (20 °C).

Define User Functions

Select the **Define user functions** checkbox to enter up to two **User-defined functions** using the Console Mode syntax.

For an example of user-defined functions, see T_07: User-Defined Functions.

Dot derivatives (e.g. Hm.T for heat capacity) should NOT be used since these are not consistent with freezing in the amount of phases.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

Select from these plot quantities:

- **Temperature**
- **Lattice parameter Gamma** (γ) (a_p): Choose a unit Meter, Micrometer, Nanometer, or Ångström.
- **Lattice parameter Gamma-Prime** (γ') (a_{gp}): Choose a unit Meter, Micrometer, Nanometer, or Ångström.
- **Lattice mismatch Gamma/Gamma-Prime** (γ/γ'): This is an unconstrained misfit between Gamma/Gamma-prime lattice parameters:

  $$100 * \frac{2*(a_{gp}-a_g)}{(a_{gp}+a_g)}$$

- **Electric resistivity (ohm m)** (Ωm)
- **Electric conductivity (S/m)**

- **Thermal conductivity (W/(mK))**
- **Thermal resistivity (mK/W)**
- **Thermal diffusivity (m^2/s)**
- **Heat capacity (J/mol K))**
- **Volume (m^3/mol)**
- **Density (g/cm^3)**
- **Linear CTE (technical) (1/K)**: Fractional change of length per unit temperature change. Calculated as (L1-L0)/(T1-T0)/L0, where L0 is the length at a reference temperature T0. T0 is by default equal to room temperature. Assumed Isotropic material.
- **Linear CTE (physical) (1/K)**: Fractional change of length per unit temperature change. Assumed Isotropic material.
- **Volumetric CTE (physical) (1/K)**: Fractional change of volume per unit temperature change.
- **User-defined function** and **2nd user-defined function**: Available when the **Define user functions** checkbox is selected and the functions are defined.

Elastic moduli is available to plot when the thermodynamic database selected includes elastic properties. However, even if the database does not have elastic constants, the quantity is visible to select from the list even. In this case there is a message in the Event Log to indicate there is no elastic data and the value will be NaN.

About the Solvus for Ordered Phase Property Model

The **Solvus for Ordered Phase - Ni** Property Model, available with the Property Model Calculator and the Nickel Model Library, calculates the solvus of ordered phases such as FCC_L12, BCC_B2, NI3TA_D0A, NI3TI_D024, TCP-phases (Sigma), and so forth.

The Model chooses the correct composition set by minimizing the Gibbs energy, which means that the correct composition set is automatically detected by the software for you.

The remarkable properties of Ni-base superalloys often rely on the formation of finely dispersed ordered phases. In order to obtain the correct microstructure, and therefore also the properties you want, it is necessary to heat treat the alloy accordingly. One important aspect of the heat treatment is the solvus temperature for the phase or phases that is expected and wanted in the microstructure. An appropriate heat treatment aims to dissolve the ordered phases in the as-cast or as-printed structure, which must be done above the respective phases' solvus temperature.

By combining the **Solvus for Ordered Phase - Ni** model with the latest TCS Ni-based Superalloys Database (TCNI) version, you can predict the solvus temperature for any ordered phase, provided that it is present in the database and that it is stable for the given alloy chemistry. As such, appropriate heat treatments may readily be designed with guidance from thermodynamic calculations, which efficiently cuts down on time spent using trial-and-error approaches.

To run calculations with the **Nickel Models** requires a valid maintenance license plus licenses for both the TCNI (version 11 and newer) and MOBNI (version 5 and newer) databases. For some Property Models, additional recommendations for the database version to use is indicated in its description. Also see our website to learn more about the Nickel Model Library.

Configuration Settings

The input parameters are entered on the **Configuration** window for the Property Model Calculator. There are also settings on the Plot Renderer where you can choose from the available and relevant axis variables.

See Solvus for Ordered Phase Property Model Settings for details.

Example

For an example, see PM_Ni_03: Critical Temperatures of Alloy 718.

Solvus for Ordered Phase Property Model Settings

About the Solvus for Ordered Phase Property Model

Configuration Settings

The settings are found on the Property Model Calculator when **Solvus for Ordered Phase- Ni** is selected under **Nickel Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

NAMING CONVENTION

Select **Conventional phase names** (the default) or **Explicit phase names**.

Select **Conventional phase names** to limit the list to commonly occurring ordered phases, which are **Gamma prime (FCC_L12)**, **Gamma double prime (BCT_D022)**, **Eta (NI3TI_D024)**, **Delta (NI3TA_D0A)**, and **Sigma (SIGMA)**. You can alternatively select a phase from the full list of **Explicit phase names**; phases available in the list are based on the selected database.

PHASE TO CALCULATE SOLVUS FOR

From the **Phase to calculate solvus for** list, choose a phase. When **Conventional phase names** is selected **Gamma prime (FCC_L12)** is the default.

Phases such as FCC_L12 and BCC_B2 normally exhibit ordering (when used with the TCS Ni-based Superalloys Database (TCNI)).

SUBSET OF PHASES

The **Subset of phases** setting allows you to select a subset of phases relevant to the material type under investigation. The purpose is to consider only phases relevant to typical commercial Ni-base alloys, for example it excludes the eta and delta phases that are normally thermodynamically stable at heat treatment temperatures but rarely form in practice due to their slow formation. Select one of these options to include the specified phases in the calculation:

- **All phases**: To include all phases in the current system.
- **Gamma and gamma prime only** (γ and γ' only): To include only disordered FCC (γ) and L12 ordered FCC (γ').

> For the **Coarsening - Ni** Property Model, you select **Gamma and selected precipitate(s)** instead and it still includes only disordered FCC (γ) and L12 ordered FCC (γ').

> For **Solvus for Ordered Phases - Ni** and **Strain-Age Cracking - Ni**, this option is **Gamma + Gamma Prime**.

- **Typical Ni-base superalloy**: To include phases typically present in Ni-base superalloys, i.e. liquid, gamma (γ), gamma prime (γ'), gamma double prime (γ'') and carbides (FCC_L12#3, HCP_A3#1, HCP_A3#2, M23C6, M6C, M7C3) along with some additional phases (BCC_A2, BCC_A2#2, BCC_B2, BCC_B2#2, BCT_D022, NI3B_D011, M2B_TETR, D5A_M3B2, M3B2, MB_B33, MB2_C32, G_PHASE, NI5ZR, NI7ZR2, CR3NI5SI2, CR3NI5SI2, SPINEL, ALPHA_SPINEL, CORUNDUM).
- **Typical Ni-base superalloy plus eta and delta**: To include the phases listed above for a **Typical Ni-base superalloy** plus eta (η) (NI3TI_D024) and delta (δ) (NI3TA_D0A) phases.
- **Typical Ni-base superalloy plus TCP phases**: To include the phases listed above for a **Typical Ni-base superalloy** plus topologically close packed (TCP) phases. TCP phases are laves (C14_LAVES), sigma (σ) (SIGMA), mu (μ) (MU_PHASE), R (R_PHASE), P (P_PHASE), Z (Z_PHASE) and CR3SI (CR3SI_A15).

Advanced Settings

Click the **Advanced settings** checkbox to edit the following settings.

UPPER AND LOWER TEMPERATURE SEARCH LIMITS (K)

The search for the solvus temperature is performed between the upper and lower limits. Enter values for the **Upper temperature search limit (K)** (default is 2000 K) and **Lower temperature search limit (K)** (default is 500 K).

FIRST AND SECOND SUBLATTICES FOR ORDERING

Depending on the phase model for the selected phase, different sets of sublattices can be used to model ordering. For example, the ordering of FCC_L12 in the TCS Ni-based Superalloys Database (TCNI) occurs on sublattice 1 and 2. Enter a number for the **First sublattice for ordering** (default is 1) and **Second sublattice for ordering** (default is 2).

NUMBER OF DECIMALS

Ordering reactions may be continuous and it is necessary to set a numerical precision. This is because the difference in site occupancy in ordered and disordered phases may be small. Enter a **Number of decimals** at which to truncate the site fractions (default is 7).

MAX NUMBER OF ITERATIONS

Limits the number of iterations. Enter any value in the **Max. number of iterations** field that is greater than 0. The default is 100.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

Select from these plot quantities:

- **Composition**
- **Solvus temperature**

About the Strain-Age Cracking Property Model

The **Strain-Age Cracking - Ni** Property Model, available with the Property Model Calculator and the Nickel Model Library, is used in applications related to welding or additively manufactured components, where there are interface strains between γ' (gamma prime) and the matrix.

To run calculations with the **Nickel Models** requires a valid maintenance license plus licenses for both the TCNI (version 11 and newer) and MOBNI (version 5 and newer) databases. For some Property Models, additional recommendations for the database version to use is indicated in its description. Also see our website to learn more about the Nickel Model Library.

For best results with this Property Model and the features it uses, it is recommended to use TCNI version 12 and newer.

Strain-age cracking (SAC) may occur in welded or additively manufactured components due to interface strains between γ' (gamma prime) and the matrix. The interface strain may be quantified as a misfit parameter, i.e.

$$\delta = \frac{2(a_{\gamma'} - a_{\gamma})}{(a_{\gamma'} + a_{\gamma})}$$

where a is the lattice parameter of each respective phase (γ matrix or γ') in conjunction with residual thermal stresses from welding or additive manufacturing. Strain-age cracking may occur at negative values of the misfit parameter in combination with thermal stresses and the risk for cracking is also related to the γ' volume fraction.

Misfit strain naturally varies with temperature (thermal expansion) and phase composition (molar volume depends on composition and temperature) and therefore an accurate assessment of the strain-age cracking risk must account for these variables. When defining this Model on the Configuration window, this is managed using either a **Single temperature** or **Temperature interval** mode.

Single Temperature Mode

When using the **Single temperature** mode, the model evaluates the misfit parameter at the temperature and composition specified. By stepping in temperature or composition (or both), it is possible to get an idea of how the misfit varies. Misfit values calculated using this mode can be compared with experiment but it is necessary to remember that comparisons are only valid if experimental data are taken from fully equilibrated alloys.

Temperature Interval Mode

The **Temperature interval** mode circumvents the issue of having to compare with fully equilibrated alloys. It provides a single parameter to describe the tendency for strain-age cracking. When using this mode, the Model searches for a temperature interval, between the lower limit (this is the **Temperature** set under *Condition Definitions*) and the upper limit (by default the calculated γ' solvus, which can also be changed by using the **Set maximum temperature** checkbox), where the misfit parameter becomes negative.

The misfit value, and the γ' volume fraction is then integrated over the interval where the misfit is negative and the risk value for strain-age cracking is thereafter calculated.

Values of the SAC risk factor close to or below 0 indicate low or no risk for strain-age cracking. Positive values indicate risk for cracking and the more positive the value, the higher the risk. The risk factor, as defined here, also incorporates all thermodynamically related factors for strain-age cracking and makes it possible to differentiate the SAC risk for various alloys using a single number for any given temperature interval.

Configuration Settings

The input parameters are entered on the **Configuration** window for the Property Model Calculator. There are also settings on the Plot Renderer where you can choose from the available and relevant axis variables.

See Strain-Age Cracking Property Model Settings for details.

Example

For an example, see PM_Ni_04: Strain Age Cracking (SAC).

Reference

[2024Kap] B. Kaplan, A comprehensive model for quantitatively predicting the comparative Strain-Age Cracking risk in welded or additively manufactured Ni-base superalloys. In press, Mater. Today Commun., 40, 109408 (2024).

Strain-Age Cracking Property Model Settings

The **Strain-Age Cracking - Ni** Property Model, available with the Property Model Calculator and the Nickel Model Library, is used in applications related to welding or additively manufactured components, where there are interface strains between γ' (gamma prime) and the matrix.

Strain-Age Cracking Property Model Settings

For an example, see PM_Ni_04: Strain Age Cracking (SAC).

Configuration Settings

These settings are found on the Property Model Calculator when **Strain-Age Cracking - Ni** is selected under **Nickel Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

SUBSET OF PHASES

The **Subset of phases** setting allows you to select a subset of phases relevant to the material type under investigation. The purpose is to consider only phases relevant to typical commercial Ni-base alloys, for example it excludes the eta and delta phases that are normally thermodynamically stable at heat treatment temperatures but rarely form in practice due to their slow formation. Select one of these options to include the specified phases in the calculation:

- **All phases**: To include all phases in the current system.
- **Gamma and gamma prime only** (γ and γ' only): To include only disordered FCC (γ) and L12 ordered FCC (γ').

For the **Coarsening - Ni** Property Model, you select **Gamma and selected precipitate(s)** instead and it still includes only disordered FCC (γ) and L12 ordered FCC (γ').

For **Solvus for Ordered Phases - Ni** and **Strain-Age Cracking - Ni**, this option is **Gamma + Gamma Prime**.

- **Typical Ni-base superalloy**: To include phases typically present in Ni-base superalloys, i.e. liquid, gamma (γ), gamma prime (γ'), gamma double prime (γ") and carbides (FCC_L12#3, HCP_A3#1, HCP_A3#2, M23C6, M6C, M7C3) along with some additional phases (BCC_A2, BCC_A2#2, BCC_B2, BCC_B2#2, BCT_D022, NI3B_D011, M2B_TETR, D5A_M3B2, M3B2, MB_B33, MB2_C32, G_PHASE, NI5ZR, NI7ZR2, CR3NI5SI2, CR3NI5SI2, SPINEL, ALPHA_SPINEL, CORUNDUM).
- **Typical Ni-base superalloy plus eta and delta**: To include the phases listed above for a **Typical Ni-base superalloy** plus eta (η) (NI3TI_D024) and delta (δ) (NI3TA_D0A) phases.
- **Typical Ni-base superalloy plus TCP phases**: To include the phases listed above for a **Typical Ni-base superalloy** plus topologically close packed (TCP) phases. TCP phases are laves (C14_LAVES), sigma (σ) (SIGMA), mu (μ) (MU_PHASE), R (R_PHASE), P (P_PHASE), Z (Z_PHASE) and CR3SI (CR3SI_A15).

CHOOSE MODE

The Strain-Age Cracking (SAC) risk can be evaluated for a single temperature or for a specified temperature interval.

For background information about these settings, see Strain-Age Cracking Property Model Settings.

From the **Choose mode** list, select **Temperature interval** or **Single temperature**.

For **Temperature interval** the following limits are applied and defined with additional settings:

- The lower limit **Temperature** is set under *Condition Definitions*.
- The upper limit is by default the γ' solvus temperature. You can also select the **Set maximum temperature** checkbox to enter a user defined maximum temperature.

SET MAXIMUM TEMPERATURE

Available when **Temperature interval** is selected as the mode.

The Strain-Age Cracking (SAC) risk is evaluated between the temperature specified in conditions and the γ' solvus.

Select the **Set maximum temperature** checkbox if a lower maximum temperature than the γ' solvus is required and thus to skip the γ' solvus calculation.

MAXIMUM TEMPERATURE

Available when **Temperature interval** is selected as the mode and the **Set maximum temperature** checkbox is selected.

Limit the search for a negative misfit to the **Maximum temperature** entered in the field.

> This should be below the γ' solvus temperature.

INITIAL STEP SIZE FOR SEARCH

Available when **Temperature interval** is selected as the mode.

The search for a negative misfit parameter is initiated with the step size entered in the **Initial step size for search** field.

> If convergence issues arise, it can be useful to adjust this parameter and increase (or decrease) the lower temperature limit.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

Depending on the set up, there are a variety of plot quantities available to choose from. For example, select from these plot quantities:

- **Temperature**
- **Composition**
- **Initial step size for search**
- **SAC risk factor**
- **Solvus of FCC_L12 (gamma prime)**
- **Misfit value at current temperature**

Noble Metal Alloys Model Library Property Models

? Property Model Calculator

In this section:

About the Noble Metal Alloys Model Library Property Models

These **Noble Metal Alloys Models** are available with the Property Model Calculator and as part of the Noble Metal Alloys Model Library.

The **General Models**are available to all users. To run calculations with the **Noble Metal Alloys Models** (as part of the Noble Metal Alloys Model Library) requires a valid maintenance license plus a license for the TCNOBL (version 3 and newer) database.

Optical Properties - Noble

The **Optical Properties - Noble** Property Model, available with the Property Model Calculator and the Noble Metal Alloys Model Library, is used to simulate the color, reflection, and transmission of light, based on modeling the alloy microstructure and the resulting optical properties. This model is currently applicable for the Au-Al-Ag-Cu-Pt system.

See About the Optical Properties - Noble Metals Property Model and Optical Properties - Noble Metals Property Model Settings for background theory and input parameter details.

About the Optical Properties - Noble Metals Property Model

The **Optical Properties - Noble** Property Model, available with the Property Model Calculator and the Noble Metal Alloys Model Library, is used to simulate the color, reflection, and transmission of light, based on modeling the alloy microstructure and the resulting optical properties. This model is currently applicable for the Au-Al-Ag-Cu-Pt system.

For an example see PM_Noble_01: Color Prediction.

In the text *CIE* is the abbreviation for *Commission internationale de l'éclairage* (International Commission on Illumination), which is the international authority on light, illumination, color, and color spaces.

To run calculations with the **Noble Metal Alloys Models** (as part of the Noble Metal Alloys Model Library) requires a valid maintenance license plus a license for the TCNOBL (version 3 and newer) database.

The input parameters are entered on the **Configuration** window for the Property Model Calculator. There are also settings on the Plot Renderer where you can choose from the available and relevant axis variables.

See Optical Properties - Noble Metals Property Model Settings

Background

The **Optical Properties - Noble** model simulates the color and optical properties such as refractive index n and extinction coefficient k for a given condition. The process to simulate those properties has four steps.

The first step is to calculate the composition and phase fractions for phases using the Equilibrium Calculator. Once that is done, you calculate the dielectric function $\epsilon(\lambda)$ of an alloy:

$$\epsilon(\lambda) = \epsilon_1(\lambda) + i\epsilon_2(\lambda)$$

where $\epsilon(\lambda)$ is the complex dielectric function of wavelength, $\epsilon_1(\lambda)$ is the real part of the dielectric function, representing the material's ability to polarize in response to an electric field, thus affecting refraction, and $\epsilon_2(\lambda)$ is the imaginary part of the dielectric function, representing the energy loss or absorption in the material.

Thermo-Calc calculates the dielectric functions of FCC_A1 and L12_FCC phases with different Al, Au, Ag, Cu, and Pt content. The TCS Noble Metal Alloys Database (TCNOBL) calculates dielectric functions that cover intermetallic phases AL2CU_C16, AL3NI2 (PT)_D513, ALPT_B20, CUPT_L11, AL2AU_C1_CAF2, PTAL2, and CU9AL4. For alloys containing multiple phases, the Bruggeman model [2001Mar] is adopted to get the effective dielectric functions based on the phase fraction and dielectric functions of each individual phase. For N different phases, the generalized Bruggeman model equation is:

[*Eq. 1*] $$\sum_{i=1}^{N} f_i \frac{\epsilon_i-\epsilon_{\text{eff}}}{\epsilon_i+(N-1)\epsilon_{\text{eff}}}=0$$

Where:

- ϵ_i is the dielectric function of the i-th phase.
- f_i is the volume fraction of the i-th phase, and $\sum_{i=1}^{N} f_i = 1$
- ϵ_{eff} is the effective dielectric constant of the composite material.

The third step is obtaining refractive index n and k from dielectric functions using Eq. 2 and Eq. 3.

[*Eq. 2*] $$n=\sqrt{\frac{\epsilon_1+\sqrt{\epsilon_1^2+\epsilon_2^2}}{2}}$$

[*Eq. 3*] $$k=\sqrt{\frac{-\epsilon_1+\sqrt{\epsilon_1^2+\epsilon_2^2}}{2}}$$

ϵ_1 and ϵ_2 are the real and imaginary parts of dielectric functions, respectively.

The fourth step is to calculate reflectivity of the material using Fresnel equations (Eq. 4 and Eq. 5) [2023Gri], which describes how much light is reflected and transmitted when it strikes from material 1 to the surface of material 2 at a specific angle. For light striking the surface at an oblique angle θ_i, the Fresnel equations differ for s-polarized and p-polarized light. For more complex situations such as thin films and multiple materials layers, the transfer matrix method (TMM) is used [2016Byr]:

[*Eq. 4*] $$R_s=\left|\frac{n_1\cos\theta_i-n_2\cos\theta_t}{n_1\cos\theta_i+n_2\cos\theta_t}\right|^2$$

[*Eq. 5*] $$R_p=\left|\frac{n_2\cos\theta_i-n_1\cos\theta_t}{n_2\cos\theta_i+n_1\cos\theta_t}\right|^2$$

Where:

- R_s: The reflectance for s-polarized light.
- R_p: The reflectance for p-polarized light.
- n_1: The complex refractive index of material 1 (include real and imaginary part). In the current version material 1 is set to be air.
- n_2: The complex refractive index of material 2 (include real and imaginary part).
- θ_i: The angle of incidence (angle between the incident light and the normal to the surface).
- θ_t: The transmission angle (or angle of refraction), calculated using Snell's law: $n_1 \sin\theta_i = n_2 \sin\theta_t$.

The last step is to calculate the color coordinates by using the CIE XYZ color space and integrating over the visible spectrum [2019Pra]:

[*Eq. 6*] $$X = k\int_{380}^{780} R(\lambda)S(\lambda)x(\lambda)d\lambda$$

[*Eq. 7*] $$Y = k\int_{380}^{780} R(\lambda)S(\lambda)y(\lambda)d\lambda\lambda$$

[*Eq. 8*] $$Z = k\int_{380}^{780} R(\lambda)S(\lambda)z(\lambda)d\lambda$$

Where:

- $R(\lambda)$ is the reflectance of the material as a function of wavelength λ, where it is calculated using the calculated materials n and k and Fresnel equations.
- $S(\lambda)$ is the spectral power distribution of the illuminant (for example, the CIE D65 illuminant represents average daylight).
- $x(\lambda)$, $y(\lambda)$, and $z(\lambda)$ are the CIE color-matching functions that model the human eye's response to different wavelengths of light.
- $d\lambda$ is the differential element over the visible spectrum (400 nm to 700 nm).
- k is a normalization constant chosen so that Y = 100 for a perfectly reflective material.

Finally, the tristimulus values for the color of the material is found and based on its reflectance spectrum.

You can further convert these tristimulus values into other color spaces, such as CIE LAB or sRGB, depending on the display or application requirements. See About Color Space.

About DeltaE (ΔE)

Delta E (ΔE, dE) is a metric to understand how the human eye perceives color difference. On a typical scale, the ΔE value ranges from 0 to 100. The larger the ΔE value, the more perceptible the color difference.

If ΔE is:

- Smaller than 2 (ΔE < 2), it is hard to find the color difference.
- In the range of 2 – 10, you can find the difference at a glance.
- Between 11 and 49, colors are more similar than opposite.
- Between 50 to 99, colors are more opposite than similar.
- 100, colors are the exact opposite.

This is a general guideline and it is possible to get a ΔE value below 1.0 for two colors that appear different. This is the case with CIE 1976 and CIE 1994 formulas, in which saturation is either not considered or not weighted properly. For the **Optical Properties** Model there are three methods for calculating ΔE. Because of inconsistencies between the three algorithms, the exact meaning of ΔE changes slightly depending on which formula is used.

ΔE Method

When you select the **Calculate ΔE value** checkbox, an additional setting, **ΔE method** is available. This section describes the options **CIE 1976**, **CIE 1994**, and **CIE 2000** (default).

Over time, several versions of ΔE have been developed to improve how accurately they represent human color perception. The most common versions are ΔE 1976, ΔE 1994, and ΔE 2000. Each one has improvements in accuracy for different use cases.

- ΔE 1976 formula (**CIE 1976**) was the first standardized method to calculate color differences and is based on the CIE 1976 Lab color space. It uses the Euclidean distance between two colors in this three-dimensional space. It is simple and easy to compute, however it has limitations. For example, it treats all changes in color as being equally perceptible, even though the human eye is more sensitive to changes in lightness and less sensitive to changes in chroma (color saturation).

- ΔE 1994 **CIE 1994** was introduced to address the limitations of ΔE 1976 by considering the non-uniformity of human color perception. It adjusts for differences in lightness, chroma, and hue. It is widely used in industrial applications such as textiles, coatings, and plastics but it still does not perfectly match human visual perception.
- ΔE 2000 **CIE 2000** is the most recent and accurate method to calculate color differences. It is designed to improve on ΔE 1994 and provides a more perceptually uniform color difference metric, considering additional corrections for viewing conditions and color perception anomalies. It is the best choice for applications where precise color matching is crucial.

About the Standard Illuminant

There are several options to choose from in the **Standard illuminant** list. These options are related to how the color of alloys is simulated under different lighting conditions. Each option represents a specific type of light source with a defined spectral power distribution (SPD), which describes the intensity of light at different wavelengths. The choice of illuminant affects the perceived color of an object.

The following is an overview of the most common standard illuminants available to select.

- **Single wavelength**: Choose this when you want to know n and k value at certain wavelengths. When selected, color is not calculated.
- **A**: Illuminant A represents typical tungsten incandescent lighting, with a color temperature ~2856 K. Use case: Indoor lighting conditions.
- **B**: Illuminant B represents noon sunlight, with a color temperature ~4874 K. Use case: Daylight conditions with direct sunlight. Often replaced by D series illuminants.
- **C**: Illuminant C represents average daylight, with a color temperature ~6774 K. Use case: Color matching in daylight, superseded by the D-series illuminants.
- Illuminant **D** Series represents different types of daylight with varying color temperatures
    - **D50**: ~5003 K, warm daylight at sunrise or sunset.
    - **D55**: ~5503 K, mid-morning or mid-afternoon daylight.
    - **D65**: ~6504 K, the most common standard for noon daylight conditions. This is the default for the Property Model.
    - **D75**: ~7500 K, used for north sky daylight, that has been largely replaced by D65.
- **E**: Illuminant E is theoretical, equal-energy illuminant, with no color temperature as it is theoretical. Use case: Represents uniform energy across all visible wavelengths, often used in colorimetric calculations as a reference.

- Illuminant **F** Series illuminants represent various types of fluorescent lighting, commonly found in offices, retail environments, and other indoor spaces. The number after "FL" corresponds to different types of fluorescent bulbs.
    - **FL1**: 6430, daylight fluorescent.
    - **FL2**: 4230, cool white fluorescent.
    - **FL3**: 3450, white fluorescent.
    - **FL4**: 2940, warm white fluorescent.
    - **FL5**: 6350, daylight fluorescent.
    - **FL6**: 4150, light white fluorescent.
    - **FL7**: 6500, D65 simulator, daylight simulator.
    - **FL8**: 5000, D50 simulator, Sylvania F40 Design 50.
    - **FL9**: 4150, cool white deluxe fluorescent.
    - **FL10**: 5000, Philips TL85, Ultralume 50.
    - **FL11**: 4000, Philips TL84, Ultralume 40.
- **LED** Illuminants represent different LED lighting sources, which are becoming more common as replacements for traditional incandescent and fluorescent lighting. They often focus on different spectral distributions.
    - **LED-B1** to **LED-B5**: Represents different types of blue-enhanced LED lights.
    - **LED-BH1** defines a blend of phosphor-converted blue and a red LE.
    - **LED-V1** and **LED-V2**: Represents different types of violet-enhanced LED lights
    - **LED-RGB1**: Represents RGB LED lights, where colors are mixed from red, green, and blue LEDs.

In summary:

- D65 is typically used to simulate daylight when designing digital displays or performing color matching in industrial settings.
- Illuminant A is used to simulate indoor lighting conditions with tungsten bulbs.
- Fluorescent (FL series) and LED illuminants are used when you need to simulate environments using these artificial light sources.

About the Viewing Angle

The **Viewing angle** options are **CIE 1931 2 Degree Standard Observer** or **CIE 1964 10 Degree Standard Observer**.

The CIE 2° and CIE 10° Standard Observers are models that describe how an average human eye perceives color. They are based on experiments that measured human color vision using color matching functions. These functions describe how different wavelengths of light are combined by the human eye to match a perceived color. The main difference between the two observers lies in the angle of view they represent, which corresponds to different parts of the eye's visual field.

- CIE 1931 2° Standard Observer model is based on experiments where subjects matched colors within a 2° field of view. This small angle represents the central vision, which is the part of the eye responsible for seeing fine detail. It is most accurate to view small objects or when details are seen up close, such as tiny pixels on a screen or small color samples.
- CIE 1964 10° Standard Observer model represents color perception over a 10° field of view, a much larger area than the 2° observer. This wider field involves more of the peripheral vision, provides a broader and more comprehensive representation of how the eye perceives color in general viewing situations. This is better for measuring color in typical situations where larger objects are viewed, such as printed materials, paints, textiles, or any larger surface.

About Color Space

A color space organizes colors to ensure consistent representation across devices. The **Color space** options are used in two sets of settings and in both you have the option to choose **LAB** (default), **sRGB**, or **XYZ**.

- CIE **LAB** (the default) includes all visible colors and is ideal for color matching, quality control, and any application where accurate perceptual color differences matter.
- CIE **XYZ** covers all perceivable colors and is best for scientific and colorimetric studies, where precise color representation and transformations are needed.
- **sRGB** has a smaller color gamut, but it is widely used for displaying on consumer electronics

CIE LAB Color Space (CIE LAB)

CIE LAB was introduced by the CIE in 1976, and was designed to overcome some of the limitations of CIE XYZ. It created a color space that is perceptually uniform, meaning that a given change in color value should correspond to a similar level of perceived difference to the human eye.

How it Works

- **L**: Lightness (ranging from 0 for black to 100 for white).
- **a**: Green-red axis (with negative values being green and positive values being red).
- **b**: Blue-yellow axis (with negative values being blue and positive values being yellow).

When to Use It

- Color matching and quality control: CIELAB is used extensively in industries like, where precise control of color is required. Like CIE XYZ, LAB is device-independent, meaning it can represent colors regardless of the device displaying or printing them.
- ΔE calculations: The LAB color space is the basis for computing ΔE values, which measure the perceptual difference between two colors. This is important for ensuring that two objects have colors that match closely.
- Easy to interpret and understand by humans: The LAB color space is designed so that small changes in color values are perceived by humans as approximately the same amount of color difference, regardless of where they occur in the color space.

Limitations

- Not well-suited for all applications: Because LAB is not tied to specific devices, it may not be as effective for applications where you're working within the constraints of a particular display or print color gamut (e.g., in digital photography).

CIE XYZ Color Space

Developed in 1931 by the CIE, which was based on tristimulus values—X, Y, and Z—that are hypothetical primaries derived from human vision experiments. It aims to represent all visible colors using a mathematical model grounded in human color perception.

How it Works

The Y value is designed to represent luminance, which corresponds to the brightness or intensity of the color, while X and Z represent the chromaticity (colorfulness) without the influence of brightness.

When to Use It

Scientific research: Since CIE XYZ can represent any perceivable color, it is used in color science and colorimetric applications where precise color measurements are required.

- Device-independent color reproduction: It is used as a foundational color space for transforming colors between different device color profiles, such as between monitors, printers, or cameras.
- Converting to other color space: It's a reference color space, which makes it useful as an intermediary when converting colors between different color spaces.

Limitations

- Not perceptually uniform: While it can represent all colors, it does not account for how humans perceive color differences. A color change of the same magnitude in different areas of the XYZ space might not be perceived as equally different to the human eye.
- Not intuitive for users: The X, Y, and Z coordinates do not correspond to human-perceptible properties like red, green, or blue, making it harder for non-technical users to interpret.

sRGB Color Space

sRGB (Standard Red Green Blue) was created by HP and Microsoft in 1996 as a standard color space for digital displays and the internet webpage. It is based on the typical capabilities of a standard CRT monitor and has become the default color space for web images, digital photography, and many consumer-level devices like cameras and printers.

How It Works

sRGB defines colors in terms of Red, Green, Blue, where each component can range from 0 to 255 or 0 to 1.

When to Use It

- Web and digital content: sRGB is the default color space for the web, and almost all images and digital media you encounter online are in sRGB. This ensures that content looks consistent across different devices.
- Consumer-level photography. Most consumer-grade cameras shoot in sRGB, and it is the standard color space used by default on screens, phones, and printers.

Limitations

sRGB covers a smaller range of colors than spaces like Adobe RGB or LAB. Highly saturated or vivid colors may not be represented accurately in sRGB, which can limit its usefulness for professional printing or design.

References

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[2016Byr] S. J. Byrnes, “Multilayer optical calculations” (2016); http://arxiv.org/abs/1603.02720.

[2019Pra] G. Prandini, G.-M. Rignanese, N. Marzari, Photorealistic modelling of metals from first principles. npj Comput. Mater. 5, 129 (2019).

[2023Gri] D. J. Griffiths, Introduction to Electrodynamics (5th Edition) (Cambridge University Press, 2023).

Optical Properties - Noble Metals Property Model Settings

The **Optical Properties - Noble** Property Model, available with the Property Model Calculator and the Noble Metal Alloys Model Library, is used to simulate the color, reflection, and transmission of light, based on modeling the alloy microstructure and the resulting optical properties. This model is currently applicable for the Au-Al-Ag-Cu-Pt system.

About the Optical Properties - Noble Metals Property Model

For an example see PM_Noble_01: Color Prediction.

Configuration Settings

The settings are found on the Property Model Calculator when **Optical Properties - Noble** is selected under **Noble Metal Alloys Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

Intercritical Annealing

The **Intercritical annealing** checkbox is selected by default. It is where the Model can either accept the given composition as a homogeneous FCC solid solution or perform an equilibrium calculation at the temperature specified under *Condition Definitions* to get the phase fractions.

This is an important setting as intermetallic phases have a very important effect on the actual color of the alloy.

- When selected, an equilibrium calculation is performed at the specified temperature and the composition and uses the calculated equilibrium phase and composition for optical property simulation.
- Click to clear the checkbox if the specified composition is used directly and the alloy contains only FCC phases without phase separation.

Calculate ΔE Value and ΔE Method Settings

Select the **Calculate ΔE value** checkbox if there is a target color and you want to know the difference between the calculated alloy color and targeting color. Then choose a **ΔE method**: **CIE 2000** (default), **CIE 1976**, or **CIE 1994**.

See About DeltaE (ΔE) in the theory section for more background detail about these settings.

Based on the ΔE method selected, further define these settings.

See About Color Space in the theory section for more detail about the options.

- **Color space of targeting color**: Select **LAB** (default), **sRGB**, or **XYZ**. Then define the index to calculate ΔE, where the range of space for each setting is: **LAB** [0, 100], **sRGB** [0, 1], and **XYZ** [0, 1].
- Enter values into the 1st, 2nd, and 3rd index fields based on the **Color space of targeting color** selection:
- **First index of targeting color**: **X** for XYZ, **L** for LAB, **R** for sRGB.
- **Second index of targeting color**: **Y** for XYZ, **a** for LAB, **G** for sRGB.
- **Third index of targeting color**: **Z** for XYZ, **b** for LAB, **B** for sRGB.

Incident Angle

Enter a value for the **Incident angle [degree]** between 0° and 90° for the incident light angle. The default is 0° (normal light). Incident angle is the angle at which light strikes a surface. This angle is measured between the incoming light ray and the normal (a perpendicular line) to the surface. The incident angle plays a crucial role in determining how light interacts with a material, which in turn affects the perceived color of the material.

Standard Illuminant

Select an option from the **Standard illuminant** list. Choose the incident light wavelength distribution, such as standard daylight illuminant **D65** (the default).

See About the Standard Illuminant in the theory section for more detail about the options.

View Angle of Observer

Select the **View angle of observer**: **CIE 1931 2 Degree Standard Observer** or **CIE 1964 10 Degree Standard Observer** (the default).

In general:

- **CIE 1931 2 Degree Standard Observer** is most accurate to view small objects or when details are seen up close, such as tiny pixels on a screen or small color samples.
- **CIE 1964 10 Degree Standard Observer** is better for measuring color in typical situations where larger objects are viewed, such as printed materials, paints, textiles, or any larger surface.

See About the Viewing Angle in the theory section for more detail about the options.

Material Thickness

Enter a value for the **Material thickness [nm]**. The default is 10000 nm.

This is and important setting when dealing with thin films or coatings.

Material thickness plays a significant role especially in the context of thin films, coatings, and transparent or semi-transparent materials. It affects how light interacts with the material, influencing reflection, transmission, absorption, and interference effects, all of which contribute to the final perceived color of the material. For example, a several nanometer thin gold film may display red or orange color, and it shows gold color when the film is thick enough. The default thickness is 10000 nm which displays bulk properties. The calculation assumes the two sides of materials are both air.

Color Space

Choose the **Color space** for the resulting color space index 1-3: **LAB** (default), **sRGB**, or **XYZ**.

See About Color Space in the theory section for more detail about the options.

- **LAB** (the default) includes all visible colors and is ideal for color matching, quality control, and any application where accurate perceptual color differences matter.
- **XYZ** covers all perceivable colors and is best for scientific and colorimetric studies, where precise color representation and transformations are needed.
- **sRGB** has a smaller color gamut, but it is widely used for displaying on consumer electronics

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

Plot Quantities

- **24-bit color**: To visualize the color, the three color channels need to be merged into a single value. For **sRGB**, 24-bit color is one way to do this.

> Merging three channels (each channel representing an independent axis) into a single value creates a non-linear scale. Thus, the legend option for the Z-axis scale can be considered irrelevant for the actual plot.

- **Color space index 1**, **Color space index 2**, and **Color space index 3**: For the **LAB**, **sRGB**, and **XYZ** color spaces, the color is described by three values (the color channels). The **Color space index 1**, **2**, and **3** result quantities correspond to these values, e.g., for **sRGB**, **1=R**, **2=G**, **3=B**.
- **n for single wavelength** or **k for single wavelength**: Provides the selected part of the refractive index when choosing a single wavelength as the illuminant. The values of **n** and **k** are material properties, but they do depend on the wavelength, wherefore if a multiwavelength illuminant is chosen, these result quantities will give NaN.

- **ΔE value**: A metric for understanding how the human eye perceives color difference. On a typical scale, the ΔE value ranges from 0 to 100. The larger the ΔE value, the more perceptible the color difference.

Steel Model Library Property Models

? Property Model Calculator

In this section:

About the Steel Model Library Property Models

These **Steel Models** are available with the Property Model Calculator. The following are available with the Steel Model Library.

Also see Steel Library CCT Diagram Template, Steel Library TTT Diagram Template, Plot Type: CCT Mode, and Plot Type: TTT Mode.

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

For the **Ferrite**, **Bainite**, and **Pearlite** Property Models, it is also useful to review the Recommended Composition Ranges for Steel Models.

Bainite

The **Bainite** Property Model describes the thermodynamics and isothermal kinetics of bainite transformation from austenite. In this Model, bainite is modeled as ferrite or a ferrite-cementite mixture.

See About the Bainite Property Model and Bainite Property Model Settings for background theory and input parameter details.

CCT Diagram

The **CCT Diagram** Property Model calculates the concurrent transformations to ferrite, pearlite, bainite, and martensite under continuous cooling conditions and is used to construct a continuous-cooling-transformation (CCT) diagram.

See About the CCT Diagram Property Model and CCT Diagram Property Model Settings for background theory and input parameter details.

Critical Transformation Temperatures

The **Critical Transformation Temperatures** Property Model calculates critical transformation temperatures for steels.

See About the Critical Transformation Temperatures Property Model and Critical Transformation Temperatures Property Model Settings for background theory and input parameter details.

Ferrite

The **Ferrite** Property Model calculates the thermodynamics and isothermal kinetics of proeutectoid ferrite forming from austenite in hypoeutectoid steels.

See About the Ferrite Property Model and Ferrite Property Model Settings for background theory and input parameter details.

Martensite Fractions

The **Martensite Fractions** Property Model calculates the fraction of athermal martensite based on available driving force.

See About the Martensite Fractions Property Model and Martensite Fractions Property Model Settings for background theory and input parameter details.

Martensite Temperatures

The **Martensite Temperatures** Property Model calculates the martensite start (Ms) temperature based on modeling of the transformation barrier. Martensite half and finish temperatures are also given according to the Martensite Fractions Property Model.

See About the Martensite Temperatures Property Model and Martensite Temperatures Property Model Settings for background theory and input parameter details.

Martensitic Steel Strength

The **Martensitic Steel Strength** Property Model calculates the strength and/or hardness of martensitic steels.

See About the Martensitic Steel Strength Property Model, Flow Stress, and Martensitic Steel Strength Property Model Settings for background theory and input parameter details.

Pearlite

The **Pearlite** Property Model calculates the thermodynamics and kinetics of pearlite formation from austenite during isothermal heat treatment.

See About the Pearlite Property Model and Pearlite Property Model Settings for background theory and input parameter details.

TTT Diagram

The **TTT Diagram** Property Model calculates the concurrent transformations to ferrite, pearlite, bainite, and martensite under isothermal conditions and is used to construct a time-temperature-transformation (TTT) diagram.

See About the TTT Diagram Property Model and TTT Diagram Property Model Settings for background theory and input parameter details.

Recommended Composition Ranges for Steel Models

The Steel Property Models (a.k.a. Steel Models or just Models) included with the Steel Model Library in Thermo-Calc calculate the process of austenite decomposition into ferrite, pearlite, bainite, and martensite. These Models are developed to satisfy the needs for a wide range of steels and are built on the thermodynamic and kinetic descriptions in the TCS Steel and Fe-alloys Database (TCFE) and TCS Steels/Fe-Alloys Mobility Database (MOBFE) databases, which are widely validated. However, the Steel Models also include their own modeling approach and parameters, which may limit the applicability to certain ranges of compositions and temperature, often due to some underlying assumptions of the modeling approaches and/or availability of calibration data.

In general, the Models for ferrite, bainite, and pearlite are for low-alloy, low-to-medium carbon steels involving austenite (Fe-rich disordered FCC_A1) transforming into ferrite (Fe-rich disordered BCC_A2) and cementite. For steels with higher Cr contents, it is also possible to select M7C3 and M23C6 to be the carbide in pearlite, and M7C3 for bainite. Otherwise, the Models are not designed for other phase relations, for example:

- Austenite transforming into a mixture of ferrite and another type of carbide (e.g. kappa carbide for high-Mn high-Al alloys).
- Precipitation (e.g. FCC-Cu, FCC-carbides due to microalloying elements Ti, V, Nb) taking place concurrently while austenite is transforming into ferrite (and possibly cementite).

If some other phases coexist with austenite prior to its transformation, the Steel Models assume these do not participate in or affect the transformations by any means (e.g. by providing extra nucleation sites). The only effect of these phases is to determine the austenite composition (which is now different from the nominal composition). In this case, the setting **Equilibrium composition at austenitizing temperature** is selected from the **Austenite composition from** list on the **Configuration** window.

For an explanation of **Austenite composition from** see the individual configuration settings for the different Steel Models (**Ferrite**, **Bainite**, and **Pearlite**). Links to these are listed in About the Steel Model Library Property Models.

Ferrite and bainite calculations rely on carbon partitioning from ferrite to austenite. Therefore, the Models are *not* suitable for the ferrite transformed from austenite in a "massive" manner (composition invariant), in some "interstitial-free" ferrous alloys with very low carbon contents.

Pearlite is assumed to be steady-state, i.e. growth rate and lamellar spacing are constant over time under isothermal conditions. This is reasonable if composition and transformation temperature lie in the ferrite-cementite two-phase region of a phase diagram. The Pearlite

Model does *not* cover the so-called "divergent pearlite", or "partitioned pearlite", which usually forms in the austenite-ferrite-cementite three-phase region with growth rate and lamellar spacing changing over time. Also, pearlite nucleation is modeled to be on austenite grain boundaries only. In practice, however, pearlite nucleation at grain edges and corners may also be considerable if the undercooling is small.

Parameters within the Steel Models are calibrated against experimental data on nucleation, growth, and overall transformation kinetics. However, the composition space covered by the calibration data, on which the Steel Models calculations are checked, is limited. As a result, together with the limitations from modeling approach discussed above, some recommended composition ranges are listed below. The Models may not give reasonable results when the composition in question is far outside the recommended ranges.

Element	*Ferrite*	*Bainite*		*Pearlite*[3]
		Bainite Start Temperature [2018Lea][1]	*Bainite Growth, Nucleation, Transformation Kinetics*[2]	
C	Max. 0.7	Max. 0.7	0.2-1.5	0.6-1
Mn	Max. 3	Max. 5.5	Max. 0.6	Max. 1.8
Ni	Max. 5	Max. 9	Max. 5.3	Max. 3
Si	Max. 2	Max. 2	Max. 1	Max. 2
Al	Max. 1.4	–	–	(unknown, assuming similar to Si)
Co	Max. 3.2	–	–	Max. 2.2
Cr	Max. 3	Max. 5.7	Max. 5	Max. 13[4]
Mo	Max. 2	Max. 4	(unknown)	Max. 0.6
W	–	–	–	Max. 0.37

[1] The model is from [2018Lea]. The supporting bainite start data is compiled and published in [2019Lea].

Element	*Ferrite*	*Bainite*		*Pearlite*[3]
		Bainite Start Temperature [2018Lea][1]	*Bainite Growth, Nucleation, Transformation Kinetics*[2]	

[2] Parameters are not assessed to be composition dependent. The listed composition ranges come from the data of growth considered in a “universal” fitting.

[3] References in [2020Yan].

[4] Requires calculation setting **Custom** for type of carbide. Estimated boundaries: CEMENTITE for <5 wt.% Cr, M7C3 for 5~10 wt. % Cr, M23C6 for >10 wt.% Cr.

References

[2018Lea] L. Leach, P. Kolmskog, L. Höglund, M. Hillert, A. Borgenstam, Critical Driving Forces for Formation of Bainite. Metall. Mater. Trans. A. 49, 4509–4520 (2018).

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About the Bainite Property Model

The **Bainite** Property Model, available with the Property Model Calculator and the Steel Model Library, describes the thermodynamics and isothermal kinetics of bainite transformation from austenite. In this Model, bainite is modeled as ferrite or a ferrite-cementite mixture.

For a given austenite composition, the bainite start temperature, WB_S, is calculated following Leach et al. [2018Lea] (see Eqs. 8 and 9 and Table 1 in the paper). At WB_S, the driving force for ferrite to precipitate out of austenite under the “para” condition (i.e. no partitioning of substitutional elements, carbon in equilibrium) is balanced by a barrier, which is modeled as a function of composition.

At a temperature below WB_S, there is a net driving force (over the barrier) for the growth of bainitic ferrite. The steady-state lengthening rate of ferrite plate is calculated based on the method from Leach et al. [2019Lea] with modifications. In the Bainite Model, unlike in [2019Lea], local equilibrium of carbon at the ferrite/austenite is sought, and a finite interfacial friction term is added to the dissipation terms. Otherwise the two methods are both based on a driving-force–dissipation balance and the Zener-Hillert equation, with a unique lengthening rate determined by maximizing it with respect to radius of curvature at the plate tip.

The Bainite Model also considers the case where cementite (under the “para” condition) can precipitate on the ferrite/austenite interface and grow into ferrite, forming a ferrite-cementite mixture. The formation of para-cementite usually accelerates lengthening, by enlarging the driving force of transformation while reducing carbon partitioning from bainite to austenite. Carbon partitioning to austenite vanishes if para-cementite forms in bainite to its maximum fraction allowed by mass balance.

Thickening of bainitic plates is usually much slower than lengthening. In the Bainite Model, it is assumed that whenever there is a positive driving force of precipitating para-cementite on the ferrite/austenite interface, the final state of the bainite transformation should be a mixture of ferrite and cementite, with austenite being completely transformed. Otherwise, the final state is a ferrite-austenite mixture with no cementite but a finite fraction of retained austenite (incomplete transformation).

The overall kinetics of bainite transformation is calculated in the extended-volume approach devised by Cahn [1956Cah] and generalized for ellipsoids. Both grain boundary (GB) nucleation and volume nucleation are considered, the former being very temperature-sensitive, the latter temperature-insensitive. This is used to model the kinks at about 350 °C in the TTT diagrams of some medium- and high-carbon steels—At higher temperatures GB nucleation is predominant, whereas at lower temperatures it is effectively suppressed, and volume nucleation becomes significant.

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Configuration Settings

The input parameters are entered on the **Configuration** window for the Property Model Calculator. There are also settings on the Plot Renderer where you can choose from the available and relevant axis variables.

See Bainite Property Model Settings for details.

Example

For an example, see PM_Fe_05: Fe-C-Mn-Si-Ni-Cr-Mo Bainite.

References

[1956Cah] J. W. Cahn, “The kinetics of grain boundary nucleated reactions”, Acta Metallurgica 4, 449–459 (1956).

[2018Lea] L. Leach, P. Kolmskog, L. Höglund, M. Hillert, and A. Borgenstam, “Critical driving forces for formation of bainite”, Metallurgical and Materials Transactions A 49, 4509–4520 (2018).

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Bainite Property Model Settings

The **Bainite** Property Model, available with the Property Model Calculator and the Steel Model Library, describes the thermodynamics and isothermal kinetics of bainite transformation from austenite. In this Model, bainite is modeled as ferrite or a ferrite-cementite mixture.

Considered elements: Fe, C, Mn, Si, Cr, Ni, Mo. Other elements in the system are neglected for bainite by mass percent.

For the **Ferrite**, **Bainite**, and **Pearlite** Property Models, it is also useful to review the Recommended Composition Ranges for Steel Models.

About the Bainite Property Model

For an example, see PM_Fe_05: Fe-C-Mn-Si-Ni-Cr-Mo Bainite.

Configuration Settings

These settings are found on the Property Model Calculator when **Bainite** is selected under **Steel Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

AUSTENITE COMPOSITION FROM

Select an option from the **Austenite composition from** list:

- **Nominal composition** uses the system composition as austenite composition.
- **Equilibrium composition at austenizing temperature**. Select to enter an **Austenitizing temperature**. The austenite composition is determined from an equilibrium calculation at the austenitizing temperature (if austenite is stable). This option is useful when austenite coexists with other phase(s), e.g. primary carbide, before the transformation(s) being calculated starts. But the Model only considers the effect of other phase(s) on austenite composition.

AUSTENTIZING TEMPERATURE

This setting is available when **Equilibrium composition at austenitizing temperature** is selected from the **Austenite composition from** list.

Enter an **Austentizing temperature** in the field. The unit is the same as that selected under *Condition Definitions*.

GRAIN SIZE

Enter the **Grain size** of the austenite in micrometers (µm). The default is `100` µm.

Plot Renderer Settings

Plot Renderer, Configuration Settings, and Plot Type: TTT Mode

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

These plot quantities are available:

- **Temperature**
- **Start time (2% bainite)**
- **Half time (50% bainite)**
- **Finish time (98% bainite)**
- **Bainite start temperature**
- **Lengthening rate [m/s]**
- **Cementite fraction in bainite**
- **Retained austenite fraction**

About the CCT Diagram Property Model

The **CCT Diagram** Property Model, available with the Property Model Calculator and the Steel Model Library, can be used to calculate a Continuous-Cooling-Transformation (CCT) diagram, with a **One Axis** calculation on **Log10(cooling rate[K/s])**. This Model calculates the kinetics of concurrent transformation of austenite into ferrite, pearlite, bainite, and martensite. The algorithms and parameters for ferrite, pearlite, bainite, and martensite are the same as in their individual Property Models (**Ferrite**, **Pearlite**, **Bainite**, **Martensite Temperatures**, and **Martensite Fractions**), but the competitive occupation of prior austenite grain boundaries and bulk volume is handled in the **CCT Diagram** Property Model.

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Configuration Settings

The input parameters are entered on the **Configuration** window for the Property Model Calculator. There are also settings on the Plot Renderer where you can choose from the available and relevant axis variables.

See CCT Diagram Property Model Settings for details.

Example

For an example, see PM_Fe_08: CCT Diagram for Fe-C-Mn-Si-Cr-V.

CCT Diagram Property Model Settings

The **CCT Diagram** Property Model, available with the Property Model Calculator and the Steel Model Library, calculates the concurrent transformations to ferrite, pearlite, bainite, and martensite under continuous cooling conditions and is used to construct a continuous-cooling-transformation (CCT) diagram.

About the CCT Diagram Property Model and Steel Library CCT Diagram Template

For an example, see PM_Fe_08: CCT Diagram for Fe-C-Mn-Si-Cr-V

Configuration Settings

These settings are found on the Property Model Calculator when **CCT Diagram** is selected under **Steel Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

AUSTENITE COMPOSITION FROM

Select an option from the **Austenite composition from** list:

- **Nominal composition** uses the system composition as austenite composition.
- **Equilibrium composition at austenizing temperature**. Select to enter an **Austenitizing temperature**. The austenite composition is determined from an equilibrium calculation at the austenitizing temperature (if austenite is stable). This option is useful when austenite coexists with other phase(s), e.g. primary carbide, before the transformation(s) being calculated starts. But the Model only considers the effect of other phase(s) on austenite composition.

Austentizing Temperature

This setting is available when **Equilibrium composition at austenitizing temperature** is selected from the **Austenite composition from** list.

Enter an **Austentizing temperature** in the field. The unit is the same as that selected under *Condition Definitions*.

Grain Size

Enter the **Grain size** of the austenite in micrometers (µm). The default is `100` µm.

Start Temperature

Enter a **Start temperature**, which is the temperature at time zero where cooling starts.

End Temperature

Enter an **End temperature**, which is the lowest possible temperature where cooling stops. Cooling may also stop before reaching this temperature if austenite has fully transformed (>98%).

Log10(cooling rate [K/s])

Enter a **Log10(cooling rate [K/s])** , which is the 10-base logarithm of cooling rate in K/s.

> The unit must be Kelvin per second, and it does NOT follow the unit selection in the GUI. This is the *Axis Quantity* if a CCT diagram is to be constructed.

Calculation Setting

Select **Quick** (the default), **Accurate**, or **Custom** to balance accuracy and calculation time. Choose **Custom** to define the numerical settings yourself, which are otherwise set in the background when **Quick** or **Accurate** is selected. See the separate section below about the details for the **Custom** settings.

QUICK CALCULATION SETTING

Quick is used for a relatively quick and rough calculation to reveal the general feature of a CCT diagram. Interpolation is used when necessary, in order to avoid calculating the growth rates and nucleation rates of pearlite and bainite at every time step. For simplicity, **Ferrite mode** is **PE** (paraequilibrium), and **Pearlite mode** is **Para-pearlite**.

⌛ Calculation times may vary between 30 minutes and several hours.

ACCURATE CALCULATION SETTING

Accurate evaluates the growth rates and nucleation rates at every time step accurately (without interpolation). The time step control is also tighter than when using the **Quick** setting.

- **Ferrite mode** is **PE if possible, otherwise OE** so as to handle any ortho-para transition.
- **Pearlite mode** is **Optimal pearlite**, but its rate calculation becomes slower if austenite contains many alloying elements.

⌛ Calculation times may vary between several hours and tens of hours.

DETAILS ABOUT THE QUICK AND ACCURATE CALCULATION SETTINGS

When you choose **Quick** or **Accurate** as the calculation setting, the following is what is automatically set in the background for each of the sections. These sections are visible to you and also can be edited when **Custom** is chosen:

Setting	*Quick*	*Accurate*
Ferrite selected	checkbox selected (yes)	checkbox selected (yes)
Pearlite selected	checkbox selected (yes)	checkbox selected (yes)

Setting	*Quick*	*Accurate*
Bainite selected	checkbox selected (yes)	checkbox selected (yes)
Martensite selected	checkbox selected (yes)	checkbox selected (yes)
Ferrite mode	PE only	Faster start (TTT); PE if possible otherwise OE (CCT)
Pearlite criterion	Maximize growth rate	Maximize growth rate
Pearlite mode	Para-pearlite	Optimal pearlite
Use interpolation when necessary	checkbox selected (yes)	checkbox NOT selected (no)
Interpolation error tolerance	0.1	(does not apply)
Maximum phase fraction change (absolute) in a time step	0.005	0.005
Maximum phase fraction change (relative) in a time step	0.05	0.05
Error tolerance for austenite fraction	1E-3	1E-4

Custom Calculation Setting

The following settings are available when **Custom** is selected as the *Calculation Setting*. Otherwise these settings are handled in the background as described above for when **Quick** or **Accurate** is selected.

FERRITE/PEARLITE/BAINITE/MARTENSITE SELECTED CHECKBOXES

By default the **Ferrite selected**, **Pearlite selected**, **Bainite selected**, and **Martensite selected** checkboxes are selected. For ferrite and pearlite, additional settings are then available.

Click to deselect as required to exclude one or more from the calculation.

FERRITE MODE

This setting is available when the **Ferrite selected** checkbox is selected.

From the **Ferrite mode** list choose an option.

- **OE only** and **PE only** are the same as in the **Ferrite** Property Model. i.e.
    - *Orthoequilibrium (OE)*: The ferrite and austenite compositions at the interface are fixed to the final equilibrium compositions
    - *Paraequilibrium (PE)*: Only carbon is allowed to partition, reaching PE at the interface
- **PE if possible, otherwise OE** means ferrite grows in PE mode if this mode has a positive driving force, otherwise ferrite grows in OE mode. This is usually useful to handle an ortho-to-para transition as temperature decreases.

PEARLITE CRITERION

This setting is available when the **Pearlite selected** checkbox is selected.

Select an option from the **Criterion** list to determine the pearlite growth condition. This list is called **Pearlite criterion** for the CCT Diagram and TTT Diagram Property Models.

- For **Maximize growth rate**, pearlite growth rate is maximized with respect to lamellar spacing (and for optimal pearlite, partition coefficients of substitutional alloying elements between ferrite and cementite). The calculation gives maximal growth rate and minimal lamellar spacing. This is the default criterion.
- For **Maximize Gibbs energy dissipation rate**, Gibbs energy dissipation rate is maximized with respect to lamellar spacing (and for optimal pearlite, partition coefficients of substitutional alloying elements between ferrite and cementite). The calculation gives a smaller growth rate than the maximal, and a larger lamellar spacing than the minimal, which may better represent the average growth rate and lamellar spacing of all pearlite colonies in the material.

PEARLITE MODE

This setting is available when the **Pearlite selected** checkbox is selected. It is used to determine how substitutional alloying elements partition between ferrite and cementite in pearlite. Select an option from the **Pearlite mode** list.

- For **Optimal pearlite**, the partitioning of substitutional alloying elements between ferrite and cementite is optimized according to the **Criterion** while keeping carbon equilibrium between the two phases. This is the default mode. This mode realizes a smooth transition between ortho-pearlite and para-pearlite.

- For **Para-pearlite**, ferrite and cementite are in para-equilibrium where substitutional alloying elements do not partition and carbon reaches equilibrium.
- For **Ortho-pearlite**, ferrite and cementite are in ortho-equilibrium.

CARBIDE IN PEARLITE

From the **Carbide in pearlite** list, select the carbide to be present in pearlite: **CEMENTITE** (default), **M7C3**, or **M23C6**. For M23C6, this usually depends on Cr content.

When M23C6 is selected, parameters optimized for stainless steels are invoked.

Recommended Composition Ranges for Steel Models

CARBIDE IN BAINITE

From the **Carbide in bainite** list, select the carbide to be present in pearlite: **CEMENTITE** (default) or **M7C3**. For M7C3, this usually depends on Cr content.

USE INTERPOLATION WHEN NECESSARY

If the **Use interpolation when necessary** checkbox is selected, and depending on alloy composition and temperature, if the code determines that an interpolation is necessary and possible to implement, then a composition grid (TTT diagram) or composition-temperature grid (CCT diagram) is generated and refined as needed.

The growth rates and nucleation rates of pearlite and bainite, as functions of composition (TTT diagram) or composition and temperature (CCT diagram), are determined by interpolation (if sufficiently accurate). This is intended to avoid direct calculations of pearlite and bainite rates for every time step, which is usually time-consuming.

INTERPOLATION ERROR TOLERANCE

This setting is available when the **Use interpolation when necessary** checkbox is selected.

The growth and nucleation rates of pearlite and bainite, if determined from interpolation, are accepted only when the relative interpolation error estimated is below the value entered here. A large number implies few grid points necessary (shorter calculation time) and lower accuracy, and a small number implies the opposite.

MAXIMUM PHASE FRACTION CHANGE (ABSOLUTE/RELATIVE) IN A TIME STEP

The **Maximum phase fraction change (absolute) in a time step** and **Maximum phase fraction change (relative) in a time step** settings are used to control time step size during time integration.

The phase fraction (X) of ferrite, pearlite, and bainite cannot change more than $atol + X * rtol$ during a time step, where $atol$ and $rtol$ are the absolute and relative maximum change, respectively. If the change is too large, the new time step is rejected, and time integration is retried with a smaller time step.

ERROR TOLERANCE FOR AUSTENITE FRACTION

The **Error tolerance for austenite fraction** setting is used to control the accuracy for austenite fraction during time integration. Finite time steps cause an error in austenite volume fraction. When the error is larger than the tolerance, time integration is backed up and retried with a smaller time step.

Plot Renderer Settings

Plot Renderer, Configuration Settings, Plot Type: CCT Mode, and Plot Type: TTT Mode

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

Each quantity is defined in both time **(t)** and temperature **(T)**:

- **Ferrite start (2%)**, time **(t)**, and temperature **(T)**
- **Pearlite start (2%)**, time **(t)**, and temperature **(T)**
- **Bainite start (2%)**, time **(t)**, and temperature **(T)**
- **Total ferrite start (2%)**, time **(t)**, and temperature **(T)**: The start of the sum of polygonal ferrite and bainitic ferrite.
- **Total ferrite+cementite start (2%)**, time **(t)**, and temperature **(T)**: The start of the sum of pearlite and cementite-containing bainite.

- **Total ferrite + cementite finish (98%)**, time **(t)**, and temperature **(T)**: 98% austenite transformed to ferrite, pearlite, and bainite.
- **Martensite start**, time **(t)**, and temperature **(T)**
- **Austenite transformed 2%**, time **(t)**, and temperature **(T)**
- **Austenite transformed 10%**, time **(t)**, and temperature **(T)**
- **Austenite transformed 50%**, time **(t)**, and temperature **(T)**
- **Austenite transformed 90%**, time **(t)**, and temperature **(T)**
- **Austenite transformed 98%**, time **(t)**, and temperature **(T)**

Fractions of transformation products at the last time step (unit-free) are also available:

- **Terminal fraction of ferrite**
- **Terminal fraction of pearlite**
- **Terminal fraction of bainite**
- **Terminal fraction of martensite**
- **Terminal fraction of total ferrite**
- **Terminal fraction of total ferrite+cementite**

The **CCT Mode** on the Plot Renderer the time-temperature pairs are automatically identified and arranged in the plot to give a CCT diagram. Selected cooling curves are also given in the CCT Mode.

About the Critical Transformation Temperatures Property Model

The **Critical Transformation Temperatures** Property Model, available with the Property Model Calculator and the Steel Model Library, calculates critical transformation temperatures for steels under equilibrium conditions.

This Property Model can output the transformation temperatures for the following:

- Liquidus: First austenite or ferrite transformation from the liquid
- Solidus: Liquid fully transformed to solid
- A0: Magnetic transition temperature (Curie temperature) of cementite. The cementite is paramagnetic above A0 and ferromagnetic below
- A1: Austenite (FCC_A1) transforms to ferrite (BCC_A2) + carbide (cementite or graphite or M23C6)
- A2: Magnetic transition temperature (Curie temperature) of ferrite (BCC_A2). Paramagnetic above A2 and ferromagnetic below
- A3: Austenite (FCC_A1) transforms to ferrite (BCC_A2)
- A4: Delta-ferrite (BCC_A2) transforms to austenite (FCC_A1)
- Acem: Austenite (FCC_A1) transforms to cementite. Requires that the **Suspend graphite** checkbox is selected on the Configuration window, which it is by default.
- Agraph: Austenite (FCC_A1) transforms to graphite. Requires that the **Suspend graphite** checkbox is NOT selected on the Configuration window, i.e. graphite is not suspended.

> To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Configuration Settings

The input parameters are entered on the **Configuration** window for the Property Model Calculator and described in Critical Transformation Temperatures Property Model Settings.

Example

For an example, see PM_Fe_04: Critical Temperatures.

Critical Transformation Temperatures Property Model Settings

The **Critical Transformation Temperatures** Property Model, available with the Property Model Calculator and the Steel Model Library, calculates critical transformation temperatures for steels under equilibrium conditions.

About the Critical Transformation Temperatures Property Model

For an example, see PM_Fe_04: Critical Temperatures.

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Configuration Settings

These settings are found on the Property Model Calculator when **Critical Transformation Temperatures** is selected under **Steel Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

CALCULATE SOLIDUS AND LIQUIDUS

Select the **Calculate solidus and liquidus** checkbox to calculate these temperatures.

CALCULATE AX TEMPERATURES

Select the **Calculate Ax temperatures** checkbox to calculate A0, A1, A3, Acem, and Agraph temperatures. Typically, only one temperature of A3, Acem, and Agraph exists. See below for additional details about these temperatures.

- A0: Magnetic transition temperature (Curie temperature) of cementite. The cementite is paramagnetic above A0 and ferromagnetic below
- A1: Austenite (FCC_A1) transforms to ferrite (BCC_A2) + carbide (cementite or graphite or M23C6)
- A2: Magnetic transition temperature (Curie temperature) of ferrite (BCC_A2). Paramagnetic above A2 and ferromagnetic below
- A3: Austenite (FCC_A1) transforms to ferrite (BCC_A2)
- A4: Delta-ferrite (BCC_A2) transforms to austenite (FCC_A1)
- Acem: Austenite (FCC_A1) transforms to cementite (requires that the **Suspend graphite** checkbox is selected, which it is by default)
- Agraph: Austenite (FCC_A1) transforms to graphite (requires that the **Suspend graphite** checkbox is NOT selected, i.e. graphite is not suspended)

SUSPEND GRAPHITE

By default the **Suspend graphite** checkbox is selected and suspends the graphite phase. Click to clear the checkbox as needed to enable the graphite.

SUSPEND GAS

By default the **Suspend gas** checkbox is selected and suspends the gas phase. Click to clear the checkbox as needed.

MANUAL TEMPERATURE SEARCH LIMITS

By default the temperature search limits are automatically defined. Select the **Manual temperature search limits** checkbox to manually change the limits for the **Lower temperature search limit**, **Upper temperature search limit**, and **Max temperature step**. Is given in the same unit as the temperature in the **Condition Definitions**.

LOWER AND UPPER TEMPERATURE SEARCH LIMITS

These settings are available when the **Manual temperature search limits** checkbox is selected.

In the **Lower temperature search limit** and **Upper temperature search limit** fields enter temperature values to search the lower and upper limits of transformation temperatures.

MAX TEMPERATURE STEP

This setting is available when the **Manual temperature search limits** checkbox is selected.

In the **Max temperature step** field, enter the largest temperature step. This is most often reduced when changes in driving force or the amount of the phases indicate a phase transformation at a shorter temperature step.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

Output the transformation temperatures:

- **Liquidus**: First austenite or ferrite transformation from the liquid
- **Solidus**: Liquid fully transformed to solid
- **A0**: Magnetic transition temperature (Curie temperature) of cementite. The cementite is paramagnetic above A0 and ferromagnetic below
- **A1**: Austenite (FCC_A1) transforms to ferrite (BCC_A2) + carbide (cementite or graphite or M23C6 or M7C3)
- **A2**: Magnetic transition temperature (Curie temperature) of ferrite (BCC_A2). Paramagnetic above A2 and ferromagnetic below
- **A3**: Austenite (FCC_A1) transforms to ferrite (BCC_A2)
- **A4**: Delta-ferrite (BCC_A2) transforms to austenite (FCC_A1)
- **Acem**: Austenite (FCC_A1) transforms to cementite (only possible if graphite is suspended)
- **Agraph**: Austenite (FCC_A1) transforms to graphite (only possible if graphite is enabled)

About the Ferrite Property Model

The **Ferrite** Property Model, available with the Property Model Calculator and the Steel Model Library, calculates the thermodynamics and isothermal kinetics of proeutectoid ferrite forming from austenite in hypoeutectoid steels.

This model is for the form of proeutectoid ferrite which forms without distinct crystallographic preferences at austenite grain boundaries. This type of ferrite is referred to as *grain boundary allotriomorph*, or *polygonal ferrite*. Another type, plate-shaped ferrite (*Widmanstätten ferrite*), is treated in the **Bainite** Property Model as a special case of bainite without cementite.

? About the Bainite Property Model

Growth Models

Growth is modeled based on a simplified diffusion-control theory with the ferrite/austenite interfacial composition determined by:

- *Orthoequilibrium (OE)*: The ferrite and austenite compositions at the interface are fixed to the final equilibrium compositions
- *Paraequilibrium (PE)*: Only carbon is allowed to partition, reaching PE at the interface
- *Negligible-partitioning local equilibrium (NPLE)*
- *Orthoprecipitate (OP)*: Austenite interfacial composition being the bulk composition, ferrite interfacial composition from the maximum driving force condition (parallel tangent construction in Gibbs energy-composition diagram)
- *Paraprecipitate (PP)*: Only carbon is allowed to partition, otherwise the same as OP

The growth is parabolic if only diffusion-controlled. The parabolic rate constant can be modified by a *phase addition* because the driving force and interfacial compositions are changed. With a finite interfacial mobility and solute drag effects, the growth is then mixed-controlled. The effect is handled in the overall transformation kinetics but not reflected in the parabolic rate constant.

Nucleation Rate and Interfacial Mobility

Nucleation rate of ferrite allotriomorph on austenite grain boundaries is calculated from classical nucleation theory assuming a pillbox shape of the ferrite nucleus [1988Lan].

When you are setting up the model, parameters for nucleation rate (site density, edge energy, and epsilon, see [1988Lan] for definition) and interfacial mobility (pre-exponential factor and activation energy) can be customized. Otherwise, default values assessed by Thermo-Calc are used. The overall kinetics of isothermal transformation is calculated in the extended-volume framework by numerical integration over time. Austenite composition changes over time due to partitioning of elements, and its effects on growth and nucleation are handled.

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Configuration Settings

The input parameters are entered on the **Configuration** window for the Property Model Calculator. There are also settings on the Plot Renderer where you can choose from the available and relevant axis variables.

See Ferrite Property Model Settings for details.

Example

For an example, see PM_Fe_09: Fe-C-Ni Ferrite.

Reference

[1988Lan] W. F. Lange, M. Enomoto, H. I. Aaronson, The kinetics of ferrite nucleation at austenite grain boundaries in Fe-C alloys. Metall. Trans. A. 19, 427–440 (1988).

Ferrite Property Model Settings

The **Ferrite** Property Model, available with the Property Model Calculator and the Steel Model Library, calculates the thermodynamics and isothermal kinetics of proeutectoid ferrite forming from austenite in hypoeutectoid steels.

About the Ferrite Property Model

For an example, see PM_Fe_09: Fe-C-Ni Ferrite.

Included Elements and Important Notes

- Austenite must contain at least Fe and C for this model to function.
- Elements that are quite soluble in both austenite and ferrite—Mn, Ni, Si, Al, Co, Cr, and Mo—have their effects on overall kinetics assessed.
- Cu and strong carbide-formers—W, V, Nb, Ta, Ti, and Zr—can be included, but only to a certain extent not to cause phases other than austenite and ferrite to form at the calculation temperature. Otherwise, the model calculation may give unrealistic results or even fail. If carbide is expected to form at an austenitizing temperature, use the setting **Equilibrium composition at austenitizing temperature** for **Austenite composition from**, then enter an austenitizing temperature.

Elements not listed above are excluded in mass percent from the austenite composition used to calculate the transformation.

For the **Ferrite**, **Bainite**, and **Pearlite** Property Models, it is also useful to review the Recommended Composition Ranges for Steel Models.

Configuration Settings

These settings are found on the Property Model Calculator when **Ferrite** is selected under **Steel Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

AUSTENITE COMPOSITION FROM

Select an option from the **Austenite composition from** list:

- **Nominal composition** uses the system composition as austenite composition.
- **Equilibrium composition at austenizing temperature**. Select to enter an **Austenitizing temperature**. The austenite composition is determined from an equilibrium calculation at the austenitizing temperature (if austenite is stable). This option is useful when austenite coexists with other phase(s), e.g. primary carbide, before the transformation(s) being calculated starts. But the Model only considers the effect of other phase(s) on austenite composition.

As per above in Included Elements and Important Notes, use the **Equilibrium composition at austenitizing temperature** setting if carbide is expected to form at an austenitizing temperature.

AUSTENTIZING TEMPERATURE

This setting is available when **Equilibrium composition at austenitizing temperature** is selected from the **Austenite composition from** list.

Enter an **Austentizing temperature** in the field. The unit is the same as that selected under *Condition Definitions*.

GRAIN SIZE

Enter the **Grain size** of the austenite in micrometers (µm). The default is `100` µm.

GROWTH MODE

Select a **Growth mode**: **Orthoequilibrium (OE)**, **Paraequilibrium (PE)**, **Negligible-partitioning local equilibrium (NPLE)**, **Orthoprecipitate (OP)**, or **Paraprecipitate (PP)**. This defines the compositions on the two sides of the ferrite-austenite interface and therefore affects growth rate.

For definitions of these modes, see About the Ferrite Property Model.

PHASE ADDITION

Enter a **Phase addition** in J/mol. This applies a Gibbs energy shift to ferrite.

SKIP TIME INTEGRATION

Click to select the **Skip time integration** checkbox to skip this step in the calculations. Time integration is required for calculating ferrite start/half/finish times, but is usually time-consuming. Skipping time integration allows you to get the other result quantities more quickly.

Custom Parameters

Select the **Custom parameters** checkbox to choose to set more advanced settings as listed below.

- **Site density**, **Edge surface energy**, and **Epsilon** are for calculating grain-boundary nucleation rate (see [1988Lan] for definition and details).
- **M0** and **Q** are to define an interfacial mobility in the Arrhenius equation.

SITE DENSITY

This setting is available when **Custom parameters** is selected. Enter a **Site density** in 1/m^2.

EDGE SURFACE ENERGY

This setting is available when **Custom parameters** is selected. Enter an **Edge surface energy** in J/m^2.

EPSILON

This setting is available when **Custom parameters** is selected. Enter a value for **Epsilon** in J/m^2.

M0

This setting is available when **Custom parameters** is selected. Enter a value for **M0** in m mol/(Js). This is the pre-exponential factor for interfacial mobility.

Q

This setting is available when **Custom parameters** is selected. Enter a value for **Q** in J/mol. This is the activation energy for interfacial mobility.

MAXIMUM PHASE FRACTION CHANGE (ABSOLUTE) IN A TIME STEP

This setting is available when **Custom parameters** is selected, and is used for time integration.

Enter the **Maximum phase fraction change (absolute) in a time step**.

MAXIMUM PHASE FRACTION CHANGE (RELATIVE) IN A TIME STEP

This setting is available when **Custom parameters** is selected, and is used for time integration.

Enter the **Maximum phase fraction change (relative) in a time step**

Plot Renderer Settings

Plot Renderer, Configuration Settings, and Plot Type: TTT Mode

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

- **Ferrite molar fraction (OE or PE)**: The ferrite molar fraction at the end of the transformation, determined from orthoequilibrium (for **Ferrite mode** “OE” or “OP”) or paraequilibrium (for **Ferrite mode** “PE”, “NPLE”, or “PP”).
- Growth Models

- **Parabolic growth rate constant [m/s(1/2)]**: The ratio of half-thickness to square root of time. This is calculated from interfacial composition and diffusion coefficients in austenite.
- **Driving force [J/mol]**
- **Nucleation rate [1/(m2 s)]**: Steady-state nucleation rate of ferrite per unit austenite grain boundary area.
- **Ferrite start**, **Ferrite half**, or **Ferrite finish**: The times at ferrite fraction being 0.02, 0.50, and 0.98, respectively.
- **Ferrite start (relative)**, **Ferrite half (relative)**, or **Ferrite finish (relative)**: The times at 2%, 50%, and 98% of the final ferrite fraction, respectively.

Reference

[1988Lan] W. F. Lange, M. Enomoto, H. I. Aaronson, The kinetics of ferrite nucleation at austenite grain boundaries in Fe-C alloys. Metall. Trans. A. 19, 427–440 (1988).

About the Martensite Fractions Property Model

The **Martensite Fractions** Property Model, available with the Property Model Calculator and the Steel Model Library, calculates fraction of athermal martensite based on an analytical equation derived in Huyan et al. [2016Huy]. It is assumed that the first forming martensite morphology is the only forming one. The first morphology is determined based on the Ms-temperatures of all morphologies.

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Configuration Settings

The input parameters are entered on the **Configuration** window for the Property Model Calculator. There are also settings on the Plot Renderer where you can choose from the available and relevant axis variables.

See Martensite Fractions Property Model Settings for details.

Example

For an example see PM_Fe_01: Fe-Cr-C Martensite with Intercritical Annealing.

Reference

[2016Huy] F. Huyan, P. Hedström, L. Höglund, A. Borgenstam, A Thermodynamic-Based Model to Predict the Fraction of Martensite in Steels. Metall. Mater. Trans. A. 47, 4404–4410 (2016).

Martensite Fractions Property Model Settings

The **Martensite Fractions** Property Model, available with the Property Model Calculator and the Steel Model Library, calculates the fraction of athermal martensite based on available driving force.

About the Martensite Fractions Property Model

For an example see PM_Fe_01: Fe-Cr-C Martensite with Intercritical Annealing.

Configuration Settings

The settings are found on the Property Model Calculator when **Martensite Fractions** is selected under **Steel Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

INTERCRITICAL ANNEALING

Click to select the **Intercritical annealing** checkbox to assume intercritical annealing. Click to clear the checkbox if the specified composition is used directly. When selected, an equilibrium calculation is performed at the specified temperature and the composition of the austenite phase is used for the martensite temperature calculation.

ANNEALING TEMPERATURE

This setting is available when the **Intercritical annealing** checkbox is selected.

Enter an **Annealing temperature** in the field. The unit is the same as that selected under *Condition Definitions*.

GRAIN SIZE [MM]

Enter the **Grain size** of the austenite in micrometers (µm). The default is `100` µm.

PARENT PHASE GIBBS ENERGY ADDITION

In the **Parent phase Gibbs energy addition [J/mol]** field enter a value in J/mol to add a Gibbs energy offset to the parent austenite phase. This can be used, for example, to correct database offsets. The default is `0` J/mol.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

These plot quantities are available:

- **Total martensite percentage**: The martensite percentage at these conditions.
- **Retained austenite percentage**: The retained austenite percentage at these conditions.

About the Martensite Temperatures Property Model

The **Martensite Temperatures** Property Model, available with the Property Model Calculator and the Steel Model Library, calculates the martensite start temperature (Ms) based on modeling the transformation barrier with fitted analytical equations. It is based on Stormvinter et al. [2012Sto] with subsequent update and extension by Gulapura Hanumantharaju [2017Gul] and Thermo-Calc internal assessment. The partitionless equilibrium temperature T_0 is calculated using the thermodynamic database. The Model also gives temperatures corresponding to 50%, 90%, and 99% transformations.

Martensite fractions are calculated with the same algorithm as in the **Martensite Fractions** Property Model.

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Configuration Settings

The input parameters are entered on the **Configuration** window for the Property Model Calculator. There are also settings on the Plot Renderer where you can choose from the available and relevant axis variables.

See Martensite Temperatures Property Model Settings.

Examples

For examples see PM_Fe_01: Fe-Cr-C Martensite with Intercritical Annealing and PM_Fe_02: Fe-Mn Martensite Morphologies.

References

[2012Sto] A. Stormvinter, A. Borgenstam, J. Ågren, Thermodynamically Based Prediction of the Martensite Start Temperature for Commercial Steels. Metall. Mater. Trans. A. 43, 3870–3879 (2012).

[2017Gul] A. K. Gulapura Hanumantharaju, Master's thesis, KTH Royal Institute of Technology (2017).

Martensite Temperatures Property Model Settings

The **Martensite Temperatures** Property Model, available with the Property Model Calculator and the Steel Model Library, calculates the martensite start (Ms) temperature based on modeling of the transformation barrier. Martensite half and finish temperatures are also given according to the Martensite Fractions Property Model.

About the Martensite Temperatures Property Model

For an example see PM_Fe_01: Fe-Cr-C Martensite with Intercritical Annealing and PM_Fe_02: Fe-Mn Martensite Morphologies.

Configuration Settings

The settings are found on the Property Model Calculator when **Martensite Temperatures** is selected under **Steel Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

INTERCRITICAL ANNEALING

Click to select the **Intercritical annealing** checkbox to assume intercritical annealing. Click to clear the checkbox if the specified composition is used directly. When selected, an equilibrium calculation is performed at the specified temperature and the composition of the austenite phase is used for the martensite temperature calculation.

ANNEALING TEMPERATURE

This setting is available when the **Intercritical annealing** checkbox is selected.

Enter an **Annealing temperature** in the field. The unit is the same as that selected under *Condition Definitions*.

GRAIN SIZE [MM]

Enter the **Grain size** of the austenite in micrometers (µm). The default is `100` µm.

PARENT PHASE GIBBS ENERGY ADDITION

In the **Parent phase Gibbs energy addition [J/mol]** field enter a value in J/mol to add a Gibbs energy offset to the parent austenite phase. This can be used, for example, to correct database offsets. The default is `0` J/mol.

Plot Renderer Settings

Plot Renderer, Configuration Settings, and Plot Type: TTT Mode

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

- **Ms temperature**: Martensite start temperature
- **Lath Ms**: Martensite start temperature of lath alpha or alpha-prime martensite
- **Plate Ms**: Martensite start temperature of plate alpha or alpha-prime martensite
- **Epsilon Ms**: Martensite start temperature of epsilon martensite
- **M50**: 50% martensite temperature
- **M90**: 90% martensite temperature
- **M99**: 99% martensite temperature

About the Martensitic Steel Strength Property Model

The **Martensitic Steel Strength** Property Model, available with the Property Model Calculator and the Steel Model Library, is available to predict the general flow stress properties of martensitic steels, such as hardness, stress at arbitrary strain, yield strength, ultimate tensile strength, Young's modulus, etc.

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

The model evaluates the following in consecutive steps:

- Martensite fraction based on composition, annealing temperature, and quench temperature
- Hardness of the as-quenched microstructure
- Effect of tempering on microstructure and hardness
- Young's modulus based on the composition of the matrix phase and contributions from precipitates
- Strain hardening response (flow stress) based on the final hardness after tempering

The hardness is evaluated by considering the individual contributions to hardness from intrinsic hardness, solid solution hardening and martensite hardening (as-quenched and tempered). The effect of tempering temperature is described on the basis of a physical model, with an applied correction using a neural network model describing the effect of tempering time. It is possible to predict precipitates forming at the tempering temperature and their individual properties will add to the total strength of the steel.

The resulting hardness forms the foundation for evaluating the flow stress by means of estimating the strain hardening response of the steel. Deviations in predicted flow stress properties can be corrected by changing key parameters in the settings, which are:

- Pre-straining (accounts for cold work the material may have been subjected to)
- Flow stress model (Ramberg-Osgood or Voce) and model specific parameters
- Young's modulus
- Constant strength addition

Graphite, Diamond, and Gas phases are all suspended throughout the calculation.

Read about the theory in Flow Stress.

Background

Steels undergoing austenitization, or at least partial austenitization (i.e., intercritical annealing), may form martensite upon quenching. The mechanical properties of martensite depend heavily on the content of interstitial elements in the parent austenite but are of course also affected by other elements and secondary phases. In general, a martensitic steel exhibits the following contributions to strength (or hardness):

[Eq. 1] $$\sigma_{tot} = \sigma_i + \sigma_{ss.} + \Delta\sigma_{mart.}$$

where σ_i is the total intrinsic hardness of the phases in the material, σ_{ss} is the contribution from solid solution hardening from each phase, and $\Delta\sigma_{mart.}$ is the additional hardening due to formation of martensite from the parent austenite.

The σ_i and σ_{ss} terms are modeled in the same way as in the **Yield Strength** Model. See About the Yield Strength Property Model.

The last term ($\Delta\sigma_{mart.}$) in Eq. 1 can further be decomposed into:

[Eq. 2] $$\Delta\sigma_{mart.} = \sigma_{mart.} \cdot f_{transf.}$$

where $\Delta\sigma_{mart.}$ is the hardening effect of the formation of martensite and $f_{transf.}$ is the fraction of parent austenite that has transformed to martensite. In the **Martensitic Steel Strength** Property Model, the fraction transformed is evaluated using the **Martensite Fractions** Model.

About the Martensite Fractions Property Model and Martensite Fractions Property Model Settings.

This means that the evaluation of the fraction of martensite is dependent on composition, austenitization temperature, quench temperature, and other parameters. These parameters are also available from within the Martensitic Steel Strength model.

Be aware of the absence of the contribution from grain size in Eq. 1. It has been shown that parent austenite grain boundaries contribute very little to the overall strength, due to the numerous other defects and interfaces that form during a martensitic transformation. The grain size may, however, affect the martensitic transformation itself in terms of the residual austenite content, which is modeled separately.

Eq. 1 is valid for the as-quenched condition, however, martensitic steels are most often tempered, which decomposes the martensite (and the residual austenite), to reduce brittleness. In the tempered condition, the martensite hardening contribution is reduced by reduction of dislocation density and precipitation of carbides. The carbides may also contribute significantly to the overall hardness and thus reduce the softening or even cause what is known as a secondary hardening peak. Eq. 2 thus becomes:

[*Eq. 3*] $$\Delta\sigma_{mart.tempered} = \sigma_{mart.} \cdot f_{transf.} \cdot \delta_{temper}$$

where δ_{temper} is a number between 0 and 1 and depends on tempering temperature and composition. In addition to this, the first two terms of Eq. 1 now also contain contributions from any tempering carbides that form. Tempering carbides are obtained from a constrained equilibrium calculation using the parent austenite composition and tempering temperature, where during set up you can select what phases are allowed on the **System Definer Configuration** window. This is justified by the abundant nucleation sites (due to very high dislocation density) and the fact that the carbides that form are very small, which implies very short diffusion distances.

The tempering behavior as function of time is modeled using a neural network trained on a large dataset covering mainly carbon and low-alloy steels, which provides a correction term to the total calculated hardness of the steel in the quench and tempered condition based on the physical model described above. For most of the steels considered, a very rapid decrease of hardness is expected with time, resulting in an asymptotic approach to an apparent stable value. Such a highly non-linear behavior, also exhibiting dependency on composition, lends itself well to machine learning (ML) based models.

The use of the predicted hardness to further predict flow stress is detailed in the theory for Flow Stress. Since the framework for evaluating flow stress is generally applicable, it is described as a separate section.

FCC_A1, BCC_A2, and Cementite must be selected on the **System Definer Configuration** window but can be suspended with settings available on the **Property Model Configuration** window. If these phases are excluded on the System Definer, the calculation does not work.

The Model only accepts phases that have had the intrinsic strength assessed. For a list of available phases see the section in the theory for Yield Strength Property Model regarding the Intrinsic Strength model.

Configuration Settings

The input parameters are entered on the **Configuration** window for the Property Model Calculator. There are also settings on the Plot Renderer where you can choose from the available and relevant axis variables.

See Martensitic Steel Strength Property Model Settings.

Example

For an example see PM_Fe_10: Martensitic Steel Strength.

Reference

[2008Pav] E. J. Pavlina, C. J. Van Tyne, Correlation of Yield Strength and Tensile Strength with Hardness for Steels. J. Mater. Eng. Perform. 17, 888–893 (2008).

Flow Stress

The **Martensitic Steel Strength** Property Model includes flow stress and is able to predict stress at arbitrary strain with these properties:

- True stress
- True strain (this requires user input)
- Engineering strain
- Engineering stress

The Model has a **Flow stress mode** to predict engineering properties such as:

- Yield strength
- Yield strain
- Ultimate tensile strength
- Uniform elongation
- Fracture strength
- Elongation at fracture
- Young's modulus

True strain is not available as an input parameter when using the *engineering properties mode* (i.e. E, σ_y and σ_{UTS}, which is selected as a **Flow stress mode**).

Additional Information

This section is specifically about the flow stress theory and is a continuation from the main theory described in About the Martensitic Steel Strength Property Model.

The input parameters are entered on the **Configuration** window for the Property Model Calculator. There are also settings on the Plot Renderer where you can choose from the available and relevant axis variables.

For details about the various settings mentioned in this theory section, see Flow Stress Settings.

You can also open an installed example to see the application of these features. See PM_Fe_12: Flow Stress 15-5PH Steel for more information.

Main Implementation

The flow stress model relies on the Ramberg-Osgood equation to predict flow stress, which can be expressed as:

$$\varepsilon = \frac{\sigma}{E} + 0.002(\frac{\sigma}{\sigma_y})^{(1/n)}$$

where

- ε is the strain,
- σ is the stress,
- E is the Young’s modulus,
- σ_y is the yield strength, and
- n is the strain hardening exponent.

To calculate stress at an arbitrary strain, the parameters E, σ_y, and n need to be determined.

The Young’s modulus of the material is obtained by averaging the Young’s moduli of individual phases.

> Elastic properties (the elastic constants and moduli) are available with the TCS Steel and Fe-alloys Database (TCFE) starting with version 14 (TCFE14). If you are using an earlier version of the database, i.e., no elastic properties are available, then the Young’s moduli of individual phases are estimated using simple rules.

The yield strength (σ_y) is determined based on its relationship with hardness, where the work by Pavlina and Van Tyne [2008Pav] is extended to consider a larger dataset. The hardness itself is predicted by the model as described in the primary theory section, About the Martensitic Steel Strength Property Model.

User-defined Flow Stress Parameters

Young's modulus (E) and the strain hardening exponent (n) can be set manually by selecting the **User-defined flow stress parameters** checkbox on the **Configuration** window. The yield strength, σ_y, is then inferred from these parameters and the known hardness.

After selecting the checkbox, you can further choose to use the **Voce** equation (select this option from the **Flow stress model** list), which is expressed as:

$$\sigma = \sigma_y + (\sigma_s - \sigma_y)(1 - e^{-k\varepsilon_p})$$

where

- σ_s is the saturation stress,
- ε_p is the plastic strain, and
- k is the hardening rate.

As the Voce equation is only expressed in terms of plastic strain, the model uses $\sigma = \varepsilon E$ for strains lower than the yield strain. To use the Voce model, you must specify the following additional settings:

- E (**Young's modulus**)
- σ_s (**Saturation stress**)
- k (**Hardening rate**)

Pre-deformed Materials

The flow stress model can be used to predict flow stress in pre-deformed materials, using the parameter **Pre-straining [%]**. The value given should correspond to the plastic strain that the material is exposed to beforehand. Pre-straining shifts the yield point and affects the yield strain, where uniform elongation and total elongation is then reduced by a corresponding amount.

Strain-rate Dependence

Strain-rate dependence on stress is implemented in the model and expressed as:

$$\sigma(\dot{\varepsilon}) = \sigma\left(\dot{\varepsilon_0}\right)\left(\frac{\dot{\varepsilon}}{\dot{\varepsilon_0}}\right)^m$$

where

- ε is the applied strain rate,
- $\dot{\varepsilon}_0$ is the reference strain rate (corresponding to quasi-static conditions), and
- m is the strain rate sensitivity, where m can be predicted by the model or user-defined.

Fracture Properties

Elongation and Fracture

Neither the Ramberg-Osgood nor Voce models can be used to predict fracture properties as they are only valid for uniform deformation. In fact, modeling, e.g., total elongation in a general manner based on some physical or empirical model is a challenging task. For this reason, the total elongation is modeled using a machine learning approach. Together with other properties, total elongation can then be used to estimate the fracture strength. In the stress vs. strain mode, any engineering stress at engineering strains beyond the predicted elongation is set to NaN, signifying that the material has fractured completely.

Post-uniform True vs. Engineering Stress and Strain

The conversion between engineering and true quantities is mathematically valid in the entire range of strain, however, the conversion assumes constant volume. This assumption is not valid in the necking regime as the deformation is not distributed evenly. Furthermore, void formation would decrease the density and cross-sectional area of the specimen. These issues are not easily corrected for as they require detailed knowledge on the geometry of the necking region as a function of strain and the progression of void formation etc. Therefore, the post-uniform elongation and total elongation are only available as engineering quantities.

Gauge Length

Total elongation is the sum of uniform elongation and elongation in the necking regime, where deformation is highly localized. Therefore, post-uniform elongation scales with cross-sectional area rather than length of the test piece. Since total elongation is expressed as a percentage of the length of the test piece, the measured value of the elongation in the necking regime is dependent on the actual length of the test-piece (so-called gauge length), and thus the same is valid for total elongation. This is an artifact of improper normalization and not a material dependence. The elongation model is trained on data mostly from tests performed on samples with 50 or 80 mm gauge lengths. For martensitic steels, the difference in total elongation between these gauge lengths would not, in most cases, exceed the experimental scatter.

Reference

[2008Pav] E. J. Pavlina, C. J. Van Tyne, Correlation of Yield Strength and Tensile Strength with Hardness for Steels. J. Mater. Eng. Perform. 17, 888–893 (2008).

Martensitic Steel Strength Property Model Settings

The **Martensitic Steel Strength** Property Model, available with the Property Model Calculator and the Steel Model Library, is available to predict the general flow stress properties of martensitic steels, such as hardness, stress at arbitrary strain, yield strength, ultimate tensile strength, Young's modulus, etc.

Background theory related to these settings is found in About the Martensitic Steel Strength Property Model and Flow Stress.

For examples see PM_Fe_10: Martensitic Steel Strength, PM_Fe_11: Steel Design Using the Parallel Coordinates Plot, and PM_Fe_12: Flow Stress 15-5PH Steel.

System Definer Configuration Settings

The following details relate to choosing the phases on the System Definer.

Then on the Property Model Calculator Configuration Settings window you can suspend as needed using the Suspend FCC, BCC, or Cementite settings described below.

FCC_A1, BCC_A2, and Cementite must be selected on the **System Definer Configuration** window but can be suspended with settings available on the **Property Model Configuration** window. If these phases are excluded on the System Definer, the calculation does not work.

The Model only accepts phases that have had the intrinsic strength assessed. For a list of available phases see the section in the theory for Yield Strength Property Model regarding the Intrinsic Strength model.

Property Model Calculator Configuration Settings

The settings are found on the Property Model Calculator when **Martensitic Steel Strength** is selected under **Steel Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

EVALUATION TEMPERATURE

The default **Evaluation temperature** is room temperature. Otherwise, select the **Evaluation temperature** checkbox to evaluate the strength at a temperature other than room temperature. The value is taken from the **Temperature** defined under *Condition Definitions*.

Also:

1. If the **Evaluation temperature** is *lower* than the tempering temperature, then the model evaluates the intrinsic and solid solution strengthening at the selected temperature.
2. Alternatively, if the **Evaluation temperature** is *higher* than the tempering temperature, then in addition to (1), the model treats the evaluation temperature as the tempering temperature.

ANNEALING TEMPERATURE

Enter an **Annealing temperature**, which is the temperature at which austenization or intercritical annealing is performed before the steel is quenched. The default is `1273.15`.

QUENCH TEMPERATURE

Enter a **Quench temperature**, which is the end temperature for quench after austenization. The default is `298.15`.

TEMPERING TEMPERATURE

The **Tempering temperature** is the temperature at which tempering is performed. This is used to estimate martensite hardness after tempering. The default is `673.15`.

TEMPERING TIME

Add a **Tempering time [s]**. The default is 3600 seconds. The time dependency is predicted using a machine learning model. If tempering time is set to a negative value, no tempering correction is applied to the total hardness.

SUSPEND FCC, BCC, OR CEMENTITE

Select the **Suspend FCC, BCC, or cementite** checkbox to choose to suspend one or more of these phases. All other phases can be deselected on the System Definer to exclude from the calculation as required.

> Austenite (FCC_A1), ferrite (BCC_A2), and Cementite phases all need to be selected on the System Definer. However, for some alloys it might be necessary to suspend one or more of these from the tempering calculation.

Then from one or more of the **FCC_A1**, **BCC_A2**, or **Cementite** lists choose **Entered** or **Suspended**.

MORE OPTIONS

Select the **More options** checkbox to adjust settings for **Grain size**, the **Parent phase Gibbs energy addition**, and **Constant strength addition**.

GRAIN SIZE

This setting is available when **More options** is selected.

Enter the **Grain size** of the austenite in micrometers (µm). The default is `100` µm.

PARENT PHASE GIBBS ENERGY ADDITION

This setting is available when **More options** is selected.

In the **Parent phase Gibbs energy addition [J/mol]** field enter a value in J/mol to add a Gibbs energy offset to the parent austenite phase. This can be used, for example, to correct database offsets. The default is `0` J/mol.

CONSTANT STRENGTH ADDITION

This setting is available when **More options** is selected.

Enter a value for the **Constant strength addition [MPa]**. You can also enter expressions such as `T*w(cr)+10` or similar.

Flow Stress Settings

For specific theory, see Flow Stress.

FLOW STRESS MODE

Select a **Flow stress mode**:

- **σ vs ϵ** to calculate the stress at a total specified strain
- **E, σ_y and σ_{UTS}** to calculate engineering properties. This is generally referred to as the *engineering properties mode* in the theory section.

TRUE STRAIN [%]

Available when **σ vs ϵ** is selected.

Enter a value for **True strain [%]** to evaluate the stress at a specified true strain (elastic plus plastic).

PRE-STRAINING [%]

Enter a value for the **Pre-straining [%]** to specify the strain the material is exposed to before calculation. This is useful in cases where prior deformation needs to be accounted for, e.g., cold work, as it affects the calculated flow stress.

The value entered does not affect the calculated hardness

USER-DEFINED FLOW STRESS PARAMETERS

Select the **User-defined flow stress parameters** checkbox to define additional parameters related to the flow stress calculation.

When the checkbox is selected also define other settings such as the **Flow stress model** and **Young's modulus**. Then based on the **Flow stress model**, also define **Strain hardening exponent**(Ramberg-Osgood) or **Saturation stress**, and **Hardening rate** (Voce). In addition, a value for the Young's modulus needs to be given.

FLOW STRESS MODEL

This is available when the **User-defined flow stress parameters** checkbox is selected.

Select a **Flow stress model** to use for the calculation: **Ramberg-Osgood** or **Voce**.

YOUNG'S MODULUS

This is available when the **User-defined flow stress parameters** checkbox is selected.

Enter a value for the **Young's modulus** in **GPa**.

STRAIN HARDENING EXPONENT

This is available when the **User-defined flow stress parameters** checkbox is selected and **Ramberg-Osgood** is the **Flow stress model**.

Enter a value for the **Strain hardening exponent**.

SATURATION STRESS

This is available when the **User-defined flow stress parameters** checkbox is selected and **Voce** is the **Flow stress model**.

Enter a **Saturation stress**, which is the stress value in MPa approached asymptotically with strain.

HARDENING RATE

This is available when the **User-defined flow stress parameters** checkbox is selected and **Voce** is the **Flow stress model**.

Enter a **Hardening rate**, which is the rate at which strain hardening progresses according to the Voce model.

APPLY STRAIN RATE

Select the **Apply strain rate** checkbox to account for the effect of strain rate on flow stress. If the checkbox is not selected (the default), flow stress is calculated for quasi-static conditions only.

When the checkbox is selected also define other settings such as **Strain rate [1/s]**, **Reference strain rate**, and **Strain rate sensitivity**.

STRAIN RATE

This is available when the **Apply strain rate** checkbox is selected.

Enter a value for the **Strain rate** in **1/s**.

REFERENCE STRAIN RATE

This is available when the **Apply strain rate** checkbox is selected.

Specify the **Reference strain rate** in 1/s. This should correspond to the strain rate at quasi-static conditions, i.e., in the range of 10^{-4} to 10^{-3}

APPLY USER-DEFINED STRAIN RATE SENSITIVITY

This is available when the **Apply strain rate** checkbox is selected.

Select the **Apply user-defined strain rate sensitivity** checkbox to enter a **Strain rate sensitivity** exponent. If the checkbox is not selected (the default), the strain rate sensitivity exponent is estimated by the model.

Plot Renderer Settings

? Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

Plot Quantities

These plot quantities are available:

- **Tempering temperature**
- **True stress**
- **Engineering strain**
- **Engineering stress**
- **Yield strength**
- **Yield strain**
- **Ultimate tensile strength**
- **Uniform elongation**
- **Fracture strength**
- **Elongation at fracture**
- **Young's modulus**
- **Constant strength addition**
- **Total martensite percentage**: The percentage of martensite after quenching.
- **Retained austenite percentage**: The percentage of retained austenite after quenching.
- **Precipitate fraction (Annealing)**: The fraction of any given phase present at the annealing temperature before quenching.
- **Precipitate fraction (Tempering**): The fraction of any given phase present after quenching and tempering (precipitates after temper are added to those at annealing, if any).
- **Martensite hardening as-quenched**
- **Martensite hardening quenched and tempered**
- **Total solid solution hardening**
- **Solid solution hardening after temper**
- **Total hardness of the as-quenched steel**
- **Total hardness of the tempered steel**

About the Pearlite Property Model

The **Pearlite** Property Model [2020Yan], available with the Property Model Calculator and the Steel Model Library, calculates the thermodynamics and kinetics of pearlite formation from austenite during isothermal heat treatment.

The **Pearlite** Model describes the thermodynamics and kinetics of pearlite formation from austenite. It is assumed that the overall composition of pearlite is the same as the austenite composition, and growth rate is constant over time. Growth rate and lamellar spacing of pearlite are determined by a criterion where either growth rate or Gibbs energy dissipation rate is maximized. The Model considers Gibbs energy dissipation due to formation of ferrite-cementite interface in pearlite, finite austenite-pearlite interfacial mobility, solute drag, and diffusion of elements within austenite and along austenite-pearlite interface.

Divergent pearlite, of which growth rate and lamellar spacing change with time, is not considered. This Model only considers the transformation from FCC_A1 phase to pearlite consisting of BCC_A2 and CEMENTITE_D011 (for TCFE9 this is CEMENTITE). Pearlite with other phases is not implemented.

Pearlite is assumed to nucleate on austenite grain boundaries. Grain boundary nucleation rate is modeled as a function of composition and temperature. The isothermal transformation kinetics follows Cahn [1956Cah]. Start, half, and finish times are taken as 2%, 50%, and 98% transformation, respectively.

Austenite composition can be taken either as the nominal composition or from an equilibrium calculation at an austenitization temperature. The latter option can be useful when austenite coexists with other phase(s), e.g. primary carbide or ferrite, before pearlite starts to form in austenite. But the Model only considers the effect of other phase(s) on austenite composition.

Model parameters have been determined from published data of maximal growth rate, minimal lamellar spacing, partition coefficients, and isothermal transformation kinetics in ternary and multicomponent systems.

The included elements in the Pearlite Property Model are Fe (dependent element), C, Mn, Cr, Mo, W, Si, Al, Ni, Co. Other elements are neglected by weight percent.

🔑 To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Configuration Settings

The input parameters are entered on the **Configuration** window for the Property Model Calculator. There are also settings on the Plot Renderer where you can choose from the available and relevant axis variables.

See Pearlite Property Model Settings.

Example

For an example see PM_Fe_03: Fe-C-Mn Pearlite.

References

[1956Cah] J. W. Cahn, The kinetics of grain boundary nucleated reactions. Acta Metall. 4, 449–459 (1956).

[2020Yan] J.-Y. Yan, J. Ågren, J. Jeppsson, Pearlite in Multicomponent Steels: Phenomenological Steady-State Modeling. Metall. Mater. Trans. A. 51, 1978–2001 (2020).

Pearlite Property Model Settings

The **Pearlite** Property Model, available with the Property Model Calculator and the Steel Model Library, calculates the thermodynamics and kinetics of pearlite formation from austenite during isothermal heat treatment.

The included elements in the Pearlite Property Model are Fe (dependent element), C, Mn, Cr, Mo, W, Si, Al, Ni, Co. Other elements are neglected by weight percent.

For the **Ferrite**, **Bainite**, and **Pearlite** Property Models, it is also useful to review the Recommended Composition Ranges for Steel Models.

About the Pearlite Property Model

For an example see PM_Fe_03: Fe-C-Mn Pearlite.

Configuration Settings

The settings are found on the Property Model Calculator when **Pearlite** is selected under **Steel Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

AUSTENITE COMPOSITION FROM

Select an option from the **Austenite composition from** list:

- **Nominal composition** uses the system composition as austenite composition.
- **Equilibrium composition at austenizing temperature**. Select to enter an **Austenitizing temperature**. The austenite composition is determined from an equilibrium calculation at the austenitizing temperature (if austenite is stable). This option is useful when austenite coexists with other phase(s), e.g. primary carbide, before the transformation(s) being calculated starts. But the Model only considers the effect of other phase(s) on austenite composition.

AUSTENTIZING TEMPERATURE

This setting is available when **Equilibrium composition at austenitizing temperature** is selected from the **Austenite composition from** list.

Enter an **Austentizing temperature** in the field. The unit is the same as that selected under *Condition Definitions*.

GRAIN SIZE [MM]

Enter the **Grain size** of the austenite in micrometers (µm). The default is `100` µm.

CRITERION

This setting is available when the **Pearlite selected** checkbox is selected.

Select an option from the **Criterion** list to determine the pearlite growth condition. This list is called **Pearlite criterion** for the CCT Diagram and TTT Diagram Property Models.

- For **Maximize growth rate**, pearlite growth rate is maximized with respect to lamellar spacing (and for optimal pearlite, partition coefficients of substitutional alloying elements between ferrite and cementite). The calculation gives maximal growth rate and minimal lamellar spacing. This is the default criterion.
- For **Maximize Gibbs energy dissipation rate**, Gibbs energy dissipation rate is maximized with respect to lamellar spacing (and for optimal pearlite, partition coefficients of substitutional alloying elements between ferrite and cementite). The calculation gives a smaller growth rate than the maximal, and a larger lamellar spacing than the minimal, which may better represent the average growth rate and lamellar spacing of all pearlite colonies in the material.

PEARLITE MODE

This setting is available when the **Pearlite selected** checkbox is selected. It is used to determine how substitutional alloying elements partition between ferrite and cementite in pearlite. Select an option from the **Pearlite mode** list.

- For **Optimal pearlite**, the partitioning of substitutional alloying elements between ferrite and cementite is optimized according to the **Criterion** while keeping carbon equilibrium between the two phases. This is the default mode. This mode realizes a smooth transition between ortho-pearlite and para-pearlite.
- For **Para-pearlite**, ferrite and cementite are in para-equilibrium where substitutional alloying elements do not partition and carbon reaches equilibrium.
- For **Ortho-pearlite**, ferrite and cementite are in ortho-equilibrium.

Plot Renderer Settings

Plot Renderer, Configuration Settings, and Plot Type: TTT Mode

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

- **Temperature**
- **Start time (2% pearlite)**
- **Half time (50% pearlite)**
- **Finish time (98% pearlite)**
- **Growth rate [m/s]**
- **Lamellar spacing [m]**
- **Cementite molar fraction in pearlite**
- **Driving force of pearlite formation [J/mol]**

About the TTT Diagram Property Model

The **TTT Diagram** Property Model, available with the Property Model Calculator and the Steel Model Library, can be used to calculate a Time-Temperature-Transformation (TTT) diagram, with a **One Axis** calculation on temperature. The Model calculates the isothermal kinetics of concurrent transformation of austenite into ferrite, pearlite, bainite, and martensite. The algorithms and parameters for ferrite, pearlite, bainite, and martensite are the same as in the individual Property Models (**Ferrite**, **Pearlite**, **Bainite**, **Martensite Temperatures**, and **Martensite Fractions**), but the competitive occupation of prior austenite grain boundaries and bulk volume is handled in the **TTT Diagram** Property Model.

If the reaction temperature is below martensite-start temperature (Ms), it is assumed that a fraction of (athermal) martensite according to the calculation forms instantaneously at time zero, prior to the formation of ferrite, pearlite, and bainite. Otherwise austenite transforms to ferrite, pearlite, and/or bainite.

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Configuration Settings

The input parameters are entered on the **Configuration** window for the Property Model Calculator. There are also settings on the Plot Renderer where you can choose from the available and relevant axis variables.

See TTT Diagram Property Model Settings.

Example

For an example see PM_Fe_06: TTT Diagram for Fe-C-Mn-Si-Cr-V.

TTT Diagram Property Model Settings

The **TTT Diagram** Property Model, available with the Property Model Calculator and the Steel Model Library, calculates the concurrent transformations to ferrite, pearlite, bainite, and martensite under isothermal conditions and is used to construct a time-temperature-transformation (TTT) diagram.

About the TTT Diagram Property Model and Steel Library TTT Diagram Template

For an example see PM_Fe_06: TTT Diagram for Fe-C-Mn-Si-Cr-V

Configuration Settings

These settings are found on the Property Model Calculator when **TTT Diagram** is selected under **Steel Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

AUSTENITE COMPOSITION FROM

Select an option from the **Austenite composition from** list:

- **Nominal composition** uses the system composition as austenite composition.
- **Equilibrium composition at austenizing temperature**. Select to enter an **Austenitizing temperature**. The austenite composition is determined from an equilibrium calculation at the austenitizing temperature (if austenite is stable). This option is useful when austenite coexists with other phase(s), e.g. primary carbide, before the transformation(s) being calculated starts. But the Model only considers the effect of other phase(s) on austenite composition.

AUSTENTIZING TEMPERATURE

This setting is available when **Equilibrium composition at austenitizing temperature** is selected from the **Austenite composition from** list.

Enter an **Austentizing temperature** in the field. The unit is the same as that selected under *Condition Definitions*.

GRAIN SIZE

Enter the **Grain size** of the austenite in micrometers (µm). The default is `100` µm.

Calculation Setting

Select **Quick** (the default), **Accurate**, or **Custom** to balance accuracy and calculation time. Choose **Custom** to define the numerical settings yourself, which are otherwise set in the background when **Quick** or **Accurate** is selected. See the separate section below about the details for the **Custom** settings.

QUICK CALCULATION SETTING

Quick is used for a relatively quick and rough calculation to reveal the general feature of a TTT diagram. Interpolation is used when necessary in order to avoid calculating the growth rates and nucleation rates of pearlite and bainite at every time step.

- For simplicity, **Ferrite mode** is **PE** (paraequilibrium), and **Pearlite mode** is **Para-pearlite**.
- Recommended temperature interval: 50-100 K.

⌛ Each temperature can take several minutes.

ACCURATE CALCULATION SETTING

Accurate evaluates the growth rates and nucleation rates at every time step accurately (without interpolation). The time step control is also tighter than when using the **Quick** setting.

- **Ferrite mode** is *faster start*, meaning the mode between OE and PE which gives a faster initial transformation.
- **Pearlite mode** is **Optimal pearlite**, but its rate calculation becomes slower if austenite contains many alloying elements.
- Recommended temperature interval: 20-50 K or even lower.

> ⌛ Calculating the whole TTT diagram may take several hours.

Details about the Quick and Accurate Calculation Settings

When you choose **Quick** or **Accurate** as the calculation setting, the following is what is automatically set in the background for each of the sections. These sections are visible to you and also can be edited when **Custom** is chosen:

Setting	*Quick*	*Accurate*
Ferrite selected	checkbox selected (yes)	checkbox selected (yes)
Pearlite selected	checkbox selected (yes)	checkbox selected (yes)
Bainite selected	checkbox selected (yes)	checkbox selected (yes)
Martensite selected	checkbox selected (yes)	checkbox selected (yes)
Ferrite mode	PE only	Faster start (TTT); PE if possible otherwise OE (CCT)
Pearlite criterion	Maximize growth rate	Maximize growth rate
Pearlite mode	Para-pearlite	Optimal pearlite
Use interpolation when necessary	checkbox selected (yes)	checkbox NOT selected (no)
Interpolation error tolerance	0.1	(does not apply)

Setting	*Quick*	*Accurate*
Maximum phase fraction change (absolute) in a time step	0.005	0.005
Maximum phase fraction change (relative) in a time step	0.05	0.05
Error tolerance for austenite fraction	1E-3	1E-4

Custom Calculation Setting

The following settings are available when **Custom** is selected as the *Calculation Setting*. Otherwise these settings are handled in the background as described above for when **Quick** or **Accurate** is selected.

FERRITE/PEARLITE/BAINITE/MARTENSITE SELECTED CHECKBOXES

By default the **Ferrite selected**, **Pearlite selected**, **Bainite selected**, and **Martensite selected** checkboxes are selected. For ferrite and pearlite, additional settings are then available.

Click to deselect as required to exclude one or more from the calculation.

PEARLITE CRITERION

This setting is available when the **Pearlite selected** checkbox is selected.

Select an option from the **Criterion** list to determine the pearlite growth condition. This list is called **Pearlite criterion** for the CCT Diagram and TTT Diagram Property Models.

- For **Maximize growth rate**, pearlite growth rate is maximized with respect to lamellar spacing (and for optimal pearlite, partition coefficients of substitutional alloying elements between ferrite and cementite). The calculation gives maximal growth rate and minimal lamellar spacing. This is the default criterion.
- For **Maximize Gibbs energy dissipation rate**, Gibbs energy dissipation rate is maximized with respect to lamellar spacing (and for optimal pearlite, partition coefficients of substitutional alloying elements between ferrite and cementite). The calculation gives a smaller growth rate than the maximal, and a larger lamellar spacing than the minimal, which may better represent the average growth rate and lamellar spacing of all pearlite colonies in the material.

CARBIDE IN PEARLITE

From the **Carbide in pearlite** list, select the carbide to be present in pearlite: **CEMENTITE** (default), **M7C3**, or **M23C6**. For M23C6, this usually depends on Cr content.

When M23C6 is selected, parameters optimized for stainless steels are invoked.

Recommended Composition Ranges for Steel Models

CARBIDE IN BAINITE

From the **Carbide in bainite** list, select the carbide to be present in pearlite: **CEMENTITE** (default) or **M7C3**. For M7C3, this usually depends on Cr content.

PEARLITE MODE

This setting is available when the **Pearlite selected** checkbox is selected. It is used to determine how substitutional alloying elements partition between ferrite and cementite in pearlite. Select an option from the **Pearlite mode** list.

- For **Optimal pearlite**, the partitioning of substitutional alloying elements between ferrite and cementite is optimized according to the **Criterion** while keeping carbon equilibrium between the two phases. This is the default mode. This mode realizes a smooth transition between ortho-pearlite and para-pearlite.
- For **Para-pearlite**, ferrite and cementite are in para-equilibrium where substitutional alloying elements do not partition and carbon reaches equilibrium.
- For **Ortho-pearlite**, ferrite and cementite are in ortho-equilibrium.

USE INTERPOLATION WHEN NECESSARY

If the **Use interpolation when necessary** checkbox is selected, and depending on alloy composition and temperature, if the code determines that an interpolation is necessary and possible to implement, then a composition grid (TTT diagram) or composition-temperature grid (CCT diagram) is generated and refined as needed.

The growth rates and nucleation rates of pearlite and bainite, as functions of composition (TTT diagram) or composition and temperature (CCT diagram), are determined by interpolation (if sufficiently accurate). This is intended to avoid direct calculations of pearlite and bainite rates for every time step, which is usually time-consuming.

INTERPOLATION ERROR TOLERANCE

This setting is available when the **Use interpolation when necessary** checkbox is selected.

The growth and nucleation rates of pearlite and bainite, if determined from interpolation, are accepted only when the relative interpolation error estimated is below the value entered here. A large number implies few grid points necessary (shorter calculation time) and lower accuracy, and a small number implies the opposite.

MAXIMUM PHASE FRACTION CHANGE (ABSOLUTE/RELATIVE) IN A TIME STEP

The **Maximum phase fraction change (absolute) in a time step** and **Maximum phase fraction change (relative) in a time step** settings are used to control time step size during time integration.

The phase fraction (X) of ferrite, pearlite, and bainite cannot change more than $atol + X * rtol$ during a time step, where $atol$ and $rtol$ are the absolute and relative maximum change, respectively. If the change is too large, the new time step is rejected, and time integration is retried with a smaller time step.

ERROR TOLERANCE FOR AUSTENITE FRACTION

The **Error tolerance for austenite fraction** setting is used to control the accuracy for austenite fraction during time integration. Finite time steps cause an error in austenite volume fraction. When the error is larger than the tolerance, time integration is backed up and retried with a smaller time step.

Plot Renderer Settings

Plot Renderer, Configuration Settings, and Plot Type: TTT Mode

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

- **Ferrite start (2%)**
- **Pearlite start (2%)**
- **Bainite start (2%)**

- **Total ferrite start (2%)**: The start of the sum of polygonal ferrite and bainitic ferrite.
- **Total ferrite + cementite start (2%)**: The start of the sum of pearlite and cementite-containing bainite.
- **Total ferrite + cementite finish (98%)**: 98% austenite transformed to ferrite, pearlite, and bainite.
- **Austenite transformed 2%**
- **Austenite transformed 10%**
- **Austenite transformed 50%**
- **Austenite transformed 90%**
- **Austenite transformed 98%**
- **Martensite start**
- **Martensite 50%**
- **Martensite 98%**

Fractions of transformation products at the last time step are also available:

- **Terminal fraction of ferrite**
- **Terminal fraction of pearlite**
- **Terminal fraction of bainite**
- **Terminal fraction of martensite**
- **Terminal fraction of total ferrite**
- **Terminal fraction of total ferrite+cementite**

Martensite start, Martensite 50%, and Martensite 98% are temperature quantities. Terminal fractions are unit-free quantities. The others are time quantities.

In the **TTT Mode** of a Plot Renderer, the three temperature quantities for martensite are plotted as horizontal lines because these are independent of time. The other time quantities are plotted as functions of temperature.

Titanium Model Library Property Models

? Property Model Calculator

In this section:

About the Titanium Model Library Property Models

These **Titanium Models** are available with the Property Model Calculator and as part of the Titanium Model Library.

To run calculations with the **Titanium Models** requires a valid maintenance license plus a license for the TCTI (version 6 and newer) database. For some Property Models, additional recommendations for the database version to use is indicated in its description. Also see our website to learn more about the Titanium Model Library.

Alloy Strength - Ti

The **Alloy Strength - Ti** Property Model, available with the Property Model Calculator and the Titanium Model Library, calculates the strength and hardness for Ti-base alloys.

See About the Alloy Strength - Ti Property Model and Alloy Strength - Ti Property Model Settings for background theory and input parameter details.

Martensite Temperatures - Ti

The **Martensite Temperatures - Ti** Property Model, available with the Property Model Calculator and the Titanium Model Library, calculates the martensite start temperature (Ms) and T-Zero temperatures for Ti-base alloys.

See About the Martensite Temperatures - Ti Property Model and Martensite Temperatures - Ti Property Model Settings for background theory and input parameter details.

About the Alloy Strength - Ti Property Model

The **Alloy Strength - Ti** Property Model, available with the Property Model Calculator and the Titanium Model Library, calculates the strength and hardness for Ti-base alloys.

To run calculations with the **Titanium Models** requires a valid maintenance license plus a license for the TCTI (version 6 and newer) database. For some Property Models, additional recommendations for the database version to use is indicated in its description. Also see our website to learn more about the Titanium Model Library.

The various forms of alpha martensite HCP (α, α', or α'') are not explicitly distinguished and are collectively described by the phase HCP_A3 in terms of thermodynamic properties.

The **Alloy Strength - Ti** model is built from individual models for four strength contributions. The effect of impurities on the strength of Ti-base alloys is very strong [1981Con; 1998Ouc] and this model has therefore been equipped with a functionality to select base grades, according to the ASTM definitions of purity, for cases where the exact impurity content is not known.

Intrinsic Strength

The *intrinsic strength* is calculated as the combination of the strength for the pure elements in the system, weighted by the mole fraction of each element. In the **Alloy Strength - Ti** model you can choose the **Titanium base grade**, which are base grades of “commercially pure” titanium and represent the impurity elements allowed in each grade. The compositions defined for the available grades are as listed:

- **Iodide Titanium**: Pure Ti with no impurity elements (the default)
- **Grade 1 (35A)**: Ti-0.2Fe-0.18O-0.08C-0.03N-0.015H (wt%)
- **Grade 2 (50A)**: Ti-0.3Fe-0.25O-0.08C-0.03N-0.015H (wt%)
- **Grade 3 (65A)**: Ti-0.3Fe-0.35O-0.08C-0.05N-0.015H (wt%)
- **Grade 4 (75A)**: Ti-0.5Fe-0.4O-0.08C-0.05N-0.015H (wt%)

The intrinsic strength for the different grades is given as the linear combination of the strength for the elements in the system plus the calculated strengthening contribution from solid solution of the impurity elements.

Grain Boundary Strengthening

For the *grain boundary strengthening*, after selecting the **Grain boundary strengthening** checkbox you can include an effect of **Grain size** on the strength/hardness. This contribution is given by the Hall-Petch equation [2016Cor]. When setting up the model, you can either specify a **User-defined Hall-Petch coefficient** or otherwise it is calculated by default.

For additional background information, see About the Yield Strength Property Model.

Solid Solution Strengthening

The *solid solution strengthening* contribution is evaluated as per the model by Walbrühl et al. [2017Wal], where the parameters for each Ti binary system are optimized against a compiled collection of experimental studies on titanium. There is no specific input required for solid solution strengthening when setting up the model. This calculation uses the composition of the alpha and/or beta phase of the system, which is automatically calculated in the model.

For additional background information, see About the Yield Strength Property Model.

Precipitation Strengthening

After selecting the **Precipitation strengthening** checkbox on the **Configuration** window, there are several settings you can define. One phase can be chosen to contribute to the alloy strength by *precipitation strengthening*, which in this Property Model is given by the model by Deschamps et al. [1998Des].

On the **Configuration** window for this setting, the following input parameters can be defined:

- **Precipitate radius**: The mean radius of the precipitates.
- **Critical radius**: The mean precipitate radius where the mechanism that dislocations pass precipitates changes from shearing ($r < r_{critical}$) to looping ($r > r_{critical}$).
- **Taylor factor**: The Taylor factor accounts for the texture of the material, normally the

value is between 2.24 and 3.06 for randomly oriented grains.

- **Shear modulus**: The shear modulus of the matrix phase, given in Pascal (Pa).
- **Burgers vector**: The burgers vector of the matrix phase, given in meters (m).

Starting with TCS Ti/TiAl-based Alloys Database (TCTI) version 6, it is possible to calculate the **Shear modulus** of individual phases. The option is enabled by default for the precipitation strengthening contribution. See the settings information or the tooltip.

Constant Strength Addition

The *Constant strength addition* contribution can be used to displace the calculated result in the *y*-direction.

Settings, Example, and References

Configuration Settings

The input parameters are entered on the **Configuration** window for the Property Model Calculator. There are also settings on the Plot Renderer where you can choose from the available and relevant axis variables.

See Alloy Strength - Ti Property Model Settings.

Example

For an example see PM_Ti_02: Alloy Strength for Ti-O.

References

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Alloy Strength - Ti Property Model Settings

The **Alloy Strength - Ti** Property Model, available with the Property Model Calculator and the Titanium Model Library, calculates the strength and hardness for Ti-base alloys.

About the Alloy Strength - Ti Property Model

For an example see PM_Ti_02: Alloy Strength for Ti-O

About the Contributions

The model can be configured to include contributions from:

- *Intrinsic strength / hardness*: The base line strength expressed as the weighted average of the strength for the pure elements in the system. If any of grade 1-4 is chosen as the base, a solid solution strengthening contribution stemming from impurities of Fe, C, N, H, and O is added to the weighted average of pure element strength.
- *Solid solution strengthening / hardening*: The contribution to strength from solid solution calculated as the sum of contributions from binary interactions.
- *Grain boundary strengthening / hardening*: The contribution to strength from grain boundaries described by the Hall-Petch relationshipis described by the Hall-Petch relation.
- *Precipitation strengthening / hardening*: The contribution to strength from precipitation, described by the model developed by Deschamps.
- *Constant strength / hardness*: This contribution is a constant addition to the overall strength. It is a true constant in the sense that it is not converted between either strength or hardness, nor between Mpa or Vickers units.

For more details about these contributions, see About the Alloy Strength - Ti Property Model.

Configuration Settings

The settings are found on the Property Model Calculator when **Alloy Strength - Ti** is selected under **Titanium Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

TITANIUM BASE GRADE

Select a **Titanium base grade** from the list. Impurities have a strong solid solution hardening effect. When you select a Ti-grade as the base for the alloys system, this effect is taken into account. The default, **Iodide Titanium**, is pure Ti with no impurity elements, i.e. this excludes this contribution to the intrinsic hardness. Otherwise choose a Ti-base grade from the list, where the compositions for the available grades are also listed:

- **Grade 1 35A**: Ti-0.2Fe-0.18O-0.08C-0.03N-0.015H (wt%)
- **Grade 2 50A**: Ti-0.3Fe-0.25O-0.08C-0.03N-0.015H (wt%)
- **Grade 3 65A**: Ti-0.3Fe-0.35O-0.08C-0.05N-0.015H (wt%)
- **Grade 4 75A**: Ti-0.5Fe-0.4O-0.08C-0.05N-0.015H (wt%)

EVALUATION TEMPERATURE

Enter an **Evaluation temperature**, which is the temperature at which the hardness is evaluated.

GRAIN BOUNDARY STRENGTHENING

Click to select the **Grain boundary strengthening** checkbox to include calculated grain boundary strengthening (σ_{gb}).

GRAIN SIZE

This setting is available when the **Grain boundary strengthening** checkbox is selected.

Enter the **Grain size [µm]**, which is the grain diameter in micrometers (µm). The default is `100` µm.

USER-DEFINED HALL-PETCH COEFFICIENT

This setting is available when the **Grain boundary strengthening** checkbox is selected. By default, a suitable default **Hall-Petch coefficient** is automatically calculated by the model.

Alternatively, select the **User defined Hall-Petch coefficient** checkbox and enter a different **Hall-Petch coefficient**: k_{h-p} in MPa µm$^{1/2}$.

PRECIPITATION STRENGTHENING

Click to select the **Precipitation strengthening** checkbox to include calculated precipitation strengthening (σ_p). Then continue to define the settings under Additional Precipitation Strengthening Settings.

CONSTANT STRENGTH ADDITION

Enter a **Constant strength addition**. This strength contribution can be used to displace the calculated result in the *y*-direction. Function input is allowed, e.g., `1000*w(Al)`.

Additional Precipitation Strengthening Settings

The following settings are available when the **Precipitation strengthening** checkbox is selected.

PRECIPITATE PHASE

Select a **Precipitate phase** from the list. One phase can be chosen to contribute to the alloy strength.

The various forms of alpha martensite HCP (α, α', or α'') are not explicitly distinguished and are collectively described by the phase HCP_A3 in terms of thermodynamic properties.

PRECIPITATE RADIUS

Enter a **Precipitate radius**, which is the mean radius of the precipitates. The default is `1.0E-8`.

CRITICAL RADIUS

Enter a **Critical radius**. This is the mean precipitate radius where the mechanism that dislocations pass precipitates changes from shearing ($r < r_{critical}$) to looping ($r > r_{critical}$). The default is `1.0E-8`.

TAYLOR FACTOR

Enter a value for the **Taylor factor**. The default is `3.0`.

The value of the Taylor factor accounts for texture in the material. Normally the value is between 2.24 and 3.06 for random orientations.

SHEAR MODULUS

Enter the word `Calculated` (not case sensitive) in this field to calculate the shear modulus of the matrix phase from the parameters in the thermodynamic TCS Ti/TiAl-based Alloys Database (TCTI) (version TCTI6 and higher), which contains the elastic properties.

Additionally, values or functions, expressed in Pa, are also accepted as input. If the shear modulus cannot be calculated or evaluated from the input, a default value of `4.5E10` Pa is used, which is close to the value for pure Ti at room temperature.

BURGERS VECTOR

Enter a value for the **Burgers vector**, which is the burgers vector of the matrix phase. The unit is meter (m) and the default is `2.5E-10`.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

The various *hardness* or *hardening* quantities are treated separately from the various *strength* or *strengthening* quantities and each (hardness and strength) are plotted on the respective axes. When setting up the simulation, the **Configuration** window (when in *Grouped Mode*) shows either *Vickers Hardness* or *Strength*. This corresponds to the labeling of axes in the **Visualizations** window when plotting two or more quantities of the same type. The legend then lists the specific quantity names selected on the **Configuration** window.

Plot Quantities

- **Temperature**
- **Total Hardness**
- **Total Yield Strength**
- **Intrinsic Hardness**
- **Total Solid Solution Hardening**
- **Solid Solution Hardening for Beta Phase**
- **Solid Solution Hardening for Alpha Phase**
- **Constant strength addition [MPa]**
- **Amount of Phases**

About the Martensite Temperatures - Ti Property Model

The **Martensite Temperatures - Ti** Property Model, available with the Property Model Calculator and the Titanium Model Library, calculates the martensite start temperature (Ms) and T-Zero temperatures for Ti-base alloys.

You can choose between **HCP** (α, α', or α'') and **B19_PRIME** or **B19_ORTHO** as the **Martensite phase**:

- The HCP (α, α', or α'') is the common choice for alloys such as Ti-6Al-4V and other structural alloys.
- The B19_PRIME and B19_ORTHO options are intended for TiNi-based shape-memory alloys. In particular, B19_ORTHO is useful for TiNiCu-based shape-memory alloys.

The various forms of alpha martensite HCP (α, α', or α'') are not explicitly distinguished and are collectively described by the phase HCP_A3 in terms of thermodynamic properties.

An initial equilibrium is calculated to set the starting composition and internal constitution (in case of ordering) of the parent phase. This should be performed at a temperature that reflects the thermal history of the studied alloy. The starting composition and constitution is held fixed throughout the calculation as it is expected that the alloy cannot equilibrate during a martensitic transformation.

The model then calculates the T_0 temperature and the associated offset to the Ms temperature, which occurs due to the thermodynamic barrier for nucleation of martensite. The offset is parameterized using conventional Redlich-Kister polynomials.

To run calculations with the **Titanium Models** requires a valid maintenance license plus a license for the TCTI (version 6 and newer) database. For some Property Models, additional recommendations for the database version to use is indicated in its description. Also see our website to learn more about the Titanium Model Library.

Configuration Settings

The input parameters are entered on the **Configuration** window for the Property Model Calculator. There are also settings on the Plot Renderer where you can choose from the available and relevant axis variables.

See Martensite Temperatures - Ti Property Model Settings.

Example

For an example see PM_Ti_01: Martensite Temperatures for Ti-Zr

Martensite Temperatures - Ti Property Model Settings

The **Martensite Temperatures - Ti** Property Model, available with the Property Model Calculator and the Titanium Model Library, calculates the martensite start temperature (Ms) and T-Zero temperatures for Ti-base alloys.

About the Martensite Temperatures - Ti Property Model

For an example see PM_Ti_01: Martensite Temperatures for Ti-Zr

Configuration Settings

The settings are found on the Property Model Calculator when **Martensite Temperatures - Ti** is selected under **Titanium Models**.

When working in the **Configuration** window, click the **Description** tab for more information about the Model.

For the details about the *Condition Definitions*, *Calculation Type*, *Timeout in minutes*, *Parallel Calculation*, and other calculation associated settings, see Configuration Window Settings.

Additionally note the following about the **Temperature** setting for this Property Model. You can also select the **Annealing** checkbox to treat this as the annealing temperature. See details below.

TEMPERATURE (IN CONDITION DEFINITIONS)

The temperature at which an initial equilibrium is calculated to set the starting composition and internal constitution (in case of ordering) of the parent phase. Should reflect the initial microstructure of the studied alloy. The starting composition and constitution is held fixed throughout the calculation as it is expected that the alloy can not equilibrate during a martensitic transformation.

MARTENSITE PHASE

Select a **Martensite phase** from the list: **HCP** (α, α', or α''), **B19_PRIME (shape-memory alloys)**, or **B19_ORTHO (shape-memory alloys)**.

- **HCP**(α, α', or α'') is the common choice for alloys such as Ti-6Al-4V and other structural alloys.
- **B19_PRIME (shape-memory alloys)** for TiNi-based shape-memory alloys.
- **B19_ORTHO (shape-memory alloys)** for TiNi-based shape-memory alloys. This setting is particularly useful for TiNiCu-based shape-memory alloys.

PARENT PHASE ENERGY ADDITION

In the **Parent phase energy addition [J/mol]** field enter a value in J/mol to add a Gibbs energy shift for the parent phase. This should normally only be used for calculating T-Zero since it might produce unpredictable results for Ms.

The expression can be a function of temperature, T, and composition, w(el) or x(el), for example:

```
50*T/1000+10*x(Cr)+5*x(Cr)^2
```

The default is `0` J/mol.

ANNEALING

The model initially calculates a global equilibrium for the bulk composition in order to identify the correct parent phase. The temperature condition for this calculation is taken from the Condition Definitions setting.

It is also possible to treat this temperature as the annealing temperature, i.e., that the composition of the parent phase is taken from the equilibrium calculation at this temperature and used as composition conditions.

If the parent phase is the only stable phase, the nominal composition is equal to the parent phase composition. However, for multiphase equilibria, the composition of the parent phase will differ from the build composition.

Select the **Annealing** checkbox to use the annealing temperature instead of the Temperature set under Condition Definitions.

Plot Renderer Settings

Plot Renderer and Configuration Settings

When setting up your calculation on the Plot Renderer and/or Table Renderer, the following axis variables are available for the conditions defined on the Property Model Calculator.

Quantities

- **Temperature**
- **Ms temperature**: Martensite start temperature
- **T-Zero temperature**

Graphical Mode Examples Guide

Thermo-Calc Version 2025b

Thermo-Calc Software

Thermo-Calc Examples Collection

These are the Graphical Mode examples. There are separate Console Mode examples also available.

In this section:

Graphical Mode Examples Listed by Product

This guide includes descriptions of the following examples.

? About the Examples

Category	*Example number*
The Thermo-Calc collection includes binary and ternary system examples, Scheil, the Equilibrium Calculator, Material to Material Calculator, plus more. Thermo-Calc Examples Collection	T_01 to T_20
General Property Models Library Thermo-Calc General Property Models Examples Collection	General Models: PM_G_01 to PM_G_17
Add-on Modules and Material Specific Property Model Libraries (in Alphabetical Order)	
Additive Manufacturing (AM) Module Examples Collection	AM_01 to AM_14
Diffusion Module (DICTRA) Examples Collection	D_01, D_02, D_03 (the Quick Start Guide Examples) D_04 to D_10
Nickel Model Library Examples Collection	Nickel Property Models: PM_NI_01 to PM_Ni_04
Noble Metal Alloys Model Library Examples Collection	Noble Metals Property Models: PM_Noble_01
Precipitation Module (TC-PRISMA) Examples Collection	P_01 to P_16
Process Metallurgy Module Examples Collection	PMET_01 to PMET_08
Steel Model Library Examples Collection	Steel Property Models: PM_Fe_01 to PM_Fe_12
Titanium Model Library Examples Collection	Titanium Property Models: PM_Ti_01 to PM_Ti_02

T_01: Calculating a Single-Point Equilibrium

This example shows the result from a single-point equilibrium calculation in the Fe-C system. It demonstrates the use of the Equilibrium Calculator and generates a Table Renderer in the **Visualizations** window. The number of equilibrium conditions is C+2 where C is the number of components, meaning that four conditions are needed in this example:

- **Temperature** is 1000 K
- **Pressure** is 100000 Pa
- **System size** is 1 mole
- **Mass percent carbon** is 0.1%

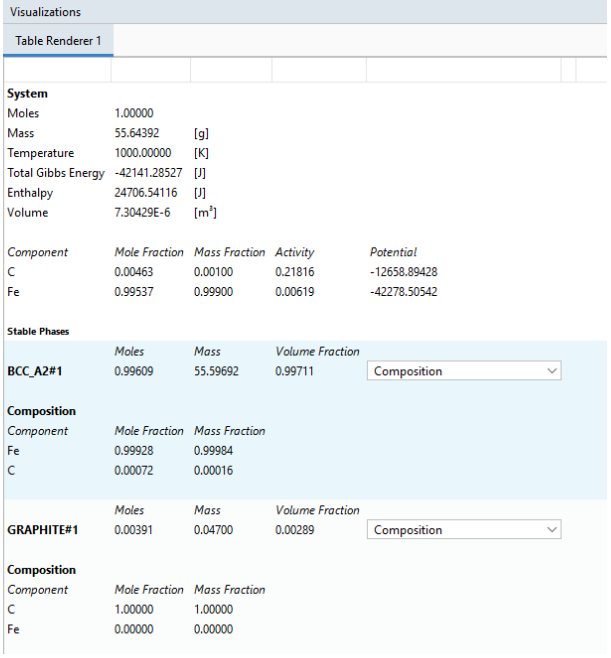
Project File Information

- Folder: **Thermo-Calc**
- File name: *T_01_Single-point_equilibrium.tcu*

Table Results

This example is included as a tutorial on our website and as part of the Graphical Mode Examples playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.



System				
Moles	1.00000			
Mass	55.64392	[g]		
Temperature	1000.00000	[K]		
Total Gibbs Energy	-42141.28527	[J]		
Enthalpy	24706.54116	[J]		
Volume	7.30429E-6	[m^3]		
Component	*Mole Fraction*	*Mass Fraction*	*Activity*	*Potential*
C	0.00463	0.00100	0.21816	-12658.89428
Fe	0.99537	0.99900	0.00619	-42278.50542
Stable Phases				
	Moles	*Mass*	*Volume Fraction*	
BCC_A2#1	0.99609	55.59692	0.99711	Composition
Composition				
Component	*Mole Fraction*	*Mass Fraction*		
Fe	0.99928	0.99984		
C	0.00072	0.00016		
	Moles	*Mass*	*Volume Fraction*	
GRAPHITE#1	0.00391	0.04700	0.00289	Composition
Composition				
Component	*Mole Fraction*	*Mass Fraction*		
C	1.00000	1.00000		
Fe	0.00000	0.00000		

Figure 1: The displayed results of the calculation show that the BCC_A2 (ferrite) and GRAPHITE phases are stable for this set of equilibrium conditions.

T_02: Stepping in Temperature in the Fe-C System

This example shows how the fractions of stable phases vary for an Fe-0.1 mass-% C alloy when the temperature is varied between 500 and 2000 K. It demonstrates the use of the Equilibrium Calculator. To allow temperature to vary, the corresponding **Axis Definition** checkbox is selected.

Project File Information

- Folder: **Thermo-Calc**
- File name: *T_02_Step_in_temperature_in_Fe-C.tcu*

Visualizations

This example is included as a tutorial on our website and as part of the Graphical Mode Examples playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

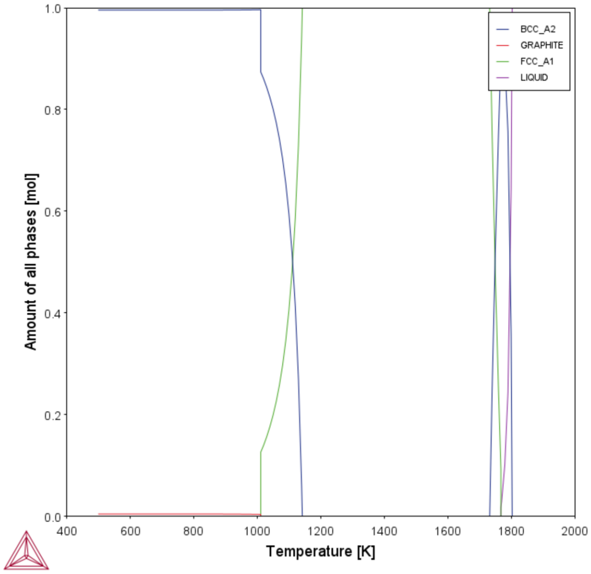
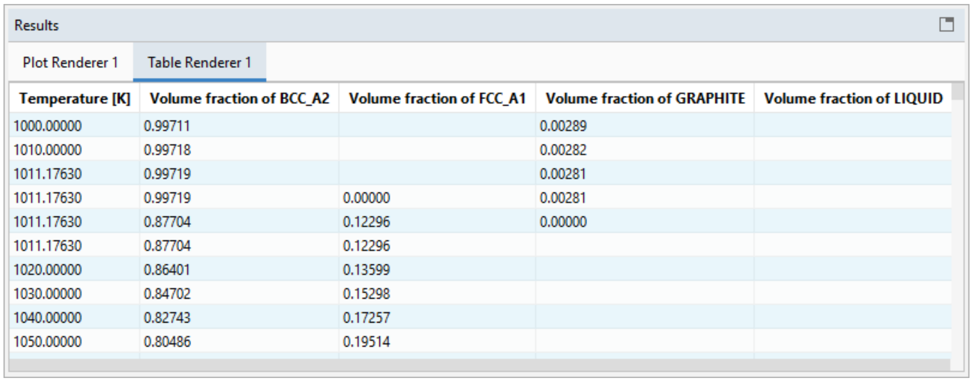


Figure 2: In this example, results are displayed graphically using a Plot Renderer activity.

For the Plot Renderer, there is an option to use the **Table View** button to convert plots to table data for all calculation types and calculators. See Plot Renderer: Convert a Plot to a Table and Export the Data.

If you want, you can also use a Table Renderer to generate text results instead, as shown in this example after adding a Table Renderer to the Equilibrium Calculator and clicking **Perform**.

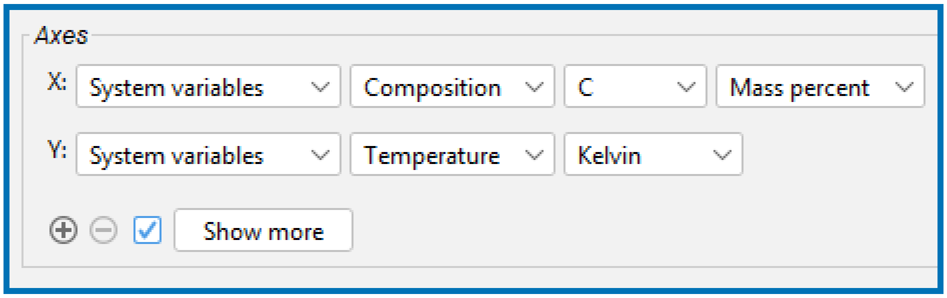


Temperature [K]	Volume fraction of BCC_A2	Volume fraction of FCC_A1	Volume fraction of GRAPHITE	Volume fraction of LIQUID
1000.00000	0.99711		0.00289	
1010.00000	0.99718		0.00282	
1011.17630	0.99719		0.00281	
1011.17630	0.99719	0.00000	0.00281	
1011.17630	0.87704	0.12296	0.00000	
1011.17630	0.87704	0.12296		
1020.00000	0.86401	0.13599		
1030.00000	0.84702	0.15298		
1040.00000	0.82743	0.17257		
1050.00000	0.80486	0.19514		

T_03: Fe-C Phase Diagrams

This example shows the stable Fe-C phase diagram (stable meaning that the graphite phase is entered in the calculation). The same diagram is calculated using the Binary Calculator activity and then using a System Definer and Equilibrium Calculator.

In both cases, a Plot Renderer is used to display results. The purpose of the **Binary Calculator** is to simplify common calculations for binary systems. In the **Equilibrium Calculator** two *Axes* are defined on the **Plot Renderer**. An axis variable must be an equilibrium condition.



Axes

X: System variables | Composition | C | Mass percent

Y: System variables | Temperature | Kelvin

In the **Plot Renderer** settings window, click **Show more** and **Show less** to toggle between viewing all or some of the available settings.

Project File Information

- Folder: **Thermo-Calc**
- File name: *T_03_Fe-C_phase_diagram.tcu*

Visualizations

This example is included as a tutorial on our website and as part of the Graphical Mode Examples playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

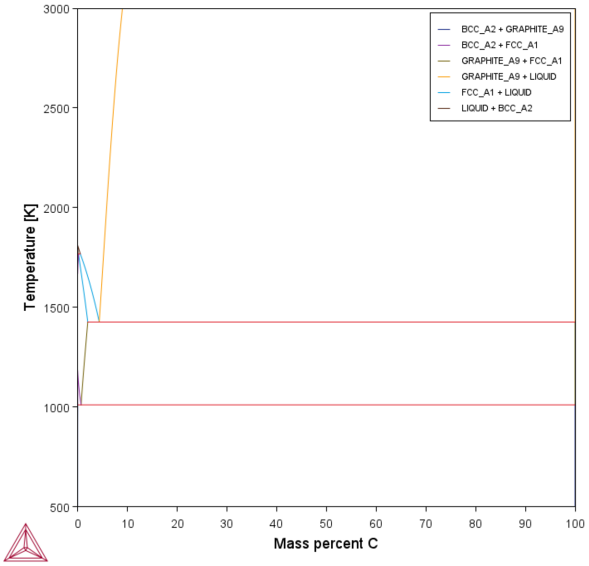


Figure 3: The plot result of the System Definer and Equilibrium Calculator.

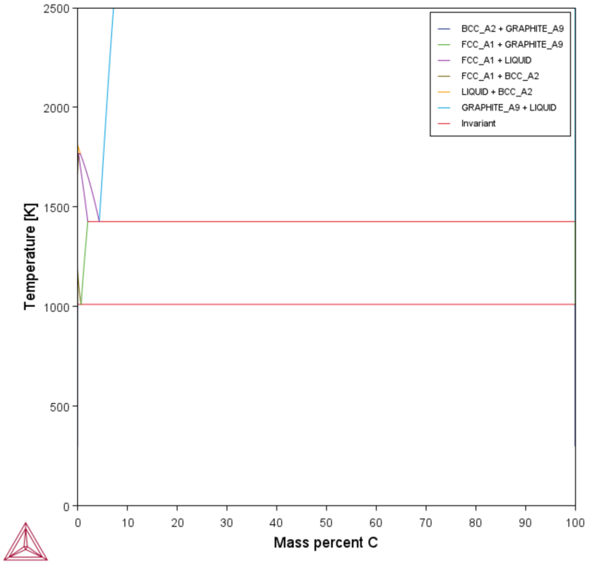


Figure 4: The plot result of the Binary Calculator simulation.

T_04: Fe-Cr-C Ternary Phase Diagram at 1000 K

This example shows a ternary phase diagram in the Fe-Cr-C system at 1000 K. Similar to example T_03: Fe-C Phase Diagrams, the same diagram is calculated using a Ternary Calculator and then using a System Definer and Equilibrium Calculator. Two Plot Renderer activities are added to create two plots.

Project File Information

- Folder: **Thermo-Calc**
- File name: *T_04_Fe-Cr-C_ternary_phase_diagram.tcu*

Visualizations

This example is included as a tutorial on our website and as part of the Graphical Mode Examples playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

In the **Plot Renderer** settings window, click **Show more** and **Show less** to toggle between viewing all or some of the available settings.

Try practicing with two features on the **Plot Renderer Configuration** window.

- To toggle between a triangular and a rectangular diagram, click the △ **Toggle Triangular/Regular Diagram** button then click **Perform** to see what happens.
- To toggle the X and Y axis variables, click the **Switch Axes** button and then click **Perform**.

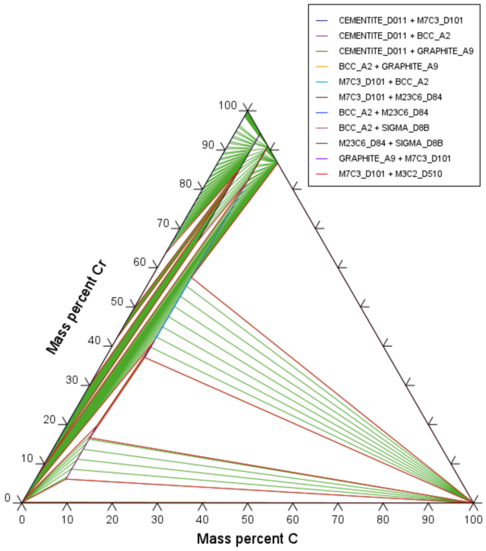


Figure 5: Ternary Calculator.

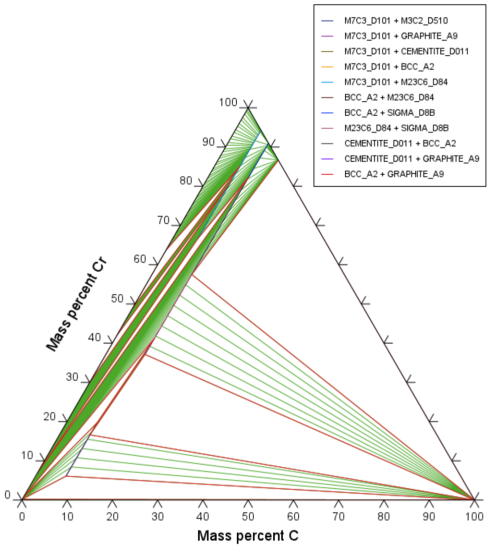


Figure 6: Equilibrium Calculator.

T_05: Stable and the Metastable Fe-C Phase Diagrams

This example shows how to overlay results from two calculations in the same plot using the Equilibrium Calculator.

Project File Information

- Folder: **Thermo-Calc**
- File name: *T_05_Fe-C_stable_and_metastable_phase_diagram.tcu*

Visualizations

This example is included as a tutorial on our website and as part of the Graphical Mode Examples playlist on our YouTube channel.

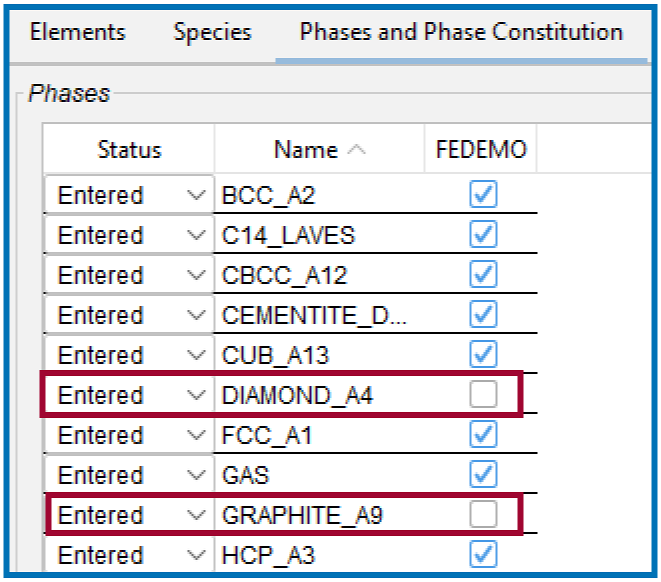
Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

Plotting Several Calculations in One Diagram

1. The Plot Renderer activity is first created as a successor to Equilibrium Calculator 1.
2. Then right-click the **Plot Renderer** node and select **Add predecessor** and the results from both equilibrium calculators are in the same plot. In **Equilibrium Calculator 1** the stable phase diagram is calculated and in **Equilibrium Calculator 2** the metastable phase.

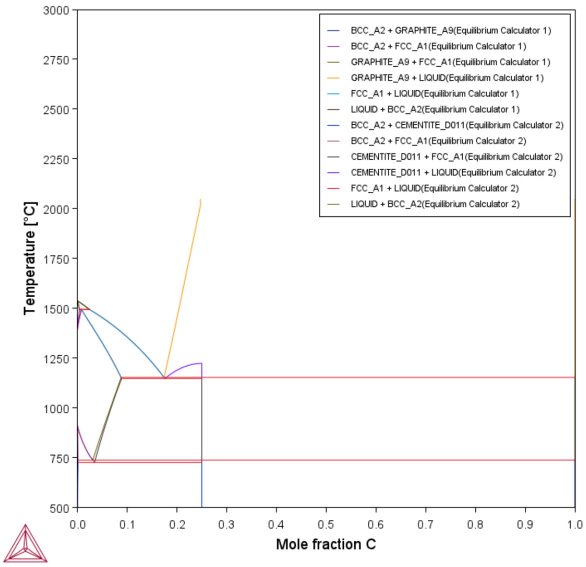
3. The metastable diagram is obtained by deselecting checkboxes for the GRAPHITE_A9 and DIAMOND_A4 phases on the **Metastable Phases** node (System Definer 2) → **Phases and Phase Constitution** tab.

To make it easier to work with your project, right-click any node and select **Rename**. In this example, System Definer 1 is renamed to **Stable System** and System Definer 2 is renamed to **Metastable System**.



Phases

Status	Name	FEDEMO
Entered	BCC_A2	☑
Entered	C14_LAVES	☑
Entered	CBCC_A12	☑
Entered	CEMENTITE_D...	☑
Entered	CUB_A13	☑
Entered	DIAMOND_A4	☐
Entered	FCC_A1	☑
Entered	GAS	☑
Entered	GRAPHITE_A9	☐
Entered	HCP_A3	☑



T_06: Serially Coupled Equilibrium Calculators

Sometimes there are multiple solutions for a given set of equilibrium conditions. In other cases the equilibrium calculation does not converge. You can then aid the final calculation by, in effect, telling the software where it should start the search for the equilibrium.

This example shows how to serially couple two Equilibrium Calculator nodes together for more complex equilibrium conditions. For each calculation, the output is to a Table Renderer.

Project File Information

- Folder: **Thermo-Calc**
- File name: *T_06_Serial_equilibrium_calculators.tcu*

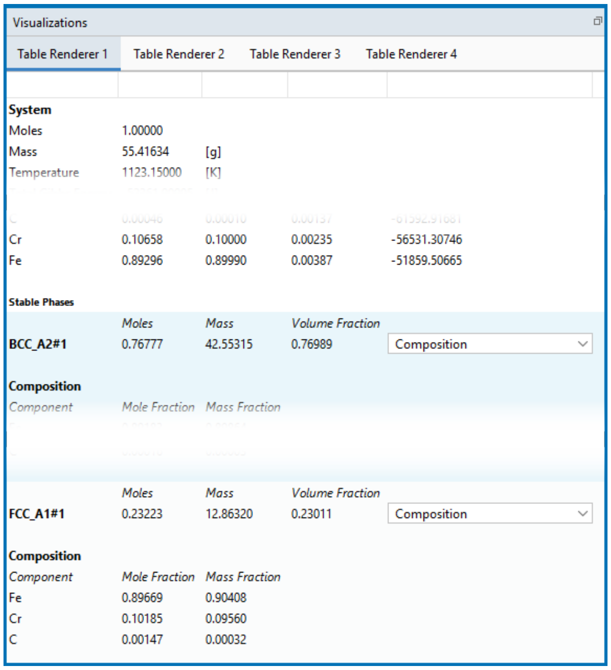
Table Renderer Results

This example is included as a tutorial on our website and as part of the Graphical Mode Examples playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

Equilibrium Calculator 1

In the first example, the objective is to calculate the equilibrium at 850° C where the mole fractions of the FCC A1 and BCC A2 phases are 0.5 each for an Fe-Cr-C steel with 10% chromium. In Equilibrium Calculator 1 a simple set of equilibrium conditions (temperature, pressure, system size and composition) are used to find a carbon content where only the FCC A1 and BCC A2 phases are stable. The results from this preliminary calculation are displayed in Table Renderer 1. Open the example to see the full table.



System				
Moles	1.00000			
Mass	55.41634	[g]		
Temperature	1123.15000	[K]		
C	0.00046	0.00010	0.00137	-61592.91681
Cr	0.10658	0.10000	0.00235	-56531.30746
Fe	0.89296	0.89990	0.00387	-51859.50665

Stable Phases

	Moles	*Mass*	*Volume Fraction*	
BCC_A2#1	0.76777	42.55315	0.76989	Composition

Composition

Component	*Mole Fraction*	*Mass Fraction*

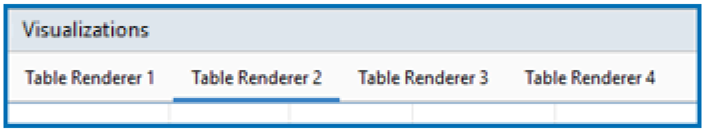
	Moles	*Mass*	*Volume Fraction*	
FCC_A1#1	0.23223	12.86320	0.23011	Composition

Composition

Component	*Mole Fraction*	*Mass Fraction*
Fe	0.89669	0.90408
Cr	0.10185	0.09560
C	0.00147	0.00032

Equilibrium Calculator 2, 3, and 4

Click each tab along the top of the **Visualizations** window to view the results associated to **Table Renderer 2**, **Table Renderer 2**, and **Table Renderer 2**.



- In Equilibrium Calculator 2 the carbon content equilibrium condition is replaced by the condition that the numbers of moles of the BCC A2 phase should be 0.5. The final result is displayed in Table Renderer 2. In this case, the final objective is to calculate the solidus temperature of an Fe-Cr-C steel with 10% Cr and 0.01% C.
- In Equilibrium Calculator 3 the state at 2000 K is calculated and the result is displayed in Table Renderer 3.
- In Equilibrium Calculator 4 the temperature equilibrium condition is replaced by the condition *Fix phase / liquid / 0.0*, meaning that liquid should be stable in an amount of zero moles, i.e. the solidus temperature. The final result is displayed in Table Renderer 4.

T_07: User-Defined Functions

This example shows how to implement user-defined functions. A series of equilibria for an Fe-Cr-C alloy are calculated by varying temperature between 500 and 3000 K. In the configuration window of the Equilibrium Calculator under the **Functions** tab, two identically meaning functions are defined, *fraction solid* and *f solid*, the values of which are plotted against temperature in two Plot Renderer activities. Functions can be entered in terms of *QuantitiesQ1*, *Q2*, *Q3* and so forth, or by using the Thermo-Calc syntax.

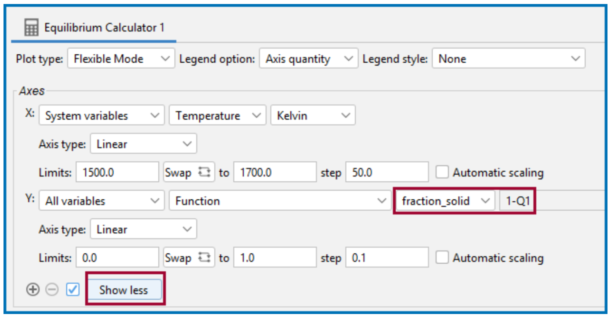
Project File Information

- Folder: **Thermo-Calc**
- File name: *T_07_User_defined_functions.tcu*

Visualizations

This example is included as a tutorial on our website and as part of the Graphical Mode Examples playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.



Equilibrium Calculator 1

Plot type: Flexible Mode Legend option: Axis quantity Legend style: None

Axes

X: System variables Temperature Kelvin

Axis type: Linear

Limits: 1500.0 Swap to 1700.0 step 50.0 ☐ Automatic scaling

Y: All variables Function fraction_solid 1-Q1

Axis type: Linear

Limits: 0.0 Swap to 1.0 step 0.1 ☐ Automatic scaling

☑ Show less

In the **Plot Renderer** settings window, click **Show more** and **Show less** to toggle between viewing all or some of the available settings.

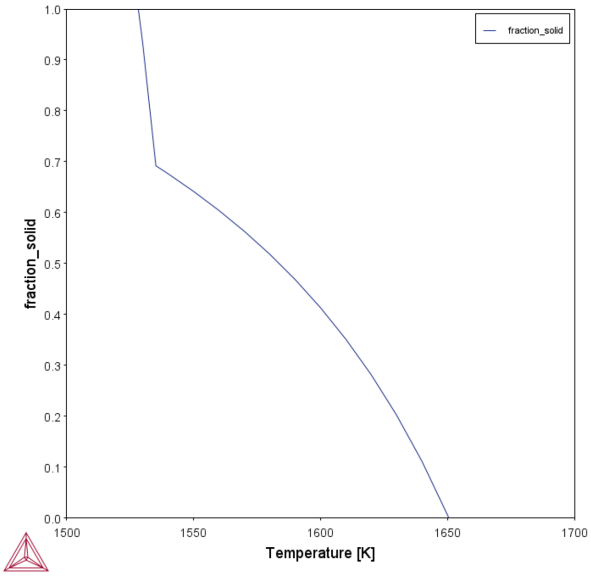


Figure 7: The result of the fraction_solid function.

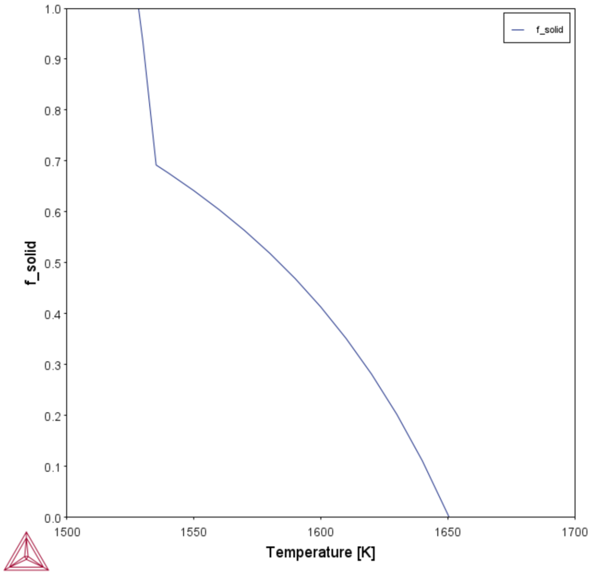


Figure 8: The result of the f_solid function.

T_08: Scheil and Equilibrium Solidification

This example shows a comparison for an Al-Si alloy solidified under full local equilibrium and under the Scheil assumptions, i.e. zero diffusion in the solidified material and infinitely fast diffusion in the liquid. The example uses the Scheil Calculator and adds a Plot Renderer and a Table Renderer.

Project File Information

- Folder: **Thermo-Calc**
- File name: *T_08_Scheil_and_equilibrium_solidification.tcu*

Visualizations

This example is included as a tutorial on our website and as part of the Scheil Solidification Simulations playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

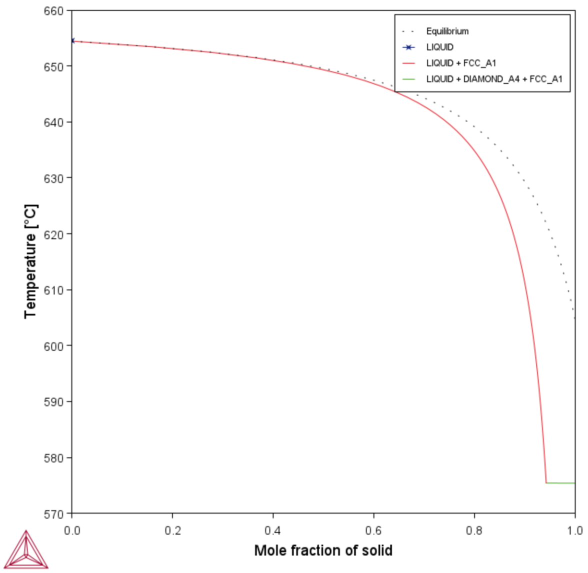
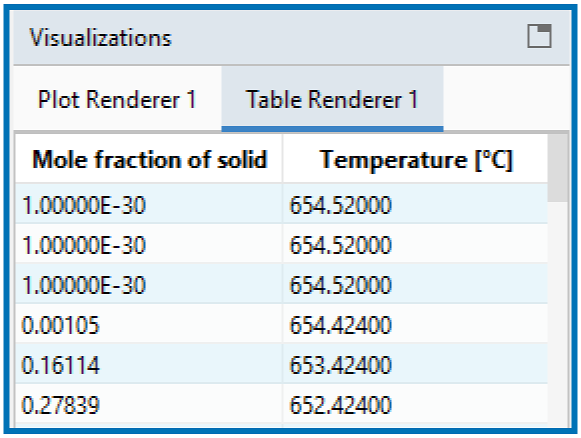


Figure 9: The plot compares the mole fraction of a solid vs temperature.



Mole fraction of solid	Temperature [°C]
1.00000E-30	654.52000
1.00000E-30	654.52000
1.00000E-30	654.52000
0.00105	654.42400
0.16114	653.42400
0.27839	652.42400

Figure 10: The table provides the data, which you can also export.

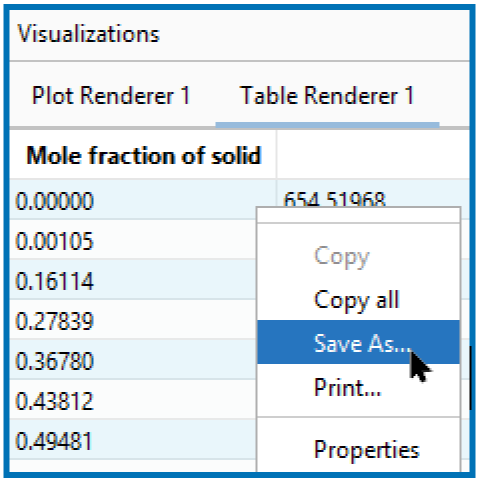
Saving the Table (via Table Renderer)

There are different ways to save the table from the Table Renderer **Visualizations** or **Configuration** windows.

For the Plot Renderer, there is an option to use the ▦ **Table View** button to convert plots to table data for all calculation types and calculators. See Plot Renderer: Convert a Plot to a Table and Export the Data.

Method 1

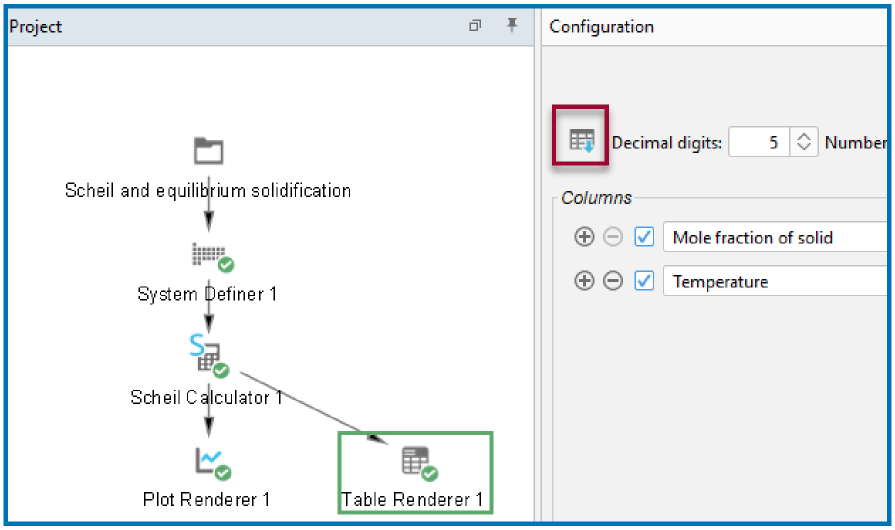
In the **Visualizations** window, right click the table and select **Save As...**



Mole fraction of solid	
0.00000	654.51968
0.00105	
0.16114	
0.27839	
0.36780	
0.43812	
0.49481	

Method 2

1. In the **Project** window, click the **Table Renderer**.
2. In the **Configuration** window, click the **Save table** button .



Decimal digits: 5 Number

Columns

☑ Mole fraction of solid

☑ Temperature

T_09: Carbide Driving Force Heat Map

This is an example of using **Grid** calculations to plot the driving force for a carbide as a function of two composition variables. With the **Grid** *Calculation Type*, a 2D grid is generated from the two calculation axes. After the calculation is done, an equilibrium is calculated in each grid point. A Plot Renderer connected to a grid calculation plots the *Z*-axis property for each equilibrium as a function of the two calculation axes. You can choose different *Plot types* such as **Heat map**, **Contour**, and **3D** to display the results.

In the **Plot Renderer** settings window, click **Show more** and **Show less** to toggle between viewing all or some of the available settings.

Project File Information

- Folder: **Thermo-Calc**
- File name: *T_09_Heat_map_of_carbide_driving_force.tcu*

Visualizations

This example is included as a tutorial on our website and as part of the Graphical Mode Examples playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

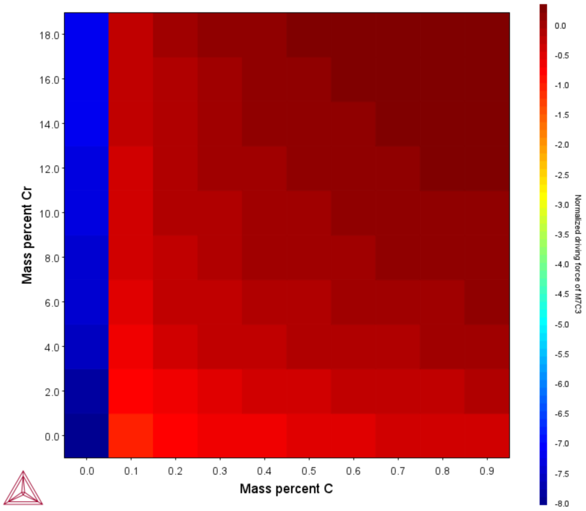


Figure 11: The results are plotted as a Heat map. Alternatively, a Contour Plot type can be selected on the Plot Renderer.

T_10: Scheil Solidification with Back Diffusion

This is an example of a Scheil solidification simulation of a Al-2.1Cu-1Si alloy including back diffusion in the primary phase.

The example uses two of the Scheil Calculator activity nodes with different cooling rates, 10 K/s and 0.005 K/s. The lower cooling rate produces a solidification curve that is closer to the equilibrium curve as shown in the plot result. Both a thermodynamic ALDEMO (aluminum demo) and mobility MALDEMO (Al-alloys mobility) database are used for this calculation.

See Scheil Calculator for an overview of the different Scheil simulation models available.

Project File and License Information

- Folder: **Thermo-Calc**
- File name: *T_10_Scheil_with_back_diffusion.tcu*

The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. this model requires the use of a mobility database.

Running the example itself does not require an additional license.

Visualizations

This example is included as a tutorial on our website and as part of the Scheil Solidification Simulations playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

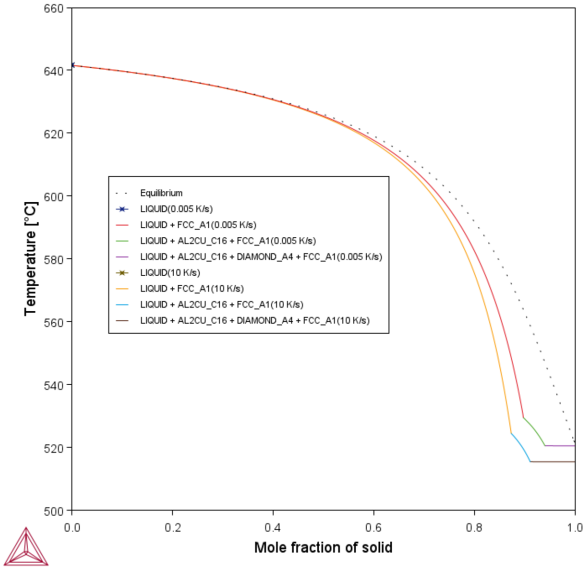


Figure 12: Scheil solidification. The lower cooling rate produces a solidification curve that is closer to the equilibrium curve .

T_11: Surface Tension in Cu-Zr

This is an example of including surface tension in the calculations.

Using the ALDEMO database, which is the free demonstration version of the TCS Al-based Alloy Database (TCAL), the surface tension of liquid metallic is plotted at 1373 K for Cu-Zr and compared to experimental data from [2005Kra].

Reference

[2005Kra] V. P. Krasovskyy, Y. V. Naidich, N. A. Krasovskaya, Surface tension and density of copper–Zirconium alloys in contact with fluoride refractories, J. Mater. Sci. 40, 2367–2369 (2005).

Project File Information

- Folder: **Thermo-Calc**
- File name: *T_11_Surface_tension_in_Cu-Zr.tcu*

The same example is also provided in Console Mode as `tcex56`.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

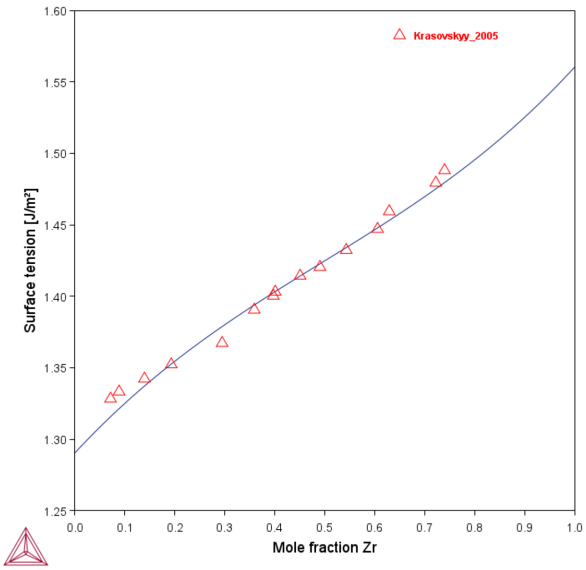


Figure 13: Surface tension of liquid metallic at 1373 K for Cu-Zr and compared to experimental data from [2005Kra].

More Information

The thermophysical properties are progressively being added to the Thermo-Calc databases starting with Thermo-Calc software version 2020a.

You can learn more about the models by searching the help (press F1 when in Thermo-Calc).

You can find information on our website about the properties that can be calculated with Thermo-Calc and the Add-on Modules.

T_12: Viscosity in Cr-Ni

This is an example of including viscosity in the calculations.

Using the FEDEMO database, which is the free demonstration version of the TCS Steel and Fe-alloys Database (TCFE), the viscosity of metallic liquids is plotted at 1873 K for Cu-Ni and compared to experimental data from [2005Sat].

Reference

[2005Sat] Y. Sato, K. Sugisawa, D. Aoki, T. Yamamura, Viscosities of Fe–Ni, Fe–Co and Ni–Co binary melts, Meas. Sci. Technol. 16, 363–371 (2005).

Project File Information

- Folder: **Thermo-Calc**
- File name: *T_12_Viscosity_in_Cr-Ni.tcu*

The same example is also provided in Console Mode as `tcex55`.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

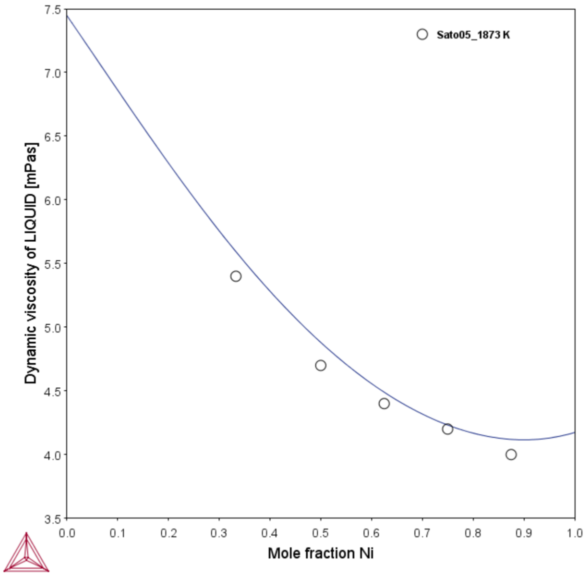


Figure 14: The viscosity of metallic liquids at 1873 K for Cu-Ni and compared to experimental data from [2005Sat].

More Information

The thermophysical properties are progressively being added to the Thermo-Calc databases starting with Thermo-Calc software version 2020a.

You can learn more about the models by searching the help (press F1 when in Thermo-Calc).

You can find information on our website about the properties that can be calculated with Thermo-Calc and the Add-on Modules.

T_13: Scheil Solidification with Solute Trapping

In Graphical Mode, you use the **Scheil Calculator** to set up the various Scheil solidification simulations outlined in more detail in Scheil-Gulliver Solidification Calculations.

For background theory see About Scheil with Solute Trapping.

This example shows the use of the *Scheil with solute trapping* option with an Al-7.5Si-0.2Cu alloy as compared to a Classic Scheil calculation. The thermodynamic ALDEMO (Aluminum demo) database, available to all users, is selected for this calculation to simulate the effect of solute trapping in the primary phase. This type of simulation is useful for additive manufacturing applications.

This example shows how the alloy starts to solidify at a lower temperature compared to a classic Scheil simulation, an effect which increases with increasing solidification speed. The solidification speed is calculated from user supplied scanning speed and angle between the solid/liquid interface and the scanning direction.

The example uses the **Aziz** model, with an **Interface driving force** of **Migration energy** and a **Maximum velocity for infinite driving force** of 2000 m/s.

Read more about Scheil Solidification Simulations on our website, including how to select the right model for your simulation. If you are in Thermo-Calc, press F1 to search the help to learn about using Scheil.

Project File Information

- Folder: **Thermo-Calc**
- File name: *T_13_Scheil_with_Solute_Trapping.tcu*

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

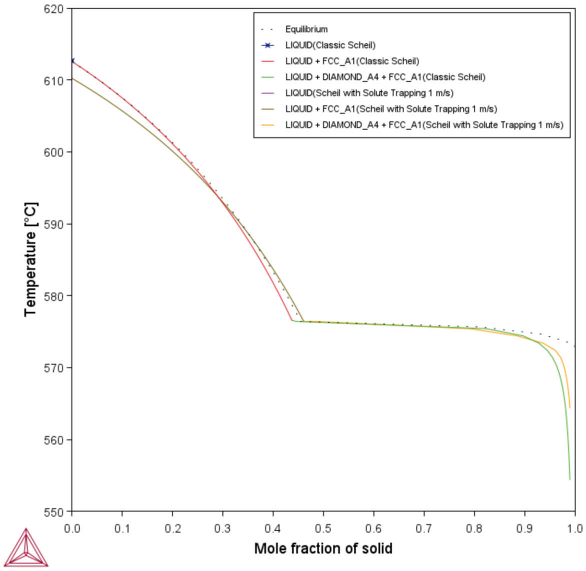


Figure 15: The effect of Scheil solidification with solute trapping of a Al-7.5Si-0.2Cu alloy compared to equilibrium and a Classic Scheil calculation.

T_14: Fe-Cr-Ni Transition Comparison Using the Material to Material Calculator

In Graphical Mode, you use the **Material to Material Calculator** to perform calculations and examine how two materials transition from one into the other. The calculations in this example search for potential deleterious phases during heat treatment of alloys joined together. In this example, the calculation steps between a model martensitic stainless steel (Fe-17Cr-2Ni) and a model Alloy 800 composition (Fe-35Ni-19Cr). Neither alloy is predicted to form the deleterious sigma phase at 600 °C. However sigma is predicted to form at a wide range of mixtures of these two materials, which could have an impact on mechanical properties if it forms.

The example, as defined when you open it, uses a **One Axis** calculation (also known as a property diagram), a temperature of 650 °C, to compare the volume fraction of all phases to the mass fraction of Alloy 800. The **Fraction of the second material** (Alloy 800) is set to 50% (0.5), which for a **One Axis** calculation is used as the start value.

> As with all the examples, you can adjust the settings to plot a variety of combinations of output to see how the Material to Material Calculator works before defining your own project.

The plot for this calculation compares the volume fraction of all phases of Material 1 (martensitic stainless steel) to the mass fraction of Material 2 (Alloy 800). In the plots you can see where each phase (FCC_A1, SIGMA_D8B, and BCC_A2) evolves. As you step from Material 1 to Material 2, the FCC_A1 phase starts forming at about 5% (0.05), SIGMA-D8B phase starts to evolve at about 19% (0.19), and the BCC_A2 transitions from Material 1 to Material 2 where it stops forming at approximately 24% (0.24). The purpose of the calculation is to determine at what fraction of Alloy 800 the deleterious sigma phase forms and this is shown for these compositions.

Project File Information

- Folder: **Thermo-Calc**
- File name: *T_14_Fe-Cr-Ni_Material_to_Material.tcu*

Visualizations

This example is included as a tutorial on our website and as part of the Graphical Mode Examples playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

In the **Plot Renderer** settings window, click **Show more** and **Show less** to toggle between viewing all or some of the available settings.

The default plot shows the volume fraction of all phases as a function of the mass fraction of the second material, which in this case, is Alloy 800. You can see that the martensitic stainless composition is BCC at this temperature, and the highly alloyed stainless is FCC. Neither material is expected to form any deleterious phase on its own at 650 °C.

However, mixtures of these two materials, which could arise from a graded transition joint, weld, or potentially a diffusion couple, show some stability for the deleterious sigma phase at this temperature. You can try to make small adjustments to the initial chemistry to reduce the potential for sigma phase to form.

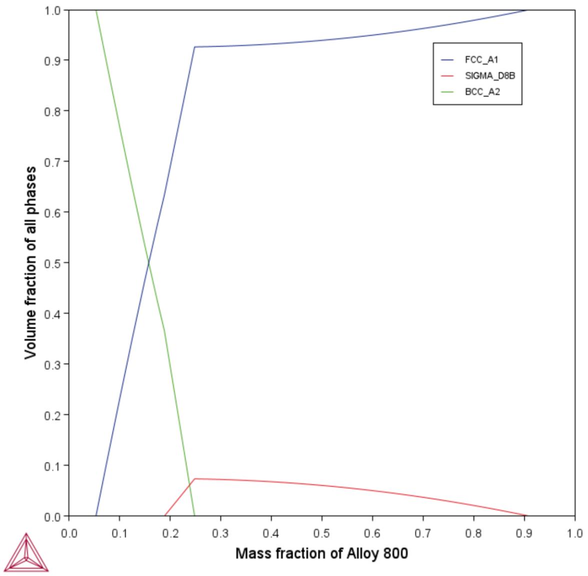


Figure 16: This plot shows the volume fraction of phases when changing composition from the Martensitic Steel (First material) to the Alloy 800 (Second material). This calculation uses the Material to Material Calculator to examine the transition of phases for two compositions of Fe-Cr-Ni. The purpose is to determine at what fraction of Alloy 800 does the deleterious sigma phase start to form. See the text for details.

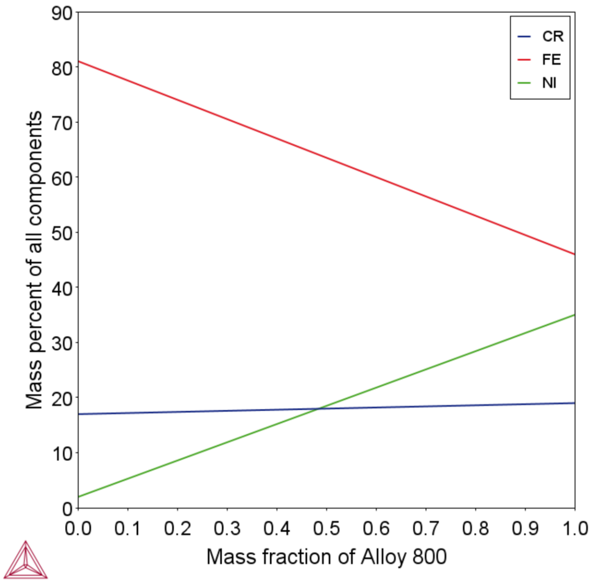


Figure 17: The composition varies linearly when the composition is changed from the Martensitic steel to the Alloy 800 using the Material to Material Calculator. See the text for details.

T_15: Molar Volume and Thermal Expansion Coefficients for L12-type Al3Sc and Al3Zr Compounds

This example calculates volumetric thermal expansion coefficients of the L12-type Al3Sc and the L12-type Al3Zr, respectively. Both Al3Zr and Al3Sc are modeled as the same phase (named as AL3SC, since Al3Sc is stable while Al3Zr is metastable).

The example uses two System Definers and Equilibrium Calculators to plot and compare the molar volume and thermal expansion coefficients of the Al3Sc and Al3Zr binary compounds. It uses the ALDEMO database, which is the free demonstration version of the TCS Al-based Alloy Database (TCAL) and an Experimental File Reader node to read the data from [2015Sah].

Project File Information

- Folder: **Thermo-Calc**
- File name: *T_15_Molar_Volume_and_Thermal_Expansion_Coefficient.tcu*

The example includes an experimental data (*.exp) file called `Al3X.exp`.

The same example is also provided in Console Mode as two separate examples: `tcex58` and `tcex59`.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

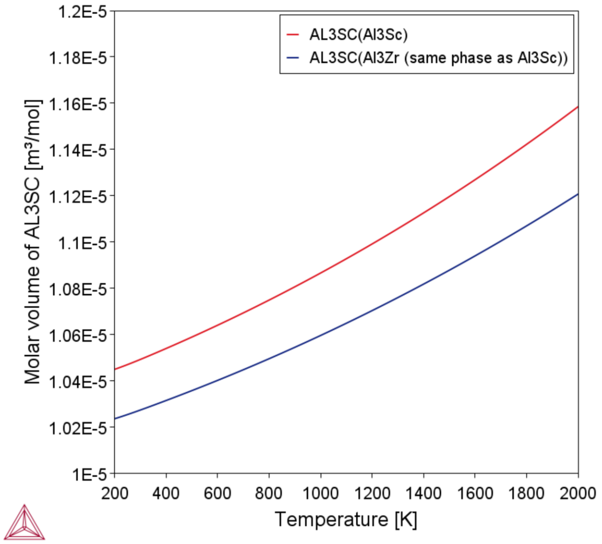


Figure 18: Compares the molar volume of both Al3Zr and Al3Sc, which are modeled as the same phase (named as AL3SC, since Al3Sc is stable while Al3Zr is metastable).

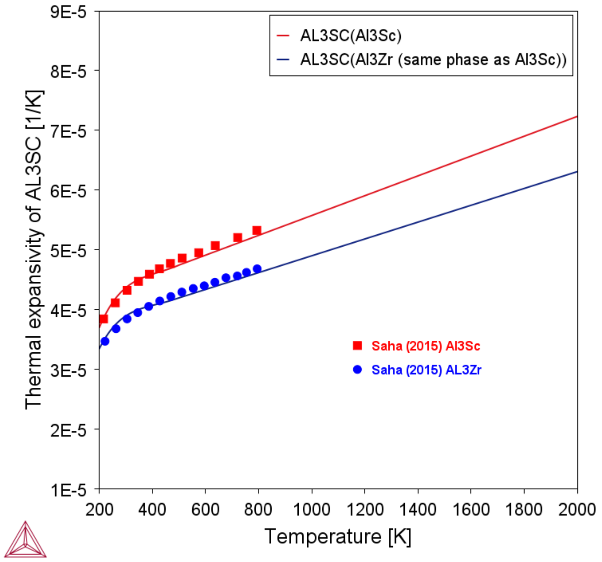


Figure 19: Compares volumetric thermal expansion coefficients of the L12-type Al3Sc and the L12-type Al3Zr using theoretical data with quasiharmonic approximation from [2015Sah].

Reference

[2015Sah] S. Saha, T. Z. Todorova, J. W. Zwanziger, Temperature dependent lattice misfit and coherency of Al3X (X=Sc, Zr, Ti and Nb) particles in an Al matrix. Acta Mater. 89, 109–115 (2015).

More Information

The thermophysical properties are progressively being added to the Thermo-Calc databases starting with Thermo-Calc software version 2020a.

You can learn more about the models by searching the help (press F1 when in Thermo-Calc).

You can find information on our website about the properties that can be calculated with Thermo-Calc and the Add-on Modules.

T_16: Electrical Resistivity and Thermal Conductivity for Pure Copper

This example calculates the electrical resistivity (ELRS) and thermal conductivity (THCD) of pure Cu. It makes a *One Axis* (step) calculation over a wide temperature range, covering both the FCC_A1 state and the liquid state. It plots thermal conductivity of the system (both FCC_A1 and liquid) and that of a single phase (taking FCC_A1 as an example), respectively. Also it plots electrical resistivity of the system and that of FCC_A1.

The example set up uses an Equilibrium Calculator combined with four Experimental File Reader nodes that take data from the included 1972Ho_cu_thcd.exp and 1981Ho_cu_elrs.exp files.

The example is available to all users as it uses the ALDEMO database, which is the free demonstration version of the TCS Al-based Alloy Database (TCAL).

Project File Information

- Folder: **Thermo-Calc**
- File name: *T_16_Electrical_Resistivity_Thermal_Conductivity_Cu.tcu*
- Experimental data files included `1972Ho_cu_thcd.exp` and `1981Ho_cu_elrs.exp`

The same example is also provided in Console Mode as `tcex60`.

Visualizations

This example is included as a tutorial on our website and as part of the Graphical Mode Examples playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

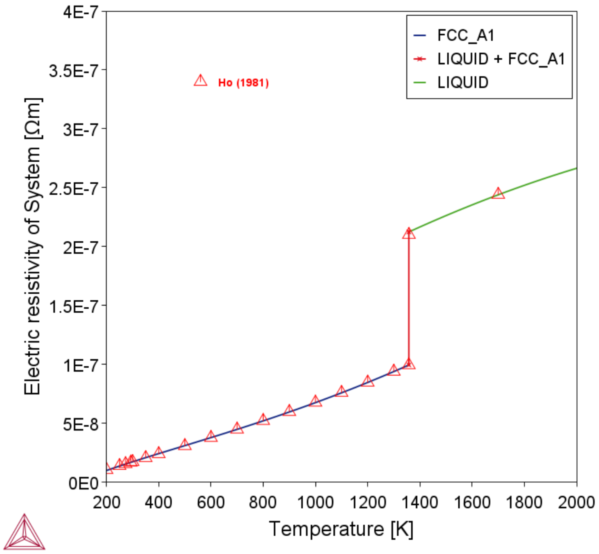


Figure 20: The electrical resistivity (ELRS) of pure Cu over a wide temperature range, covering both the FCC_A1 state and the liquid state. The data was recommended by [1981Ho].

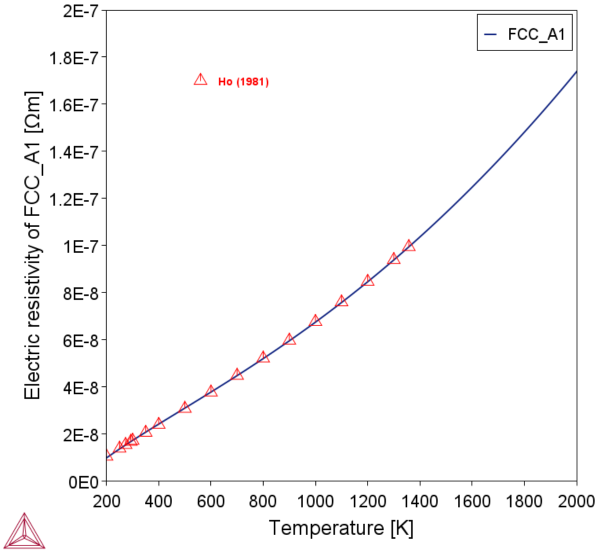


Figure 21: The electrical resistivity (ELRS) of a single phase (FCC_A1) vs. temperature. The data was recommended by [1981Ho].

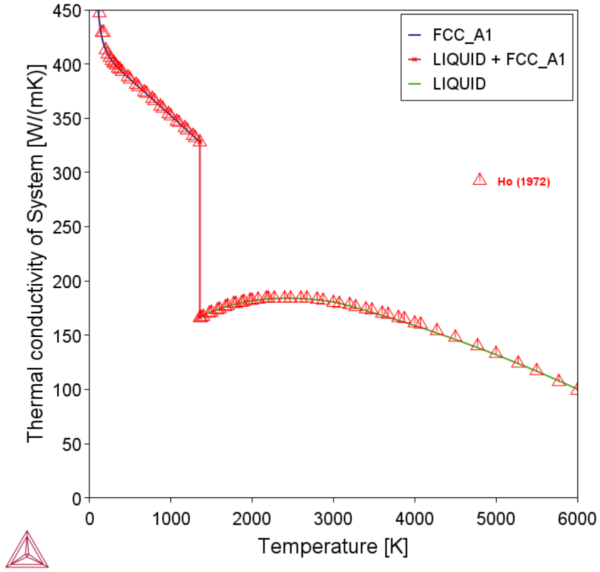


Figure 22: The thermal conductivity of pure Cu over a wide temperature range, covering both the FCC_A1 state and the liquid state. The data was recommended by [1972Ho].

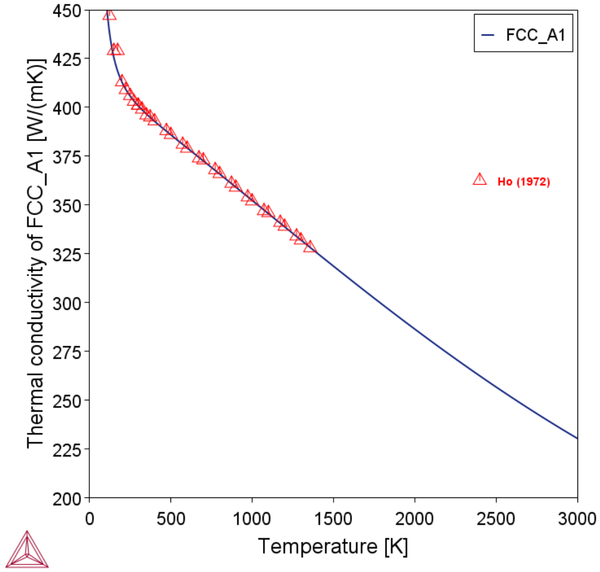


Figure 23: The thermal conductivity (THCD) of a single phase (FCC_A1) vs. temperature. The data was recommended by [1972Ho].

References

[1972Ho] C. Y. Ho, R. W. Powell, P. E. Liley, Thermal Conductivity of the Elements. J. Phys. Chem. Ref. Data. 1, 279–421 (1972).

[1981Ho] C. Y. Ho, M. W. Ackerman, K. Y. Wu, T. N. Havill, R. H. Bogaard, R. A. Matula, S. G. Oh, and H. M. James. Electrical resistivity of ten selected binary alloy systems. CINDAS report 59, for Office of standard reference data National Bureau of Standards, Department of Commerce (1981).

More Information

For more advanced examples using the TCAL database, see PM_G_10: Freeze-in Thermal Conductivity and PM_G_11: Freeze-in Electrical Resistivity.

The thermophysical properties are progressively being added to the Thermo-Calc databases starting with Thermo-Calc software version 2020a.

You can learn more about the models by searching the help (press F1 when in Thermo-Calc).

You can find information on our website about the properties that can be calculated with Thermo-Calc and the Add-on Modules.

T_17: Al_2O_3-MgO Phase Diagram

Al_2O_3-MgO is one of the basic systems to understand metallurgical slags and refractories. This example uses an Equilibrium Calculator to calculate a phase diagram of the pseudo-binary system Al_2O_3-MgO. It also demonstrates how to change components in the System Definer. In this case, the components AL_2O_3 and MgO are defined instead of the elements Al, Mg, and O.

In the **Plot Renderer** settings window, click **Show more** and **Show less** to toggle between viewing all or some of the available settings.

Project File and License Information

- Folder: **Thermo-Calc**
- File name: *T_17_Al2O3-MgO_phase_diagram.tcu*

The TCS Metal Oxide Solutions Database (TCOX) is used in this example. A valid license for version 11 (TCOX11) or newer is required to run the example.

Visualizations

This example is included as a tutorial on our website and as part of the Graphical Mode Examples playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

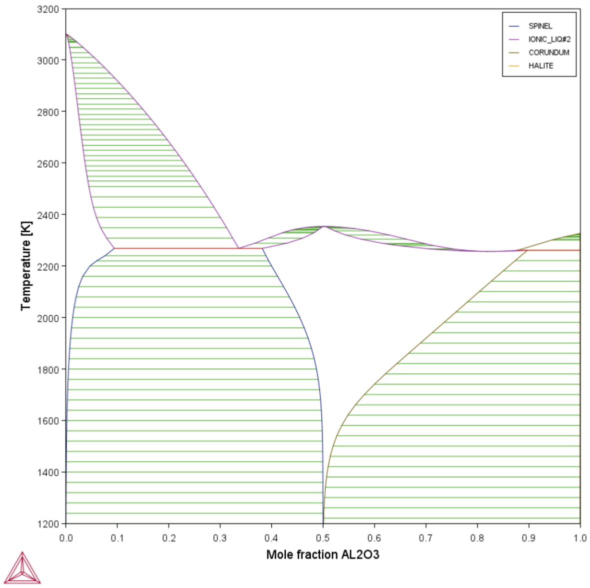


Figure 24: Phase diagram of the pseudo-binary system Al_2O_3*-MgO.*

More Information

This example is also included in the *TCS Metal Oxide Solutions Database (TCOX) Validation and Calculation Examples Collection*.

There is a similar example provided in Console Mode that uses the OXDEMO database, which is available to all users. See `tcex17`.

Go to the Metal Slag and Oxides Database page on our website where you can access a Validation and Calculation Examples Collection and the Technical Information plus learn about its many applications with the Process Metallurgy Module. Also explore further applications of Thermo-Calc to Refractory Oxides and Slags including links to resources such as examples, publications, and more.

T_18: Scheil with Delta Ferrite to Austenite Transition

This is a example of a Scheil solidification simulation using an Fe-0.23C-0.19Si-0.47Mn-0.92Cr-0.09Ni-0.3Mo (wt%) alloy (Steel P) [2015Sch], which is a steel that undergoes the peritectic transformation.

The result of a Scheil Calculator with the default **Classic Scheil** calculation type is compared to a the result of a calculator where the setting **Allow delta ferrite to austenite transition in steel** is selected. Carbon (C) is set as a **Fast diffuser** in both. A comparison to experimental solidus temperature from Schaffnit et al. [2015Sch] shows that for this steel, using the **Allow delta ferrite to austenite transition in steel** option gives a much better agreement with experiment than the standard **Classic Scheil**.

See Scheil Calculator for an overview of the different Scheil simulation models available.

Project File and License Information

- Folder: **Thermo-Calc**
- File name: *T_18_Scheil_with_Delta_Ferrite_to_Austenite_Transition.tcu*

This uses the TCFE database. A license is required to run the example.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

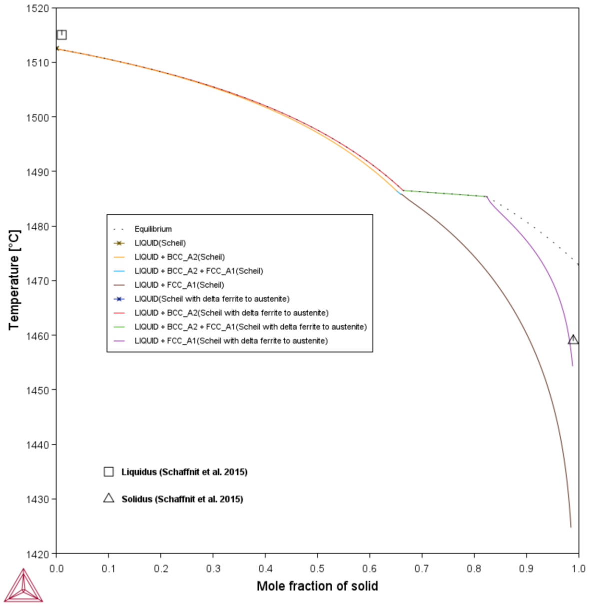


Figure 25: Mole fraction of solid as a function of temperature comparing the liquidus and solidus from experimental data [2015Sch].

Reference

[2015Sch] P. Schaffnit, C. Stallybrass, J. Konrad, F. Stein, M. Weinberg, A Scheil–Gulliver model dedicated to the solidification of steel. Calphad. 48, 184–188 (2015).

T_19: Young's Modulus for Ti-O with Elastic Properties

This is an example which shows the effect of oxygen concentration at three temperatures on an elastic property, Young's modulus, for the HCP_A3 phase in a Ti-O system.

It is well established in the literature that mechanical properties of titanium and its related alloys are sensitive to the presence of even dilute concentrations of interstitial solutes such as carbon, hydrogen, nitrogen and oxygen. It is therefore important to adequately model the effects of impurities in the host lattice when calculating mechanical properties, such as the elastic constants and the corresponding moduli determined from these constants.

> Only the elastic constants are assessed, and then used to derive the elastic moduli, meaning the experimental data in the plot are completely standalone from the assessment process.

In this example, three **Equilibrium Calculators** are used with **One Axis** calculations at different temperatures (298 K, 533 K, and 672 K) to show the Young's modulus of an HCP_A3 phase as a function of mole percent of O and compared to experimental data from [1957Gra; 1966Fed; 1971Hsu].

Project File and License Information

- Folder: **Thermo-Calc**
- File name: *T_19_Elastic_Properties_YoungsModulus_Ti-O.tcu*

> The TCS Ti/TiAl-based Alloys Database (TCTI) is used in this example. A valid license is required to run the example.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

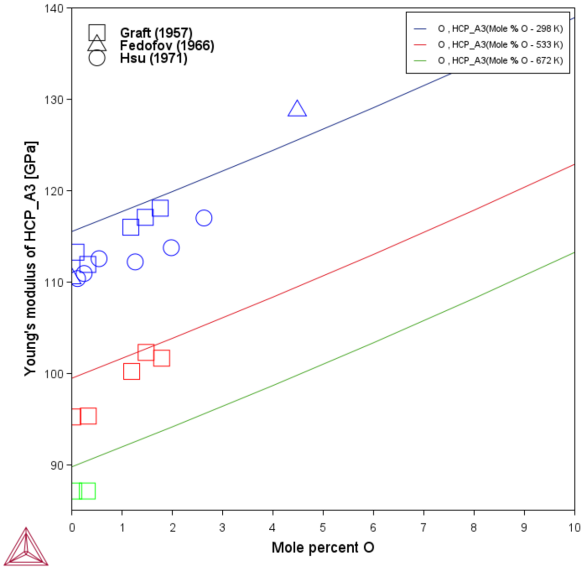


Figure 26: Effect of oxygen on Young's modulus in HCP_A3 titanium compared to experimental data [1957Gra; 1966Fed; 1971Hsu].

References

[1957Gra] W. H. Graft, D. W. Levinson and W. Rostoker, The influence of alloying on the elastic modulus of titanium alloys, Trans. Am. Soc. Met. 49, 263-279 (1957).

[1966Fed] S. G. Fedofov, Titanium and Its Alloys, Publ. No. lO, I. I. Kornilov Editor, Israel Prog. Sci. Trans., 199 (1966).

[1971Hsu] N. Hsu, H. Conrad, Ultrasonic wave velocity measurements on titanium-oxygen alloys. Scr. Metall. 5, 905–908 (1971).

More Information

As of Thermo-Calc version 2025b, elastic properties are available with Thermo-Calc and the TCS Ti/TiAl-based Alloys Database (TCTI) (TCTI6 and newer), TCS Steel and Fe-alloys Database (TCFE) (TCFE14 and newer), TCS High Entropy Alloys Database (TCHEA) (TCHEA8 and newer), and TCS Ni-based Superalloys Database (TCNI) (TCNI13 and newer). These elastic properties will be added to additional databases over time. Subscribe to our newsletter to be kept up-to-date on the latest product releases, webinars, user group meetings, applications examples, and more.

For more information about the theory about the elastic properties, which includes constants and moduli, see About the Elastic Properties.

T_20: Ternary Diagram with Clockwise Plot Axes

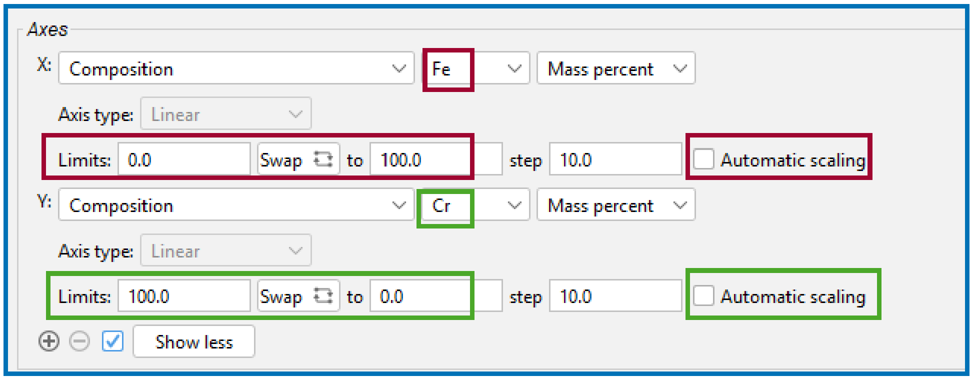
This **Ternary Calculator** example for a Cr-Fe-Ni system shows how to use different plot axis combinations on the **Plot Renderer** representing clockwise and counterclockwise axes. This example uses the FEDEMO database and is available to all users.

A ternary phase diagram is fully defined by the elements in the corners of the diagram. See Figure 27 for the Cr-Fe-Ni 1000 K isothermal section when plotted as a ternary diagram. To plot this diagram in Thermo-Calc you define the X- and Y-axes instead of the corner elements.

Define the X- and Y- Plot Axes

The same diagram can therefore be defined with different combinations of the plot axes. In this example, there is Cr in the bottom left corner and Fe in the lower right corner. Then you can define the X-axis by **Fe** *increasing* from `0` to `100` (these numbers are entered in the **Limits** fields). It is also possible to define the X-axis by *decreasing* **Cr** from `100` to `0`. The main reason for defining a decreasing plot axis in Thermo-Calc is when comparing with experimental diagrams that can be visualized in this way.

To define a decreasing plot axis, on the **Plot Renderer**, click to deselect the **Automatic scaling** checkbox. Then either change the limits as described above by entering `100.0` and `0.0` in the fields, or click the **Swap** button to swap the lower (0.0) and upper (100.0) limits.



Axes

X: Composition, Fe, Mass percent

Axis type: Linear

Limits: 0.0 to 100.0, step 10.0, ☐ Automatic scaling

Y: Composition, Cr, Mass percent

Axis type: Linear

Limits: 100.0 to 0.0, step 10.0, ☐ Automatic scaling

The **Flexible Mode** plot type is used in this example as it allows you to individually work with the axes.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

Project File Information

- Folder: **Thermo-Calc**
- File name: *T_20_Ternary_Cr-Fe-Ni_Clockwise_Axes.tcu*

In the installed example the Plot Renderer node is renamed to **Counterclockwise x:+Fe y:-Cr**. As above, the settings are completed on the **Configuration** window to plot the **Composition** of **Fe** on the X-axis and **Cr** decreasing on the Y-axis. Click **Perform** to display the result of Figure 27.

You can continue on the Plot Renderer to plot different combinations of axes variables in order to represent clockwise and counterclockwise plot axes.

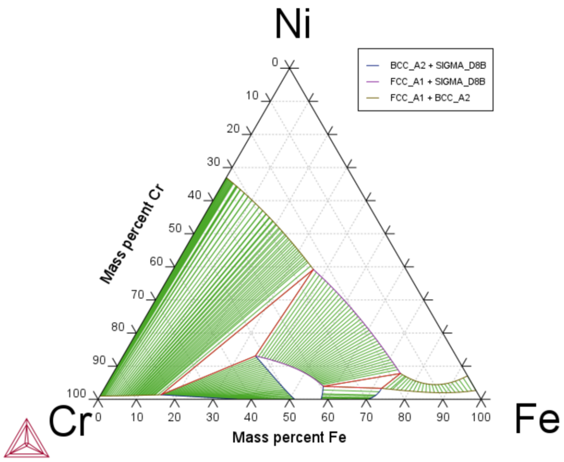


Figure 27: Counterclockwise x:+Fe y:-Cr. Increasing Mass percent Fe (X-axis). Decreasing Mass percent Cr (Y-axis).

Then for the other plot examples, the settings on each **Plot Renderer Configuration** window (for renamed nodes **Clockwise x:-Cr y:+Ni** and **Counterclockwise x:+Fe y:+Ni**) are also changed to show the different combinations of plot axes.

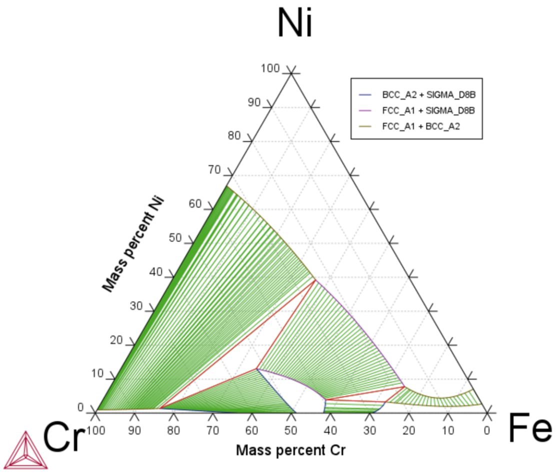


Figure 28: Clockwise x:-Cr y:+Ni: Decreasing Mass percent Cr (X-axis). Increasing Mass percent Ni (Y-axis).

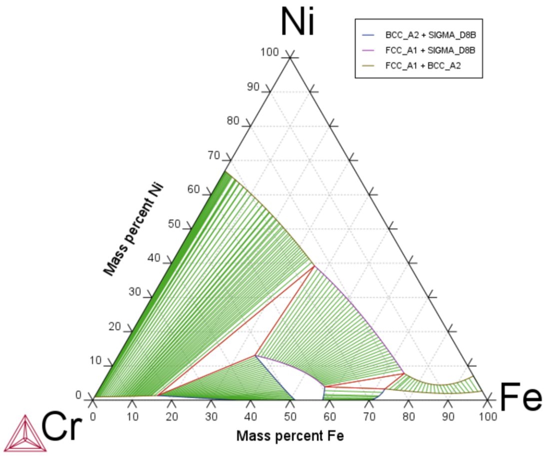


Figure 29: Counterclockwise x:+Fe y:+Ni: Increasing Mass percent Fe (X-axis). Increasing Mass percent Ni (Y-axis).

Thermo-Calc General Property Models Examples Collection

The **General Models** are available to all users.

> To run calculations with the Add-on Property Model Libraries all require a valid maintenance license plus a license for the specific database version: **Nickel Models** (TCNI11 and newer and MOBNI5 and newer; **Noble Metal Alloys Models** (TCNOBL3 and newer); **Steel Models** (TCFE9 and newer + MOBFE4 and newer); **Titanium Models** (TCTI6 and newer).

These examples use the **Property Model Calculator**, an activity available with Thermo-Calc.

About the Examples

In this section:

PM_G_01: Phase Transition

The example uses the **Property Model Calculator** to predict the transition temperature to the unwanted brittle sigma phase. The example shows how the temperature is influenced by changes to a steel alloy's composition using the **Uncertainty** *Calculation Type* and then you can choose to use either a **Histogram** (frequency diagram) or **Probability** plot after choosing the **Statistical** *Plot type* on the **Plot Renderer**.

Phase Transition Property Model Settings

Project File Information

- Folder: **Property Models → General**
- File name: *PM_G_01_Phase_Transition.tcu*

Visualizations

This example is included as a Property Model tutorial on our website and as part of the Property Model Calculator playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

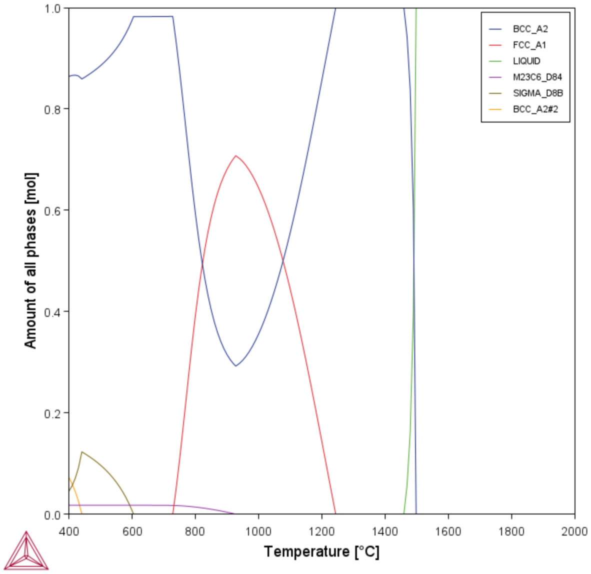


Figure 30: A property diagram as a result of using the Equilibrium Calculator with a One Axis calculation to determine a good starting temperature of the SIGMA phase.

Once you set up the Property Model Calculator, but before running a **Grid** calculation, it is recommended you run a **Single** calculation to make sure the calculation is valid.

- If the subprocess worked, it displays in the **Event Log**. The **Event Log** also has the result `Relaxed condition`, referring to the variable, which in this case is temperature.
- If the calculation did not work, `NaN` (not a number) displays instead. Check your configuration set up and run the calculation again before moving on to the more complicated calculation.

About the Uncertainty Calculations

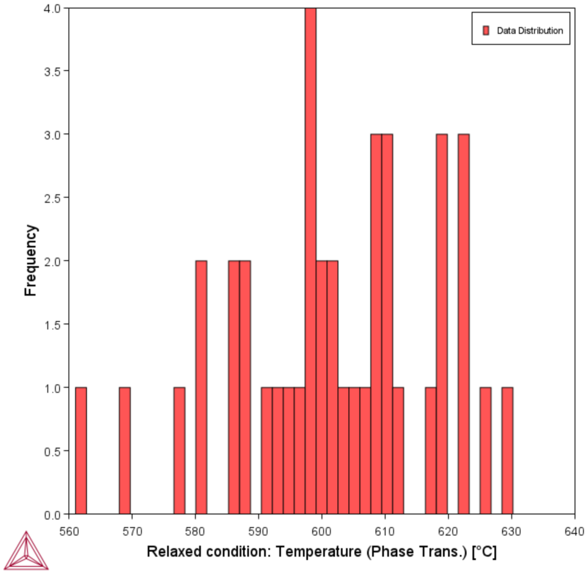


Figure 31: Using the Property Model Calculator with the Phase Transition Model to plot a histogram showing how the transition temperature of sigma varies when you vary the composition. The plot changes each time you run the calculation because it is taking a random sampling from the composition range set.

The X-axis is labeled the **Relaxed Condition: Temperature (Phase Trans.)**, which you can see on the **Plot Renderer 1 Configuration** window. The Y-axis shows the **Frequency**, which is the number of samples out of 40 where the composition transitions at each temperature. You can see that the transitions occur more frequently near the 600 °C starting point and less frequently at the edges.

Since only one variable can serve as a **Relaxed condition** per calculation, the quantity that is not relaxed has a NaN result in its corresponding result quantity. The **Temperature** result quantity inherits the unit set in the conditions while the **Composition** result quantity inherits the normalization (mole or mass) but always returns a fraction.

PM_G_02: Coarsening and Interfacial Energy

The example uses the **Property Model Calculator** and both thermodynamic (FEDEMO) and kinetic (MFEDEMO) demonstration steel databases. Using a **Grid** *Calculation Type* it produces these plot types: a **Heat map**, a **Contour plot** and an overlaid plot combining a cross plot with a contour plot (where both the interfacial energy and coarsening rate is shown). It also creates a diagram to show the phase fractions vs time and a **3D** *Plot type* comparing the coarsening rate coefficient.

Coarsening Property Model Settings

Project File Information

- Folder: **Property Models → General**
- File name: *PM_G_02_Coarsening_and_Interfacial_energy.tcu*

Visualizations

This example is included as a Property Model tutorial on our website and as part of the Property Model Calculator playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

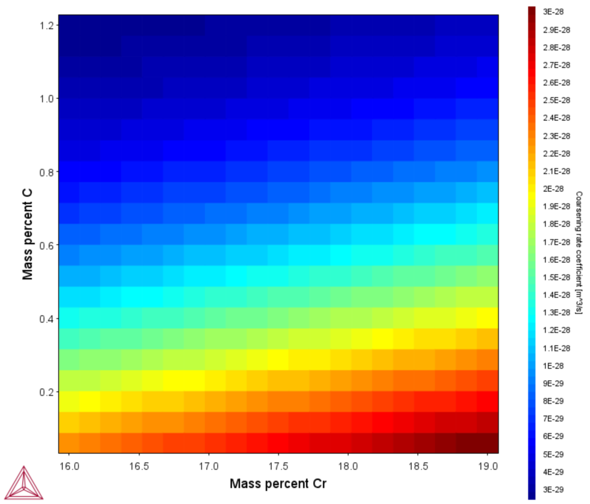


Figure 32: Uses a Property Model Calculator with a Grid Calculation type to plot the coarsening rate coefficient as a Heat map.

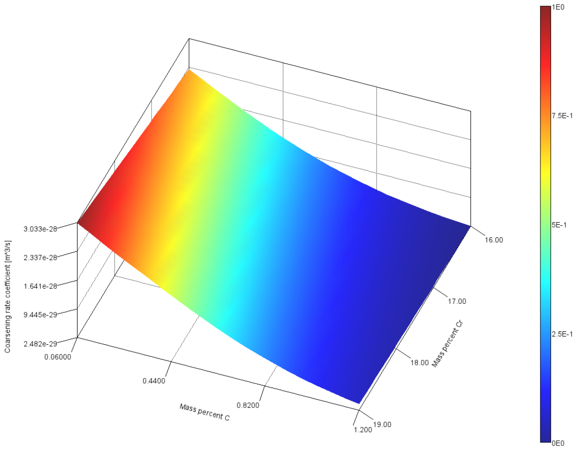


Figure 33: Uses a Property Model Calculator with a Grid Calculation type to plot the coarsening rate coefficient as a 3D plot.

When in the Thermo-Calc help (press F1), go to Rotating 3D Plots to watch a short video showing you how to rotate this plot in the Visualizations window.

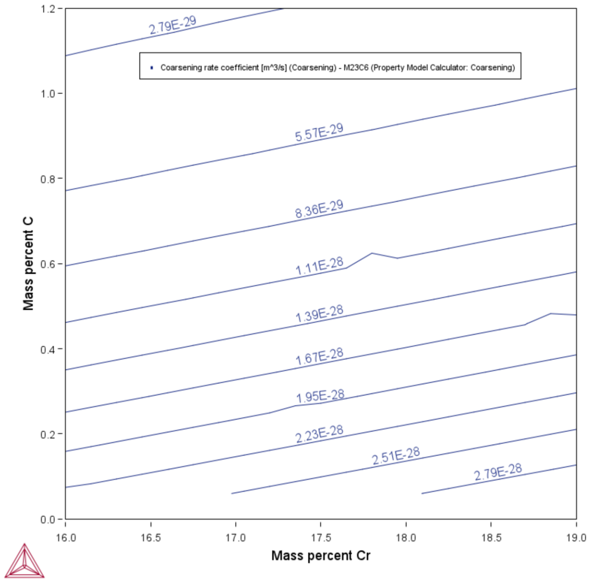


Figure 34: Uses a Property Model Calculator with a Grid Calculation type to plot the coarsening rate coefficient as a Contour plot.

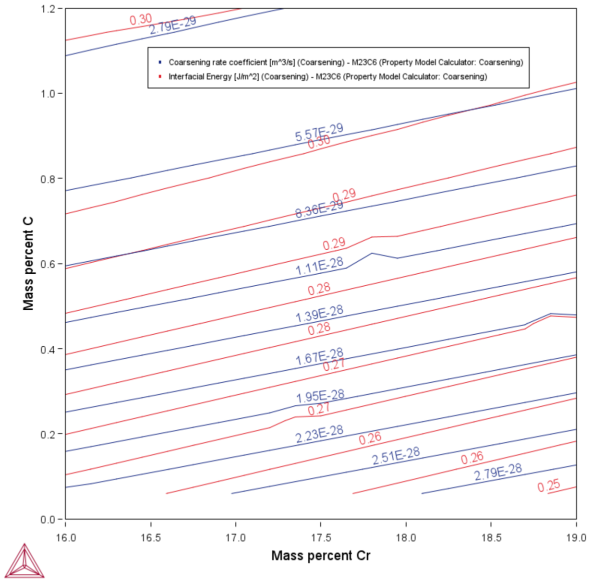


Figure 35: Comparing the coarsening rate coefficient and interfacial energy in overlaid plots.

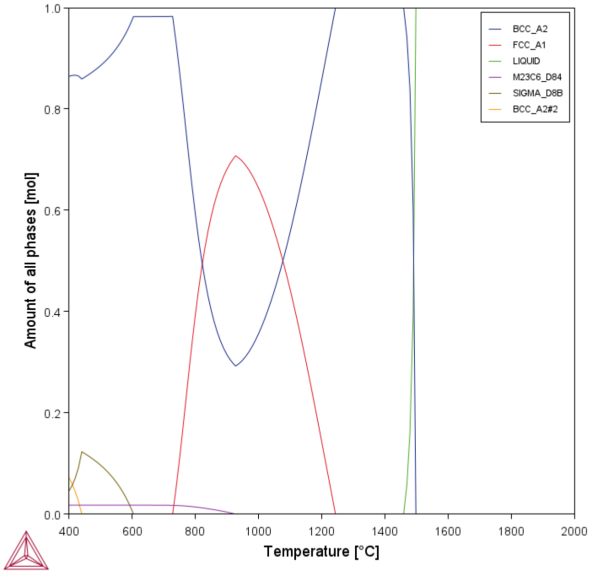


Figure 36: A One Axis Equilibrium calculation showing the phase fractions vs T (with a Flexible Mode plot type).

PM_G_03: Driving Force and Interfacial Energy

The example uses the **Property Model Calculator** and a thermodynamic demonstration steel database (FEDEMO). Using a **Grid** *Calculation type* it produces a **Contour** plot comparing the driving force and interfacial energy.

Driving Force Property Model Settings and Interfacial Energy Property Model Settings

Project File Information

- Folder: **Property Models → General**
- File name: *PM_G_03_Driving_force_and_Interfacial_energy.tcu*

Visualizations

This example is included as a Property Model tutorial on our website and as part of the Property Model Calculator playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

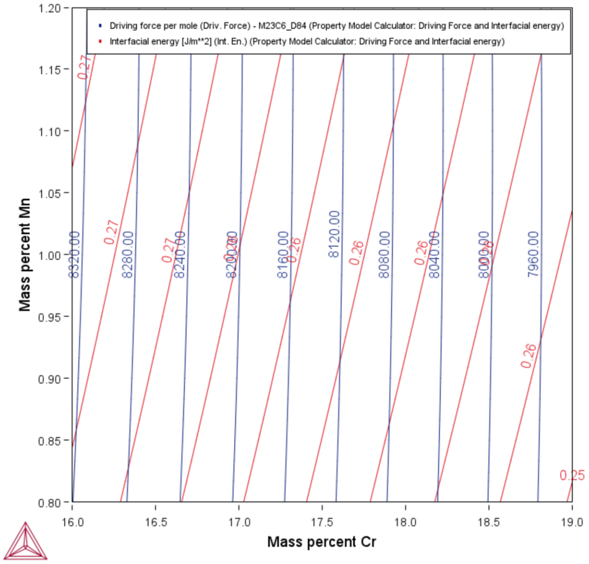


Figure 37: An overlaid Contour plot comparing the driving force and interfacial energy.

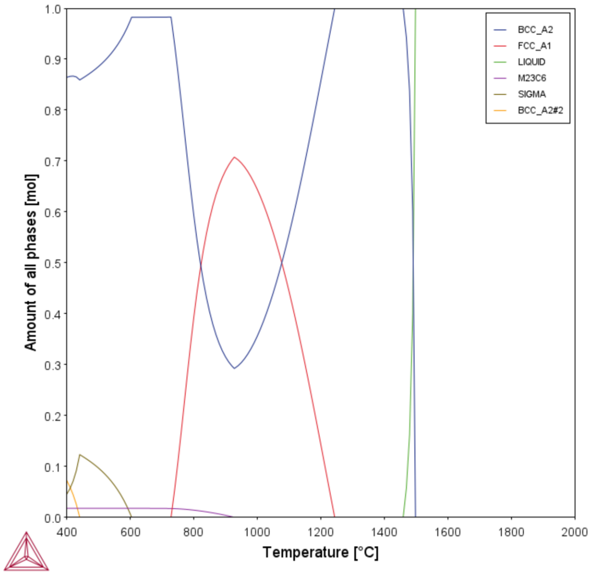


Figure 38: A One Axis Equilibrium calculation showing the Phase fractions vs T.

PM_G_04: Yield Strength

The example uses the **Property Model Calculator** and the **Yield strength** Property Model with a thermodynamic demonstration aluminum database (ALDEMO).

Using default options for the precipitation strengthening models, this example compares the **Simplified model (general)**, **Seidman model (Al-base)** and **Deschamps model (Al-base)** yield strength versus precipitate radius to experimental data for an Al-0.3wt%Sc alloy homogenized at 648 °C for 24 hours and subsequently aged at 350 °C.

For more settings information, see Yield Strength Property Model: Simplified Mode Settings or Yield Strength Property Model: Advanced Mode Settings. For additional theoretical information about the models, see About the Yield Strength Property Model.

The Seidman model [2002Sei] considers a combination of a shearing mechanism and Orowan dislocation bypass mechanism. For the shearing mechanism, the increase in yield strength results from the contributions of ordering strengthening, coherency strengthening, and modulus mismatch strengthening.

When **Seidman model (Al-base)** is selected as the *Precipitation strengthening model*, the setting for α is a constant related to the coherency strengthening of precipitates, which usually varies from 2 to 3. In this example, the default α is 2.6 [1985Ard]. The *m* setting is the parameter that relates to the modulus mismatch strengthening and the default is set as 0.85 [1985Ard]. This model is applied in the study of precipitation hardening in dilute Al(Sc) alloys containing coherent Al_3Sc precipitates. The model parameters described above can be adjusted to work for hardenable aluminum alloy calculations from the 2000 (Al–Cu and Al–Cu–Mg), 6000 (Al–Mg–Si), and 7000 (Al–Zn–Mg) series.

As a comparison, the **Simplified model** [2008Zan] only considers the general mechanisms of cutting and looping (Orowan mechanism) without regard to any detailed dislocation mechanisms.

When **Simplified model (general)** is selected as the *Precipitation strengthening model*, the default *Critical radius* (the critical size r_c) is optimized against experimental results for dilute Al-Sc. If the precipitates are smaller than a critical size (approximately 5–10 nm) the dislocations cut the precipitates. The strength of the obstacle is then proportional to the square root of the average radius. If the particles are larger than the critical size, r_c, it is less costly for the dislocations to bow round the particles and the strengthening contribution is inversely proportional to r. Since the **Simplified model (general)** only depends on generic material constants (k_p and r_c) it may be applied to any precipitation strengthened material.

The **Deschamps model (Al-base)** model [1998Des], is for precipitation strengthening, mainly intended for use with Al-base alloys. The Deschamps model includes use of Friedel or Kock's statistics for particle size distribution. Default parameters are used to match a dilute Al-Sc alloy with Al_3Sc precipitates. As is done for the other precipitation strengthening models, a critical radius, describing the transition from cutting to looping, must be specified when you are setting up the configuration.

Project File Information

- Folder: **Property Models → General**
- File name: *PM_G_04_Yield_Strength.tcu*

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

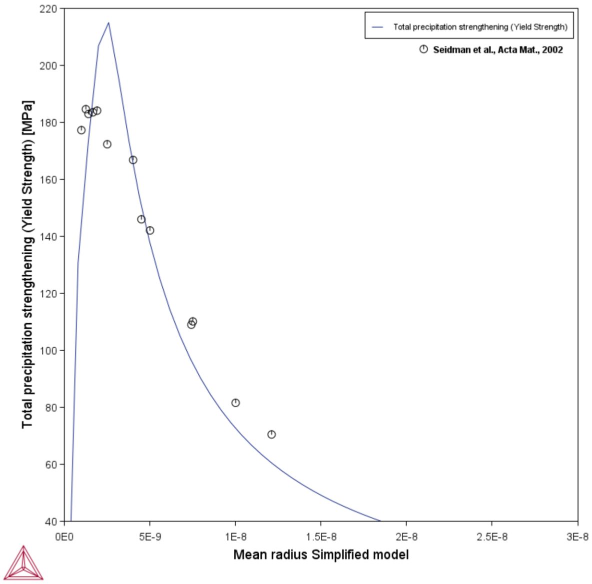


Figure 39: Strength vs Radius - Simplified compared to experimental data from [2002Sei].

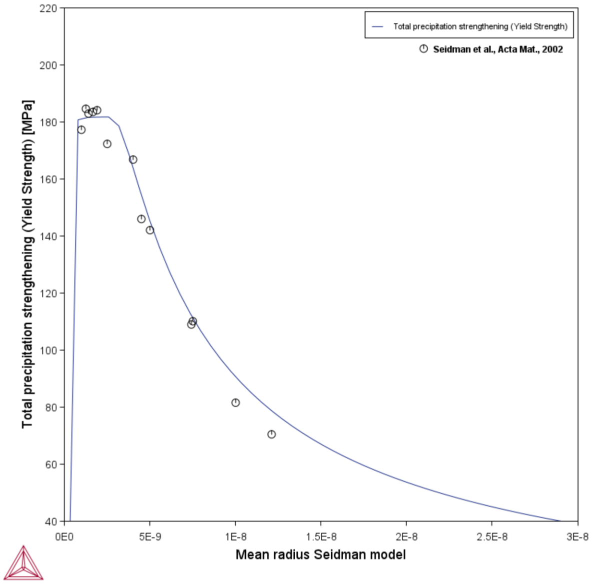


Figure 40: Strength vs Radius - Seidman compared to experimental data from [2002Sei].

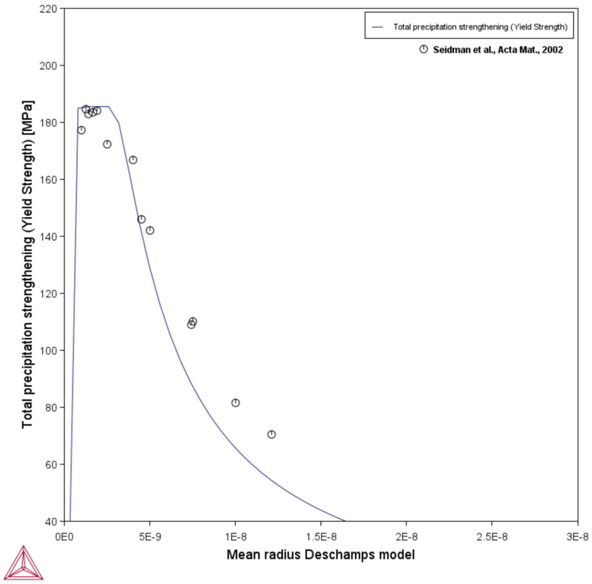


Figure 41: Strength vs Radius - Deschamps compared to experimental data from [2002Sei].

References

[1985Ard] A. J. Ardell, Precipitation hardening. Metall. Trans. A. 16, 2131–2165 (1985).

[1998Des] A. Deschamps, Y. Brechet, Influence of predeformation and ageing of an Al–Zn–Mg alloy—II. Modeling of precipitation kinetics and yield stress. Acta Mater. 47, 293–305 (1998).

[2002Sei] D. N. Seidman, E. A. Marquis, D. C. Dunand, Precipitation strengthening at ambient and elevated temperatures of heat-treatable Al(Sc) alloys. Acta Mater. 50, 4021–4035 (2002).

[2008Zan] J. Zander, R. Sandström, One parameter model for strength properties of hardenable aluminium alloys. Mater. Des. 29, 1540–1548 (2008).

PM_G_05: Yield Strength NiAlCr

The example uses the **Property Model Calculator** and the **Yield strength** Property Model with a thermodynamic demonstration nickel database (NIDEMO).

The Reppich model is developed for calculation of precipitation strengthening in Ni-based super alloys consisting mainly of gamma prime (γ') precipitates in a gamma matrix. The example shows a calculation of the precipitation strengthening vs precipitate radius in a Ni-10at%Al-10at%Cr alloy.

This example uses the Reppich model [1982Rep] which is developed and rests on existing hardening models estimating the increase of the yield stress due to pairwise particle cutting and antiphase domain boundary (APB) formation. The effect of the anisotropy on the dislocation line tension of two-phase material and on the Orowan stress is taken into account. Compared to conventional APB hardening theories, this model can be applied to large volume fraction of precipitates in the anisotropic systems.

For more settings information, see Yield Strength Property Model: Simplified Mode Settings and for additional theoretical information about the models, see About the Yield Strength Property Model.

For the settings input of the **Reppich model (Ni-base)**:

- *A* is a numerical factor depending on the morphology of the precipitates. For spherical particles, *A* equals to 0.72.
- *w* represents the elastic repulsion between the strongly paired dislocations, which can be determined by the experimental data [1979Hüt].

  In this example, *A* and *w* are set by default to 0.7639 and 0.2919, respectively. The *C* factor default of 0 is not changed.

Project File Information

- Folder: **Property Models → General**
- File name: *PM_G_05_Yield_Strength_NiAlCr.tcu*

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

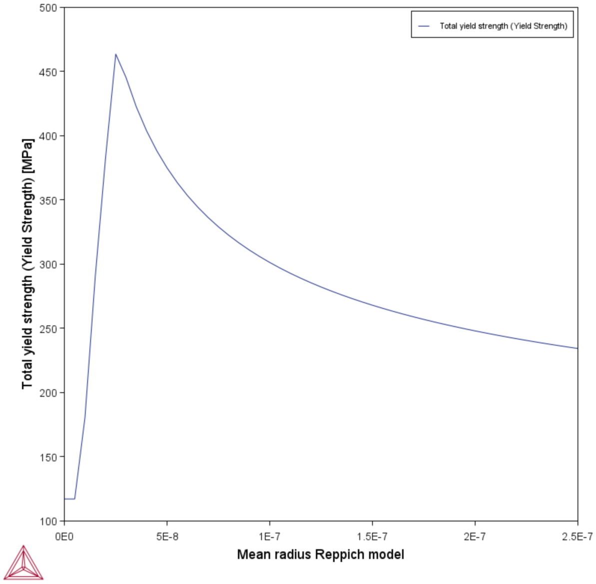


Figure 42: Reppich model plotted with results and experimental data for PE16, all data is normalized with the square root of the volume fraction of precipitate.

References

[1979Hüt] W. Hüther, B. Reppich, Order hardening of MgO by large precipitated volume fractions of spinel particles. Mater. Sci. Eng. 39, 247–259 (1979).

[1982Rep] B. Reppich, Some new aspects concerning particle hardening mechanisms in γ’ precipitating Ni-base alloys—I. Theoretical concept. Acta Metall. 30, 87–94 (1982).

PM_G_06: Yield Strength HEA

The example uses the **Property Model Calculator** and the **Yield strength** Property Model with the thermodynamic TCS High Entropy Alloys Database (TCHEA). It is an example of solid solution strengthening, which is the contribution to total strength due to the elastic strains in the crystal lattice caused by alloying elements of a lattice parameter differing from the main constituent. The example shows the solid solution strengthening at 300 K and 411 K over the full solubility range for the Mo-Ta system as compared to experimental data [1972Ste].

For more settings information, see Yield Strength Property Model: Simplified Mode Settings and for additional theoretical information about the models, see About the Yield Strength Property Model.

Project File and License Information

- Folder: **Property Models → General**
- File name: *PM_G_06_Yield_Strength_HEA.tcu*

This example requires the use of the TCS High Entropy Alloys Database (TCHEA). A license is required to run the example.

This example is configured to run with BCC_A2 selected and BCC_B2/BCC_B2#2 deselected in the **System Definer → Phases and Phase Constitution** tab, when using version 8 (TCHEA8) or higher. If the database is changed to an earlier version, this selection is reset by the software and you need to either manually re-apply these settings on the System Definer or reopen the example.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

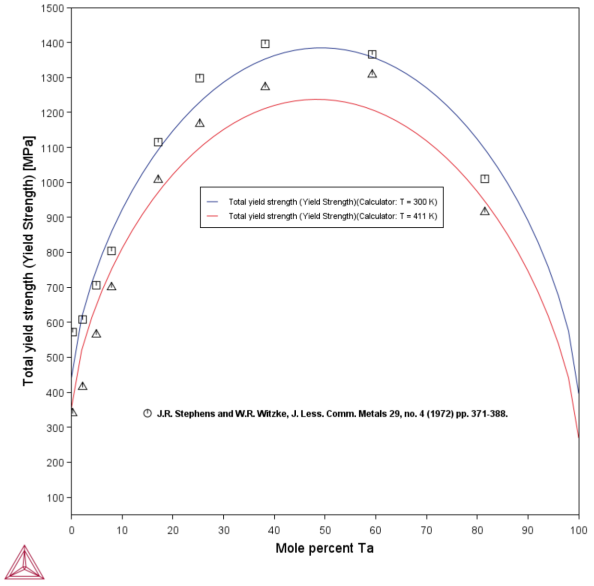


Figure 43: The solid solution strengthening over the full solubility range for the Mo-Ta system as compared to experimental data [1972Ste].

Reference

[1972Ste] J. R. Stephens, W. R. Witzke, Alloy hardening and softening in binary molybdenum alloys as related to electron concentration. J. Less Common Met. 29, 371–388 (1972).

PM_G_07: Hot Crack Susceptibility

The example uses the **Property Model Calculator** and the **Crack Susceptibility Coefficient** Property Model to calculate the hot tearing tendency during solidification for an Al-Si alloy. The **ALDEMO: Aluminum Demo Database** is used and this example is available to all users.

Hot tearing is one of the most common and serious defects encountered during the casting of, for example, aluminum alloys. In general, it is defined by the formation of a macroscopic fissure in a casting as a result of stress and the associated strain, generated during cooling, at a temperature above the non-equilibrium solidus.

The Model is based on the publication by Yan and Lin [2006Yan] and uses experimental data [1955Pum; 1976Feu; 2004Bar] from this paper.

The experimental hot cracking susceptibility of an alloy is defined as the ratio between the cracking length for that alloy and the maximum cracking length in the alloy system studied. Considering the uncertainties and difficulties in hot tearing measurements, the calculated hot tearing tendencies are in excellent agreement with the experimental data. The typical L-shaped curve is well reproduced in the current prediction. It rapidly increases at a low solute content and has a maximum at a composition of around 0.5 wt pct Si.

See About the Crack Susceptibility Coefficient Property Model for background information about this Property Model.

Project File Information

- Folder: **Property Models → General**
- File name: *PM_G_07_Hot_Crack_Susceptibility.tcu*

Visualizations

This example is included as a Property Model tutorial on our website and as part of the Property Model Calculator playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

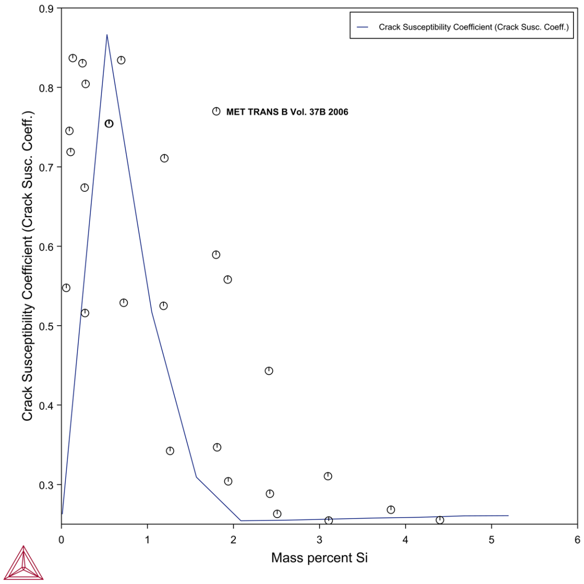


Figure 44: The plot compares the predicted cracking susceptibility/composition curve for the Al-Si system with the experimental hot tearing tendencies [1955Pum; 1976Feu; 2004Bar].

References

[1955Pum] W.I. Pumphrey: ‘‘The Aluminum Development Association Report No. 27,’’ Aluminum Development Association, London, 1955.

[1976Feu] U. Feurer, Mathematical Model by the Hot Cracking Tendency of Binary Aluminum Alloys. Giessereiforschung. 28, 75–80 (1976).

[2004Bar] S. R. Barnett, J. A. Taylor, and D. H. St. John: Solidification of Aluminum Alloys, M.G. Chu, D.A. Granger, and Q. Han, eds., TMS, Warrendale, PA, 2004, pp. 201-09.

[2006Yan] X. Yan and J. C. Lin, “Prediction of hot tearing tendency for multicomponent aluminum alloys,” Metall. Mater. Trans. B, vol. 37, no. 6, pp. 913–918, Dec. 2006.

PM_G_08: Spinodal

The example uses the **Property Model Calculator** and the **Spinodal** Property Model to calculate the so-called spinodal curve for the BCC_A2 miscibility gap in the system Fe-Cr. The **FEDEMO: Iron Demo Database** is used and this example is available to all users.

Two Property Model Calculators are used in this example. The spinodal curve (a **One Axis** calculation), is overlaid on top of a the Fe-Cr **Phase diagram** calculation. As can be seen in the plot, the spinodal curve for BCC goes through the one-phase region for Sigma. This is because the spinodal curve for a phase is calculated when all other phases are suspended.

About the Spinodal Property Model

Project File Information

- Folder: **Property Models → General**
- File name: *PM_G_08_Spinodal.tcu*

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

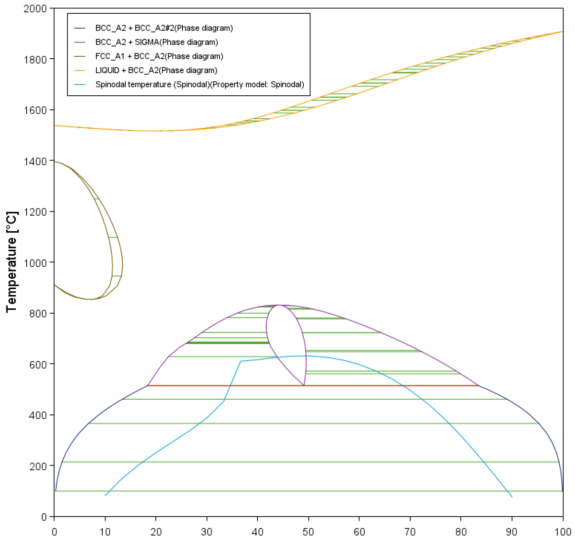


Figure 45: An Fe-Cr spinodal curve for BCC goes through the one-phase region for Sigma.

PM_G_09: T-Zero Temperature

The example uses the **Property Model Calculator** and the **T-Zero Temperature** Property Model to calculate the so-called T_0 line for the two-phase field FCC_A1 and BCC_A2 in the Fe-Ni system. The line is plotted together with the phase diagram for the same Fe-Ni system. The **FEDEMO: Iron Demo Database** is used and this example is available to all users.

The T_0 temperature is defined as the temperature where two phases of identical chemical composition have the same molar Gibbs free energy. This temperature is an important quantity in the field of diffusionless phase transformations, e.g. martensitic transformation, since it is the upper limit where diffusionless phase transformations can occur.

Two Property Model Calculators are used in this example. The T_0 line (a **One Axis** calculation) for the two-phase field FCC_A1 and BCC_A2 is overlaid on top of a the Fe-Ni **Phase diagram** calculation.

About the T0 Temperature Property Model

Project File Information

- Folder: **Property Models → General**
- File name: *PM_G_09_T-Zero_temperature.tcu*

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

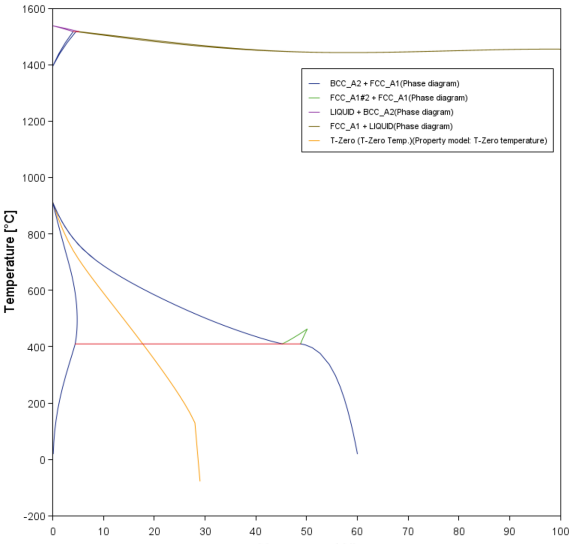


Figure 46: In this plot for the Fe-Ni system, the T_0 line for the FCC_A1 and BCC_A2 phases is located in the middle of the two-phase region. No solution for the T_0 temperature exists above about 30 mass% Ni.

PM_G_10: Freeze-in Thermal Conductivity

The example uses the **Property Model Calculator** and the **Equilibrium with Freeze-in Temperature** Property Model to compare the use of the model with thermal conductivity with and without grain boundary (GB) phase scattering being included in the calculation.

The TCS Al-based Alloy Database (TCAL) is used to evaluate a 7075_T6 alloy (Al-1.6Cu-2.5Mg-5.6Zn-0.25Fe-0.15Mn-0.23Cr-0.2Ti-0.2Si) mass%. The "T6" in the alloy name means that the alloy has been artificially peak-aged, i.e. the matrix is almost depleted. The heating is assumed to be at a typical artificial aging temperature of 150 °C. The temperature has then been increased for measuring of the reported values thermal conductivity at 400, 500, and 532 °C.

The thermal conductivity due to grain boundary phase scattering is approximated as a scattering constant times the total volume fraction of the grain boundary phases. The contribution to thermal conductivity is assumed to be related to that to electrical resistivity, following the Wiedemann-Franz law.

The calculation set up assumes that the alloy reaches equilibrium at the peak-age temperature, i.e. that the amounts of phases and their composition freeze-in at 150 °C and that these do not change for the evaluation of thermal conductivity at the temperatures 400, 500, and 532 °C. Calculations are compared between accounting and ignoring contributions from grain boundary (GB) phase scattering.

As can be seen in Figure 47, the calculation including the approximate effect of grain boundary phase scattering is close to the experimentally measured values. Excluding the effect of grain boundary phase scattering slightly overestimates the thermal conductivity. Experimental data is from [2008ASM].

About the Equilibrium with Freeze-in Temperature Property Model

Project File and License Information

- Folder: **Property Models → General**
- File name: *PM_G_10_Freeze_In_Thermal_Conductivity.tcu*

The TCS Al-based Alloy Database (TCAL) is used in this example. A valid license for version 7 (TCAL7) or newer is required to run the example.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

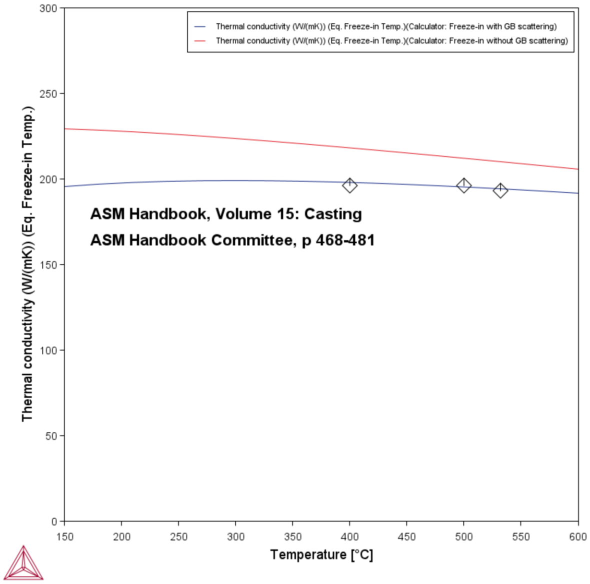


Figure 47: Comparing the freeze-in temperature for the 7075_T6 alloy with and without grain boundary (GB) scattering included in the calculations.

Reference

[2008ASM] ASM Handbook Committee, ASM Handbook Volume 15: Casting. ASM International, p. 468-481, 2008, ISBN 978-0-87170-711-6.

PM_G_11: Freeze-in Electrical Resistivity

The example uses the **Property Model Calculator** and the **Equilibrium with Freeze-in Temperature** Property Model to compare the use of the model for electrical resistivity with and without grain boundary (GB) scattering being included in the calculation.

The TCS Al-based Alloy Database (TCAL) is used to evaluate a 4032-O alloy (Al-0.9Cu-1.0Mg-0.9Ni-12.2Si) mass%. The "O" in the alloy name means that the Al alloy has been heat-treated at a typical temperature of 350 °C. The measurement of electric resistivity is usually performed at room temperature.

The electrical resistivity due to grain boundary phase scattering is approximated as a scattering constant times the total volume fraction of the grain boundary phases.

The calculation set up assumes that the alloy reaches equilibrium at the "O" heat-treated temperature, i.e. that the amounts of phases and their composition freeze-in at 350 °C and that these do not change for the evaluation of electrical resistivity at the room temperature. Calculations are compared between accounting and ignoring contributions from grain boundary (GB) scattering.

As can be seen from Figure 48, the calculated electrical resistivity at room temperature, including grain boundary phase scattering, is very close to the experimentally measured value (4.3E-8) for the alloy. Excluding the grain boundary phase scattering somewhat underestimates the electrical resistivity for the alloy. Experimental data is from [1993Dav].

About the Equilibrium with Freeze-in Temperature Property Model

Project File and License Information

- Folder: **Property Models → General**
- File name: *PM_G_11_Freeze_In_Electric_Conductivity.tcu*

The TCS Al-based Alloy Database (TCAL) is used in this example. A valid license for version 7 (TCAL7) or newer is required to run the example.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

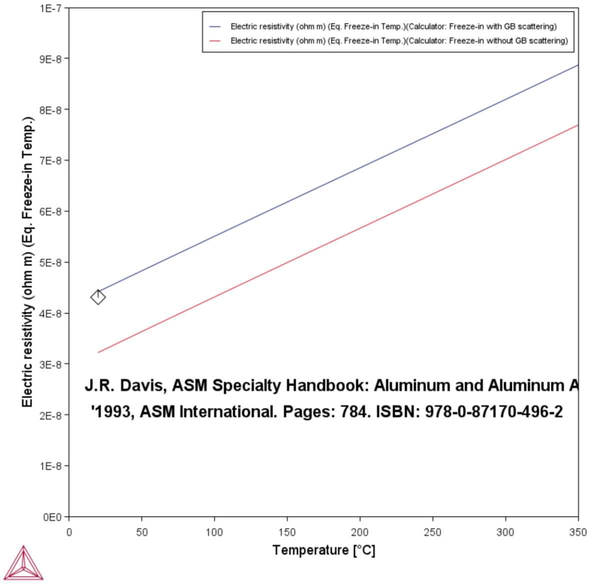


Figure 48: Comparing the freeze-in temperature for the 4032-O alloy with and without grain boundary (GB) scattering included in the calculations.

Reference

[1993Dav] J.R. Davis, ASM Specialty Handbook: Aluminum and Aluminum Alloys, 1993, ASM International. Pages: 784. ISBN: 978-0-87170-496-2.

PM_G_12: Solidus and Liquidus Batch Calculation

The example uses the **Property Model Calculator** and the **Liquidus and Solidus Temperature** Property Model to demonstrate the use of the **Batch** *Calculation Type*.

The thermodynamic demonstration steel database (FEDEMO) is used along with a randomized set of experimental data points that are shown on the **Configuration** window in a table. The data showing in this example is imported from a data file prepared with specific data entry requirements.

A variety of compositions for an Fe-Cr-Mn-Ni-C alloy is used for the calculations; these compositions are also taken from the same data file. When the heading includes `Exp`, then these columns are considered experimental data by Thermo-Calc, where in this example it is the columns titled `Exp Liq temp C` and `Exp Sol temp C`. This experimental data can then be plotted as a function of the calculated solidus/liquidus temperature and compared on the plot using a **Cross plot**, which is selected on the **Plot Renderer**. The limits are shown using the setting RMS (root mean square).

> The experimental data entered into the batch data file is unitless even though the actual experimental data unit is Celsius (as written in the header text). In order for the plot and calculations to match, Celsius is chosen as the temperature unit when defining the **Solidus/Liquidus** Property Model and all the axes manually scaled to the same limits (1360 → 1520).

> Working with Batch Calculations

Project File Information

- Folder: **Property Models → General**
- File name: *PM_G_12_Solidus_and_Liquidus_Batch_Calculation.tcu*

Visualizations

This example is included as a Property Model tutorial on our website and as part of the Property Model Calculator playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

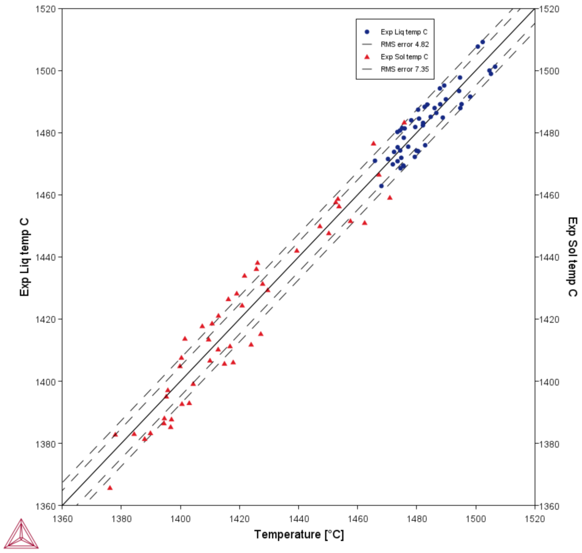


Figure 49: A comparison of experimental liquidus and solidus data using a Cross plot with a Batch calculation. A root mean square (RMS) setting shows the distribution of the data points.

PM_G_13: Ti Alloy Design for Additive Manufacturing

This in-depth example, which is available on our website, uses the **Property Model Calculator** to find the optimal composition for a titanium-based alloy to be used for additive manufacturing applications.

Additive manufacturing provides new opportunities to fabricate complex parts. However, traditional alloys may not be readily printable using techniques such as laser powder bed fusion. As such, the development of new alloys may be necessary to fully realize the benefits of additive manufacturing technologies.

In this example, inspired by the work of Ackers et al. [2021Ack], **Batch** calculations within the Property Model Calculator are used to identify candidate titanium alloy chemistries for biomedical implant applications using the thermodynamic TCS Ti/TiAl-based Alloys Database (TCTI). To optimize printability and material weight, the liquidus temperature, solidus temperature, and density of 2000 randomized titanium alloy chemistries from the Ti-Nb-Zr-Sn-Ta-Fe-Mo system are calculated. An estimate of alloy cost is also made for each alloy. Taken together, this methodology can be used to identify compositions of interest and accelerate material development activities.

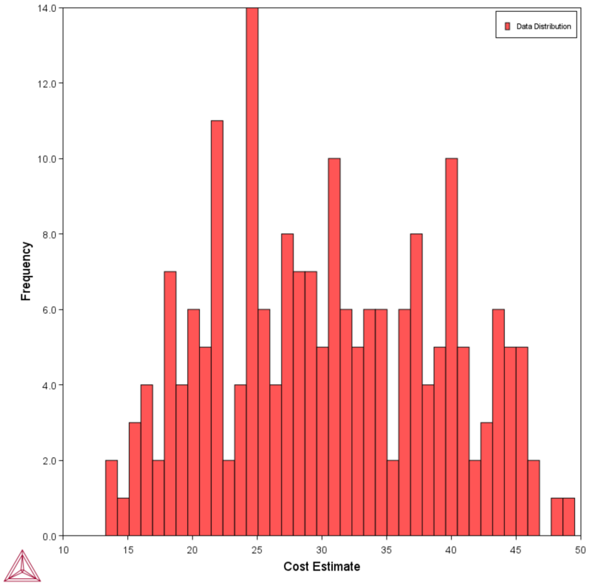


Figure 50: Cost estimate histogram for 2000 randomized chemistries from the Ti-Nb-Zr-Sn-Ta-Fe-Mo system. The cost estimate was calculated using a user-defined function in the Property Model Calculator.

Project File and License Information

- Folder: **Property Models → General**
- File name: *PM_G_13_Ti_Alloy_Design_for_AM.tcu*

A license for Thermo-Calc 2022b or newer and the TCS Ti/TiAl-based Alloys Database (TCTI) version 4 (TCTI4) or newer, is required to run the example.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

The resulting plots and details related to setting up this example are available to download via the dedicated web page.

Reference

[2021Ack] M. A. Ackers, O. M. D. M. Messé, U. Hecht, Novel approach of alloy design and selection for additive manufacturing towards targeted applications. J. Alloys Compd. 866, 158965 (2021).

PM_G_14: Ti-Fe T-Zero Martensite

The example uses the **Property Model Calculator** and the **T-Zero Temperature** Property Model to demonstrate the martensitic BCC → HCP transformation for a binary Ti-Fe system. A setting is used to include a Gibbs energy addition to the second phase, which allows for the inclusion of an energy barrier for martensitic phase transformations.

About the T0 Temperature Property Model

Project File and License Information

- Folder: **Property Models → General**
- File name: *PM_G_14_Ti_Fe_T-Zero_Martensite.tcu*

The TCS Ti/TiAl-based Alloys Database (TCTI) is used in this example. A valid license is required to run the example.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

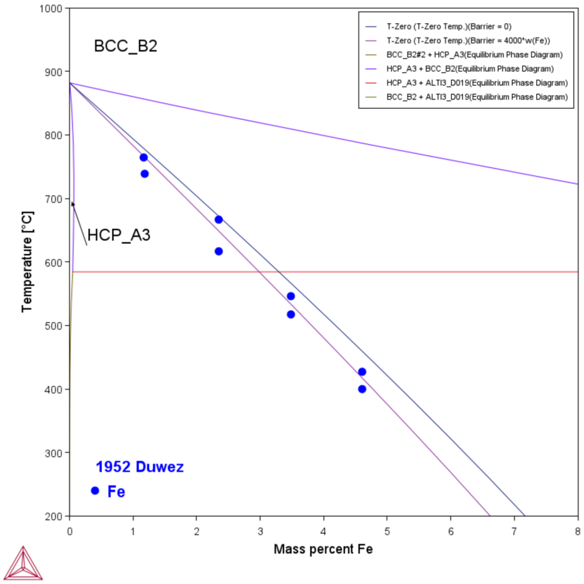


*Figure 51: The T-Zero (barrier = 0) line is the temperature without energy addition, the solid blue line is the T-Zero temperature with an energy addition of 4000*w(Fe) [J/mol], that well reproduces the experimental data from Duwez (1952).*

Reference

[1952Duw] P. Duwez, “The Martensite Transformation Temperature in Titanium Binary Alloys, Third Technical Report” (U.S. Atomic Energy Commission, 1952).

PM_G_15: Columnar to Equiaxed Transition (CET) of a NiAlCr Alloy

This example uses the **Property Model Calculator** and the **Columnar to Equiaxed Transition** Property Model with nickel demo databases to mimic the result of CMSX-4 alloy, which compares the tip radius and undercooling with growth velocity.

A Ni-26Al-9Cr (at.%) alloy is used so that its calculated undercooling is close to that of a 10-component CMSX-4 alloy. A **One Axis** calculation for the FCC_L12 primary phase is done using the CET parameters entered on the **Property Model Calculator Configuration** window.

The settings used are the same as those from the literature [2001Gäu], i.e.:

- **Number of nucleation sites**: `2.0E15`/m^3
- **Equiaxed exponent**: `3.4`
- **Nucleation undercooling**: `2.5` K
- **Solve for**: **Thermal gradient**
- **Equiaxed fractions**: `0.0066 0.1`

About the Columnar to Equiaxed Transition (CET) Property Model

Project File Information

- Folder: **Property Models → General**
- File name: *PM_G_15_Ni-Al-Cr_Columnar_Equiaxed_Transition.tcu*

The NIDEMO and MNIDEMO databases are used in this example and it is available to all users.

Also see these examples that use the same Property Model. However, these examples require licenses as they use the TCS Ni-based Superalloys Database (TCNI) and TCS Ni-alloys Mobility Database (MOBNI): PM_G_16: Columnar to Equiaxed Transition of a CMSX-4 Alloy and PM_G_17: Columnar to Equiaxed Transition of an IN718 Alloy.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

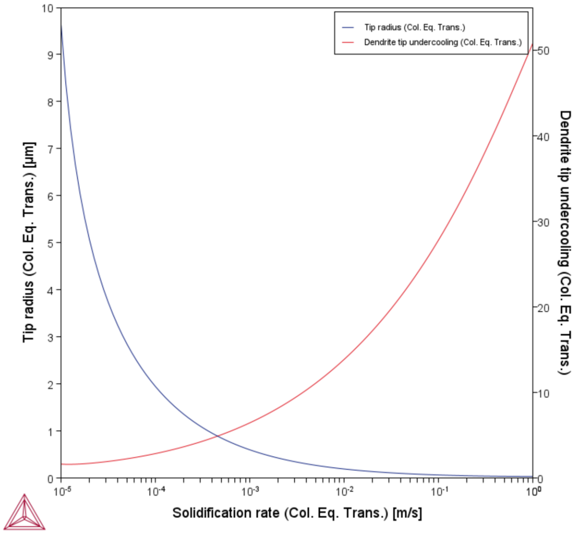


Figure 52: Tip radius and undercooling vs growth velocity for a Ni-26Al-9Cr alloy.

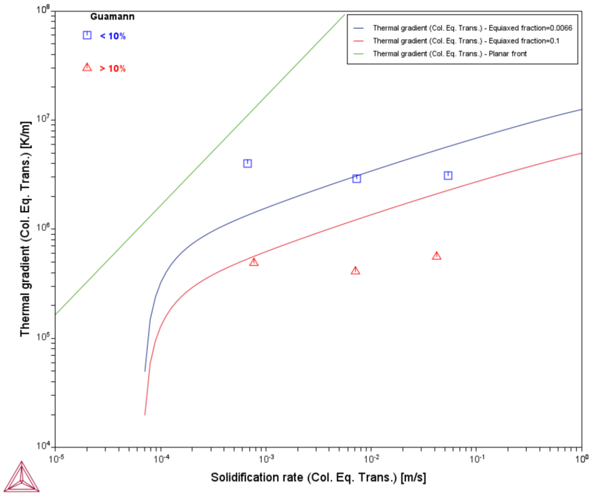


Figure 53: CET curves for a Ni-26Al-9Cr alloy using experimental data from [2001Gäu]. Also see PM_G_16 to compare the results to the CMSX-4 alloy results.

Reference

[2001Gäu] M. Gäumann, C. Bezençon, P. Canalis, W. Kurz, Single-crystal laser deposition of superalloys: processing–microstructure maps. Acta Mater. 49, 1051–1062 (2001).

PM_G_16: Columnar to Equiaxed Transition of a CMSX-4 Alloy

This example uses the **Property Model Calculator** and the **Columnar to Equiaxed Transition** Property Model with a CMSX-4 alloy to compare calculated CET curves to experimental data.

About the Columnar to Equiaxed Transition (CET) Property Model

A 10-component system, with a composition from Gäumann et al. [2001Gäu], is used for this simulation of a CMSX-4 alloy.

Alloy composition of CMSX-4 [2001Gäu].

	Co	*Cr*	*Al*	*Ti*	*W*	*Ta*	*Re*	*Hf*	*Mo*	*Ni*
wt.%	9.0	6.5	5.6	1.0	6.0	6.5	3.0	0.1	0.6	Bal
at.%	9.262	7.581	12.587	1.267	1.979	2.178	0.977	0.034	0.379	Bal

The results are compared with literature data (epitaxial laser metal forming) and the original model [1999Gäu; 2001Gäu].

A **One Axis** calculation for the FCC_L12 primary phase is done using the CET parameters entered on the **Property Model Calculator Configuration** window.

The settings entered include:

- **Interfacial energy**: `0.25` J/m^2, which gives a Gibbs-Thomson coefficient of 1.87 x 10^{-7} mK, in agreement with the literature [2001Gäu].
- **Number of nucleation sites:** `2.0E15`/m^3
- **Nucleation undercooling** : `3.0` K
- **Equiaxed exponent:** `3.4`
- **Solve for**: **Thermal gradient**
- **Equiaxed fractions**: `0.0066 0.1`

In the calculation, the nucleation undercooling is slightly larger than originally used (2.5 K) [2001Gäu], since it has been found that at a low speed limit, the Property Model gives an undercooling close to 3 K.

The original value is arbitrary and does not affect the results at a high speed range.

Project File and License Information

- Folder: **Property Models → General**
- File name: *PM_G_16_CMSX-4_Columnar_Equiaxed_Transition.tcu*

To run this example requires a license for the TCS Ni-based Superalloys Database (TCNI) version 12 (TCNI12) or newer and the TCS Ni-alloys Mobility Database (MOBNI) version 6 (MOBNI6) or newer.

Example PM_G_15: Columnar to Equiaxed Transition (CET) of a NiAlCr Alloy uses demo databases available to everyone and mimics this alloy in its results.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

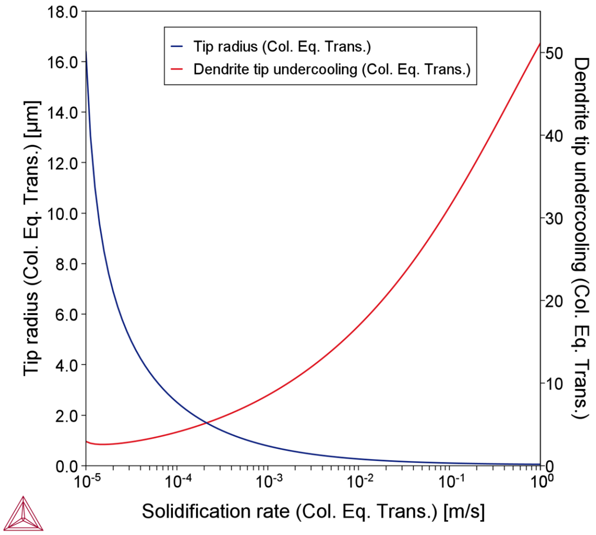


Figure 54: Tip radius and undercooling vs growth velocity for a CMSX-4 alloy.

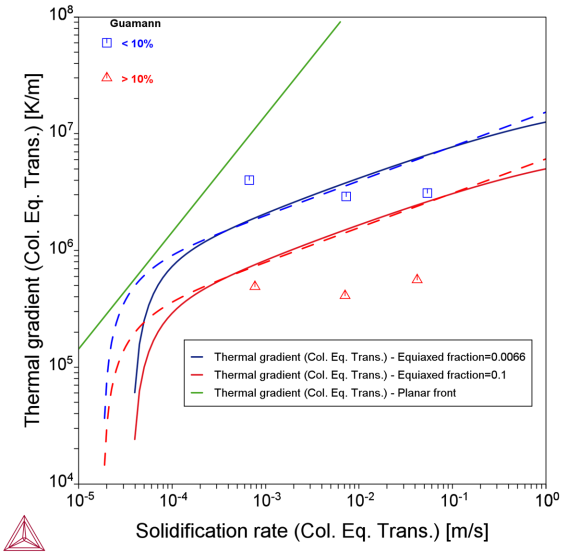


Figure 55: Calculated CET curves (solid lines) in comparison to experimental data (data points) and calculations (dashed lines) from the literature [2001Gäu].

References

[1999Gäu] M. Gäumann, PhD thesis, Epitaxial laser metal forming of a single crystal superalloy, École polytechnique fédérale de Lausanne (EPFL) (1999).

[2001Gäu] M. Gäumann, C. Bezençon, P. Canalis, W. Kurz, Single-crystal laser deposition of superalloys: processing–microstructure maps. Acta Mater. 49, 1051–1062 (2001).

More Information

Also see these examples that use the same Property Model: PM_G_15: Columnar to Equiaxed Transition (CET) of a NiAlCr Alloy and PM_G_17: Columnar to Equiaxed Transition of an IN718 Alloy.

PM_G_17: Columnar to Equiaxed Transition of an IN718 Alloy

The example uses the **Property Model Calculator** and the **Columnar to Equiaxed Transition** Property Model to compare calculated CET curves for an IN718 alloy to experimental data.

About the Columnar to Equiaxed Transition (CET) Property Model

A **One Axis** calculation for the FCC_L12 primary phase is done using the CET parameters entered on the **Property Model Calculator Configuration** window.

The settings entered include:

- **Interfacial energy**: `0.5` J/m^2.
- **Number of nucleation sites**: `4.0E11`/m^3
- **Nucleation undercooling** : `4.0` K
- **Equiaxed exponent**: `3.13`
- **Solve for**: **Thermal gradient**
- **Equiaxed fractions**: `0.01 0.49 0.99`

The literature data from Polonsky et al. [2020Pol] are not purely experimental data, but rather combined with experimental equiaxed evidence and model calculations with numerical values of thermal gradients, growth velocity as well as tip undercooling. Polonsky et al. estimated tip undercooling based on a Scheil calculation, which smeared out the composition inhomogeneity at the dendrite front, hence underestimating the undercooling. Since both tip undercooling and nucleation site density promotes the formation of equiaxed crystals, an increase in undercooling in this example calculation leads to a decrease in nucleation site density compared to the results in [2020Pol] if one were fitting the same set of data.

Project File and License Information

- Folder: **Property Models → General**
- File name: *PM_G_17_IN718_Columnar_Equiaxed_Transition.tcu*

To run this example requires a license for the TCS Ni-based Superalloys Database (TCNI) version 12 (TCNI12) or newer and the TCS Ni-alloys Mobility Database (MOBNI) version 6 (MOBNI6) or newer.

Example PM_G_15: Columnar to Equiaxed Transition (CET) of a NiAlCr Alloy uses demo databases available to everyone.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

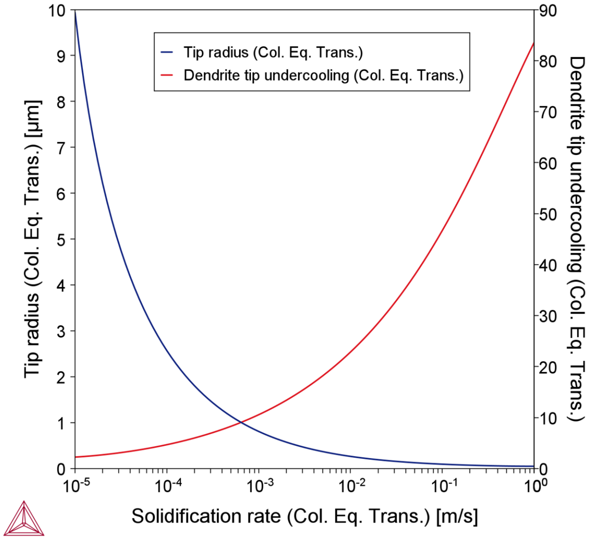


Figure 56: Tip radius and undercooling vs growth velocity for an IN718 alloy.

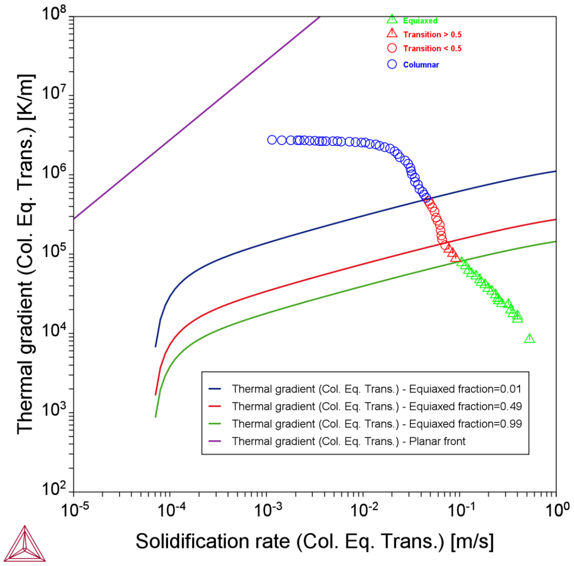


Figure 57: Calculated CET curves for IN718 in comparison with literature data [2020Pol].

Reference

[2020Pol] A. T. Polonsky, N. Raghavan, M. P. Echlin, M. M. Kirka, R. R. Dehoff, T. M. Pollock, 3D Characterization of the Columnar-to-Equiaxed Transition in Additively Manufactured Inconel 718, in Superalloys 2020 (2020), pp. 990–1002.

More Information

Also see these examples that use the same Property Model: PM_G_15: Columnar to Equiaxed Transition (CET) of a NiAlCr Alloy and PM_G_16: Columnar to Equiaxed Transition of a CMSX-4 Alloy.

Additive Manufacturing (AM) Module Examples Collection

A separate license is required to perform calculations with the Additive Manufacturing (AM) Module. Without a license you are in *Demo Mode* where you can, for example, open and view example set ups, run some examples, add templates and nodes to the Project window, adjust some Configuration settings, and preview some functionality on the Visualizations window.

Read more about the Additive Manufacturing (AM) Module on our website including the details about database compatibility or to watch an introductory webinar. You can also use the Getting Started Guide to learn about the key features available.

In this section:

AM_01: Transient Simulation of a Single Track

The following example is part of a series showing some of the features of the Additive Manufacturing (AM) Module and the **AM Calculator**. In this example, a single track simulation is performed using the **Transient** model of the AM Calculator.

Project File and License Information

- Folder: **Additive Manufacturing**
- File name: `AM_01_Transient_DE_No_Marangoni.tcu`

A separate license is required to perform calculations with the Additive Manufacturing (AM) Module. Without a license you are in *Demo Mode* where you can, for example, open and view example set ups, run some examples, add templates and nodes to the Project window, adjust some Configuration settings, and preview some functionality on the Visualizations window.

Some examples (AM_01, AM_02, AM_03, and AM_06b) are available to all users. These examples can be run without an additional Additive Manufacturing license when you are in DEMO (demonstration) mode. However, the AM Module is not available with the Educational version of Thermo-Calc. Search the help for Available Options with the Additive Manufacturing (AM) Module. See Available Options for details.

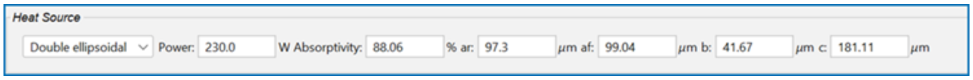
Material Properties

These properties are the same for both AM_01 and AM_02 [2021Gra].

- Inconel 738LC: Ni-15.8 Cr-8.6 Co-2.7 W-3.3 Ti-3.6 Al-1.8 Ta-1.8 Mo-0.04 Fe-0.8 Nb-0.002 Mn-0.1 C Mass percent.
- Database: TCNI12
- The material property was pre-calculated, and stored as a built-in material library of the Additive Manufacturing (AM) Module.

Model Configuration

The transient model solves for the heat equation in the entire 3D domain, including the melt pool, and is therefore, computationally expensive to solve. The fluid flow inside the melt pool due to the Marangoni effect is not included in this example. The double ellipsoidal, or the so-called Goldak heat source model, is used to predict melt pool size and temperature distribution during single track scanning. The parameters for the double ellipsoidal heat source are computed using optimization in a steady-state case for the given process parameters (power and scanning speed) and the melt pool size reported in the paper by Grange et al. [2021Gra]. The resulting parameters are shown in Figure 58.


Heat Source

Double ellipsoidal | Power: 230.0 W | Absorptivity: 88.06 % | ar: 97.3 µm | af: 99.04 µm | b: 41.67 µm | c: 181.11 µm

Figure 58: Optimized heat source parameters entered on the AM Calculator for the experiment given in Grange et al. [2021Gra] with power = 230 W and scanning speed = 960 mm/s.

The geometry for a transient simulation, as given in the paper by Grange et al. [2021Gra], is shown in Figure 59. The base plate is 2 mm in length, 0.5 mm in width, and with a thickness of 0.95 mm. A layer of powder with a thickness of 55 µm is deposited on the solid substrate. The powder layer, however, has the same material properties as the solid substrate. The laser beam with a power of 230 W develops linear scanning with constant velocity 960 mm/s. The trajectory evolves from initial position (x, y) = (0.25, 0.25) mm to final position (1.75, 0.25) mm on the top surface.

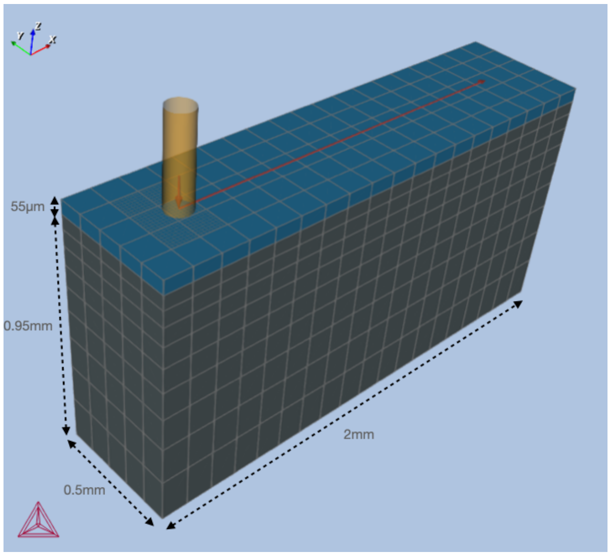
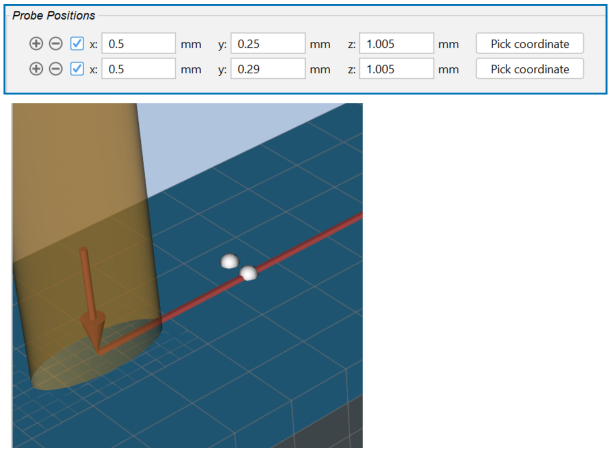


Figure 59: The geometry used for the Additive Manufacturing (AM) Module examples AM_01 and AM_02.

Two probes monitor the temporal evolution of temperature at positions shown in Figure 60. The results can be presented by tabulated data or as 2D graph plots.



Probe Positions

☑ x: 0.5 mm y: 0.25 mm z: 1.005 mm

☑ x: 0.5 mm y: 0.29 mm z: 1.005 mm

Figure 60: Probe positions for Probes P1 and P2, where P1 is placed exactly on the scanning track while P2 is placed at a distance of 0.04 mm from the track, as shown in a close up of the probes on the Visualizations window.

Visualizations

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

⌛ When you run (Perform) this example, it takes at least 30 minutes for the calculations to complete.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation(s).

- **Geometry**: View the geometry and adjust parameters visually by changing inputs on the Configuration window. Add probes needed.
- Melt pool and other dynamically changing features can also be visualized and changed.

- **Plot** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, click a **Plot Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

In the surface plot it shows the temperature distribution after the scanning process is completed. It is noted that the melt pool shape reaches a steady-state when the laser beam approaches the end of the scanning track. The melt pool dimensions at the end of scanning track is given in the table.

Melt Pool Dimension	*Size (mm)*
Width	0.125
Depth	0.144
Length	1.12

If you are in the project file, click the **Probe plot** node in the Project window and the **3D Plot** tab in the Visualizations window.

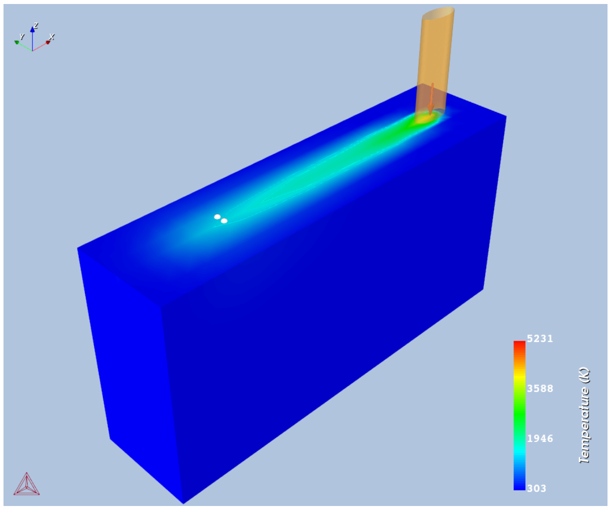


Figure 61: Surface plot of temperature distribution after the single track scan is completed. Probes P1 and P2 can also be seen on the top surface.

It is also possible to plot quantities at different cross-sections inside the domain by selecting the **Slice** checkbox on the **Plot Renderer Configuration** window under the **3D Plot** tab. The next figure shows the temperature slices plotted at cross-sections orthogonal to the scanning direction.

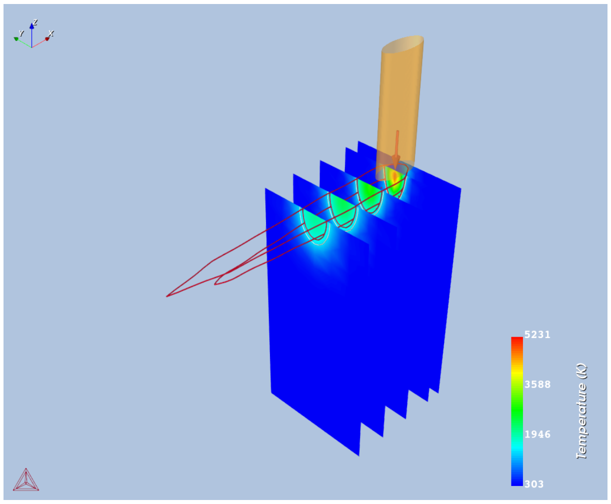


Figure 62: Slices of the computational domain, orthogonal to the scanning direction, showing temperature distribution at different cross-sections. Red tubes show the contour of the melt pool (at liquidus temperature).

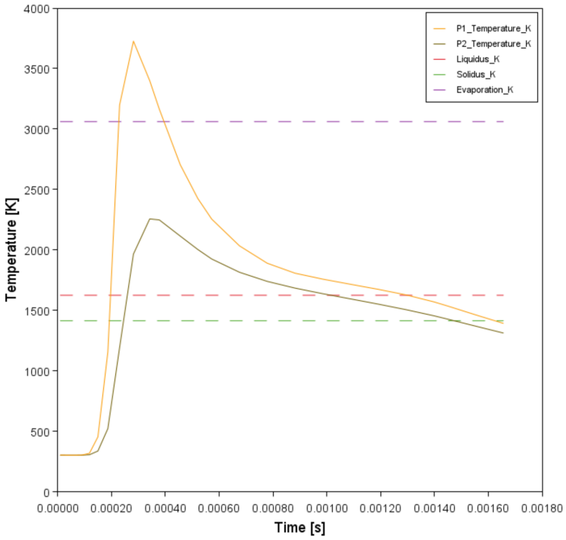


Figure 63: 2D probe plot showing temperature evolution as a function of time at probes P1 and P2.

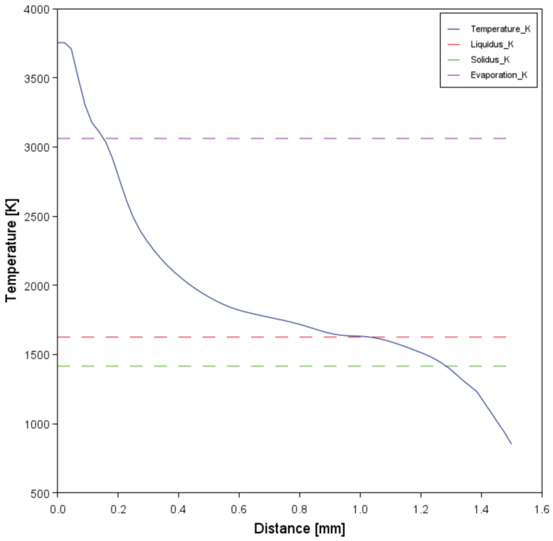


Figure 64: 2D plot over line showing temperature in the tail of the melt pool as a function of distance plotted along the scanning track.

Reference

[2021Gra] D. Grange, A. Queva, G. Guillemot, M. Bellet, J.-D. Bartout, C. Colin, Effect of processing parameters during the laser beam melting of Inconel 738: Comparison between simulated and experimental melt pool shape. J. Mater. Process. Technol. 289, 116897 (2021).

Other Resources

Read more about the Additive Manufacturing (AM) Module on our website including the details about database compatibility or to watch an introductory webinar. You can also use the Getting Started Guide to learn about the key features available.

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

AM_02: Transient and Steady-state Simulations of a Single Track

The following example is part of a series showing some of the features of the Additive Manufacturing (AM) Module and the **AM Calculator**. This example builds on the work done by Grange et al. [2021Gra] and is similar to example AM_01. The difference however is that in this example a single track simulation is performed using **Transient with heat source from Steady-state** model instead of the **Transient** model.

The **Transient with heat source from Steady-state** model exploits the assumption that the melt pool size and temperature distribution reaches a steady-state almost instantly and thus first solves for a **Steady-state** case with the given process parameters. The result from the **Steady-state** in the form of temperature distribution in the melt pool is then mapped as a heat source in the transient simulation. This novel approach is much faster and efficient than the approach used in example AM_01 where the heat equation is solved in the entire 3D domain.

Project File and License Information

- Folder: **Additive Manufacturing**
- File name: `AM_02_TransientSS_DE.tcu`

A separate license is required to perform calculations with the Additive Manufacturing (AM) Module. Without a license you are in *Demo Mode* where you can, for example, open and view example set ups, run some examples, add templates and nodes to the Project window, adjust some Configuration settings, and preview some functionality on the Visualizations window.

Some examples (AM_01, AM_02, AM_03, and AM_06b) are available to all users. These examples can be run without an additional Additive Manufacturing license when you are in DEMO (demonstration) mode. However, the AM Module is not available with the Educational version of Thermo-Calc. Search the help for Available Options with the Additive Manufacturing (AM) Module. See Available Options for details.

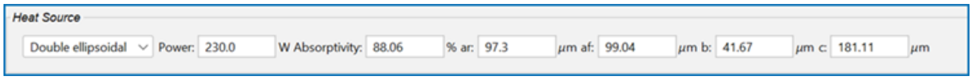
Material Properties

These properties are the same for both AM_01 and AM_02 [2021Gra].

- Inconel 738LC: Ni-15.8 Cr-8.6 Co-2.7 W-3.3 Ti-3.6 Al-1.8 Ta-1.8 Mo-0.04 Fe-0.8 Nb-0.002 Mn-0.1 C Mass percent.
- Database: TCNI12
- The material property was pre-calculated, and stored as a built-in material library of the Additive Manufacturing (AM) Module.

Model Configuration

The transient model solves for the heat equation in the entire 3D domain, including the melt pool, and is therefore, computationally expensive to solve. The fluid flow inside the melt pool due to the Marangoni effect is not included in this example. The double ellipsoidal, or the so-called Goldak heat source model, is used to predict melt pool size and temperature distribution during single track scanning. The parameters for the double ellipsoidal heat source are computed using optimization in a steady-state case for the given process parameters (power and scanning speed) and the melt pool size reported in the paper by Grange et al. [2021Gra]. The resulting parameters are shown in Figure 65.



Double ellipsoidal
Power: 230.0 W
Absorptivity: 88.06 %
ar: 97.3 µm
af: 99.04 µm
b: 41.67 µm
c: 181.11 µm

Figure 65: Optimized heat source parameters entered on the AM Calculator for the experiment given in Grange et al. [2021Gra] with power = 230 W and scanning speed = 960 mm/s.

The geometry for a transient simulation, as given in the paper by Grange et al. [2021Gra], is shown in Figure 66. The base plate is 2 mm in length, 0.5 mm in width, and with a thickness of 0.95 mm. A layer of powder with a thickness of 55 µm is deposited on the solid substrate. The powder layer, however, has the same material properties as the solid substrate. The laser beam with a power of 230 W develops linear scanning with constant velocity 960 mm/s. The trajectory evolves from initial position (x, y) = (0.25, 0.25) mm to final position (1.75, 0.25) mm on the top surface.

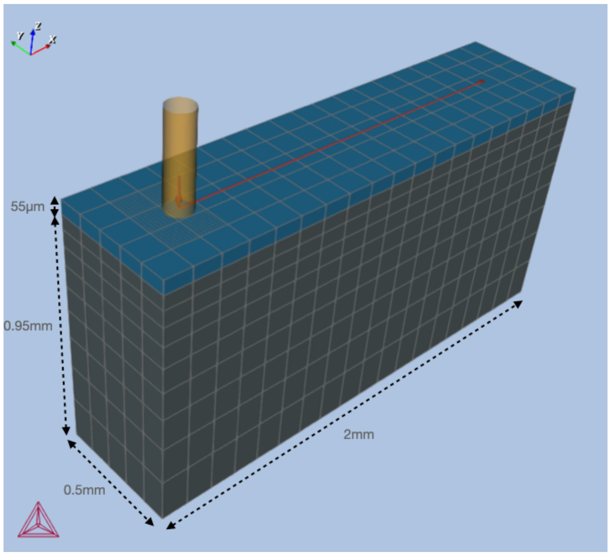
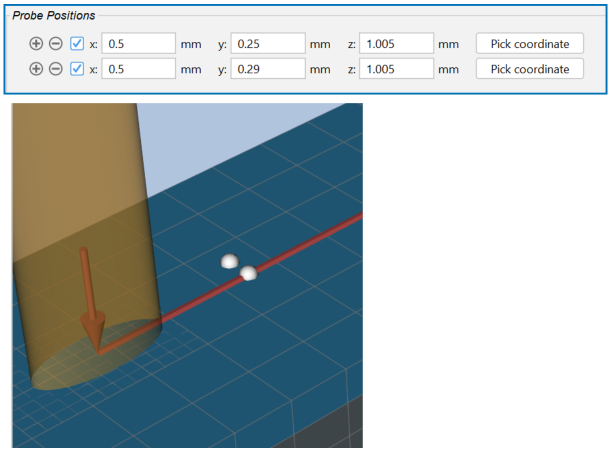


Figure 66: The geometry used for the Additive Manufacturing (AM) Module examples AM_01 and AM_02.

Two probes monitor the temporal evolution of temperature at positions shown in Figure 67. The results can be presented by tabulated data or as 2D graph plots.



Probe Positions

☑ x: 0.5 mm y: 0.25 mm z: 1.005 mm Pick coordinate
☑ x: 0.5 mm y: 0.29 mm z: 1.005 mm Pick coordinate

Figure 67: Probe positions for Probes P1 and P2, where P1 is placed exactly on the scanning track while P2 is placed at a distance of 0.04 mm from the track, as shown in a close up of the probes on the Visualizations window.

Visualizations

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects,

you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation(s).

- **Geometry**: View the geometry and adjust parameters visually by changing inputs on the Configuration window.
- Melt pool and other dynamically changing features can also be visualized and changed.
- **Plot** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, click a **Plot Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

With the example open and after it is run, the following is a summary of what is visible on the **Visualizations**window.

The figure below shows the surface plot of temperature distribution after the single track scanning is completed. The temperature profile is qualitatively similar to the one in example AM_01, however the maximum temperature is slightly lower in example AM_02. This could be due to selection of a coarse mesh in both examples which sometimes could affect the maximum temperature.

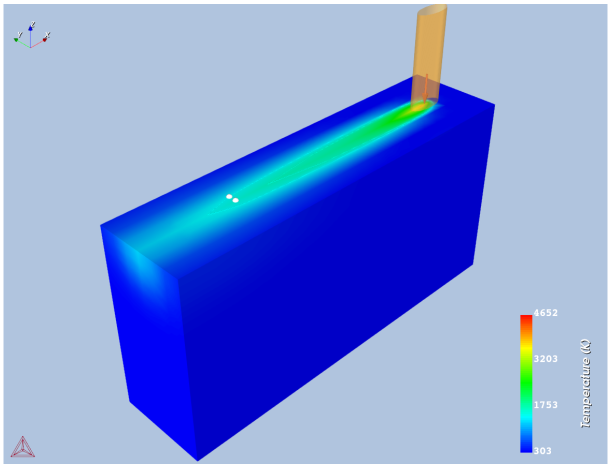


Figure 68: Surface plot of temperature distribution after the single track scan is completed. Probes P1 and P2 can also be seen on the top surface.

The melt pool dimensions for AM_02 are given in the following table, which are very similar to the melt pool dimensions obtained in example AM_01.

Melt Pool Dimension	***Size (mm)***
Width	0.127
Depth	0.129
Length	1.12

A qualitative comparison between AM_01 and AM_02 can also be made by looking at probe plots. The probe plot for AM_02 is given in Figure 69.

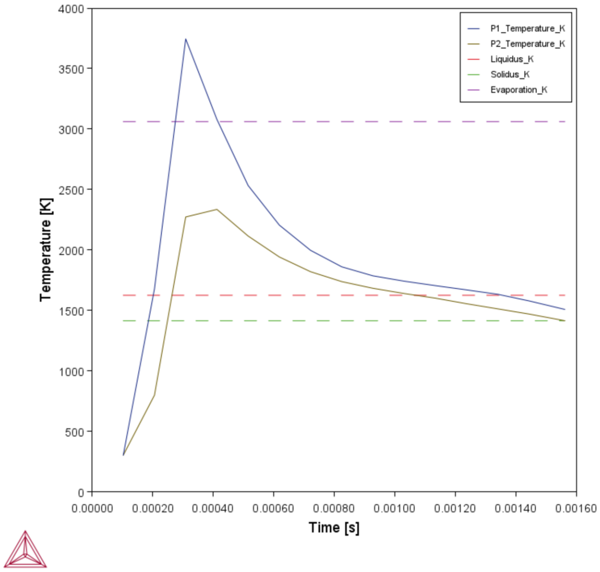


Figure 69: 2D probe plot showing temperature evolution as a function of time at probes P1 and P2.

Despite the fact that maximum temperature is higher in AM_01, the temperature profile in the tail of the melt pool and close to the melt pool is very similar. This can also be concluded by comparing plot over lines for the two examples, where the plot over line for AM_02 is given in Figure 70.

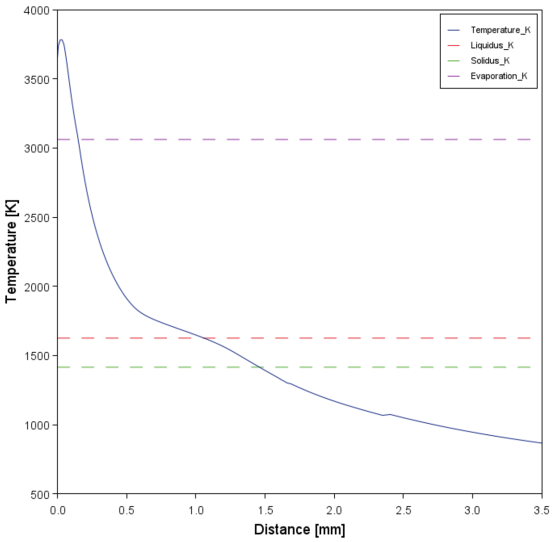


Figure 70: 2D plot over line showing temperature in the tail of the melt pool as a function of distance plotted along the scanning track.

Reference

[2021Gra] D. Grange, A. Queva, G. Guillemot, M. Bellet, J.-D. Bartout, C. Colin, Effect of processing parameters during the laser beam melting of Inconel 738: Comparison between simulated and experimental melt pool shape. J. Mater. Process. Technol. 289, 116897 (2021).

Other Resources

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AM_03: Steady-state Simulations

The following example is part of a series showing some of the features of the Additive Manufacturing (AM) Module and the **AM Calculator**.

In this example steady-state simulations are performed for IN625 with different conditions i.e.

i. without fluid flow in the melt pool,
ii. with fluid flow in the melt pool due to Marangoni effect, and
iii. using separate material properties for the powder.

and then the results are compared to demonstrate the effects of fluid flow and separate material properties for the powder on the temperature distribution as well as on the shape of the melt pool.

> For the first two simulations, the same material properties are used for both powder and solid substrate while for the third simulation no fluid flow is included in the melt pool.

> In steady-state simulations it is assumed that the heat source (laser beam) moves with a uniform speed relative to the base plate. In this case, the model is solved by modifying governing equations to a reference frame attached to a moving heat source. Furthermore, in steady-state mode you can make use of symmetry along the width of the geometry and solve for only half of the domain.

Project File and License Information

- Folder: **Additive Manufacturing**
- File name: `AM_03_Steady.tcu`

A separate license is required to perform calculations with the Additive Manufacturing (AM) Module. Without a license you are in *Demo Mode* where you can, for example, open and view example set ups, run some examples, add templates and nodes to the Project window, adjust some Configuration settings, and preview some functionality on the Visualizations window.

Some examples (AM_01, AM_02, AM_03, and AM_06b) are available to all users. These examples can be run without an additional Additive Manufacturing license when you are in DEMO (demonstration) mode. However, the AM Module is not available with the Educational version of Thermo-Calc. Search the help for Available Options with the Additive Manufacturing (AM) Module. See Available Options for details.

Visualizations

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation(s).

- **Geometry**: View the geometry and adjust parameters visually by changing inputs on the Configuration window.
- Melt pool and other dynamically changing features can also be visualized and changed.
- **Plot** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, click a **Plot Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

Results Discussion

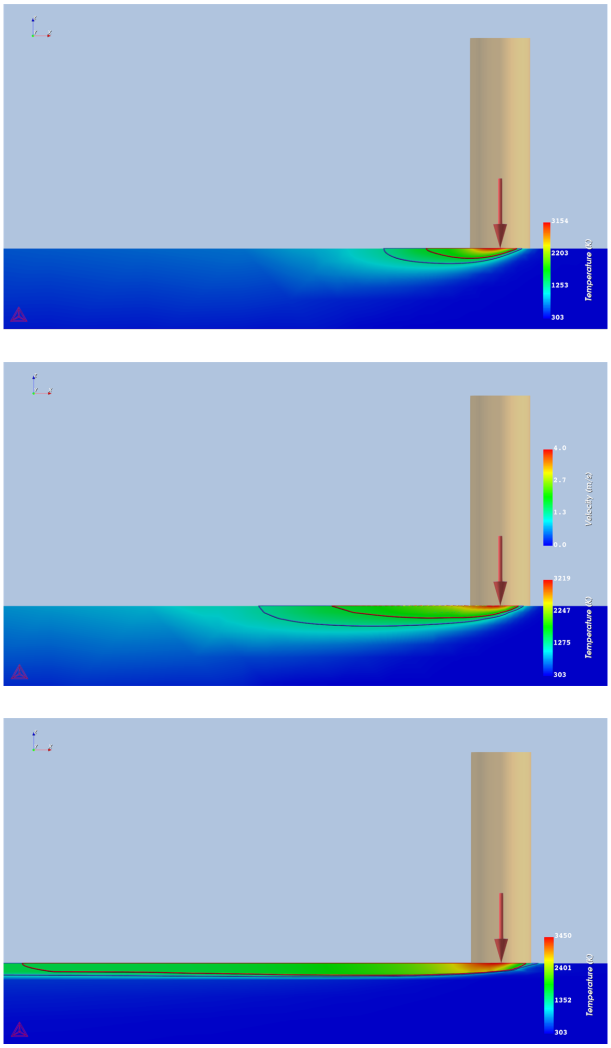

Figure 71: A comparison of the melt pool depth for different simulation conditions; (top) without fluid flow, (middle) with fluid flow in the melt pool and (bottom) with different material properties for the powder layer. Isocontours show the boundaries of (inner) melt pool and (outer) mushy zone.

The table shows a comparison of the melt pool dimensions for different simulation conditions.

Simulation set up	***Melt Pool Dimensions (mm)***		
	Width	***Depth***	***Length***
Without fluid flow	0.156	0.032	0.300
With fluid flow	0.188	0.040	0.619
Separate powder material properties	0.250	0.039	1.670

Figure 71 shows the effect of fluid flow on temperature distribution and size of the melt pool for the given process parameters. A quantitative comparison is also given in the table. It can be seen that with the addition of fluid flow due to gradient in surface tension (Marangoni effect), the melt pool tends to increase its dimensions in all three directions. This is because the negative gradient in surface tension with respect to the temperature creates an outward flow on the surface of the melt pool which consequently increases the width and length of the melt pool, as shown in Figure 72.

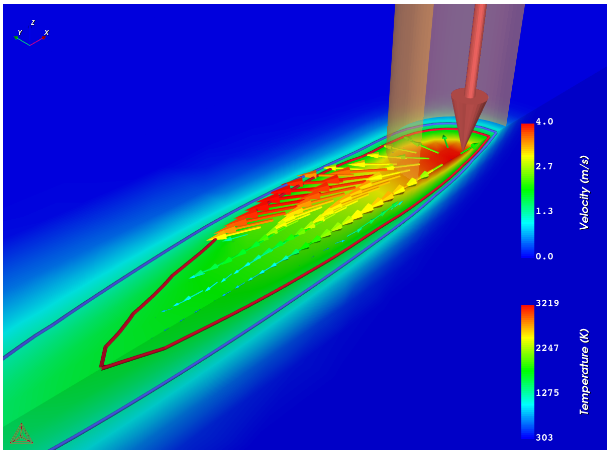

Figure 72: Vectors showing flow field in the melt pool due to gradient in surface tension. The colours of the vectors represent the magnitude of the velocity. Surface colormap shows the temperature distribution.

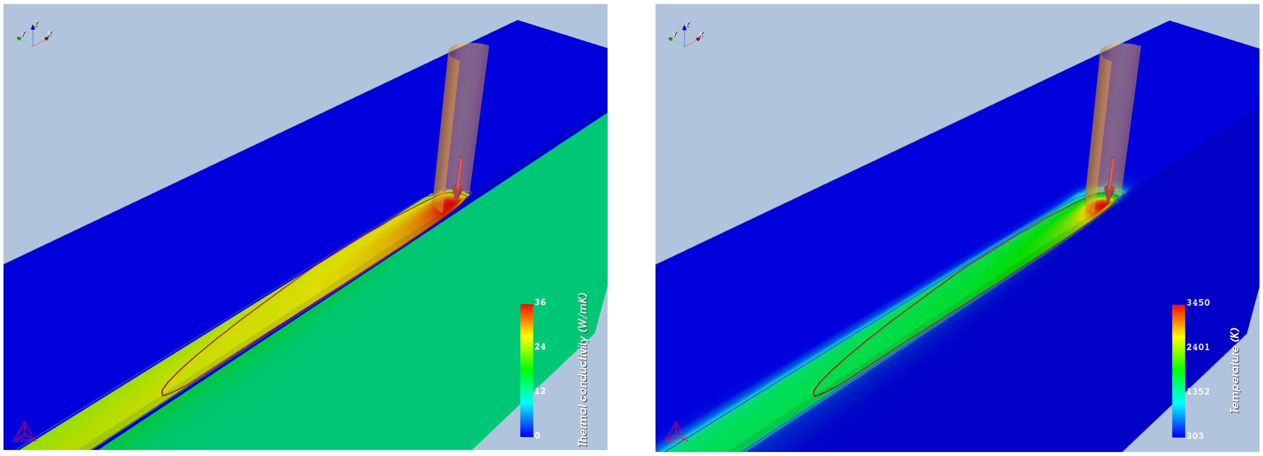

Figure 73: (left) Surface colormap of temperature dependent thermal conductivity showing different values in powder and liquid/solid and (right) the corresponding temperature distribution.

Using separate material properties for powder has a significant effect on both the temperature distribution and the size of the melt pool. This is because a lower thermal diffusivity in the powder makes the temperature to diffuse more towards the length of the melt pool hence causing a significant increase in the length of the melt pool (shown in Figure 73) as compared to the first two cases. There is also an obvious increase in the width of the melt pool while the depth of the melt pool is almost the same as with the fluid flow. Furthermore, the maximum temperature is also highest in the case with separate material properties.

Other Resources

Read more about the Additive Manufacturing (AM) Module on our website including the details about database compatibility or to watch an introductory webinar. You can also use the Getting Started Guide to learn about the key features available.

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AM_04: Scheil Transient Steady-state

In this example, three different simulations are performed: Steady-state, Transient Single track, and Transient Multilayer. Both Transient Single track and Transient Multilayer use **Transient with heat source from Steady-state** model to compute time-dependent temperature distribution in the given geometry. The primary difference between this example and the previous examples (AM_01 to AM_03) is that, in this case, the material properties data is retrieved from the Scheil Calculator whereas in the previous examples the material properties are taken from the preinstalled material library. Furthermore, this example simulates scanning of two layers of powder where the second layer is spread on the top of the first layer when scanning of the first layer is completed.

Project File and License Information

- Folder: **Additive Manufacturing**
- File name: `AM_04_Scheil_TransientSS.tcu`

Material chosen for this example is Ti-6Al-4V. To run this example requires both version TCTI5.0 and newer of the TCS Ti/TiAl-based Alloys Database (TCTI) in addition to a license for the Additive Manufacturing (AM) Module. Some portions of this example are also covered in the Getting Started Guide on our website.

Visualizations

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

When you run (Perform) this example, it takes at least 30 minutes for the calculations to complete.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation(s).

- **Geometry**: View the geometry and adjust parameters visually by changing inputs on the Configuration window.
- Melt pool and other dynamically changing features can also be visualized and changed.
- **Plot** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, click a **Plot Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

Steady-state

The Steady-state calculator of this example computes temperature distribution in a steady state for the power of 100 W and scanning speed of 600 mm/s. The beam radius in this example is taken as 100 µm. For the geometry, the steady-state model only needs the height of the solid substrate as the input, which is taken as 2.0 mm. The solid substrate is covered with a powder layer of thickness 55 µm. This example also takes into account the effect of fluid flow due to Marangoni forces inside the melt pool.

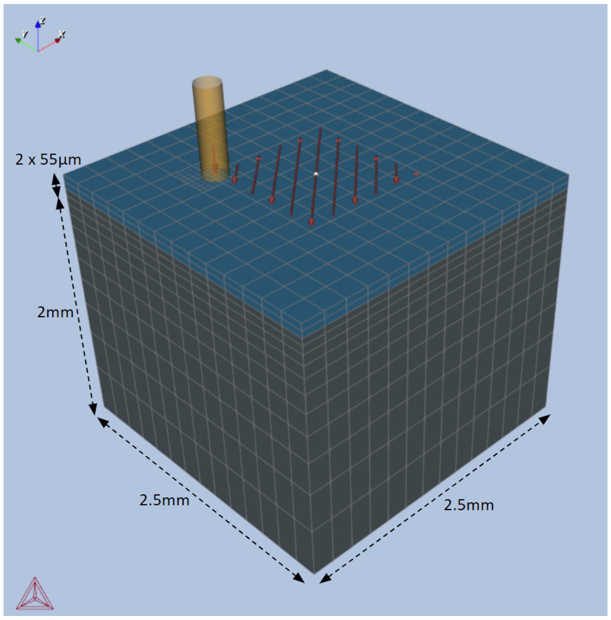

Figure 74: Geometry definition for Transient Multilayer. The scanning strategy shows the scanning pattern on the top most layer.

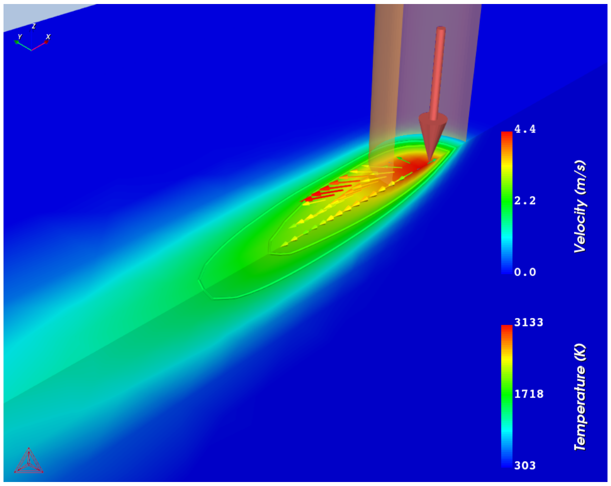

Figure 75: Temperature distribution around the melt pool and mushy zone for the Steady-state case. Velocity vectors representing the fluid flow inside the melt pool can also be seen.

Transient Single Track

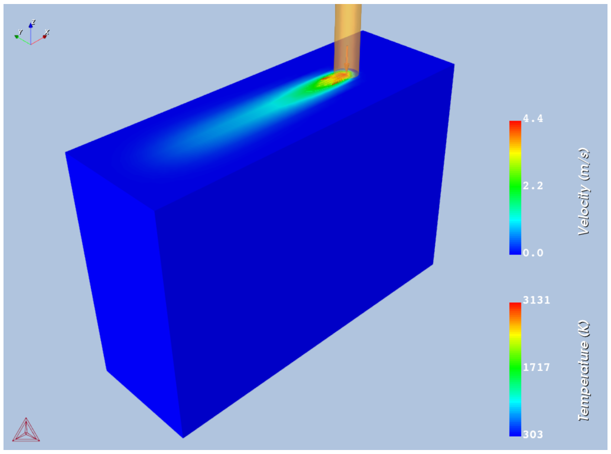

Figure 76: 3D Surface colormap showing temperature distribution at the end of single track transient simulation. The velocity vectors around the heat source show the direction of fluid flow in the melt pool.

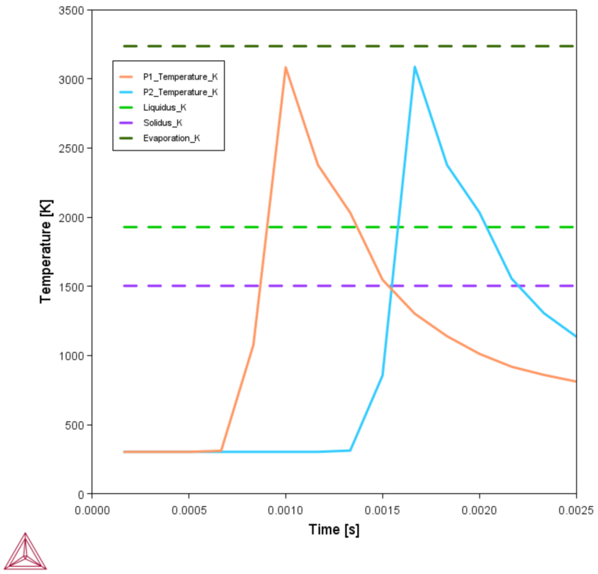

Figure 77: 2D Plot showing temperature as a function of time from Probe 1 (orange) and Probe 2 (blue) after the single track scan is completed.

Transient Multilayer

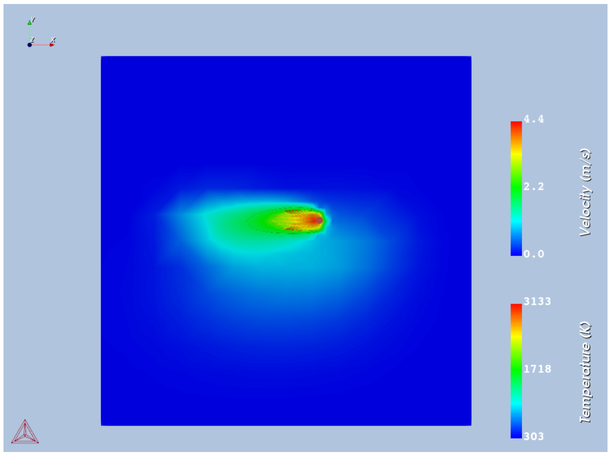

Figure 78: Temperature distribution on the top surface of the workpiece during scanning of the first layer.

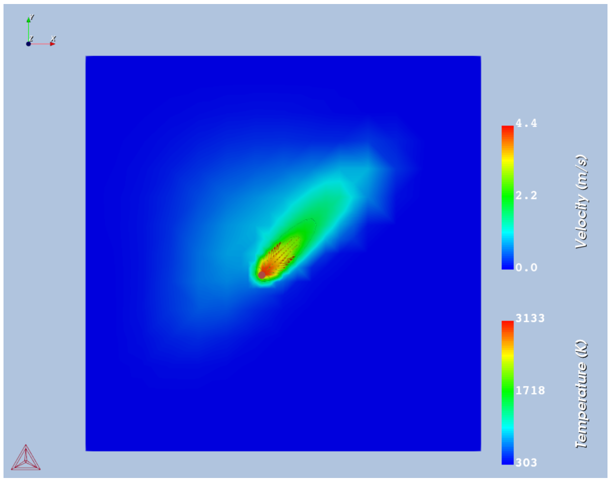

Figure 79: Temperature distribution on the top surface of the workpiece during scanning of the second layer.

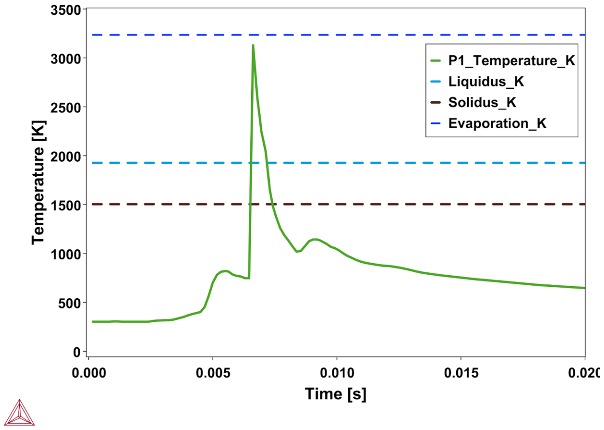

Figure 80: 2D Plot showing temperature as a function of time from Probe 1 after scanning the first layer.

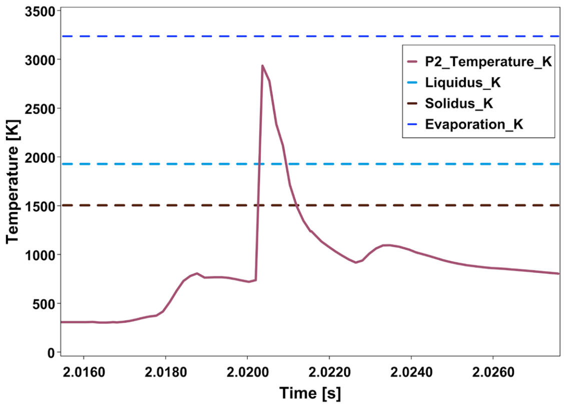

Figure 81: 2D Plot showing temperature as a function of time from Probe 2 after scanning the second layer.

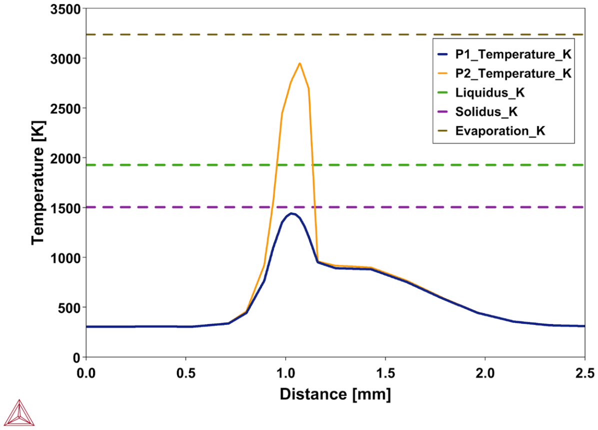

Figure 82: 2D Plot Over Line showing temperature profiles plotted along the lines, parallel to the width of the geometry placed on the top of the first layer (P1) and the second layer (P2).

Other Resources

Read more about the Additive Manufacturing (AM) Module on our website including the details about database compatibility or to watch an introductory webinar. You can also use the Getting Started Guide to learn about the key features available.

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AM_05: Using AM Calculator Probe Data with the Diffusion Module (DICTRA)

The microstructure of a hot-work tool steel additively manufactured using laser powder-bed fusion (L-PBF) is studied in detail by microstructure characterization and computational thermodynamics and kinetics by C.-Y. Chou et al. [2021Cho].

This example demonstrates the application of adding probes to an AM Calculator and then using this data via the Thermal Profile that is set up on a connected Diffusion Calculator. The example also uses a Scheil Calculator to collect some materials data that is then further used with the AM Calculator prior to using the probe data generated by the AM Calculator.

Project File and License Information

- Folder: **Additive Manufacturing**
- File name: `AM_05_AM_Probe_to_Diffusion.tcu`

A separate license is required to perform calculations with the Additive Manufacturing (AM) Module. This example also requires a license for the Diffusion Module (DICTRA), plus additional database licenses for the TCS Steel and Fe-alloys Database (TCFE) (TCFE13 and newer), and the TCS Steels/Fe-Alloys Mobility Database (MOBFE) (MOBFE8 and newer).

Background

According to the thermodynamics of this steel, δ-ferrite is the solid phase stable at the highest temperature and would be the first solid phase to form during solidification from a thermodynamic point of view, see Figure 83.

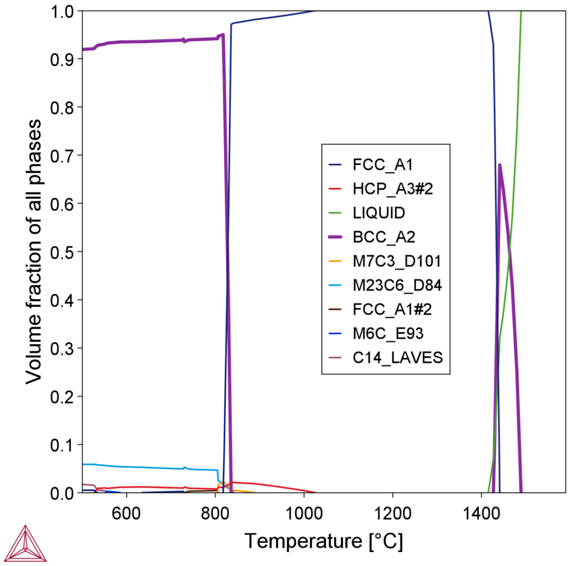


Figure 83: Equilibrium property diagram calculated in Thermo-Calc of the tool steel showing δ-ferrite would be the first solid phase to form during solidification according to equilibrium.

However, the high solidification and cooling rates during the L-PBF process lead to suppression of δ-ferrite and instead solidification of an austenite phase directly containing a cellular substructure where the alloying elements have segregated to the inter-cellular regions.

The microsegregation can be predicted by reducing the complex solidification behavior to a diffusion problem in one dimension enabling comparisons with the measured segregation profiles quantified at a nanometer scale.

Configuration and Calculation Set Up

For all calculations, the simplified composition Fe-0.35C-4.93Cr-0.45Mn-2.24Mo-0.25Si-0.54V (mass%) was used with δ-ferrite suspended on the System Definer.

The **Additive Manufacturing** template was used to first add the **System Definer**, **Scheil Calculator**, **AM Calculator**, and **Plot Renderer** to the **Project** window tree. Additionally, a **Diffusion Calculator** was added as a successor to the AM Calculator in order to automatically import the time-temperature profile from the AM simulation into the diffusion simulation. See Figure 84 (or refer to the example if you have it open) to see the layout.

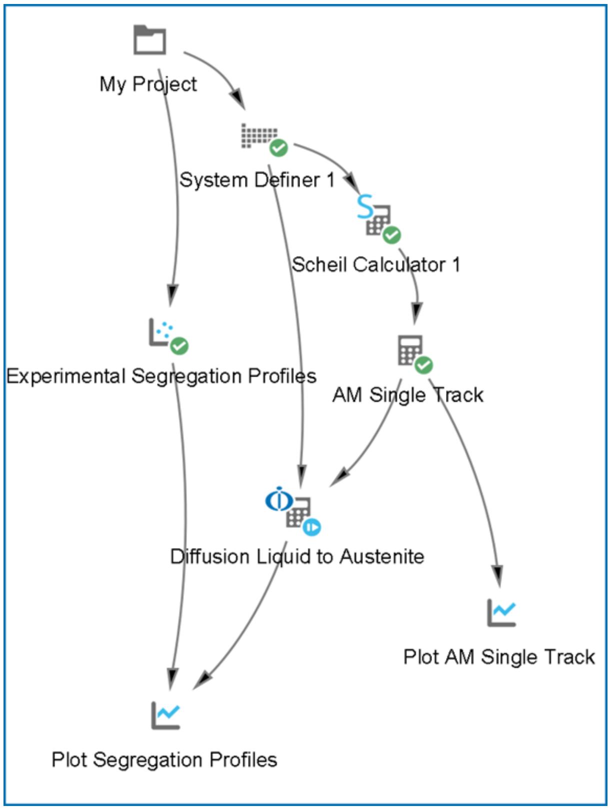
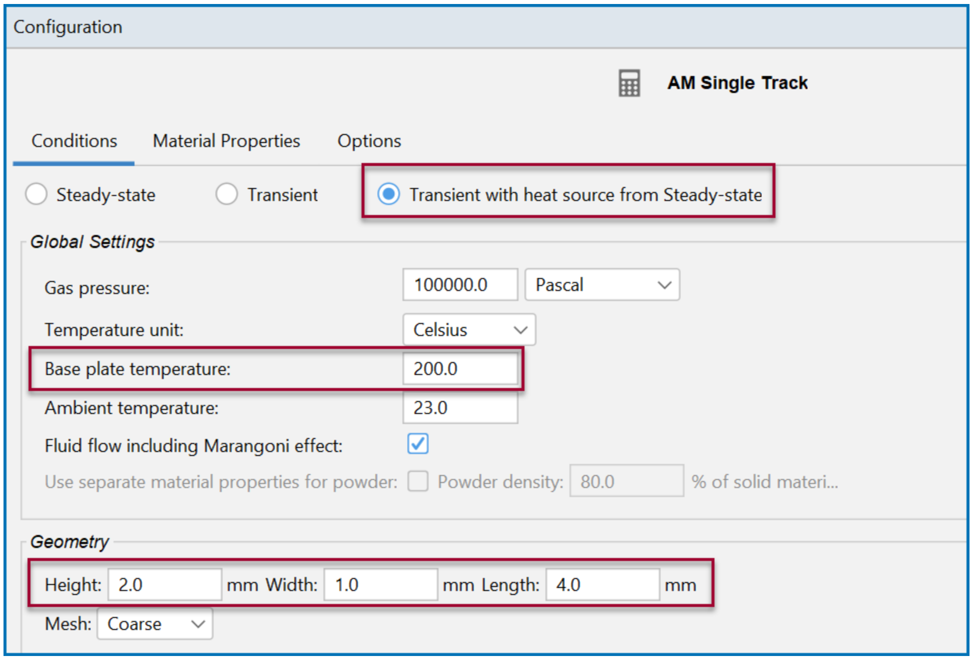


Figure 84: Project tree of the example containing activities from the default Additive Manufacturing template with additional Diffusion Calculator and Experimental File Reader nodes added, where the segregation profiles datasets are pulled from the Experimental File Reader.

On the **AM Calculator Configuration** window, the calculation type **Transient with heat source from Steady-state** is selected with a single track scan pattern and a **Geometry** of 2 mm x 1 mm x 4 mm (height x width x length). The **Base plate temperature** is set to 200 °C.



○ Steady-state ○ Transient ● Transient with heat source from Steady-state

Global Settings

Gas pressure: 100000.0 Pascal

Temperature unit: Celsius

Base plate temperature: 200.0

Ambient temperature: 23.0

Fluid flow including Marangoni effect: ☑

Use separate material properties for powder: ☐ Powder density: 80.0 % of solid materi...

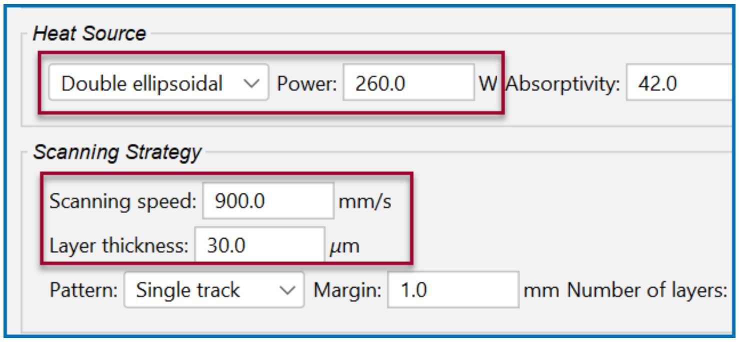
Geometry

Height: 2.0 mm Width: 1.0 mm Length: 4.0 mm

Mesh: Coarse

Additional settings are then made on the **Configuration** window as follows.

The **Double ellipsoidal** volume heat source was previously assessed as a function of linear energy density for a similar material and directly applied to the experimental conditions of a volumetric energy density of 80 J/mm^3. The laser **Power** is entered at 260 W, **Scanning speed** at 900 mm/s, and powder **Layer thickness** 30 µm. Below is a snapshot of the settings.



Heat Source

Double ellipsoidal Power: 260.0 W Absorptivity: 42.0

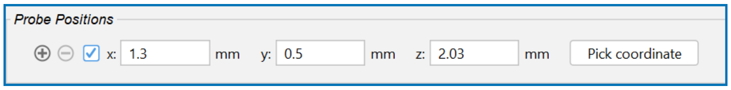
Scanning Strategy

Scanning speed: 900.0 mm/s

Layer thickness: 30.0 µm

Pattern: Single track Margin: 1.0 mm Number of layers:

A probe was then added in the center of the scan track at a distance of 1.3 mm from the edge. The **Probe Positions** can either be entered directly on the Configuration window or click the **Pick coordinate** button and then click on the geometry in the **Visualizations** window to directly choose the probe point (or points if there is more than one probe added).



☑ x: 1.3 mm y: 0.5 mm z: 2.03 mm

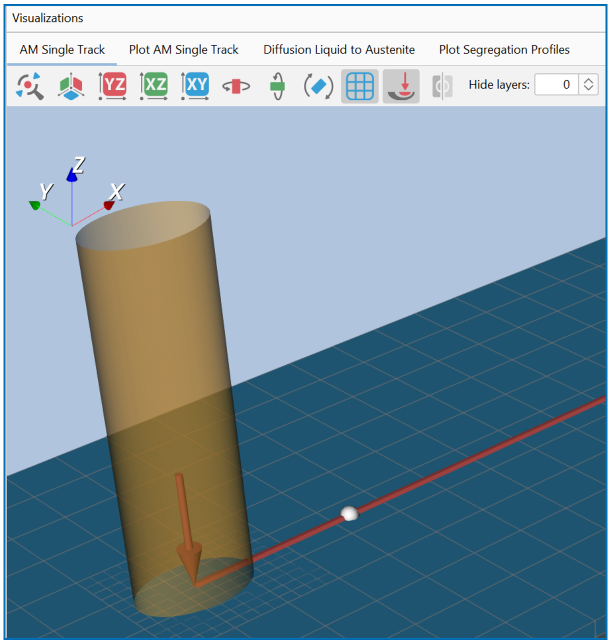


Figure 85: Close up of the probe point added to the geometry for the single track AM simulation.

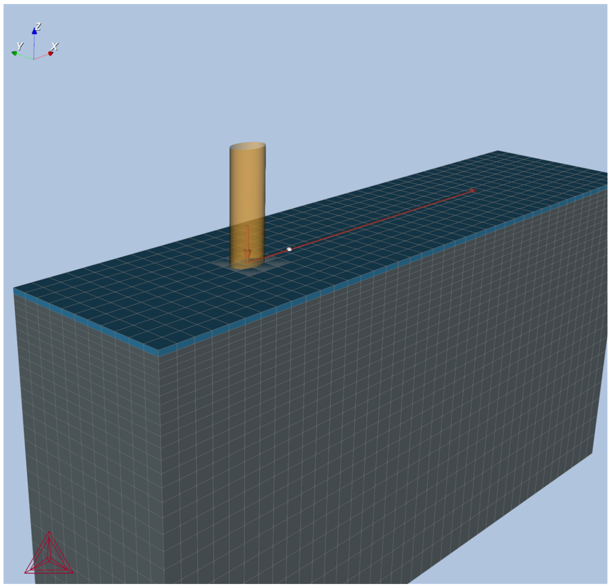
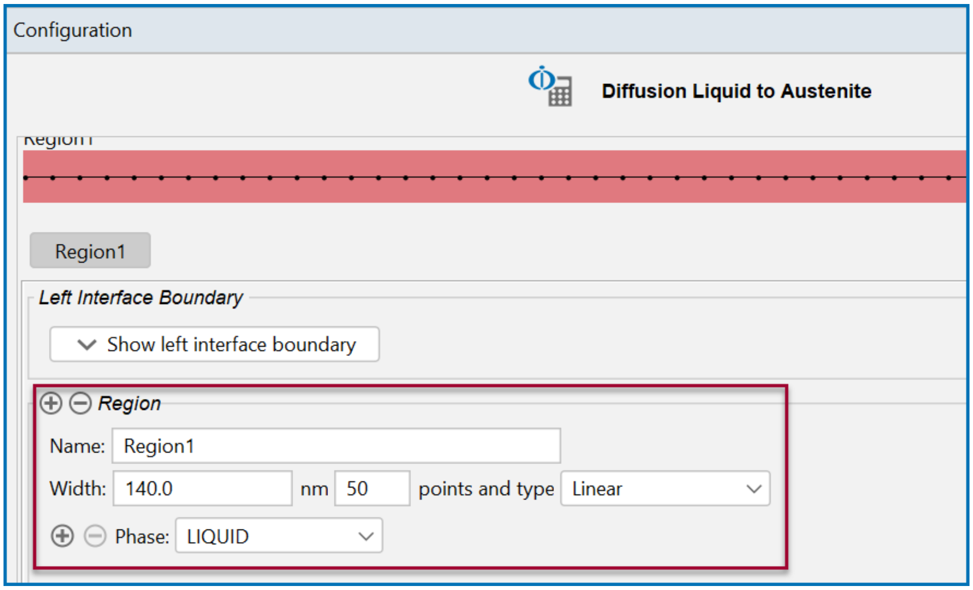


Figure 86: The full geometry set up for the single track AM simulation with a probe point added to the middle of the scan. Open the example to better see the set up and to try working within the window.

Diffusion Calculations

For the Diffusion Module (DICTRA) solidification calculations using the **Diffusion Calculator**, only the liquid to austenite (FCC) transformation was simulated. On the **Diffusion Calculator Configuration** window, a **Region** of 140 nm with liquid and FCC allowed to form at the right boundary is set.

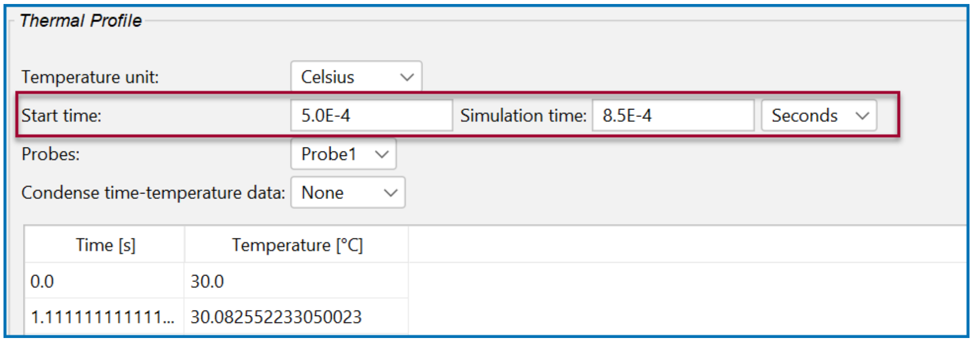


Name: Region1

Width: 140.0 nm 50 points and type Linear

Phase: LIQUID

In the *Thermal Profile* section, the time temperature from the probe was selected between a **Start time** of 5.0E-4 and **Simulation time** of 8.5.0E-4 s in order to only simulate the solidification, which can be viewed on the **Visualizations** window as in Figure 87. Note that the probes need to be added and then run in the AM Calculator to make this data available in for this part of the calculation.



Temperature unit: Celsius

Start time: 5.0E-4 Simulation time: 8.5E-4 Seconds

Probes: Probe1

Condense time-temperature data: None

Time [s]	Temperature [°C]
0.0	30.0
1.111111111111...	30.082552233050023

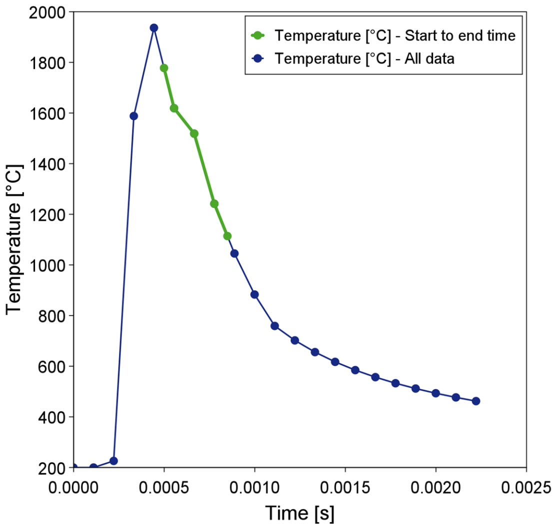


Figure 87: Time temperature profile of the probe in the AM simulation. The green curve show the part of the profile used during the diffusion simulation with the Diffusion Calculator.

The calculated segregation profiles are finally compared with the STEM-EDS line scans as shown in Figure 88.

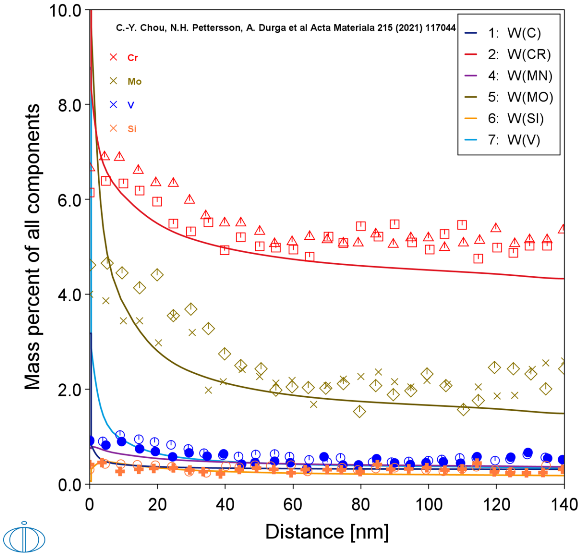


Figure 88: The simulated segregation profile with overlaid experimental STEM-EDS line scans from C.-Y. Chou et al. [2021Cho].

Visualizations

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

> When you run (Perform) this example, it can take over three hours to complete the calculations.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation(s). This example highlights some of these capabilities:

- **Probes**: Probes are added to the AM Calculator during the set up either by entering coordinates or directly adding these to the geometry. See Figure 85 and Figure 86 for example.
- **Thermal Profile**: The Diffusion Calculator Thermal Profile settings automatically include the probe data and you can visualize to help you continue the simulation. See Figure 87.
- **Plot** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, click a **Plot Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window. See Figure 88.

Reference

[2021Cho] C.-Y. Chou, N. H. Pettersson, A. Durga, F. Zhang, C. Oikonomou, A. Borgenstam, J. Odqvist, G. Lindwall, Influence of solidification structure on austenite to martensite transformation in additively manufactured hot-work tool steels. Acta Mater. 215, 117044 (2021).

Other Resources

Read more about the Additive Manufacturing (AM) Module on our website including the details about database compatibility or to watch an introductory webinar. You can also use the Getting Started Guide to learn about the key features available.

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AM_06a: Calibrating a Heat Source for a 316L Steel

This example demonstrates the calibration of the heat source using the Gaussian as well as Double ellipsoidal heat sources. In this example, experimental data is taken from Hu. et al. [2019Hu] where the authors performed single-track experiments using the selective laser melting (SLM) process on 316L stainless steel for varying processing conditions. The power ranges from 50 W to 100 W while the scanning speed varies from 400 mm/s to 2800 mm/s. The data imported from [2019Hu], consisting of 21 experimental points, is saved in the project file.

Also see the companion example, AM_06b: Using the Calibrated Heat Source for a 316L Steel.

Project File and License Information

- Folder: **Additive Manufacturing**
- File name: `AM_06a_Calibrate_Heat_Sources_316L.tcu`

An Additive Manufacturing Module license is needed to run AM_06a.

Some examples (AM_01, AM_02, AM_03, and AM_06b) are available to all users. These examples can be run without an additional Additive Manufacturing license when you are in DEMO (demonstration) mode. However, the AM Module is not available with the Educational version of Thermo-Calc. Search the help for Available Options with the Additive Manufacturing (AM) Module. See Available Options for details.

Material Properties

- SS316L: Fe-17.0Cr-12.0Ni-2.5Mo-0.03C Mass percent
- Database: TCFE13
- The material properties are precalculated, and stored as a built-in material library with the Additive Manufacturing (AM) Module.

AM Calculator Configuration Settings

The AM_06a example contains two AM Calculators, which are renamed to **AM Calibration Gaussian** and **AM Calibration Double Ellipsoidal**.

- **AM Calibration Gaussian** uses a **Gaussian** *Heat Source* with the **keyhole model**.
- **AM Calibration Double Ellipsoidal** uses a **Double ellipsoidal** *Heat Source*.
- The heat source parameters for both heat sources are calibrated for the given experimental data.
- For both AM Calculators, the **Base plate temperature** and the **Ambient temperature** use a value of 353 K and the **Layer thickness** is 10 µm. The rest of the Configuration settings keep the original defaults.

For **AM Calibration Gaussian**, all of the 21 experimental points that are imported to the *Experiment Data* table are selected to be used in the calibration. This is because, for the Gaussian heat source with the keyhole model, one wants to obtain a single constant value for beam radius as well as absorptivity to correctly predict the melt pool size for a range of power and scanning speed. It is also in order to obtain the best possible value it is good to include as many experiments as you can to calibrate the heat source parameters.

For this AM Calculator, other settings include:

- **Constant (calibrated)**, which means the absorptivity is not a function of temperature or angle, and a constant value is calibrated for each experiment.
- The **Beam radius** is set to **Calibrated**, which means that both beam radius and absorptivity are calibrated.
- **Calibrate for** is set to **Width and depth**, which means that the experimental values for both width and depth are used for calibration.

For **AM Calibration Double Ellipsoidal**, only five (5) experiment points are selected to perform the calibration. Two experiments are selected from the lower energy density, two from the higher energy density, and then one experiment is selected in the middle region of the two extremes.

Visualizations

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

When you run (Perform) this example, it can take about an hour to complete the calculations.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation(s).

See Visualizing Heat Source Calibrations for an extended overview of what is available and how to navigate the many options for visualizing the heat source calibration data.

Calibrated Functions

For **AM Calibration Gaussian**, a comparison of the melt pool dimensions from the experiments and calibration simulation is shown in Figure 89.

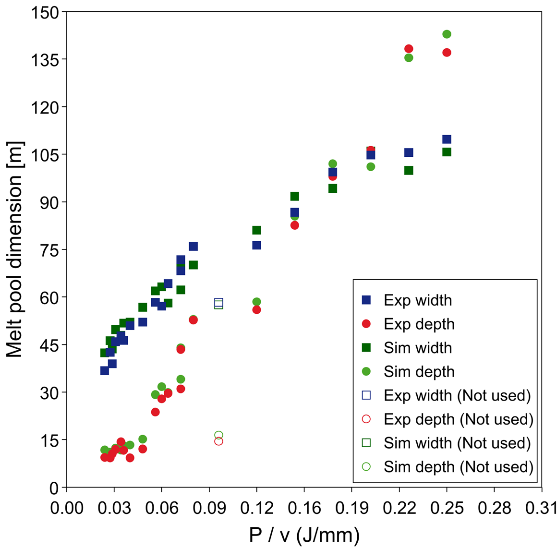

Figure 89: A comparison of melt pool dimension for Gaussian heat source calibration. The "Not used" points shown in the legend are because a checkbox is not selected in the 'Use' column for row 10 on the Plot Renderer Configuration window.

The resulting calibrated heat source parameters for **AM Calibration Gaussian**, are shown in Figure 90.

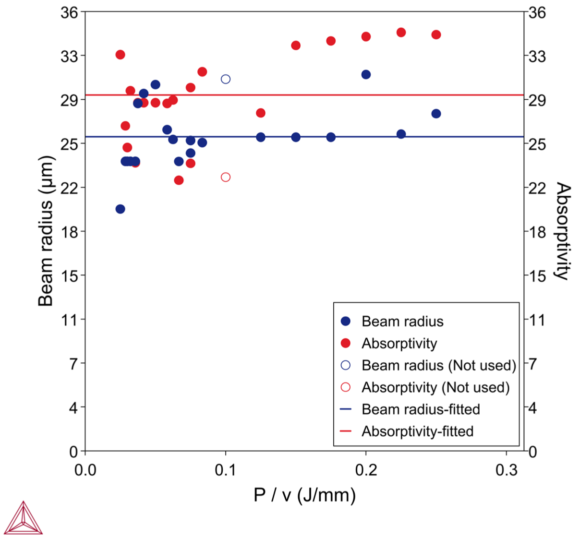

Figure 90: Calibrated heat source parameters for Gaussian heat source calibration.

In order to obtain the expressions for **Absorptivity** and **Beam radius**, one of the experiments (*Experiment # 10*) is not included. This is because *Experiment # 10* is an outlier and you can see that the values for *Exp width* and *Exp depth* (hollow square) then the *Sim width* and *Sim depth* (hollow circle) are excluded in Figure 89.

For both **Absorptivity** and **Beam radius** the **Constant function of P/v** is chosen to be saved as a calibrated heat source. Absorptivity of the material at the printing conditions is usually unknown in these experiments which is why it is regarded as a fitting parameter. Beam radius, on the other hand, is most often known, but does not match the definition of beam radius in the Gaussian heat source model used in the simulation, which is why a different value is obtained as compared to the one used in the experiment.

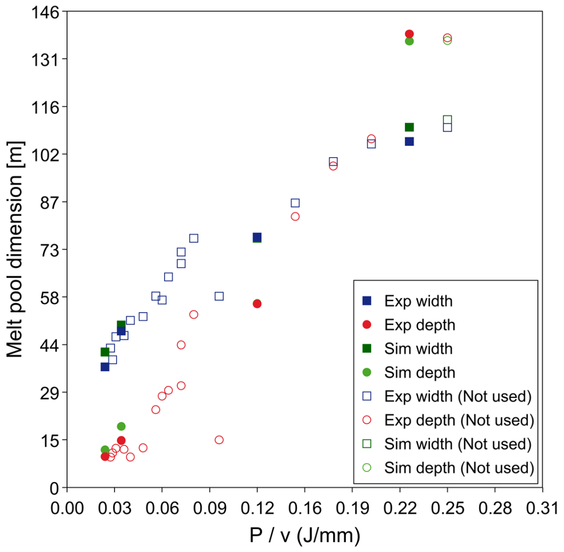

Figure 91: A comparison of melt pool dimension for double ellipsoidal heat source calibration.

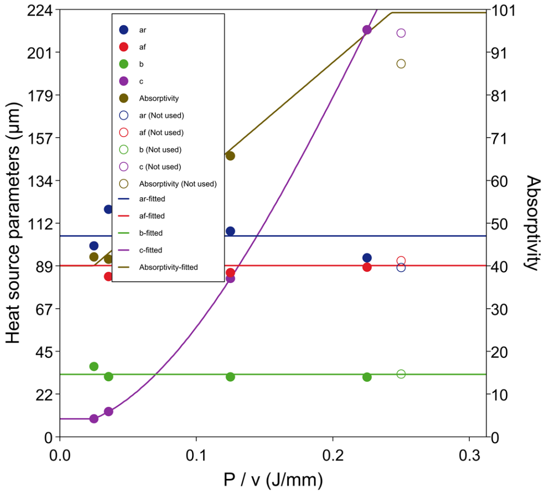

Figure 92: Calibrated heat source parameters for double ellipsoidal heat source calibration.

While selecting the functions for heat source parameters for double ellipsoidal, it was seen that **ar**, **af**, and **b** remained almost unchanged for all the experiments. Therefore the **Constant function of P/v for ar, af, and b** is used. For **Absorptivity**, a **Linear function of P/v** gave the best R2 value while for **c** a **Cubic function of P/v** gave the best R2 value. One of the experiments (experiment # 21) was excluded (i.e. the checkbox is deselected) to get a suitable curve for all functions.

Reference

[2019Hu] Z. Hu, B. Nagarajan, X. Song, R. Huang, W. Zhai, J. Wei, Formation of SS316L Single Tracks in Micro Selective Laser Melting: Surface, Geometry, and Defects. Adv. Mater. Sci. Eng. 2019, Article ID 9451406, 1–9 (2019).

Other Resources

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AM_06b: Using the Calibrated Heat Source for a 316L Steel

This example demonstrates the use of the two calibrated heat sources that are saved in the example AM_06a. One heat source is of the Gaussian type while the other heat source is Double ellipsoidal. For both heat sources, expressions are saved as a function of energy density (P/v) for all heat source parameters as well as the absorptivity. The example consists of four AM Calculators, two of which use a Gaussian heat source while the other two use a Double ellipsoidal heat source, and where the processing conditions for all four AM Calculators are taken from Hu et al [2019Hu].

AM_06a: Calibrating a Heat Source for a 316L Steel

Project File and License Information

- Folder: **Additive Manufacturing**
- File name: `AM_06b_Use_Calibrated_Heat_Sources_316L.tcu`

> Other than an Additive Manufacturing (AM) Module license, this example does not require an additional license to run it, although its companion example, AM_06a, does.

Material Properties

- SS316L: Fe-17.0Cr-12.0Ni-2.5Mo-0.03C Mass percent
- Database: TCFE13
- The material properties are precalculated, and stored as a built-in material library with the Additive Manufacturing (AM) Module.

Configuration and Calculation Set Up

There are four AM Calculators where all the calculators use the **Steady-state** simulation type and the **Single point** *Calculation Type*. The purpose of this example is to use the saved heat sources from AM_06a and then validate the results by comparing the melt pool size from the simulations with the experimental melt pool dimensions as given in Hu et. al [2019Hu].

The saved heat sources are selected from the *Heat Source* list on the AM Calculator, where a subsection called **Users heat sources** includes all previously saved heat sources. In the example, two calculators use the **Gaussian - 316L - beam d 15um** user-defined heat source, and two use the **Double ellipsoidal - 316L - beam d 15um** user-defined heat source. The **Base plate temperature** and **Ambient temperature** is set to 353 K, while the **Layer thickness** is set to 10 µm.

Visualizations

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

> ⌛ When you run (Perform) this example, it takes a few minutes for the calculations to complete.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation(s).

> For this example, it is best to open and run this simulation to be able to view all the different plots and outputs to various tabs on both the various Configuration windows as well as the Visualizations window.

> See Visualizing Heat Source Calibrations for an extended overview of what is available and how to navigate the many options for visualizing the heat source calibration data.

Gaussian Heat Source and Keyhole Model

The different processing conditions are selected to simulate both the conduction mode as well as the keyhole mode. For **Gaussian - 316L - beam d 15 um** heat source, with P = 100 W and scanning speed = 2800 mm/s, the dominant mode of heat transfer is conduction, which is why a shallow melt pool is obtained. The results from the simulations are fairly close to the ones from the experiments, as can be seen in *Table 1*.

With P = 80 W and scanning speed = 400 mm/s, a keyhole mode is observed in the experiments. This is also predicted from the simulations as can be seen in Figure 93.

A comparison of the melt pool depth from the simulations and the experiments for the latter case shows that the calibrated Gaussian heat source with the keyhole model predicts the melt pool depth with reasonable accuracy. However, it underpredicts the melt pool width. This is because fluid flow due to Marangoni forces is not included in these simulations, which probably causes the melt pool to widen in the experiments.

Calculator Name	***Power [W]***	***Scanning Speed [mm/s]***	***Melt Pool Width***		***Melt Pool Depth***	
			Simulation [µm]	***Experiment [µm]***	***Simulation [µm]***	***Experiment [µm]***
AM use calibrated Gaussian P100 u2800	100	2800	53.30	47.82	12.93	14.36
AM use calibrated Gaussian P80 u400	80	400	93.25	105	102.71	106.57

Table 1: A comparison of the melt pool dimensions from the simulations and experiments using the calibrated Gaussian heat source.

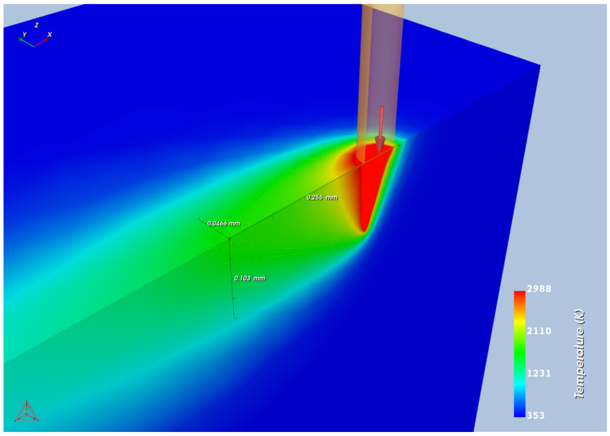

Figure 93: Steady-state temperature distribution around the melt pool for SS316L with P = 80 W and scanning speed = 400 mm/s using the calibrated Gaussian heat source with the keyhole model. A keyhole can also be seen formed just below the location of the heat source.

Double Ellipsoidal Heat Source

For the **Double ellipsoidal - 316L - beam d 15 um** heat source, two different processing conditions are selected to simulate both the conduction mode as well as the keyhole mode. For both processing conditions, the prediction of the melt pool size from the simulations is in fairly good agreement with the results from the experiments as can be seen in *Table 2*.

The temperature distribution using the calibrated double ellipsoidal heat source with P = 80 W and scanning speed = 400 mm/s is shown in Figure 94.

Calculator Name	***Power [W]***	***Scanning Speed [mm/s]***	***Melt Pool Width***		***Melt Pool Depth***	
			Simulation [µm]	***Experiment [µm]***	***Simulation [µm]***	***Experiment [µm]***
AM use calibrated DE P80 u1200	100	1200	65.07	64.34	31.63	29.68
AM use calibrated DE P80 u400	80	400	103.65	105	112.29	106.57

Table 2: A comparison of the melt pool dimensions from the simulations and experiments using the calibrated double ellipsoidal heat source.

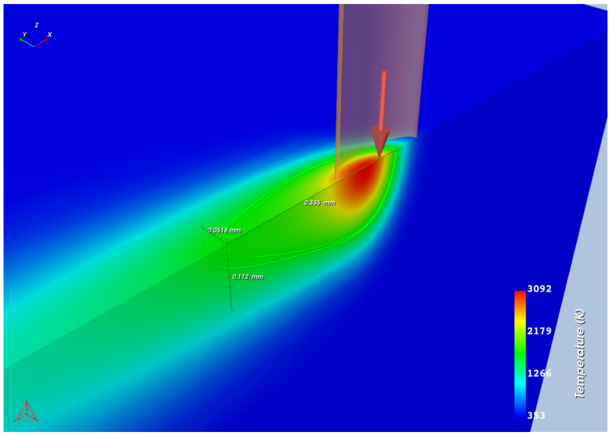

Figure 94: Steady-state temperature distribution around the melt pool for SS316L with P = 80 W and scanning speed = 400 mm/s using the calibrated double ellipsoidal heat source.

Reference

[2019Hu] Z. Hu, B. Nagarajan, X. Song, R. Huang, W. Zhai, J. Wei, Formation of SS316L Single Tracks in Micro Selective Laser Melting: Surface, Geometry, and Defects. Adv. Mater. Sci. Eng. 2019, Article ID 9451406, 1–9 (2019).

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AM_07: Batch Calculations for an IN718 Alloy

This example shows the use of the **AM Calculator** with a **Steady-state** mode and **Batch** *Calculation Type* where it compares calculated and measured melt pool dimensions. The experimental data are from the 2022 NIST AM-Bench Test Series [2022NIST] where single track experiments were performed on a IN718 bare plate at different power and scan speeds.

The use of different **Plot types** in this example include a **Parity plot**, **3D plot** showing the keyhole, and **Printability map**.

This example is part of a set using a **Steady-state** simulation with a **Gaussian** heat source, plus the **Keyhole model** including **Fluid flow**. These examples collectively show the use of **Batch** and **Grid** calculation types plus various plot types such as **Printability maps**, **Parity plots**, and **Melt pool vs energy density**. The examples are numbered AM_07 to AM_09b.

Project File and License Information

- Folder: **Additive Manufacturing**
- File name: `AM_07_Batch_IN718.tcu`

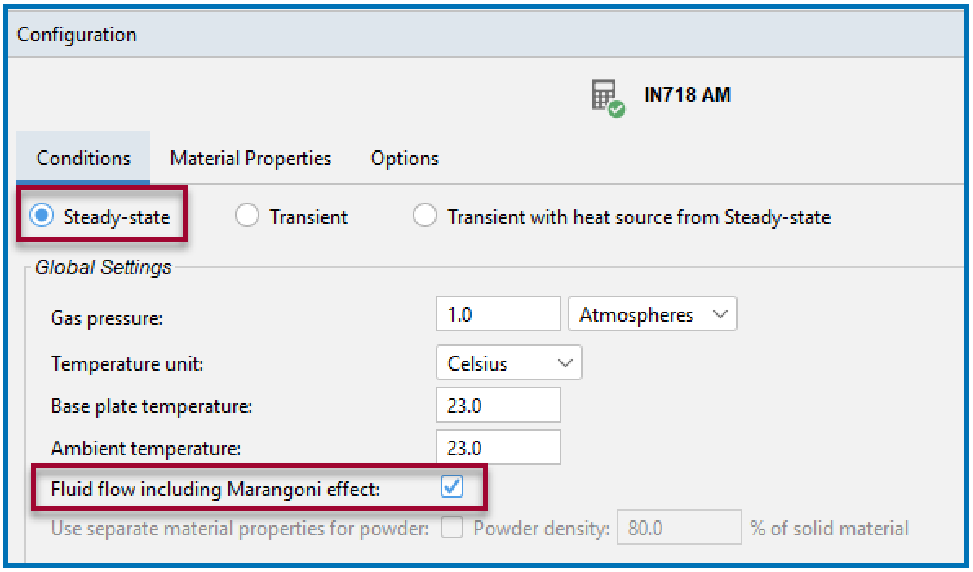
This example requires an Additive Manufacturing (AM) Module license.

Some examples (AM_01, AM_02, AM_03, and AM_06b) are available to all users. These examples can be run without an additional Additive Manufacturing license when you are in DEMO (demonstration) mode. However, the AM Module is not available with the Educational version of Thermo-Calc. Search the help for Available Options with the Additive Manufacturing (AM) Module. See Available Options for details.

Configuration and Calculation Set Up

Below highlights the main settings for this example.

The **Steady-state** simulation is selected and the **Fluid flow including Marangoni effect** checkbox is selected.



● Steady-state ○ Transient ○ Transient with heat source from Steady-state

Gas pressure: 1.0 Atmospheres

Temperature unit: Celsius

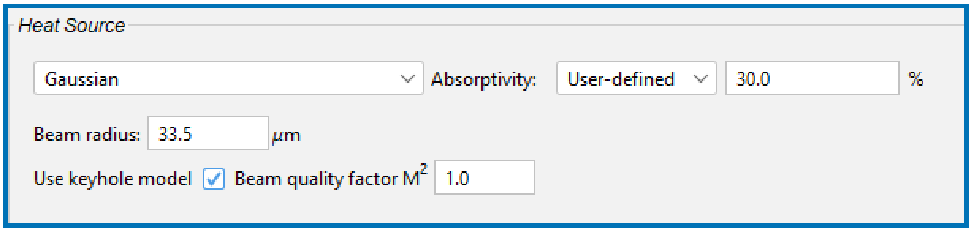
Base plate temperature: 23.0

Ambient temperature: 23.0

Fluid flow including Marangoni effect: ☑

Use separate material properties for powder: ☐ Powder density: 80.0 % of solid material

The *Heat Source* is set to **Gaussian** and uses the **Keyhole model**. The printers in the experiments had a beam diameter of `67` µm so the Gaussian **Beam radius** is set to `33.5` µm. The **Absorptivity** is set to `30.0` %.

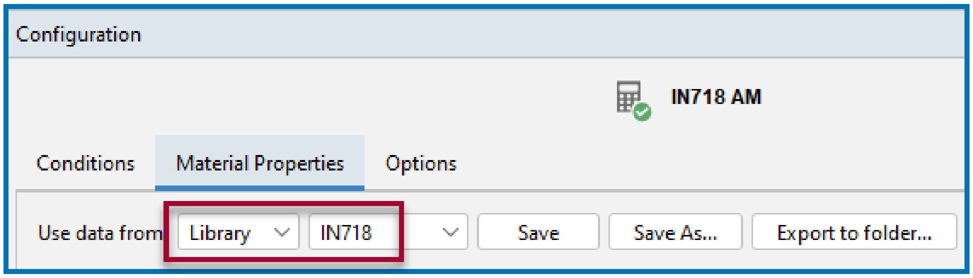


Gaussian Absorptivity: User-defined 30.0 %

Beam radius: 33.5 µm

Use keyhole model ☑ Beam quality factor M^2 1.0

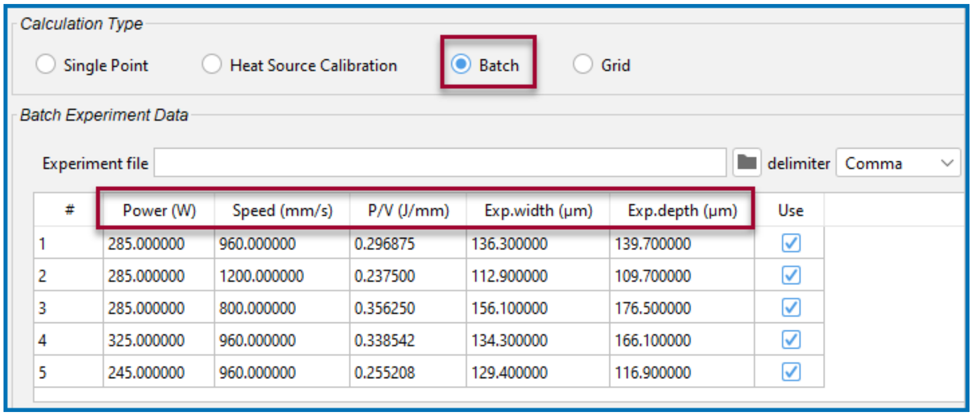
The **IN718** material is selected from the **Material Properties** library. The material properties are precalculated and stored as a built-in material **Library**.



Use data from Library IN718

The **Batch** *Calculation Type* is used to set up all the conditions from the multiple experiments in a single calculation. The experimental *Power* and scan *Speed* as well as the measured melt pool *Width* and *Depth* were collected in a CSV file and read into the software. This data is then saved in the project file.

In the *Batch Experiment Data* table you can see that the power ranges between `245` W to `285` W and the scan speed ranges between `800` mm/s to `1200` mm/s.



Calculation Type

○ Single Point ○ Heat Source Calibration ● Batch ○ Grid

Batch Experiment Data

Experiment file: delimiter Comma

#	Power (W)	Speed (mm/s)	P/V (J/mm)	Exp.width (µm)	Exp.depth (µm)	Use
1	285.000000	960.000000	0.296875	136.300000	139.700000	☑
2	285.000000	1200.000000	0.237500	112.900000	109.700000	☑
3	285.000000	800.000000	0.356250	156.100000	176.500000	☑
4	325.000000	960.000000	0.338542	134.300000	166.100000	☑
5	245.000000	960.000000	0.255208	129.400000	116.900000	☑

Visualizations

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

When you run (Perform) this example, it takes at least 30 minutes for the calculations to complete.

There is a wide variety of information shown both in the **Visualizations** and **Plot Renderer Configuration** windows that can be viewed during configuration and after performing the calculation(s). Not all views, such as the **Geometry** or previews, nor all additional output (i.e. plots) are shown in this section and it is recommended that you open and run the example to review all available options and results.

Parity Plot

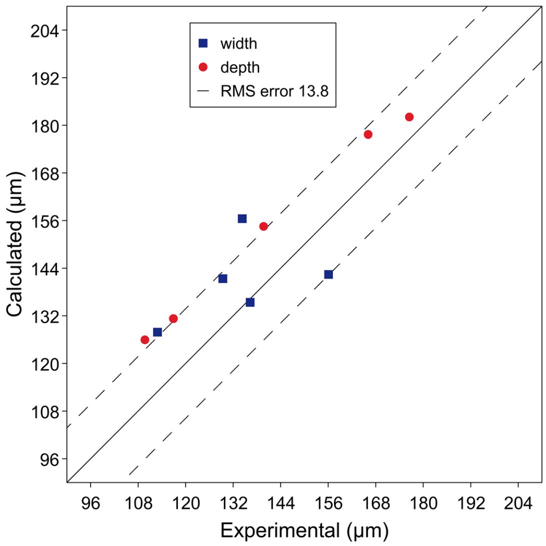
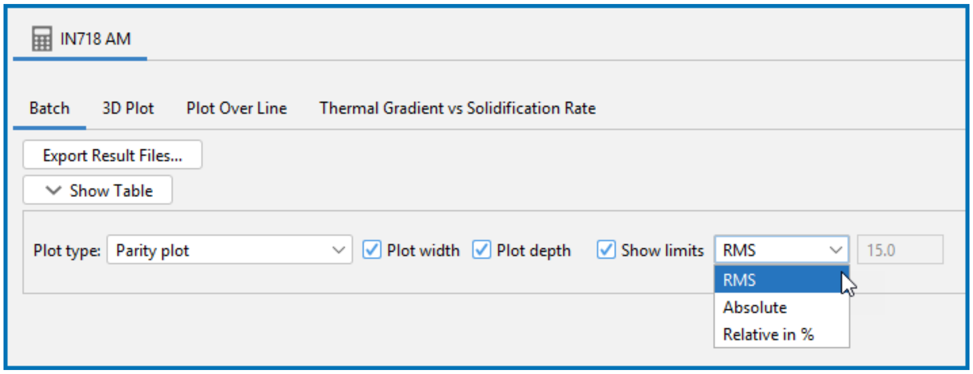


Figure 95: Parity plot comparing experimental versus calculated melt pool width and depth for all the experiments. The experiments are single tracks on bare plate IN718 with varied power and scan speed. The Root Mean Square (RMS) error can also be shown as a dashed line.



Plot type: Parity plot ☑ Plot width ☑ Plot depth ☑ Show limits RMS 15.0

Figure 96: Alternatively, lines for user-defined Absolute or Relative in % error can be shown instead by selecting these options on the Configuration window.

3D Plot with Surface Colormap

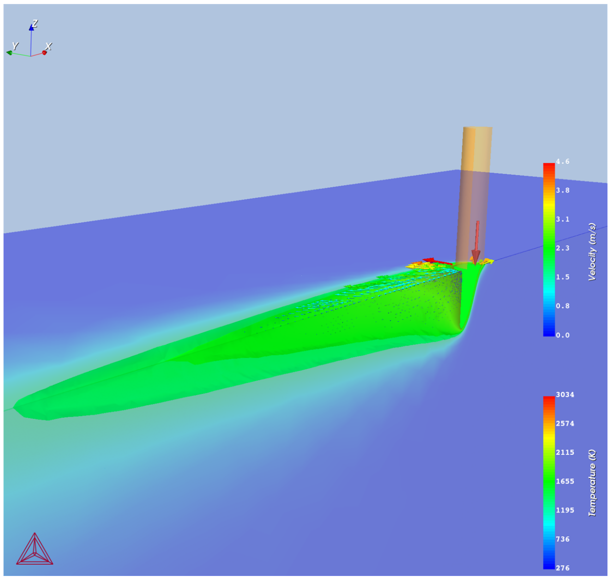
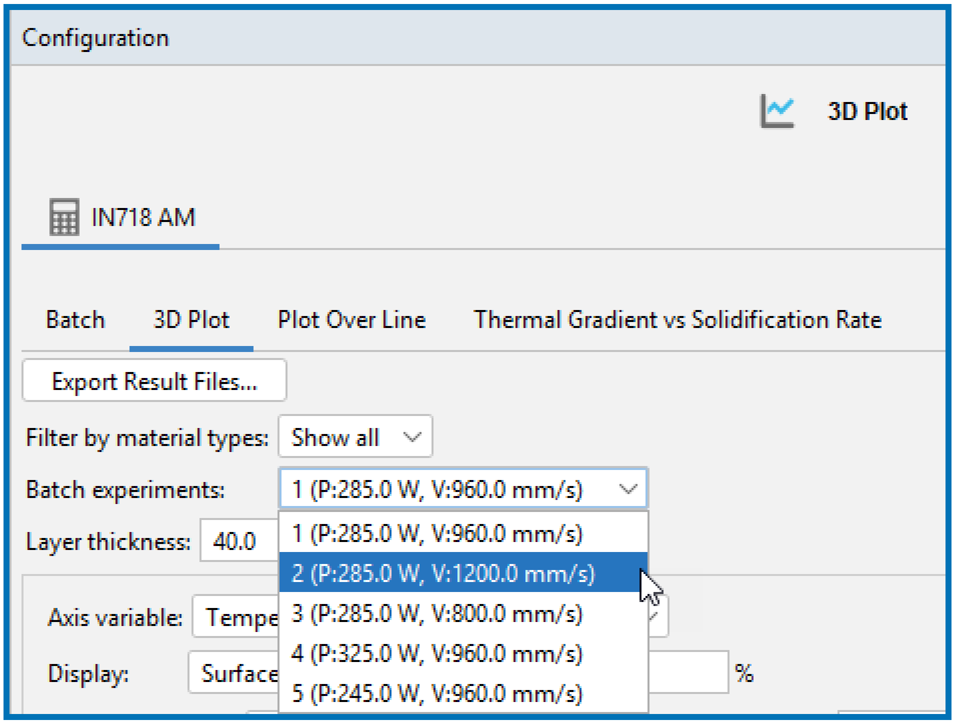


Figure 97: 3D plot showing a keyhole for the second simulation that uses power 285 W and scan speed 1200 mm/s.



Filter by material types: Show all

Batch experiments: 1 (P:285.0 W, V:960.0 mm/s)

- 1 (P:285.0 W, V:960.0 mm/s)
- 2 (P:285.0 W, V:1200.0 mm/s)
- 3 (P:285.0 W, V:800.0 mm/s)
- 4 (P:325.0 W, V:960.0 mm/s)
- 5 (P:245.0 W, V:960.0 mm/s)

Layer thickness: 40.0

Axis variable: Tempe

Display: Surface

%

Figure 98: Selecting the Batch experiment number to display in the Visualizations window for the 3D plot shown in Figure 97.

Visualizing Batch Calculations in the AM Module

Reference

[2022NIST] National Institute of Standards and Technology (NIST), Additive Manufacturing Benchmark Test Series (AM-Bench) (2022), (available at https://www.nist.gov/ambench).

Other Resources

Read more about the Additive Manufacturing (AM) Module on our website including the details about database compatibility or to watch an introductory webinar. You can also use the Getting Started Guide to learn about the key features available.

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

AM_08a: Grid Calculation for a Ti64 Alloy

This example shows the use of the **AM Calculator** with a **Steady-state** mode and **Grid** *Calculation Type* where it compares the calculated and measured printability map. Printability maps are also known as *process maps*. The experiments are from Dilip *et. al* [2017Dil] where they performed single track experiments with the alloy Ti64 at different power and scan speeds. They also printed cubes and performed measurements of the porosity amounts for each experimental condition.

The use of different **Plot types** in this example include a **Printability map** and a **3D plot** with surface colormap.

This example is part of a set using a **Steady-state** simulation with a **Gaussian** heat source, plus the **Keyhole model** including **Fluid flow**. These examples collectively show the use of **Batch** and **Grid** calculation types plus various plot types such as **Printability maps**, **Parity plots**, and **Melt pool vs energy density**. The examples are numbered AM_07 to AM_09b.

Project File and License Information

- Folder: **Additive Manufacturing**
- File name: `AM_08a_Printability_Map_Ti64.tcu`

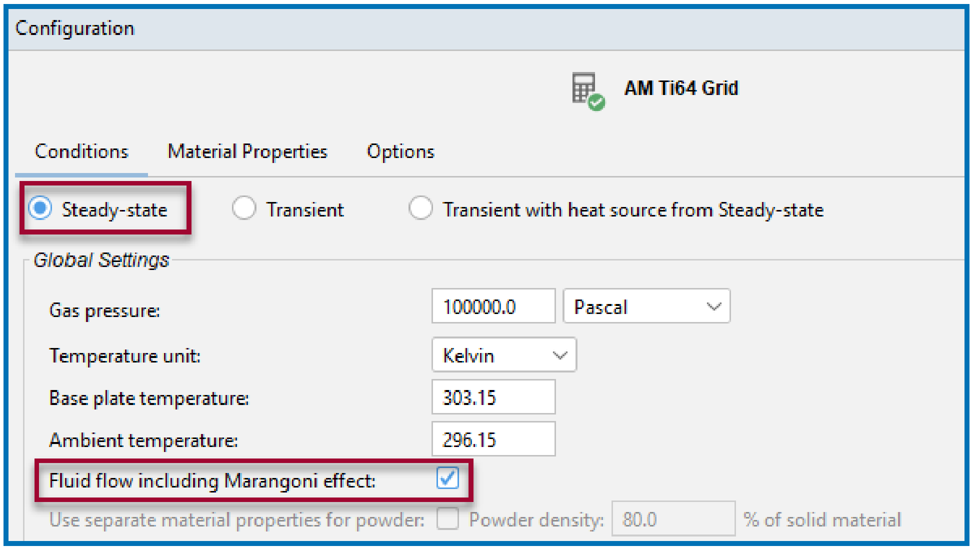
This example requires an Additive Manufacturing (AM) Module license.

Configuration and Calculation Set Up

Below highlights some of the settings for this example to compare with experimental data of Ti64.

This example builds on the previous one (AM_07) and it is recommended to review this and to open the example file to locate and follow along for the settings described here and found on the **Configuration** window.

The **Steady-state** calculation includes **Fluid flow**.



● Steady-state ○ Transient ○ Transient with heat source from Steady-state

Gas pressure: 100000.0 Pascal

Temperature unit: Kelvin

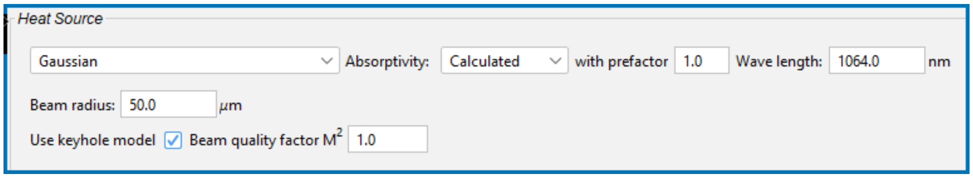
Base plate temperature: 303.15

Ambient temperature: 296.15

Fluid flow including Marangoni effect: ☑

Use separate material properties for powder: ☐ Powder density: 80.0 % of solid material

The *Heat Source* is set to **Gaussian** and uses the **Keyhole model**. The printers in the experiments had a beam diameter of `100` µm so the Gaussian **Beam radius** is set to `50` µm. The **Absorptivity** is set to **Calculated**.

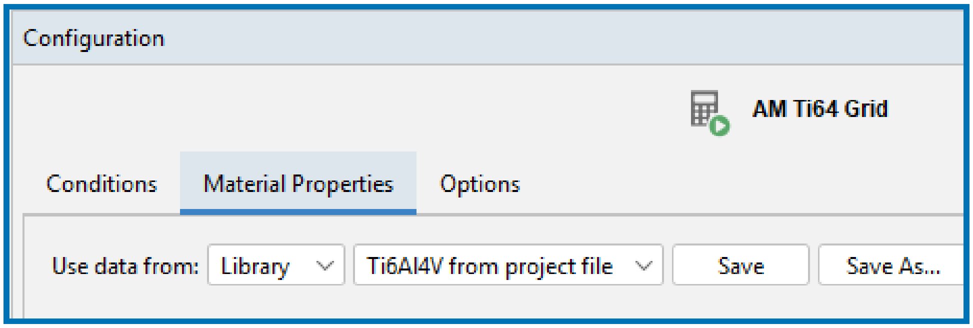


Gaussian Absorptivity: Calculated with prefactor 1.0 Wave length: 1064.0 nm

Beam radius: 50.0 µm

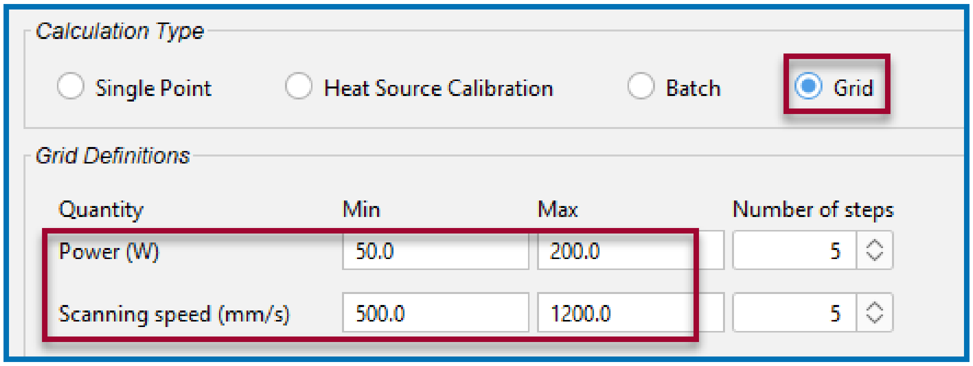
Use keyhole model ☑ Beam quality factor M^2 1.0

The **Ti6Al4V from project file** material is selected from the **Material Properties** library. The material properties are precalculated and stored as a built-in material **Library**.



Use data from: Library Ti6Al4V from project file

The **Grid** *Calculation Type* is used to cover all the conditions from the experiments in a single calculation. The **Power** ranges between `50–200` W and the **Scanning speed** ranges between `500–1200` mm/s.



Calculation Type

○ Single Point ○ Heat Source Calibration ○ Batch ● Grid

Grid Definitions

Quantity	Min	Max	Number of steps
Power (W)	50.0	200.0	5
Scanning speed (mm/s)	500.0	1200.0	5

Visualizations

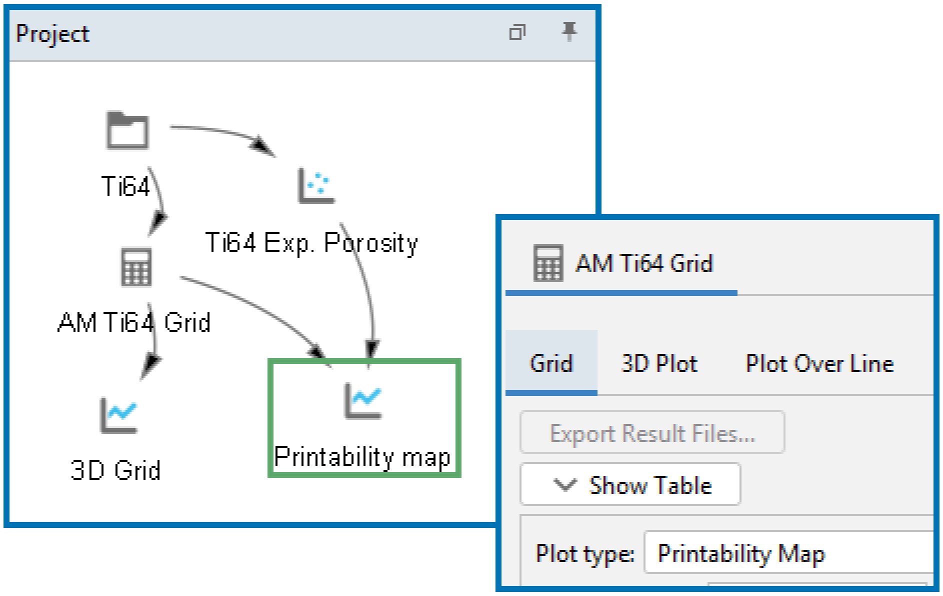
Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

⌛ When you run (Perform) this example, it can take around two hours to complete the calculations.

There is a wide variety of information shown both in the **Visualizations** and **Plot Renderer Configuration** windows that can be viewed during configuration and after performing the calculation(s). Not all views, such as the **Geometry** or previews, nor all additional output (i.e. plots) are shown in this section and it is recommended that you open and run the example to review all available options and results.

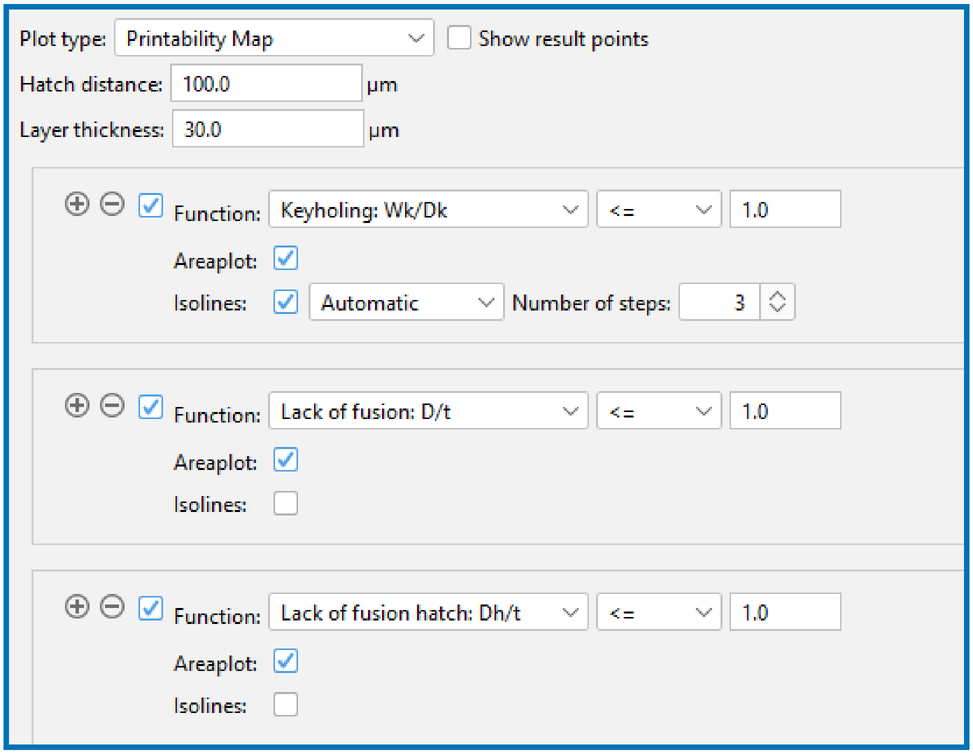
Plot Renderer Configuration Window

The combined results from the **Grid** calculation can be viewed under the matching **Grid** tab on the Plot Renderer **Configuration** window where it is set to use the **Printability map** plot type. In this example, the **Plot Renderer** node is renamed to **Printability map** in the **Project** window.



Plot type: Printability Map

The experimental value of `30` µm powder thickness (**Layer thickness**) and `100` µm for the **Hatch distance** seems to be too big to produce dense builds according to this lack of fusion criteria. Full density can then in principle only be achieved by melting the regions between tracks by shifting the layers printed on top so the full depth of the melt pool covers unmelted regions.



Plot type: Printability Map ☐ Show result points
Hatch distance: 100.0 µm
Layer thickness: 30.0 µm

☑ Function: Keyholing: Wk/Dk <= 1.0
Areaplot: ☑
Isolines: ☑ Automatic Number of steps: 3

☑ Function: Lack of fusion: D/t <= 1.0
Areaplot: ☑
Isolines: ☐

☑ Function: Lack of fusion hatch: Dh/t <= 1.0
Areaplot: ☑
Isolines: ☐

Printability Map and 3D Plot

There is a video tutorial about the **Printability Map** on our website and on our YouTube channel. It is also included in the Additive Manufacturing Module YouTube playlist.

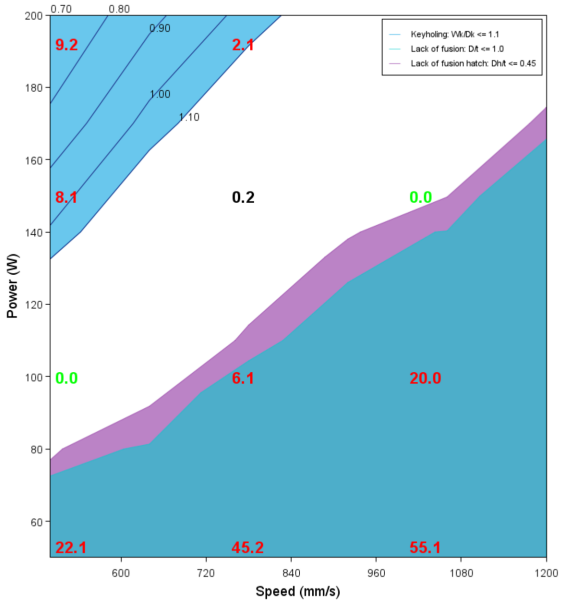


Figure 99: The calculated printability map for Ti64 showing the regions for keyholing porosity (upper left) and lack of fusion porosity to the lower right. The labels show the measured amount of porosity. Labels in red show regions with severe amounts of porosity and labels in black/green show regions with little or no defects.

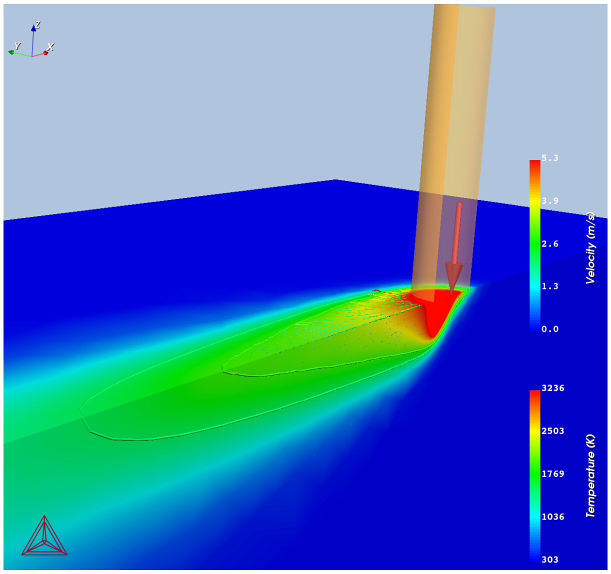


Figure 100: 3D plot showing a keyhole for the simulation that uses power 200 W and scan speed 1200 mm/s.

Reference

[2017Dil] J. J. S. Dilip, S. Zhang, C. Teng, K. Zeng, C. Robinson, D. Pal, B. Stucker, Influence of processing parameters on the evolution of melt pool, porosity, and microstructures in Ti-6Al-4V alloy parts fabricated by selective laser melting. Prog. Addit. Manuf. 2, 157–167 (2017).

Other Resources

Read more about the Additive Manufacturing (AM) Module on our website including the details about database compatibility or to watch an introductory webinar. You can also use the Getting Started Guide to learn about the key features available.

AM_08b: Batch Calculations for a Ti64 Alloy

This example shows the use of the **AM Calculator** with a **Steady-state** mode and **Batch** *Calculation Type* where it compares the calculated and measured melt pool dimensions. The experiments are from Dilip *et. al* [2017Dil] where they performed single track experiments with the alloy Ti64 at different power and scan speeds.

The use of different **Plot types** in this example include a **Parity plot**, **Melt pool vs energy density**, **3D plot** showing the keyhole, and **Printability map**.

This example is part of a set using a **Steady-state** simulation with a **Gaussian** heat source, plus the **Keyhole model** including **Fluid flow**. These examples collectively show the use of **Batch** and **Grid** calculation types plus various plot types such as **Printability maps**, **Parity plots**, and **Melt pool vs energy density**. The examples are numbered AM_07 to AM_09b.

Project File and License Information

- Folder: **Additive Manufacturing**
- File name: `AM_08b_Batch_Ti64.tcu`

This example requires an Additive Manufacturing (AM) Module license.

Configuration and Calculation Set Up

Below highlights some of the settings for this example. This example builds on the previous ones (AM_07 and AM_08a) and it is recommended to review these and to open the example file to locate and follow along for the settings described here and found on the **Configuration** window.

The **Steady-state** calculation is configured with the **Gaussian** *Heat Source* with the **Keyhole model** and includes **Fluid flow**. The printers had a beam diameter of 100 µm so the Gaussian **Beam radius** is set to `50` µm. The **Absorptivity** is set to `27` %.

The **Ti6Al4V** material is selected from the **Material Properties** library. The material properties are precalculated and stored as a built-in material **Library**.

The **Batch** *Calculation Type* is used to set up all the conditions from the experiments in a single calculation. The experimental *Power* and scan *Speed* as well as the measured melt pool *Width* and *Depth* were collected in a CSV file and read into the software. This data is then saved in the project file.

In the *Batch Experiment Data* table (see Visualizing the Batch Calculation Experimental Data) you can see that the power ranges between `50-195` W and the scan speed ranges between `500-1200` mm/s.

Visualizations

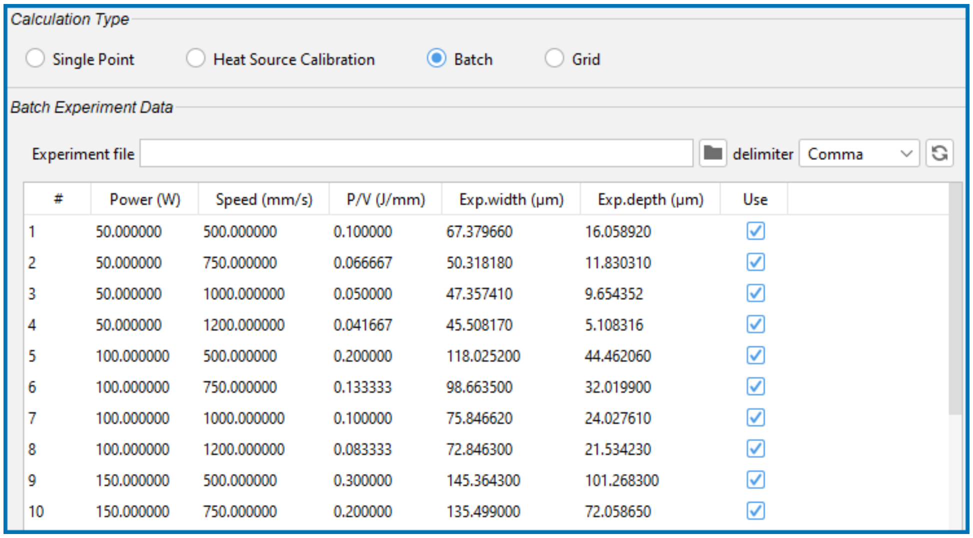
Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

⌛ When you run (Perform) this example, it takes at least 30 minutes for the calculations to complete.

There is a wide variety of information shown both in the **Visualizations** and **Plot Renderer Configuration** windows that can be viewed during configuration and after performing the calculation(s). Not all views, such as the **Geometry** or previews, nor all additional output (i.e. plots) are shown in this section and it is recommended that you open and run the example to review all available options and results.

Visualizing the Batch Calculation Experimental Data

During the set up of a calculation, the *Batch Experiment Data* is imported into the **AM Calculator Configuration** window, where you can review the data and choose to include or exclude data points by selecting and deselecting the checkboxes as needed in the **Use** column (see Figure 101). At the same time, you can observe the change as this is updated in the **Visualizations** window (see Figure 102). Data can also be entered directly into the table.



Calculation Type

○ Single Point ○ Heat Source Calibration ● Batch ○ Grid

Batch Experiment Data

Experiment file: delimiter: Comma

#	Power (W)	Speed (mm/s)	P/V (J/mm)	Exp.width (μm)	Exp.depth (μm)	Use
1	50.000000	500.000000	0.100000	67.379660	16.058920	☑
2	50.000000	750.000000	0.066667	50.318180	11.830310	☑
3	50.000000	1000.000000	0.050000	47.357410	9.654352	☑
4	50.000000	1200.000000	0.041667	45.508170	5.108316	☑
5	100.000000	500.000000	0.200000	118.025200	44.462060	☑
6	100.000000	750.000000	0.133333	98.663500	32.019900	☑
7	100.000000	1000.000000	0.100000	75.846620	24.027610	☑
8	100.000000	1200.000000	0.083333	72.846300	21.534230	☑
9	150.000000	500.000000	0.300000	145.364300	101.268300	☑
10	150.000000	750.000000	0.200000	135.499000	72.058650	☑

Figure 101: The experimental data used for the Batch calculation for the single track experiments of Ti64 is imported to the AM Calculator table where you can review the data points and include or exclude as needed using the checkboxes.

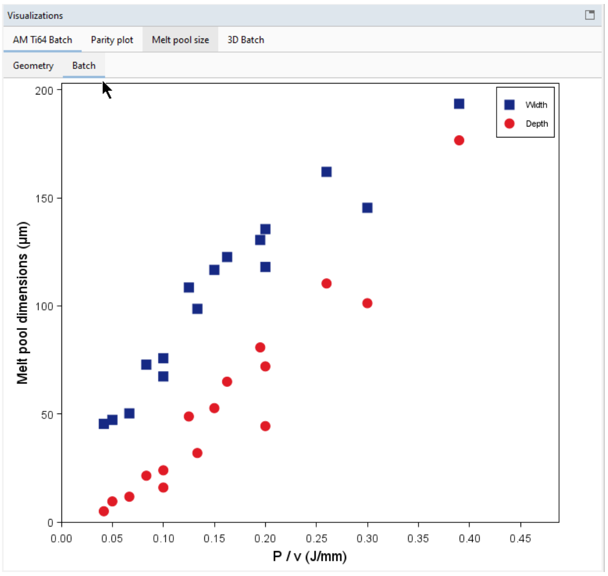


Figure 102: The visualization of the experimental melt pool dimensions are shown as a function of the energy density P/v. You can adjust the selected points in the Batch Experiment Data table and watch the updates dynamically in this window.

Parity, Melt Pool, and 3D Plot

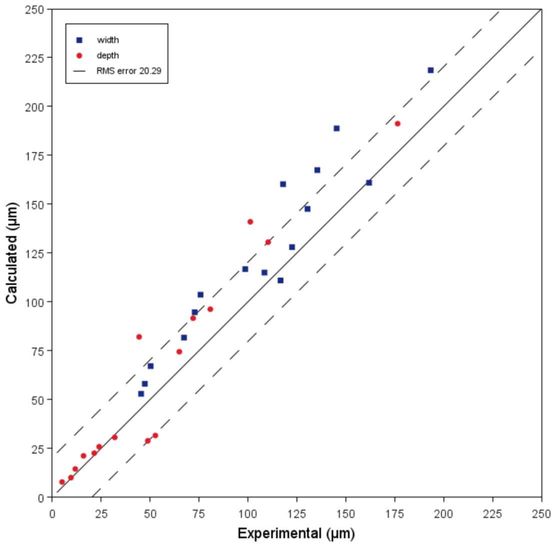


Figure 103: Parity plot comparing experimental versus calculated melt pool width and depth for all the Batch calculations. The experiments are single tracks with Ti64 with varied power and scan speed.

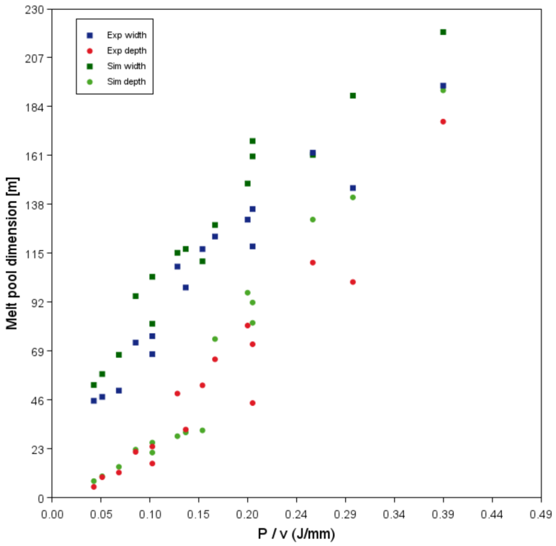


Figure 104: Plot comparing experimental versus calculated melt pool dimensions for all the Batch calculations. The experiments are single tracks with Ti64 with varied power and scan speed. The melt pool width and depth are shown on the Y-axis and the energy density (P/v) on the X-axis.

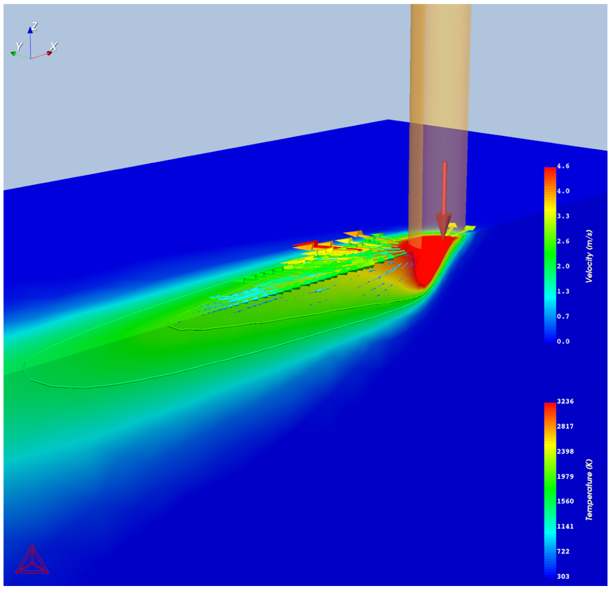


Figure 105: 3D plot showing a keyhole for the 15th simulation that uses power 195 W and scan speed 1000 mm/s.

Visualizing Batch Calculations in the AM Module

Reference

[2017Dil] J. J. S. Dilip, S. Zhang, C. Teng, K. Zeng, C. Robinson, D. Pal, B. Stucker, Influence of processing parameters on the evolution of melt pool, porosity, and microstructures in Ti-6Al-4V alloy parts fabricated by selective laser melting. Prog. Addit. Manuf. 2, 157–167 (2017).

Other Resources

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AM_09a: Grid Calculation for an SS316L Alloy

This example shows the use of the **AM Calculator** with a **Steady-state** mode and **Grid** *Calculation Type* where it compares the calculated and measured printability map. Printability maps are also known as *process maps*. The experiments are from Hu *et. al* [2019Hu] where they performed single track experiments with the alloy SS316L at different power and scan speeds.

The use of different **Plot types** in this example include a **Printability map** and a **3D plot** with surface colormap.

This example is part of a set using a **Steady-state** simulation with a **Gaussian** heat source, plus the **Keyhole model** including **Fluid flow**. These examples collectively show the use of **Batch** and **Grid** calculation types plus various plot types such as **Printability maps**, **Parity plots**, and **Melt pool vs energy density**. The examples are numbered AM_07 to AM_09b.

Project File and License Information

- Folder: **Additive Manufacturing**
- File name: `AM_09a_Printability_Map_316L.tcu`

This example requires an Additive Manufacturing (AM) Module license.

Configuration and Calculation Set Up

Below highlights some of the settings for this example. This example builds on the previous ones (AM_07, AM_08a, and AM_08b) and it is recommended to review these and to open the example file to locate and follow along for the settings described here and found on the **Configuration** window.

The **Steady-state** calculation is configured with the **Gaussian** *Heat Source* with the **Keyhole model** and includes **Fluid flow**.

The Gaussian **Beam radius** is set to `22` µm. The **Absorptivity** is set to `30` % and in the *Scanning Strategy* section, the powder **Layer thickness** is set to `10` µm.

The **SS316L** material is selected from the **Material Properties** library. The material properties are precalculated and stored as a built-in material **Library**.

The **Grid** *Calculation Type* is used to cover all the conditions from the experiments in a single calculation. The **Power** ranges between `40-100` W and the **Scanning speed** ranges between `400-3000` mm/s.

Visualizations

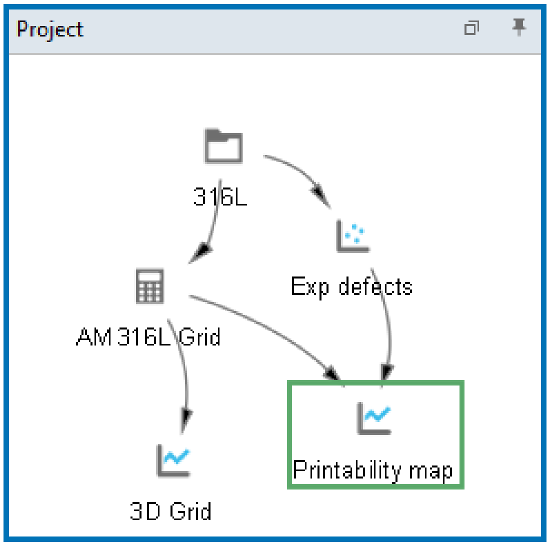
Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

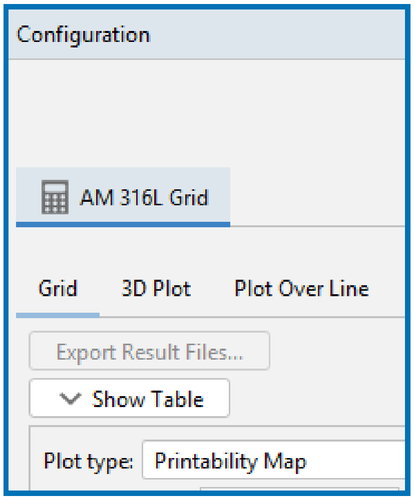
⌛ When you run (Perform) this example, it can take around two hours to complete the calculations.

There is a wide variety of information shown both in the **Visualizations** and **Plot Renderer Configuration** windows that can be viewed during configuration and after performing the calculation(s). Not all views, such as the **Geometry** or previews, nor all additional output (i.e. plots) are shown in this section and it is recommended that you open and run the example to review all available options and results.

Plot Renderer Configuration Window

The combined results from the **Grid** calculation can be viewed under the matching **Grid** tab on the Plot Renderer **Configuration** window where it is configured to use the **Printability map** plot type. In this example, the **Plot Renderer** node is renamed to **Printability map** in the **Project** window.

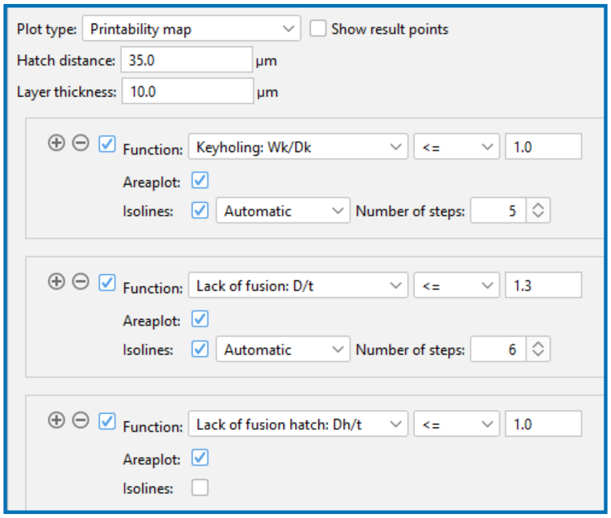




Plot type: Printability Map

Next each **Function** is defined and limits were adjusted to match the experimental regions of keyholing and lack of fusion porosity.

- The keyholing limit (**Keyholing: Wk/Dk**) is kept at default `1.0`.
- The **Lack of fusion: D/t** is increased from default of `1.0` to `1.3`.
- The experiments were only single-track and the lack of fusion at half of the hatch distance (**Lack of fusion hatch: Dh/t**) is kept at default `1.0` and only included together with the **Hatch distance** of `35` µm for demonstration purposes.



Plot type: Printability map ☐ Show result points

Hatch distance: 35.0 µm

Layer thickness: 10.0 µm

☑ Function: Keyholing: Wk/Dk <= 1.0
Areaplot: ☑
Isolines: ☑ Automatic Number of steps: 5

☑ Function: Lack of fusion: D/t <= 1.3
Areaplot: ☑
Isolines: ☑ Automatic Number of steps: 6

☑ Function: Lack of fusion hatch: Dh/t <= 1.0
Areaplot: ☑
Isolines: ☐

Figure 106: The settings for the printability map with the Function limits defined for keyholing, lack of fusion, and lack of fusion at half of the hatch distance (as described in the text).

Printability Map and 3D Plot

There is a video tutorial about the **Printability Map** on our website and on our YouTube channel. It is also included in the Additive Manufacturing Module YouTube playlist.

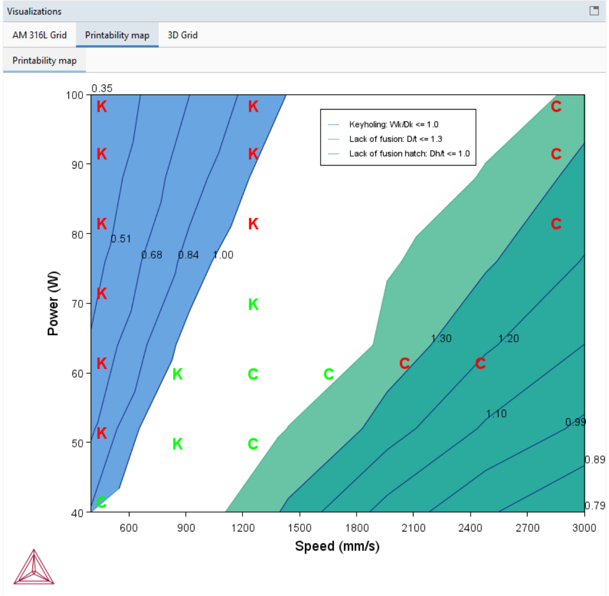


*Figure 107: Printability map for 316L showing regions of keyholing and lack-of-fusion. Experimental information from Hu et. al. [2019Hu] overlaid as coloured labels showing keyhole porosity (**K**), conduction mode with lack-of-fusion porosity (**C**). Green labels showing experiments without defects for conduction mode (**C**) and keyhole mode (**K**).*

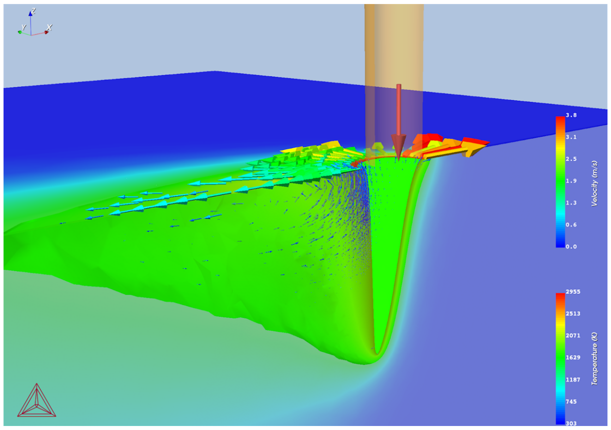


Figure 108: 3D plot showing a keyhole for the simulation that uses power 100 W and scan speed 400 mm/s.

Reference

[2019Hu] Z. Hu, B. Nagarajan, X. Song, R. Huang, W. Zhai, J. Wei, Formation of SS316L Single Tracks in Micro Selective Laser Melting: Surface, Geometry, and Defects. Adv. Mater. Sci. Eng. 2019, 1–9 (2019).

Other Resources

Read more about the Additive Manufacturing (AM) Module on our website including the details about database compatibility or to watch an introductory webinar. You can also use the Getting Started Guide to learn about the key features available.

AM_09b: Batch Calculations for an SS316L Alloy

This example shows the use of the **AM Calculator** with a **Steady-state** mode and **Batch** *Calculation Type* where it compares the calculated and measured melt pool dimensions. The experiments are from Hu *et. al* 2019 where they performed single track experiments with the alloy SS316L at different power and scan speeds.

The use of different **Plot types** in this example include a **Parity plot**, **Melt pool vs energy density**, **3D plot** showing the keyhole, and **Printability map**.

This example is part of a set using a **Steady-state** simulation with a **Gaussian** heat source, plus the **Keyhole model** including **Fluid flow**. These examples collectively show the use of **Batch** and **Grid** calculation types plus various plot types such as **Printability maps**, **Parity plots**, and **Melt pool vs energy density**. The examples are numbered AM_07 to AM_09b.

Project File and License Information

- Folder: **Additive Manufacturing**
- File name: `AM_09b_Batch_316L.tcu`

This example requires an Additive Manufacturing (AM) Module license.

Configuration and Calculation Set Up

Below highlights some of the settings for this example. This example builds on the previous ones (AM_07, AM_08a, AM_08b, and AM_09a) and it is recommended to review these and to open the example file to locate and follow along for the settings described here and found on the **Configuration** window.

The **Steady-state** calculation is configured with the **Gaussian** *Heat Source* with the **Keyhole model** and includes **Fluid flow**.

The Gaussian **Beam radius** is set to `22` µm. The **Absorptivity** is set to `30` % and in the *Scanning Strategy* section, the powder **Layer thickness** is set to `10` µm.

The **SS316L** material is selected from the **Material Properties** library.The material properties are precalculated and stored as a built-in material **Library**.

The **Batch** *Calculation Type* is used to set up all the conditions from the experiments in a single calculation. The experimental *Power* and scan *Speed* as well as the measured melt pool *Width* and *Depth* were collected in a CSV file and read into the software. This data is then saved in the project file.

In the *Batch Experiment Data* table the power ranges between `50-100` W and the scan speed ranges between `400-2800` mm/s.

Visualizations

There is a video tutorial about the **Printability Map** on our website and on our YouTube channel. It is also included in the Additive Manufacturing Module YouTube playlist.

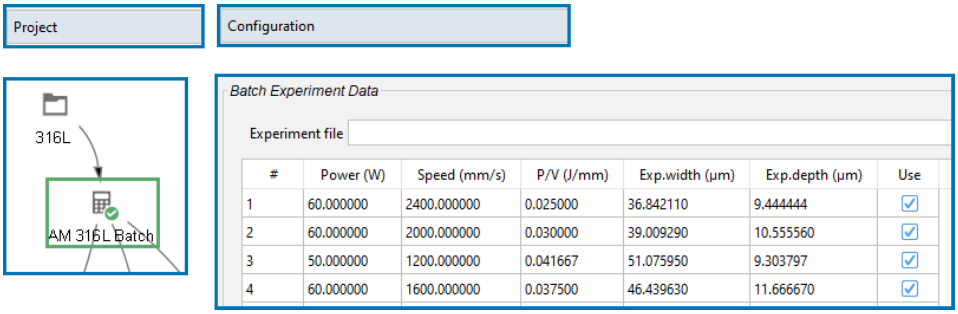
Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

When you run (Perform) this example, it can take about an hour to complete the calculations.

There is a wide variety of information shown both in the **Visualizations** and **Plot Renderer Configuration** windows that can be viewed during configuration and after performing the calculation(s). Not all views, such as the **Geometry** or previews, nor all additional output (i.e. plots) are shown in this section and it is recommended that you open and run the example to review all available options and results.

Visualizing the Batch Calculation Experimental Data

During the set up of this calculation, the *Batch Experiment Data* is imported into the AM Calculator **Configuration** window, where you can review the data and choose to include or exclude data points by selecting and deselecting the checkboxes as needed in the **Use** column. At the same time, you can observe the change as this is updated in the **Visualizations** window.



Batch Experiment Data

Experiment file

#	Power (W)	Speed (mm/s)	P/V (J/mm)	Exp.width (µm)	Exp.depth (µm)	Use
1	60.000000	2400.000000	0.025000	36.842110	9.444444	☑
2	60.000000	2000.000000	0.030000	39.009290	10.555560	☑
3	50.000000	1200.000000	0.041667	51.075950	9.303797	☑
4	60.000000	1600.000000	0.037500	46.439630	11.666670	☑

Figure 109: The experimental data used for the Batch calculation for the single track experiments of SS316L is imported to the AM Calculator table where you can review the data points and include or exclude as needed using the checkboxes.

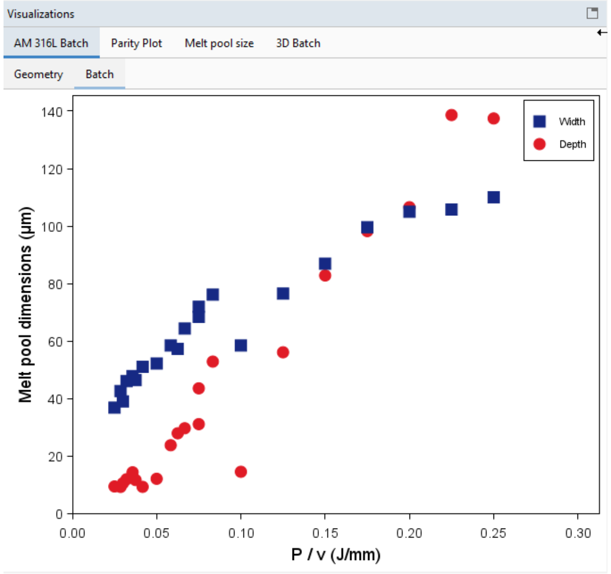


Figure 110: The visualization of the experimental melt pool dimensions are shown as a function of the energy density P/v. You can adjust the selected points in the Batch Experiment Data table and watch the updates dynamically in this window.

Parity, Melt Pool, and 3D Plot

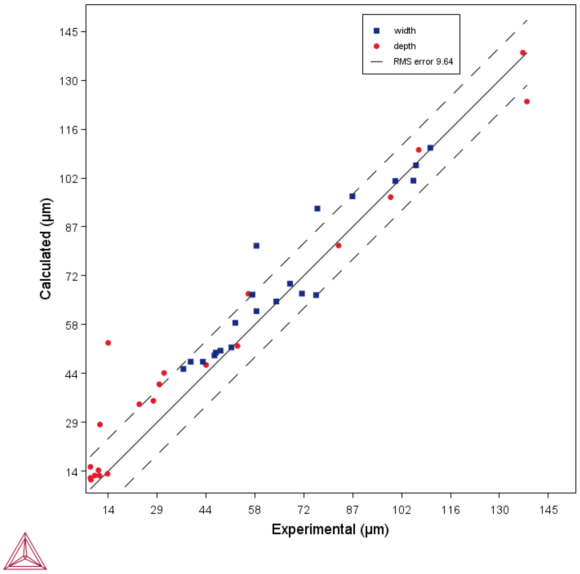


Figure 111: Parity plot comparing experimental versus calculated melt pool width and depth for all the Batch calculations. The experiments are single tracks with SS316L with varied power and scan speed.

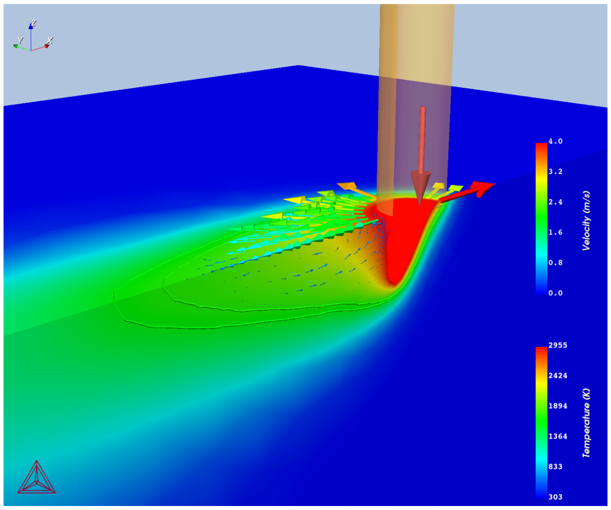


Figure 112: 3D plot showing a keyhole for the 12th simulation that uses power 60 W and scan speed 800 mm/s.

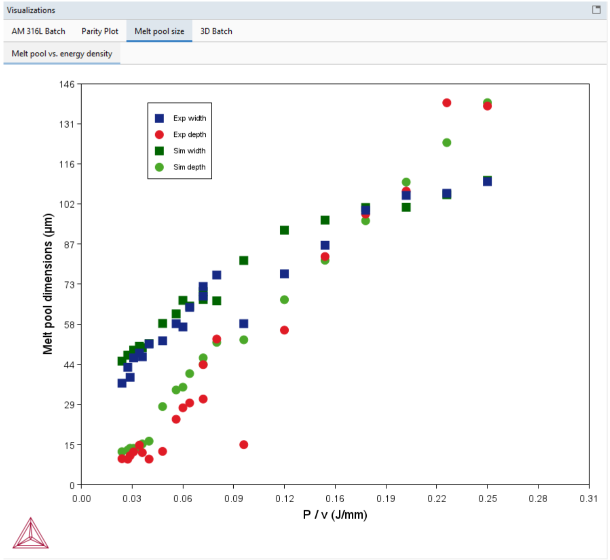
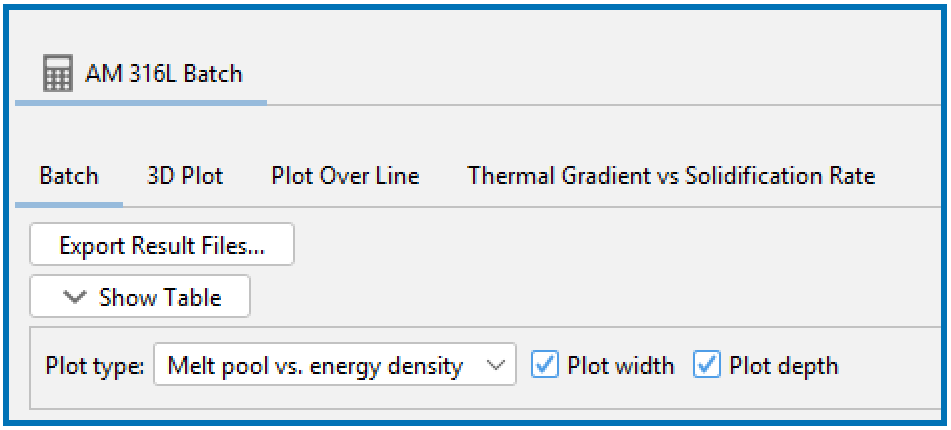


Figure 113: Plot comparing experimental versus calculated melt pool dimensions for all the Batch calculations. The experiments are single tracks with SS316L with varied power and scan speed. The melt pool width and depth are shown on the Y-axis and the energy density (P/v) on the X-axis.



Plot type: Melt pool vs. energy density ☑ Plot width ☑ Plot depth

Figure 114: For the plot, you can choose what to include on the plot, to show width and/or depth by selecting the relevant checkboxes on the Configuration window.

Visualizing Batch Calculations in the AM Module

Reference

[2019Hu] Z. Hu, B. Nagarajan, X. Song, R. Huang, W. Zhai, J. Wei, Formation of SS316L Single Tracks in Micro Selective Laser Melting: Surface, Geometry, and Defects. Adv. Mater. Sci. Eng. 2019, 1–9 (2019).

Other Resources

Read more about the Additive Manufacturing (AM) Module on our website including the details about database compatibility or to watch an introductory webinar. You can also use the Getting Started Guide to learn about the key features available.

AM_10: CET Transition in an IN718 Alloy

The example uses a **Scheil Calculator**, **AM Calculator**, and the **Property Model Calculator** with the **Columnar to Equiaxed Transition** Property Model to compare calculated CET curves for an IN718 alloy (from example PM_G_17) with the solidification conditions of the melt pool in the AM simulation.

For more background about this Property Model, search the Help or the main Thermo-Calc documentation set for *About the Columnar to Equiaxed Transition (CET) model*.

This example is similar to, and based on, example *PM_G_17: Columnar to Equiaxed Transition of an IN718 Alloy*. This is available from the **Property Models → General** folder.

A Scheil with solute trapping calculation is done first on the **Scheil Calculator** to generate thermophysical properties data to the **AM Calculator**. A steady-state AM simulation is done to predict the solidification conditions in the melt pool, the solidification rates, and thermal gradients.

Then using the **Property Model Calculator** with the **Columnar to Equiaxed Transition (CET)** model, the calculated CET curves for an IN718 alloy are fed into the **AM + CET** node (the renamed Plot Renderer), where together the data from the AM and Property Model calculations are combined and overlaid on one plot.

The literature data from Polonsky et al. [2020Pol] are not purely experimental data, but rather combined with experimental equiaxed evidence and model calculations with numerical values of thermal gradients, growth velocity as well as tip undercooling. Polonsky et al. estimated tip undercooling based on a Scheil calculation, which smeared out the composition inhomogeneity at the dendrite front, hence underestimating the undercooling. Since both tip undercooling and nucleation site density promotes the formation of equiaxed crystals, an increase in undercooling in this example calculation leads to a decrease in nucleation site density compared to the results in [2020Pol] if one were fitting the same set of data.

Project File and License Information

- Folder: **Additive Manufacturing**
- File name: `AM_10_Columnar_to_Equiaxed_Transition_IN718.tcu`

A separate license is required to perform calculations with the Additive Manufacturing (AM) Module. This example also requires additional database licenses for the TCS Ni-based Superalloys Database (TCNI) (TCNI12 and newer), and the TCS Ni-alloys Mobility Database (MOBNI) (MOBNI6 and newer).

Configuration and Calculation Set Up

On the **Scheil Calculator** (renamed to *Scheil with solute trapping*) , the **Scheil with solute trapping** is used with these specific settings:

- Trans-interface diffusivity: **Same for all elements**
- Prefactor: `5.0E-9`
- Maximum velocity for infinite driving force: `2000` m/s
- Model: **Aziz**
- Interface driving force: **Driving energy**

For the **AM Calculator** (renamed to *AM Steady-state*), the **Steady-state** calculation is configured as a **Gaussian** *Heat Source* with the **Keyhole model** and includes **Fluid flow**. It also uses a **Single Point** calculation with the **Calculated Absorptivity**.

On the **Property Model Calculator** (renamed to *Columnar to Equiaxed Transition*) a **One Axis** calculation for the **FCC_L12** primary phase is done using the CET parameters entered on the **Configuration** window.

The settings on the Property Model Calculator include:

- Interfacial energy: `0.5` J/m^2.
- Number of nucleation sites: `4.0E11`/m^3
- Nucleation undercooling : `4.0` K
- Equiaxed exponent: `3.13`

- Solve for: **Thermal gradient**
- Equiaxed fractions: `0.01 0.49 0.99`
- Solidification rate: `log10(v)`

Visualizations

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a wide variety of information shown both in the **Visualizations** and **Plot Renderer Configuration** windows that can be viewed during configuration and after performing the calculation(s). Not all views, such as the **Geometry** or previews, nor all additional output (i.e. plots) are shown in this section and it is recommended that you open and run the example to review all available options and results.

The thermal gradients and solidification rate can be visualized in 2D or 3D. Figure 115 shows the thermal gradient along the melt pool boundary in a 3D plot. Only the data corresponding to solidification conditions are shown. The thermal gradients corresponding to melting conditions are filtered out and only the tail part of the meltpool are shown.

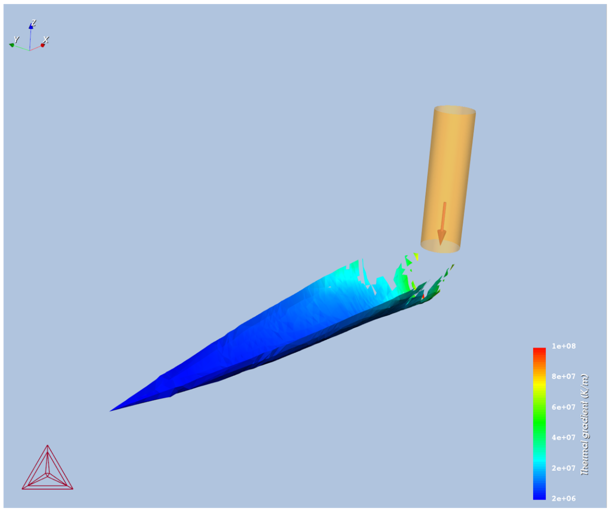


Figure 115: The 3D Plot for the 3D Thermal Gradient Plot Renderer.

Both the thermal gradients and solidification rates from the melt pool can be visualized at the same time in a 2D scatter plot when the Plot Renderer tab **Thermal Gradient vs Solidification Rate** is selected.

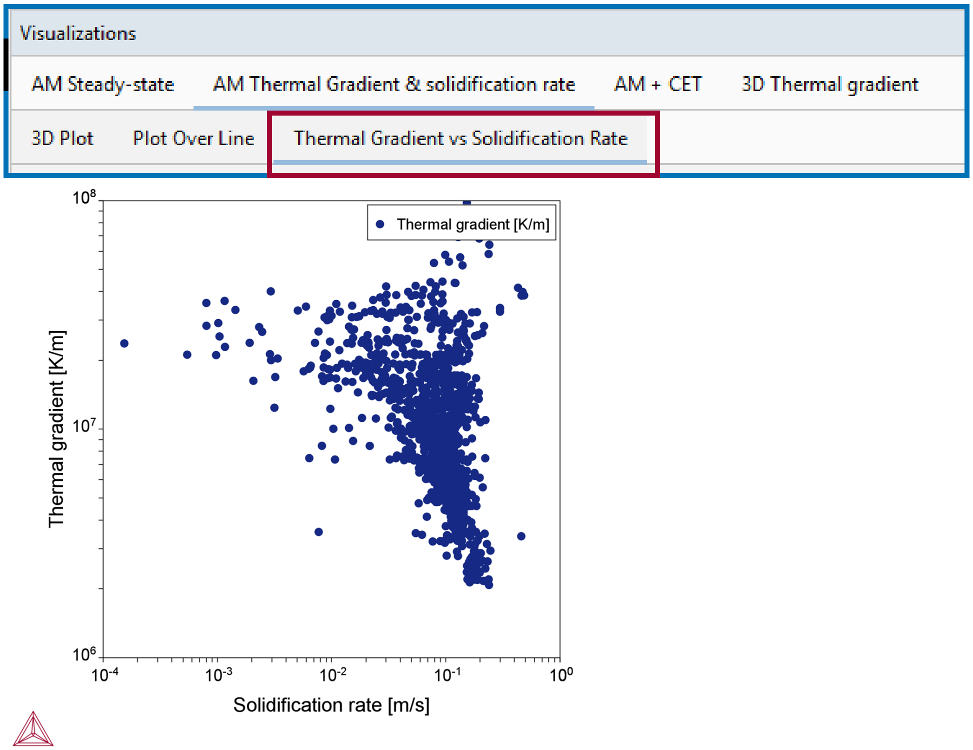


Figure 116: The solidification rate vs thermal gradient is shown on the AM Thermal Gradient & Solidification Rate Plot Renderer.

Figure 117 is an example of a plot where the results from both the AM simulation and the CET model for the IN718 thermal gradient vs solidification rate are overlaid on the same plot. The blue, red, and green lines show the increasing equiaxed fraction from the CET Property Model and the points show the solidification conditions at the melt pool calculated with the Additive Manufacturing (AM) Module. When the results are overlaid like this, you can see that nearly all the points (those below the purple line) exist in a fully columnar region.

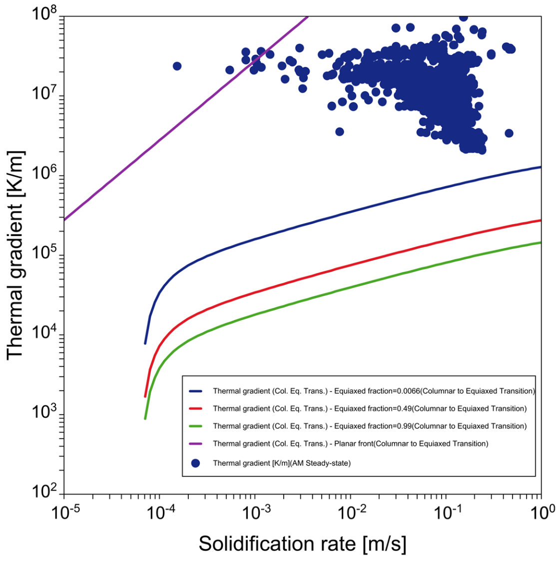


Figure 117: The solidification rate vs the thermal gradient overlaying both plots from the AM Calculator and Property Model Calculator (via the AM + CET Plot Renderer).

Reference

[2020Pol] A. T. Polonsky, N. Raghavan, M. P. Echlin, M. M. Kirka, R. R. Dehoff, T. M. Pollock, 3D Characterization of the Columnar-to-Equiaxed Transition in Additively Manufactured Inconel 718, in Superalloys 2020 (2020), pp. 990–1002.

Other Resources

Read more about the Additive Manufacturing (AM) Module on our website including the details about database compatibility or to watch an introductory webinar. You can also use the Getting Started Guide to learn about the key features available.

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

AM_11: Comparing Single Tracks Printed on Casted and LPBF Substrates

Bogdonova et al. [2024Bog] performed single track experiments with the alloy Al10SiMg. The study compared the printing of single tracks on two types of substrates—one fabricated with traditional casting and the other with laser powder bed fusion (LPBF).

Project File and License Information

- Folder: **Additive Manufacturing**
- File name: `AM_11_Batch_Al10SiMg.tcu`

A separate license is required to perform calculations with the Additive Manufacturing (AM) Module. This example also requires an additional database license for the TCS Al-based Alloy Database (TCAL) (TCAL9 and newer).

Background

It is well known that the thermal conductivity of the alloy Al10SiMg is drastically reduced in the as-printed condition when fabricated by LPBF compared to conventionally manufactured counterparts [2022Gha].

Thermal conductivity in Thermo-Calc is modeled as a temperature- and composition-dependent property per phase, and the conductivity of the alloy is taken as an average over the stable phases. The composition of the primary phase can change greatly depending on the fabrication method where the LPBF method results in rapid solidification and solute trapping of solute alloy elements.

Thermal conductivity can generally be reduced by different scattering phenomena (pores, defects, phase interfaces) within the microstructure and can therefore be lower than the calculated conductivity averaged over the phases.

The electrical resistivity due to phase interface scattering is evaluated as the scattering constant times sum of the interaction between the volume fraction of all the phases. The default value for the phase interface scattering constant is found to be 4.0e-8 Ωm for aluminum alloys. The contribution to thermal conductivity is assumed to be related to that of electrical resistivity, following the Wiedemann-Franz law.

The rapid solidification during LPBF generally results in a much finer microstructure compared to traditional casting. LPBF fabricated Al10SiMg solidifies with a cellular primary FCC structure and a eutectic structure between the cells [2021Lef]. An increased interface scattering constant more than 4.0E-8 can be argued given the much finer structure that has a large number of phase interfaces.

In this example the effect on material properties and melt pool dimensions is compared when printing single tracks on the two types of substrates. The material properties for the traditionally cast alloy is calculated using regular Scheil and the default interface scattering constant of `4.0E-8`. The material properties for the LBPF fabricated alloy is calculated using Scheil with solute trapping and the effect of increasing the interface scattering is shown.

Visualizations

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a wide variety of information shown both in the **Visualizations** and **Plot Renderer Configuration** windows that can be viewed during configuration and after performing the calculation(s). Not all views, such as the **Geometry** or previews, nor all additional output (i.e. plots) are shown in this section and it is recommended that you open and run the example to review all available options and results.

When you run (Perform) this example, it can take around two hours to complete the calculations.

Material Properties for the As-cast Substrate Material

The TCS Al-based Alloy Database (TCAL) is selected on the **System Definer** (renamed to *Scheil As-cast*). The as-cast Al10SiMg alloy has the composition of Al-10.8Si-0.3Mg-0.1Cu-0.1Fe.

The **Scheil Calculator** (renamed to *Scheil As-cast*) is configured with default settings for AM with an evaluation of thermophysical properties from 5000 K down to room temperature. The **Calculation type** is set to **Classic Scheil**.

Material Properties for the LPBF Printed Substrate Material

The TCS Al-based Alloy Database (TCAL) is selected in the **System Definer** (renamed to *Scheil printed*). The LPBF Al10SiMg alloy has almost the same composition (Al-10.8Si-0.3Mg-0.1Cu-0.2Fe) with only a small difference in Fe content.

The **Scheil Calculator** (renamed to *Scheil Solute-Trapping*) is configured with the default settings for AM with an evaluation of thermophysical properties from 5000 K down to room temperature. The **Calculation type** is set to **Scheil with solute trapping**.

Comparing Material Properties Between the Substrates

Two plots overlay results from the two Scheil Calculators in Figure 118. The Plot Renderer, renamed to *Si in primary FCC*, shows the Si content in the primary FCC phase. The classic Scheil calculation gives less than 1.5 at% Si. The solute trapping simulation results in twice the Si content with about 3 at% Si in the primary FCC phase. Atom probe experiments for a LPBF printed Al10SiMg alloy measured 3.08 at% Si in the FCC cell structure for the as-printed condition [2021Lef].

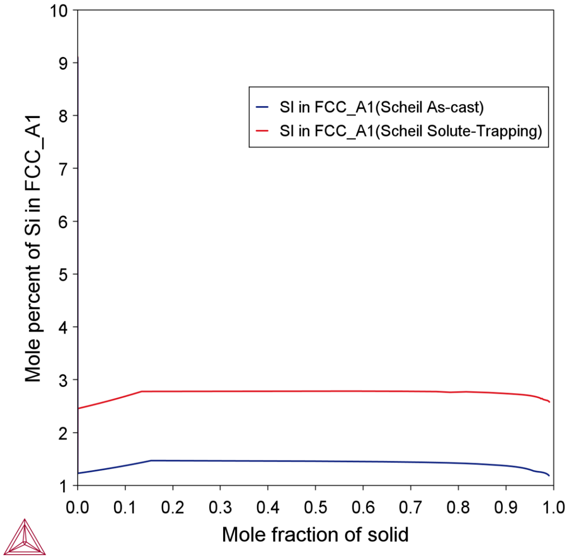


Figure 118: Silicon content in the primary FCC phase comparing regular (classic) Scheil with Scheil and solute trapping. The solute trapping almost doubles the Si content in the primary FCC phase.

Figure 119 is another overlaid plot that takes the results from two Scheil Calculator predecessors to show how the thermal conductivity varies with temperature. The conductivity for the as-cast substrate (blue line), that uses classic Scheil and the default setting for the phase interface scattering constant (`C = 4.0E-8`), naturally gives the highest thermal conductivity. The red line shows the reduction in conductivity due to solute trapping and the increased Si content in the primary phase. The green line shows further reduction in thermal conductivity due to the increased interface scattering when the scattering constant was increased (`C = 1.0E-7`).

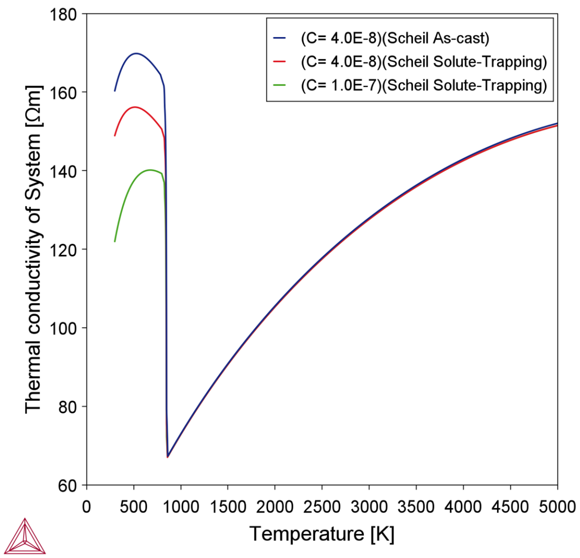


Figure 119: Thermal conductivity for as-cast substrate and printed substrate. Blue line shows conductivity for as-cast structure using the default setting for the interface scattering constant (C = 4.0E-8). The red line shows the reduced conductivity due to the solute trapping. Finally, the green line shows further reduction in thermal conductivity due to increased interface scattering where C = 1.0E-7.

Batch AM Steady-State Simulations

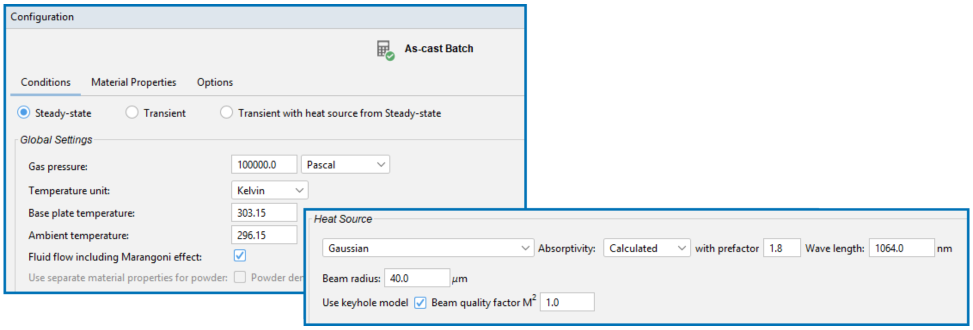
Two AM Calculators are next set up. These are renamed to *As-cast Batch* and *AM Batch*. These AM batch steady-state simulations are configured with similar settings, except for the interface scattering and the measured experimental melt pool dimensions that are different for the as-cast and LPBF fabricated substrates. The interface scattering settings are found on the **Material Properties** tab for both AM Calculators:

- The as-cast substrate uses the default interface scattering (`C = 4.0E-8`).
- The LPBF as-printed substrate uses the increased value for interface scattering (`C = 1.0E-7`).

The shared settings in the AM Calculator configuration (on the **Conditions** tab) are:

- Uses **Fluid flow including Marongoni effect** and the **keyhole model**.
- **Absorptivity** is selected as **Calculated** and the **with prefactor** is set to `1.8` times the calculated value in order to match the experimental melt pool dimensions.

The need to use a large prefactor is probably related to surface oxides and that the calculated absorptivity is for an oxide free liquid surface. The stable oxide Al_2O_3 often forms at the surfaces of Al-alloys where it remains in solid form to above 2000 °C and evaporates well above 3000 °C.



● Steady-state ○ Transient ○ Transient with heat source from Steady-state

Global Settings

Gas pressure: 100000.0 Pascal

Temperature unit: Kelvin

Base plate temperature: 303.15

Ambient temperature: 296.15

Fluid flow including Marangoni effect: ☑

Use separate material properties for powder: ☐ Powder der

Heat Source

Gaussian Absorptivity: Calculated with prefactor 1.8 Wave length: 1064.0 nm

Beam radius: 40.0 µm

Use keyhole model ☑ Beam quality factor M^2 1.0

Figure 120: The settings window for an AM steady-state simulation for the As-cast Batch calculator. Fluid flow and Gaussian heat source with keyhole model are enabled, plus it uses a calculated absorptivity with a prefactor set to 1.8.

To reduce total calculation time, for each AM Calculator only 5 of the 12 experiments are selected on the Plot Renderer (click **Show Table** to see the details). However, the example still takes about two hours to perform.

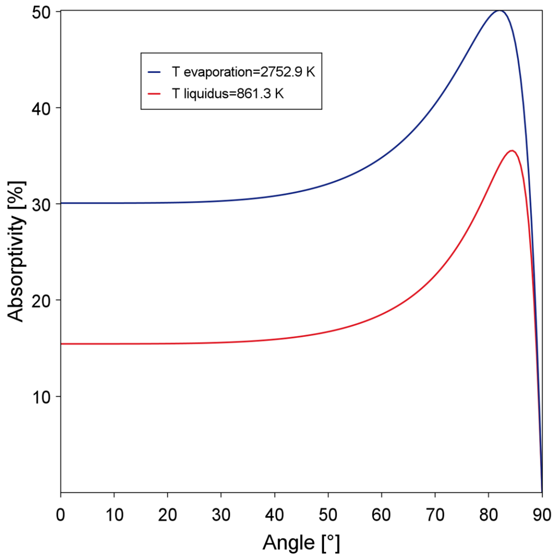
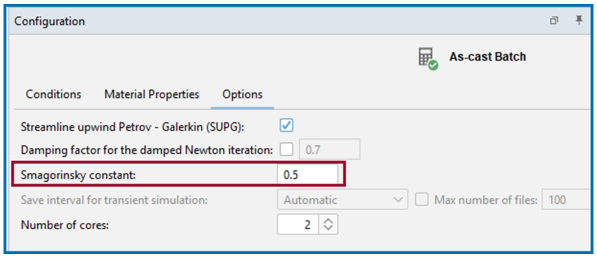


Figure 121: The temperature- and incident angle-dependent absorptivity. Red curve shows the absorptivity as a function of incident angle at the liquidus temperature, the blue curve shows the corresponding absorptivity at the evaporation temperature.

Turbulent Flow - Large Eddy Simulations

Al-alloys have in general lower viscosity compared to other metallic alloys (e.g. Ti-, Fe- or Ni-based alloys). The low viscosity in combination with high fluid flow rates can result in turbulent flows. This happens in this example for the simulations at the higher energy densities. The turbulent flow model implemented in the AM simulation is based on *Large Eddy Simulations* (LES) where the large-scale motions are represented directly and smaller-scale motions are modeled. A larger Smagorinsky constant filters more small-scale motions to be modeled. The example increases the Smagorinsky constant to `0.5`. The simulations with the highest energy densities will otherwise fail to converge with the default value of `0.18`.



Streamline upwind Petrov - Galerkin (SUPG): ☑

Damping factor for the damped Newton iteration: ☐ 0.7

Smagorinsky constant: 0.5

Save interval for transient simulation: Automatic ☐ Max number of files: 100

Number of cores: 2

Figure 122: On the Options tab for the AM Steady-State simulation (As-cast Batch) with an increased Smagorinsky constant to handle the high turbulent flows.

The following parity plot examples compare the experimental versus calculated melt pool dimensions. In general a good trend can be seen for both the simulations with the as-cast and LPBF fabricated substrates. The experimental melt pools are in general deeper than the simulated with an increasing error with increasing depth of the melt pool.

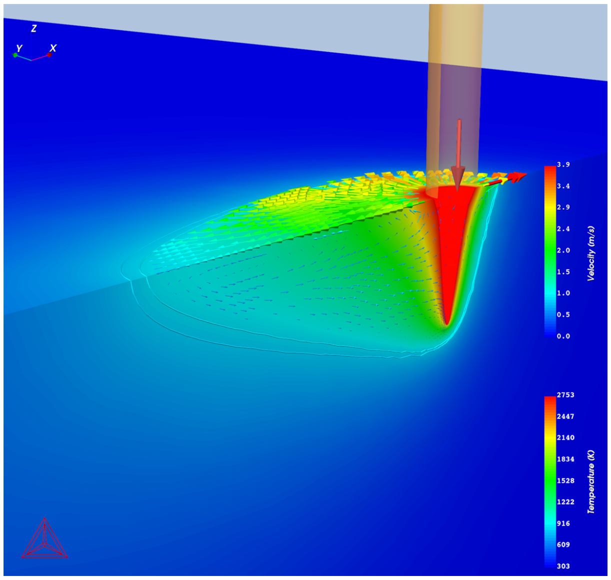


Figure 123: 3D plot of melt pool for as-cast substrate where P = 325 W and scanning speed = 600 mm/s.

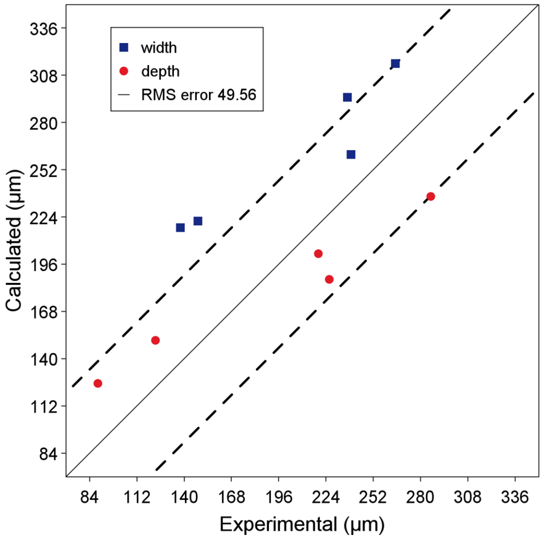


Figure 124: Parity plot for as-cast substrate when 5/12 experiments are calculated.

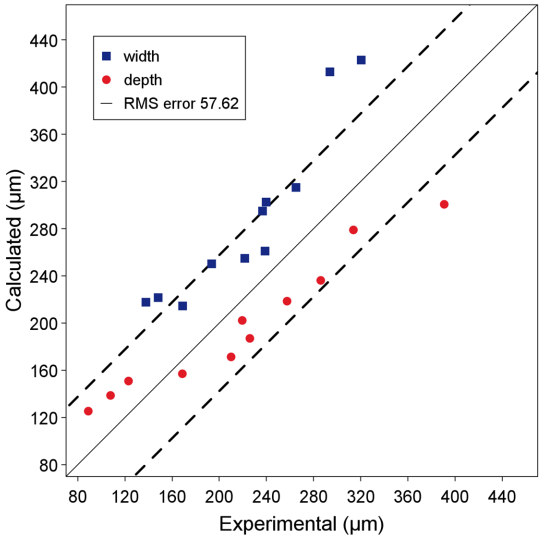


Figure 125: Parity plot for as-cast substrate when all 12 experiments are calculated.

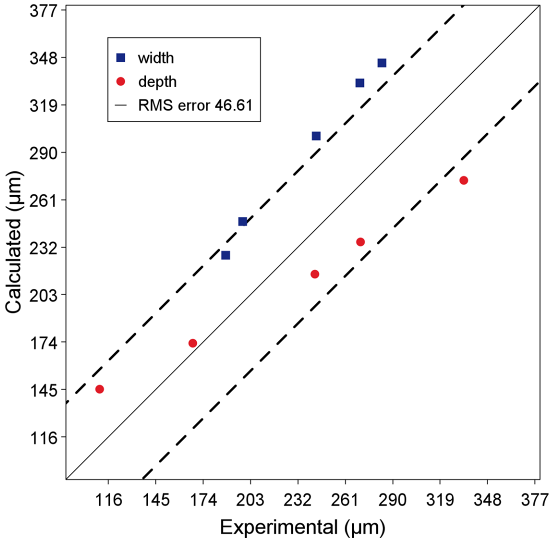


Figure 126: Parity plot for LPBF printed substrate when 5/12 experiments are calculated.

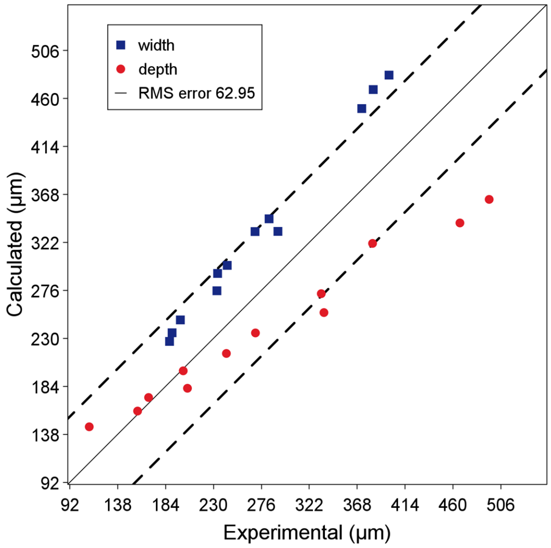


Figure 127: Parity plot for LPBF printed substrate when all 12 experiments are calculated.

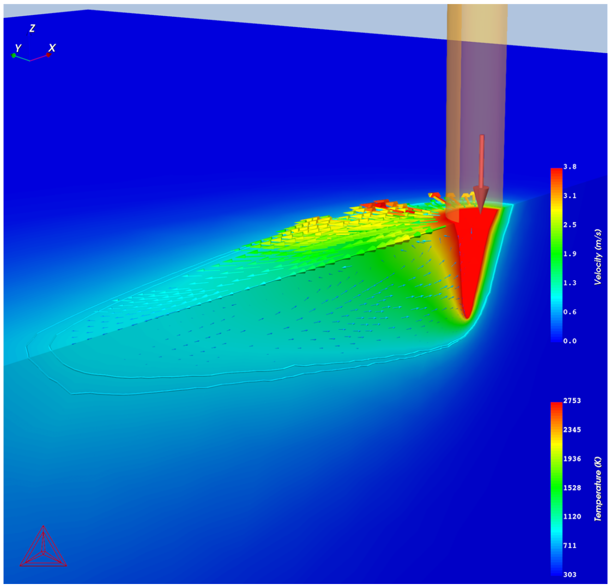


Figure 128: 3D plot of melt pool for LPBF printed substrate where P = 325 W and scanning speed = 1200 mm/s.

References

[2021Lef] W. Lefebvre, G. Rose, P. Delroisse, E. Baustert, F. Cuvilly, A. Simar, Nanoscale periodic gradients generated by laser powder bed fusion of an AlSi10Mg alloy. Mater. Des. 197, 109264 (2021).

[2022Gha] A. Ghasemi, E. Fereiduni, M. Balbaa, M. Elbestawi, S. Habibi, Unraveling the low thermal conductivity of the LPBF fabricated pure Al, AlSi12, and AlSi10Mg alloys through substrate preheating. Addit. Manuf. 59, 103148 (2022).

[2024Bog] M. Bogdanova, S. Chernyshikhin, A. Zakirov, B. Zotov, L. Fedorenko, S. Belousov, A. Perepelkina, B. Korneev, M. Lyange, I. Pelevin, I. Iskandarova, E. Dzidziguri, B. Potapkin, A. Gromov, Mesoscale Simulation of Laser Powder Bed Fusion with an Increased Layer Thickness for AlSi10Mg Alloy. J. Manuf. Mater. Process. 8, 7 (2024).

Other Resources

Read more about the Additive Manufacturing (AM) Module on our website including the details about database compatibility or to watch an introductory webinar. You can also use the Getting Started Guide to learn about the key features available.

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

AM_12: Using AM Calculator Probe Data with the Precipitation Module (TC-PRISMA)

This example demonstrates the coupling of the **AM Calculator** with the **Precipitation Calculator** via probe data from an AM simulation. Both a thermodynamic and mobility database is needed for the precipitation calculation, so the AM Material Library cannot be used. Instead, a **Scheil Calculator** is used to calculate the material properties used in the AM simulation.

The example simulates the incipient melting and re-precipitation of gamma prime in CMSX-4 during Selective Electron Beam Melting (SEBM) during a single pass of the beam. The SEBM process is simulated using a Gaussian heat source. A transient simulation of a single track is simulated, with a cooling time of 150 s. The bed and ambient temperature is elevated to 950 °C. The process parameters are taken from Ramsperger et al. [2016aRam].

Project File and License Information

- Folder: **Additive Manufacturing**
- File name: *AM_12_AM_Probe_to_Precipitation.tcu*

A separate license is required to perform calculations with the Additive Manufacturing (AM) Module. This example also requires a license for the Precipitation Module (TC-PRISMA), plus additional database licenses for the TCS Ni-based Superalloys Database (TCNI) (TCNI12 and newer), and the TCS Ni-alloys Mobility Database (MOBNI) (MOBNI6 and newer).

Background

Ramsperger and Körner [2016bRam] demonstrated that it is possible to print single crystal CMSX-4 components using SLBM with an elevated bed temperature. The main challenge encountered is fracture during printing. The formation of gamma prime may incur a drop in ductility that contributes to fracture. Understanding the precipitation kinetics of gamma prime during 3D printing is important with regards to identifying optimum process parameters, and determining how best to heat treat the final component.

Wahlmann et al. [2019Wah] studied gamma prime kinetics in emulated SLBM thermal conditions, indirectly measuring the size of the gamma prime using X-ray diffraction during repeated nucleation and dissolution thermal cycles imitating the thermal history of an SLBM build. Figure 129 shows the calibration of the Precipitation Calculator to capture the measured kinetics.

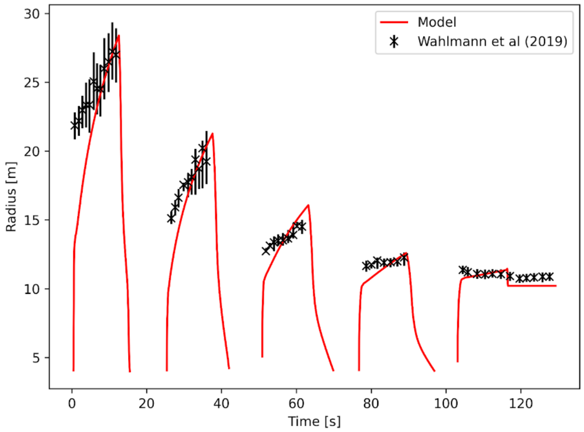


Figure 129: A comparison of the indirectly measured gamma prime size evolution during thermal heat treatment emulated an SLBM process with predictions from the Precipitation Calculator using the Thermo-Calc Ni-based superalloys databases (TCNI12 and MOBNI6) [2019Wah].

This AM Calculator to Precipitation Calculator example uses the calibrated parameters for gamma prime kinetics shown in Figure 129. The Precipitation Calculator includes the possibility for incipient melting of the gamma prime, which is predicted to occur during the first pass of the electron beam. Incipient melting describes the phenomena where solid-state precipitates are heated rapidly to a high temperature beyond their solvus temperature. The precipitates reach a temperature where they melt before the parent matrix phase. The Precipitation Calculator removes the gamma prime dispersion upon melting.

Configuration and Calculation Set Up

The **Additive Manufacturing** template was used to first add the **System Definer**, **Scheil Calculator**, **AM Calculator**, and **Plot Renderer** to the **Project** window tree. Additionally, a **Precipitation Calculator** was added as a successor to the AM Calculator in order to automatically import the time-temperature profile from the AM simulation into the precipitation simulation.

Open the example to see the **Project** tree layout and review the settings for each activity. It is useful to click around in the interface to understand where the settings are located and configured. This section highlights the relevant settings for this example.

System Definer

On the **System Definer**, the nickel-based superalloy CSMX-4 composition was approximated by Ni-9.8Co-6.4Ta-6.5Cr-6.4W-5.7Al-2.8Re-0.97Ti-0.62Mo-0.086Hf, (mass%). The thermodynamic (TCNI) and mobility (MOBNI) nickel-based superalloy databases were selected, with the phase **DIS_FCC_A1** included.

You can include or exclude phases from the **Phases and Phase Constitution** tab on the System Definer.

AM Calculator

On the **AM Calculator Configuration** window, the calculation type **Transient** is selected with a single track scan pattern and **Geometry** of 5 mm x 5 mm x 5 mm (height x width x length). The **Base plate temperature** and **Ambient temperature** is set to 950 °C.

Additional settings are then made on the **Configuration** window as follows.

- In the *Heat Source* section, **Gaussian** is selected with a **Power** of `180` W, and a **User-defined Absorptivity** of `85` %.
- In the *Scanning Strategy* section, the **Scanning speed** is `300` mm/s and the **Layer thickness** is `50` µm. A **Cooling time** of `150` s is included.
- In the *Top Boundary Conditions* section, the **Evaporation** checkbox is selected to include this in the model.
- In the *Probe Positions* section, a single probe is added to the center of the top surface of the component, below the powder layer. See the **Geometry** tab as shown in Figure 130.

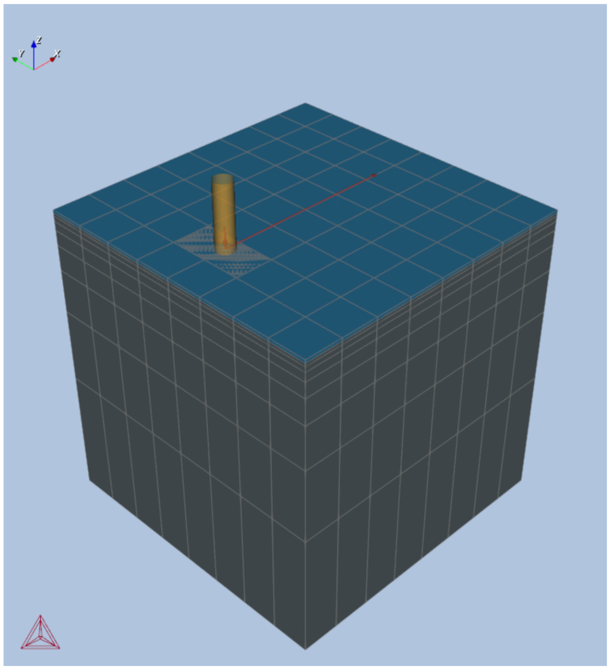


Figure 130: The full geometry set up for the single track AM simulation with a probe point added to the middle of the scan. Open the example to better see the set up and try working in the Visualizations window.

Precipitation Calculator

The following highlights the relevant settings to make on the **Configuration** window for this example.

On the **Options** tab:

- Both the **Preprocess equilibrium data** and **Include incipient melting** checkboxes are selected.

On the **Conditions** tab, under *Matrix Phase*:

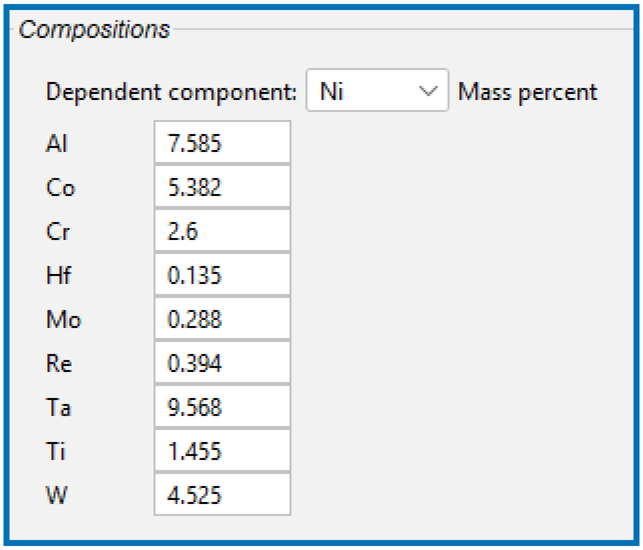
- **DIS_FCC_A1** is selected.

  Also see "Selecting the Disordered Phase as a Matrix Phase" in the *Precipitation Module User Guide*, or search for this in the help.

- Click **Show Details**, then for **Mobility adjustment > Prefactor**, keep **Same for all elements** and enter `6.0` for the **Prefactor**.

On the **Conditions** tab, under *Precipitate Phase*:

- **FCC_L12#2** is selected.
- **Nucleation sites** = **Bulk**
- **Interfacial energy** = `0.035` J/m^2
- Click **Show Details**, then:
    - **Phase energy addition** = `-55.0` J/mol
    - Select the **Preexisting size distribution** checkbox.
    - Click **Edit Particle Size Distribution**, and note the *Compositions* entered.



Compositions

Dependent component: Ni Mass percent

Al	7.585
Co	5.382
Cr	2.6
Hf	0.135
Mo	0.288
Re	0.394
Ta	9.568
Ti	1.455
W	4.525

In the **Preexisting Particle Size Distribution** window you can also adjust other settings. In this case, the size distribution is approximated by a Weibull distribution function with a mean radius of 200 nm, an Alpha of 2.0, and a fraction offset of 0.5 Search for "Particle Size Distribution (PSD)" in the *Precipitation Module User Guide*, or in the help.

On the **Conditions** tab, under *Calculation Type*:

- **Temperature unit** = **Kelvin**
- **Start time** = `0.0`
- **Simulation time** = `150.01` **Seconds**
- **Probes**: **Probe1**
- **Condense time-temperature data** = **None**

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation(s).

Figure 131 and Figure 132 show the predicted evolution of the precipitate dispersion including the change in mean radius and volume fraction, respectively. The second Y axis in both figures shows the temperature. The initial gamma prime size distribution describes the gamma prime that has formed during the production of the AM powder. It is too large to dissolve during the rapid heating as the electron beam heats the component, and melts before the matrix. The gamma prime re-precipitates upon resolidification and cooling below the gamma prime solvus, and coarsens whilst held at elevated temperature. The incipient melting of the initial size distribution is clearly evident.

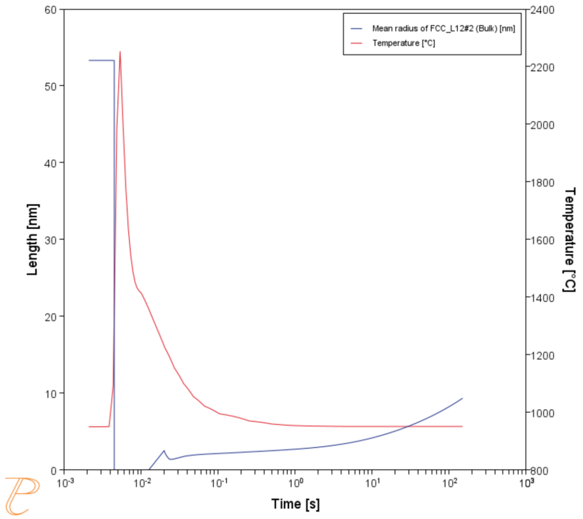


Figure 131: The mean radius and temperature as a function of temperature, with the mean radius on the left axis, and the temperature on the right axis.

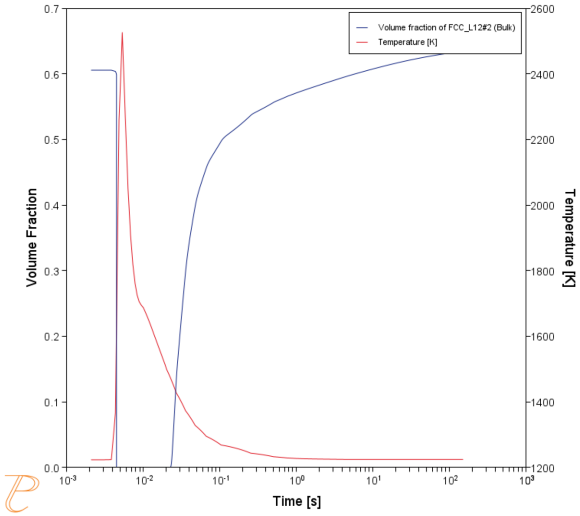


Figure 132: The volume fraction and temperature as a function of temperature, with the volume fraction on the left axis, and the temperature on the right axis.

The gamma prime distribution just prior to incipient melting is observed at 0.004 s. It has not dissolved significantly during the rapid heating as the electron beam passes. At 1 s the material has solidified and cooled to a temperature where gamma prime has nucleated and grown. The size distribution at the end of the simulation is shown at 150.1 s. Figure 133 shows the size distributions at these times during the single track AM simulation.

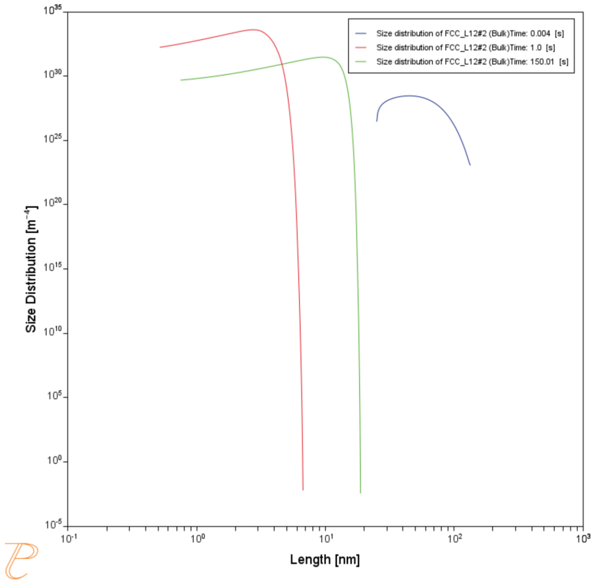


Figure 133: The size distributions of gamma prime at key points during the simulation.

References

[2016aRam] M. Ramsperger, R. F. Singer, C. Körner, Microstructure of the Nickel-Base Superalloy CMSX-4 Fabricated by Selective Electron Beam Melting. Metall. Mater. Trans. A 47, 1469–1480 (2016).

[2016bRam] M. Ramsperger, C. Körner, “Selective Electron Beam Melting of the Single Crystalline Nickel-Base Superalloy CMSX-4®: From Columnar Grains to a Single Crystal” in Superalloys 2016 (John Wiley & Sons, Inc., Hoboken, NJ, USA, 2016), pp. 341–349.

[2019Wah] B. Wahlmann, F. Galgon, A. Stark, S. Gayer, N. Schell, P. Staron, C. Körner, Growth and coarsening kinetics of gamma prime precipitates in CMSX-4 under simulated additive manufacturing conditions. Acta Mater. 180, 84–96 (2019).

Other Resources

Read more about the Additive Manufacturing (AM) Module on our website including the details about database compatibility or to watch an introductory webinar. You can also use the Getting Started Guide to learn about the key features available.

AM_13: Using the Core-ring Beam Shape

This **Steady-state** example demonstrates the use of **Core-ring** *Heat Source* model available in the AM Module with **Batch** calculations.

The heat source parameters for the **Core-ring** heat source, as well as the processing parameters (power and speed), are taken from Holla et al. [2024Hol]. The example also compares the predicted melt pool dimensions with the experimental data from this paper.

For TC-Python users, there is an example using **Core-ring**: `pyex_AM_09_CoreRing_BeamShape.py`.

There is a companion example in Graphical Mode using **Top-hat**: AM_14: Using the Top-hat Beam Shape.

Project File and License Information

- Folder: **Additive Manufacturing**
- File name: *AM_13_CoreRing_BeamShape.tcu*

This example requires an Additive Manufacturing (AM) Module license.

Background

In a core-ring heat source, the energy is distributed between the central core and the surrounding ring, allowing for more precise control of heat input and a more uniform temperature distribution, reducing the risk of unstable keyhole formation [2023Bi]. Furthermore, a wider melt pool with the **Core-ring** beam shape as compared to a Gaussian profile allows enlargement of the hatch distances and together with the possibility of using higher scanning speeds, results in faster printing process and increased productivity [2021Grü].

About the Heat Source Models

The inclusion of a **Core-ring** heat source model in the AM Module, together with the keyhole model, allows you to predict the temperature evolution and melt pool shape along with the transition from conduction mode to keyhole mode for a **Core-ring** heat source. The experimental data taken from the literature [2024Hol] demonstrates the use of a **Core-ring** heat source for single track experiments on stainless steel 316L bare plates. A wide range of process parameters (power = 200 W – 900 W and scanning speed = 200 mm/s – 800 mm/s) also shows different cases for both conduction as well as the keyhole mode, which are correctly predicted in this example by the simulation results.

Material Properties

- SS316L: Fe-17.0Cr-12.0Ni-2.5Mo-0.03C Mass percent
- Database: TCFE13 and with interface scattering = 1e-07.
- The material properties are precalculated, and stored as a built-in material library with the Additive Manufacturing (AM) Module.

AM Calculator Configuration Settings

This example contains one AM Calculator, which is renamed to **Core-ring_20/80**. On the **Configuration** window, **Conditions** tab, this **Steady-state** calculation is configured with the **Core-ring** *Heat Source* with the **Keyhole model** and includes **Fluid flow**.

The **Custom Mode** is used in order to set all the heat source parameters as given in Table 2 of [2024Hol]. Individual settings are entered to match:

- **Beam radius-Core**: 47.6 µm
- **Beam radius-Ring**: 25.29 µm
- **Ring radius**: 68.4 µm

The **Amount of power in the ring** is set to **80%**, which is equivalent to 20/80 beam shape in [2024Hol].

The **Absorptivity** is set to **Calculated** with a **prefactor** of `1.2`. It uses the **keyhole model** where the **Beam quality factor M^2** is kept as `1.0`.

The **Batch** *Calculation Type* is used to set up all the conditions from the experiments in a single calculation. In the *Batch Experiment Data* section, the experimental **Power** and scan **Speed** as well as the measured melt pool Width (**Exp width**) and Depth (**Exp. depth**) were collected in a CSV file and imported into the software. This data is then saved in the project file.

In the *Batch Experiment Data* table, the **Power** ranges between 200 W to 900 W, and the scan **Speed** ranges between 200 mm/s to 800 mm/s.

AM Calculator Conditions Settings and AM Calculator Heat Source Settings

Visualizations

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

When you run (Perform) this example, it takes a few minutes for the calculations to complete.

For more information also see Working with AM Visualizations.

Parity Plot

This specific **Parity** plot is shown by clicking the **Parity Plot** node in the **Project** window. Then you can see on the **Visualizations** window it is in the tab of the same name. The settings are located on the **Configuration** window on the **Batch** tab.

The plot compares experimental and calculated melt pool width and depth for all experiments. The experiments are single tracks on bare plate SS316L with varied power and scan speed using a **Core-ring** heat source.

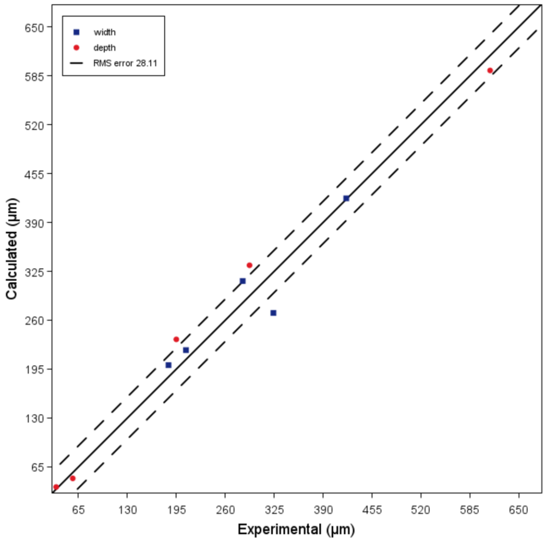


Figure 134: Parity plot comparing experimental and calculated melt pool width and depth for all the experiments when using a Core-ring heat source. The Root Mean Square (RMS) error can also be seen as a dashed line.

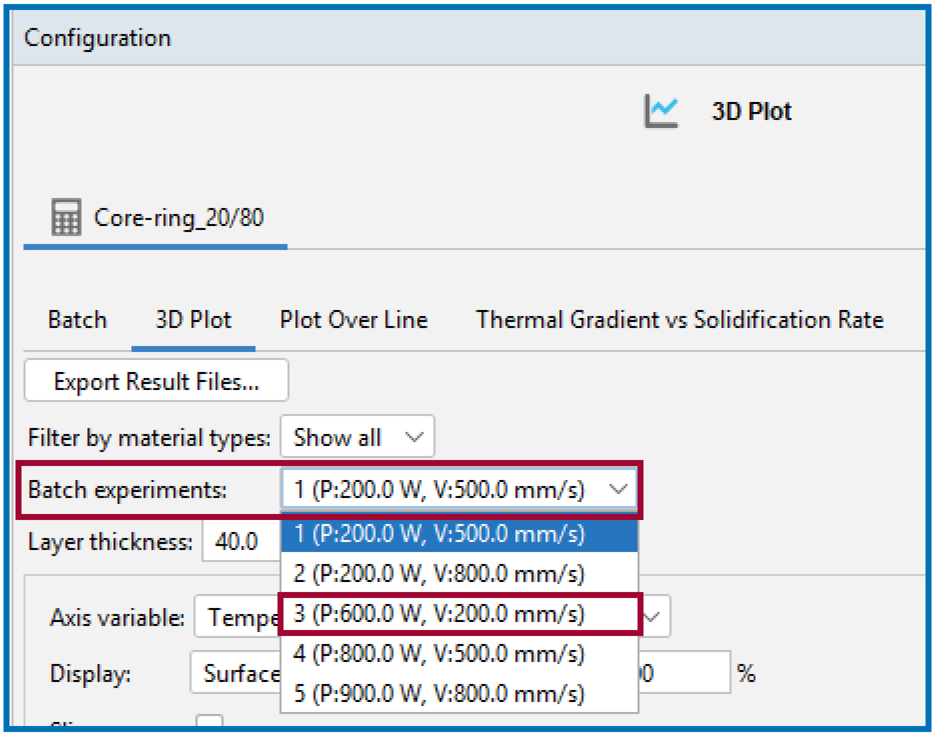
3D Plots

The specific **3D Plot** that is highlighted in this section is shown by clicking the **3D Plot** node in the **Project** window. Then on the **Visualizations** window on the tab of the same name, you can use various toolbar buttons to navigate and experiment with the views, for example:

Zoom to Heat Source position

In Figure 135, and using a combination of the **Plot Renderer Configuration** window settings on the **3D Plot** tab and the **Visualizations** window, different zoom levels and adjusting the **Glyph scale factor** setting helps to clearly show the melt pool and velocity vectors.

Further, the plot on the left is displayed by choosing the applicable **Batch experiments** results from the list (P=200 W, V=500 mm/s) and this set of experiments undergoes melting in conduction mode. Then the plot on the right is displayed by choosing the applicable **Batch experiments** results (P=600 W, V=200 mm/s) and that one forms a keyhole.



Configuration

3D Plot

Core-ring_20/80

Filter by material types: Show all

Batch experiments: 1 (P:200.0 W, V:500.0 mm/s)

- 1 (P:200.0 W, V:500.0 mm/s)
- 2 (P:200.0 W, V:800.0 mm/s)
- 3 (P:600.0 W, V:200.0 mm/s)
- 4 (P:800.0 W, V:500.0 mm/s)
- 5 (P:900.0 W, V:800.0 mm/s)

Layer thickness: 40.0

Axis variable: Tempe

Display: Surface

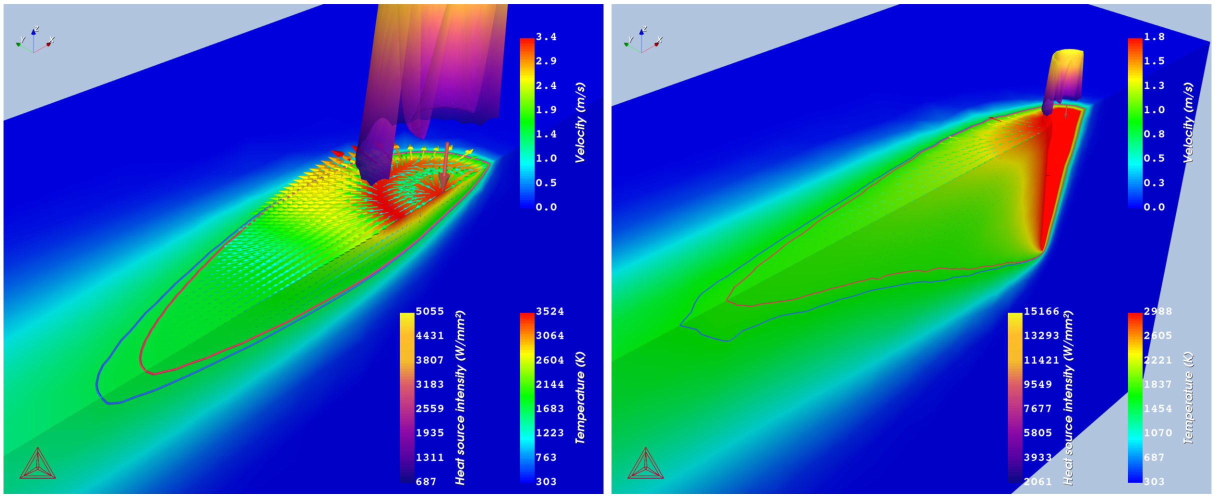


Figure 135: A comparison of the melt pools for two different processing conditions: Red and blue isocontours show liquidus and solidus temperatures, respectively. See the text for details.

In Figure 136 you can click the **Set View** button plus **Mirror Geometry** button to obtain this top view of a **Surface colormap**.

In general, you can play around with the **3D Plot Configuration** window settings. For example, for the right-hand side figure, you can view the **Flow velocity field** with different **Display** types such as an **Arrow** (shown).

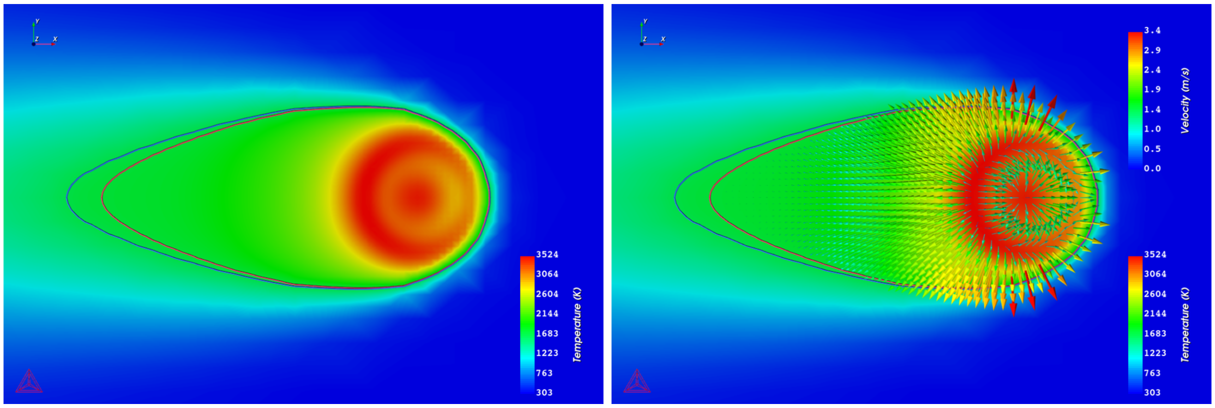


Figure 136: Top view (XY) of the surface colormap showing (left) temperature distribution due to the 20/80 Core-ring beam shape, and (right) velocity field caused by the distinctive temperature profile, resulting in widening of the melt pool. P=200 W, V=500 mm/s. Red and blue isocontours show liquidus and solidus temperatures, respectively.

In Figure 137, this cross-section compares the melt pool shape and size for **Batch experiment 1** (P=200 W, V=500 mm/s) to the experimental results as shown in Figure 9 in the paper by [2024Hol].

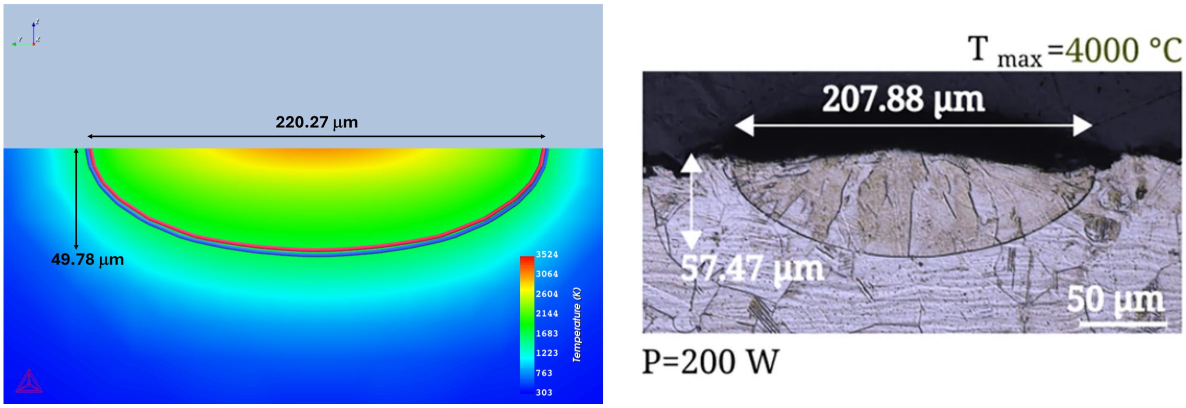


Figure 137: A cross-section comparing melt pool shape and size for P=200 W, V=500 mm/s from (left) simulation and (right) experiments [2024Hol-Fig9]. Red and blue isocontours in the simulation result show liquidus and solidus temperatures, respectively.

In Figure 138, the formation of the meltpool is shown on the left and compared to a cross-section that is taken from **Batch experiment 3** (P=600 W, V=200 mm/s) to show the formation of a keyhole and the maximum melt pool size, where you can also see the widening of the melt pool due to fluid flow. Compare this to Figure 139, which are the experimental results as shown in Figure 9 in the paper by [2024Hol].

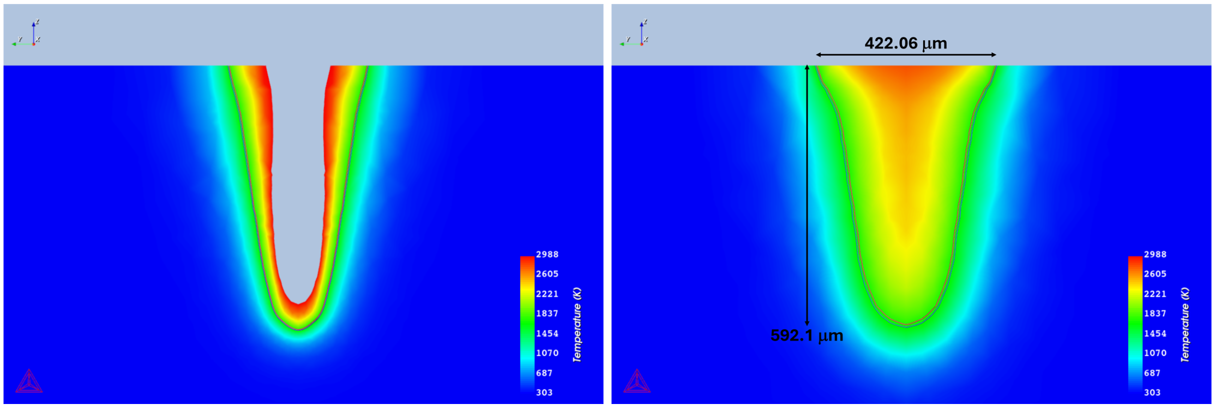


Figure 138: Cross-sections at different locations along the scanning direction showing (left) formation of keyhole and (right) maximum melt pool dimensions for P=600 W, V=200 mm/s. See the text for more.

Figure 139: Cross-section showing the experimental melt track for the same processing conditions shown in Figure 138. From [2024Hol-Fig9].

Other Resources

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References

[2021Grü] J. Grünewald, F. Gehringer, M. Schmöller, K. Wudy, Influence of Ring-Shaped Beam Profiles on Process Stability and Productivity in Laser-Based Powder Bed Fusion of AISI 316L. Metals (Basel). 11, 1989 (2021).

[2023Bi] J. Bi, L. Wu, S. Li, Z. Yang, X. Jia, M. D. Starostenkov, G. Dong, Beam shaping technology and its application in metal laser additive manufacturing: A review. J. Mater. Res. Technol. 26, 4606–4628 (2023).

[2024Hol] V. Holla, J. Grünewald, P. Kopp, P. M. Praegla, C. Meier, K. Wudy, S. Kollmannsberger, Validity of Thermal Simulation Models for Different Laser Beam Shapes in Bead-on-Plate Melting. Integr. Mater. Manuf. Innov. 13, 969–985 (2024).

[2024Hol-Fig9]: V. Holla et. al, Validity of Thermal Simulation Models for Different Laser Beam Shapes in Bead-on-Plate Melting. Integr. Mater. Manuf. Innov. 13, 969–985 (2024). Creative Commons Attribution 4.0 International License, Figure 9, accessed May 2025, cropped individual images from source. https://link.springer.com/article/10.1007/s40192-024-00382-2/figures/9

AM_14: Using the Top-hat Beam Shape

This **Steady-state** example demonstrates the use of **Top-hat** *Heat Source* model in the AM Module with **Batch** calculations.

The processing parameters (power and speed) and other processing conditions such as the layer thickness are taken from Sow et al. [2020Sow]. The example also compares the predicted melt pool dimensions with the experimental data.

For TC-Python users, there is an example using **Top-hat**: `pyex_AM_10_TopHat_BeamShape.py`.

There is a companion example in Graphical Mode using **Core-ring**: AM_13: Using the Core-ring Beam Shape.

Project File and License Information

- Folder: **Additive Manufacturing**
- File name: *AM_14_TopHat_BeamShape.tcu*

This example requires an Additive Manufacturing (AM) Module license.

Background

The primary benefit of the Top-hat heat source beam shape, in comparison to the Gaussian beam shape, is uniform energy distribution across the beam spot, leading to even heating of the material surface. With lower peak intensity as compared to the Gaussian beam, a Top-hat beam also allows the use of larger beam size that not only increases productivity but also reduces vapor-induced instabilities [2020Sow]. The inclusion of Top-hat heat source model in the AM Module, together with the keyhole model, allows you to predict the temperature evolution and melt pool shape along with the transition from conduction mode to keyhole mode for a Top-hat heat source. The example uses experimental data taken from the literature [2020Sow] and demonstrates the use of Top-hat heat source with a rather large beam size for single track experiments on an IN625 alloy.

About the Heat Source Models

Material Properties

- IN625: Ni-21.5Cr-5.0Fe-0.5Si-0.5Mn-9.0Mo-0.4Ti-1.0Co-1.8Nb-1.8Ta-0.4Al Mass percent
- Database: TCNI12 and with solute trapping and interface scattering = 1e-07.
- The material properties are precalculated, and stored as a built-in material library with the Additive Manufacturing (AM) Module.

AM Calculator Configuration Settings

This example contains one AM Calculator, which is renamed to **Top-hat**. On the **Configuration** window, **Conditions** tab, this **Steady-state** calculation is configured with the **Top-hat** *Heat Source* with the **Keyhole model**.

Fluid flow is not used in this example (the **Fluid flow including Marangoni effect** checkbox is not selected). Although fluid flow plays a crucial role in determining the shape and size of the melt pool, in this case it was found that it overestimates the melt pool width for most cases when fluid flow is included.

In the *Geometry* section, the **Height** of the base plate is set to `3.0` mm and in the *Scanning Strategy* section the **Layer thickness** is changed to 50.0 µm.

In the *Heat Source* section, the **Beam radius** is set to `450` µm.

In the [2020Sow] paper, it is mentioned that the beam diameter for the top-hat distribution is 500 µm. However, in Figure 2 of this paper, where intensity is plotted against the distance for the top-hat beam, the actual diameter looks much larger than that. In order to match the intensity distribution, the beam radius is therefore set to 450 µm.

Also in the *Heat Source* section, the **Absorptivity** is set to **Calculated** with a **prefactor** of `1.0` and in the keyhole model, **Beam quality factor M^2** is kept as `1.0`.

The **Batch** *Calculation Type* is used to set up all the conditions from the experiments in a single calculation. In the *Batch Experiment Data* section, the experimental **Power** and scan **Speed** as well as the measured melt pool Width (**Exp width**) and Depth (**Exp. depth**) were collected in a CSV file and imported into the software. This data is then saved in the project file.

Data with the error bars is also read and stored in the project file, that is later used to plot error bars together with the experimental values of melt pool width and depth.

In the *Batch Experiment Data* table, the **Power** is always 1000 W and the scan **Speed** ranges between 25 mm/s to 500 mm/s.

AM Calculator Conditions Settings and AM Calculator Heat Source Settings

Visualizations

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

When you run (Perform) this example, it takes a few minutes for the calculations to complete.

For more information also see Working with AM Visualizations.

Parity Plot

This specific **Parity** plot is shown by clicking the **Parity Plot** node in the **Project** window. Then you can see on the **Visualizations** window it is in the tab of the same name. The settings are located on the **Configuration** window on the **Batch** tab.

The plot compares experimental and calculated melt pool width and depth. It can be seen that the calculated melt pool width shows a fairly good agreement with the measured values. A mixed trend is however, seen for the melt pool depth. For lower energy densities, the calculated and measured melt pool depth matches quite well, however it starts to deviate once the melting appears to happen in the keyhole mode in the experiments, while it is still in the conduction mode in the calculations. For the last three points, where the calculations also predict a keyhole mode, the melt pool depth matches quite well with the measured value, except for the very last point where it is somehow overpredicted. The difference in depth could be attributed to the uncertainty in the actual beam size of the top-hat beam.

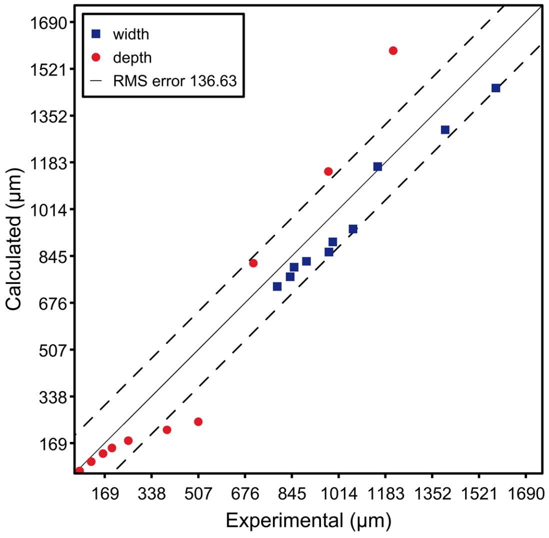


Figure 140: Parity plot comparing experimental and calculated melt pool width and depth for all the experiments. The experiments are single tracks on IN625 with constant power and varied scan speed using the Top-hat heat source. The Root Mean Square (RMS) error can also be seen as a dashed line.

Melt Pool Dimensions

This **Melt Pool vs Energy Density** plot is shown by clicking the **Melt Pool Dimensions** node in the **Project** window. Then you can see on the **Visualizations** window it is in the tab of the same name. The settings are located on the **Configuration** window on the **Batch** tab.

The plot shows a comparison of the experimental and calculated melt pool width and depth, where the error bars are also plotted with the measured data. Rather large error bars, especially for the higher energy density cases, show that the overall trend for the calculated values of melt pool width and depth is in good agreement with the measured values. Some improvements are however needed for the low energy density cases where a huge deviation is found between the calculated and measured values.

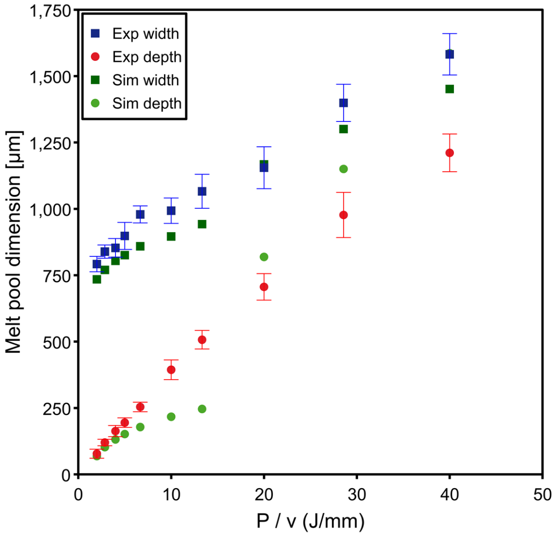


Figure 141: A comparison of the experimental and calculated melt pool width and depth for all the experiments. The error bars on the experimental data are also shown.

3D Plots

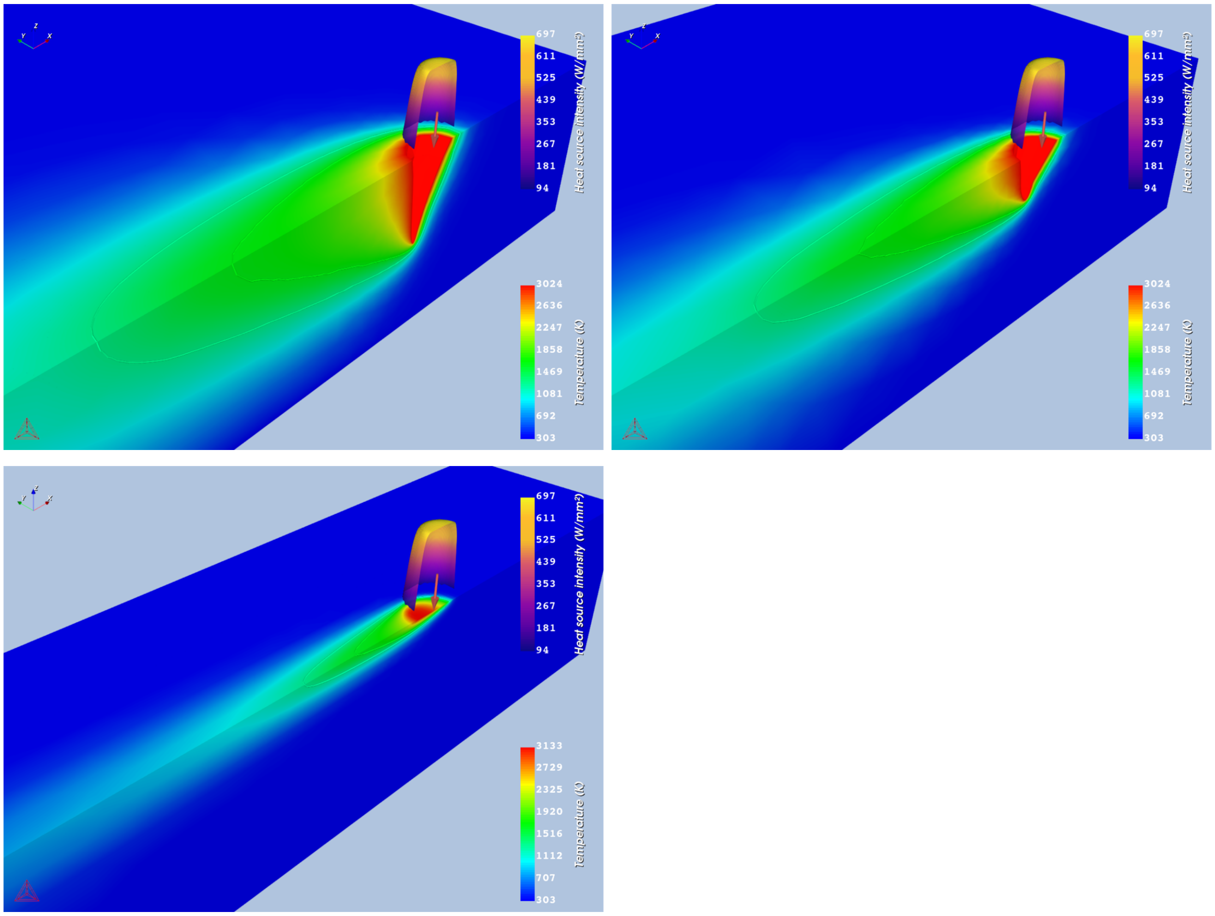


Figure 142: A comparison of the temperature distribution for three different processing conditions: (top-left) P=1000 W, V=25 mm/s, (top-right) P=1000 W, V=50 mm/s, both of which form keyhole during melting and (bottom-left) P=1000 W, V=250 mm/s that undergoes melting in conduction mode.

For the comparisons in Figure 143, all cross-sections are taken where the melt pools attain maximum width and depth. Red and blue isocontours show liquidus and solidus temperatures, respectively.

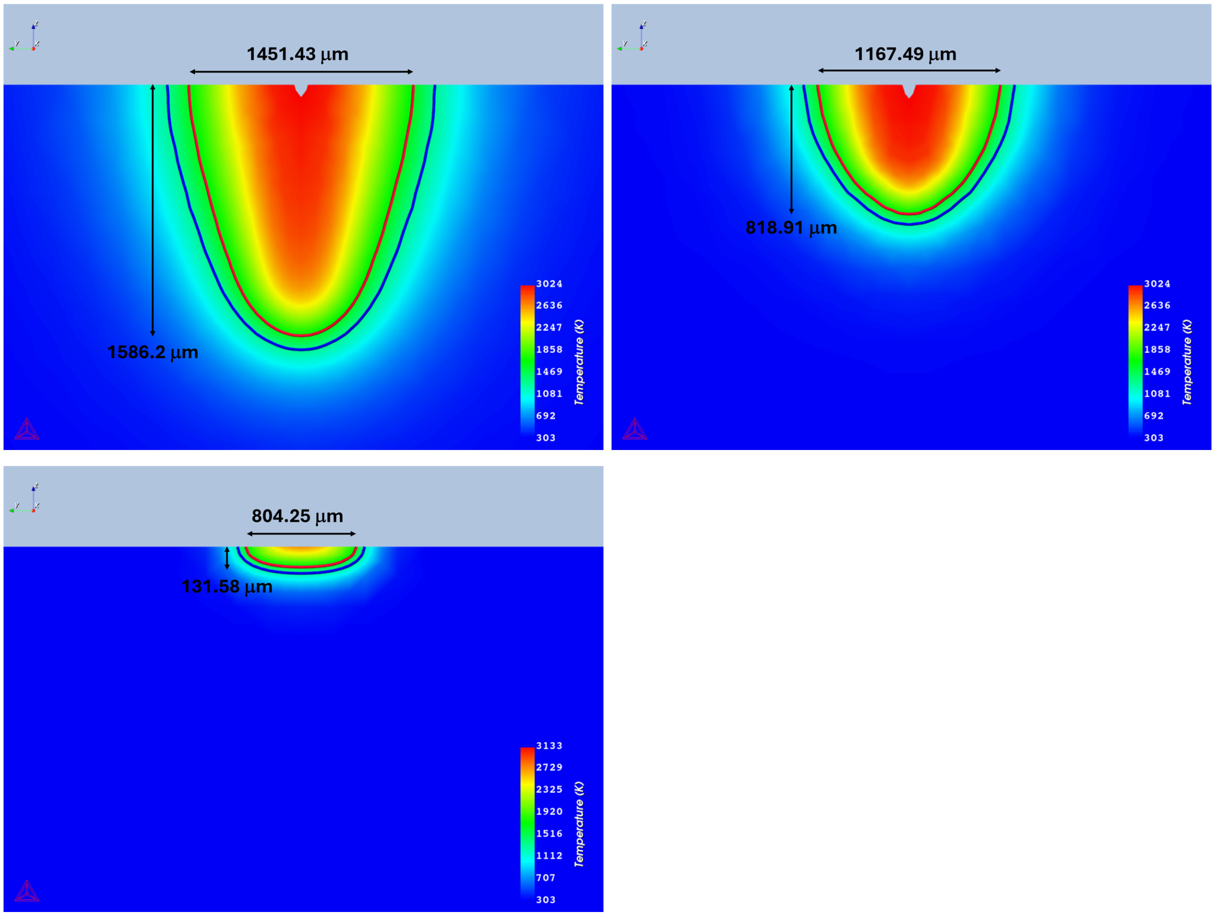


Figure 143: Cross-sections comparing melt pool shape and size for (top-left) P=1000 W, V=25 mm/s, (top-right) P=1000 W, V=50 mm/s and (bottom-left) P=1000 W, V=250 mm/s.

Other Resources

Read more about the Additive Manufacturing (AM) Module on our website including the details about database compatibility or to watch an introductory webinar. You can also use the Getting Started Guide to learn about the key features available.

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Reference

[2020Sow] M. C. Sow, T. De Terris, O. Castelnau, Z. Hamouche, F. Coste, R. Fabbro, P. Peyre, Influence of beam diameter on Laser Powder Bed Fusion (L-PBF) process. Addit. Manuf. 36, 101532 (2020).

Diffusion Module (DICTRA) Examples Collection

These are the Graphical Mode examples. There are separate Console Mode examples also available.

Examples using up to three elements are available to all users. The other examples require a Diffusion Module (DICTRA) license to calculate and plot results.

The Role of Diffusion in Materials: A Tutorial is available for download on our website. It is intended for engineers interested in using the Diffusion Module (DICTRA), as well as students learning about the role of diffusion in materials. It is designed to be useful at many levels, from undergraduate studies to someone with a PhD and experience in a related field.

These examples use the **Diffusion Calculator**. All examples use demonstration database packages included with your installation no matter what licenses you have.

About the Examples

In this section:

D_01: Homogenization of a Binary Fe-Ni Alloy

The single phase example simulates the diffusion of Fe and Ni at a temperature of 1400 K in a planar domain. At this temperature the material is fully austenitic, i.e. the only phase present is the so-called fcc (face centered cubic) phase. Initially, there is a linear variation in Ni going from 10 mass-% on the left-hand side to 50 mass-% on the right-hand side.

Project File Information

- Folder: **Diffusion Module - DICTRA**
- File name: `D_01_Diffusion_Single_Phase.tcu`

This example is part of the *Diffusion Module (DICTRA) Quick Start Guide* available to all users. A version of the example is also available for Console Mode.

Visualizations

This example is included as a Diffusion Module (DICTRA) tutorial on our website and as part of the playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Composition Profiles** and **Thermal Profile**: When setting up a calculator on a **Configuration** window you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.
- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

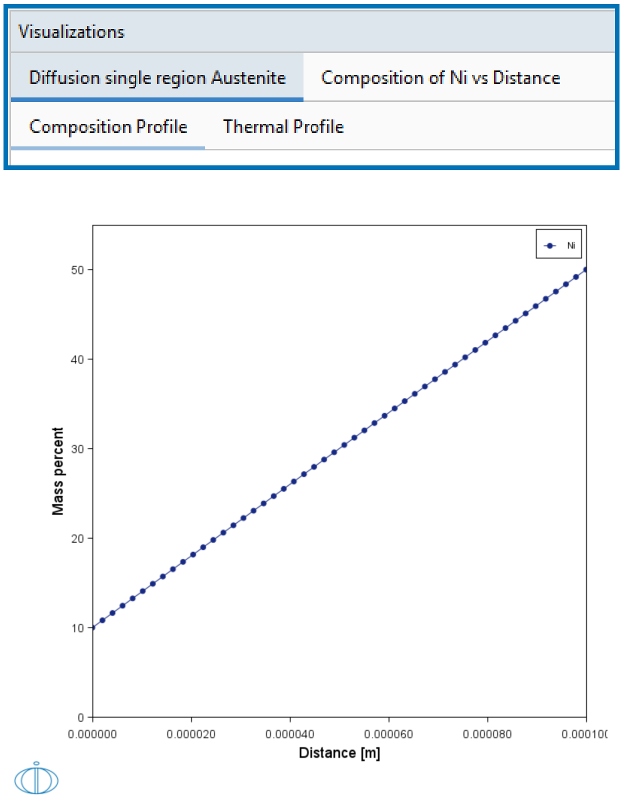


Figure 144: During set up of the calculation, you can preview the Composition Profile (shown) or Thermal Profile. Click the tab(s) in the Visualizations window to switch between these previews and adjust settings on the Diffusion Calculator Configuration window. For an Isothermal Thermal Profile this shows the constant temperature as entered.

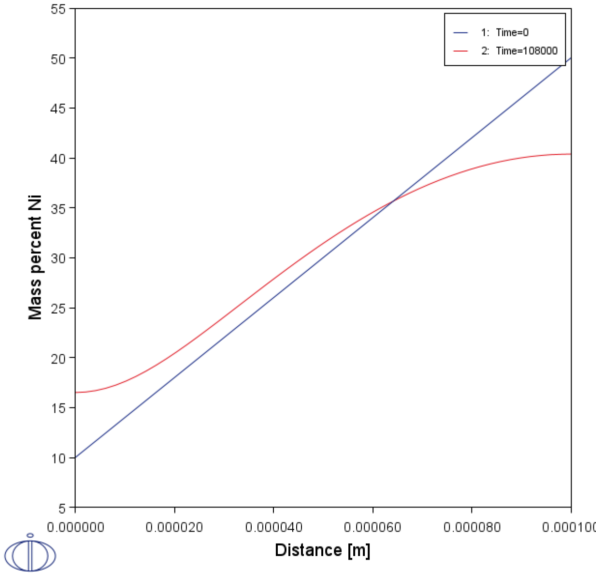


Figure 145: After performing the calculation, you can view the result on the Composition of Ni vs Distance tab, which shows the initial and final Ni profile. In this example, the Plot Renderer is renamed and this matches the tab name in the Visualizations window.

D_02: Ferrite(bcc)/Austenite(fcc) Transformation in a Binary Fe-C Alloy

The moving phase boundary example simulates the growth of ferrite (bcc) into austenite (fcc). The austenite is assumed to be initially homogeneous with the composition Fe-0.15 mass-% C. The transformation temperature is 1050 K. The initial thickness of the austenite is 2 mm and an initially very thin ferrite (1 nm) is also present at the start of the simulation.

Project File Information

- Folder: **Diffusion Module - DICTRA**
- File name: `D_02_Diffusion_Moving_Boundary.tcu`

This example is part of the *Diffusion Module (DICTRA) Quick Start Guide* available to all users. A version of the example is also available for Console Mode.

Visualizations

This example is included as a Diffusion Module (DICTRA) tutorial on our website and as part of the playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Composition Profiles** and **Thermal Profile**: When setting up a calculator on a **Configuration** window you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.
- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

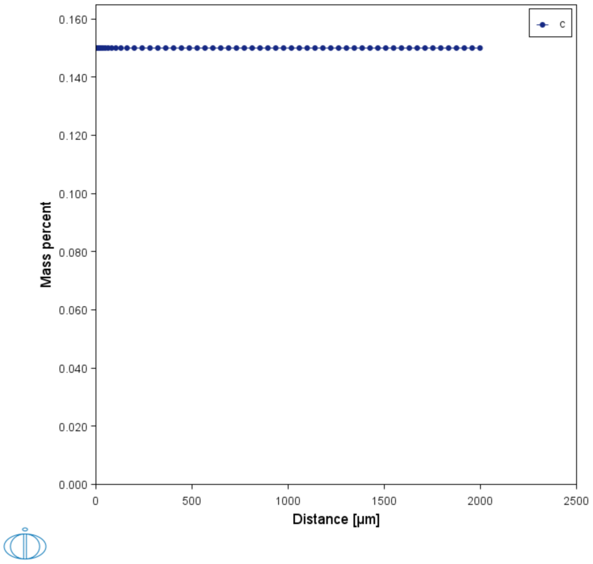


Figure 146: During set up of the calculation, you can preview the Composition Profile (shown) or Thermal Profile. Click the tab(s) in the Visualizations window to switch between these previews and adjust settings on the Diffusion Calculator Configuration window. For an Isothermal Thermal Profile this shows the constant temperature as entered.

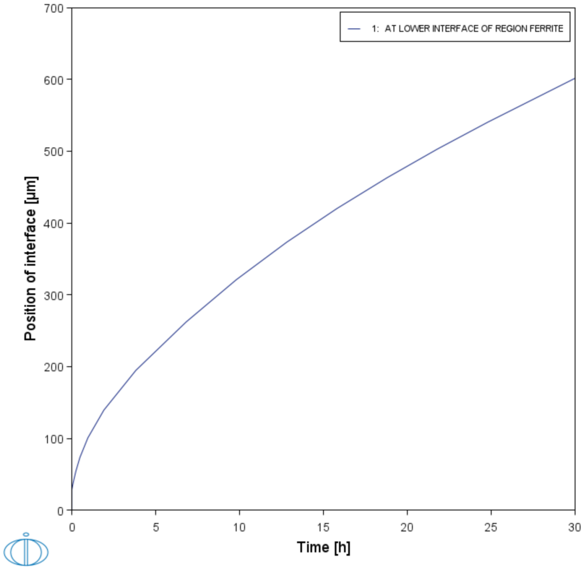


Figure 147: After performing the calculation, you can view the result on the Position of interface vs time tab. In this example, the Plot Renderer is renamed and this matches the tab name in the Visualizations window.

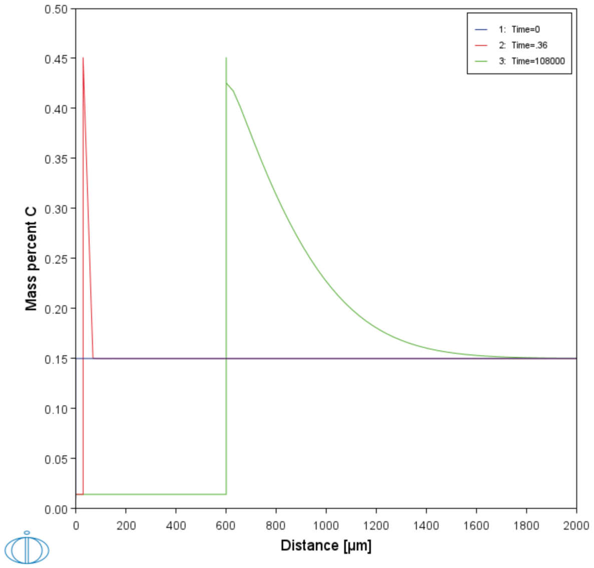


Figure 148: After performing the calculation, you can view the result on the Composition profile C tab. In this example, the Plot Renderer is renamed and this matches the tab name in the Visualizations window.

D_03: Evolution of an Fe-Cr-Ni Diffusion Couple

The multiphase example simulates the evolution of an Fe-Cr-Ni diffusion couple during a 100 hour heat treatment at 1100° C (1373.15 K). Both end members of the diffusion couple are duplex ferrite plus austenite, but the majority phase is ferrite on the left-hand side and austenite on the right.

With this type of simulation it is assumed that the material is fully equilibrated at each grid point, i.e. the local phase fractions, phase compositions and so forth are obtained from an equilibrium calculation with the local overall composition as a condition.

More details about the homogenization model for multiphase simulations can be found in Larsson and Engström [2006Lar] and Larsson and Höglund [2009Lar]. Experimental data is from Engström [1995Eng].

Project File Information

- Folder: **Diffusion Module - DICTRA**
- File name: `D_03_Diffusion_Multiphase.tcu`

This example is part of the *Diffusion Module (DICTRA) Quick Start Guide* available to all users. A version of the example is also available for Console Mode.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Composition Profiles** and **Thermal Profile**: When setting up a calculator on a **Configuration** window you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.
- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

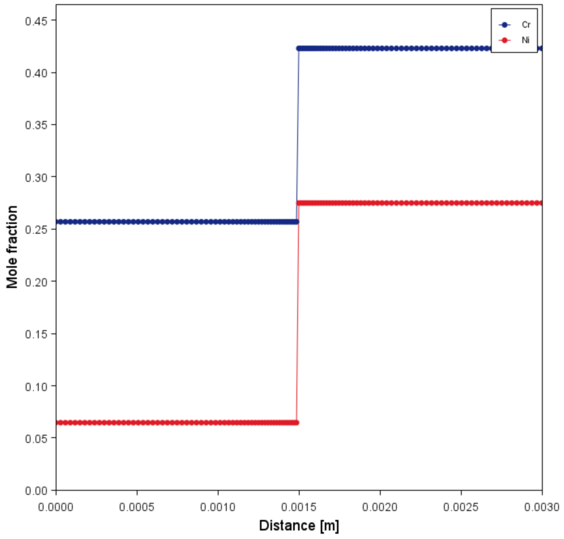


Figure 149: During set up of the calculation, you can preview the Composition Profile (shown) or Thermal Profile. Click the tab(s) in the Visualizations window to switch between these previews and adjust settings on the Diffusion Calculator Configuration window. For an Isothermal Thermal Profile this shows the constant temperature as entered.

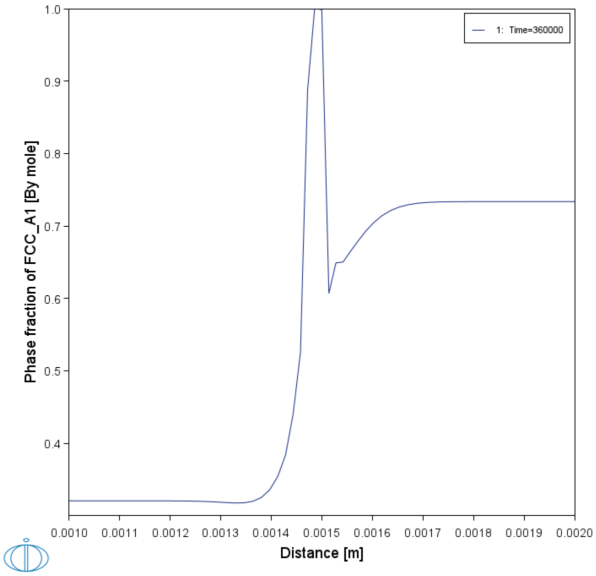


Figure 150: After performing the calculation, you can view the result on the Phase fraction of FCC tab. In this example, the Plot Renderer is renamed and this matches the tab name in the Visualizations window.

References

[1995Eng] A. Engström, Interdiffusion in multiphase, Fe-Cr-Ni diffusion couples. Scand. J. Metall. 24, 12–20 (1995).

[2006Lar] H. Larsson, A. Engström, A homogenization approach to diffusion simulations applied to α+γ Fe–Cr–Ni diffusion couples. Acta Mater. 54, 2431–2439 (2006).

[2009Lar] H. Larsson, L. Höglund, Multiphase diffusion simulations in 1D using the DICTRA homogenization model. Calphad. 33, 495–501 (2009).

D_04: Fe-C Moving Boundary - Austenite to Ferrite

This example simulates the austenite to ferrite transformation in a Fe-0.01 mass% C steel during continuous cooling. The simulation starts at a temperature where only austenite is stable, ferrite nucleates and grows into the austenite during cooling in the two phase region. Plots of thermal and carbon composition profiles are generated.

Project File Information

- Folder: **Diffusion Module - DICTRA**
- File name: `D_04_Diffusion_Fe-C_Moving_Boundary_Austenite_to_Ferrite.tcu`

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Composition Profiles** and **Thermal Profile**: When setting up a calculator on a **Configuration** window you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.
- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

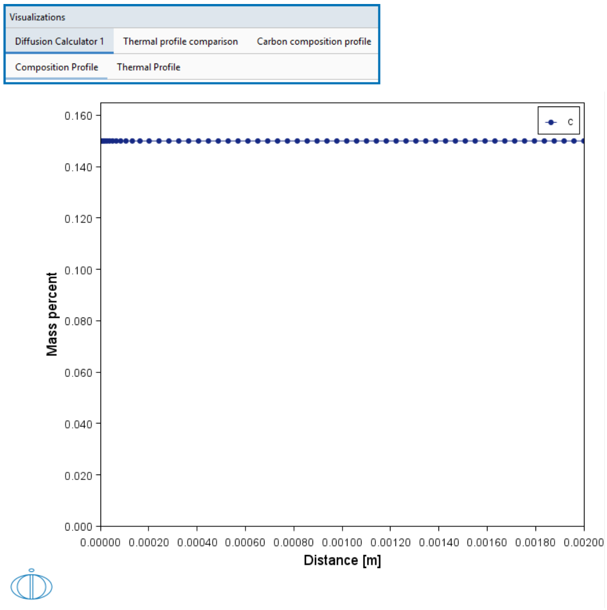


Figure 151: During set up of the calculation, preview the Composition Profile. Click the tab in the Visualizations window to switch between these previews and adjust settings on the Diffusion Calculator Configuration window.

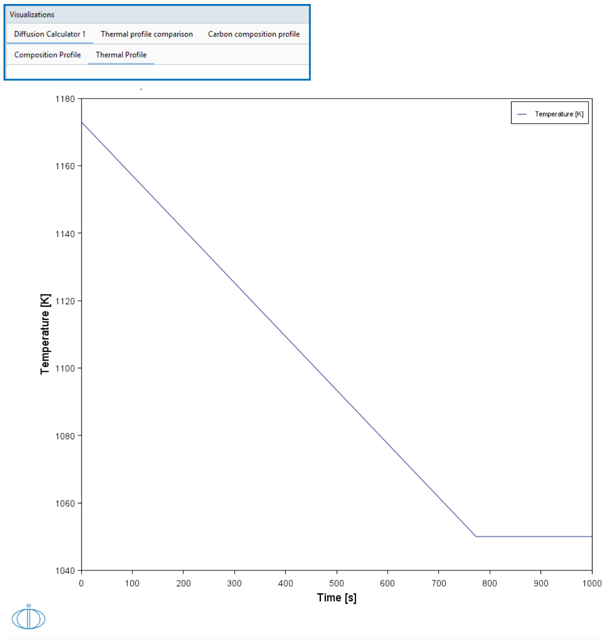


Figure 152: During set up of the calculation, preview the non-isothermal Thermal Profile. Click the tab in the Visualizations window to switch between these previews and adjust settings on the Diffusion Calculator Configuration window. Also see the plot result comparing the thermal profile for the two regions.

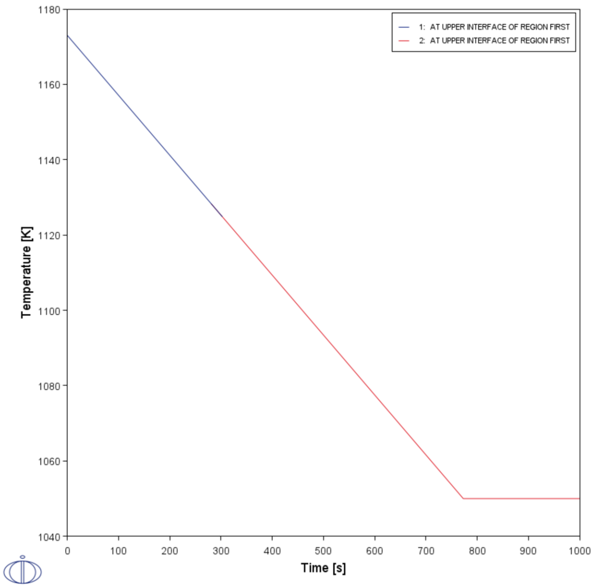


Figure 153: After performing the calculation, view the result on the Thermal profile tab. In this example, the Plot Renderer is renamed and this matches the tab name in the Visualizations window. Note that this Thermal Profile is slightly different than what you can preview during set up.

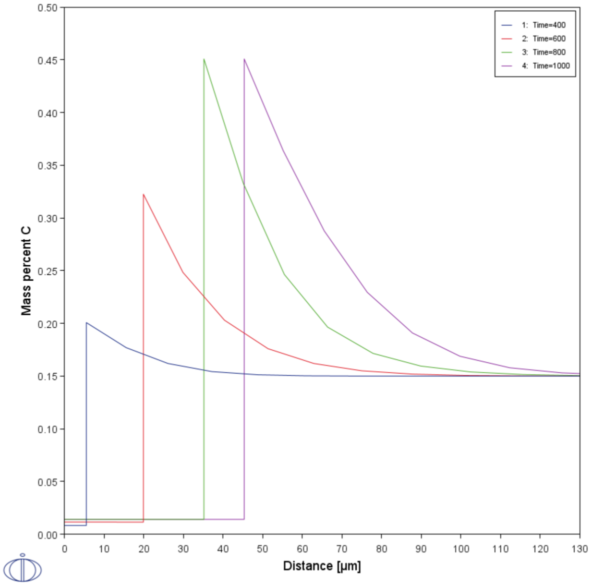
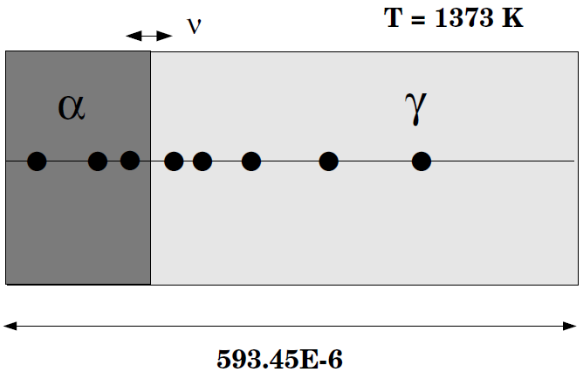


Figure 154: After performing the calculation, view the result on the Carbon composition profile tab. In this example, the Plot Renderer is renamed and this matches the tab name in the Visualizations window.

D_05: γ/α/γ Diffusion Couple of Fe-Ni-Cr alloys

This example demonstrates the evolution of a ternary Fe-Cr-Ni diffusion couple. A thin slice of ferrite (α phase) (38%Cr,0%Ni) is clamped between two thicker slices of austenite (γ phase) (27%Cr, 20%Ni). The assembly is subsequently heat treated at 1373 K.

This set up corresponds to diffusion couple in Kajihara et al. [1993aKaj] and Kajihara and Kikuchi [1993bKaj].



Project File Information

- Folder: **Diffusion Module - DICTRA**
- File name: `D_05_Diffusion_Fe_Ni_Cr_Moving_Boundary_Diffusion_Couple.tcu`

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

⌛ When you run (Perform) this example, it takes a few minutes for the calculations to complete.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Composition Profiles** and **Thermal Profile**: When setting up a calculator on a **Configuration** window you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.
- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

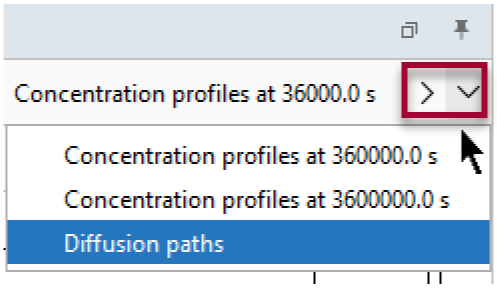


Figure 155: In this example, all Plot Renderer nodes are renamed and each match a tab name in the Visualizations window. Use the left and right arrows in the Visualizations window to move through the tabs and the down arrow to choose by name when a tab is not visible.

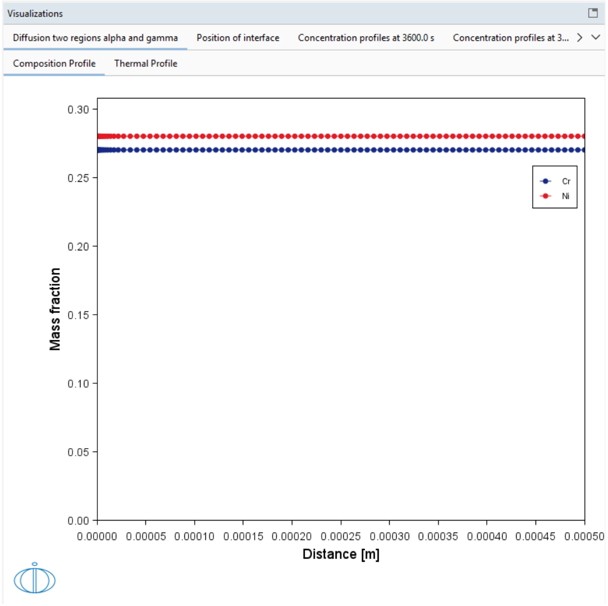


Figure 156: During set up of the calculation, preview the Composition Profile (shown) or Thermal Profile. Click the tab(s) in the Visualizations window to switch between these previews and adjust settings on the Diffusion Calculator Configuration window. For an Isothermal Thermal Profile this shows the constant temperature as entered.

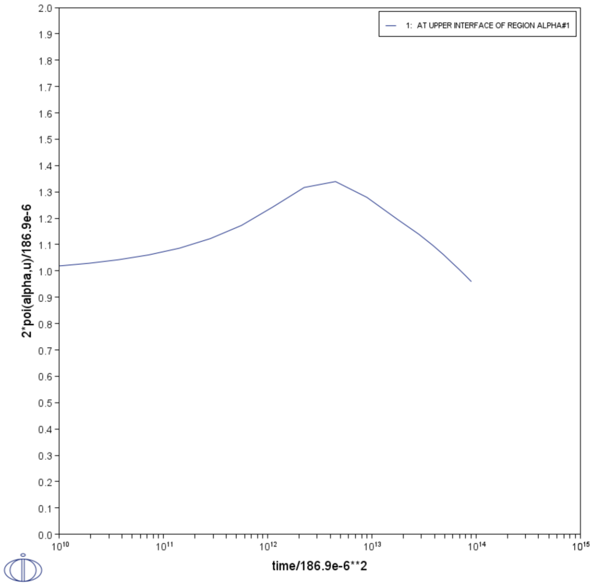


Figure 157: After performing the calculation, view the result on the Interface position tab.

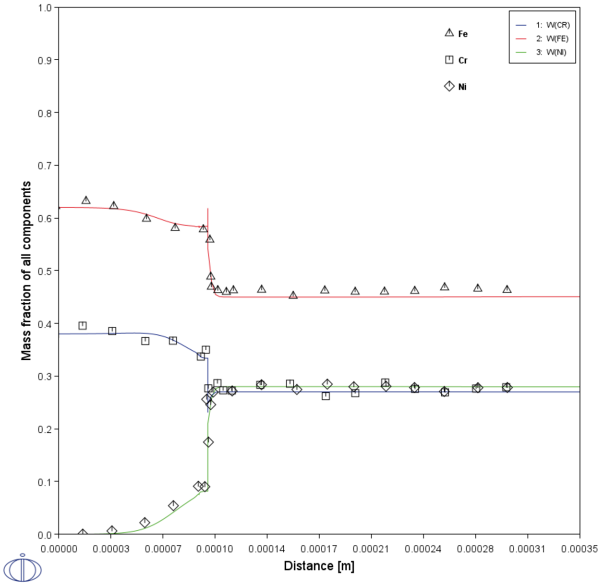


Figure 158: After performing the calculation, view the result on the Concentration profiles at 3600 s tab.

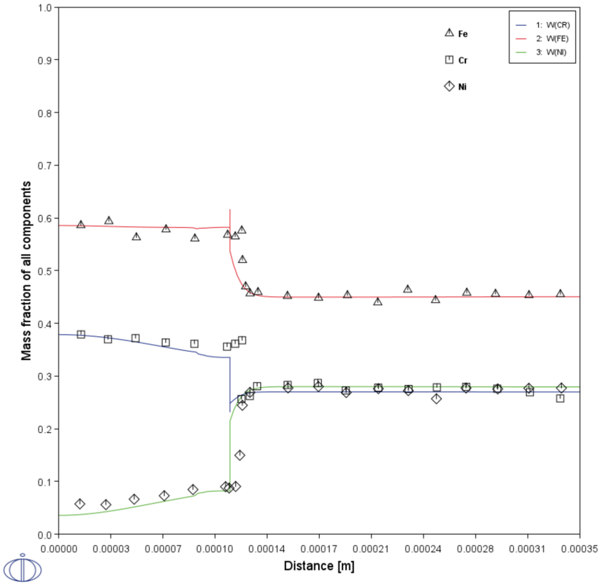


Figure 159: After performing the calculation, view the result on the Concentration profiles at 36 000 s tab.

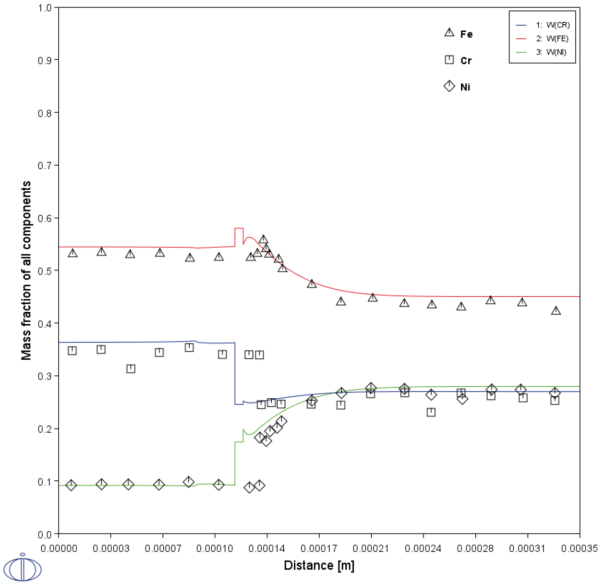


Figure 160: After performing the calculation, view the on the Concentration profiles at 360 000 s tab.

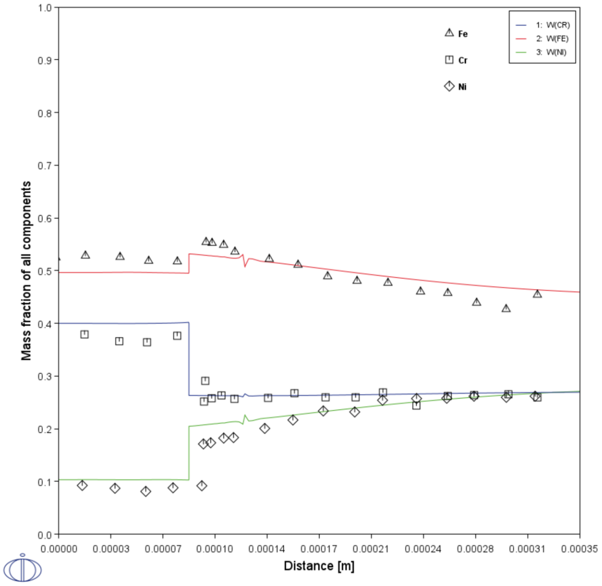


Figure 161: After performing the calculation, view the result on the Concentration profiles at 3 600 000 s tab.

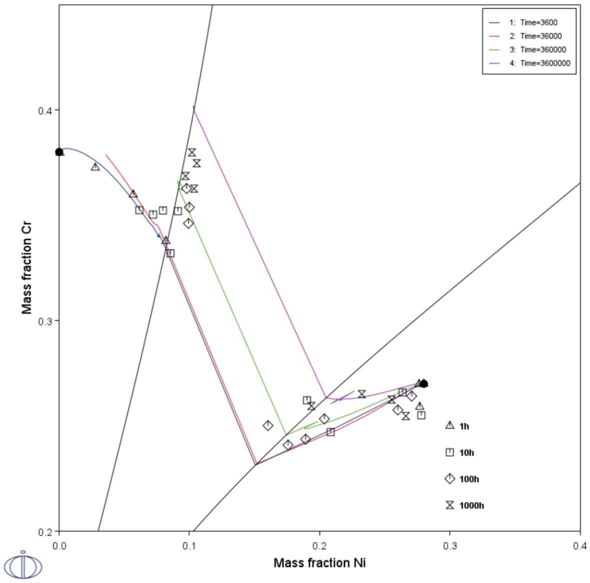


Figure 162: After performing the calculation, view the result on the Diffusion paths tab.

References

[1993aKaj] M. Kajihara, C.-B. Lim, M. Kikuchi, Experimental Study on Dissolution of ALPHA Phase in GAMMA/ALPHA/GAMMA Diffusion Couples of the Fe-Cr-Ni System. ISIJ Int. 33, 498–507 (1993).

[1993bKaj] M. Kajihara, M. Kikuchi, Numerical analysis of dissolution of α phase in γ/α/γ diffusion couples of the Fe-Cr-Ni system. Acta Metall. Mater. 41, 2045–2059 (1993).

D_06: Diffusion Through a Tube Wall

This is a simple example of diffusion through a tube wall. The tube material is an Fe-0.06Mn-0.05C alloy. Two plots comparing distance to the U-fraction of manganese and composition of carbon are generated to visualize the austenite region. A *cylindrical* geometry is used with *mixed zero flux and activity* boundary conditions.

On the inside wall a carbon activity of 0.9 is maintained whereas on the outside the carbon activity is very low. This example demonstrates the use of boundary conditions, advanced plotting and tables.

Project File Information

- Folder: **Diffusion Module - DICTRA**
- File name: `D_06_Diffusion_Carburization_Tube.tcu`

This example is based on Console Mode exab6. When in Console Mode, you can open the example from Thermo-Calc (**File → Examples Files → Diffusion Module**).

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Composition Profiles** and **Thermal Profile**: When setting up a calculator on a **Configuration** window you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

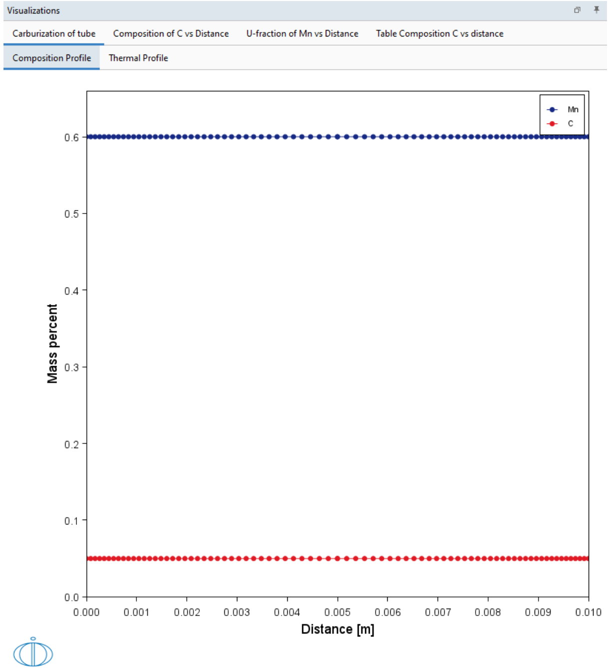


Figure 163: During set up of the calculation, you can preview the Composition Profile (shown) or Thermal Profile. Click the tab(s) in the Visualizations window to switch between these previews and adjust settings on the Diffusion Calculator Configuration window. For an Isothermal Thermal Profile this shows the constant temperature as entered.

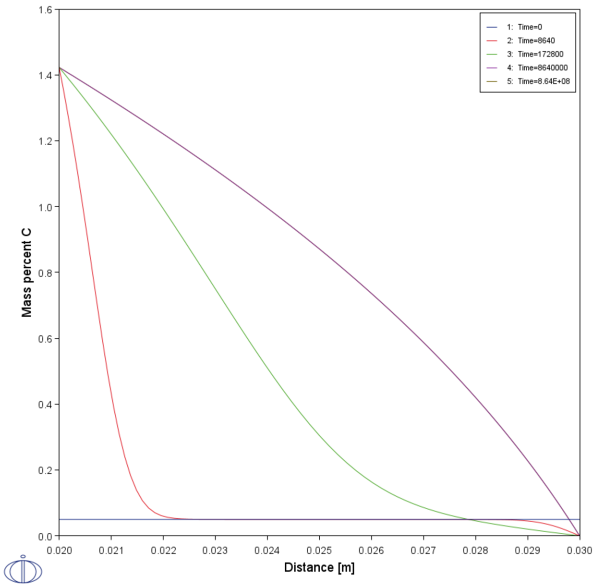


Figure 164: After performing the calculation, you can view the result on the Composition of C vs Distance tab. In this example, the Plot Renderer is renamed and this matches the tab name in the Visualizations window.

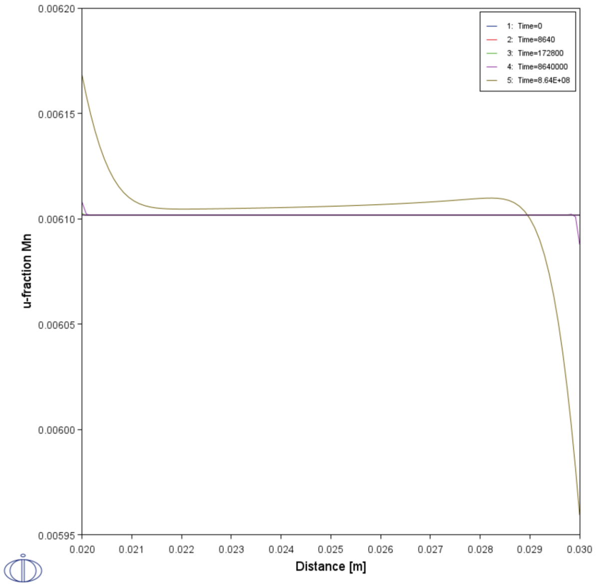
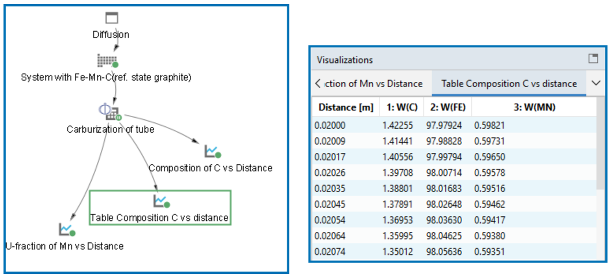


Figure 165: After performing the calculation, you can view the result on the U-fraction of Mn vs Distance tab. In this example, the Plot Renderer is renamed and this matches the tab name in the Visualizations window.



Distance [m]	1: W(C)	2: W(FE)	3: W(MN)
0.02000	1.42255	97.97924	0.59821
0.02009	1.41441	97.98828	0.59731
0.02017	1.40556	97.99794	0.59650
0.02026	1.39708	98.00714	0.59578
0.02035	1.38801	98.01683	0.59516
0.02045	1.37891	98.02648	0.59462
0.02054	1.36953	98.03630	0.59417
0.02064	1.35995	98.04625	0.59380
0.02074	1.35012	98.05636	0.59351

Figure 166: After performing the calculation, you can view the result on the Table Composition C vs Distance tab. In this example, the Table Renderer is renamed and this matches the tab name in the Visualizations window.

D_07: Multiphase Carburization of an Alloy

This example is based on Engström et al. [1994Eng] and is about carburization of a Ni-25Cr-0.0001C alloy. In this case the M7C3 and M3C2 carbides are entered as spheroid phases in an FCC_A1 matrix. It is similar to Graphical Mode example D_06 except the default simulation condition is automatically set to use the homogenization model.

The isothermal calculation is run for 1000 hours at a temperature of 1123 K using the mixed zero flux and activity left boundary condition. Results are plotted using two Plot Renderers and a Table Renderer.

Project File Information

- Folder: **Diffusion Module - DICTRA**
- File name: `D_07_Diffusion_Carburization_Multiphase.tcu`

This example is based on Console Mode exd1b. When in Console Mode, you can open the example from Thermo-Calc (**File → Examples Files → Diffusion Module**).

Visualizations

This example is included as a Diffusion Module (DICTRA) tutorial on our website and as part of the playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

When you run (Perform) this example, it takes a few minutes for the calculations to complete.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Composition Profiles** and **Thermal Profile**: When setting up a calculator on a **Configuration** window you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.
- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

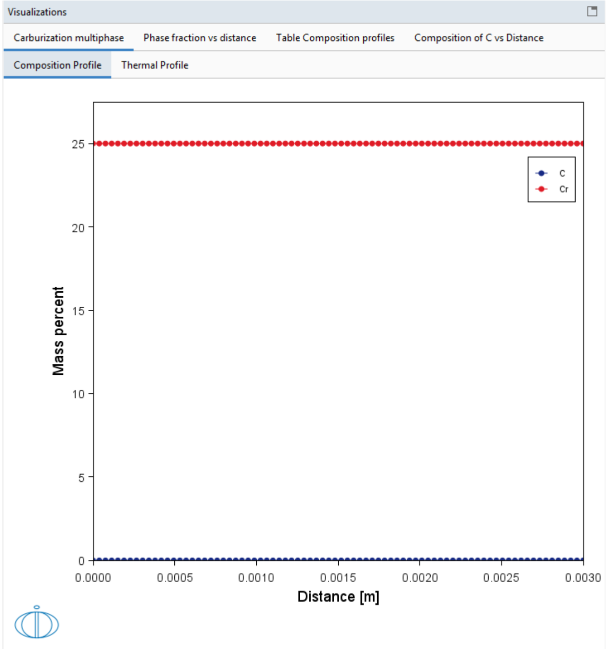


Figure 167: During set up of the calculation, you can preview the Composition Profile (shown) or Thermal Profile. Click the tab(s) in the Visualizations window to switch between these previews and adjust settings on the Diffusion Calculator Configuration window. For an Isothermal Thermal Profile this shows the constant temperature as entered.

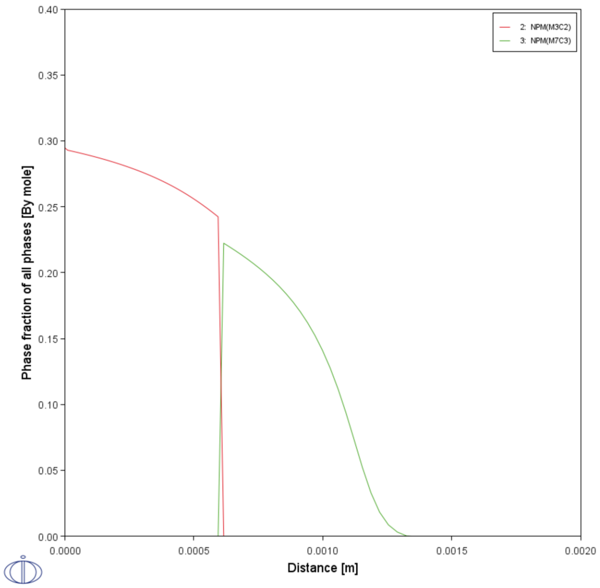
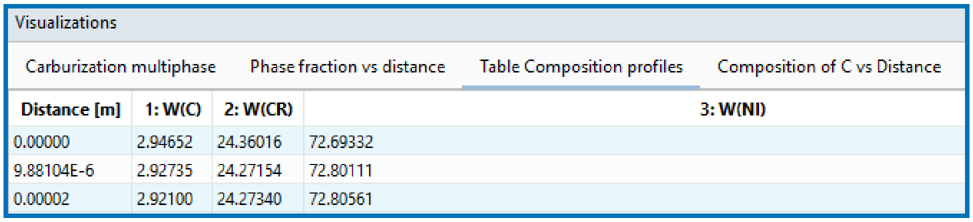


Figure 168: After performing the calculation, you can view the result on the Phase fraction vs distance tab. In this example, the Plot Renderer is renamed and this matches the tab name in the Visualizations window.



Distance [m]	1: W(C)	2: W(CR)	3: W(NI)
0.00000	2.94652	24.36016	72.69332
9.88104E-6	2.92735	24.27154	72.80111
0.00002	2.92100	24.27340	72.80561

Figure 169: After performing the calculation, you can view the result on the Table of Composition profiles tab. In this example, the Table Renderer is renamed and this matches the tab name in the Visualizations window.

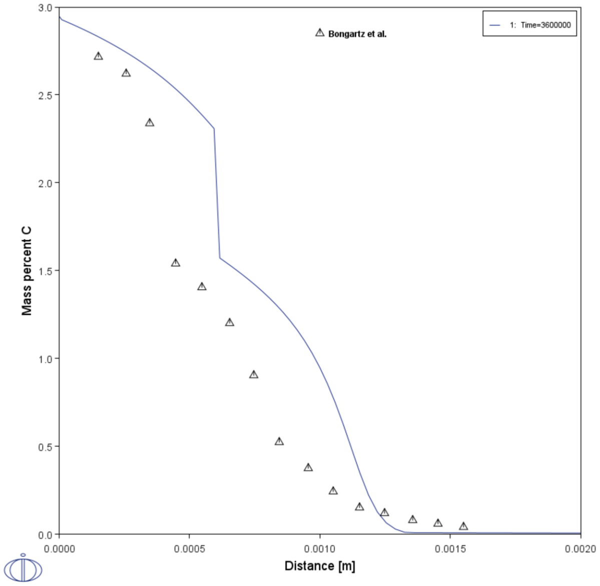


Figure 170: After performing the calculation, you can view the result on the Composition of C vs distance tab. In this example, the Plot Renderer is renamed and this matches the tab name in the Visualizations window.

Reference

[1994Eng] A. Engström, L. Höglund, J. Ågren, Computer simulation of diffusion in multiphase systems. Metall. Mater. Trans. A. 25, 1127–1134 (1994).

D_08: Microsegregation During Solidification

This application example, which is available on our website, shows how Thermo-Calc together with the Diffusion Module (DICTRA) can be used to investigate and predict microsegregation (solute redistribution) during solidification.

The example is based on a real case where the elemental distribution of a continuously cast steel was measured revealing the concentration of the elements Si, Mn, and P as sketched in Figure 1. The profile results from the well-known segregation across secondary dendrite arms. The interesting point is that the elements Si and Mn show the expected positive segregation (higher concentrations) in the interdendritic regions. The peak of the P content, on the other hand, is shifted compared to Si and Mn, and, in fact, shows negative segregation in the interdendritic region. This is unexpected and counterintuitive.

The calculations are based on ones performed in the frame of a research project funded by the European Union called VESPISM – Virtual Experiments to Solve Problems in Metallurgy – conducted from 2001 to 2004.

Project File and License Information

- Folder: **Diffusion Module - DICTRA**
- File name: `D_08_Diffusion_Microsegregation_During_Solidification.tcu`

Running this calculation requires licenses for the Add-on Diffusion Module (DICTRA) plus the steels thermodynamic database (TCFE) and mobility database (MOBFE). For best results, TCFE14 and MOBFE8.1 and newer (as of 2025a) are recommended.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects,

you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

> When you run (Perform) this example, it takes a few minutes for the calculations to complete.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Composition Profiles** and **Thermal Profile**: When setting up a calculator on a **Configuration** window you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.
- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

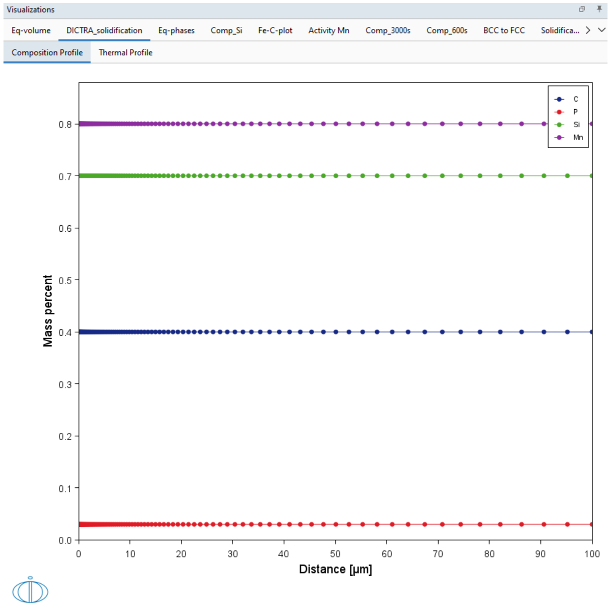


Figure 171: During set up of the calculation, you can preview the Composition Profile. Click the tab in the Visualizations window to switch between these previews and adjust settings on the Diffusion Calculator Configuration window.

The other resulting plots and details related to setting up this example are available to download via the dedicated web page.

D_09: Ni Post Weld Heat Treatment

In this example, a Ni-based alloy (Ni-Al-Co-Cr-Mo-Ti) post weld heat treatment analysis is completed. It shows how to import an initial composition profile from a file into the Diffusion Calculator. Then the calculation is run and plotted to show the composition of Al vs distance compared to experimental data from [2017She]. Such simulations can be used to design the heat treatment such that the desired homogenization of the weld is achieved. The initial composition profile needs to be determined by suitable experimental techniques, for example microprobe.

This example highlights the dual purpose of the **Visualizations** window where you can enter or import *Composition profiles* via the Diffusion Calculator **Configuration** window as well as being able to view and analyze results via the Plot Renderer after a calculation runs.

Project File Information

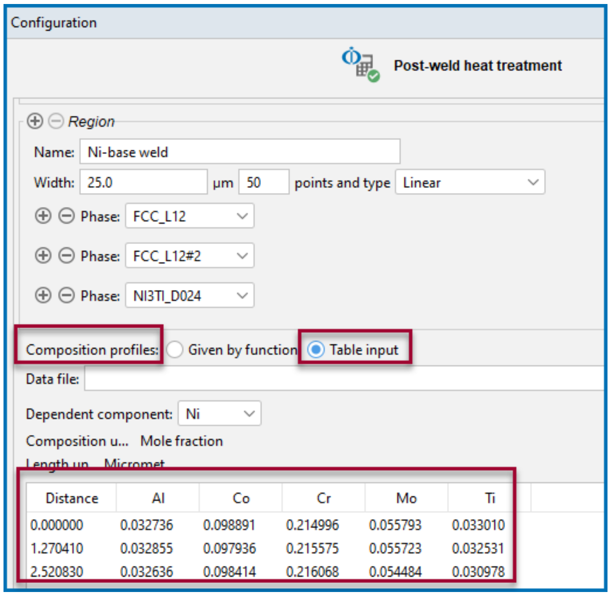
- Folder: **Diffusion Module - DICTRA**
- File name: `D_09 Ni_Post_Weld_Heat_Treatment_From_File.tcu`

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

On the Diffusion Calculator, when defining its setup, the **Composition profiles** are imported using the **Table input** option. A prepared file, in this case a csv file, is set up with the correct data columns, which then are included on the **Configuration** window. After import the **Composition Profiles** are further able to be seen via the **Visualizations** window, at which point adjustments can be made as needed. In this isothermal example, you can also see that the constant temperature of the **Thermal Profile** is previewed.



Name: Ni-base weld

Width: 25.0 µm 50 points and type Linear

Phase: FCC_L12

Phase: FCC_L12#2

Phase: NI3TI_D024

Composition profiles: ○ Given by function ● Table input

Data file:

Dependent component: Ni

Composition u... Mole fraction

Length un... Micromet...

Distance	Al	Co	Cr	Mo	Ti
0.000000	0.032736	0.098891	0.214996	0.055793	0.033010
1.270410	0.032855	0.097936	0.215575	0.055723	0.032531
2.520830	0.032636	0.098414	0.216068	0.054484	0.030978

Figure 172: The Diffusion Calculator Configuration window showing the composition profile data, which is then compiled and displayed on the Visualizations window.

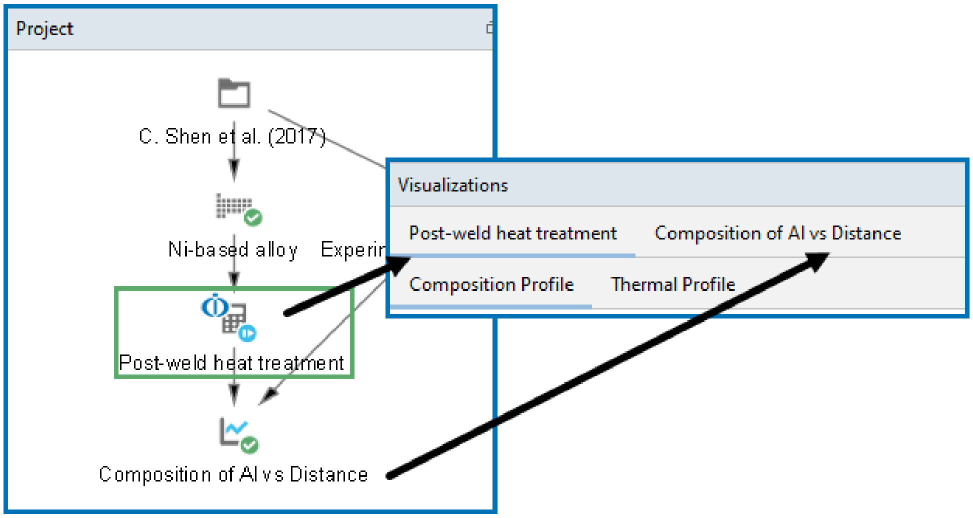


Figure 173: The Visualizations window displays details from both the Diffusion Calculator node (renamed to Post-weld heat treatment) via the Composition Profile and Thermal Profile tabs as well as the Plot Renderer node (renamed to Composition of Al vs Distance).

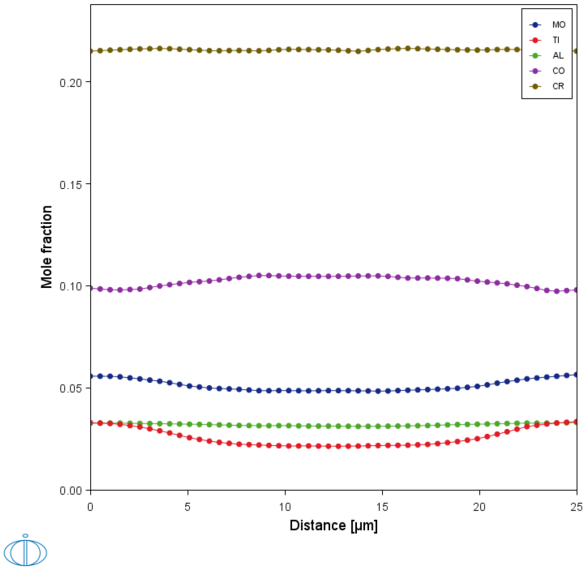


Figure 174: The Composition Profiles as shown in the Visualizations window after data is prepared and then imported into the Diffusion Calculator Configuration window.

An **Experimental File Reader** node is used to supply experimental data from [2017She] to the Plot Renderer to validate the composition of, for example, Al vs distance on the Plot Renderer. The plot shows the content of Al along the cross-section of the weld, both before and after the post weld heat treatment. There is good agreement between the diffusion simulation and the data measured in the literature.

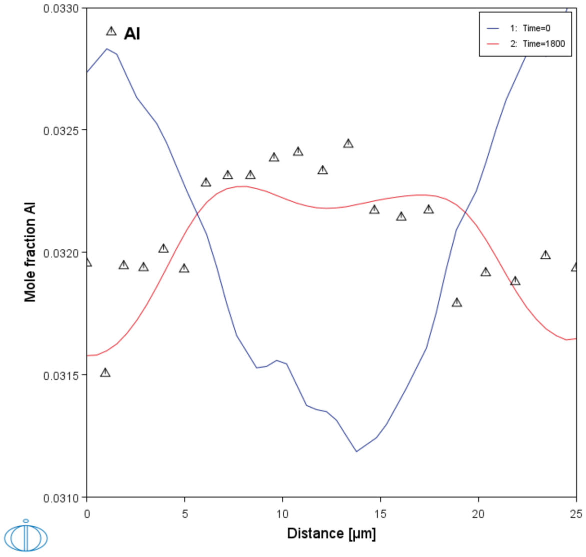


Figure 175: Plot results showing the mole fraction of Al before and after the heat treatment as a function of distance for a Ni-based alloy compared to experimental data [2017She].

Other plots can be added to investigate further details of the simulations, such as phase fractions or compositions.

Reference

[2017She] C. Shen, V. Gupta, S. Huang, M. Soare, P. Zhao, Y. Wang, “Modeling Long-term Creep Performance for Welded Nickel-base Superalloy Structures for Power Generation Systems” (Pittsburgh, PA, and Morgantown, WV (United States), 2017).

D_10: Iron (Fe) Homogenization in Scheil

This example models the homogenization of a cast Ni-Cr steel and compares predictions with the experimental data collated by Fuchs and Roósz [1975Fuc]. The conditions studied have a dendritic half spacing of 200 µm and are heat treated to temperatures of 1120 °C and 1235 °C. The data has been un-normalized to allow comparison using wt.% composition values.

The composition of the steel is 0.4C, 0.65Mn, 0.35Si, 0.015S, 0.01P, 1.9Ni, 0.95Cr, and 0.3 Mo (wt.%). The diffusion of Cr and Ni are modeled using a simplified chemistry of 0.4C, 0.65Mn, 1.9Ni, and 0.95Cr.

Project File and License Information

- Folder: **Diffusion Module - DICTRA**
- File name: `D_10_Fe _Homogenization_from_Scheil.tcu`

The Diffusion Module (DICTRA) Console Mode example `exa7` is available to show the use of Scheil segregation profiles in Console Mode.

The FEDEMO thermodynamic and MFEDEMO mobility databases are used with this example. Users with a Diffusion Module (DICTRA) license can run the example. Other users can read the documentation as a DEMO license only allows the use of up to three components.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Composition Profiles** and **Thermal Profile**: When setting up a calculator on a **Configuration** window you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.
- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

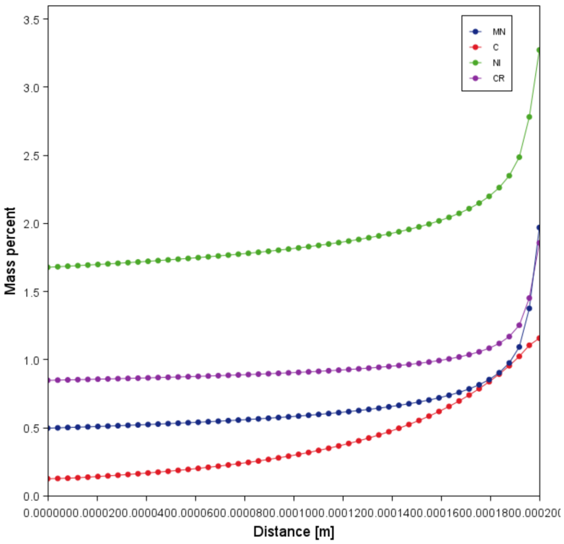


Figure 176: The predicted chemical segregation using the Scheil calculation, with a dendritic half spacing of 200 µm. This is the Composition Profile that is set up on the Diffusion Calculator and then previewed in the Visualizations window.

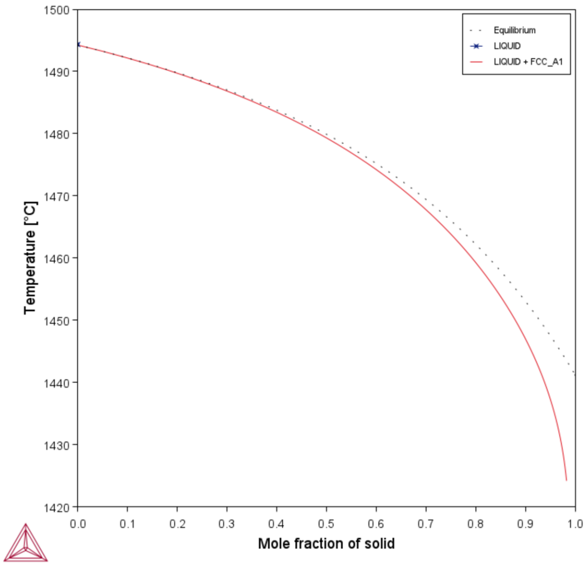


Figure 177: The solidification behavior predicted from the Scheil calculation compared with the equilibrium solid fraction.

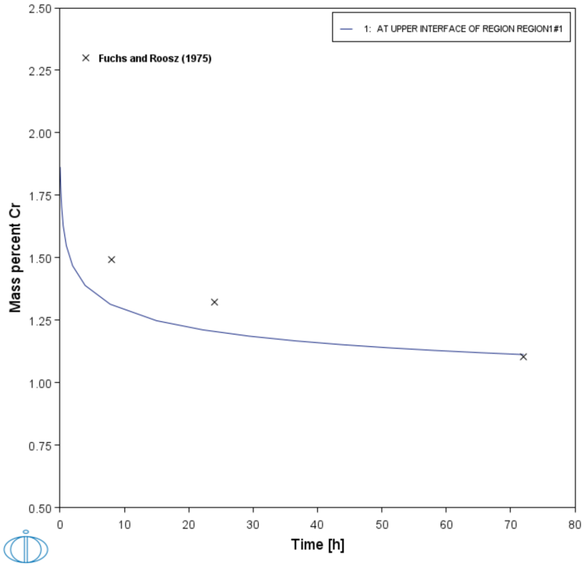


Figure 178: A comparison of the predicted and measured maximum Cr across the dendrites during homogenization at 1120 °C.

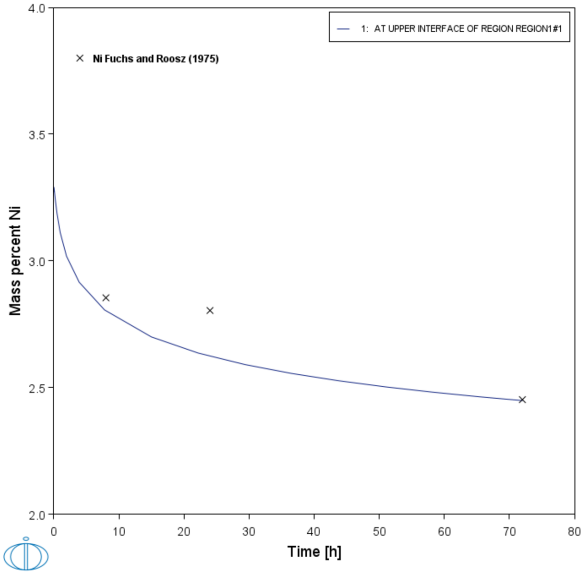


Figure 179: A comparison of the predicted and measured maximum Ni across the dendrites during homogenization at 1120 °C.

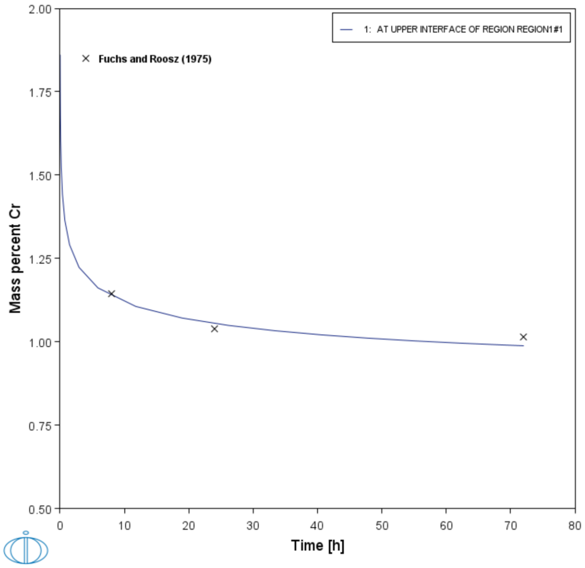


Figure 180: A comparison of the predicted and measured maximum Cr across the dendrites during homogenization at 1235 °C.

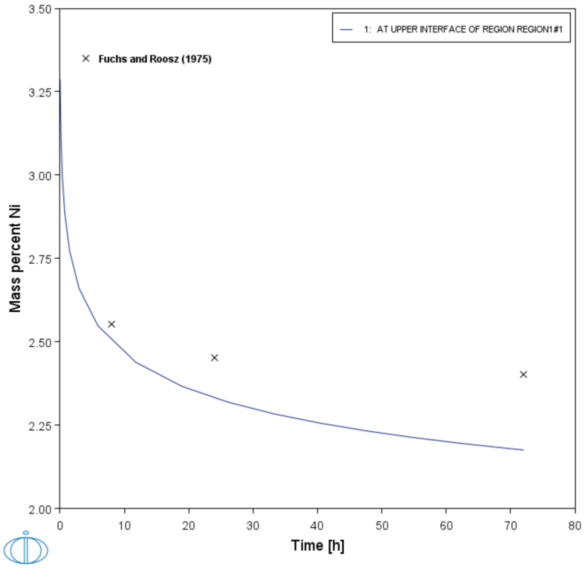


Figure 181: A comparison of the predicted and measured maximum Ni across the dendrites during homogenization at 1235 °C.

Reference

[1975Fuc] E. G. Fuchs, A. Roósz, Homogenization of Iron-Base Cast Alloys. Met. Sci. 9, 111–118 (1975).

Precipitation Module (TC-PRISMA) Examples Collection

Examples that use up to three elements are available to all users. Other examples require a Precipitation Module (TC-PRISMA) license to calculate and plot results.

When an example uses a demonstration (demo) database package, this is included with your installation.

Unless specified in tables for each example, all the numerical parameters are assumed default values.

In this section:

P_01: Isothermal Precipitation of Al_3Sc

This example simulates the kinetics of precipitation of Al_3Sc from an FCC_A1 solution phase. The simulation results can be compared with experimental data collected from Marquis and Seidman [2001Mar] and Novotny and Ardell [2001Nov].

This example also includes a plot using the **Yield strength** Property Model. This demonstrates how you can use the results from a Precipitation Module (TC-PRISMA) simulation as input to the Yield Strength Model, i.e. the calculated precipitate radius/radii for each time step is used to calculate the precipitation strengthening, and similarly, the matrix composition for each time step is used to calculate the solid solution strengthening when this is selected in the **Configuration** on the Plot Renderer. The experimental data for the Yield Strength Model is from Seidman et al. [2002Sei]. In this example, the *Precipitation strengthening model* used is **Seidman model (Al-base)**. This is selected on the Plot Renderer configuration panel that is connected to the Property Model.

Project File and Step-By Step Instructions

- Folder: **Precipitation Module - TC-PRISMA**
- File name: `P_01_Precipitation_Al-Sc_AL3SC.tcus`

Example Settings

System (System Definer)	
Database package	Demo: Aluminum-based alloys (ALDEMO, MALDEMO)
Elements	Al, Sc
Conditions (Precipitation Calculator)	
Composition	Al-0.18Sc Mole percent
Matrix phase	FCC_A1
Precipitate phase	AL3SC
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk

Interfacial energy	Calculated
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	350° C
Simulation time	1.0E7 seconds
Experimental File Reader 1 and 2	
There are two Experimental File Reader nodes used. One for the mean radius plot and one to demonstrate the *Yield Strength Property Model*.	

Visualizations

This example is included as a Precipitation Module (TC-PRISMA) tutorial on our website and as part of the playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

> For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

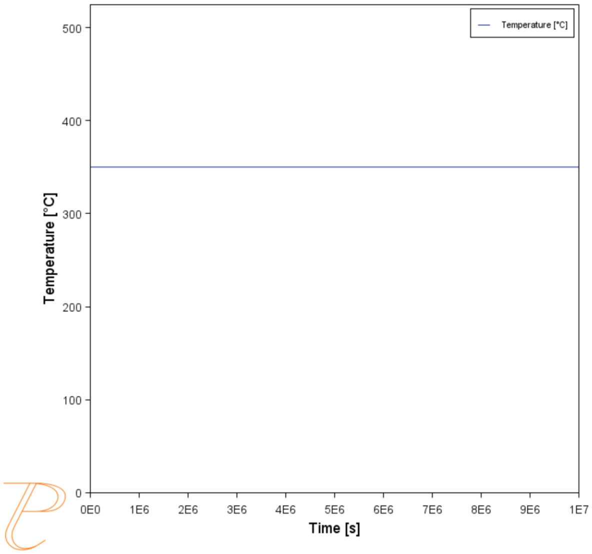


Figure 182: During set up of the calculation, preview the Thermal Profile. Click the tab in the Visualizations window to preview it. For an Isothermal Thermal Profile this shows the constant temperature as entered.

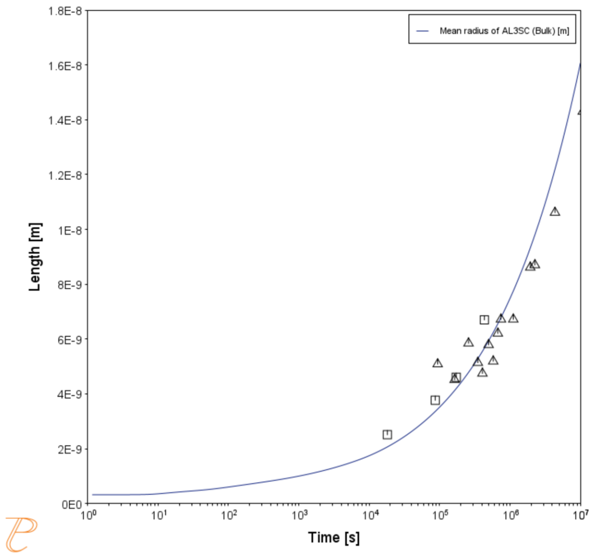


Figure 183: After performing the calculation, you can view the result on the applicable tab. This plot shows the mean radius of the AL3SC precipitate as a function of time.

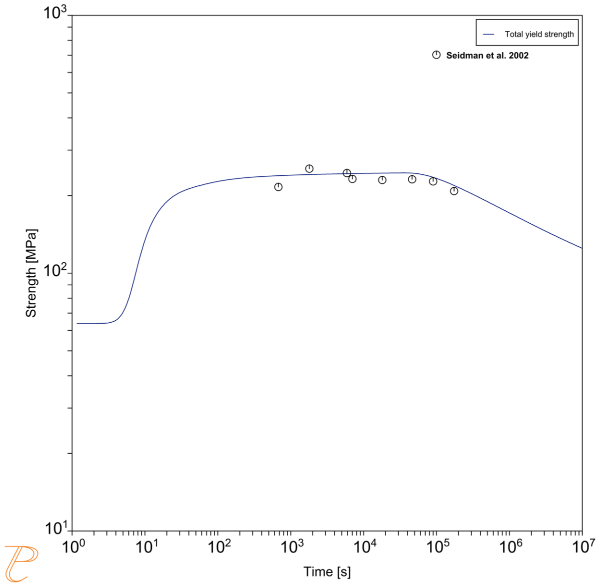


Figure 184: After performing the calculation, you can view the result on the applicable tab. This plot shows the total yield strength of the AL3SC precipitate as a function of time compared to experimental data from Siedmen et al. [2002Sei]. The model captures the over-tempering behavior from excessive coarsening of the strengthening precipitates.

References

[2001Mar] E. A. Marquis, D. N. Seidman, Nanoscale structural evolution of Al3Sc precipitates in Al(Sc) alloys. Acta Mater. 49, 1909–1919 (2001).

[2001Nov] G. M. Novotny, A. J. Ardell, Precipitation of Al3Sc in binary Al–Sc alloys. Mater. Sci. Eng. A Struct. Mater. Prop. Microstruct. Process. 318, 144–154 (2001).

[2002Sei] D. N. Seidman, E. A. Marquis, D. C. Dunand, Precipitation strengthening at ambient and elevated temperatures of heat-treatable Al(Sc) alloys. Acta Mater. 50, 4021–4035 (2002).

P_02: Stable and Metastable Carbides - Isothermal

This example simulates the kinetics of precipitation of both stable and metastable carbides from ferrite phase. It demonstrates that metastable carbides (cementite, M7C3) may first emerge and then disappear and the stable phase (M23C6) prevails.

This example uses the Equilibrium Calculator and a one axis calculation to determine how the phases change with temperature. We are interested in the carbide precipitation at 1053 K where only the carbide M23C6 is stable according to the equilibrium calculation. The Precipitation Calculator is used to do an isothermal calculation of the three phases (cementite, M23C6, and M7C3) where cementite and M7C3 are metastable phases.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: `P_02_Precipitation_Fe-C-Cr_Cementite-M7C3-M23C6.tcu`

Example Settings

System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO,MFEDEMO)
Elements	Fe, C, Cr
Conditions (Precipitation Calculator)	
Composition	Fe-0.1C-12Cr Mass percent
Matrix phase	BCC_A2
Precipitate phases	Cementite, M23C6 and M7C3
Matrix Phase Data Parameters (Precipitation Calculator)	
Grain size (click **Show Details** to display this setting)	1.0E-4 m
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Grain boundaries
Interfacial energy	Cementite 0.167 J/m^2, M23C6 0.252 J/m^2, M7C3 0.282

	J/m^2
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	1053 K
Simulation time	400 000 seconds

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

  For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

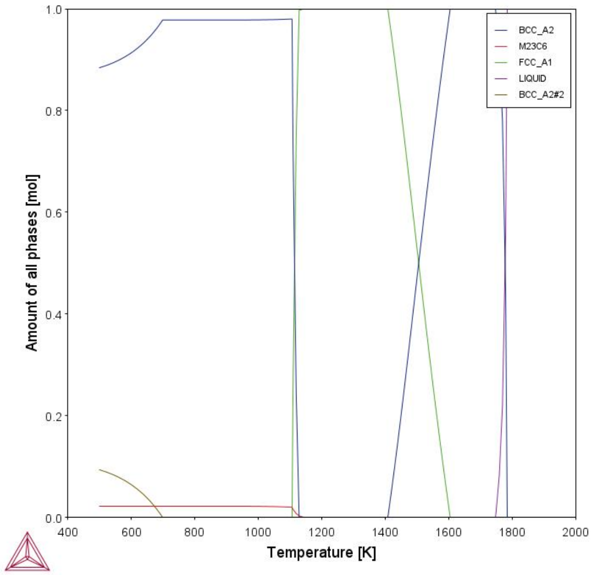


Figure 185: After performing the calculation, you can view the result on the applicable tab. This shows the equilibrium property diagram for the Fe-C-Cr alloy, highlighting what phases are predicted to be at equilibrium for a range of temperatures. The calculation shows that at 1053 K, M23C6 is the stable carbide.

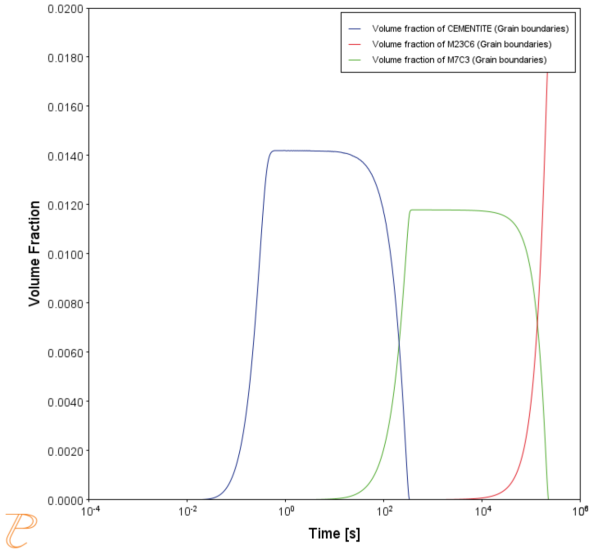


Figure 186: After performing the calculation, you can view the result on the applicable tab. This shows the evolution of the volume fraction of cementite, M7C3, and M23C6 during an isothermal heat treatment of an Fe-C-Cr alloy at 1073 K. The cementite and M7C3 are metastable at this temperature, however their nucleation kinetics are faster than the stable phase, allowing them to form and then dissolve when the next more thermodynamically stable phase nucleates.

P_03: Stable and Metastable Carbides - TTT Diagram

In this example, the kinetics of precipitation of both stable and metastable carbides is calculated from the ferrite phase. It demonstrates that metastable carbides may first emerge and then disappear and the stable phase prevails.

This example uses the Equilibrium Calculator and a one axis calculation type to determine how the phases change with temperature. Using this result, the Precipitation Calculator is used to do a TTT (Time-Temperature-Transformation) diagram calculation of the three phases (cementite, M23C6 and M7C3) at the grain boundaries.

For a TTT diagram calculation, select **TTT diagram** in **Calculation Type**, then enter **Min**, **Max**, and **Step** of **Temperature**, as well as **Max annealing time**. In **Stop criterion**, choose **Volume fraction of phase** and enter the value.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: `P_03_Precipitation_Fe-C-Cr_TTT_Cementite-M7C3-M23C6.tcu`

Example Settings

System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO)
Elements	Fe, C, Cr
Conditions (Precipitation Calculator)	
Composition	Fe-0.1C-12Cr Mass percent
Matrix phase	BCC_A2

Precipitate phases	Cementite, M23C6 and M7C3
Matrix Phase Data Parameters (Precipitation Calculator)	
Grain size (click **Show Details** to display this setting)	1.0E-4 m
Precipitate Phase Data Parameters	
Nucleation sites	Grain boundaries
Interfacial energy	Cementite 0.167 J/m^2, M23C6 0.252 J/m^2, M7C3 0.282 J/m^2
Calculation Type (Precipitation Calculator)	
Calculation type	TTT diagram
Temperature	500° to 800° C with 25° C steps
Max. annealing time	1.0E8 seconds
Stop criteria	Volume fraction of phase is set to 0.0001
Options > Numerical Parameters	
No. of grid points over one order of magnitude in radius	150
Max no. of grid points over one order of magnitude in radius	200
Min no. of grid points over one order of magnitude in radius	100

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects,

you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

> For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

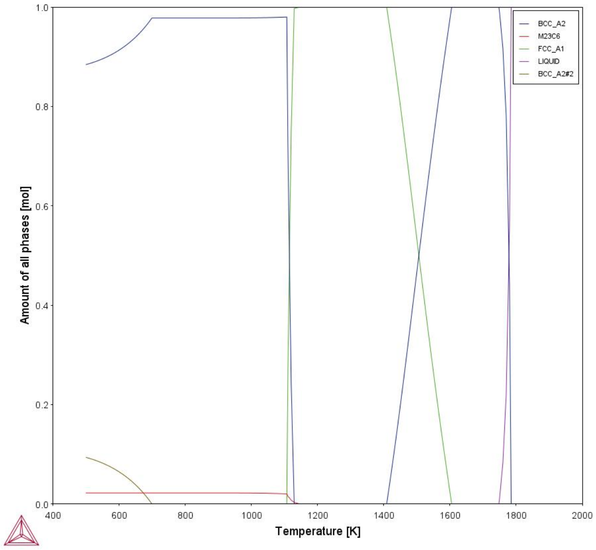


Figure 187: After performing the calculation, you can view the result on the applicable tab. Here the results from the equilibrium calculator are shown, which assesses the stability of phases across the temperature range of interest.

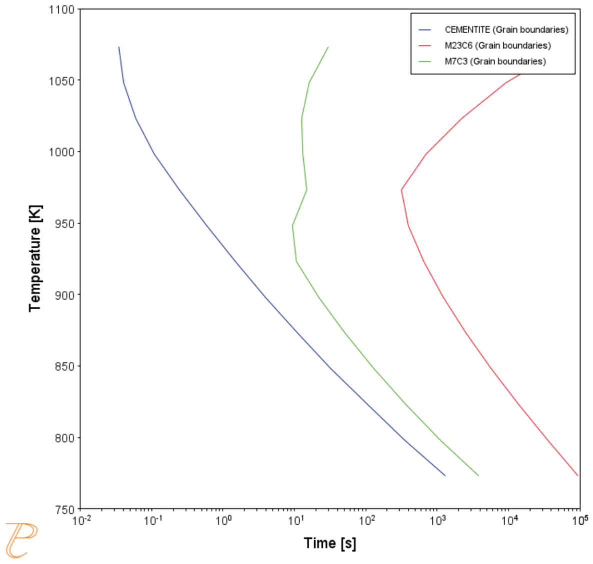


Figure 188: After performing the calculation, you can view the result on the applicable tab.This shows results from a TTT (Temperature-Transformation) simulation using the Precipitation Calculator to examine the sequence of phase transitions considering the formation of cementite, M7C3, and M23C6 carbide phases. The previous Equilibrium Calculator reveals the temperatures where the cementite and M7C3 are metastable.

P_04: Precipitation of Iron Carbon Cementite

This example is based on [1949Wer] and simulates the kinetics of precipitation of carbides from a BCC Fe solution phase. This isothermal calculation example uses the Precipitation Calculator plus two Experimental File Reader activities to plot the volume fraction of the cementite phase.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: `P_04_Precipitation_Fe-C_Cemetite.tcu`

Example Settings

System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO)
Elements	Fe, C
Conditions (Precipitation Calculator)	
Composition	Fe-0.016C mass percent
Matrix phase	BCC_A2
Precipitate phase	Cementite
Matrix Phase Data Parameters (Precipitation Calculator)	
Grain aspect ratio (click **Show Details** to display this setting)	1.0
Dislocation density (click **Show Details** to display this setting)	1.5e11m^{-3}
Precipitate Phase Parameters (Precipitation Calculator)	
Nucleation sites	Dislocations
Interfacial energy	0.24 J/m^2

Growth rate model (click **Show Details**)	Advanced
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	102° C
Simulation time	600 000 seconds

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

When you run (Perform) this example, it takes a few minutes for the calculations to complete.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

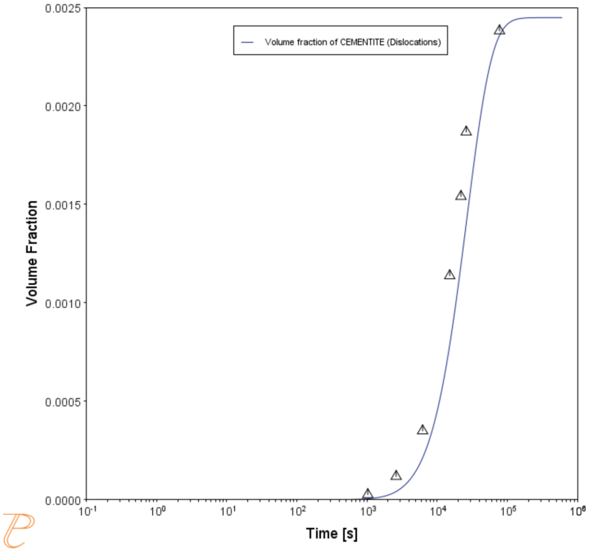


Figure 189: After performing the calculation, you can view the result on the applicable tab. The result compares the predicted evolution of the volume fraction of cementite with the measurements of [1949Wer].

Reference

[1949Wer] C. A. Wert, Precipitation from Solid Solutions of C and N in α-Iron. J. Appl. Phys. 20, 943 (1949).

P_05: Precipitation of γ’ in Ni Superalloys - Isothermal

This example simulates the kinetics of precipitation of gamma prime (γ’) phase from gamma (γ) phase. The simulation results can be compared with experimental data collected from Sudbrack et al. [2008Sud].

This example uses three Experimental File Reader activities with the Precipitation Calculator. It does an isothermal calculation to plot the volume fraction, mean radius, and number density of the cementite phase.

> DIS_FCC_A1 needs to be selected on the System Definer. See Selecting the Disordered Phase as a Matrix Phase for details.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: `P_05_Precipitation_Ni-Al-Cr_Isothermal_Gamma-Gamma_prime.tcu`

Example Settings

System (System Definer)	
Database package	Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO)
Elements	Ni, Al Cr
Conditions (Precipitation Calculator)	
Composition	Ni-9.8Al-8.3Cr Mole percent
Matrix phase	DIS-FCC_A1 See Selecting the Disordered Phase as a Matrix Phase
Precipitate phase	FCC_L12#2
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk

Interfacial energy	0.012 J/m^2
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	800° C
Simulation time	1 000 000 seconds

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

  For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

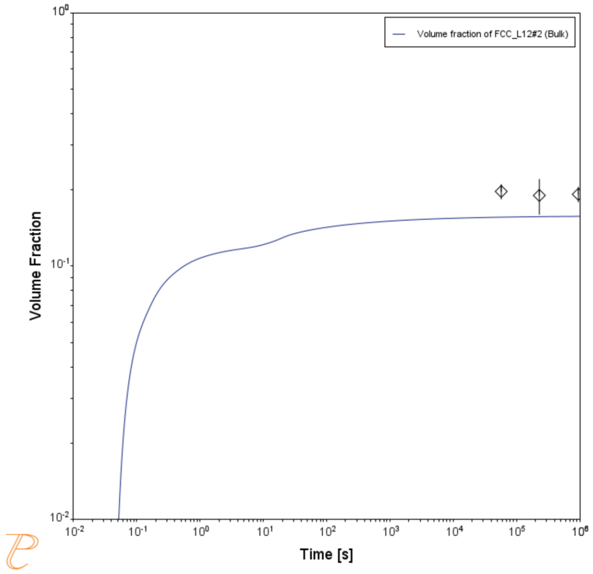


Figure 190: After performing the calculation, you can view the result on the applicable tab. This plot compares the predicted evolution of the volume fraction of gamma prime with the measurements of [2008Sud].

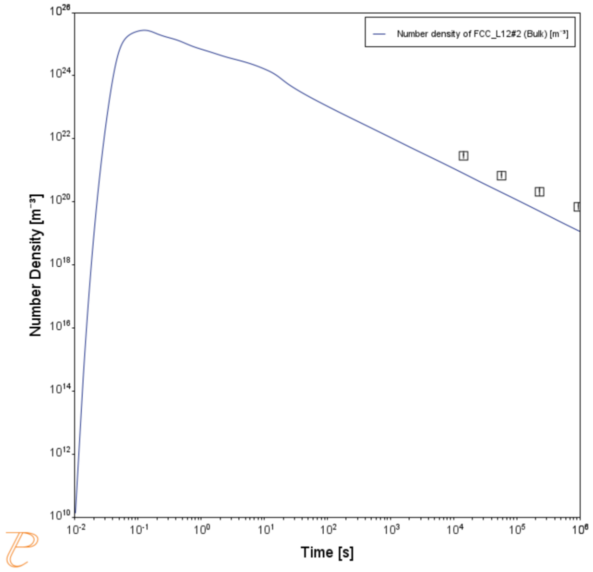


Figure 191: After performing the calculation, you can view the result on the applicable tab. This plot compares the predicted evolution of the number density of gamma prime with the measurements of [2008Sud].

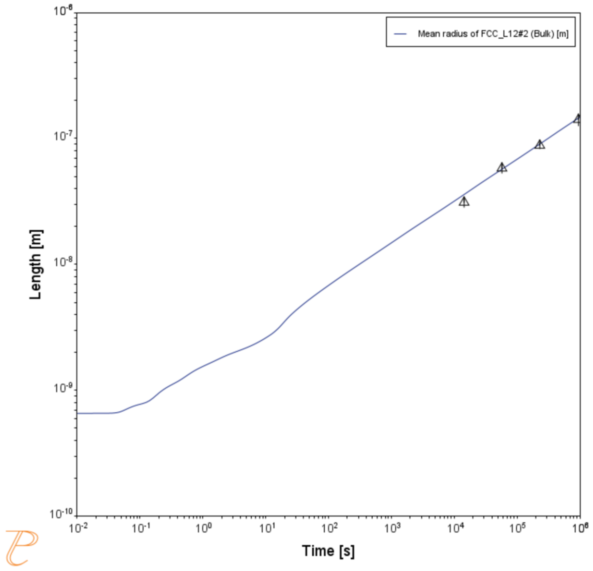


Figure 192: After performing the calculation, you can view the result on the applicable tab. This plot compares the predicted evolution of the mean particle radius of gamma prime with the measurements of [2008Sud].

Reference

[2008Sud] C. K. Sudbrack, T. D. Ziebell, R. D. Noebe, D. N. Seidman, Effects of a tungsten addition on the morphological evolution, spatial correlations and temporal evolution of a model Ni–Al–Cr superalloy. Acta Mater. 56, 448–463 (2008).

P_06: Precipitation of γ’ in Ni Superalloys - Non-isothermal

This example simulates the kinetics of precipitation of gamma prime (γ’) phase from gamma (γ) phase in Ni-8Al-8Cr and Ni-10Al-10Cr at.% alloys during continuous cooling from a super-solvus temperature. The simulation results can be compared with experimental results from Rojhirunsakool et al. [2013Roj].

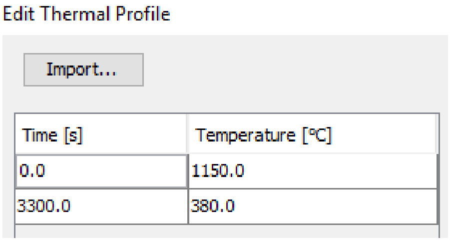
DIS_FCC_A1 needs to be selected on the **System Define**r for both the thermodynamic and mobility databases. See Selecting the Disordered Phase as a Matrix Phase for details.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: `P_06_Precipitation_Ni-Al-Cr_Non-isothermal_Gamma-Gamma_prime.tcu`

Example Settings

System (System Definer)	
Database package	Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO)
Elements	Ni, Al, Cr
Conditions (Precipitation Calculator)	
Composition (Ni-8Al-8Cr)	Ni-8Al-8Cr Mole percent
Composition (Ni-10Al-10Cr)	Ni-10Al-10Cr Mole percent
Matrix phase	DIS_FCC_A1 See Selecting the Disordered Phase as a Matrix Phase
Precipitate phase	FCC_L12#2
Matrix Phase Data Parameters (Precipitation Calculator)	
Mobility adjustment > Prefactor (click **Show Details**	Keep the default, Same for all elements, then enter

to display this setting)	5.0 for the Prefactor.
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk
Interfacial energy	0.023 J/m^2
Calculation Type (Precipitation Calculator)	
Calculation type	Non-isothermal
Temperature unit	Celsius
Time unit	Seconds
Temperature	1150 - 380 °C  Edit Thermal Profile Import... Time [s] — Temperature [°C] 0.0 — 1150.0 3300.0 — 380.0
Simulation time (Ni-8Al-8Cr)	3300 s
Simulation time (Ni-10Al-10Cr)	3300 s
Multimodal PSD (Plot Renderer)	
Separate multimodal PSD checkbox is selected for 8Al-8Cr for both the Mean radius and PSD plots.	- Mean Radius and PSD plots: The **Inflection neighbors** and **Smoothing interactions** defaults are kept. - Mean Radius plot: The **Points** are set to `15`.
Separate multimodal PSD checkbox is selected for 10Al-10Cr for both the Mean radius and PSD plots.	- Mean Radius and PSD plots: The **Inflection neighbors** and **Smoothing interactions** defaults are kept. - Mean Radius plot: The **Points** are set to `50`.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

When you run (Perform) this example, it takes a few minutes for the calculations to complete.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

  For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

In this example, all nodes are renamed in the **Project** window, and this matches each of the tab names in the **Visualizations** window.

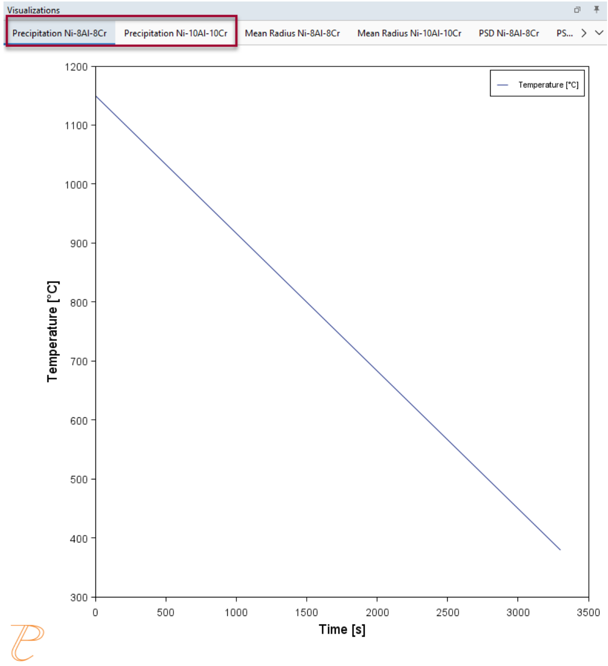


Figure 193: During set up of the calculation, you can preview the non-isothermal Thermal Profile (s). Click the tab in the Visualizations window to adjust settings on the Precipitation Calculator Configuration window. In this case the heat treatment is a continuous cooling curve, however any thermal profile can be modeled using the Non-isothermal Calculation Type.

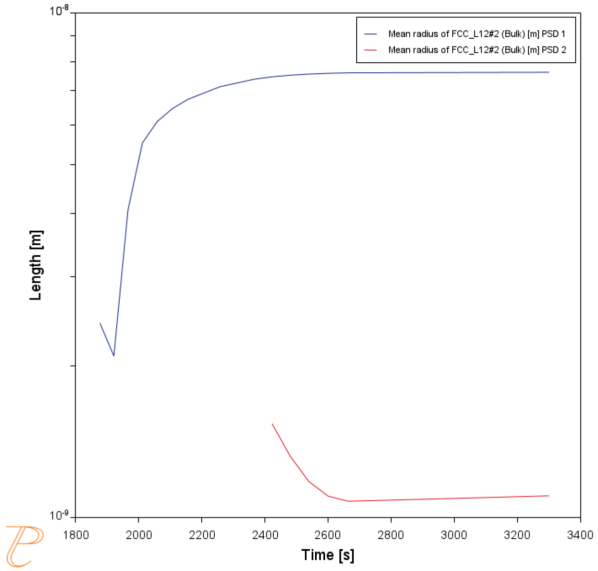


Figure 194: These results show the predicted evolution of the mean radius of gamma prime populations nucleating during the quench for the Ni-8Al-8Cr alloy. Note that the tertiary particles (second particle population) are very small, and this dispersion would appear monomodal without TEM characterization.

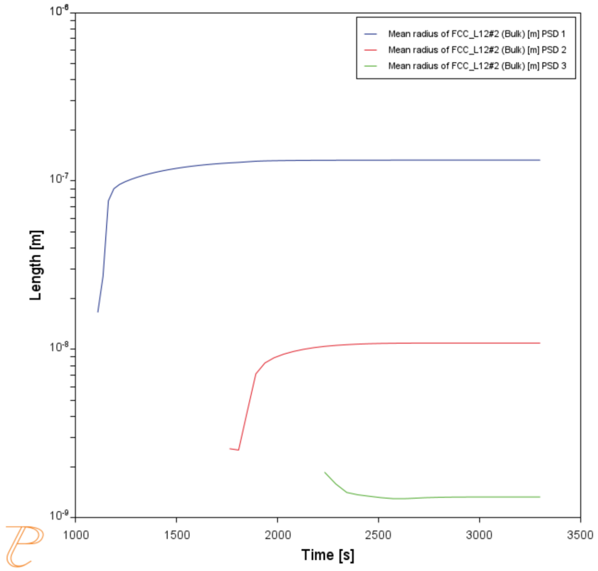


Figure 195: These results show the predicted evolution of the mean radius of gamma prime populations nucleating during the quench for the Ni-10Al-10Cr alloy. In this case three distinct particle populations are simulated to form, agreeing with [2013Roj].

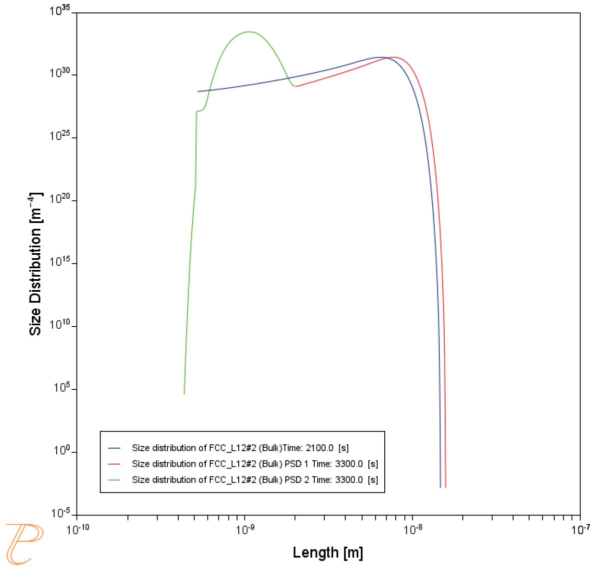


Figure 196: These results show the predicted size distributions of precipitates at different times during the quench of the for the Ni-8Al-8Cr alloy. The individual particle populations are distinguished using the "Separate multimodal PSD" option showing a bimodal distribution with very small nano-meter sized tertiary particles.

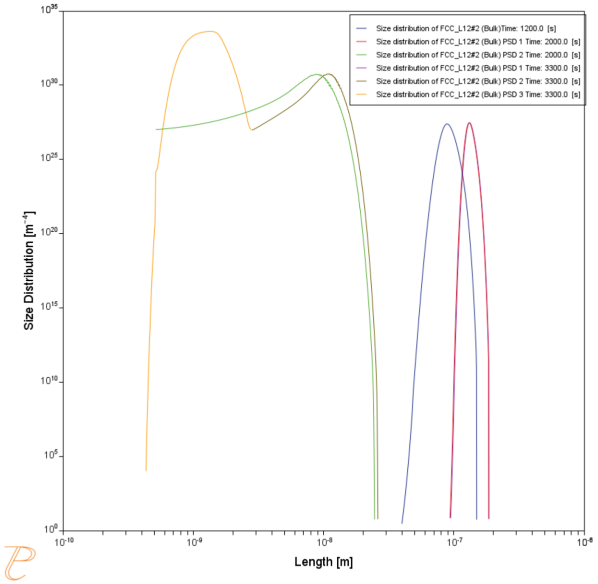


Figure 197: These results show the predicted size distributions of precipitates at different times during the quench for the Ni-10Al-10Cr alloy. The individual particle populations are distinguished using the "Separate multimodal PSD" option showing the formation of a tri-modal dispersion.

Reference

[2013Roj] T. Rojhirunsakool, S. Meher, J. Y. Hwang, S. Nag, J. Tiley, R. Banerjee, Influence of composition on monomodal versus multimodal γ′ precipitation in Ni–Al–Cr alloys. J. Mater. Sci. 48, 825–831 (2013).

P_07: Continuous Cooling Transformation (CCT) Diagram of Ni-Al-Cr γ-γ’

This example shows you how to simulate a CCT (Continuous Cooling Transformation) diagram for gamma prime (γ’) precipitation in a Ni-Cr-Al alloy using the Precipitation Calculator. A CCT calculation maintains the same cooling rate the entire time.

The system is a Ni-10Al-10Cr γ - γ’ alloy and it is calculated and plotted with superimposition of the cooling rate values.

Project File and Step-By Step Instructions

- Folder: **Precipitation Module - TC-PRISMA**
- File name: `P_07_Precipitation_Ni-Al-Cr_CCT_Gamma-Gamma_prime.tcu`

Example Settings

System (System Definer)	
Database package	Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO)
Elements	Ni, Al, Cr
Conditions (Precipitation Calculator)	
Composition	Ni-10Al-10Cr Mole percent
Matrix phase	DIS_FCC_A1
Precipitate phase	FCC_L12#2
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk
Interfacial energy	0.023 J/m^2
Calculation Type (Precipitation Calculator)	
Calculation type	CCT Diagram
Temperature Min to Max	500 to 1200 Kelvin

Cooling rate(s)	.01 .1 1 10 100 K/s
Stop criteria	Volume fraction of phase 1.0E-4

Visualizations

This example is included as a Precipitation Module (TC-PRISMA) tutorial on our website and as part of the playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

When you run (Perform) this example, it takes a few minutes for the calculations to complete.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

  For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

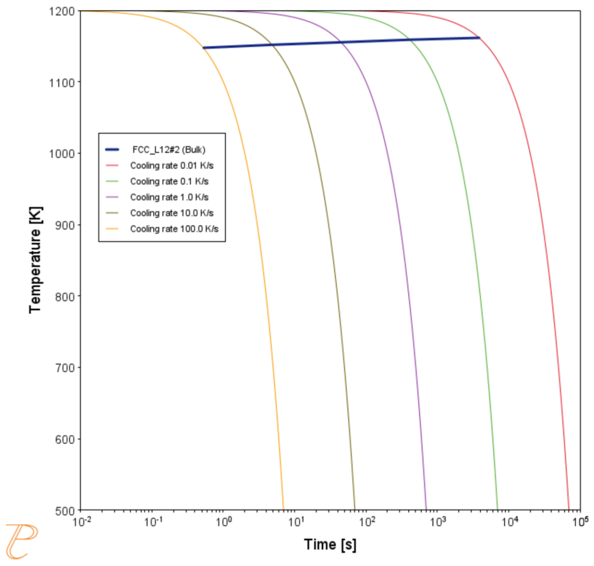
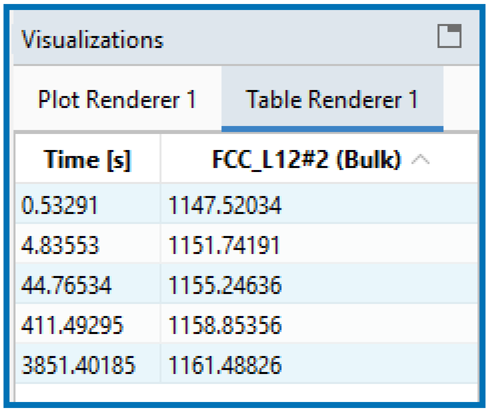


Figure 198: In this plot, the blue horizontal line shows the time it takes for γ' to transform at each of the cooling rates according to the stop criteria, which is set as 1e-4 volume fraction. The cooling rates are represented by the multicoloured curved lines.

If you hover your mouse over the intersection of the blue line and any of the vertical lines, a yellow box shows the approximate time it takes for γ' to transform according to the stop criteria, which is a volume fraction of 1e-4, followed by the approximate temperature.



Time [s]	FCC_L12#2 (Bulk)
0.53291	1147.52034
4.83553	1151.74191
44.76534	1155.24636
411.49295	1158.85356
3851.40185	1161.48826

Figure 199: An example of the table shown in the Visualizations window, which shows the same information as in the plot - for each cooling rate the temperature and the time it takes for γ' to transform according to the stop criteria, which is a volume fraction of 1e-4.

P_08: Precipitation of Cu-Ti CU4TI with Assumptions of Sphere and Needle Morphologies

In this isothermal calculation example, the precipitation of Cu4Ti phase in a Cu-Ti binary alloy is calculated. To make a comparison, two separate simulations are performed, one assuming spherical morphology without elastic strain energy, and the other assuming needle morphology whose shape, determined by competition between interfacial energy and elastic strain energy, is changed during the simulation. The transformation strain is obtained from Borchers [1999Bor]. The results are compared with experiment results from Kampmann et al. [1987Kam].

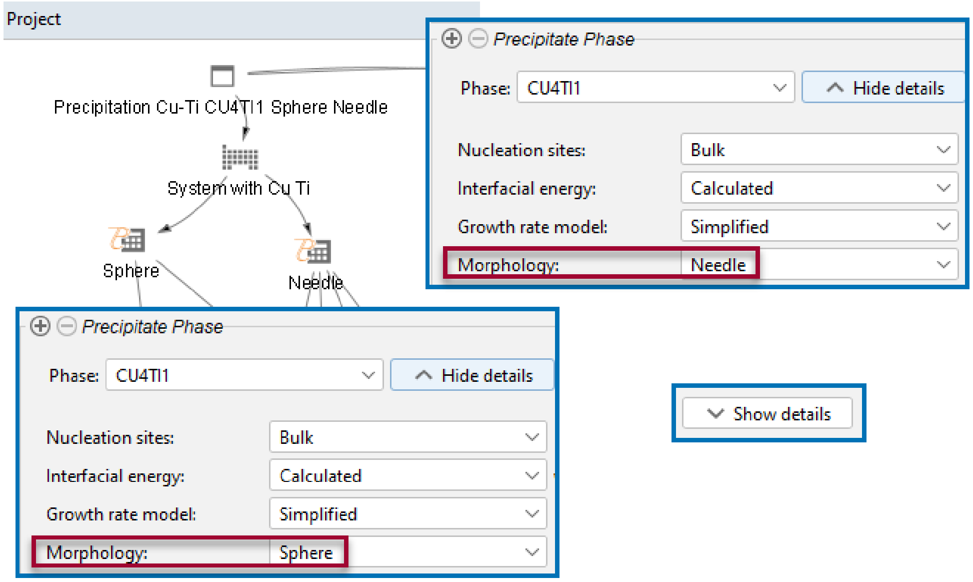
For more details about the background theory, see Precipitation Morphology.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: `P_08_Precipitation_Cu-Ti_CU4TI1_Sphere_Needle.tcu`

Example Settings

To ensure that the settings are done on the correct Precipitation Calculators, the **Sphere** and **Needle** nodes are renamed from **Precipitation Calculator** to match their morphology. The morphology is set in the **Precipitate Phase** section when you click **Show Details**.



Precipitate Phase

Phase: CU4TI1 — Hide details

Nucleation sites: Bulk

Interfacial energy: Calculated

Growth rate model: Simplified

Morphology: Needle

Precipitate Phase

Phase: CU4TI1 — Hide details

Nucleation sites: Bulk

Interfacial energy: Calculated

Growth rate model: Simplified

Morphology: Sphere

System (System Definer)	
Database package	Demo: Copper-based alloys (CUDEMO and MCUDEMO)
Elements	Cu, Ti
Sphere and Needle Conditions (Precipitation Calculator)	
Composition	Cu-1.9Ti Mole percent
Matrix phase	FCC_L12
Precipitate phase	CU4TI1
Matrix Phase Data Parameters (Precipitation Calculator)	
Mobility adjustment > Prefactor (click **Show Details** to display this setting)	Keep the default, Same for all elements, then enter 100 for the Prefactor.
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk
Interfacial energy	The default
Morphology (click **Show Details** to display this setting)	For the **Sphere** node (renamed from Precipitation Calculator), keep the default. For the **Needle** node (renamed from Precipitation Calculator), **Needle** is

	selected.
Transformation strain (click **Show Details** to display this setting)	For the **Sphere** node (renamed from Precipitation Calculator), keep the default. For the **Needle**node (renamed from Precipitation Calculator), **User defined** is selected. In this example, the following settings are defined: • ε11 and ε22 are set to **0.022** • ε33 is set to **0.003**
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	350° C
Simulation time	10,000 seconds
Datasets (Experimental File Reader)	
Borchers Mean radius vs Time and Borchers Number density vs Time	Data sets included with this example and imported to two Experimental File Readers. These data sets are used for the Mean Radius and Number Density plots, respectively.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

When you run (Perform) this example, it takes a few minutes for the calculations to complete.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

  For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

In this example, all nodes are renamed in the **Project** window, and this matches each of the tab names in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

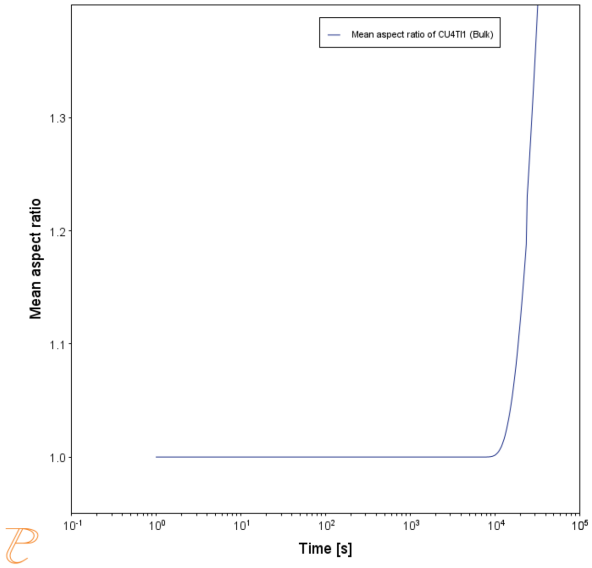


Figure 200: The predicted evolution of the morphology of needle shaped precipitates, showing how the mean aspect ratio changes during the isothermal heat treatment.

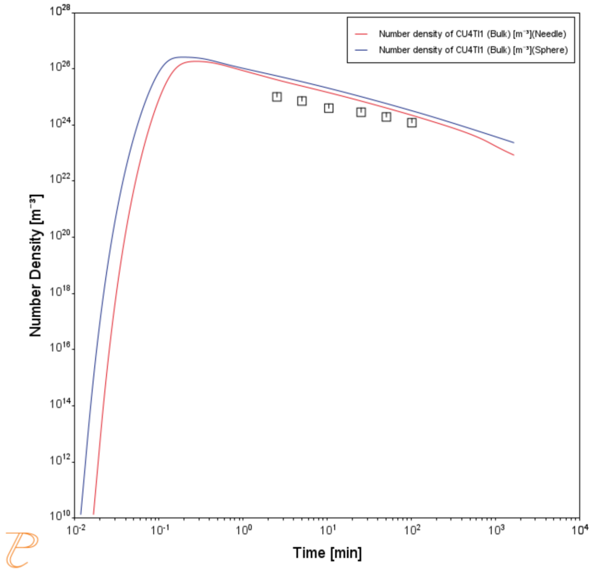


Figure 201: The results compare the predicted evolution of the mean size of precipitates with the experimental data from [1987Kam], comparing the spherical and needle shaped approximations of the precipitate morphology. Note how the needle shape approximation is closer to the experimental data.

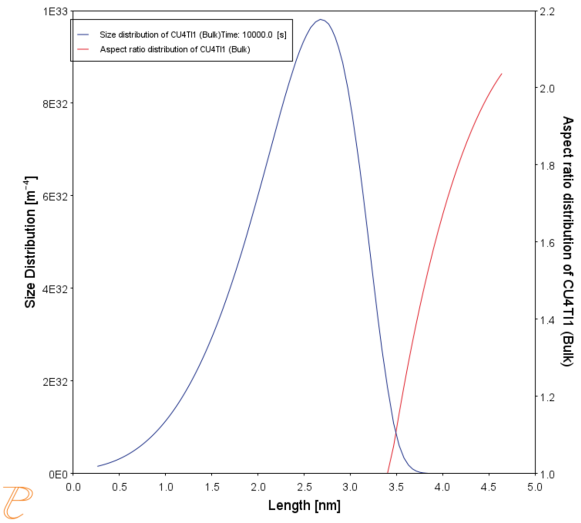


Figure 202: These results show both the predicted final particle size distribution from the needle shape simulation and the predicted relationship between the length of the precipitate and the needle aspect ratio.

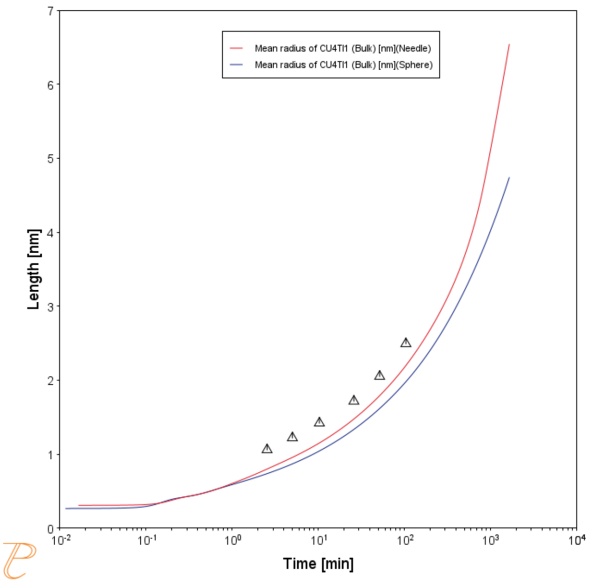


Figure 203: This shows the approximates the size of the needle shaped precipitates as a sphere of equivalent volume, and compares the experimental results of [1987Kam] with those obtained from a spherical and needle shaped approximation.

References

[1987Kam] R. Kampmann, H. Eckerlebe, R. Wagner, 1987. "Precipitation Kinetics in Metastab le Solid Solutions - Theoretical Considerations and Application to Cu-Ti Alloys." Mat. Res. Soc. Symp. Proc. 57: 525-542.

[1999Bor] C. Borchers, Catastrophic nucleation during decomposition of Cu-0.9at.% Ti. Philos. Mag. A. 79, 537–547 (1999).

P_09: Precipitation of Al-Sc AL3SC with Assumption of Sphere and Cuboid Morphologies

In this isothermal calculation example, the precipitation of Al_3Sc phase from FCC_A1 matrix phase in an Al-Sc binary alloy is simulated. To make a comparison, two separate calculations are performed, one assuming spherical morphology without elastic strain energy, and the other assuming cuboid morphology whose shape is determined by competition between interfacial energy and elastic strain energy. The simulation results are compared with experimental data collected from Marquis and Seidman [2001Mar] and Novotny and Ardell [2001Nov]. In addition, mean cubic factor and cubic factor distribution are also plotted for cuboid shape to illustrate the spherical-cuboidal transition during precipitation.

> For more details about the background theory, see Precipitation Morphology.

Project File and Step-By Step Instructions

- Folder: **Precipitation Module - TC-PRISMA**
- File name: `P_09_Precipitation_Al-Sc_AL3SC_Sphere_Cuboid.tcu`

Example Settings

> To ensure that the settings are done on the correct Precipitation Calculators, the **Sphere** and **Cuboid** nodes are renamed from **Precipitation Calculator** to match their morphology. The morphology is set in the **Precipitate Phase** section when you click **Show Details**. See P_08 for an example of this.

System (System Definer)	
Database package	Demo: Aluminum-based alloys (ALDEMO, MALDEMO)
Elements	Al, Sc
Sphere and Cuboid Conditions (Precipitation Calculator)	
Composition	Al-0.18Sc Mole percent

Matrix phase	FCC_A1
Precipitate phase	AL3SC
Matrix Phase Data Parameters (Precipitation Calculator)	
Elastic properties (click **Show Details** to display this setting)	For the **Sphere** node (renamed from Precipitation Calculator), the default, **Disregard** is kept. For the **Cuboid** node (renamed from Precipitation Calculator), choose **Cubic**. Then enter the elastic constants accordingly. Default elastic constants are given based on the major element of the alloy system. In this example that is • c11 is **108.2** GPa • c12 is **61.3** GPa • c44 is **28.5** GPa
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk
Interfacial energy	The default
Morphology (click **Show Details** to display this setting)	For the **Sphere** node (renamed from Precipitation Calculator), keep the default. For the **Cuboid** node (renamed from Precipitation Calculator), **Cuboid** is selected.
Transformation strain (click **Show Details** to display this setting)	For the **Sphere** node (renamed from Precipitation Calculator), keep the default. For the **Cuboid** node (renamed from Precipitation Calculator), **Calculate from molar volume** is selected to obtain a purely dilatational strain.
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	350° C
Simulation time	1.0E9 seconds
Datasets (Experimental File Reader)	
Dataset 1 and Dataset 2	Data sets included with this example and imported to one Experimental File Reader. It is used for the Mean Radius plot.

Visualizations

This example is included as a Precipitation Module (TC-PRISMA) tutorial on our website and as part of the playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

  For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

In this example, all nodes are renamed in the **Project** window, and this matches each of the tab names in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

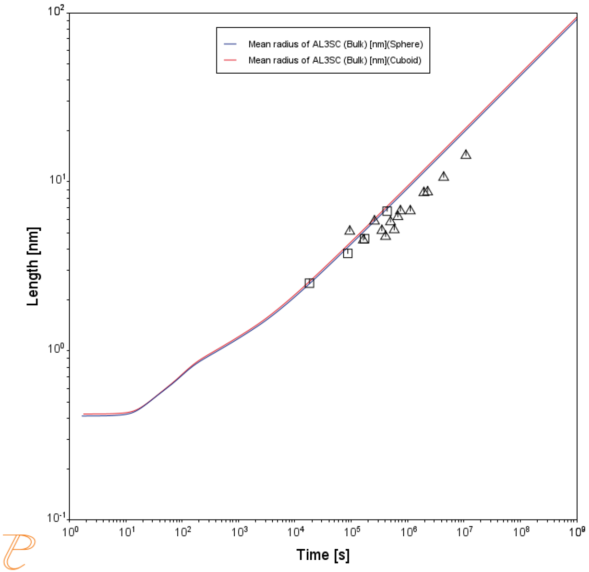


Figure 204: This shows the predicted evolution of the mean size of precipitates with the experimental data from [2001Mar, 2001Nov], comparing the spherical and cuboidal shaped approximations of the precipitate morphology. Although there is not significant difference in the results, capturing the correct geometry of the precipitate is important in subsequent calculations of precipitate spacing used in property calculations.

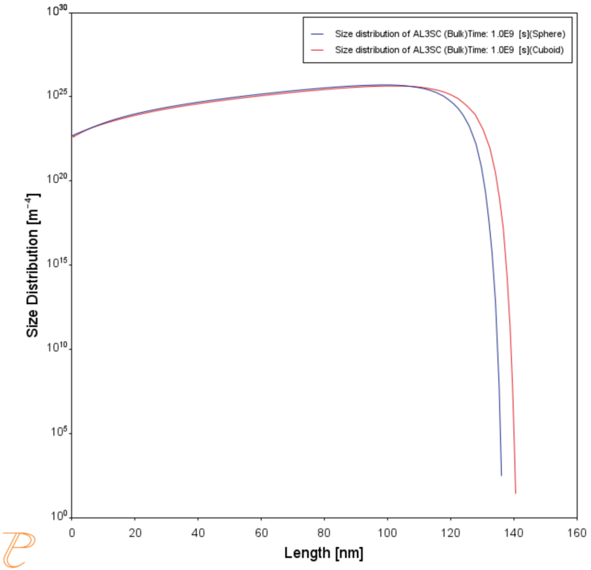


Figure 205: These results compare the predicted size distributions after heat treatment considering the spherical and cuboidal approximations of the precipitate morphology.

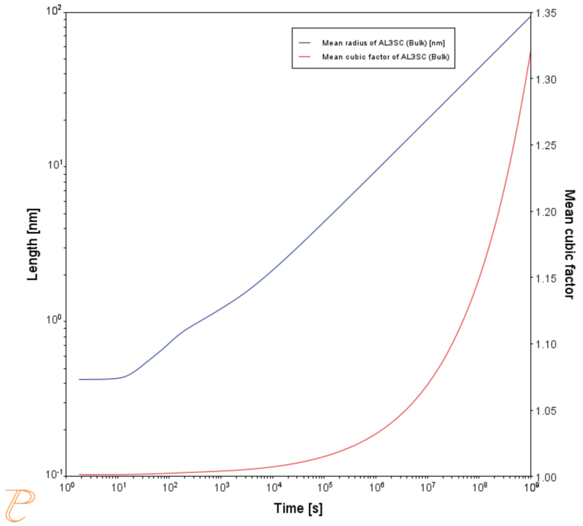


Figure 206: These results compare the predicted evolution of the mean particle radius and mean aspect ratio from using the cuboidal approximation of the precipitate morphology. In this case, the radius of a sphere of equivalent volume to the cuboidal precipitate is shown.

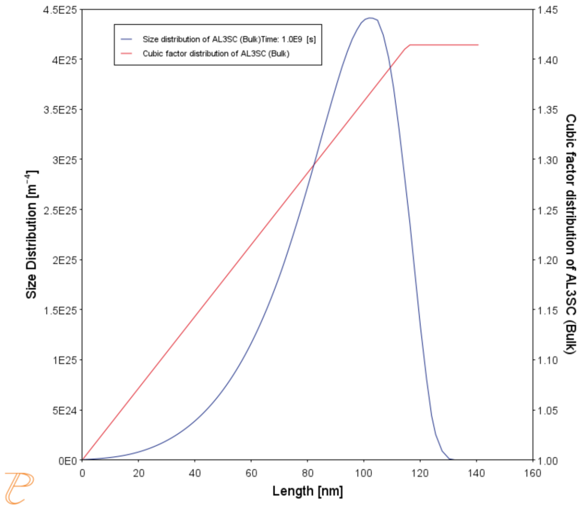


Figure 207: These results show the predicted size distribution of the precipitates obtained from the cuboidal approximation of the precipitate morphology. Also shown is the calculated size dependent cubic factor of the cuboids associated with this dispersion.

References

[2001Mar] E. A. Marquis, D. N. Seidman, Nanoscale structural evolution of Al3Sc precipitates in Al(Sc) alloys. Acta Mater. 49, 1909–1919 (2001).

[2001Nov] G. M. Novotny, A. J. Ardell, Precipitation of Al3Sc in binary Al–Sc alloys. Mater. Sci. Eng. A Struct. Mater. Prop. Microstruct. Process. 318, 144–154 (2001).

P_10: Initial Particle Size Distribution of Fe-Cr-C

This example demonstrates the effect of initial particle size distribution (PSD) of the precipitate phases on the overall precipitation kinetics. It uses two Precipitation Calculators to simulate and compare carbide precipitations from a ferritic BCC_A2 matrix in a Fe-0.1C-12Cr alloy. Three carbides, CEMENTITE, M23C7, and M7C3 are included in the calculations simulating a complex precipitation sequence with stable and meta-stable precipitate phases. The results show a large difference in predicted behaviour, with meta-stable precipitates dissolving earlier as a result of the stable precipitates existing in the initial condition.

This example also shows the different ways to create the initial size distribution.

- **Generate 3D PSD from distribution function**: CEMENTITE's PSD is approximated from an LSW distribution.
- **From File**: M23C6's PSD is loaded from a file.
- **Approximate the 3D PSD from experimental data**: M7C3's PSD is approximated from 1D experimental data descriptive of halved linear intercepts.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: `P_10_Precipitation_Initial_PSD_FeCrC.tcu`

There are also two *.csv files available for you to use as a template for when you are importing data from a file.

- Input data for M23C6: `P_10_Precipitation_Initial_PSD_FeCrC_psd_3D_M23C6.csv`
- Input data for M7C3: `P_10_Precipitation_Initial_PSD_FeCrC_psd_1D_M7C3.csv`

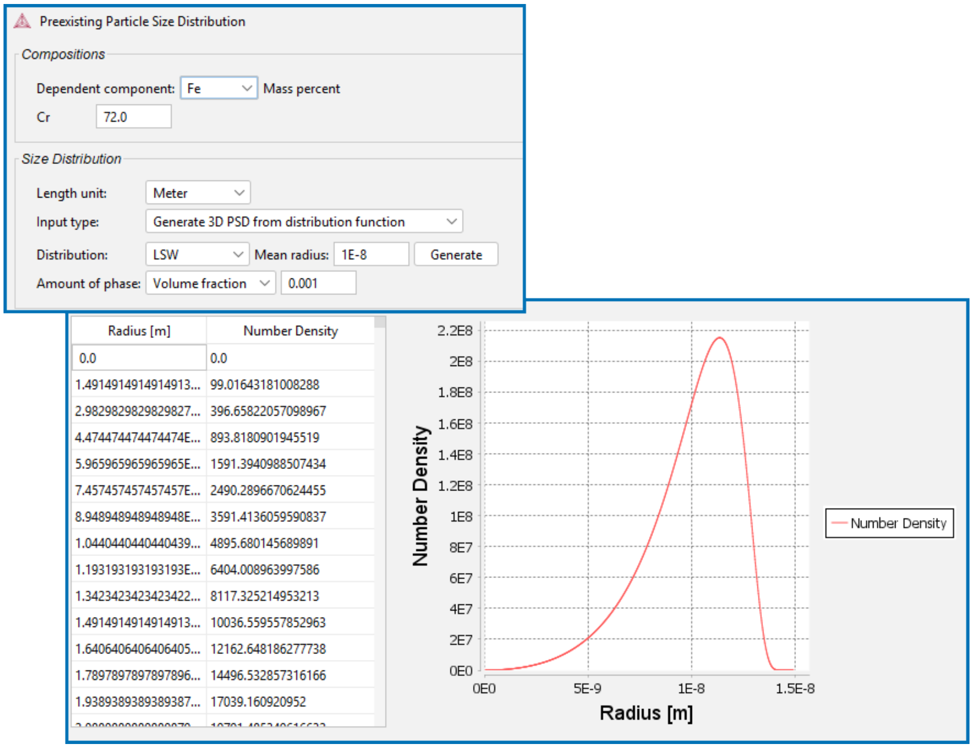
Preexisting Particle Size Distribution

The **Preexisting Particle Size Distribution** window shown in Figure 208 is a graphical representation of the radius versus corresponding number densities, with fields available to enter the initial precipitate composition and volume fraction. An editable table is also provided for the particle size distribution.

Particle Size Distribution (PSD)

Cementite

The amount of Fe and Cr must be defined for Cementite for this alloy. Fe is set to the dependent component, and 72 mass percent of Cr is set. The option **Generate 3D PSD from distribution function** is chosen to create the PSD for Cementite. The initial volume fraction of 0.001 % is assumed. An LSW distribution is selected with a mean radius of 1E-8m.



Preexisting Particle Size Distribution

Compositions

Dependent component: Fe Mass percent

Cr: 72.0

Size Distribution

Length unit: Meter

Input type: Generate 3D PSD from distribution function

Distribution: LSW

Mean radius: 1E-8

Amount of phase: Volume fraction 0.001

Radius [m]	Number Density
0.0	0.0
1.4914914914914913...	99.01643181008288
2.9829829829829827...	396.65822057098967
4.474474474474474E...	893.8180901945519
5.965965965965965E...	1591.3940988507434
7.457457457457457E...	2490.2896670624455
8.948948948948948E...	3591.4136059590837
1.0440440440440439...	4895.680145689891
1.193193193193193E...	6404.008963997586
1.3423423423423422...	8117.325214953213
1.4914914914914913...	10036.559557852963
1.6406406406406405...	12162.648186277738
1.7897897897897896...	14496.532857316166
1.9389389389389387...	17039.160920952

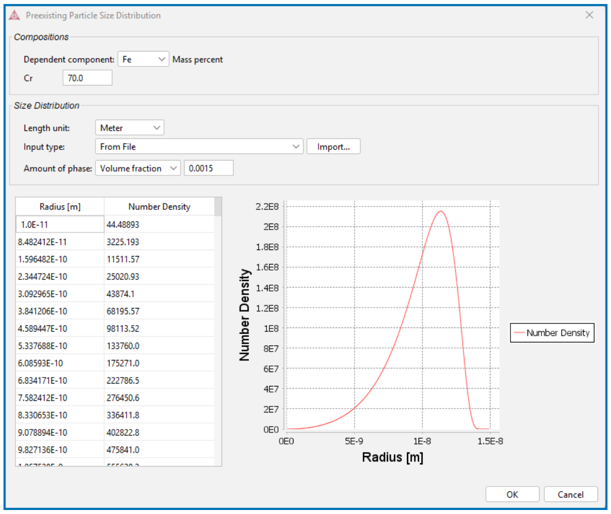
Figure 208: An LSW distribution with a mean radius of 1E-8m is used.

M23C6

The amount of Fe and Cr must be defined for M23C6 for this alloy. Fe is set to the dependent component, and 70 mass percent of Cr is set. The **From File** option is used to create the PSD.

The file loaded for M23C6 is available from the **Example files → Precipitation Module - TC-PRISMA** folder and is named `P_10_Precipitation_Initial_PSD_FeCrC_psd_3D_M23C6.csv`.

You can import data from a spreadsheet or text file (.xls, .xlsx, .csv, or .txt formats are acceptable). The initial volume fraction of 0.15 % is assumed.



Preexisting Particle Size Distribution

Compositions

Dependent component: Fe Mass percent

Cr 70.0

Size Distribution

Length unit: Meter

Input type: From File

Amount of phase: Volume fraction 0.0015

Radius [m]	Number Density
1.0E-11	44.48893
8.482412E-11	3225.193
1.596482E-10	11511.57
2.344724E-10	25020.93
3.092965E-10	43874.1
3.841206E-10	68195.57
4.589447E-10	98113.52
5.337688E-10	133760.0
6.08593E-10	175271.0
6.834171E-10	222786.5
7.582412E-10	276450.6
8.330653E-10	336411.8
9.078894E-10	402822.8
9.827136E-10	475841.0

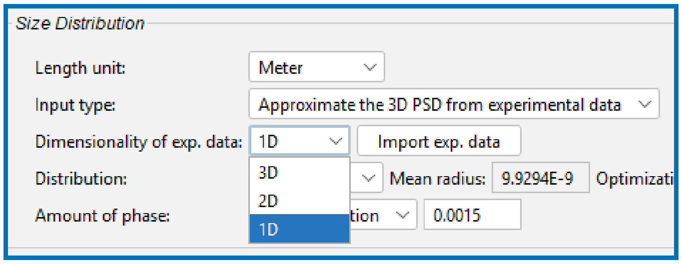
M7C3

The amount of Fe and Cr must be defined for M7C3 for this alloy. Fe is set to the dependent component, and 83 mass percent of Cr is set. The Approximate the 3D PSD from experimental data option is used to create the PSD.

In this example, the linear intercept method is used to measure the size distribution of M7C3 from micrographs descriptive of sectioning the dispersion. A size distribution of halved linear intercepts is created and is available as a file you can use as a template.

> The file loaded for M7C3 is available from the **Example files** → **Precipitation Module - TC-PRISMA** folder and is named `P_10_Precipitation_Initial_PSD_FeCrC_psd_1D_M7C3.csv`.

The **Dimensionality of the exp. data** is set to 1D. The experimental data is loaded by importing the above named *.csv file. An **LSW Distribution** is used. When you click **Generate**, it calibrates the chosen distribution and stereology description to the experimental data. The initial volume fraction of 0.15 % is assumed.



Size Distribution

Length unit: Meter

Input type: Approximate the 3D PSD from experimental data

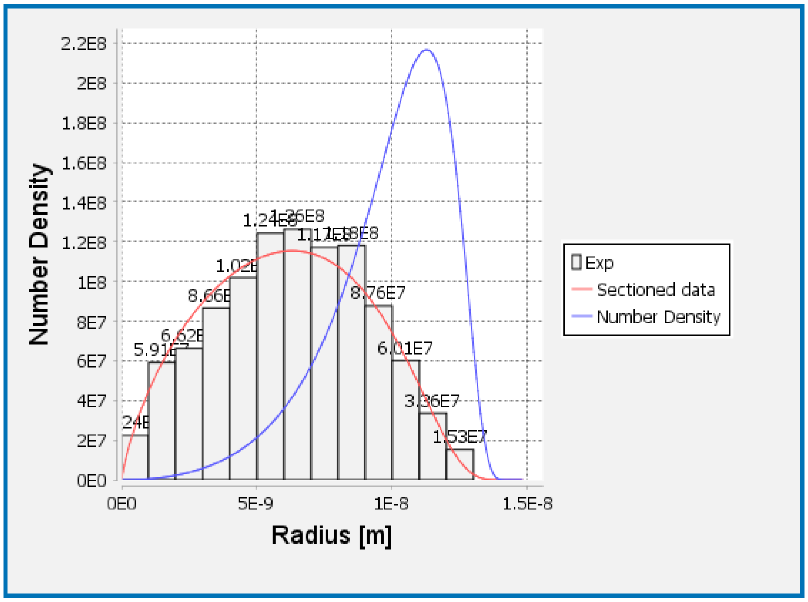
Dimensionality of exp. data: 1D

Distribution:

Mean radius: 9.9294E-9

Amount of phase:

0.0015



Example Settings

System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO)
Elements	Fe, C, Cr
Conditions (Precipitation Calculator)	
Composition	Fe-0.1C-12Cr Mass percent
Matrix phase	BCC_A2 All other defaults are kept.

Precipitate phases	CEMENTITE, M23C6 and M7C3
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Grain boundaries (all calculations): Calculated from the matrix settings with a wetting angle of 90°
Interfacial energy	User-defined function f(r,T) (all calculations): • CEMENTITE: 0.167 J/m^2 • M23C6 0.252 J/m^2 • M7C3 0.282 J/m^2
Preexisting size distribution (click **Show Details** to display this setting)	For the Precipitation Calculator including particle size distribution (PSD), and for all precipitate phases, this checkbox is selected. For each precipitate phase (CEMENTITE, M23C6 and M7C3), click **Edit Particle Size Distribution** to make changes to the parameters. A window opens with a graphical representation of the radius vs number density. **Input type** • Generate 3D PSD from distribution function - CEMENTITE uses this option in the example • From File - M23C6 uses this option in the example • Approximate the 3D PSD from experimental data - M7C3 uses this option in the example.
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	1053 K
Simulation time	400 000 seconds

Visualizations

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Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

  For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

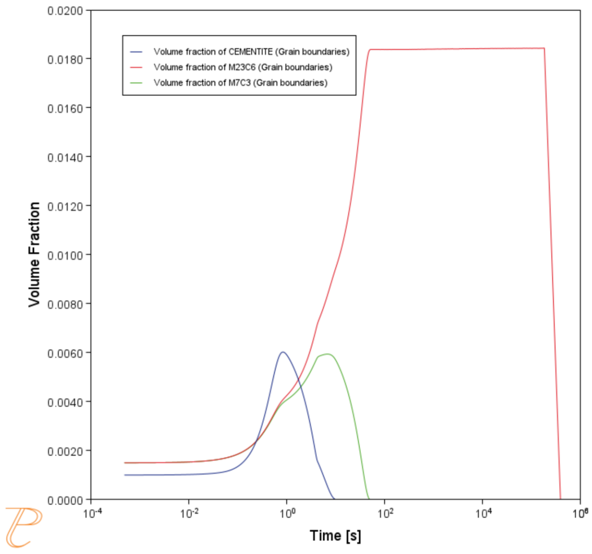


Figure 209: These results show the predicted volume fraction of cementite, M23C6, and M7C3 during an isothermal aging with an initial particle size distribution of each precipitate phase. The predicted kinetics are sensitive to the initial size, volume fraction, and composition of these precipitates.

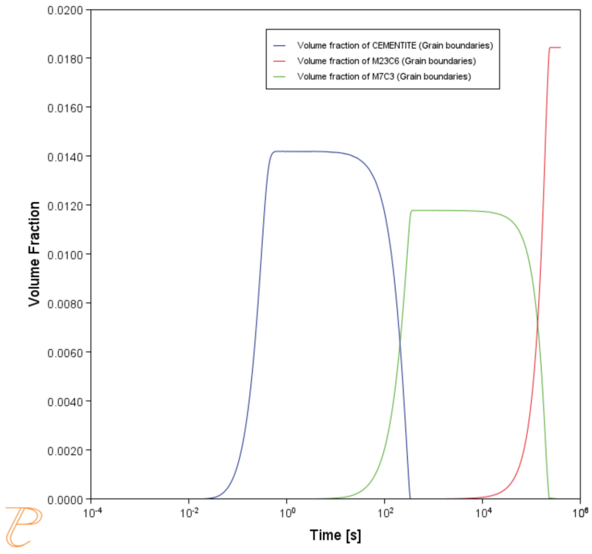


Figure 210: The predicted volume fraction of cementite, M23C6, and M7C3 during an isothermal aging with no precipitates in solution in the initial condition.

P_11: Interfacial Energy Function

In some cases, interfacial energy may be a function of temperature and/or particle radius. This example uses four Precipitation Calculators at four temperature points in 30 K increments: 673 K, 703 K, 733 K, and 763 K. It is an isothermal calculation to examine the mean radius of an Al-0.12Sc system. It uses an FCC_A1 matrix phase and AL3SC precipitate phase with bulk nucleation sites and user-defined interfacial energy function. The user defined interfacial energy function uses an error function to set a smooth transition of the interfacial energy from 0.065 J/m^2 to 0.085 J/m^2 for particle radii below and above 1e^{-8}m and 5e^{-8}m, respectively.

A dataset based on Iwamura and Miura [2004Iwa] data is compared with the calculated results.

Interfacial Energy Anisotropy

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: `P_11_Interfacial_energy_function.tcu`

Example Settings

System (System Definer)	
Database package	Demo: Aluminum-based Alloys (ALDEMO, MALDEMO)
Elements	Al, Sc
Conditions (Precipitation Calculator)	
Composition	Al-0.12Sc Mole percent
Matrix phase	FCC_A1 All other defaults are kept.
Precipitate phase	AL3SC Nucleation sites (all calculations): Bulk (6.025E28 m^{-3})

	Interfacial energy (all calculations): User-defined function f(r,T): 0.075+0.011*erf ((r-3e-8)/1e-8 J/m^2)
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal (all calculations)
Temperature	Four temperature points in 30 K increments: 673 K, 703 K, 733 K, and 763 K.
Simulation time	1 000 000 seconds (all calculations)
Datasets (Experimental File Reader)	
Wamura 2004 (Dataset 1)	Data set included with this example and imported to one Experimental File Reader.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

When you run (Perform) this example, it takes a few minutes for the calculations to complete.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

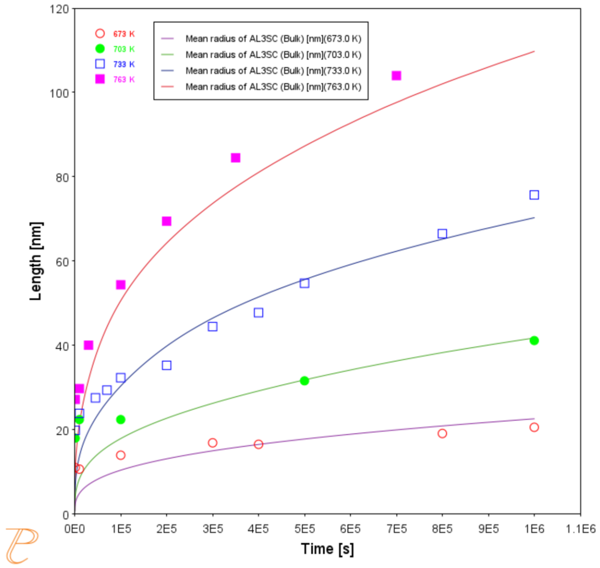


Figure 211: The results of an isothermal calculation to examine the mean radius of an Al-0.12Sc system with experimental data from [2004Iwa].

Reference

[2004Iwa] S. Iwamura, Y. Miura, Loss in coherency and coarsening behavior of Al3Sc precipitates. Acta Mater. 52, 591–600 (2004).

P_12: Comparing Growth Rate Models for an Al-Zr System

This example compares the **Simplified**, **General**, and **Advanced** growth rate models for an Al-Zr system. The resulting plot compares the mean radius of the spheres for each AL3ZR_D023 precipitate phase calculated for each type of growth rate model.

All models treat a spherical particle (precipitate) of stoichiometric composition or with negligible atomic diffusivity. Local equilibrium at the precipitate-matrix interface is assumed.

When you use the *Advanced* model, the velocity of a moving phase interface and the operating tie-line are solved together from flux-balance equations. This model can treat both high supersaturation and cross diffusion rigorously. It can also capture the transition between NPLE (non-partitioning local equilibrium) and PLE (partitioning local equilibrium) without any *ad hoc* treatment.

The *Simplified* model is based on the quasi-steady state diffusion approximation, and estimates solute partitioning with matrix composition and nuclei composition instead of time-consuming stepwise tie-line calculations. It also neglects cross diffusion for simplicity.

The *General* model can be considered the same theoretical approximation as, but an improvement over, the *Simplified* model, with cross-diffusion terms taken into account, as well as adjustment of Gibbs-Thomson effect and effective diffusivity implemented. A dataset based on Knipling et al. [2008Kni] data is compared with the calculated results.

For more background information, see the theory described in Growth.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: `P_12_Precipitation_Al-Zr_GrowthRateModel_comparison.tcu`

Example Settings

System (System Definer)	
Database package	Demo: Aluminum-based Alloys (ALDEMO, MALDEMO)

Elements	Al, Zr
Conditions (Precipitation Calculator)	
Composition	Al-0.2Zr Mole percent
Matrix phase	FCC_A1 All other defaults are kept.
Precipitate phase	AL3ZR_D023 Click **Show Details** to select the **Growth rate model** (**Simplified**, **Advanced** and **General**). All other defaults are kept.
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	425 Celsius
Simulation time	400 hours
Datasets (Experimental File Reader)	
2008 Knipling	Data set included with this example and imported to one Experimental File Reader.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

When you run (Perform) this example, it takes a few minutes for the calculations to complete.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

  For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

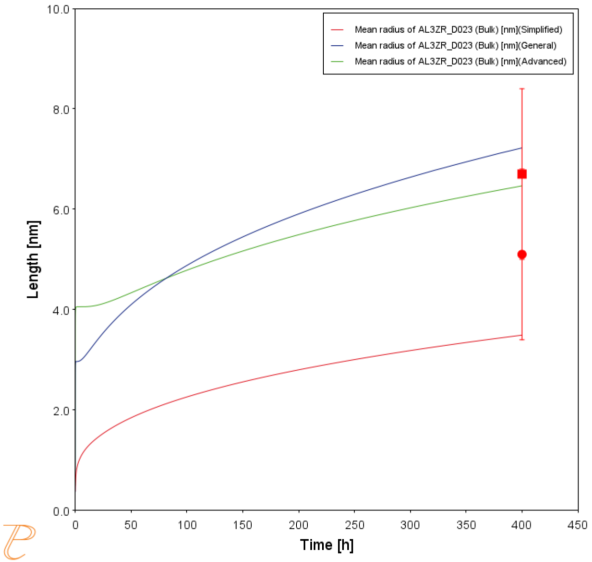


Figure 212: This shows the impact of the available growth rate settings options and compares the mean radius measurements of [2008Kni] with results obtained from the simplified, general, and advanced growth rate models. The experimental data includes measurements taken from different dendrites.

Reference

[2008Kni] K. E. Knipling, D. C. Dunand, D. N. Seidman, Precipitation evolution in Al–Zr and Al–Zr–Ti alloys during isothermal aging at 375–425 °C. Acta Mater. 56, 114–127 (2008).

P_13: Paraequilibrium Precipitation of Cementite Fe-C-Cr

In this example, the precipitation of cementite during tempering of a Fe-Cr-C steel is simulated considering two interface conditions: one is the usual ortho-equilibrium condition; the other is the para-equilibrium condition. The simulation results are compared with the experimental data from Sakuma et al. [1980Sak].

This example demonstrates that the early stage of the cementite precipitation can only be accounted for by a simulation applying the para-equilibrium condition, under which the precipitation kinetics are controlled by the diffusion of C. The comparison also shows a later stage gradual transition from the para-equilibrium condition to the ortho-equilibrium condition, and if the tempering time is long enough the diffusion of Cr has a dominating effect on the coarsening of cementite.

For more background information, see the theory described in Growth.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: `P_13_Precipitation_Fe-C-Cr_Paraequilibrium_Precipitation_of_Cementite.tcu`

Example Settings

System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)
Elements	Fe, Cr, C
Conditions (Precipitation Calculator)	
Composition	Fe-0.95Cr-1.065C Mass percent
Matrix phase	BCC_A2 All other defaults are kept.
Precipitate phase	CEMENTITE_D011

	Click **Show Details** to select the **Growth rate model** (**Simplified** (OE) and **Para-eq**) (PE). All other defaults are kept.
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	773 Kelvin
Simulation time	20 hours for the paraequilibrium model and 600 hours for the simplified model.
Datasets (Experimental File Reader)	
1980 Sakuma	Data set included with this example and imported to one Experimental File Reader.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

When you run (Perform) this example, it can take over two hours to complete the calculations.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

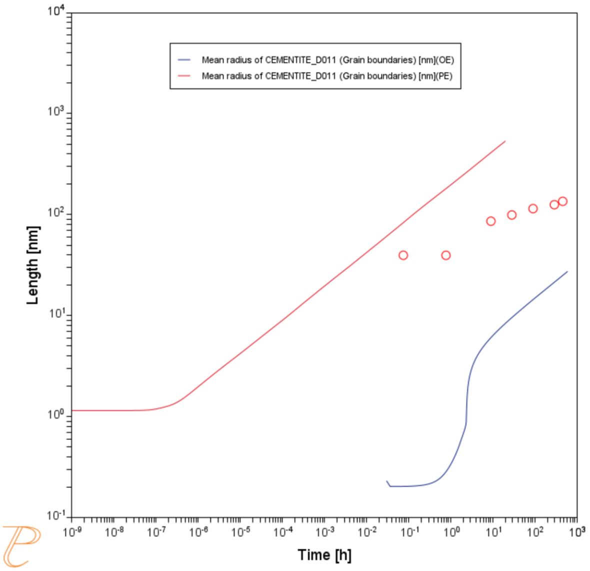


Figure 213: These results compare the predicted and measured evolution of the mean radius of cementite with the experimental data from [1980Sak] to simulation predictions obtained from the ortho-equilibrium (OE), and para-equilibrium (PE) approximations of the precipitate composition. The precipitate growth kinetics exhibited by cementite can be rationalized by the transition from PE to OE.

Reference

[1980Sak] T. Sakuma, N. Watanabe, T. Nishizawa, The Effect of Alloying Element on the Coarsening Behavior of Cementite Particles in Ferrite. Trans. Japan Inst. Met. 21, 159–168 (1980).

P_14: Grain Growth and the Zener Pinning Effect

This example demonstrates the simulation of normal grain growth and the pinning effect [1948Smi; 1998Man] of precipitated second-phase particles on the grain boundary motion.

To investigate the grain growth and Zener pinning effect, an Fe-0.2C (wt.%) binary alloy, with a BCC_A2 matrix phase and CEMENTITE precipitate phase, is simulated and uses the demonstration steel databases, FEDEMO and MFEDEMO. These databases are available to all users (i.e. you do not need a license for the Precipitation Module (TC-PRISMA)) and contain the necessary thermodynamic and kinetic data needed for the calculation.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: `P_14_Precipitation_Fe-C-Ferrite-Grain_Growth_with_Zener_Pinning.tcu`

Example Settings

System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO)
Elements	Fe, C
Conditions (Precipitation Calculator)	
Composition	Fe-0.2C Mass percent
Matrix phase	BCC_A2 • Grain boundary energy (J/m^2): 0.5 • Grain boundary mobility: Prefactor(m^4/Js): 2 x 10^{-15} • Click to **Edit grain size distribution**. Then Initial grain size distribution: Hillert distribution with average radius of 3.2 x 10^{-6} m • Mobility adjustment: Same for all elements. Prefactor 0.08.

Precipitate phase	CEMENTITE - Zener pinning parameters: Cutoff size (m): 8.0×10^{-7}
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	722 °C
Simulation time	35 hours
Datasets (Experimental File Reader)	
[1975Hel]	Data sets included with this example and imported to two Experimental File Readers.

Visualizations

This example is included as a Precipitation Module (TC-PRISMA) tutorial on our website and as part of the playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

> For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

The calculated equilibrium volume fraction of CEMENTITE at 722 °C (0.02786), using FEDEMO, matches that (0.02787) of a Fe-0.2C-0.004S-0.0004O-0.001N-0.001Al (wt.%) multicomponent commercial alloy, calculated using the latest version of the TCS Steel and Fe-alloys Database (TCFE), an alloy that was studied by Hellman and Hillert [1975Hel]. The mobility adjustment assures the precipitation kinetics of CEMENTITE phase in Fe-C system matches that of experimental data [1975Hel] of the commercial counterpart (and shown in Figure 214)

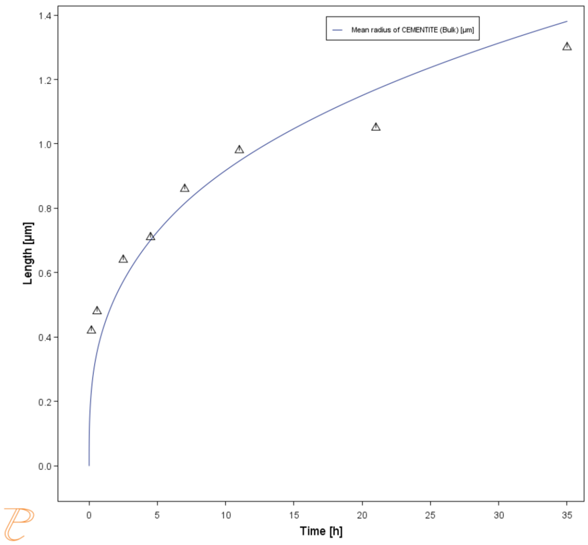


Figure 214: The evolution of the mean radius of cementite comparing the experimental data from [1975Hel] with the Precipitation Calculator results.

The grain boundary energy was chosen to be a reasonable value of 0.5 J/m^2. There is a large discrepancy, in several orders of magnitude, among experimental data regarding the grain boundary mobility. In the present calculation, a value of 2x10^{-15} m^4/Js was chosen.

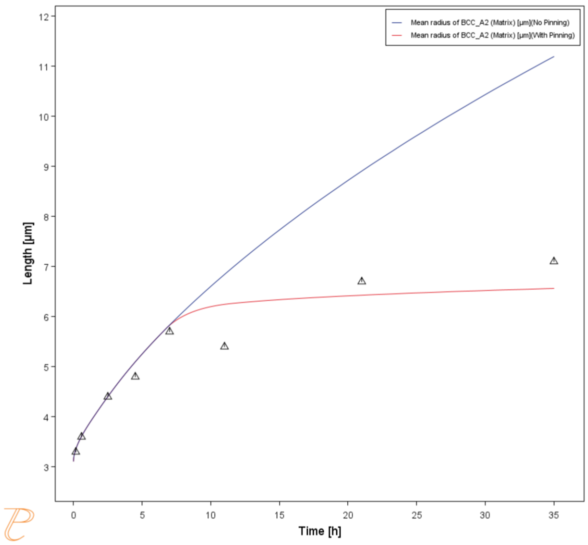


Figure 215: The evolution of the mean grain radius of ferrite comparing the experimental data from [1975Hel] with predictions made with and without Zener pinning from an evolving dispersion of cementite precipitates.

References

[1948Smi] C. S. Smith, Grains, Phases, and Interfaces - an Interpretation of Microstructure. Trans. AIME. 175, 15–51 (1948).

[1975Hel] P. Hellman, M. Hillert, On the Effect of Second-Phase Particles on Grain Growth. Scand. J. Metall. 4, 211–219 (1975).

[1998Man] P. A. Manohar, M. Ferry, T. Chandra, Five Decades of the Zener Equation. ISIJ Int. 38, 913–924 (1998).

P_15: Smooth Transition from Paraequilibrium to Ortho-equilibrium

In this example, the precipitation of cementite during tempering of an Fe-Mn-C steel is simulated considering three interface conditions: the usual ortho-equilibrium (OE) condition; paraequilibrium (PE) condition; and a smooth transition from paraequilibrium to ortho-equilibrium condition (PE-OE). The simulation results are compared with the experimental data from Miyamoto et al. [2007Miy].

> The Precipitation Calculator nodes are renamed in the example to match the abbreviations for the three interface conditions considered: OE, PE, and PE-OE. Also see the video to learn how to create this example.

This example demonstrates that the early stage of the cementite precipitation follows a PE condition, under which the precipitation kinetics is controlled by the diffusion of C. At a later stage, gradual transition from PE condition to OE condition occurs, and if the tempering time is long enough the diffusion of Mn has a dominating effect on the coarsening of cementite. While a *Simplified* model follows the OE condition and a *Para-eq* model follows PE condition, the *PE Automatic* model enables the smooth transition from PE condition at early stage to OE condition at a late stage.

The example uses the demonstration steel databases, FEDEMO and MFEDEMO. These databases are available to all users (i.e. you do not need a license for the Precipitation Module (TC-PRISMA)) and contain the necessary thermodynamic and kinetic data needed for the calculation.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: `P_15_Precipitation_Fe-C-Mn_PE-OE_Precipitation_of_Cementite.tcu`

Example Settings

System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO)

Elements	Fe, Mn, C
Conditions (Precipitation Calculator)	
Composition	Fe-1.96Mn-0.61C mass percent
Matrix phase	BCC_A2 Click **Show Details**: • Grain size: Average radius 1.0E-7m • Grain aspect ratio: 100.0 • Mobility adjustment: Keep the default, Same for all elements, then enter 0.008 for the Prefactor, and -7e4 J/mol for the Activation energy. All other defaults are kept.
Precipitate phase	CEMENTITE_D011 Click **Show Details** to select the Growth rate model (**Simplified**, **Para-eq**, and **PE Automatic**). All other defaults are kept.
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	923.15 Kelvin
Simulation time	1E6 seconds for Simplified and PE Automatic models, and 5 seconds for Para-eq model
Datasets (Experimental File Reader)	
Mean Radius Exp	Data set including experimental mean radius of cementite
Mn Concentration	Data set including experimental Mn composition in cementite

Visualizations

▶ This example is included as a Precipitation Module (TC-PRISMA) tutorial on our website and as part of the playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

⌛ When you run (Perform) this example, it takes a few minutes for the calculations to complete.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

  For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

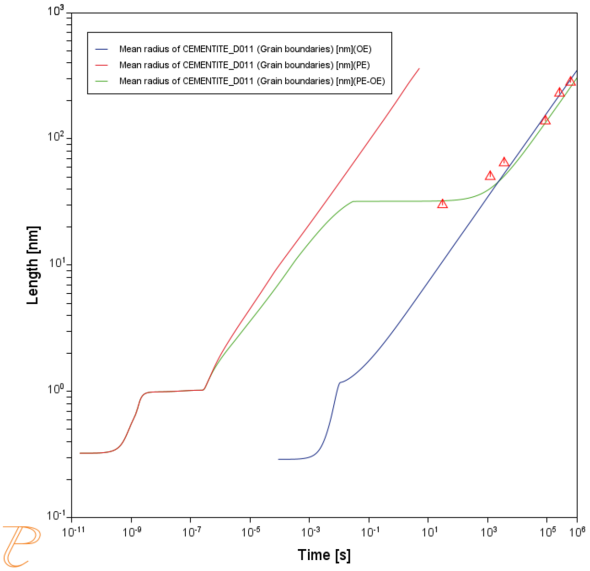


Figure 216: A comparison between the measurements of mean cementite radius from [2007Miy] with the simplified (OE), para-eq (PE), and PE Automatic (PE-OE) growth models. The PE-OE model is needed to capture the nucleation, growth, and coarsening behavior of cementite.

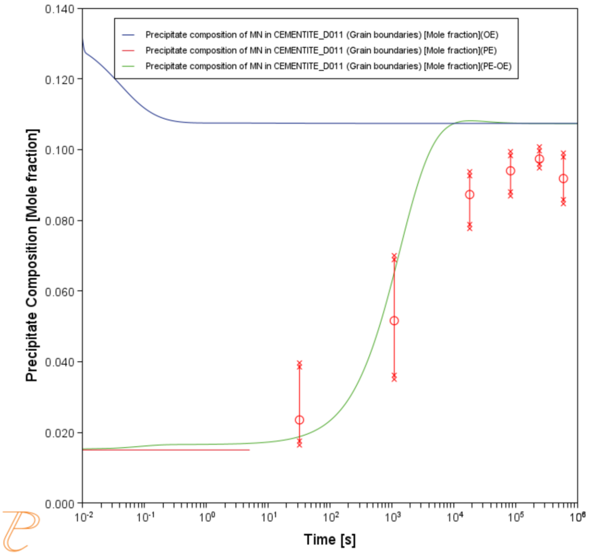


Figure 217: A comparison of the evolution of the cementite Mn composition during isothermal aging at 923.15 K between the experimental data from [2007Miy] with model predictions obtained from the simplified (OE) growth model, the para-eq (PE) growth model, and the PE Automatic (PE-OE) growth model. The PE-OE model captures the behavior shown in the experimental data, where the Mn composition transitions from the initial ferrite composition towards the equilibrium cementite composition.

Reference

[2007Miy] G. Miyamoto, J. Oh, K. Hono, T. Furuhara, T. Maki, Effect of partitioning of Mn and Si on the growth kinetics of cementite in tempered Fe–0.6 mass% C martensite. Acta Mater. 55, 5027–5038 (2007).

P_16 Isothermal Coarsening and a 3D to 2D Stereological Conversion

This example demonstrates the use of the **3D → 2D** stereological conversion functionality to compare Precipitation Module (TC-PRISMA) predictions with experimental data obtained from Scanning Electron Micrographs (SEM).

> The **3D → 2D** setting is available on a **Plot** or **Table Renderer** that is a successor to the **Precipitation Calculator**, and when certain axis variables are selected for a spherical morphology.

> For more background information, see the theory described in Stereology.

The isothermal coarsening kinetics of γ' precipitates in a Ni-Al-Cr alloy is modeled. The experimental data is from [2008Sud], which investigates isothermal coarsening kinetics at a temperature of 873 K for up to 264 h.

It is assumed that there are no precipitates in solution at the beginning of the isothermal heat treatment.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: `P_16_Precipitation_Ni-Al-Cr_Stereology.tcu`

Example Settings

> The example also includes an Equilibrium Calculator and Table Renderer to first confirm the stability of the precipitate phase for this system (FCC_L12#2), then determine particle composition at 1073 K, and this information is used with the Precipitation Calculator set up.

System (System Definer)	
Database package	Demo: Nickel-based superalloys (NIDEMO and MNIDEMO)
Elements	Ni, Al, Cr
Conditions (Precipitation Calculator)	
Composition	Ni-10l-8.5Cr Mole percent
Matrix Phase	FCC_L12 - Click **Show Details** and for the **Mobility adjustment** enter `0.5` for the **Prefactor**. - All other defaults are kept.
Precipitate Phase	FCC_L12#2 Click **Show Details** and adjust the default settings as indicated: - **Interfacial energy**: Select **User-defined** and enter `0.01` J/m^2.
Calculation Type (Precipitation Calculator)	
Calculation Type	Isothermal
Temperature	1073 Kelvin
Simulation time	300 h
Datasets (Experimental File Reader)	
2008 Sudbrack et al	Data sets are included with this example and are imported using the Experimental File Reader activity. There are 2D size distributions comparing results after a total of 16 h aging, 64 h aging, and 264 h of aging, and a comparison of the experimental and predicted 2D mean radius versus time.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

  For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

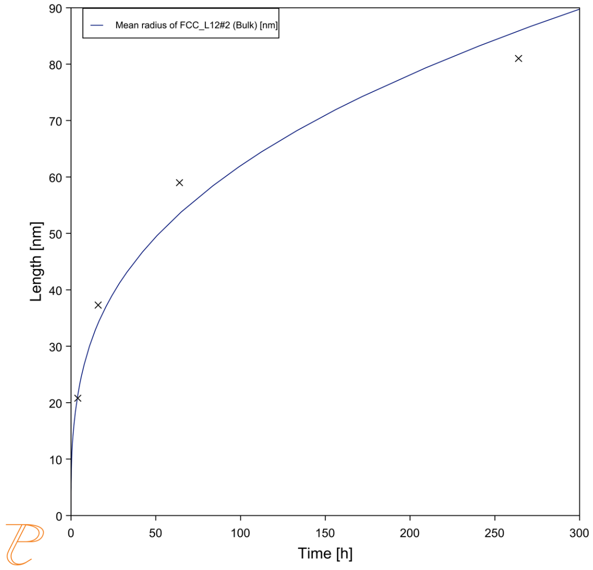


Figure 218: A comparison of the evolution of the mean 2D precipitate radius measurements of [2008Sud] with model predictions.

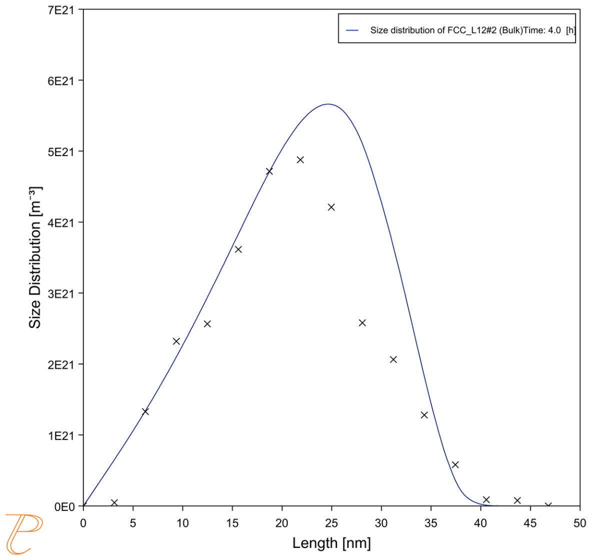


Figure 219: A comparison of the predicted and measured 2D size distribution after 4 h of aging.

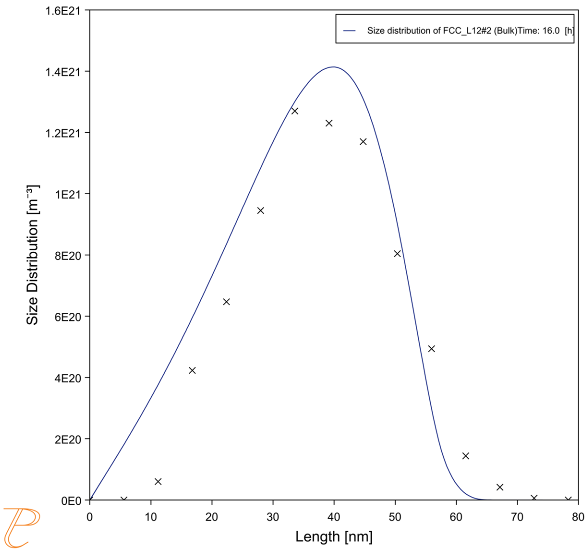


Figure 220: A comparison of the predicted and measured 2D size distribution after 16 h of aging.

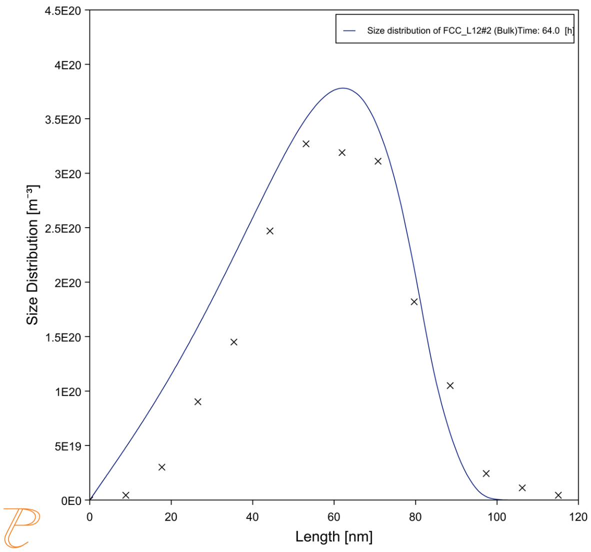


Figure 221: A comparison of the predicted and measured 2D size distribution after 64 h of aging.

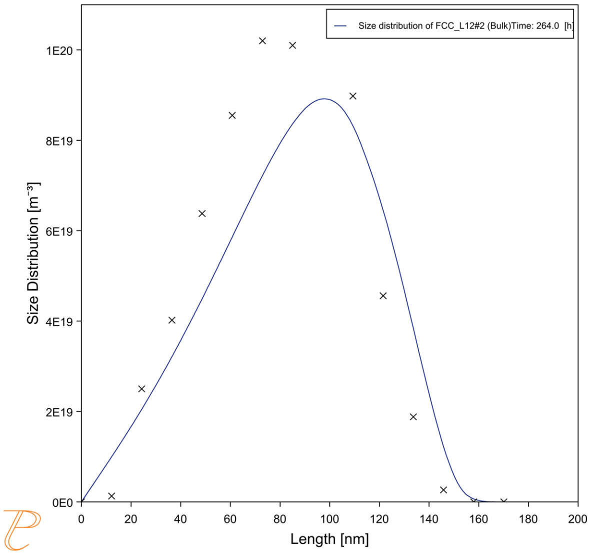


Figure 222: A comparison of the predicted and measured 2D size distribution after 264 h of aging.

Reference

[2008Sud] C. K. Sudbrack, T. D. Ziebell, R. D. Noebe, D. N. Seidman, Effects of a tungsten addition on the morphological evolution, spatial correlations and temporal evolution of a model Ni–Al–Cr superalloy. Acta Mater. 56, 448–463 (2008).

Process Metallurgy Module Examples Collection

The Process Metallurgy Module requires both a valid Maintenance and Support Subscription (M&SS) and a license for the TCS Metal Oxide Solutions Database (TCOX8 or newer).

All users can test the Process Metallurgy Module with the included OXDEMO database, which is limited to these elements: Al, C, Ca, Fe, O, S, and Si. For more information about this and other products visit our website.

The Process Metallurgy Module

About the Examples

In this section:

PMET_01: Basic Oxygen Furnace (BOF)

The example uses the **Process Metallurgy Calculator** to demonstrate a simplified steelmaking process in a Basic Oxygen Furnace (BOF).

This application example in its various forms is available on our website. There are two application examples (one equilibrium, one kinetic) showing how the Process Metallurgy Module can be used to calculate the BOF process.

This basic example uses equilibrium calculations to gain a general understanding of your BOF process and help you determine optimal operation conditions and predict and optimize costs of raw materials and recycling. The other set of examples gives detailed instructions on how to simulate the kinetics of the BOF process using the kinetic process simulation (see PMET_04: Basic Oxygen Furnace (BOF) Kinetics).

Project File and License Information

- Folder: **Process Metallurgy**
- File name: `PMET_01_Basic_Oxygen_Furnace.tcu`

Choose a, b, or c versions of the example based on your license.

- **PMET_01a_Basic_Oxygen_Furnace** is included in a regular Thermo-Calc installation as well as the free Educational version of Thermo-Calc. This is a highly simplified example and uses the OXDEMO database, and only considers the elements Fe, C, and O.
- **PMET_01b_Basic_Oxygen_Furnace** is also a simplified calculation but uses the OXDEMO database. It requires a full license of Thermo-Calc 2021b and newer.
- **PMET_01c_Basic_Oxygen_Furnace** requires the TCOX11 database and newer and a full license of Thermo-Calc 2021b and newer.

Visualizations

This example is included as a Process Metallurgy tutorial on our website and as part of the playlist our YouTube channel.

One way to learn how to work with the Process Metallurgy Calculator is to use the project files as templates to help you set up your own simulation. For example, you can examine the settings available on the **Configuration** window and that are described in Process Simulation: Conditions Tab and the Options Tab.

The resulting plots and details related to setting up this example are available to download via the dedicated web page.

PMET_02: Desulphurization in a Ladle Furnace (LF)

The example, which is also available on our website, uses the **Process Metallurgy Calculator** to demonstrate the use of a Ladle Furnace (LF) with the Process Metallurgy Module.

The ladle furnace (LF) fulfils many purposes in the steelmaking process. Desulphurization, which we will focus on in this example, is merely one of them.

Desulphurization is usually performed by transferring S that is dissolved in the liquid metal to a CaO-rich slag phase. For this process to be successful, two conditions need to be fulfilled:

1. The slag must be fully liquid (liquid fraction > 0.9). This is required for kinetic reasons. The slag phase must be fluid so that it can emulsify with the liquid steel and form a large surface area where the reaction between steel and slag can take place.
2. The slag must take up a large amount of S from the liquid steel (have a “high sulphur capacity”) so that a significant amount of sulphur will move from the liquid steel to the slag phase.

The example demonstrates how the Process Metallurgy Module in Thermo-Calc can be used to explore these two conditions for an equilibrium between liquid steel and slag in a ladle furnace, trying to find good slag compositions. We also investigate why excessive slag carry-over from the BOF or EAF is detrimental for desulphurization in the LF and who how slag conditioning with CaC_2 as fluxing agent can recover the desulphurizing ability of the slag.

Project File and License Information

- Folder: **Process Metallurgy**
- File names: `PMET_02a_Ladle_Furnace.tcu` or `PMET_02b_Desulphurization_in_Ladle_Furnace.tcu`.

Choose a or b versions of the example based on your license

- `PMET_02a_Ladle_Furnace.tcu` can be run with OXDEMO database but requires the full license for Thermo-Calc 2021b and newer.
- `PMET_02b_Desulphurization_in_Ladle_Furnace.tcu` requires the TCOX11 database and a full license for Thermo-Calc 2021b and newer.

Visualizations

This example is included as a Process Metallurgy tutorial on our website and as part of the playlist our YouTube channel.

One way to learn how to work with the Process Metallurgy Calculator is to use the project files as templates to help you set up your own simulation. For example, you can examine the settings available on the **Configuration** window and that are described in Process Simulation: Conditions Tab and the Options Tab.

The resulting plots and details related to setting up this example are available to download via the dedicated web page.

PMET_03: Argon Oxygen Decarburization (AOD)

The Argon Oxygen Decarburization (AOD) process is a converter process applied in stainless steel making. In this process the oxidation of chromium in the steel melt needs to be prevented while carbon is oxidized. This is achieved by reducing the oxygen partial pressure by having a high Ar-content in the blowing gas. It is a highly exothermic process that requires adiabatic modeling. In this example the conversion of carbon-rich steel scrap is modeled together with additions of Ferronickel and Ferrochrome to a stainless steel. The example uses the **Process Metallurgy Calculator**.

Visit the website Application Examples → Process Metallurgy page for more background information as well as more in depth analyses of this and other examples. Also visit the Process Metallurgy Module page to access resources such as training videos, presentations, publications, webinars, and much more.

Project File and License Information

- Folder: **Process Metallurgy**
- File name: `PMET_03_Argon_Oxygen_Decarburization.tcu`

This example requires a license to run the simulation. It works with TCS Metal Oxide Solutions Database (TCOX) versions 8 and newer.

Visualizations

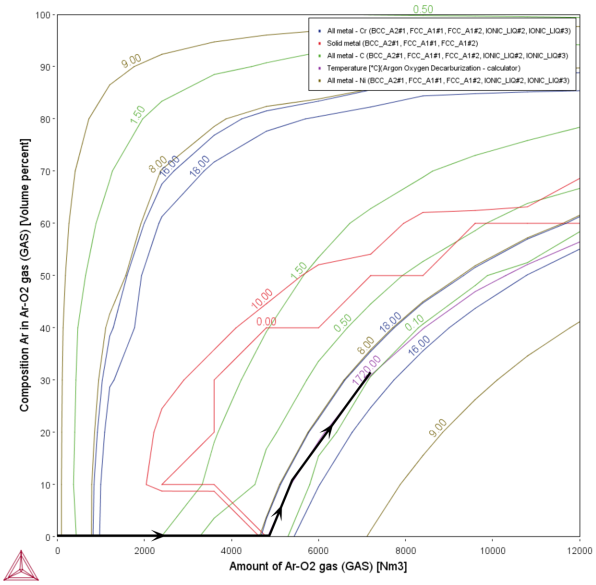
Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

⌛ When you run (Perform) this example, it takes a few minutes for the calculations to complete.

Background Description

The AOD-process is characterized by an initially high O_2-content of the blowing gas, which is gradually replaced by Ar. The maximum temperature of the process is typically around 1720 °C. A grid plot of an adiabatic calculation is well suited to model the required simultaneous change of amount of gas and its composition during this process. The black line in the plot above indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.



In principle, this plot could be used to control the blowing gas flow in a plant process. However, note that the simulation only considers a global gas phase, i.e. additional gas is added but never removed. This means that the given gas phase composition is an average one and not identical to the composition of the gas flowing in at each point in time. Additionally there is a certain impact on the resulting equilibria from the fact that all gas remains in the system and is not removed.

Slag Basicity

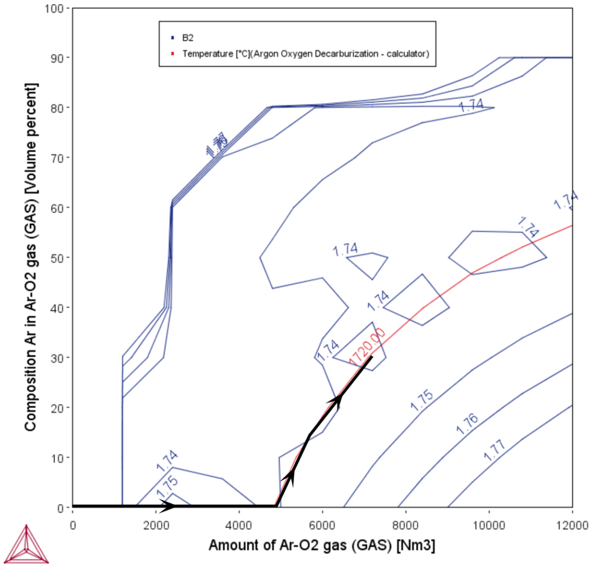


Figure 223: The Slag Basicity plot shows the basicity of the slag (which is a measure for the sulphur capacity of the slag). The process achieves a final basicity of 1.74 which is typical for an AOD-process. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

S Content in Steel

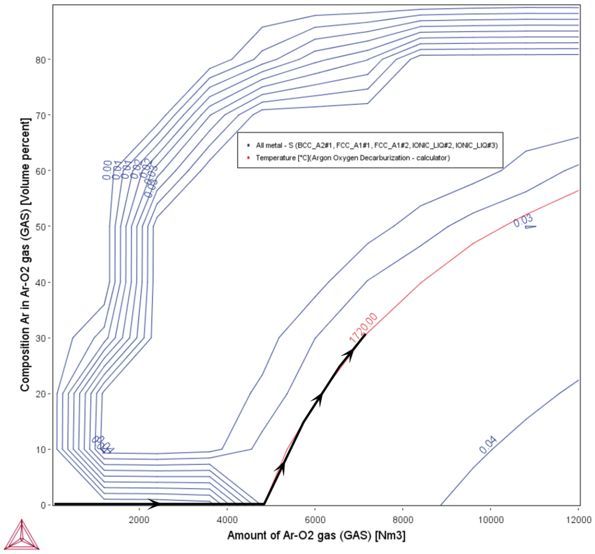


Figure 224: In the S Content in Steel plot, the sulphur content in the steel melt is slightly reduced during the process from 0.056% in the initial steel scrap to finally ca. 0.035%. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

Cr Content in Slag

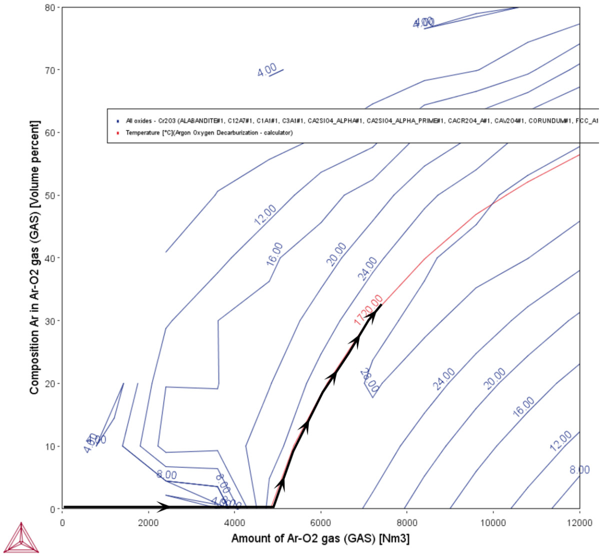


Figure 225: In the Cr Content in Slag plot, the Cr2O3-content in the slag reaches at the end of the process ca. 26 wt-%. This is typical for the AOD-process and requires an additional Cr-recovery step after the conversion to reduce the loss of chromium. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

Amount of Slag

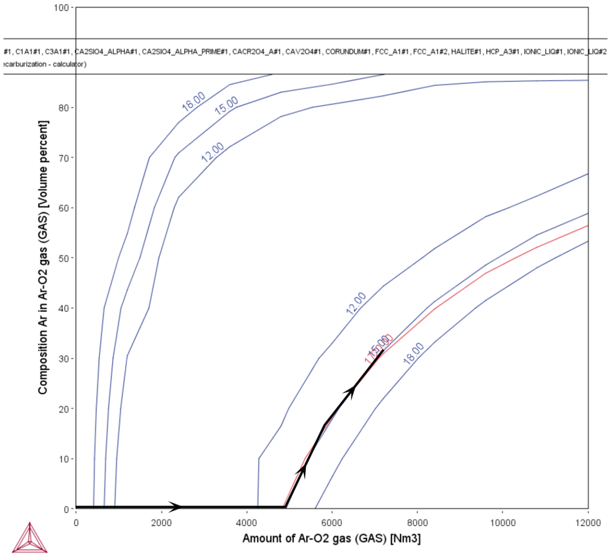


Figure 226: In the Amount of Slag plot, you can see that the process generates about 15 tons of slag in the total. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

Liquid Slag Fraction

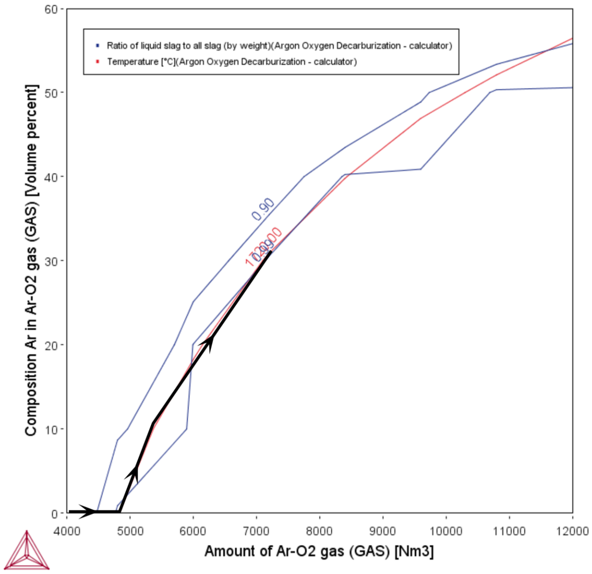


Figure 227: In the Liquid Slag Fraction plot, you can see that towards the end of the process the slag is calculated to be mostly liquid. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

PMET_04: Basic Oxygen Furnace (BOF) Kinetics

The example uses the **Process Metallurgy Calculator** to simulate the kinetics of the Basic Oxygen Furnace (BOF) process. This application example in its various forms is available on our website.

Metallurgical processes such as the BOF process rarely reach equilibrium. Therefore, a model description must include kinetics if meaningful results are to be obtained. In recent years, a simple but powerful model termed the Effective Equilibrium Reaction Zone (EERZ) model has been developed and widely applied to simulate various metallurgical processes.

This example shows you how to set up a kinetic simulation of the BOF process in the Process Metallurgy Module and includes a description of the EERZ model. For information about the equilibrium examples, see PMET_01: Basic Oxygen Furnace (BOF).

Project File Information

- Folder: **Process Metallurgy**

Choose a, b, or c versions of the example based on your license.

- `PMET_04a_Basic_Oxygen_Furnace_Kinetics` is included in a regular Thermo-Calc installation as well as the free Educational version of Thermo-Calc. This only considers the elements Fe, C, and O.
- `PMET_04b_Basic_Oxygen_Furnace_Kinetics` needs a full license of Thermo-Calc 2021b or newer, but uses the free OXDEMO database. It considers the elements Fe, C, O, Ca, Al, Si, and S.
- `PMET_04c_Basic_Oxygen_Furnace_Kinetics` requires both a full license of Thermo-Calc 2021b or newer and a license for the TCOX11 database and newer. This simulation corresponds pretty much to a real BOF process with the elements Fe, Mn, C, O, Ca, Al, Mg, Si, S, and P considered.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

The resulting plots and details related to setting up this example are available to download via the dedicated web page.

PMET_05: Lab Scale Ladle Furnace (LF) Kinetics

Using the **Process Metallurgy Calculator** and the **Process simulation** branch, this example is based on the publication by Piva et al [2017Piv] where a lab scale sample of pure iron is first deoxidized with Si-Mn and then a synthetic top slag is added to the steel. Generally, by using the project file and the information below, you can get an idea about how to set up a ladle furnace simulation using the Process Metallurgy Module.

Visit the website Application Examples → Process Metallurgy page for more background information as well as more in depth analyses of this and other examples. Also visit the Process Metallurgy Module page to access resources such as training videos, presentations, publications, webinars, and much more.

Setting Up a Process Metallurgy Simulation

Defining the Process Simulation

Project File and License Information

- Folder: **Process Metallurgy**
- File name: `PMET_05_Lab_Scale_Ladle_Furnace_Kinetics.tcu`

This example is best run with the TCS Metal Oxide Solutions Database (TCOX) version 13 or newer and a full license of Thermo-Calc 2024a or newer. Running the example with earlier versions of the database is possible but the results are not consistent with the referenced paper.

Visualizations

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

When you run (Perform) this example, it takes a few minutes for the calculations to complete.

About the Plot Results

Many different aspects of the reactions taking place in the LF can be plotted and analyzed. After you run the project file and obtain the plots, you can experiment by adjusting the settings on each Plot Renderer to see what happens in each case. There is more analysis about this and other examples available at the links to our website.

For an example of a more realistic industry scale, see PMET_06: Ladle Furnace (LF) Kinetics.

Setting Up the LF Process Simulation

In the paper by Piva et al. [2017], it is experimentally investigated how the steel and inclusion composition changes in function of time as the Si-Mn killed steel reacts with the slag. This experiment can serve as a model for the production of SiMn killed steel with subsequent top-slag deoxidation.

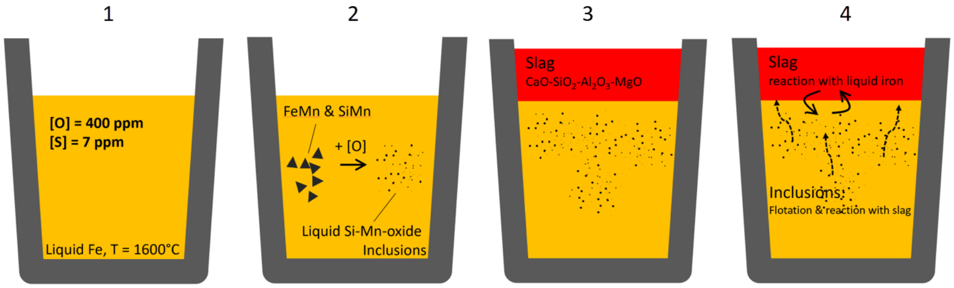


Figure 228: Diagram of the experiment performed by Piva et al. [2017]. The sequence as described in the text is: (1) liquid Fe with dissolved oxygen; (2) FeMn and SiMn added to deoxidize Fe; (3) top slag added after 360s; and (4) gradual reaction between steel, slag and inclusions.

According to the publication the following reaction sequence is expected as shown in the diagram:

1. In the initial state the steel contains 400 ppm of dissolved oxygen.
2. The deoxidizing agents are added. They dissolve and react with the oxygen in the steel forming oxide inclusions, thereby reducing the amount of dissolved oxygen ("killing" the steel). The kinetics are fast, and it can be assumed that the reaction proceeds to thermodynamic equilibrium.

3. On adding the slag (360 s after step 2, killing the steel) the liquid steel starts reacting with the slag.
4. According to the authors the most important reaction that takes place is the dissolution of Al out of the slag and its transferal into the liquid steel, where it reacts with the inclusions and changes their chemistry. Flotation of the inclusions is assumed to be negligible, due to the small size of the crucible and lack of stirring.

In this example only the last reaction is simulated after adding the slag. The kinetic parameters, compositions of all materials and process schedule are all taken from the publication.

Results and Experimental Analysis

The plots below compare the Al content in the liquid steel with the experimentally determined amount. The bottom plot shows how the Al_2O_3 from the slag phase is gradually reduced to metallic Al that dissolves in the liquid steel.

In this example, only part of the Al in the liquid steel is dissolved as metallic Al. With the Process Metallurgy Module, it is possible to plot both dissolved Al and also total Al.

In the steel industry this fraction of Al in the liquid steel is often termed *dissolved Al*. The rest of the Al reacts with the oxygen in the liquid steel and forms oxide inclusions. The amount of dissolved Al plus the Al bound up in oxide inclusions is often termed *total Al*. The difference between total Al minus dissolved Al is an important measure for the steel cleanness.

Total Al is what was measured by Piva et al. [2017] and their experimental data are compared to the calculated values below.

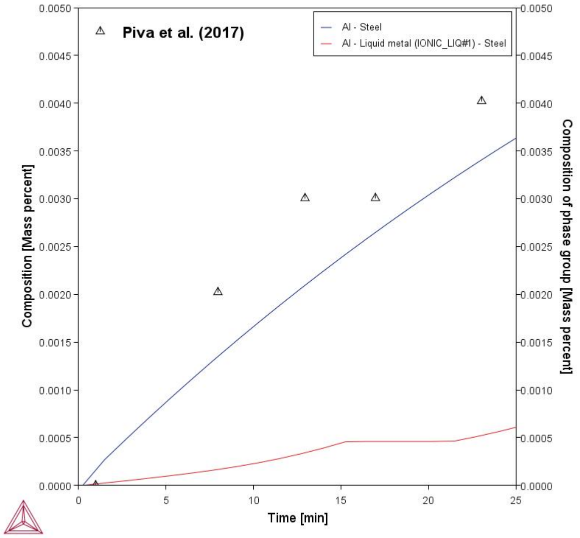


Figure 229: Total Al in the steel compared with experimental data (blue/top curve). Additionally the amount of dissolved Al is plotted (red/bottom curve), this is done by selecting "Composition of phase group" and "Liquid metal". Note that the red/bottom curve is not available with the example.

Immediately after killing the steel with SiMn and FeMn, the liquid steel contains liquid Si-Mn-oxide inclusions only. As the liquid steel picks up Al from the slag phase in function of time, the inclusions get richer and richer in Al. This experimentally verified change in inclusion chemistry is well reproduced by this simulation.

In the experiment, only the average composition of all inclusions could be measured; the type of inclusion (liquid / solid) was not determined.

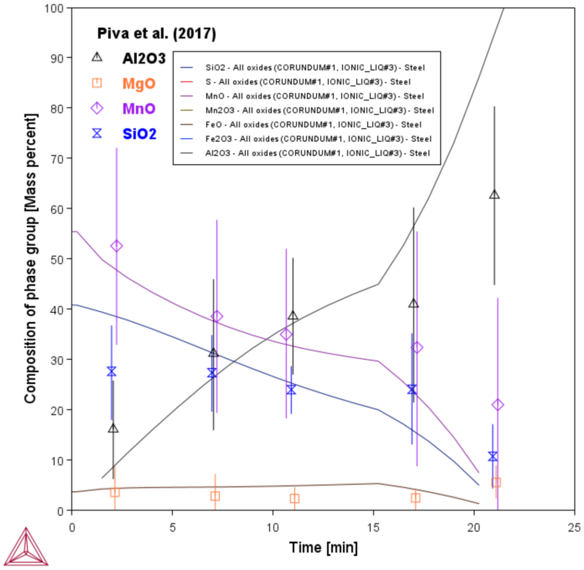


Figure 230: Calculated composition of non-metallic inclusions in function of processing time compared to experimental data [2017Piv].

With this simulation it is also possible to calculate the amount and type of inclusions present in the liquid steel. At the beginning of the process all the inclusions are liquid oxides, that gradually get richer in Al_2O_3 as the steel picks up Al from the slag. After 20 minutes processing time, the first solid corundum (Al_2O_3) inclusions start appearing. After 25 minutes almost no liquid inclusions remain.

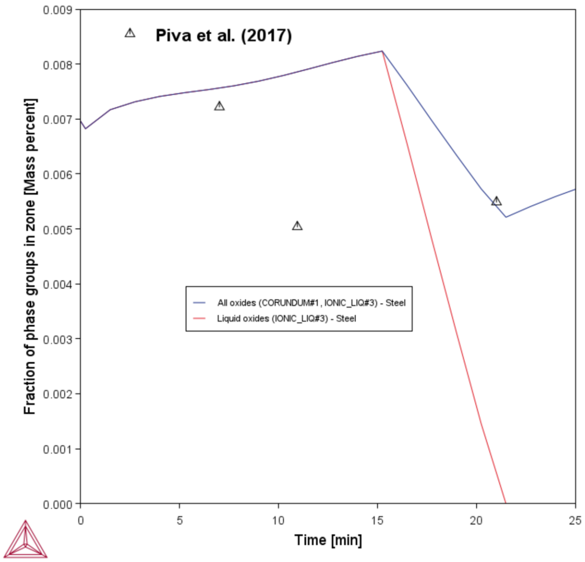


Figure 231: Amount of inclusions in the liquid steel in function of processing time. The total amount of inclusions (red line) and liquid oxide inclusions (blue line) are plotted. Up to about 20 min all inclusions are liquid oxide type, then they are replaced by solid corundum (Al_2O_3) inclusions. Experimental data from [2017Piv].

Reference

[2017Piv] Piva, S. P. T., Kumar, D. & Pistorius, P. C. "Modeling Manganese Silicate Inclusion Composition Changes during Ladle Treatment Using FactSage Macros," Metall. Mater. Trans. B 48, 37–45 (2017).

PMET_06: Ladle Furnace (LF) Kinetics

This in-depth example, which is also showcased on our website, uses the **Process Metallurgy Calculator** to show how to set up a full kinetic simulation of steel refining in a ladle furnace using the Process Metallurgy Module in Thermo-Calc. The Process Metallurgy Module uses the Effective Equilibrium Reaction Zone model (EERZ) to simulate the kinetics of the process. In this example, a full kinetic simulation of the LF refining process is set up using the Process Metallurgy Module.

For a simpler process that describes a lab-scale ladle furnace process, see PMET_05: Lab Scale Ladle Furnace (LF) Kinetics.

Background Overview

After steelmaking, which is mostly performed in a basic oxygen furnace (BOF) or electric arc furnace (EAF), the steel is usually tapped into a ladle where certain additions are made (deoxidation agents, slag formers, certain alloying elements) and then transferred to the ladle furnace (LF). The LF fulfils many purposes in the steel refining process, the most important being:

- Temperature control / heating by an electrical arc.
- Mixing by Ar or N2 bubbling through porous plugs in the bottom of the ladle to achieve homogeneous temperature and composition throughout the ladle.
- Removal of unwanted non-metallic phases / inclusions such as corundum (Al2O3), liquid oxide inclusions, spinel, on so on, by flotation, aided by Ar or N2 bubbling.
- Modification / engineering of non-metallic inclusions so that they are not detrimental for the downstream processing and/or the final product.
- Removal of unwanted volatile elements such as Pb, Zn, Sn, and so on. Due to their high vapor pressure, these elements are enriched in the rising Ar or N2 bubbles. After the gas escapes out of the ladle and cools, they condense, forming copious amounts of dust.
- Removal of unwanted elements such as sulphur by liquid steel / slag reactions.
- Lowering of the dissolved gas content. In the LF this is mainly achieved through chemical reactions. For direct removal of dissolved gas, vacuum degassing (VD) is usually required.
- Alloying and trimming of the steel to achieve the exact alloy composition required by the specification of the steel that is to be produced.

The reactions taking place in a LF are a complex interplay between equilibrium thermodynamics that define the direction of chemical reactions, and kinetics that define how fast the equilibrium state is approached.

Project File and License Information

- Folder: **Process Metallurgy**
- File name: `PMET_06_Ladle_Furnace_Kinetics.tcu`

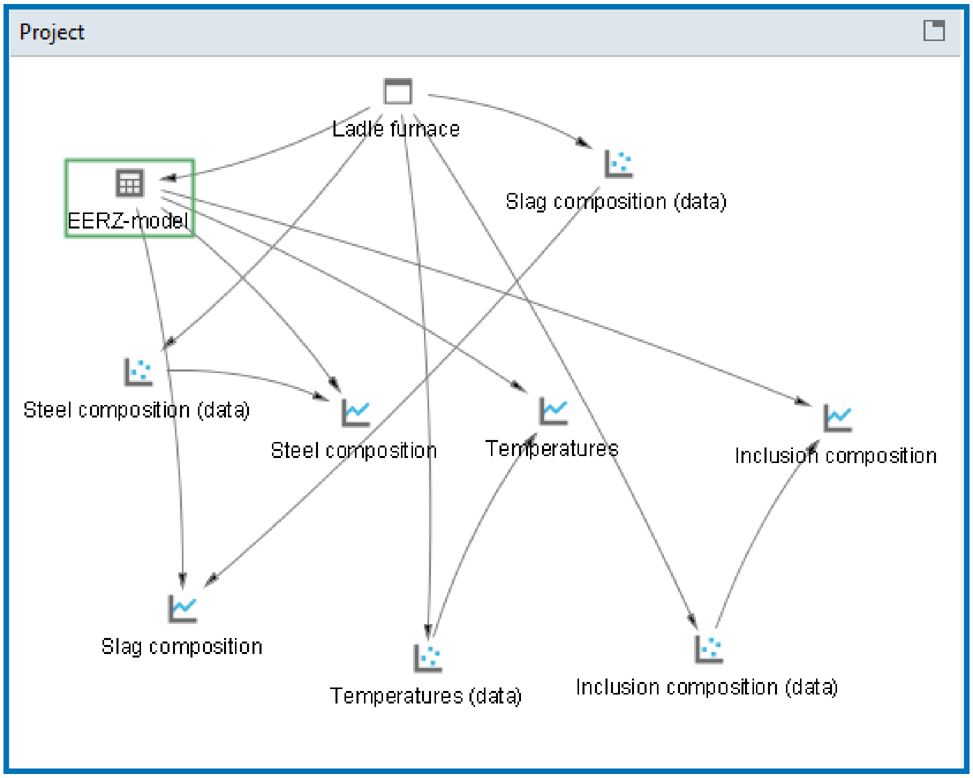
This example requires the database TCOX10 or newer, a full license of Thermo-Calc 2020b or newer, plus a license for the Process Metallurgy Module.

Visualizations

This example is included as a Process Metallurgy tutorial on our website and as part of the playlist our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

The resulting plots and details related to setting up this example are available to download via the dedicated web page.



The nodes in the Project window for this example. The Process Metallurgy Calculator is renamed to EERZ model. If you click this node the Configuration window opens, which is where all the settings for the process simulation are located. This advanced example also uses three Experimental Data Reader nodes to read the experimental data that is included in the simulation results. After setting up the system and accessing the experimental data, you then add Plot Renderers to the calculator to generate the output in the Visualizations window.

PMET_07: Vacuum Oxygen Decarburization Kinetics

The vacuum oxygen decarburization (VOD) process is used to lower the carbon content in a stainless steel without compromising on the Cr yield.

This application example, which is available on our websiteand uses the **Process Metallurgy Calculator**, shows how the Process Metallurgy Module in Thermo-Calc can be used to simulate the Vacuum Oxygen Decarburization (VOD) process for a stainless steel.

In this example, based on data of a real vacuum oxygen decarburization (VOD) process published by Ding et al. [2000Din], we show how to set up the VOD process in Thermo-Calc's Process Metallurgy Module. Use of the following features in the Process Metallurgy Module are highlighted in this example:

- Change of pressure as a function of time during the process
- Change of reaction kinetics as a function of time during the process
- Selection of zone where degassing is allowed

Project File and License Information

- Folder: **Process Metallurgy**
- File name: `PMET_07_Vacuum_Oxygen_Decarburization_Kinetics.tcu`

This example requires a license for Thermo-Calc 2024a or newer, the database TCOX13 or newer, and a license for the Process Metallurgy Module.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

The resulting plots and details related to setting up this example are available to download via the dedicated web page.

Reference

[2000Din] R. Ding, B. Blanpain, P. T. Jones, P. Wollants, Modeling of the vacuum oxygen decarburization refining process. Metall. Mater. Trans. B. 31, 197–206 (2000).

PMET_08: Steel Deoxidation on Tapping

This application example, which is available on our website and uses the **Process Metallurgy Calculator**, shows a few of the ways the Process Metallurgy Module in Thermo-Calc can be used to investigate steel deoxidation (killing) on tapping.

About Deoxidation or "Killing" of Steel

Deoxidation of steel, also known as killing of steel, occurs toward the end of the steelmaking process, but before desulphurization. After primary steelmaking, for example in a basic oxygen furnace (BOF) or electric arc furnace (EAF), the liquid steel contains a large amount of dissolved oxygen [O] (400 to over 1000 ppm.) (see PMET_04: Basic Oxygen Furnace (BOF) Kinetics).

This oxygen must be removed from the liquid steel for several reasons, including:

- Desulphurization is not effective with high oxygen content in the steel
- Continuous casting of un-killed steel is not possible and will result in "boiling" of the steel in the mould and massive porosity.

The two most widely applied methods of deoxidizing or killing the steel are adding Al to the steel (Al-killed steel) and adding Si to the steel (Si-killed steel). In this example we look at how the Process Metallurgy Module in Thermo-Calc can be used to investigate these two widely applied methods of deoxidizing or killing the steel.

The two most widely applied methods of deoxidizing or killing the steel are adding Al (Al-killed steel) to the steel and adding Si (Si-killed steel) to the steel. These elements readily react with oxygen to form oxides that precipitate within the liquid steel. This does not reduce the total amount of oxygen in the liquid steel; it simply transforms the dissolved oxygen into an oxide precipitate. This oxide precipitate then needs to be removed from the steel by flotation during secondary metallurgy in the ladle furnace (LF).

This, however, can result in the formation of damaging inclusions that cause problems during further processing, so we go on to look at two simple and very common processes that are used to transform the solid SiO_2 and Al_2O_3 inclusions into liquid oxides so that they are less damaging.

Project File and License Information

- Folder: **Process Metallurgy**
- File name: `PMET_08_Steel_Deoxidation_on_Tapping.tcu`

Choose a or b versions of the example based on your license.

- `PMET_08a_Steel_Deoxidation_on_Tapping.tcu` is included in a regular Thermo-Calc installation as well as the free Educational version of Thermo-Calc. It is a simplified version that uses the OXDEMO database.
- `PMET_08b_Steel_Deoxidation_on_Tapping.tcu` requires a full license of Thermo-Calc version 2021b or newer and database TCOX11 or newer.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

The resulting plots and details related to setting up this example are available to download via the dedicated web page.

Nickel Model Library Examples Collection

The **General Models**are available to all users. To run calculations with the **Nickel Models** (as part of the Nickel Model Library) requires a valid maintenance license plus licenses for both the TCNI (version 11 and newer) and MOBNI (version 5 and newer) databases.

These examples use the **Property Model Calculator**, an activity available with Thermo-Calc plus the available Property Models in the Nickel Model Library.

About the Examples

In this section:

PM_Ni_01: Lattice Parameter of γ/γ'

The example uses the **Property Model Calculator** with the **Equilibrium with Freeze-in Temperature - Ni** Model.

Property Model Calculator and About the Equilibrium with Freeze-in Temperature Nickel Property Model

The lattice parameters are measured experimentally for γ/γ' in a Ni0.6Mo0.92Ta12.5Al1.83Ti10.5Cr3.3W alloy.

The thermodynamically stable equilibrium will not be reached for this alloy during the experimental heat treatment; only the phases γ and γ' are noticed in the experiment. The γ/γ' microstructure is in this calculation example assumed to freeze-in at 1000 °C where the phase compositions do not change during cooling to room temperature.

Some of the key settings to note in this example:

- The **Subset of phases** is selected as **Gamma and gamma-prime only** to match the experimental observations.
- The **Freeze-in temperature** is set to 1000 °C.
- A **One Axis** calculation is used where the evaluation temperatures are within a range of 20 °C to 1000 °C.

Project File and License Information

- Folder: **Property Models → Nickel**
- File name: `PM_Ni_01_Lattice_Parameter_of_Gamma_Gamma_Prime.tcu`

To run calculations with the **Nickel Models** requires a valid maintenance license plus licenses for both the TCNI (version 11 and newer) and MOBNI (version 5 and newer) databases. For some Property Models, additional recommendations for the database version to use is indicated in its description. Also see our website to learn more about the Nickel Model Library.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

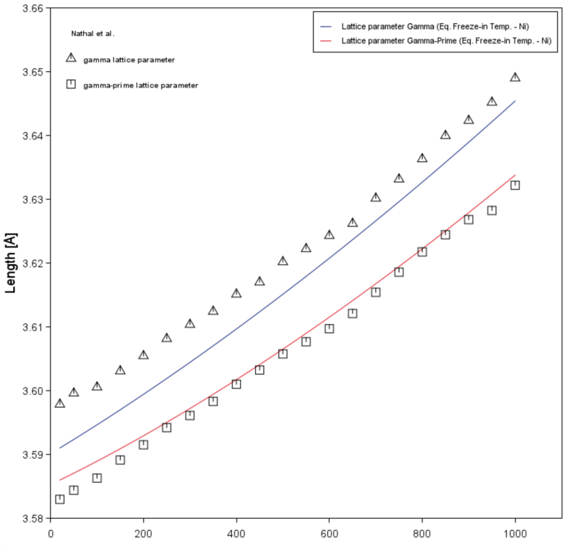


Figure 232: The lattice parameters for γ and γ' are plotted against experimental data from [1985Nat].

Reference

[1985Nat] M. V. Nathal, R. A. Mackay, R. G. Garlick, Temperature dependence of γ-γ’ lattice mismatch in Nickel-base superalloys. Mater. Sci. Eng. 75, 195–205 (1985).

PM_Ni_02: Antiphase Boundary Energy of γ'

The example uses the **Property Model Calculator** with the **Antiphase Boundary Energy - Ni** Model.

Property Model Calculator and About the Antiphase Boundary Energy Property Model

This example shows a calculation of the antiphase boundary energy for an Al75Ni alloy at room temperature with increasing amounts of Ti. The plot shows the (111) APB energy in $Ni_3Al_{1-x}Ti_x$ over the whole compositional range together with first-principle calculations from Chandran and Sondhi [2011Cha] and Vamsi and Karthikeyani [2012Vam] evaluated at 0 K. The trend with increasing 111 APBE with an increasing amount of Ti is predicted by all calculations but the absolute values between the first principle calculations are quite different.

Some of the key settings to note in this example:

- γ' is the only stable phase for these compositions. FCC_L12 is therefore selected as the only phase in the System Definer.
- The **Freeze-in temperature** and evaluation temperature are both set at 20 °C with the **Subset of phases** for **All phases**.
- A **One Axis** calculation is used with **Mole percent Ti** between 0 and 25 in 20 steps.
- The plotting quantity **APBE for 111 plane (1/2)** is then compared with the first principle calculations.

Project File and License Information

- Folder: **Property Models → Nickel**
- File name: `PM_Ni_02_Antiphase_Boundary_Energy_of_Gamma_Prime.tcu`

To run calculations with the **Nickel Models** requires a valid maintenance license plus licenses for both the TCNI (version 11 and newer) and MOBNI (version 5 and newer) databases. For some Property Models, additional recommendations for the database version to use is indicated in its description. Also see our website to learn more about the Nickel Model Library.

Visualizations

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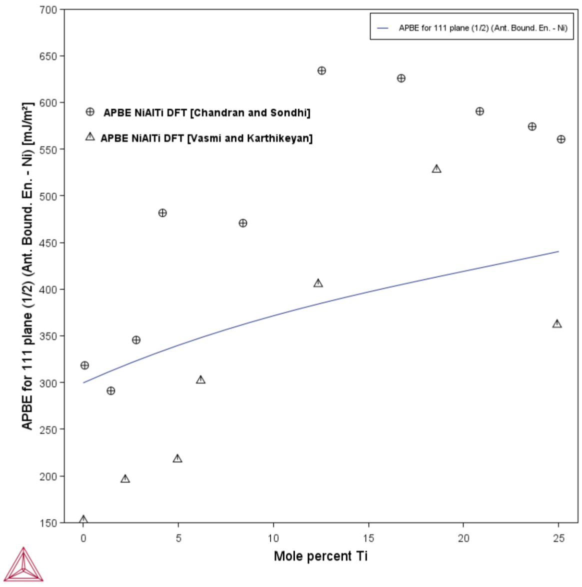

Figure 233: Composition of Ti (mole %) compared to antiphase boundary surface energy for 111 plane and experimental data from [2011Cha; 2012Vam].

References

[2011Cha] M. Chandran, S. K. Sondhi, First-principle calculation of APB energy in Ni-based binary and ternary alloys. Model. Simul. Mater. Sci. Eng. 19, 025008 (2011).

[2012Vam] K. V. Vamsi, S. Karthikeyan, Effect of Off-Stoichiometry and Ternary Additions on Planar Fault Energies in Ni3Al, in Superalloys 2012 (John Wiley & Sons, Inc., Hoboken, NJ, USA, 2012; pp. 521–530.

PM_Ni_03: Critical Temperatures of Alloy 718

The example uses the **Property Model Calculator** with the **Solvus for Ordered Phase-Ni** Model.

Property Model Calculator and About the Solvus for Ordered Phase Property Model

In this example, the respective solvus temperatures of the Delta and Gamma double-prime phases are calculated.

For the Delta phase, the **Subset of phases** is set to **All phases** but the result varies very little with the selected subset (provided that the Delta phase is included). For the Gamma double-prime phase, which is a metastable phase, it is necessary to use the **Typical Ni-base superalloy** phase subset.

The resulting solvus temperatures are compared with experimental data from [2010Fra].

Project File and License Information

- Folder: **Property Models → Nickel**
- File name: `PM_Ni_03_Critical_Temperatures_Alloy_718.tcu`

To run calculations with the **Nickel Models** requires a valid maintenance license plus licenses for both the TCNI (version 11 and newer) and MOBNI (version 5 and newer) databases. For some Property Models, additional recommendations for the database version to use is indicated in its description. Also see our website to learn more about the Nickel Model Library.

Visualizations

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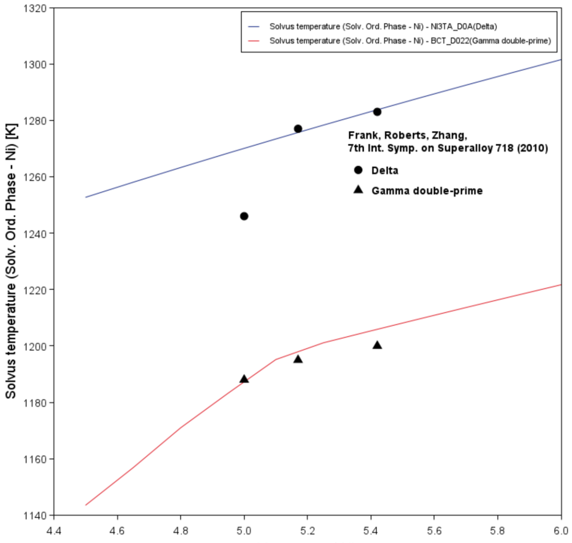

Figure 234: Solvus temperatures for NI3TA_D0A (Delta) and BCT_D022 (Gamma double-prime) compared to experimental data [2010Fra].

Reference

[2010Fra] R. B. Frank, C. G. Roberts, J. Zhang, Effect of Nickel Content on Delta Solvus Temperature and Mechanical Properties of Alloy 718, in 7th International Symposium on Superalloy 718 and Derivatives (2010) (TMS (The Minerals, Metals & Materials Society), 2010, pp. 725–736.

PM_Ni_04: Strain Age Cracking (SAC)

The example uses the **Property Model Calculator** with the **Strain-Age Cracking - Ni** Model.

For additional information, see About the Strain-Age Cracking Property Model.

Welding or additive manufacturing (AM) of Ni-base alloys has so far been strongly limited by various cracking issues during processing or post-processing. Strain-age cracking (SAC) occurs when the combination of thermal stresses and coherency stresses between the γ matrix and γ′ precipitates exceed the local strength of the alloy structure. Thermal residual stresses originate from the initial processing (welding or AM), while coherency stresses form during post-processing heat treatments, when γ′ re-precipitates in the matrix. Coherency stresses may be tensile or compressive depending on the sign of the lattice misfit.

Furthermore, coherency stresses scale with the fraction of γ′, making conventional high-γ′ alloys virtually impossible to weld or shape via AM. At the same time, high-γ′ fraction alloys offer attractive properties, such as high strength at high service temperatures. In order for such alloys to be processable, it is necessary to reduce the cracking tendency.

Thermal stresses are very difficult to alleviate, as this requires heating, which in turn triggers re-precipitation of γ′. Therefore, an alternative strategy may be to target the coherency stresses, which are determined by the respective lattice parameters of the matrix and precipitate. Such a strategy was adopted by Zhou et al. [2020Zho], where they optimized the composition of the Ni-base alloy to fulfill the above criteria, i.e., high fraction of γ′ and no strain-age cracking tendency.

In this example, the experimental alloys from [2020Zho] are analyzed based on the **Strain-Age Cracking - Ni** Property Model to compare the tendency for cracking using an SAC risk factor.

Project File and License Information

- Folder: **Property Models → Nickel**
- File name: `PM_Ni_04_Strain_Age_Cracking.tcu`

To run calculations with the **Nickel Models** requires a valid maintenance license plus licenses for both the TCNI (version 11 and newer) and MOBNI (version 5 and newer) databases. For some Property Models, additional recommendations for the database version to use is indicated in its description. Also see our website to learn more about the Nickel Model Library.

This example uses TCNI12, but in general can be run with version 11 (TCNI11) and newer databases.

Visualizations

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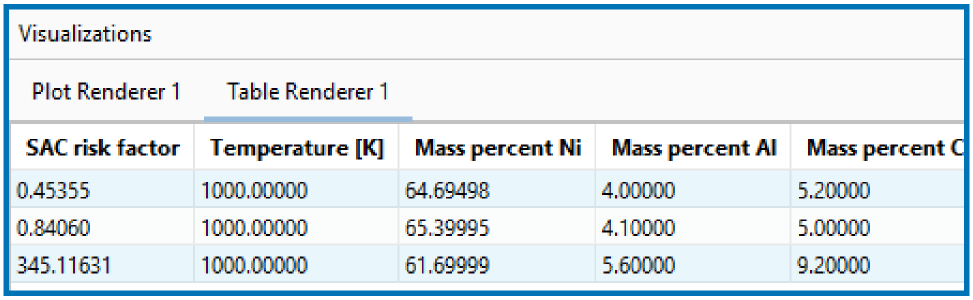
Performing the calculation for the two experimental alloys, along with the CM247LC benchmark alloy and using the temperature interval setting produces a set of relevant output results as shown in a table (Figure 235) and **Parallel coordinates** plot (Figure 236). CM247LC is considered to be very difficult to weld, which is evidenced by the very high value of the SAC risk factor. Comparatively, the two experimental alloys, ExpAM and ExpAMmod, show values very close to zero. Low or negative values of the SAC risk factor can be interpreted as low or no risk for strain-age cracking.

Conventionally, the *weldability* of a given Ni-base alloy has been assessed based on the Ti and Al contents, which correlate with the fraction of γ’. However, such an approach neglects the fact that it is the coherency stresses that cause cracking, and these are also dependent on the lattice misfit. By tailoring an alloy to have low misfit, in relation to the γ’ fraction and in the relevant temperature range, it is possible to design a high-γ’ fraction alloy with very low risk for SAC, as shown in [2020Zho]. The SAC model used here captures all of these effects and can be used as a design tool for the purpose of eliminating this cracking tendency.



SAC risk factor	Temperature [K]	Mass percent Ni	Mass percent Al	Mass percent C
0.45355	1000.00000	64.69498	4.00000	5.20000
0.84060	1000.00000	65.39995	4.10000	5.00000
345.11631	1000.00000	61.69999	5.60000	9.20000

Figure 235: There are a two ways to view the data in table format. In this example, there is a Table Renderer node added to the Project window that lists the data points in the Visualizations window.

> You can also access the same information via the Plot Renderer Configuration window by clicking the **Table View** button followed by clicking **Perform**. This converts the **Parallel coordinates** plot type to the same table of information.

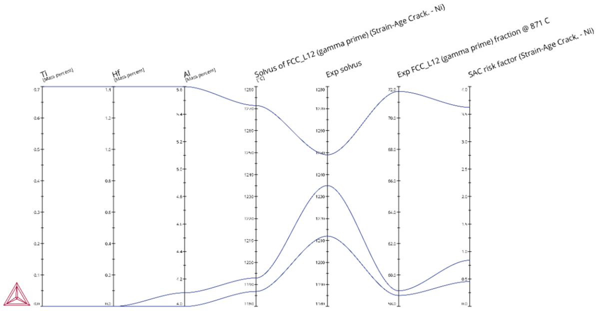


Figure 236: Parallel plot of the resulting SAC risk factor along with experimental and calculated solvus of γ’ for the three alloys compared in [2020Zho].

Plot Type: Parallel Coordinates

Reference

[2020Zho] N. Zhou, A. D. Dicus, S. A. J. Forsik, T. Wang, G. A. Colombo, M. E. Epler, Development of a New Alumina-Forming Crack-Resistant High-γ’ Fraction Ni-Base Superalloy for Additive Manufacturing, in Superalloys 2020, pp. 1046–1054.

Noble Metal Alloys Model Library Examples Collection

These examples use the **Property Model Calculator**, an activity available with Thermo-Calc plus the available Property Models in the Noble Metal Alloys Model Library.

The **General Models**are available to all users. To run calculations with the **Noble Metal Alloys Models** (as part of the Noble Metal Alloys Model Library) requires a valid maintenance license plus a license for the TCNOBL (version 3 and newer) database.

About the Examples

In this section:

PM_Noble_01: Color Prediction

The **Optical Properties - Noble** Property Model, available with the Property Model Calculator and the Noble Metal Alloys Model Library, is used to simulate the color, reflection, and transmission of light, based on modeling the alloy microstructure and the resulting optical properties. This model is currently applicable for the Au-Al-Ag-Cu-Pt system.

> For more information about the Property Model, see About the Optical Properties - Noble Metals Property Model and Optical Properties - Noble Metals Property Model Settings.

This example uses the **Property Model Calculator** with the **Optical Properties - Noble** Property Model.

The example demonstrates three use cases for simulating color in the Ag-Au-Cu alloy system (1) screening the color of the alloy system (2) designing a green-gold alloy by adjusting Ag content, and (3) visualizing the impact of alloy thickness and light incident angle on color.

Project File and License Information

- Folder: **Property Models → Noble Metals**
- File name: `PM_Noble_01_Color_Prediction.tcu`

> To run calculations with the **Noble Metal Alloys Models** (as part of the Noble Metal Alloys Model Library) requires a valid maintenance license plus a license for the TCNOBL (version 3 and newer) database.

Visualizations

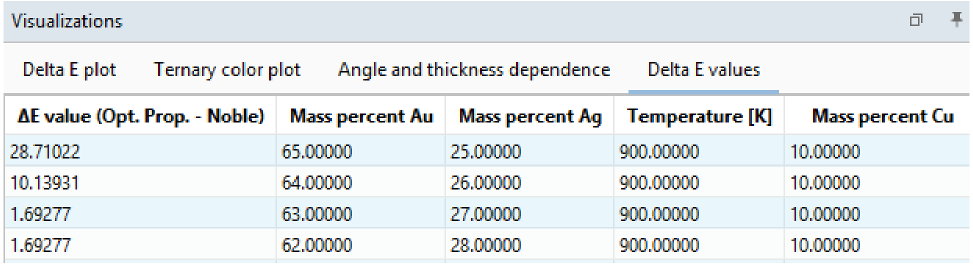
Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

⌛ When you run (Perform) this example, it takes a few minutes for the calculations to complete.

Screening the Color of the Ag-Au-Cu Alloy System

- The entire composition space was screened with a 2 wt.% step size.
- Alloys were annealed at 873.15 K to reach equilibrium phases and compositions for accurate color prediction.
- The standard illuminant is D65 noon daylight, with a 2˚standard observer. The material is assumed to be opaque with a thickness of 10,000 nm.
- Some color predictions near the 20–40 wt.% Cu region require model accuracy improvements.



ΔE value (Opt. Prop. - Noble)	Mass percent Au	Mass percent Ag	Temperature [K]	Mass percent Cu
28.71022	65.00000	25.00000	900.00000	10.00000
10.13931	64.00000	26.00000	900.00000	10.00000
1.69277	63.00000	27.00000	900.00000	10.00000
1.69277	62.00000	28.00000	900.00000	10.00000

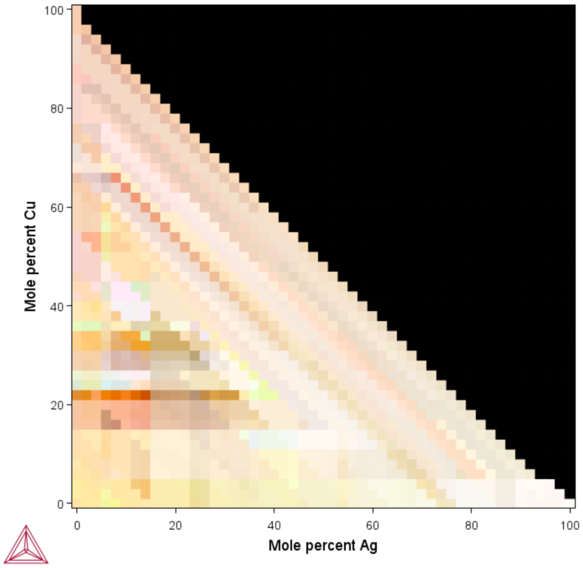


Figure 1: Color prediction for Ag-Au-Cu alloy.

Designing a Green Gold Alloy by Adjusting Ag Content in Au-10Cu-xAg Alloys

- ΔE calculation box was chosen to enable the measurement of color differences.
- Target color in Lab color space is [95, -13, 25], representing a light green shade.

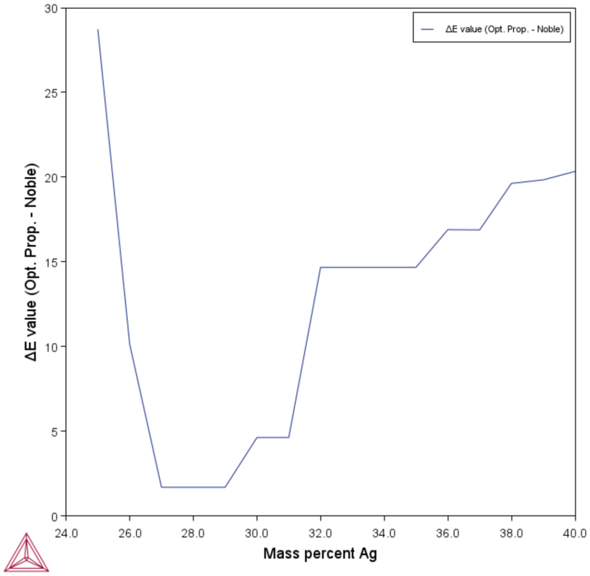


Figure 2: Change of color difference (ΔE) between the targeting light green gold and the simulated alloy when changing Ag content.

Visualizing the Impact of Alloy Thickness and Light Incident Angle on Color

- Intercritical annealing was not selected, as pure gold is in the FCC phase and does not require equilibrium calculations.
- As material thickness increases, the color of gold tends to approach the bulk gold color observed in macroscopic samples.

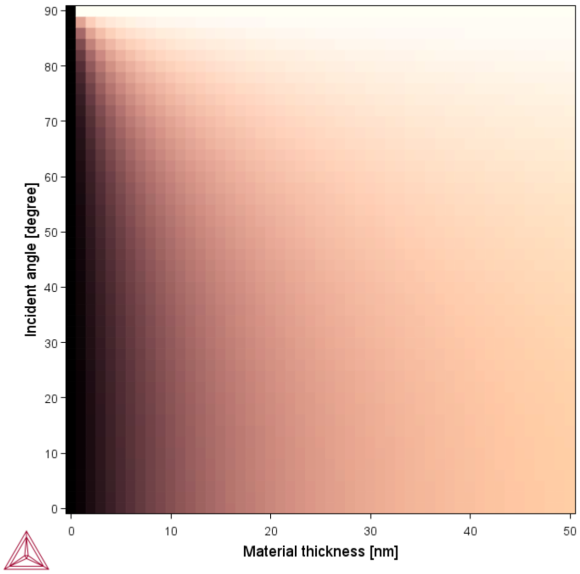


Figure 3: Color of pure gold varies with different light incident angles and material thicknesses.

Steel Model Library Examples Collection

The **General Models**are available to all users. To run calculations with the **Steel Models** (as part of the Steel Model Library) requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases.

These examples use the **Property Model Calculator**, an activity available with Thermo-Calc plus Property Models in the Steel Model Library.

About the Examples

In this section:

PM_Fe_01: Fe-Cr-C Martensite with Intercritical Annealing

The example uses the **Property Model Calculator** with the **Martensite Fractions** and **Martensite Temperatures** Models to calculate martensite fractions and martensite temperatures [martensite start (Ms) and 90% transformation temperature (M90)].

The alloy is first intercritically annealed and then quenched. Austenite composition is determined by an equilibrium calculation at the annealing temperature. Martensite fraction is calculated as a function of temperature which the alloy is quenched to. The example also shows how Cr content in the alloy influences Ms and M90 after intercritical annealing.

Property Model Calculator, About the Martensite Temperatures Property Model, and About the Martensite Fractions Property Model

Project File and License Information

- Folder: **Property Models → Steel**
- File name: `PM_Fe_01_Fe-Cr-C_martensite_intercritical_annealing.tcu`

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Visualizations

This example is included as a Property Model tutorial on our website and as part of the Property Model Calculator playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

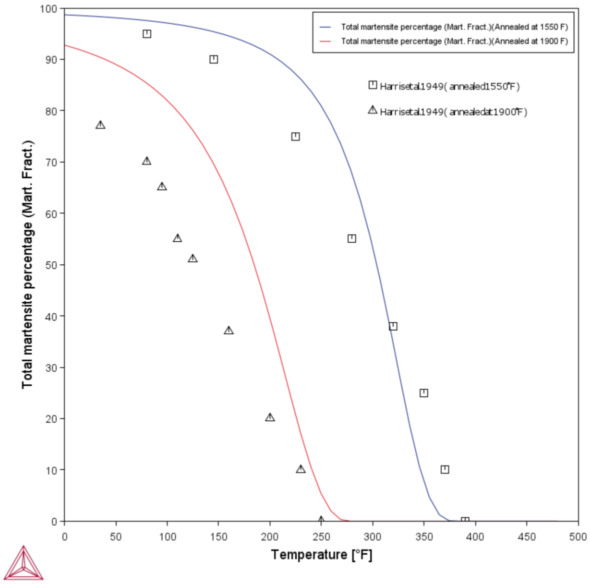


Figure 4: The transformation curves plot showing Fe-Cr-C martensite with intercritical annealing.

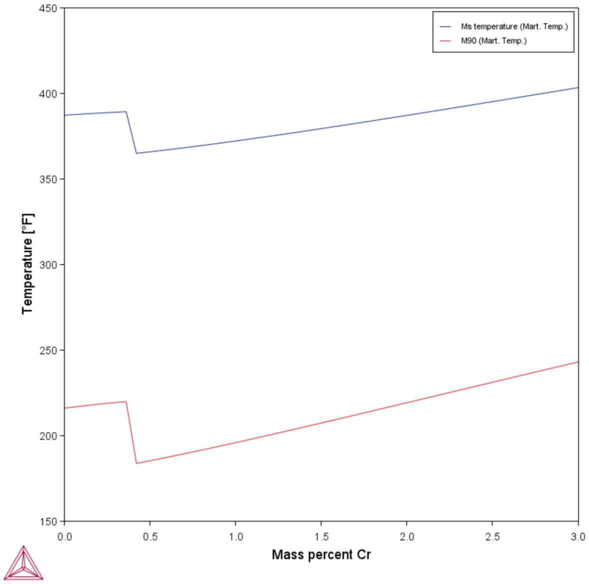


Figure 5: Comparing Martensite start (Ms) to Martensite finish (Mf).

Reference

[1949Har] W. J. Harris, M. Cohen, Stabilization Of The Austenite-Martensite Transformation. Trans. AIME. 180, 447–470 (1949).

PM_Fe_02: Fe-Mn Martensite Morphologies

The example uses the **Property Model Calculator** with the **Martensite Temperatures** Property Model to calculate the Ms temperatures of different types of martensites: lath, plate, and ε (HCP), compared with experimental ε Ms values taken from several sources.

Property Model Calculator and About the Martensite Temperatures Property Model

Project File and License Information

- Folder: **Property Models → Steel**
- File name: `PM_Fe_02_Fe-Mn_Martensite_Morphologies.tcu`

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Visualizations

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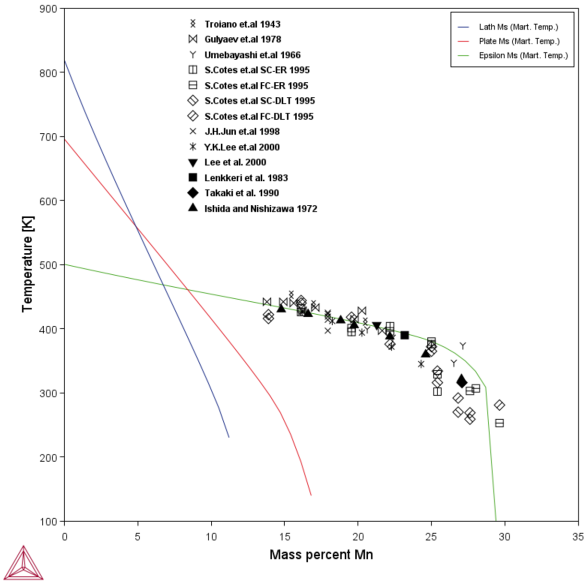

Figure 6: A diagram showing all the Ms temperatures of different types of martensite morphologies (lath, plate and epsilon (HCP) compared with experimental epsilon Ms values.

PM_Fe_03: Fe-C-Mn Pearlite

The example uses the **Property Model Calculator** and with the **Pearlite** Property Model and shows how to calculate pearlite growth rate, lamellar spacing, and times of start (2% transformation) and finish (98% transformation) as functions of isothermal heat treating temperature in an Fe-0.69C-1.80Mn alloy (mass %). With *maximize growth rate* set as the *criterion*, the model gives maximal growth rate and minimal lamellar spacing. With *optimal pearlite* as the *pearlite mode*, the model optimizes partitioning of substitutional alloying element(s) (Mn in this example) according to the criterion, which realizes a smooth transition between ortho-pearlite at high temperature and para-pearlite at low temperature.

Property Model Calculator and About the Pearlite Property Model

Project File and License Information

- Folder: **Property Models → Steel**
- File name: `PM_Fe_03_Fe-C-Mn_Pearlite.tcu`

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

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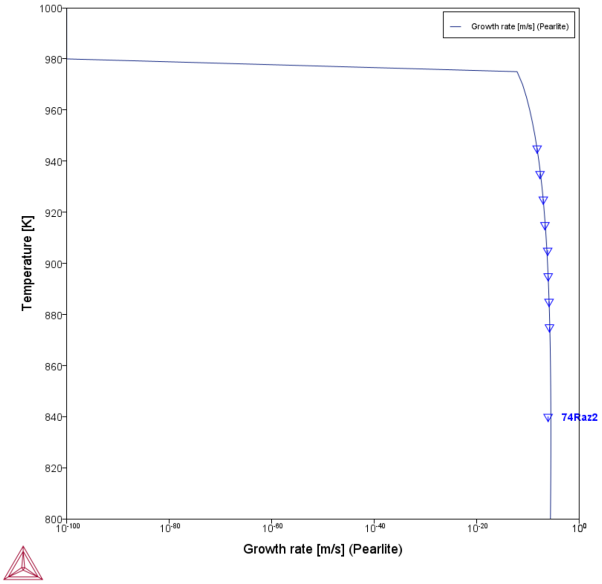

Figure 7: Growth rate as a function of temperature.

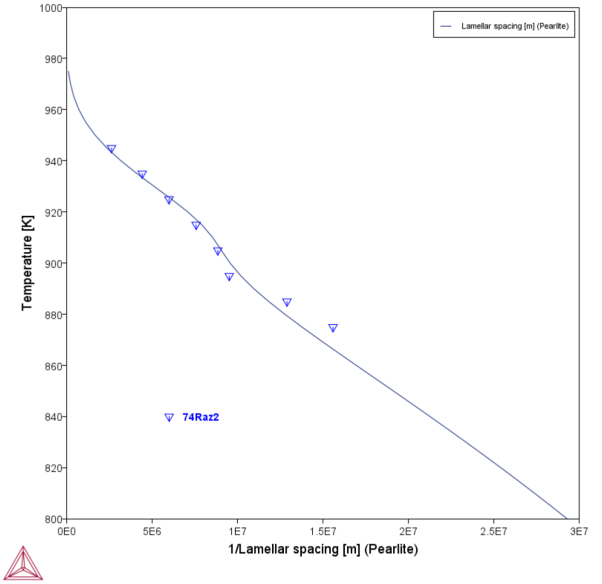

Figure 8: Lamellar spacing as a function of temperature.

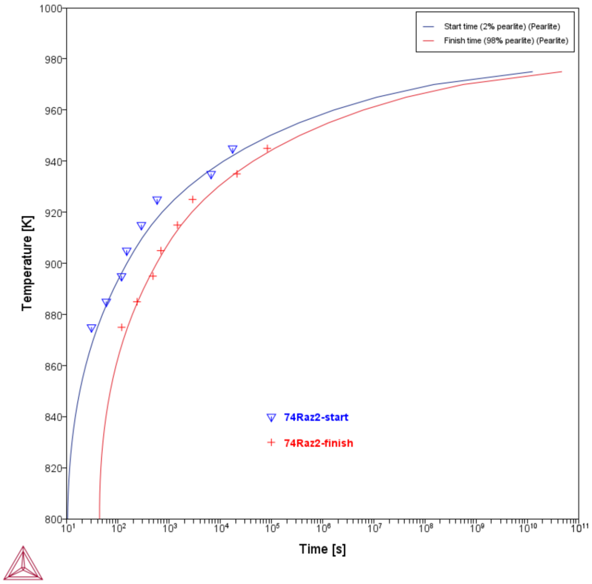

Figure 9: The TTT (time-temperature-transformation) diagram showing times of start (2% transformation) and finish (98% transformation) as functions of isothermal heat treating temperature in an Fe-0.69C-1.80Mn alloy (mass %).

Reference

[1974Raz] N. Razik, G. Lorimer, N. Ridlley, An investigation of manganese partitioning during the austenite-pearlite transformation using analytical electron microscopy. Acta Metall. 22, 1249–1258 (1974).

PM_Fe_04: Critical Temperatures

The example uses the **Property Model Calculator** and the **Critical Transformation Temperatures** Model to calculate the distribution of the typical phase transition temperatures for a low alloy steel (Fe-0.3Cr-1.0Mn-0.3Mn-0.18C) when the composition is varied within the specification for the alloy.

In the set up of the example, the **Critical Transformation Temperatures** model is used with a Property Model Calculator **Uncertainty** calculation to plot a histogram showing the distribution of A1- and A3-temperatures (Figure 10). As a comparison, an Equilibrium Calculator, **One Axis** calculation results in a property diagram showing the phase transitions for the nominal composition (Figure 11).

The phase transition temperatures are defined as:

- Liquidus: First austenite or ferrite transformation from the liquid
- Solidus: Liquid fully transformed to solid
- A0: Magnetic transition temperature (Curie temperature) of cementite. The cementite is paramagnetic above A0 and ferromagnetic below
- A1: Austenite (FCC_A1) transforms to ferrite (BCC_A2) + carbide (cementite or graphite or M23C6)
- A2: Magnetic transition temperature (Curie temperature) of ferrite (BCC_A2). Paramagnetic above A2 and ferromagnetic below
- A3: Austenite (FCC_A1) transforms to ferrite (BCC_A2)

Property Model Calculator and About the Critical Transformation Temperatures Property Model

Project File and License Information

- Folder: **Property Models → Steel**
- File name: `PM_Fe_04_Critical_Temperatures.tcu`

The **FEDEMO: Iron Demo Database** is used and this example is available to all users. However, in general a license is required to run the Steel Models.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

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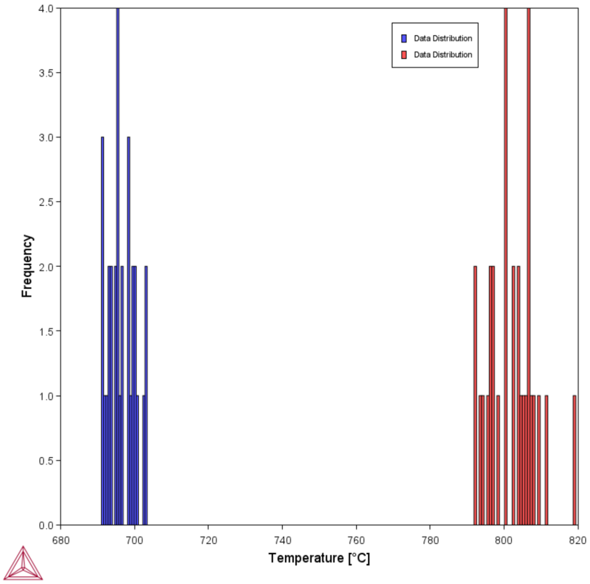

Figure 10: The distribution of the A1 and A3 phase transition temperatures for a low alloyed steel (Fe-0.3Cr-1.0Mn-0.3Mn-0.18C) when the composition is varied within the specification. This plot uses the Critical Transformation Temperatures model with the Property Model Calculator.

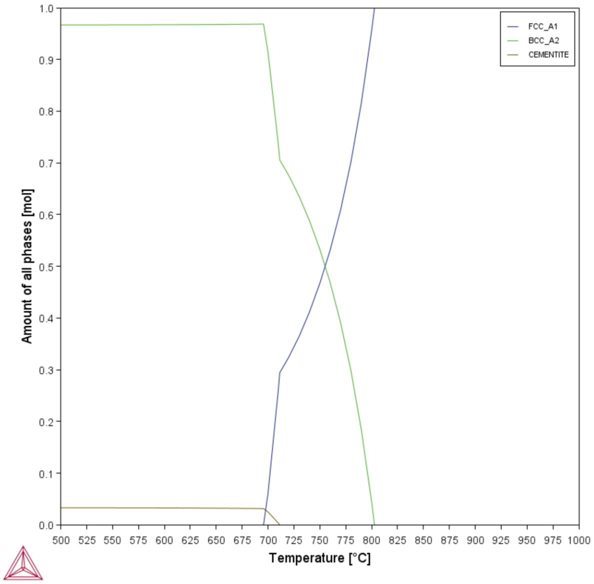

Figure 11: This plot uses an Equilibrium Calculator to show an alternate visualization of the phase transitions in a property diagram for the nominal composition.

PM_Fe_05: Fe-C-Mn-Si-Ni-Cr-Mo Bainite

The example uses the **Property Model Calculator** and the **Bainite** Steel Model to calculate a Time-Temperature-Transformation (TTT) diagram for an Fe-0.97C-0.72Mn-0.32Si-1.54Ni-0.8Cr-0.26Mo alloy. The result is compared to experimental results from [1948Jaf]. Other elements with low amount in the experimental alloy are omitted for the calculation.

Considered elements: Fe, C, Mn, Si, Cr, Ni, and Mo. Other elements in the system are neglected for bainite by mass percent.

A Property Model Calculator is used with a *One Axis* calculation and the *TTT mode* selected on the Plot Renderer to plot the TTT diagram.

For more information see About the Bainite Property Model, Plot Type: TTT Mode, and Plot Types.

Project File and License Information

- Folder: **Property Models → Steel**
- File name: `PM_Fe_05_Fe-C-Mn-Si-Ni-Cr-Mo_Bainite.tcu`

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

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⌛ When you run (Perform) this example, it takes a few minutes for the calculations to complete.

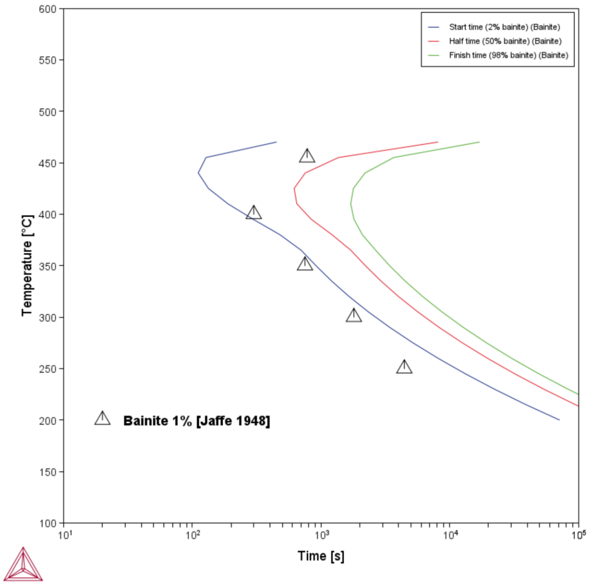

Figure 12: The bainite TTT diagram for an Fe-0.97C-0.72Mn-0.32Si-1.54Ni-0.8Cr-0.26Mo alloy.

Reference

[1948Jaf] L. D. Jaffe, Anisothermal formation of bainite and proeutectoid constituents in steels, Trans. AIME, vol. 176, pp. 343–383 (1948).

PM_Fe_06: TTT Diagram for Fe-C-Mn-Si-Cr-V

The example uses the **Property Model Calculator** and the **TTT Diagram** Property Model to calculate a Time-Temperature-Transformation (TTT) diagram for an Fe-C-Mn-Si-Cr-V alloy (Steel 42CrV6). The calculation is compared to an experimental TTT diagram for the same steel (with some other impurities) from data in [1958Wev].

A **One Axis** *Calculation Type* is selected on the Property Model Calculator and then the **TTT Mode** selected on the Plot Renderer as the *Plot type* in order to plot the final TTT diagram.

A second plot also shows the calculated terminal fractions of ferrite, pearlite, and bainite.

For more information see About the TTT Diagram Property Model, TTT Diagram Property Model Settings, and Plot Type: TTT Mode.

Project File and License Information

- Folder: **Property Models → Steel**
- File name: `PM_Fe_06_Fe-C-Mn-Si-Cr-V_TTT.tcu`

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

⌛ When you run (Perform) this example, it takes several hours to complete the calculations.

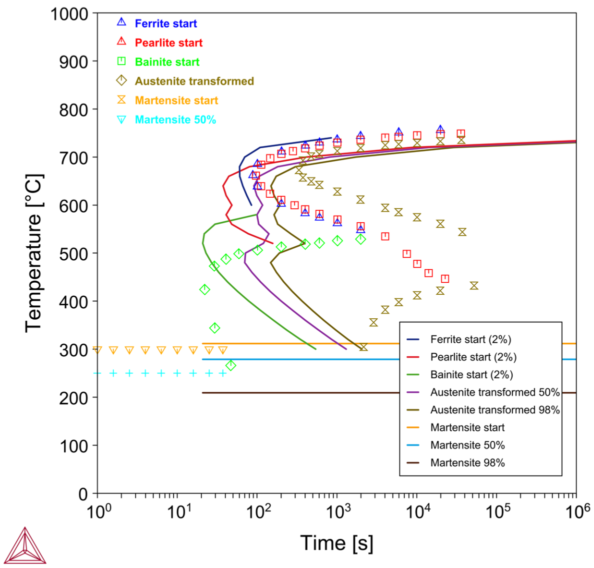

Figure 13: The TTT diagram for an Fe-C-Mn-Si-Cr-V alloy comparing the calculation with experimental data from [1958Wev].

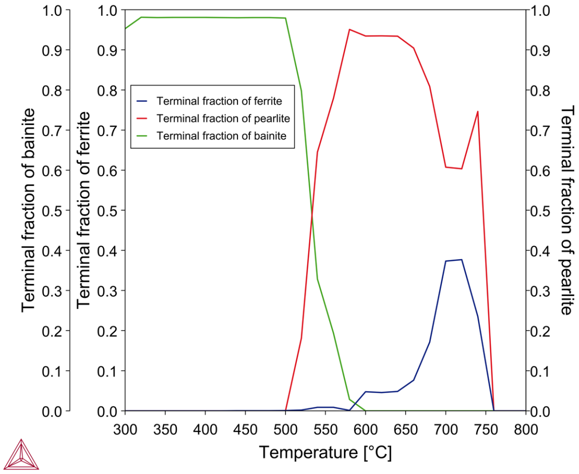

Figure 14: The terminal fractions quantities for bainite, ferrite, and pearlite are plotted against the cooling rate for the Fe-C-Mn-Si-Cr-V alloy.

Reference

[1958Wev] F. Wever, A. Rose, Atlas zur Wärmebehandlung der Stähle: 1954/56/58 (Verlag Stahleisen, Düsseldorf, 1958), p. II-112.

PM_Fe_07: Hardenability Design of Steel

This application example, which is available on our website, shows how the Steel Model Library in Thermo-Calc can be used to find the optimal compositions for an Fe-Mn-C steel to achieve high hardenability for the purpose of strength.

Hardenability of steel is an important aspect of steel design because it affects the ability of the steel to develop optimum strength and toughness. Hardenability refers to the ability of steel to form martensite on quenching. It is a measure of the capacity of a steel to be hardened in depth when quenched from its austenitizing temperature, meaning that the steel forms martensite not only at the surface of the steel, but throughout the interior. This is usually a prerequisite for the subsequent tempering treatment for an optimal combination of strength and toughness. Insufficient hardenability can make the tempering treatment ineffective and lead to low uniformity of mechanical properties in a steel component. The two most important factors that influence hardenability of steel are grain size and composition, and in this example, we will investigate composition.

Project File and License Information

- Folder: **Property Models → Steel**
- File name: `PM_Fe_07_Hardenability_Design_of_Steel.tcu`

Although this example uses the FEDEMO and MFEDEMO databases, running the calculation requires a license for Thermo-Calc 2022b or newer and for the Steel Model Library.

Visualizations

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

When you run (Perform) this example, it takes several hours to complete the calculations.

The resulting plots and details related to setting up this example are available to download via the dedicated web page.

PM_Fe_08: CCT Diagram for Fe-C-Mn-Si-Cr-V

The example uses the **Property Model Calculator** and the **CCT Diagram** Property Model to calculate a Continuous-Cooling-Transformation (CCT) diagram for an Fe-C-Mn-Si-Cr-V alloy (Steel 42CrV6). The calculation is compared to an experimental CCT diagram for the same steel (with some other impurities) from data in [1958Wev].

A **One Axis** *Calculation Type* is selected on the Property Model Calculator and then the **CCT Mode** selected as the *Plot type* on the Plot Renderer in order to plot the final CCT diagram.

A second plot also shows the calculated terminal fractions of ferrite, pearlite, bainite, and martensite.

For more information see About the CCT Diagram Property Model, CCT Diagram Property Model Settings, and Plot Type: CCT Mode.

Project File and License Information

- Folder: **Property Models → Steel**
- File name: `PM_Fe_08_Fe-C-Mn-Si-Cr-V_CCT.tcu`

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

When you run (Perform) this example, it takes several hours to complete the calculations.

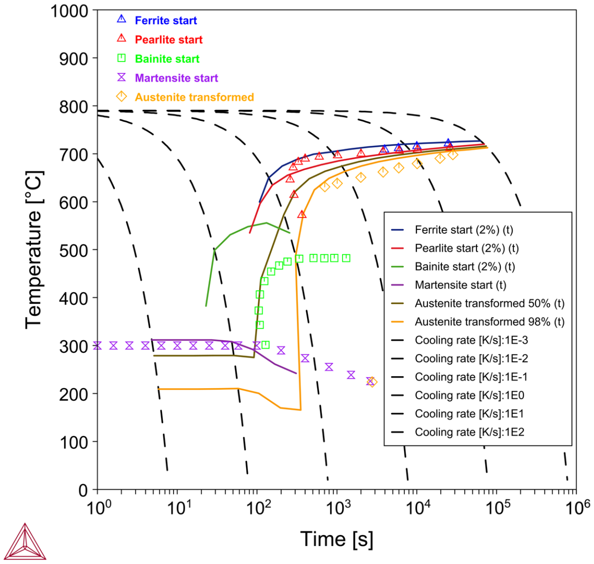

Figure 15: The CCT diagram for an Fe-C-Mn-Si-Cr-V alloy comparing the calculation with experimental data from [1958Wev].

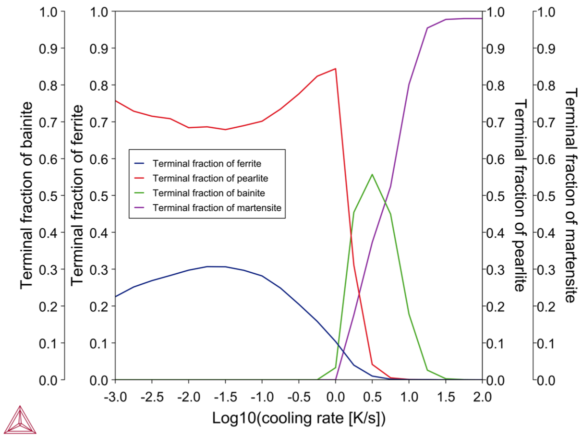

Figure 16: The terminal fractions quantities for bainite, ferrite, martensite, and pearlite are plotted against the cooling rate for the Fe-C-Mn-Si-Cr-V alloy.

Reference

[1958Wev] F. Wever, A. Rose, Atlas zur Wärmebehandlung der Stähle: 1954/56/58 (Verlag Stahleisen, Düsseldorf, 1958), p. II-112.

PM_Fe_09: Fe-C-Ni Ferrite

The example uses the **Property Model Calculator** and the **Ferrite** Property Model to calculate the ferrite fraction parabolic rate constant and ferrite start time for an Fe-0.12C-3.28Ni alloy.

Two growth modes—Orthoequilibrum (OE) and Paraequilibrium (PE)—are used with a *One Axis* calculation type to compare the ferrite molar fraction and to determine the ferrite start time for each growth mode.

The experimental data for the ferrite start is taken from [1966Aar]. For the parabolic rate constant experimental data is from [1981Bra].

> For more information about the Property Model, see About the Ferrite Property Model and Ferrite Property Model Settings.

Project File and License Information

- Folder: **Property Models → Steel**
- File name: `PM_Fe_09_Fe-C-Ni_Ferrite.tcu`

> To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

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⌛ When you run (Perform) this example, it takes a few minutes for the calculations to complete.

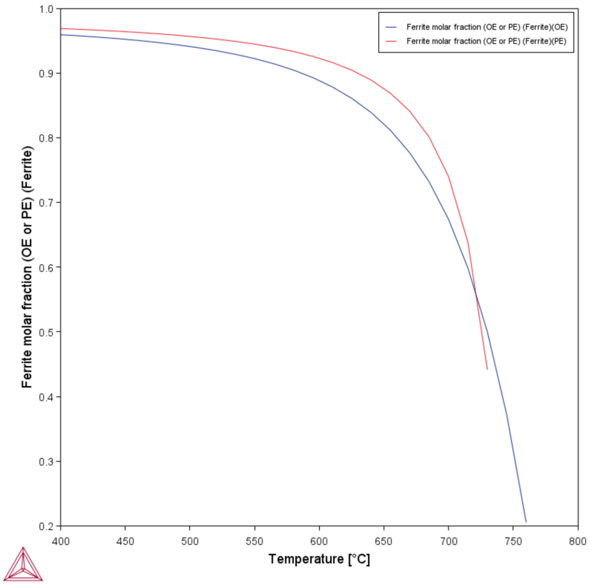

Figure 17: Ferrite fraction at the end of the transformation, under orthoequilibrium (OE) or paraequilibrium (PE).

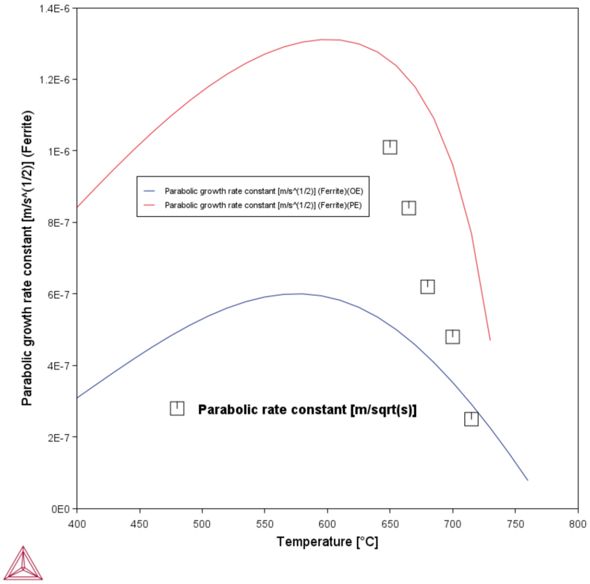

Figure 18: Parabolic rate constant. Experimental data is from [1981Bra].

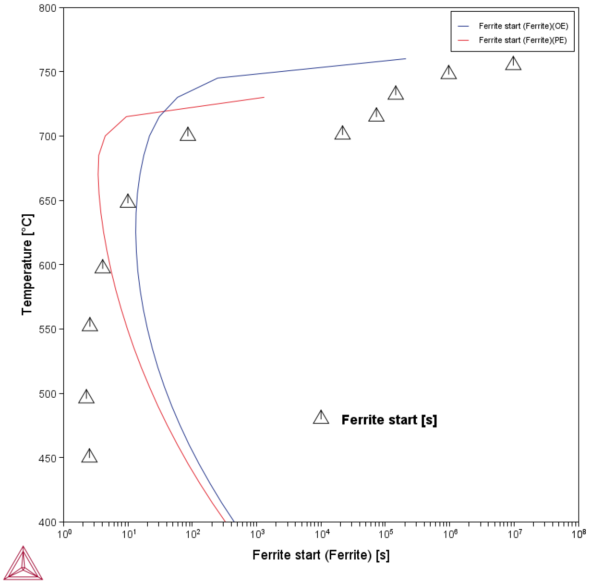

Figure 19: Ferrite start time. This plot also uses the TTT mode. Experimental data from [1966Aar].

References

[1966Aar] H. I. Aaronson, H. A. Domian, Partition of alloying elements between austenite and proeutectoid ferrite or bainite. AIME MET SOC TRANS. 236, 781–796 (1966).

[1981Bra] J. R. Bradley, H. I. Aaronson, Growth kinetics of grain boundary ferrite allotriomorphs in Fe-C-X alloys. Metall. Trans. A. 12, 1729–1741 (1981).

PM_Fe_10: Martensitic Steel Strength

The **Martensitic Steel Strength** Property Model, available with the Property Model Calculator and the Steel Model Library, is available to predict the general flow stress properties of martensitic steels, such as hardness, stress at arbitrary strain, yield strength, ultimate tensile strength, Young's modulus, etc.

In this example, data for AISI4068 from [1956Gra] are compared to calculations using the **Martensitic Steel Strength** model. In the set up, one **System Definer** and two **Experimental File Reader** activities are used along with four **Property Model Calculators**. The **Martensitic Steel Strength** Property Model is used in all cases with **One Axis** calculations to produce two plots that compare the tempering temperature and time to the total hardness of tempered steels.

For more information about the Property Model, see About the Martensitic Steel Strength Property Model and Martensitic Steel Strength Property Model Settings.

Project File and License Information

- Folder: **Property Models → Steel**
- File name: `PM_Fe_10_Martensitic_Steel_Strength.tcu`

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

This example uses TCFE13. Earlier versions of this database can be used although there may be slight differences in the results.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help →** **Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

For some Windows-based systems, performing the full calculation from the top **My Project** node can result in out of memory issues due to the number of calculators. If this happens, perform individual calculations for each Property Model Calculator (e.g. right-click the node and select **Perform Now**). This produces the full plots that are output to the Visualizations window.

When you run (Perform) this example, it takes a few minutes for the calculations to complete.

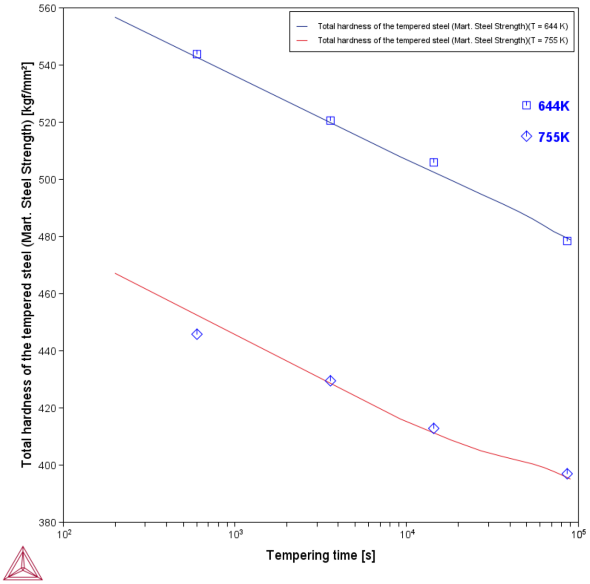

Figure 20: Total hardness of the tempered steel versus tempering time, for two tempering temperatures, compared to data from [1956Gra].

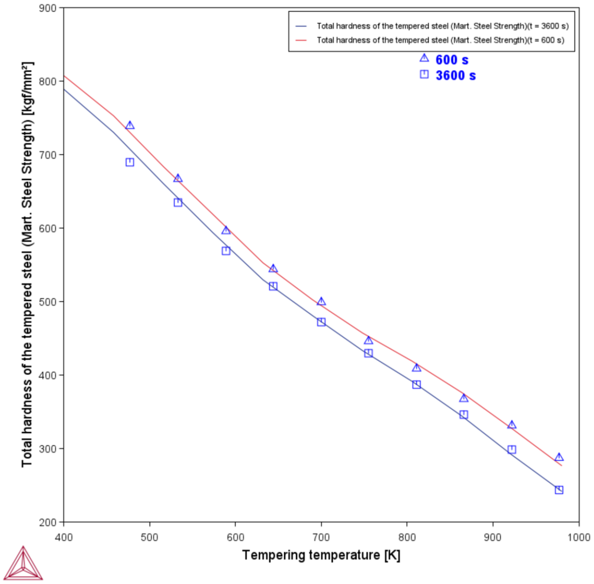

Figure 21: Total hardness of the tempered steel versus tempering temperature, for two tempering times, compared to handbook data from [1956Gra].

Reference

[1956Gra] R.A. Grange and R.W. Baughman. Hardness of tempered martensite in carbon and low alloy steels, Transactions of American Society for Metals, Vol. XLVIII, 165–197 (1956).

PM_Fe_11: Steel Design Using the Parallel Coordinates Plot

The example uses the **Property Model Calculator** and three Property Models to plot a property diagram and a **Parallel coordinates** plot for chemistries centered around an Fe1.5Cr2.0Ni0.31C1.0Mn alloy. The Ni, Cr, and C chemistries are varied to understand their influence on some key properties. This can be used to optimize a material chemistry to meet specific design criteria.

A **One Axis** calculation using the **Equilibrium Calculator** produces a property diagram to show the equilibrium fractions of the alloy.

A second calculation uses a **Grid** calculation with the Property Model Calculator and the **Driving Force**, **Martensite Temperatures**, and **Martensitic Steel Strength** models to demonstrate the use of the **Parallel coordinates** plot type. The driving force model in this example calculates the driving force for Cementite to form at 500 °C (tempering temperature). The driving force gives a good idea of how fine a dispersion of carbides could form. Higher driving force means a finer distribution.

When using a parallel coordinates plot type, you can interpret multidimensional data to compare how different parameters affect each other. In this example this includes the *composition of Ni, Cr, and C* (each in mass percent), the *Driving force per mole*, the *Total hardness of the tempered steel*, and the *Ms temperature*.

? Plot Type: Parallel Coordinates

Project File and License Information

- Folder: **Property Models → Steels**
- File name: `PM_Fe_11_Steel_Design_Using_Parallel_Plot.tcu`

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

This example uses TCFE13. Earlier versions of this database can be used although there may be slight differences in the results.

Visualizations

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Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

When you run (Perform) this example, it takes a few minutes for the calculations to complete.

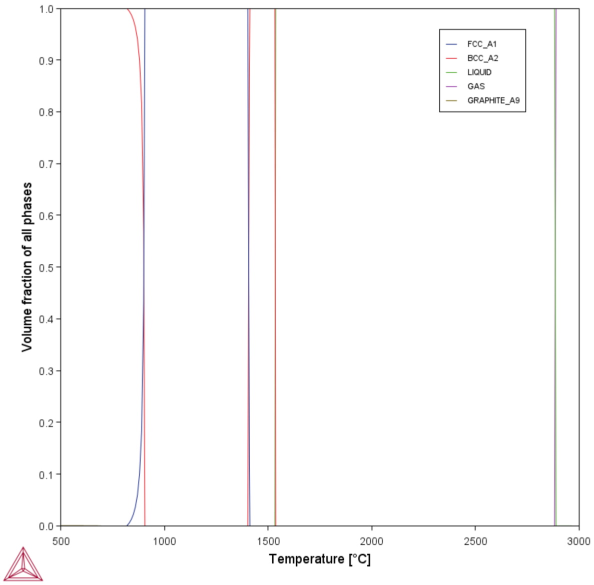

Figure 22: A Property Diagram to observe the change in volume fraction of all phases as the temperature increases.

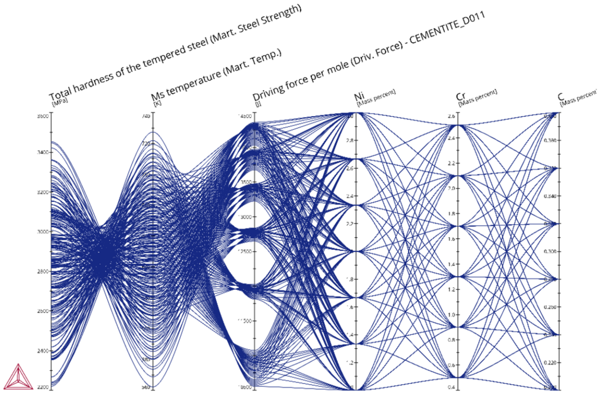

Figure 23: A parallel coordinates plot with multidimensional data comparing the Ni, Cr, and C compositions, the Driving force per mole, the Total hardness of the tempered steel, and the Ms temperature.

Tips to Interpret the Plot Data

- When most lines between two parallel axes are somewhat parallel to each other, there is a positive relationship between these two dimensions.
- When lines cross in a kind of superposition of X-shapes, that is a negative relationship.
- When lines cross randomly it means that there is no particular relationship.

PM_Fe_12: Flow Stress 15-5PH Steel

The example uses the **Property Model Calculator** and the **Martensitic Steel Strength** model to calculate the flow stress curves for a 15-5PH steel alloy, with samples tempered for 2, 5, and 50 hours. The example shows the use of flow stress with this Property Model.

An **Experimental File Reader** is used with data from Croné et al. [2022Cro]. Three Property Model Calculators are used with a **Flow stress mode** of **σ vs ϵ** and a **One Axis** calculation is used.

The **Tempering time** is set for each Property Model Calculator to 2 h, 5 h, and 50 h (the settings themselves are entered in seconds).

Read about the theory in Flow Stress.

Project File and License Information

- Folder: **Property Models → Steels**
- File name: `PM_Fe_12_Flow_Stress_15-5PH_Steel.tcu`

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

This example uses TCFE14. Earlier versions of this database can be used although there may be slight differences in the results.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

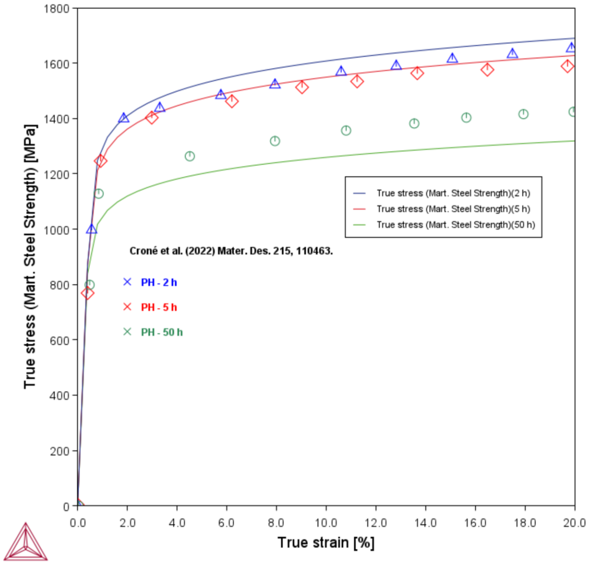

Figure 24: The calculation plots the True strain [%] to the True stress [MPa] as flow stress curves and compares it to experimental data taken from [2022Cro].

Reference

[2022Cro] P. Croné, T. Zhou, P. Hedström, J. Odqvist, P. Gudmundson, J. Faleskog, Continuum plasticity modelling of work hardening for precipitation-hardened martensitic steel guided by atom probe tomography. Mater. Des. 215, 110463 (2022).

Titanium Model Library Examples Collection

The **General Models**are available to all users. To run calculations with the **Titanium Models** (as part of the Titanium Model Library) requires a valid maintenance license plus a license for the TCTI (version 6 and newer) database.

These examples use the **Property Model Calculator**, an activity available with Thermo-Calc plus the available Property Models in the Titanium Model Library.

? About the Examples

In this section:

PM_Ti_01: Martensite Temperatures for Ti-Zr

The **Martensite Temperatures - Ti** Property Model, available with the Property Model Calculator and the Titanium Model Library, calculates the martensite start temperature (Ms) and T-Zero temperatures for Ti-base alloys.

> For more information about the Property Model, see About the Martensite Temperatures - Ti Property Model and Martensite Temperatures - Ti Property Model Settings.

This example uses the **Martensite Temperatures - Ti** Property Model with a simple Ti-Zr system to show the use of this model. A **One Axis** calculation is used to plot the Ms and T-Zero temperatures as a function of mole fraction of Zr with experimental data from [1952Du, 1965McM, and 1970Hua].

Project File and License Information

- Folder: **Property Models → Titanium**
- File name: `PM_Ti_01_Martensite_Temperatures_Ti-Zr.tcu`

> To run calculations with the **Titanium Models** requires a valid maintenance license plus a license for the TCTI (version 6 and newer) database. For some Property Models, additional recommendations for the database version to use is indicated in its description. Also see our website to learn more about the Titanium Model Library.

Visualizations

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⌛ When you run (Perform) this example, it takes a few minutes for the calculations to complete.

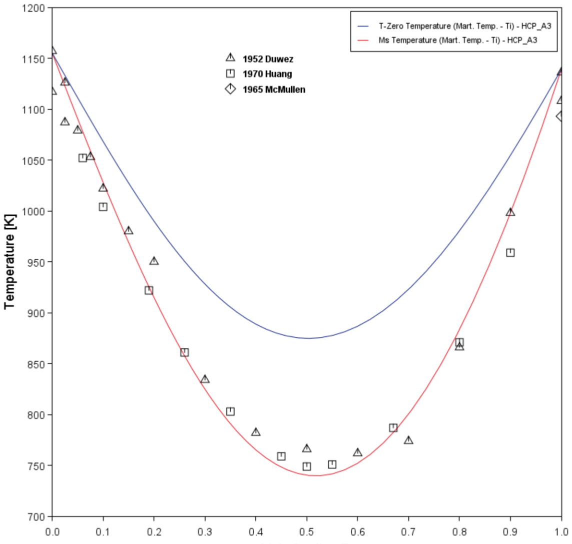


Figure 25: Ms and T-Zero temperatures as a function of mole fraction of Zr with experimental data from [1952Du, 1965McM, and 1970Hua].

References

[1952Du] P. Duwez, Allotropic transformation in titanium-zirconium alloys. J. Inst. Met. 80, 525–527 (1952).

[1965McM] A. G. McMullen, J. Gordon Parr, The Transformation in Zirconium-Niobium Alloys with an Appendix on Thermocouple Alloying with Zirconium. Can. Metall. Q. 4, 117–128 (1965).

[1970Hua] Y.C. Huang, S. Suzuki, H. Kaneko, T. Sato, Thermodynamics of the Ms points in titanium alloys, in: R.I. Jaffee, N.E. Promisel (Eds.) The Science, Technology and Application of Titanium, Pergamon Press, 1970, pp. 691-693.

PM_Ti_02: Alloy Strength for Ti-O

The **Alloy Strength - Ti** Property Model, available with the Property Model Calculator and the Titanium Model Library, calculates the strength and hardness for Ti-base alloys.

For more information about the Property Model, see About the Alloy Strength - Ti Property Model and Alloy Strength - Ti Property Model Settings.

This example uses the **Alloy Strength - Ti** Property Model to determine the total hardness of a Ti-0.04Fe-0.03C-0.005N-0.01O alloy.

A **One Axis** calculation is done using the latest version of the TCTI database to compare the total hardness vs oxygen content (in mole %). Two **Experimental File Readers** provide the data from [1950Fin] and [1973Oka] for comparison with the calculated values.

As is clearly illustrated in this example, the effect of typical impurity elements on the strength and hardness of Ti is very large. It is therefore important to keep in mind that the impurity elements and their respective contents should be included in the calculation, either explicitly, as is done in this example, or by selecting an appropriate base grade with a pre-defined impurity content for the calculation.

Project File and License Information

- Folder: **Property Models → Titanium**
- File name: `PM_Ti_02_Alloy_Strength_Ti-O.tcu`

To run calculations with the **Titanium Models** requires a valid maintenance license plus a license for the TCTI (version 6 and newer) database. For some Property Models, additional recommendations for the database version to use is indicated in its description. Also see our website to learn more about the Titanium Model Library.

Visualizations

Many of our Graphical Mode examples have video tutorials, which you can access in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

When you run (Perform) this example, it takes a few minutes for the calculations to complete.

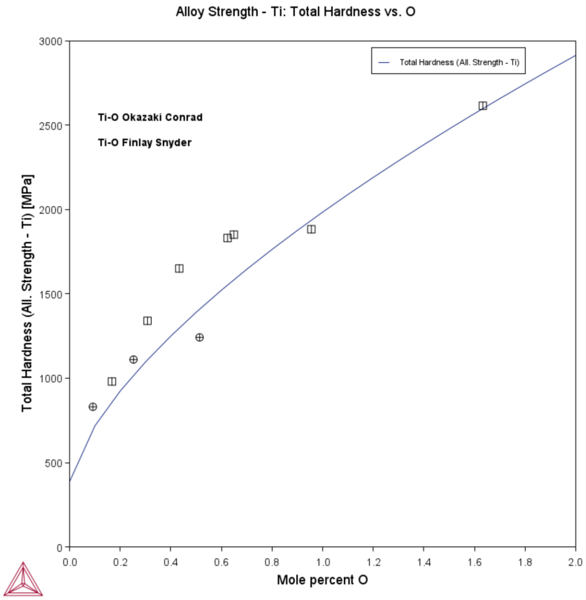


Figure 26: The total hardness vs O (in mole %) is shown with data from [1950Fin] and [1973Oka].

References

[1950Fin] W. L. Finlay, J. A. Snyder, Effects of three interstitial solutes (nitrogen, oxygen, and carbon) on the mechanical properties of high-purity, alpha titanium. JOM. 2, 277–286 (1950).

[1973Oka] K. Okazaki, H. Conrad, Effects of interstitial content and grain size on the strength of titanium at low temperatures. Acta Metall. 21, 1117–1129 (1973).

Thermo-Calc User Guide: Console Mode

Thermo-Calc Version 2025b

Working in Console Mode

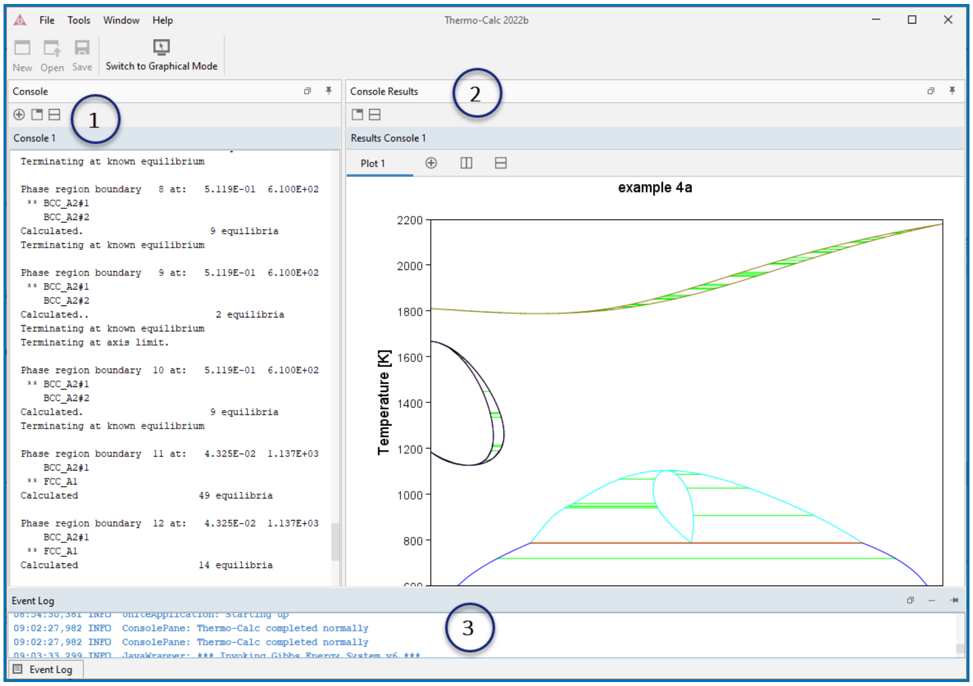
In this section:

Console Mode Layout

By default the first time you launch Thermo-Calc it opens in Graphical Mode. After this, the mode defaults to the most recent one. You can switch back and forth between modes. To open the Console Mode interface, click **Switch to Console Mode** on the toolbar.

[Keyboard Shortcuts to Navigate Between Tabs](#)

The Console Mode User Interface



```
 Terminating at known equilibrium

 Phase region boundary   8 at:   5.119E-01  6.100E+02
  ** BCC_A2#1
     BCC_A2#2
 Calculated.                      9 equilibria
 Terminating at known equilibrium

 Phase region boundary   9 at:   5.119E-01  6.100E+02
  ** BCC_A2#1
     BCC_A2#2
 Calculated..                      2 equilibria
 Terminating at known equilibrium
 Terminating at axis limit.

 Phase region boundary  10 at:   5.119E-01  6.100E+02
  ** BCC_A2#1
     BCC_A2#2
 Calculated.                      9 equilibria
 Terminating at known equilibrium

 Phase region boundary  11 at:   4.325E-02  1.137E+03
     BCC_A2#1
  ** FCC_A1
 Calculated                     49 equilibria

 Phase region boundary  12 at:   4.325E-02  1.137E+03
     BCC_A2#1
  ** FCC_A1
 Calculated                     14 equilibria
```

```
09:02:27,982 INFO  ConsolePane: Thermo-Calc completed normally
09:02:27,982 INFO  ConsolePane: Thermo-Calc completed normally
```

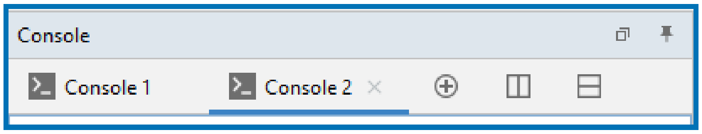
The currently selected window is called the *active* window. This has a darker title bar than the other windows. The windows are:

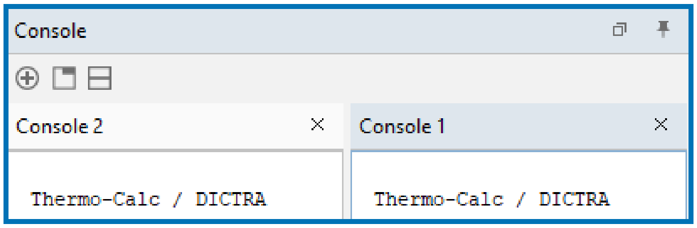
1. **Console**, with a **Console 1** tab.
2. **Console Results**, with a **Results Console 1** tab as well as a sub-tab (**Plot 1**), which is what is displayed in the window in the figure.
3. **Event Log**.

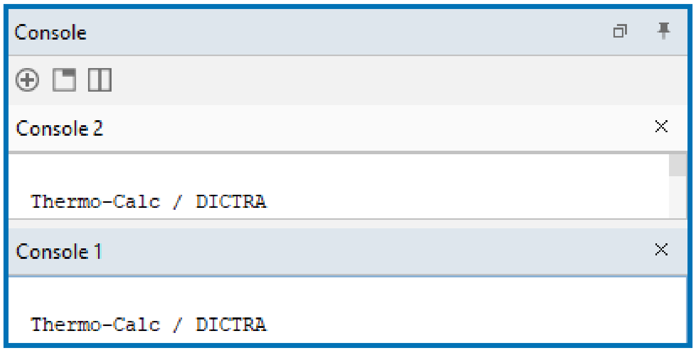
Console Tabs

By default, the tabs are side-by-side. You can toggle to view the tabs

- Click the ⊟ button to display both windows side by side where you can see the information in all windows at the same time.
- Click the ◫ button to stack the windows top to bottom where you can see the information in all windows at the same time.
- Click the ☐ button to return to the default layout with tabs side by side and the focus on one window at a time.

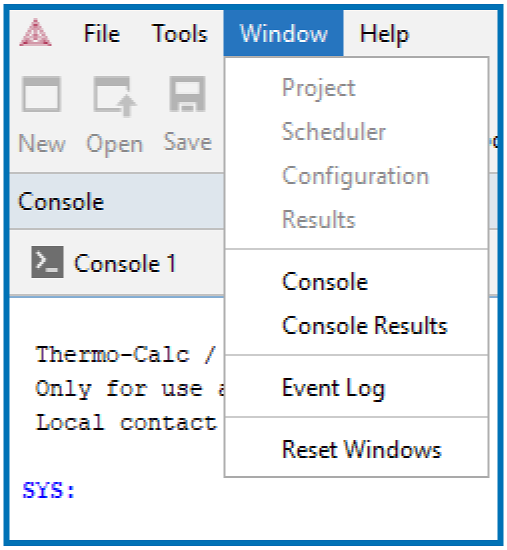






How to Open Console Windows

Open a specific window from the **Window** main menu, or select **Reset Windows** to return to the default window layout.



```
Thermo-Calc /
Only for use a
Local contact

SYS:
```

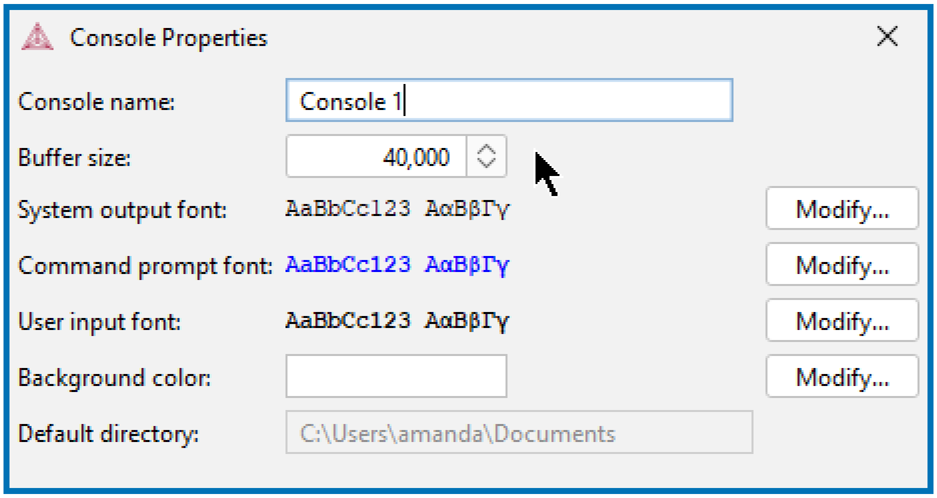
Console Window and Tabs

By default the Console window is on the left-hand side of the console. This is where you enter commands and within the window there can be several Console tabs open at a time. When you right-click the tab, there are options available from the menu to edit the tab properties, open and close tabs, and view, copy, and save a command history.

Edit the Console Tab Properties

Right-click any tab and select **Properties** from the menu to edit the Console tab properties.

Global Settings: Console Mode Default Appearance



Console name: Console 1

Buffer size: 40,000

System output font: AaBbCc123 AαBβΓγ

Command prompt font: AaBbCc123 AαBβΓγ

User input font: AaBbCc123 AαBβΓγ

Background color:

Default directory: C:\Users\amanda\Documents

- Change the tab name in the **Console name** field to make it more descriptive for the work you are doing.
- Increase or decrease the buffer size.
- Edit fonts, sizes, and colors for various Console window text. Click **Modify** next to **System output**, **Command prompt**, and **User input**.
- Click **Modify** next to **Background color** to change the color for each Console window.
- To globally set the **Default directory** file path to where the various file types are saved, go to **Tools > Options > Console Mode**.

Open and Close Console Tabs

There are options to add a **New Console** tab, **Close** one, or **Close all** tabs in the Console window.

Open One or More Console Tabs

- Click the ⊕ button.
- Press <Ctrl+T> when the Console window is active.
- Right-click a tab header and select **New Console**.

Close One or More Console Tabs

- Click the X button.
- Press <Ctrl+W> or <Ctrl+F4>.
- Right-click the tab header and select **Close**.
- To close all tabs except one, right-click the header of the tab you want to keep and select **Close Other**.
- To close all tabs and open a new one, right-click the header of any tab and select **Close All**.

Copy all Text to Clipboard

- Right-click any tab and select **Copy All Text to Clipboard** from the menu. Paste in a text editor as required.
- The shortcut for this command is to press <Ctrl+Alt+C> (Windows and Linux) or ⌥⌘C (macOS).

View, Copy, or Save a Command History

There are commands available to enter at the command line prompt as well as other ways to save or copy the full set of commands in any Console window tab.

Copy Commands to a Clipboard

- Press `CTRL + Shift + C` in the window or tab where you want to copy the command history. Paste in a text editor as required.
- Right-click any tab and select **Command History** from the menu to open the **Command History** window. Then click the **Copy** button (⧉) to copy all the commands to the clipboard. Paste in a text editor as required.

- Right-click any tab and select **Copy Command History to Clipboard** from the menu. Paste in a text editor as required.
    - The shortcut for this command is to press <Ctrl+Shift+C> (Windows and Linux) or ⇧⌘C (macOS).

View or Save Commands to a Macro File

Right-click any tab and select **Command History** from the menu to open the **Command History** window. Then click the **Save** button (💾), enter a file name and path to save all the commands in a `.TCM` file format.

Enter Commands to View the History

- To scroll through the last twenty commands used, at the command line prompt enter two exclamation marks (`!!`) and press <Enter>.
- To repeat the last *n* commands, at the command line prompt enter `!` followed by the number of previous commands to be repeated.
- `!<text>`executes the most recent command starting with `<text>`. The `< >` is not entered at the prompt.
- `!*<n>` or `!*<text>` makes the command available for editing before execution. The `< >` is not entered.
- To scroll through previous performed commands, use the Up (↑) or Down arrow (↓) keys.
- To read more information about the command history functionality in Thermo-Calc, enter `! ?` at the command line prompt.

Results Window in Console Mode

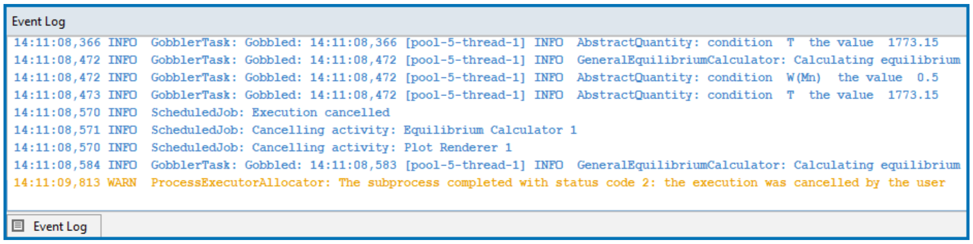
By default, the Console Results window is on the right-hand side of the screen. This is where plotted diagrams display. Each Console has its own Results tab in the Console Results window. All the plots and tables generated are presented in the Results tab.

- To open new **Plot** tabs press <Ctrl+Shift+T> or click the add ⊕ button.
- To open a new Plot tab for the currently active Console tab, press <Ctrl+Shift+T>. To close the Plot tab, press <Ctrl+Shift+W> or <Ctrl+Shift+F4>.

Event Log Window

The **Event Log** window is closed by default. Information about what Thermo-Calc is processing or doing is in blue text, an error message is in red text, and caution/warning information is in yellow text.

Global Settings



```
14:11:08,366 INFO  GobblerTask: Gobbled: 14:11:08,366 [pool-5-thread-1] INFO  AbstractQuantity: condition  T  the value  1773.15
14:11:08,472 INFO  GobblerTask: Gobbled: 14:11:08,472 [pool-5-thread-1] INFO  GeneralEquilibriumCalculator: Calculating equilibrium
14:11:08,472 INFO  GobblerTask: Gobbled: 14:11:08,472 [pool-5-thread-1] INFO  AbstractQuantity: condition  W(Mn)  the value  0.5
14:11:08,473 INFO  GobblerTask: Gobbled: 14:11:08,472 [pool-5-thread-1] INFO  AbstractQuantity: condition  T  the value  1773.15
14:11:08,570 INFO  ScheduledJob: Execution cancelled
14:11:08,571 INFO  ScheduledJob: Cancelling activity: Equilibrium Calculator 1
14:11:08,570 INFO  ScheduledJob: Cancelling activity: Plot Renderer 1
14:11:08,584 INFO  GobblerTask: Gobbled: 14:11:08,583 [pool-5-thread-1] INFO  GeneralEquilibriumCalculator: Calculating equilibrium
14:11:09,813 WARN  ProcessExecutorAllocator: The subprocess completed with status code 2: the execution was cancelled by the user
```

- To open the Event Log window: Click the **Event Log** window once to expand it or select it from the **Window → Event Log**menu. Double-clicking the window maximizes it.
- To clear all messages in the window, right-click in the text area and select **Clear**.
- To specify the level of detail in the Event Log, open the **Options** window:
  - Windows: Select **Tools → Options**.
  - Mac: Select **Thermo-Calc** *<version>* **→ Preferences** or **Settings** or press <⌘> on the keyboard.

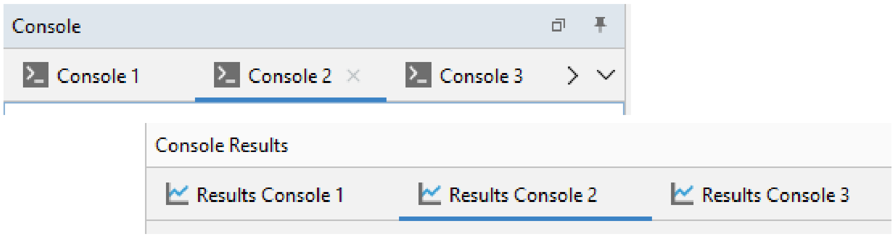
  then click the **General** tab and set the **Log level** slide bar to anything between **Debug** (most detailed) and **Error** (least detailed).

Keyboard Shortcuts to Navigate Between Tabs

Use keyboard shortcuts to move between the tabs available in the Console and Results windows.

Windows

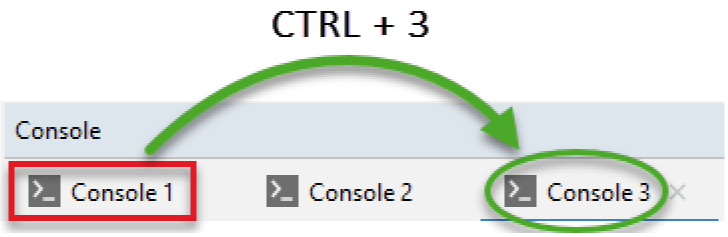
- Press CTRL + TAB to move forward sequentially through each open tab. When you are focused on the Console window, you move forward simultaneously through the Console Results tabs, e.g. If you are on Console 1 and press CTRL + TAB, you move forward to Console 2 and Results Console 2 and so forth.



- Press CTRL + SHIFT + TAB to move back through the open tabs. This is useful if you have multiple tabs open, otherwise you can use the CTRL + TAB to cycle through the windows.
- Press CTRL + [tab number 1 to 9] to move directly to the numbered tab. For example, if you are focused on Console 1 and want to move to Console 3, press CTRL+3 and the focus jumps to that tab.

The tab number corresponds to the order of the tabs, not necessarily the name. That is, if Console 4 is first, then it is what is highlighted when CTRL + 1 is used.

For **EXAMPLE**, press CTRL + 3 on the keyboard to move focus from Console 1 to Console 3.



When you are focused on the **Console Results** window and use any of the shortcuts this only moves you through the open tabs on this window.

Linux and macOS

The same **Windows** keyboard shortcuts are used but must be pressed twice to move forward and backward.

Modules and Commands

In this section:

Console Mode Workflow

Working with Thermo-Calc involves moving between different modules. The workflow differs depending on the type of calculation:

- If you want to perform a calculation using the POLY module, you typically first retrieve thermodynamic data in the DATA module, perform the calculation in POLY, and visualize the results in the POST module. It is possible to define a system directly in POLY using the DEFINE_MATERIAL and DEFINE_DIAGRAM commands.
- If you want to calculate and plot a diagram using a response-driven module, such as POTENTIAL or SCHEIL, then you can go directly to that module. Response-driven modules prompt you to go through the steps to do the calculation and the required post-processing. These modules include BIN, TERN, POTENTIAL, POURBAIX, and SCHEIL. You typically end up in the POST module after having used a response-driven module. In the POST module you can modify the plots and save the diagram.
- If you want to tabulate a chemical substance, phase, or reaction, go directly to the TAB module.

The basic workflow is:

1. You are in the **SYS** module when you start Thermo-Calc in Console Mode.
2. In the **DATA** module define the system. Before performing a calculation, you must define the system and retrieve thermodynamic data. The data is retrieved from a database file (*.TDB or *.TDC).
3. The data needed to describe a system is then sent to the **GIBBS** module. This data is accessed by the **POLY** module when you instruct it to perform calculations.
4. In the **POLY** module, perform the calculations.
    - In POLY, the conditions are set for an equilibrium calculation (temperature, pressure, system composition, etc.), then an equilibrium calculation is done.
    - If you want to make a property or phase diagram, you set the conditions for a stepping or mapping operation and perform that operation.
    - This generates data that can be used to plot a property diagram (if a stepping operation is performed) or a phase diagram (if a mapping operation is performed).

5. In the **POST** module plot and visualize your data.
    - If a stepping or mapping operation is performed, then you can go to the POST module and plot a property or phase diagram.
    - The diagram can be plotted quickly using default settings, but you can also modify which variables to plot of the diagram axes and change the appearance of the diagram.
    - You can save the diagram either as a plain text file with data about all the coordinates or as an image file.

Defining a System in Console Mode

Defining a system means to select the chemical components and to retrieve thermodynamic data about those components from an appropriate database in order to do the calculations. You use database(s) with thermodynamic data and then define what system elements as components. Once the system is defined, you retrieve the system's thermodynamic data from the database(s).

- If you use a *response-driven module* to perform your calculation, such as BIN or POURBAIX, then the module prompts you to select database(s) and define the system.
- When doing calculations in the POLY module, you typically have to manually select databases and define the system in the DATA module. However, it is also possible to define the system directly in POLY using the DEFINE_MATERIAL and DEFINE_DIAGRAM commands.

? Database (TDB) Module Commands

How to Define a System in Console Mode

1. Go to the DATA (TDB) module. At the `SYS` prompt, use GOTO_MODULE and enter `Data`.
2. Change the default database unless you directly specify the name of the database as a parameter to the command. Type `SWITCH_DATABASE` and follow the prompts.

   The second part of the command prompt indicates the current default database. For example, if the prompt is `TDB_TCFE10`, then the current database is TCFE10.

3. Use DEFINE_ELEMENTS followed by a list of the elements that you want in your system. (To list the elements that are available in your current database, use LIST_DATABASE and choose `Elements`). For example, if you want to have Fe and C in your system, type:

   ```
   DEFINE_ELEMENTS Fe C
   ```

4. Use REJECT and choose `Phases` if you want to avoid retrieving any phases from the database. (To list the phases that are available in your current database, use LIST_DATABASE and choose `Phases`. To list the phases that can form in the defined system, use LIST_SYSTEM and choose `Constituent`.) For example, if you do not want the graphite phase to be retrieved, you type:

   ```
   REJECT PHASES GRAPHITE
   ```

If the number of phases to include is much lower than the total number of phases, then it can be convenient to first `Reject Phases *` and then restore the phases to include using `Restore Phases`.

5. Use GET_DATA to search the database and send the thermodynamic data about your system to the GIBBS workspace.

   At this point you can proceed to the POLY module (with GOTO_MODULE POLY). However, you may want to add elements, phases and species to the GIBBS workspace from other databases. If so, then proceed to the next step.

6. Use APPEND_DATABASE to select the (additional) database from which you want to retrieve data. This command works exactly in the same way as the SWITCH_DATABASE command, with the exception that it does not reinitialize the DATA module and the GIBBS workspace, but instead appends or replaces the data that has already been retrieved with new data from the additional database.
7. Define your elements and specify whether to reject and restore any phases. Do this in exactly the same way when using the SWITCH_DATABASE command (see steps 2 and 3).
8. Use GET_DATA to search the database and add the thermodynamic data to the data that already exists in the GIBBS workspace.
9. Use APPEND_DATABASE again if you want to add data from yet another database. When you have retrieved all the data you need, you can proceed to the POLY module.

Console Mode Modules

Graphical Mode Activities vs Console Mode Modules

Below are each of the available modules you access in Console Mode. Most of the modules have commands, some are the same no matter what module you are in (e.g. general commands like BACK. GO TO MODULE, EXIT, HELP and so forth). Other commands have different prompts based on the module you are in how you define the system and so forth.

Most modules have several commands available. The exceptions are the BINARY, TERNARY, SCHEIL, POURBAIX and POTENTIAL modules which do not have any additional commands once you access the modules. These are response-driven modules that prompt you with a series of questions and then build the diagram automatically based on your responses.

System Utilities (SYS)

This is the module where you start. It also has several commands. Throughout the other modules there are some general commands, both of which are listed together.

System Utilities (SYS) Commands

Gibbs Energy System (GES)

The Gibbs Energy System (GES) module is an important Thermo-Calc Console Mode module and consists of a comprehensive subroutine package for various thermochemical calculations. The module is interactively connected with all basic and advanced modules in Thermo-Calc and the add-on Diffusion Module (DICTRA). Most users will not directly use the GES module and commands unless you perform assessments.

The GES module is in essence the Thermo-Calc calculation engine, sometimes referred to as the *calculation core*. When working in Graphical Mode you are using the GES calculation engine behind the scenes, whereas in Console Mode, and if you are performing assessments, you are directly interacting with the module. This is also applicable if you are working with any of the software development kits (SDKs).

- About the Gibbs Energy System (GES) Module
- Gibbs Energy System (GES) Commands

POLY3 (POLY) (Equilibrium)

With the equilibrium calculation module, POLY3, it is possible to calculate many different kinds of equilibria and diagrams, in particular multicomponent phase diagrams.

- The Equilibrium Calculation Module (POLY3)
- POLY Module Commands

Database (TDB)

The Database module (full name is Database Retrieval) is where you select and retrieve various types of thermodynamic and kinetic information from the selected databases you are going to use for your system. Once you enter the module the short name is `TDB`.

- Database (TDB) Module Commands
- Defining a System in Console Mode
- Also see the Database Manager User Guide and the available information for the specific databases.

POST - A POLY3 Submodule

The POST module (post-processor) is a submodule to the POLY module and has its own set of commands. The TAB, BIN, TERN, POT, SCHEIL and POURBAIX modules use the POST module features as part of the automatic generation of the plots.

Using the POST Module

POST Module Commands

Scheil (SCHEIL) Simulations

The available Scheil-Gulliver solidification simulations are *classic* Scheil, Scheil with *back diffusion* in the primary phase, or Scheil with *solute trapping*. There are also configuration options available with *fast diffusers* for the classic and back diffusion models.

There is also connectivity to the Diffusion Module (DICTRA) and *homogenization* where you collect data from a Scheil solidification calculation, which is then used as part of the kinetic homogenization simulation of segregated composition profiles.

Scheil in Graphical Mode vs Console Mode

The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. this model requires the use of a mobility database.

In Thermo-Calc, the Scheil calculation allows the calculation of:

- The solidification range of an alloy.
- Depression of the solidus temperature due to segregation.
- Composition of the last liquid to disappear in segregation pockets.
- Phases formed on final solidification in segregation pockets.
- The composition gradient in the primary solid phase(s) (segregation profile).
- Solute trapping to simulate deviation from local equilibrium for the primary phase
- Kinetic homogenization simulation of segregated composition profile (diffusion calculations)

About the Scheil-Gulliver Solidification Simulations

SCHEIL Module Commands

Pourbaix Diagram (POURBAIX)

The POURBAIX module lets you construct Pourbaix diagrams and other types of property diagrams for heterogeneous interaction systems with aqueous solution phases. Once you have calculated the Pourbaix diagram, you can also use the saved results of the calculation (the POLY3-file), and make a property diagram based on stepping calculation. You can also plot additional diagrams based on the results of the same calculation, but with different axis variables than Ph and Eh.

About Aqueous Solutions and the Pourbaix Diagram

Potential Diagram (POT)

The POTENTIAL_DIAGRAM module (short name, the POTENTIAL module) is a potential phase diagram calculation module. A potential diagram uses the activities of two major species in the gaseous mixture phase as mapping variables.

About Potential Diagrams

Binary Diagram (BIN)

The BINARY_DIAGRAM module (short name, the BIN module) enables you to quickly calculate a simple binary phase diagram. Binary phase diagrams are by far the most common found in the literature and calculated by computers. However, most real systems have more than two components and thus binary diagrams are more a kind of exercise in order to calculate more realistic phase diagrams.

About Binary Phase Diagrams

Ternary Diagram (TERN)

The TERNARY_DIAGRAM module (short name, the TERN module) enables you to quickly calculate a simple ternary phase diagram. There are many types of ternary phase diagrams but perhaps the most common is the isothermal section. In this case, the temperature is constant, which means that the tie-lines are in the plane of the calculation.

About Ternary Phase Diagrams

PARROT (Optimization)

The PARROT module makes use of the GES module to handle the models of the various phases that might form in a multicomponent system, as well as of the POLY module to store and calculate complex heterogeneous equilibria.

PARROT Module Commands

Also see the Data Optimization User Guide.

Tabulation Reaction (TAB)

The TABULATION_REACTION (TAB) module can be used to tabulate thermodynamic functions of any type of substance, stoichiometric phase or solution phase, or reaction. The module can tabulate thermodynamic functions of pure stoichiometric phases or solution phases at fixed composition, as well as various kinds of partial derivatives for a pure stoichiometric phase or solution phase at a given composition.

About the Tabulation Reaction Module

Tabulation Reaction (TAB) Commands

Reactor Simulator (REACTOR)

Simulate chemical reaction processes in several feed-forward steady-state stages or in several dynamic stages.

REACTOR (REACTOR_SIMULATOR) Commands

DICTRA Monitor (DICTRA)

DICTRA Monitor (DICTRA) and DIC Parrot (optimization for DICTRA): These are available with the add-on Diffusion Module.

Moving Between Modules and Submodules

To go to a specific module, you typically use GOTO_MODULE (or just GOTO) followed by the name of the module. For example, to go to the DATA module, type `GOTO DATA`.

The exceptions are the submodules POST and ED-EXP:

- To go to the POST module, you must enter the POST command from within the POLY module or DICTRA module (if you have the add-on license).
- To go to the Edit Experiments module you must enter the ED-EXP command from within the PARROT module.

To go back to the previous module type `Back`. For example, if you are in the DATA module and entered it from the SYS module, when you type `Back`, you return to the SYS prompt. This command is also available to exit from the submodules POST and ED-EXP.

Without a valid Thermo-Calc license, you cannot leave the SYS module. To enter the DICTRA and DIC_PARROT modules, you also need a valid Diffusion Module (DICTRA) license key.

Entering Command Names or Abbreviations

The name of a command typically consists of terms linked with underscores, for example, LIST_EQUILIBRIUM. Note the following:

- UPPER or lower case letters are OK.
- Hyphens (-) instead of underscores (_) are OK, e.g. LIST-EQUILIBRIUM.
- You can abbreviate commands as long as it is unambiguous, e.g. when more than one command begins with LIST_, you need to type the next letter or word to distinguish between the commands.
- Each word can be abbreviated e.g., L_E for LIST_EQUILIBRIUM.

Examples

Examples of how to abbreviate commands at the command line prompt in Console Mode.

Command Name	*Abbreviation*
CALCULATE_EQUILIBRIUM	C-E
CALCULATE_ALL_EQUILIBRIA	C-A
LIST_EQUILIBRIUM	L-E
LIST_INITIAL_EQUILBRIUM	LI-I-E
LOAD_INITIAL_EQUILBRIUM	LO-I-E
LIST_PHASE_DATA CBCC	L-P-D CBC
LIST_PHASE_DATA CEMENTITE	L-P-D CEM
SET_ALL_START_VALUES	S-A-SS-AL
SET_AXIS_VARIABLE 1 X(FCC,FE) 0 0.89 0.025	S-A-V 1 X(F,FE) 0 .89 .025
SET_START_CONSTITUENT	S-S-C
SET_START_VALUE	S-S-V
SET_AXIS_PLOT_STATUS	S-A-P
SET_AXIS_TEXT_STATUS	S-A-T-SS-A-TE

Command Name	**Abbreviation**
SET_AXIS_TYPE	S-A-TY
SET_OPTIMIZING_CONDITION	S-O-C
SET_OPTIMIZING_VARIABLE	S-O-V
SET_OUTPUT_LEVEL	S-O-LS-OU

Using the Command Line Prompt

The command line prompt in the Console window tells you which module you are currently in. When Thermo-Calc is first opened in Console Mode, you are in the SYS module, which is indicated with the command line prompt `SYS`.

To use Console Mode, you type in commands at the command line prompt. The available commands depend on which module you are in. You can list the commands by typing `?` at the prompt and then press <Enter>.

Console Window and Tabs also includes information about saving or copying the Command history.

- Moving Between Modules and Submodules
- Entering Command Names or Abbreviations
- Specifying Parameters
- Wild Card Characters
- Keyboard Shortcuts to Navigate Between Tabs
- Working with the Console Mode Output

Main Menu Commands

In Console Mode you use commands to access these menu options. If there is an equivalent command, it is listed below.

The **File** menu and toolbar are reserved for Graphical Mode. The **Tools**, **Window** and **Help** menus are described in Menu, Toolbar, and Keyboard Shortcuts.

How to Open Files

- In the SYS module: MACRO_FILE_OPEN
- In the SYS module: OPEN_FILE

Opening Console Mode Macro Files

Drag and drop files into the Console window to open or run a macro, for example. File types that can be opened this way are macro files (*.TCM and *.DCM), database files (*.TDB), and workspace files (*.POLY3, *.GES5,*.PAR, and *.DIC). Note that *.DCM and *.DIC file extensions are applicable to the Diffusion Module (DICTRA).

Save (Workspace)

This command depends on the module you are in. Type `?` at the prompt to look for a command such as SAVE_GES_WORKSPACE (GIBBS module).

Exit

In any module: EXIT

Close

In the SYS module: CLOSE_FILE

Display License Info

In the SYS module: DISPLAY_LICENSE_INFO

Wild Card Characters

You can sometimes use the asterisk (`*`) as a wild card character to, for example, refer to all components, phases, or species, when showing calculated properties in the POLY module, or when you set axis variables for plotting diagrams in the POST module.

When showing calculated properties in the POLY module, you can also use the dollar sign (`$`) to refer to all stable phases.

! For activity and/or chemical potential properties, the `*`and `$` normally do not work properly as wild card characters.

Examples

These are examples of the wild card characters you can use to search commands at the command line prompt.

Command	*Action*
SHOW_VALUE B(*)	Lists mass (gram) of all components in the system.
SET_AXIS_VAR Y B(*) *	Sets mass (gram) of all components in the system as Y-axis variable.
SHOW_VALUE MUR(*)	Lists chemical potentials of all components in the system.
SET_AXIS_VAR Y ACR(*) *	Sets activities of all components in the system as Y-axis variable.
SHOW_VALUE HM(*).T	Lists heat capacities of all phases.
SET_AXIS_VAR Y GM(*) *	Sets molar Gibbs free energies of all phases as Y-axis variable.
SHOW_VALUE TC($)	Lists curie temperature of all stable phases.
SHOW_VALUE W(*,*)	Lists mass fractions of all components in all phases.
SHOW_VALUE W($,*)	Lists mass fractions of all components in all stable phases.
SHOW_VALUE W(FCC,*)	Lists mass fractions of all components in the FCC phase.
SHOW_VALUE W(*,FE)	Lists mass fractions of the Fe component in all phases.

Command	***Action***
SHOW_VALUE W($,FE)	Lists mass fractions of the Fe component in all stable phases.
SHOW_VALUE Y(*,*)	Lists site fractions of all species in all sublattices of all phases.
SHOW_VALUE Y($,*)	Lists site fractions of all species in all sublattices of all stable phases.
SHOW_VALUE Y(*,*)	Lists site fractions of all species in all sublattices of all phases.

File Types

In this section:

Working with the Console Mode File Types

For DICTRA Console Mode see *File Formats* in the *Diffusion Module (DICTRA) User Guide*

In Console Mode, Thermo-Calc uses different types of files, including:

- Macro Files and Log Files both with the file extension *.TCM. Log files are created using the SET_LOG_FILE command.
- Workspace Files in POLY (*.POLY3), GIBBS module (*.GES5), and the PARROT module (*.PAR). (For the GIBBS module, this cannot currently be done with GES6).
- Experimental Data Files (*.POP, *.DOP) are a type of workspace file available with the PARROT module and have the file extension of *.POP. In the Diffusion Module (DICTRA), you work with .DOP files instead of .POP. These .POP and .DOP files are referred to as experimental data files.

Another type of experimental data file with the *.EXP file extension are also generated when working with DATAPLOT. See About the DATAPLOT Graphical Language.

A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

Drag and drop files into the Console window to open or run a macro, for example. File types that can be opened this way are macro files (*.TCM and *.DCM), database files (*.TDB), and workspace files (*.POLY3, *.GES5,*.PAR, and *.DIC). Note that *.DCM and *.DIC file extensions are applicable to the Diffusion Module (DICTRA).

Opening Console Mode Macro Files

The macro files (with the extension *.`TCM`) include comments, which you can either run in Thermo-Calc or open and read in a text editor.

You can open the macro files (*.TCM or *.DCM files) in different ways.

- From the main menu,
- Using a command,
- By dragging and dropping the file into the Console window, or
- Navigate to the file location on your computer and double-click to open it. If you already have Thermo-Calc open, the macro opens in a new tab. Otherwise a new instance of Thermo-Calc is launched.

> If you are using the advanced pipe or redirect option (Technical Note: Pipe or Redirect Output Data from Console Mode) then a new instance of Thermo-Calc is always started.

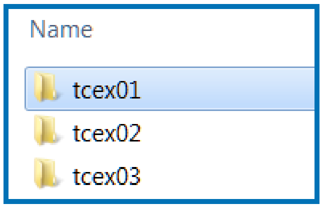
- You can also read the commands listed in the macro file using a text editor.

> If you only open and read the macro file in a text editor, you do not see the output that Thermo-Calc gives in response to the commands stored in the macro file.

Opening a Macro from the Main Menu

To open a Thermo-Calc example macro file:

1. Open Thermo-Calc.
2. Confirm you are in Console Mode. If not, click the **Switch to Console Mode**button.
3. From the main menu, select **File →** or **Help → Examples Files**. The Console Mode folder opens.
4. Open the **Thermo-Calc** folder to see the available examples contained in separate folders.



Name

tcex01

tcex02

tcex03

For the Diffusion Module (DICTRA) examples (*.`DCM` macro files), open the **Diffusion Module - DICTRA** folder.

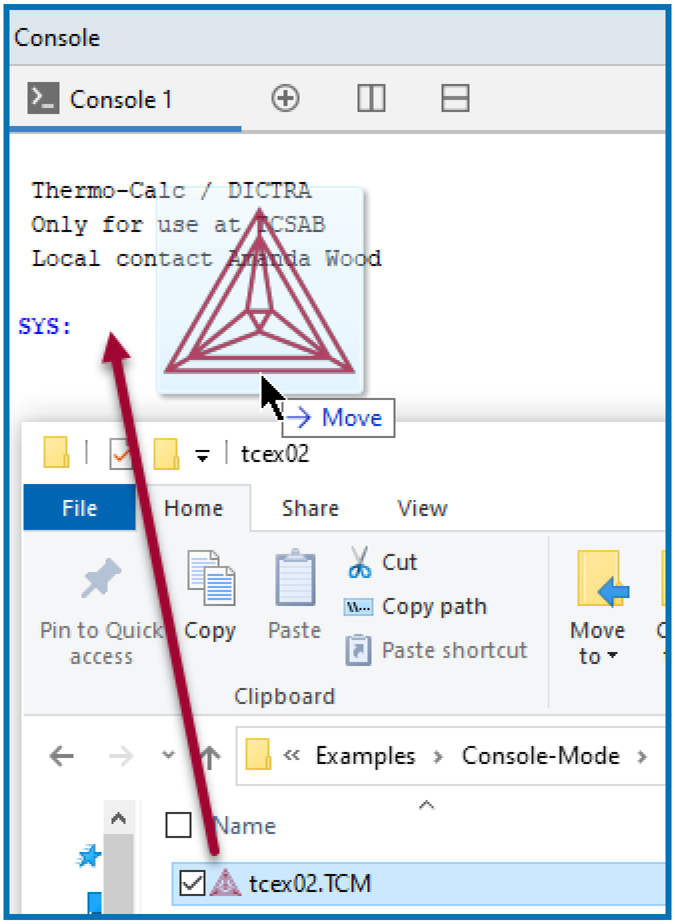
5. In the folder, double-click the *.`TCM` file or click **Open**.
6. Follow the prompts in the Console window i.e. keep pressing <Enter> to run the macro and produce a plot in the **Console Results** window.

Opening a Macro Using a Command

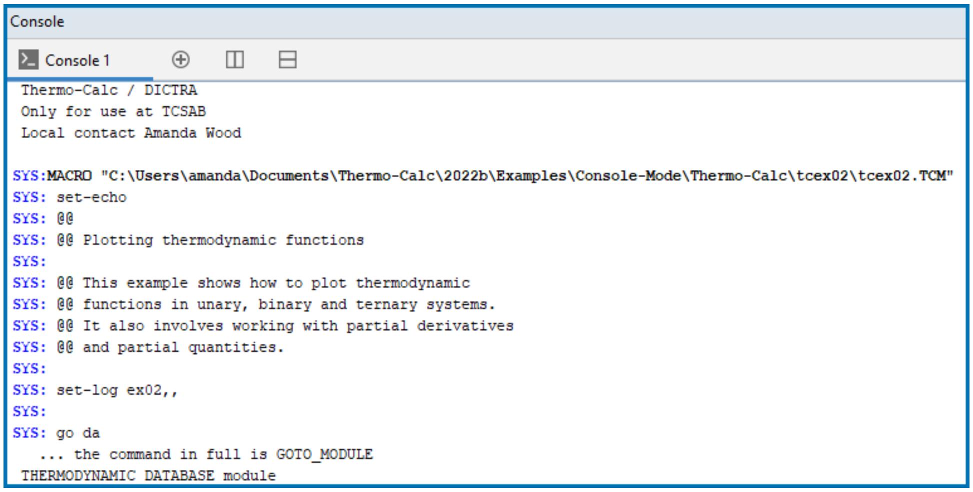
At the `SYS` prompt, type MACRO_FILE_OPEN and press <Enter>. In the file dialogue window that opens, navigate to and select the macro file to open.

Drag and Drop a Macro File into the Console Window

For example, on your computer, navigate to the examples folder. Drag the file from its location into the Thermo-Calc Console window. When you release (drop) the file, the macro starts running. Follow the prompts in the Console window i.e. keep pressing <Enter> to run the macro and produce a plot in the **Console Results** window.



```
Thermo-Calc / DICTRA
Only for use at TCSAB
Local contact Amanda Wood

SYS:
```



```
 Thermo-Calc / DICTRA
 Only for use at TCSAB
 Local contact Amanda Wood

SYS:MACRO "C:\Users\amanda\Documents\Thermo-Calc\2022b\Examples\Console-Mode\Thermo-Calc\tcex02\tcex02.TCM"
SYS: set-echo
SYS: @@
SYS: @@ Plotting thermodynamic functions
SYS:
SYS: @@ This example shows how to plot thermodynamic
SYS: @@ functions in unary, binary and ternary systems.
SYS: @@ It also involves working with partial derivatives
SYS: @@ and partial quantities.
SYS:
SYS: set-log ex02,,
SYS:
SYS: go da
   ... the command in full is GOTO_MODULE
 THERMODYNAMIC DATABASE module
```

Drag and drop files into the Console window to open or run a macro, for example. File types that can be opened this way are macro files (*.TCM and *.DCM), database files (*.TDB), and workspace files (*.POLY3, *.GES5,*.PAR, and *.DIC). Note that *.DCM and *.DIC file extensions are applicable to the Diffusion Module (DICTRA).

Log Files

Log files with the file extension *.`TCM` are plain text files used to save a sequence of commands. Log files can be edited in a text editor.

- To start saving your input into such a file, use SET_LOG_FILE in the SYS module, followed by the name of the file that you want to save your command sequence to.
- If you want to save the output in the log file as well, use SET_ECHO before the SET_LOG_FILE command. Doing this is useful if you want use the log file later as a macro file.

Macro Files

Macro files (with the file extension of either *.`TCM` or *.`LOG`) are plain text files used to save a sequence of commands that can be loaded and executed. Macro files can be edited in a text editor. When creating a command sequence, you add comments to the file by starting a line with @@.

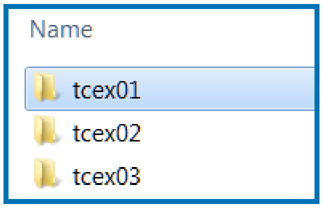
Macro files include comments, which you can either run in Thermo-Calc or open and read in a text editor.

> If you only open and read the macro file in a text editor, you do not see the output that Thermo-Calc gives in response to the commands stored in the macro file. It is recommended you run the macro to view all the details.

How to Open a Console Mode Example Macro File

To open a Thermo-Calc example macro file:

1. Open Thermo-Calc.
2. Confirm you are in Console Mode. If not, click the **Switch to Console Mode**button.
3. From the main menu, select **File →** or **Help → Examples Files**. The Console Mode folder opens.
4. Open the **Thermo-Calc** folder to see the available examples contained in separate folders.



Name
tcex01
tcex02
tcex03

> For the Diffusion Module (DICTRA) examples (*.`DCM` macro files), open the **Diffusion Module - DICTRA** folder.

5. In the folder, double-click the *.`TCM` file or click **Open**.
6. Follow the prompts in the Console window i.e. keep pressing <Enter> to run the macro and produce a plot in the **Console Results** window.

Macro File Commands

Action	*Command*	*Description and Comments*
To load a macro file	In the SYS module, MACRO_FILE_OPEN followed by the name of the macro file.	Thermo-Calc starts the command sequence that the file contains.
Regain control of the console	SET_INTERACTIVE	End a macro file with this command to have control of the Console returned to you.
Add comments to a macro file	Start a line with @@, or enclose it between an @ (-line and a @)-line.	When lines are enclosed the software ignores them when running the macro.
Open a macro file	MACRO_FILE_OPEN	When creating the log file, you can make a macro file load up to five other macro files.
Nest macro files inside of each other	MACRO_FILE_OPEN SET_INTERACTIVE	If a nested macro file ends with SET_INTERACTIVE, then Thermo-Calc resumes with the higher-level macro file at the command immediately following the MACRO_FILE_OPEN command that loaded and executed macro file that has just been terminated. If a nested macro file doesn't end with SET_INTERACTIVE (but with an end-of-file character), then the console shuts down and the macro is stopped.

Macro File Control Characters

The `@?` character allows you to make a macro interactive by allowing input. At the @? character, which is placed where a parameter value or argument is normally put, Thermo-Calc prompts to input the value of a parameter or argument. You can enter a string immediately following the @? character. This string is presented to the user when prompted to enter the parameter value or argument. The entered value is used by Thermo-Calc as input to the command in question. For example, you can request the user to specify the temperature range of a stepping calculation by entering the following in a macro file:

```
SET_AXIS_VARIABLE 1 T @?Low-temperature-limit: @?High-temperature-
limit:
```

You can also use up to nine variables in your macro file and prompt the user to enter values that can be assigned to these variables. Use the `@#n` character when you want to prompt the user to provide a value to the variable, where the n is a digit between `1` and `9`. You can then use this value by with the `##n` character. For example, you can request the user to provide the first element of a system by entering the following in the macro file:

```
@#3First-element?
```

You can then use this variable with the entering the character ##3 later in the macro file. For example, you can write:

```
SET_AXIS_VARIABLE 1 x(##3) 0 1,,,
```

Finally, there is the `@&` pause character. Thermo-Calc pauses and waits for input from the user when this pause character is read from a macro file. Inserting pause characters is useful if you want to allow the user to monitor what is happening when Thermo-Calc is running the macro.

Response-Driven Modules and Macros

Macro files that are created while you use a *response-driven module* begin with the module-entering command (for example, `Goto_Module Scheil)` followed by a number of lines with responses to the module's questions and requests. The file terminates with the commands POST or SET_INTERACTIVE (this command gives you back control of the Console). An empty line cannot be edited with any input rather than the default answer (to a specific question). Comment lines, commands to open other macro files, pause characters or input-controlling characters cannot be inserted between these empty lines (otherwise the response-driven module cannot be executed properly).

Workspace Files

For DICTRA Console Mode see *File Formats* in the *Diffusion Module (DICTRA) User Guide*

Workspaces files allow you to save all the data in your current workspace. A workspace contains all the data, specified settings and the result of any calculations performed. The saved data includes original and modified thermodynamic data, the last set of conditions and options, and the results of any simulations. You use the command SAVE_WORKSPACES to create this file type, which is available in the POLY, GIBBS and PARROT modules.

When in Thermo-Calc Console Mode these are the workspace file extensions:

- POLY module (*.POLY3)
- GIBBS (GES) module (*.GES5)
- PARROT module (*.PAR and *.POP)

For DICTRA in Console Mode, the PARROT module file extension is *.DOP.

The workspace has all the settings specified and the result of any stepping or mapping operations performed after using SAVE_WORKSPACES. Consequently, the command opens a workspace in which all data is saved which is generated after the SAVE_WORKSPACE command is executed. The saved data includes original and modified thermodynamic data, the last set of conditions and options, and calculation results.

To load the data and calculation results of a workspace file, use the READ_WORKSPACES command available in the POLY module. The file can be used for calculation in POLY, visualization in POST, or data manipulation in GES. You are also given the option in the POURBAIX and SCHEIL modules to open a previously saved workspace file. This allows you to make new POURBAIX or SCHEIL calculations on the same chemical system as before but with different temperature, pressure, and composition conditions, or to plot new property diagrams based on the previous calculations.

A reminder that Linux and macOS are case sensitive; when applicable ensure you enter file extensions with capital letters.

Drag and drop files into the Console window to open or run a macro, for example. File types that can be opened this way are macro files (*.TCM and *.DCM), database files (*.TDB), and workspace files (*.POLY3, *.GES5,*.PAR, and *.DIC). Note that *.DCM and *.DIC file extensions are applicable to the Diffusion Module (DICTRA).

Links to Workspace Commands

POLY module

- READ_WORKSPACES
- SAVE_WORKSPACES

Gibbs (GES) module

- READ_GES_WORKSPACE
- READ_WORKSPACES
- SAVE_GES_WORKSPACE
- SAVE_WORKSPACES

PARROT module

- READ_PARROT_WORKSPACES
- SAVE_PARROT_WORKSPACES

ED-EXP module (submodule to PARROT)

- READ_WORKSPACES
- SAVE_WORKSPACES

Reactor module

- READ_WORKSPACE
- SAVE_WORKSPACES

Important Information About Map and Step Commands and the Save_ Workspaces Command

❗ A STEP or MAP command automatically saves the workspace with the most recently specified name. Do not use the SAVE_WORKSPACES command after a MAP or STEP command.

The results from the STEP or MAP commands are destroyed by the SAVE_WORKSPACE command. You can append several results obtained by sequential STEP or MAP calculations without destroying the previous results, whilst SAVE_WORKSPACE erases them all. Keeping this in mind is important and useful particularly for calculating various isothermal (or isoplethal) sections and plotting them on the same diagram in a single Thermo-Calc run.

To suspend some of the STEP or MAP results, use the AMEND_STORED_EQUILIBRIA command.

Editing the Default Console Directory

You can add a startup parameter to a shortcut when launching Thermo-Calc on any of the platforms. When you launch the revised shortcut, the file path is set to a user-defined default directory. An example of why you might want to have a custom directory path is if you use batch projects or if you have macro files for batch jobs. The custom directory file path can also be viewed from within Console Mode.

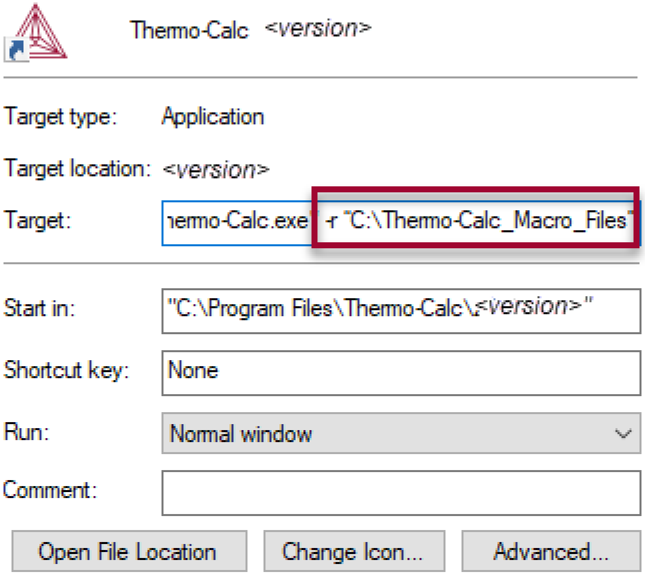
> The shortcut is only valid throughout the existing session; it is not saved as a default. Each time you want to use this file path you must launch Thermo-Calc from the customized shortcut.

The following uses Windows for the example.

How to Set up the Default Console Directory

1. Right-click a shortcut to Thermo-Calc and click **Properties**.
2. In the **Thermo-Calc 2025b Properties** dialog, **Target** field, add the following to the end of the string: **–r** plus the *"path to the default directory"*. Include a space between the –r and path, and use quotation marks around the full file path. A simple example:

   -r "C:\Thermo-Calc_Macro_Files"



Thermo-Calc <version>

Target type: Application

Target location: <version>

Target: ıermo-Calc.exe -r "C:\Thermo-Calc_Macro_Files"

Start in: "C:\Program Files\Thermo-Calc\<version>"

Shortcut key: None

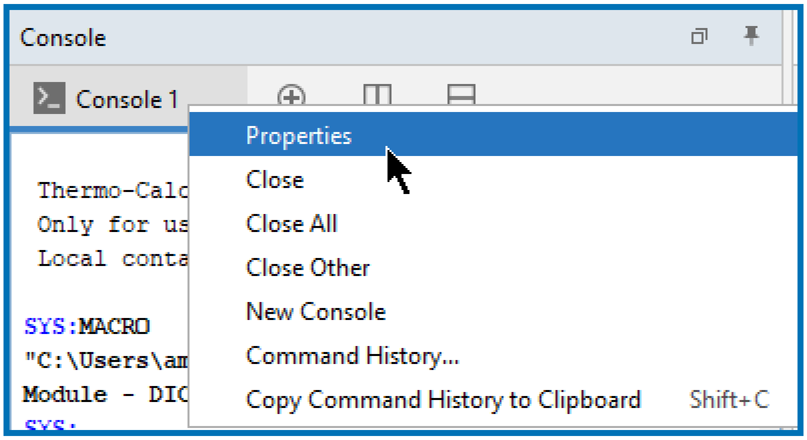
Run: Normal window

Comment:

3. Click **Apply** and **OK**.
4. Launch Thermo-Calc from the shortcut where you added the parameter. You can confirm that it is set correctly from within Thermo-Calc.

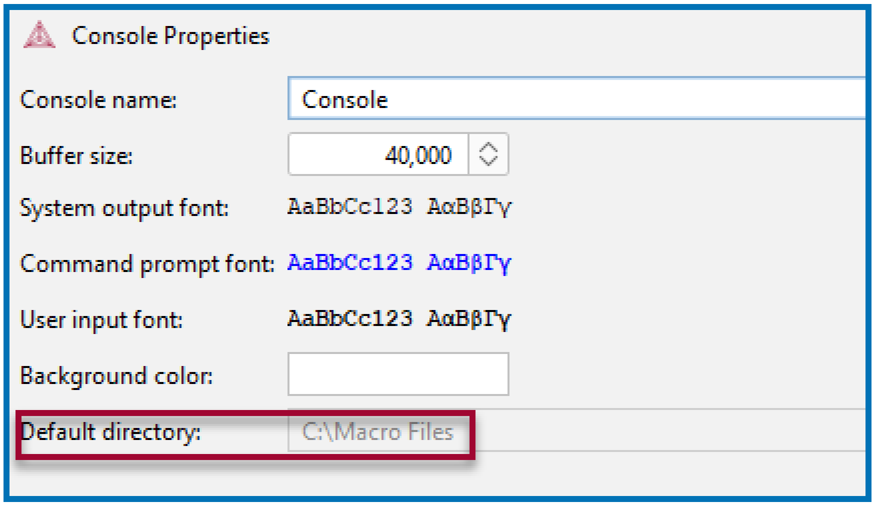
How to View the File Path in Thermo-Calc

1. Launch Thermo-Calc from the short cut where you added the parameter.
2. In Console Mode, right click the **Console** window and choose **Properties**.



```
Thermo-Calc
Only for us
Local conta

SYS:MACRO
"C:\Users\am
Module - DIC
SYS:
```

3. In the **Console Properties** window the **Default directory** section displays the custom file path. This default is set in the **Options** window, Console Mode section.



Console name: Console
Buffer size: 40,000
System output font: AaBbCc123 AαBβΓγ
Command prompt font: AaBbCc123 AαBβΓγ
User input font: AaBbCc123 AαBβΓγ
Default directory: C:\Macro Files

To open the **Options** window:

- Windows: Select **Tools → ☰ Options**.
- Mac: Select **Thermo-Calc** *<version>* **→ Preferences** or **Settings** or press <⌘> on the keyboard.

Experimental Data Files (*.POP, *.DOP)

There is also another type of experimental data file (*.EXP) generated when working with DATAPLOT. See About the DATAPLOT Graphical Language.

If you are using Graphical Mode, the Experimental File Reader activity node is used to plot experimental data on one or more plots.

See the Tips and Tricks: How to Plot Experimental Data blog post on our website for useful guidance about this topic.

In order to conduct an assessment for a system, the experimental data is described with a syntax, which is similar to the way that one calculates an equilibrium in the POLY module or you edit an experimental point in the ED_EXP module. Similar to a Thermo-Calc macro file (*.TCM), an experimental data file (i.e. the *.POP or *.DOP file) is a basic text file and can be opened and edited by any text editor. For this reason, a *.POP or *.DOP file is not hardware dependent.

A POP or DOP file consists of various commands from the POLY and ED_EXP modules, as well some special commands which can only be used in such experimental data files. Various experimental information can be inputted in an *.POP or *.DOP file as different tables; the same type of experimental data are usually documented in the same table (see below).

A *.POP or *.DOP file is used in the PARROT module to provide experimental information for the optimization process, and is checked by a *syntax checker* when the PARROT command COMPILE_EXPERIMENTS is proceeded.

The special commenting identifier, i.e. a dollar sign $ which starts a line, is used to document comment lines at any position in a *.POP or *.DOP file. You may remember that this feature is universally the same as in almost all kinds of text files in Thermo-Calc software, e.g. in *.TDB, *.DAT, *.TCM, *.POP/*.DOP and *.EXP files. Such a sign and all information afterwards in the same comment line is skipped and ignored by the syntax checker.

Many POLY and ED_EXP commands can be directly used in a POP or DOP file. But there are some differences with the set of POLY or ED_EXP commands, and some specially designed commands as described in this topic can only be used in the *.POP or *.DOP files.

Frequently Used POLY Commands

Most of the commands in the experimental data file are the same as in the POLY module. The most frequently used are listed below:

❗ The last command in an *.POP or *.DOP file must always be the SAVE command.

- CREATE_NEW_EQUILIBRIUM
- CHANGE_STATUS
- SET_CONDITION
- SET_REFERENCE_STATE
- ENTER_SYMBOL
- SAVE_WORKSPACES

Less Often Used POLY Commands

Other legal commands from the POLY module that are used less often are:

❗ The DEFINE-COMPONENTS command must be always used as the first command in an *.POP or *.DOP file, as it automatically reinitiates the whole workspace.

- DEFINE_COMPONENTS
- EVALUATE_FUNCTIONS
- SET_ALL_START_VALUES
- SET_NUMERICAL_LIMITS
- SET_START_VALUE
- ADVANCED_OPTIONS

Frequently Used Edit Experiments (ED_EXP) Commands

Most of the special commands for the ED_EXP module are also often used in an *.POP or *.DOP file. For example:

- EXPERIMENT
- EXPORT
- IMPORT
- LABEL_DATA
- SET_ALTERNATE_CONDITION
- SET_WEIGHT

Do not use these Edit Experiment (ED_EXP) Commands

The following special ED_EXP commands are illegal and should not be used in any *.POP or *.DOP file:

- COMPUTE-ALL-EQUILIBRIA
- MAKE-POP-FILE
- READ (READ-BLOCK OR READ-WORKSPACE)
- TRANSFER-START-VALUES

Calculations

? [Graphical Mode vs Console Mode: Calculation Types]

In this section:

About the Gibbs Energy System (GES) Module

The Gibbs Energy System (GES) module is an important Thermo-Calc Console Mode module and consists of a comprehensive subroutine package for various thermochemical calculations. The module is interactively connected with all basic and advanced modules in Thermo-Calc and the add-on Diffusion Module (DICTRA). Most users will not directly use the GES module and commands unless you perform assessments.

The GES module is in essence the Thermo-Calc calculation engine, sometimes referred to as the *calculation core*. When working in Graphical Mode you are using the GES calculation engine behind the scenes, whereas in Console Mode, and if you are performing assessments, you are directly interacting with the module. This is also applicable if you are working with any of the software development kits (SDKs).

The objective of the GES module is to provide a unified set of subroutines to be used in any application program that needs thermochemical data. All kinds of thermodynamic models for various types of substances are implemented. However, most model-dependent features are hidden inside the module, and the application programmer can use a standardized set of subroutines, i.e. using the Thermo-Calc SDKs such as TC-Python, TQ-Interface, and TC-Toolbox for MATLAB® to calculate the integral Gibbs energy or any partial derivative thereof for each phase at any composition, temperature and pressure.

There are subroutines to analytically calculate the first and second partial derivatives of integral Gibbs energy with respect to any variable. You can enter and modify phase descriptions, model connections, basic thermodynamic parameters, and so on.

POLY and all other basic and special modules, as well as the add-on Diffusion Module (DICTRA), interactively call the subroutines within the GES module to calculate any thermodynamic quantities.

Calculation Engine: GES5 vs GES6

❗ GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features. However, not all GES5 functionality is implemented in GES6. In such cases (except for the POURBAIX module), GES6 falls back silently and uses functionality from GES5 in the background.

To globally set the default from GES6 back to GES5, go to the **Tools → Options** →Global General Settings tab and click **Version 5** for the *Preferred Gibbs Energy System* setting. This is useful if you are using the POURBAIX module (aqueous solutions), or if you have a custom database that is not compatible with GES6. The SET_GES_VERSION Console Mode command can also be used to change GES versions for a single Thermo-Calc session.

Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.

Equilibrium Calculations

In this section:

The Equilibrium Calculation Module (POLY3)

An equilibrium describes what the composition of the end state of a system is, given a full specification of state variables such as temperature, pressure, initial composition, system size, etc. An equilibrium calculation is normally done in POLY-3 according to the *Global Minimization Technique*, which ensures that the most stable minimum under the specified conditions is computed.

For an equilibrium calculation to be performed, the state variables must all be set as conditions for the calculations. Such conditions include, for example, temperature, pressure, and system composition. When you calculate an equilibrium in the POLY module, you have to set these conditions manually.

Knowledge of the thermodynamic equilibrium is an important factor for understanding properties of materials and processes. With a database of thermodynamic model parameters, it is possible to predict such properties and also to obtain driving forces for diffusion-controlled phase transformations and other dynamic processes.

With the equilibrium calculation module, POLY3, it is possible to calculate many different kinds of equilibria and diagrams, in particular multicomponent phase diagrams.

Different types of databases can be used with the POLY module, and it can be used for alloys or ceramic systems, as well as gaseous equilibria, aqueous solution involved heterogeneous interaction systems. Up to 40 elements and 1000 species can be defined into a single system for equilibrium calculations.

All normal thermodynamic state variables can be used to set as conditions in calculating equilibria, and as axes in plotting diagrams. You can set the composition or any property of an individual phase as a condition. Any state variable can be varied along an axis in order to generate a diagram. During calculations of a diagram, complete descriptions of all calculated equilibria are stored, and in the diagram any state variable can be used as an axis.

The *Global Minimization Technique* is used to ensure that the present minimum in an equilibrium calculation is the most stable minima for the specified conditions. This is based on the traditional GEM (Gibbs Energy Minimization) technique.

A direct global minimization can be performed on conditions: N, n(comp), B, b(comp), w (comp), x(comp), T, and P, but not when combined conditions as e.g. w(a)-3*w(b)=1 are used or when an activity or potential condition is used. For all other types of conditions where regular minimization converges, Indirect Global Minimization, i.e. global test and corrections, if necessary, are performed until the lowest minimum is found.

- Direct Global Minimization: From the mesh of Gibbs energy, find the set of grid points that gives the lowest energy solution under the specified conditions. This set of grid points provides starting combination of phases and their constitutions for regular minimization to find the exact equilibrium solution. This solution is then subject to a global test as described below.

- Indirect Global Minimization: Under certain conditions, a direct approach is impossible. In this case, regular minimization is performed first and then a check is performed in order to see if the found local minimum is a global one by checking if all grid points are above the equilibrium Gibbs energy plane. If not, then recalculate by including these grid points until no grid point is above the equilibrium Gibbs energy plane from the previous step.

The full-scale and full-scope usage of the *Global Minimization Technique* has been extended from for only single-point calculations for all types of calculations (of single-points, property diagram stepping and phase diagram mapping)in Thermo-Calc.

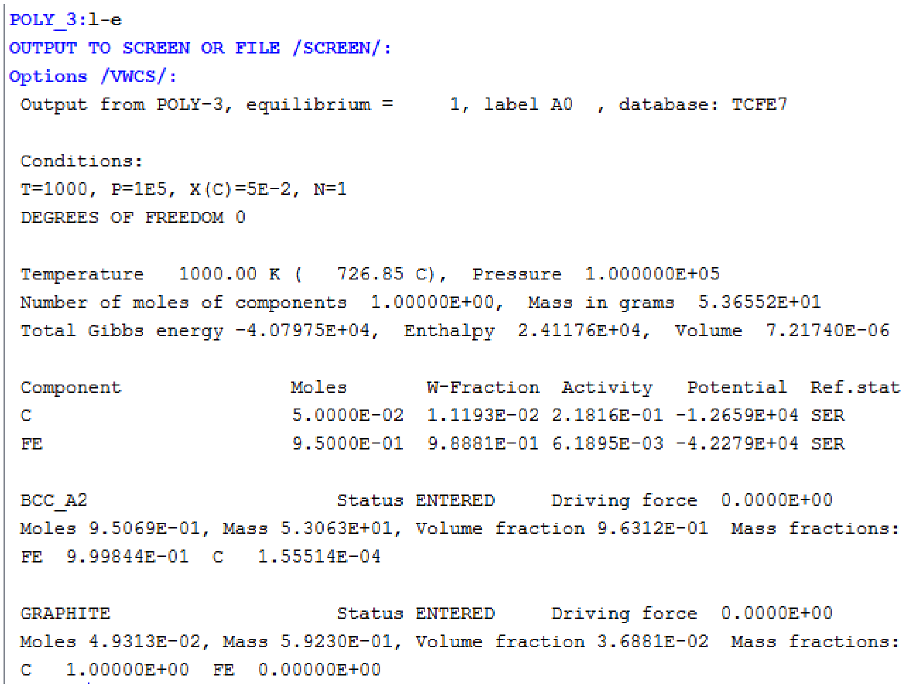
The use of *Global Minimization Technique* may increase the computation time. The main cost in time comes from the calculation of Gibbs energy at each grid point generated by properly meshing the composition space for each entered phase. An additional (but much smaller) cost in time comes from finding the set of grid points in the above mesh that give the lowest energy solution. This solution is where POLY starts its ordinary minimization. When POLY has found an equilibrium, the equilibrium Gibbs energy surface is compared to the mesh to assure that no grid point is below the surface, i.e. a global minimization has been reached.

Global minimization is performed by default in single-point or stepping or mapping equilibrium calculations.

Together with the PARROT module, the POLY module is also used for critical assessment of experimental data in order to develop thermodynamic databases. The POLY module uses the Gibbs Energy System (GES) for modeling and data manipulations of the thermodynamic properties of each phase.

Setting Conditions for Equilibrium Calculations

Setting a condition normally involves giving a single state variable a specific value. For example, you can set the temperature to 1273.5 Kelvin (T=1273.5). Alternatively, setting a condition can involve giving a linear expression with more than one state variable a specific value. For example, you can set the mole fraction of the S component to be the same in the liquid and the pyrrohotite phases (`X(LIQ,S)-X(PYRR,S)=0`).



```
POLY_3:l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: TCFE7

 Conditions:
 T=1000, P=1E5, X(C)=5E-2, N=1
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.36552E+01
 Total Gibbs energy -4.07975E+04,  Enthalpy  2.41176E+04,  Volume  7.21740E-06

 Component                Moles      W-Fraction  Activity   Potential  Ref.stat
 C                        5.0000E-02  1.1193E-02 2.1816E-01 -1.2659E+04 SER
 FE                       9.5000E-01  9.8881E-01 6.1895E-03 -4.2279E+04 SER

 BCC_A2                       Status ENTERED     Driving force  0.0000E+00
 Moles 9.5069E-01, Mass 5.3063E+01, Volume fraction 9.6312E-01  Mass fractions:
 FE  9.99844E-01  C   1.55514E-04

 GRAPHITE                     Status ENTERED     Driving force  0.0000E+00
 Moles 4.9313E-02, Mass 5.9230E-01, Volume fraction 3.6881E-02  Mass fractions:
 C   1.00000E+00  FE  0.00000E+00
```

The number of state variables that need to set is determined by the *Gibbs Phase Rule*. Typically, the state variables to give values to are:

- temperature (in K)
- pressure (in Pascal)
- system size in number of moles (in mole) or mass (in grams)
- the fraction of each component (in number of moles or mass)

If you fix the phase of the equilibrium and all but one of the state variables, you can discover the value of the other state variable at equilibrium.

It is possible to specify a set of conditions that does not have any equilibrium and the program detects this by failing to reach equilibrium during the calculation.

State Variables

The table lists some of the available state variables you can use to set conditions.

State Variable	SET_CONDITION Parameter
temperature in the system (in K)	T
pressure in the system (in Pascal)	P
system size (mole number in moles)	N
system size (mass in grams)	B
number of moles of a component in the system	N(<component>)
mole fraction of a component in the system	X(<component>)
mass fraction of a component in the system	W(<component>)
activity of a component in the system	ACR(<component>)
chemical potential of a component in the system	MUR(<component>)
mole fraction of a component in a phase	X(<phase>,<component>)
mass fraction of a component in a phase	W(<phase>,<component>)
activity of a species referred to a phase at ambient temperature and pressure	ACR(<species>,<phase>)
chemical potential of a species referred to a phase at ambient temperature and pressure	MUR(<species>,<phase>)
enthalpy in the system (in J)	H
enthalpy of a phase (in J/mol)	HM(<phase>)

Calculating an Equilibrium

This topic explains how to calculate an equilibrium in POLY. To calculate an equilibrium means to calculate the equilibrium composition of your system, given a full specification of conditions that reduce the degrees of freedom of the calculation to zero.

If you are running a network client installation of Thermo-Calc and cannot enter the POLY module, this may be because all the license instances on that the license server makes available have been checked out.

POLY Module Commands

1. Define your system.

   Defining a System in Console Mode

2. Go to the POLY module. At the SYS prompt, type `GOTO_MODULE` and enter `POLY`.
3. Use SET_CONDITION followed by conditions and value assignments to set the conditions of your calculation. For example, to set temperature, pressure, initial composition and system size for a Fe-Cr-C system, you might enter the following:

   ```
   SET_CONDITION T=1200 P=1E5 W(CR)=0.18 W(C)=0.0013 N=1
   ```

   This sets the temperature (T) to 1200 K, the pressure to 1 bar (100,000 Pascal), the mass fraction of Cr to 18 mole percent, the mass fraction of C to 0.13 weight percent, and the total amount of material to 1 mole. The fraction of Fe in the system is calculated from the fractions of Cr and C. You have to set the fraction of all the components in your system except one.

4. Use COMPUTE_EQUILIBRIUM to run the calculation.
5. Use LIST_EQUILIBRIUM to see the results of the calculation.

Calculating an Equilibrium with a Fixed Phase

There are many ways to calculate equilibriums in Thermo-Calc. The following is one example.

You can calculate an equilibrium that has a certain amount of a certain stable phase. Use CHANGE_STATUS and choose `Phase` to specify the phase and the amount of that phase (in normalized mole number) that you want to set as fixed. For example, if you want to find out at what temperature a system starts to melt, enter the following:

```
CHANGE_STATUS PHASE LIQUID=FIX 0
```

You must leave the state variable whose equilibrium value you are interested in unspecified. However, if you have already specified that state variable, you can make it unspecified again by using SET_CONDITION and set that state variable to `NONE`. For example, if you have given temperature a value, you can type:

```
SET_CONDITION T=NONE
```

The calculated equilibrium includes the value of the unspecified variable at which the equilibrium enters the phase that is fixed.

For an example where an equilibrium is calculated with a fixed phase, see Console Mode example tcex07.

Calculating an Equilibrium with Suspended or Dormant Phases

You can calculate an equilibrium under the assumption that one or several phases are `SUSPENDED` or `DORMANT` using CHANGE_STATUS and choose `Phase`. For example, to specify that all phases except one should be suspended, you can first suspend all phases and then enter a single phase in the following way:

```
CHANGE_STATUS PHASE *=SUSPENDED
CHANGE_STATUS PHASE FE_LIQUID=ENTERED
```

For an example where this is done, as well as where the status of phases is set to be dormant, see the Single Equilibrium Calculation Examples.

Property Diagrams

In this section:

About Property Diagrams

When you calculate and plot a property diagram, there is only one independent state variable. Many different properties can be plotted as a function of this independent variable. For example, if the independent state variable is temperature, then the mole fractions of all phases can be plotted as a function of temperature. Or the composition of a specific phase may be plotted relative to temperature, or the activity of a component in the system as a whole or in a specific phase may be plotted relative to it.

A property diagram is plotted based on a series of equilibria that is computed while the value of one state variable is varied between a minimum and a maximum value. This variable is referred to as the stepping axis variable. In Thermo-Calc, first calculate one initial equilibrium, and then new equilibria are calculated at incremental steps in both directions on the stepping axis from the initial equilibrium. This continues until the stepping operation has covered the length of the axis between a minimum and a maximum value that is specified.

For an example of the calculation of a property diagram, see tcex08.

Calculating and Plotting a Property Diagram

This topic explains how to calculate a property diagram in POLY. To calculate a property diagram means to calculate a series of equilibria while the value of the stepping axis variable varies between a minimum and a maximum value. With the exception of the stepping axis variable, all the state variables that you set when you calculate the initial equilibrium retain the values when the new equilibria are calculated.

POLY Module Commands

1. Calculate an initial equilibrium in the POLY module.

2. Use SET_AXIS_VARIABLE to set the axis variable, the minimum and the maximum stepping variable values and the step length. The first parameter of SET_AXIS_VARIABLE is the axis number. Since a property diagram only has one axis variable, this is set to 1. For example, if you want to set the axis variable to temperature, and calculate an equilibrium at every 50 K between a minimum temperature of 100 K and a maximum temperature of 2000 K, enter

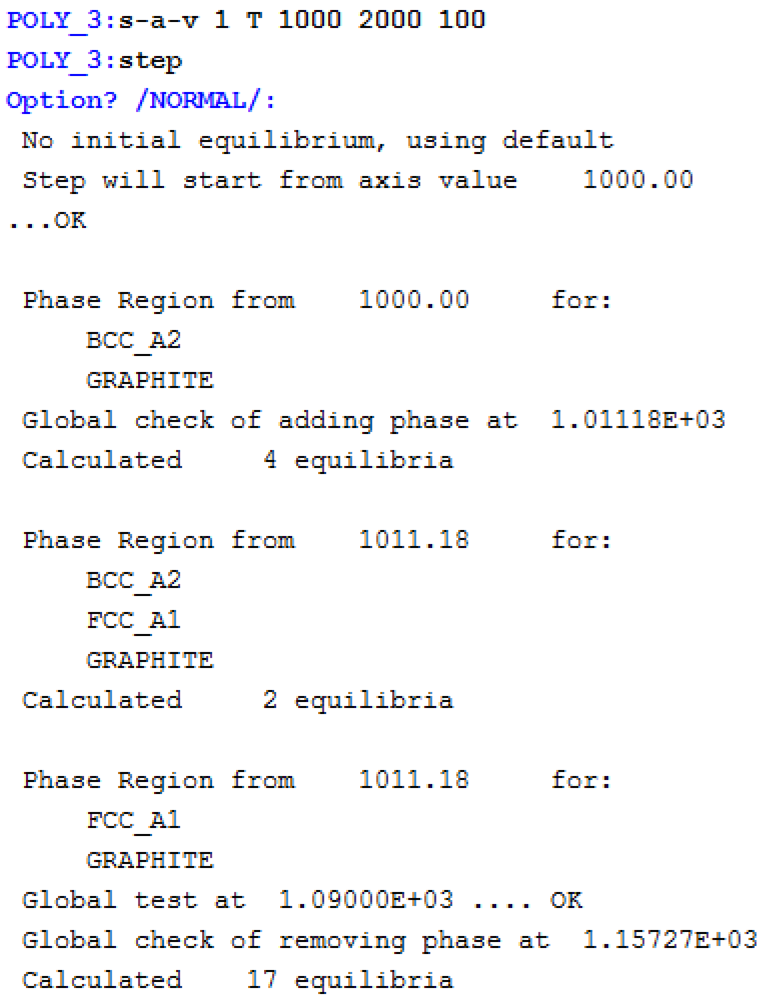
```
SET_AXIS_VARIABLE 1 T 100 2000 50
```

An axis variable must be a state variable that is set when you calculated the initial equilibrium. For example, if you set the fraction of a component in number of moles, then you cannot set the mass fraction of this component as an axis variable. Also, the minimum stepping variable value must be smaller than, and the maximum value larger than, the value that you set the state variable to when calculating the initial equilibrium.

3. Use STEP_WITH_OPTIONS and choose `Normal` to perform the stepping operation.

   The phase regions are listed along the stepping axis, the phases contained in each region, and the number of equilibria calculated in that region. Each region is defined by the phases it contains.

The number of equilibria calculated is not just the number of steps that are performed according to the step length and the minimum and maximum values on the axis variable. This is because Thermo-Calc calculates extra equilibria when a new phase is discovered in order to determine the phase region boundary more precisely.



```
POLY_3:s-a-v 1 T 1000 2000 100
POLY_3:step
Option? /NORMAL/:
 No initial equilibrium, using default
 Step will start from axis value    1000.00
...OK

 Phase Region from    1000.00     for:
     BCC_A2
     GRAPHITE
 Global check of adding phase at  1.01118E+03
 Calculated     4 equilibria

 Phase Region from    1011.18     for:
     BCC_A2
     FCC_A1
     GRAPHITE
 Calculated     2 equilibria

 Phase Region from    1011.18     for:
     FCC_A1
     GRAPHITE
 Global test at  1.09000E+03 .... OK
 Global check of removing phase at  1.15727E+03
 Calculated    17 equilibria
```

4. To plot the diagram, open the POST module and then use PLOT_DIAGRAM. By default, the X-axis represents the stepping axis variable and Y-axis represents the sum of the mole fractions of all phases (NP(*)).

Calculating a Property Diagram One Phase at a Time

There are many ways to calculate property diagrams in Thermo-Calc. One example is where you can calculate a property diagram with a separate stepping operation being performed for each phase at a time in its default most stable composition (the major constitution). This is useful if you want to create a property diagram for a heterogeneous system with both ordered phases and their disordered pairs.

To calculate a property diagram one phase at a time, use STEP_WITH_OPTIONS and when prompted choose `One_phase_at_time` to perform the stepping operation.

Calculating Several Properties in the Same Diagram

There are many ways to calculate property diagrams in Thermo-Calc. The following is another example. If you perform several stepping calculations after each other, the results of these calculations are all saved in your workspace file. This allows you to the following:

- Calculate (and then plot) missing parts of a specific property inside the first property diagram. These parts are calculated inside the range of the stepping variable with a different control condition.
- Calculate (and then plot) two or more sets of a specific property on the same property diagram for the same system. These can be calculated under different control conditions with stepping operations being performed across the same stepping axis variable range.
- Calculate phase boundary lines and then plot them in a corresponding phase diagram for the same system. This can be especially useful for some defined secondary phase-transformations. For example, if you want to find the phase boundary between BCC_A1 and BCC_B2, or the equal-Gm for two specific phases, or the equal-fraction or equal-activity for two specific phases of a certain species, then this can be useful.

Unless you have opened a new workspace file previously using SAVE_WORKSPACES , the results of the stepping calculations are saved in a RESULT.POLY3 file. To save the results of several stepping calculations in a file different from the workspace file that your results are currently saved to, then use SAVE_WORKSPACES before you perform the first stepping calculation.

SAVE_WORKSPACES overwrites and deletes the results of all previous stepping calculations.

A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

Phase Diagrams

In this section:

About Phase Diagrams

Phase diagrams have two or more independent axis variables. Any state variable that has already been set can be used as the mapping variable for a mapping calculation and then as the axis variable for a phase diagram. From a mapping calculation, many types of phase diagrams can be plotted, with one of the mapped variables as one axis variable, and with other mapped variables or any varied property (state or derived variables) or entered symbol (variables, functions or table values) as the other axis variables.

All phase diagrams consist of zero phase fraction lines. There are two distinct types of phase diagrams: those with the tie-lines in the plane of the diagram and those where the tie-lines are not in the plane. The former includes binary phase diagrams and ternary isotherms. The latter includes more general isopleth diagrams with one or more fixed extensive variables (normally, this is a composition).

- The BIN and TERN modules calculate binary and ternary phase diagrams.
- The POTENTIAL and POURABIX modules calculate the more general isopleth diagrams and other related diagrams.

The following topics describe how to calculate the types of phase diagrams in the POLY_3 module. In POLY, you can calculate phase diagram for systems with up to 40 components and with thousands of phases. You can combine activity conditions and fixed phase status and fraction conditions in any way. Thermo-Calc can calculate any arbitrary 2D section through composition space.

> There is no guarantee that the conditions set will result in a calculation that reaches an equilibrium.

Binary Phase Diagram Examples

Ternary Phase Diagram Examples

Potential Diagram Example

Pourbaix Diagram Examples

Calculating and Plotting a Phase Diagram

This topic describes how to calculate a phase diagram in the POLY module.

POLY Module Commands and POST Module Commands

1. Calculate an initial equilibrium in the POLY module.

2. Use SET_AXIS_VARIABLE to set the first axis variable, its minimum and maximum mapping value and the length of each incremental step on this axis. The first parameter of SET_AXIS_VARIABLE is the axis number and is set to 1. For example, suppose you want the mass fraction of C as your first axis variable. You want it to vary between 0 and 0.1, with the length of each incremental step being no more than 0.002. Then enter:

   ```
   SET_AXIS_VARIABLE 1 W(C) 0 .1 0.002
   ```

   > An axis variable must be a state variable that is set when you calculated the initial equilibrium. For example, if you set the fraction of a component in number of moles, then you cannot set the mass fraction of this component as an axis variable.

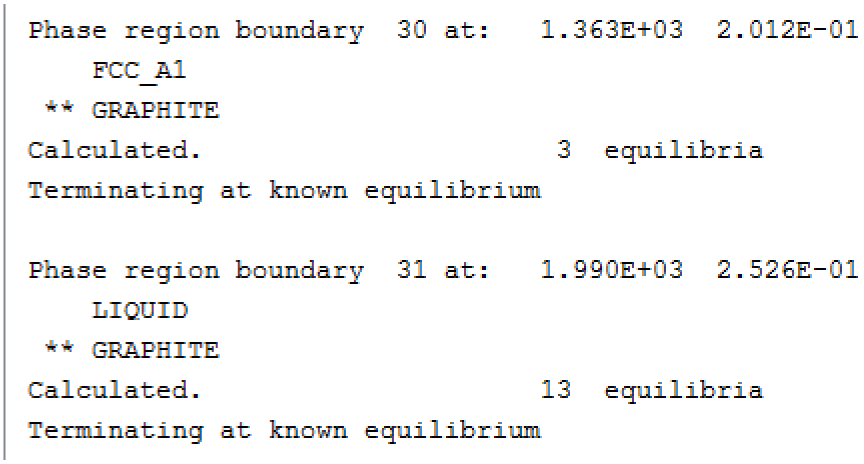
3. Use SET_AXIS_VARIABLE to set the second axis variable and specify its minimum, maximum, and step length values. The axis number is set to 2. For example, suppose you want temperature as your second axis variable and you want it to vary between 900 K and 1900 K, with an incremental step of 25 K. Then enter:

   ```
   SET_AXIS_VARIABLE 2 T 900 1900 25
   ```

4. If you want more than two axis variables, then use SET_AXIS_VARIABLE until you have set all the axis variables. You can set up to five axis variables. Axis variables 3, 4 and 5 must be set temperature, pressure or to the chemical potentials of components.

   You may want to save your workspace with SAVE_WORKSPACESbefore you perform the mapping calculation. This saves the axis variables you have set. However, it overwrites the results of any previous stepping or mapping calculations done.

5. Use MAP to perform the mapping calculation. The console lists the phase region boundaries and the phases contained on one side of each boundary.



```
Phase region boundary  30 at:   1.363E+03  2.012E-01
    FCC_A1
 ** GRAPHITE
Calculated.                      3  equilibria
Terminating at known equilibrium

Phase region boundary  31 at:   1.990E+03  2.526E-01
    LIQUID
 ** GRAPHITE
Calculated.                     13  equilibria
Terminating at known equilibrium
```

6. To plot the diagram, use POST to open the POST module and then use PLOT_DIAGRAM. By default, the X-axis represents mapping axis variable 1 and the Y-axis represents mapping axis variable 2.

About Binary Phase Diagrams

Binary phase diagrams are by far the most common found in the literature and calculated by computers. However, most real systems have more than two components and thus binary diagrams are more a kind of exercise in order to calculate more realistic phase diagrams.

You can calculate many types of binary phase diagrams with POLY, but the traditional one has one composition axis and the temperature on the other axis. This is calculated by first specifying a single equilibrium by setting conditions such as

```
SET_CONDITION T=1200, P=1E5, W(C)=.02, N=1
```

This means that the temperature should be 1200 K, pressure 1 bar, mass fraction of C is 0.02 (i.e., 2 weight percent) and the system contains one mole of atoms. Note that one does not set a condition on the amount of the second component. This is simply taken to be the rest of the system.

After setting these conditions one can calculate the equilibrium by giving the command:

```
CALCULATE_EQUILIBRIUM
```

When the calculation has converged, one continues by setting the axes for the diagram calculation. In most cases, one is interested in the complete composition range but the temperature range may vary.

```
SET_AXIS_VARIABLE 1 W(C) 0 .1 0.002
SET_AXIS_VARIABLE 2 T 900 1900 25
```

This means that the axis number 1 is taken to be the mass fraction of C which may vary between 0 and 0.1 with a maximum increment of 0.002. The axis number 2 is the temperature varied between a minimum 900 and maximum 1900 K with a maximum increment of 25.

Before starting the mapping, it is a good rule to SAVE the workspaces. If this is done just before the MAP command, and the MAP command fails for some reason, the user can restart from the situation just before mapping and try to find a better start point.

```
SAVE

MAP
```

The diagram is plotted in the post-processor. The post-processor will automatically set the same axes for plotting as used for mapping.

```
POST

PLOT
```

BINARY_DIAGRAM

The BINARY_DIAGRAM module (short name, the BIN module) enables you to quickly calculate a simple binary phase diagram. Access to specific databases designed for BIN, such as TCBIN, is required.

To enter the module, at the SYS prompt type `GOTO_MODULE BINARY`. There are no other commands for this module. Follow the prompts to plot a diagram.

Syntax	BINARY_DIAGRAM
Prompts	`Database: /TCBIN/`
	`First element` `Second element`
	`Phase diagram, Phase fraction (FE), G- OR A-curves (G/A): /Phase_Diagram/`

About Ternary Phase Diagrams

There are many types of ternary phase diagrams but perhaps the most common is the isothermal section. In this case, the temperature is constant, which means that the tie-lines are in the plane of the calculation. Isothermal sections and monovariant lines on the liquidus surface can be calculated in traditional way. They can also be calculated in the TERN module, but this requires a special database (such as PTERN).

In order to set up calculation of a ternary isothermal section in the system Al-Mg-Si, do the following (after retrieving the data from the database (TDB) module):

```
SET_CONDITION T=823,P=1E5,N=1,X(MG)=.01,X(SI)=.01
```

```
C_E
```

Note that there is no condition on the amount of Al as that is the "rest". N=1 specifies that the system is closed. This calculation gives one point inside the system. Now define the axis:

```
S-A-V 1 X(MG) 0 1 0.01

S-A-V 2 X(SI) 0 1 0.01
```

Of course, you might not be interested in the whole section, and in such cases specify different lower and upper limits for the axes. Then give a SAVE command before the MAP command:

```
SAVE almgsi-823

MAP
```

The result can be plotted in the POST module. Ternary isopleths are equally simple to calculate. Use the same conditions as above if you are interested in a section of Al-Si at 1 mole percent of Mg, just define a different set of axis:

```
S-A-V 1 X(SI) 0 1 .01

S-A-V 2 T 500 2000 25

SAVE almgsi-1mg

MAP
```

In the resulting diagrams, the tie-lines are not in the plane of the diagram, thus the lever rule etc. cannot be applied. But you can calculate more elaborate sections. An interesting diagram is the section from pure Al to Mg2Si, which is almost a quasi-binary section. In order to calculate this, set up the conditions differently:

```
SET-CONDITION T=823, P=1e5, N=1, X(MG)-2*X(SI)=0, W(MG)=.01

C-E
```

Note that there is no condition on the amount of Si as this is given by the relation X(MG)-2*X(SI)=0. Also note that you can mix conditions in X and in W. Then set the axis, save the workspace and map.

```
S-A-V 1 W(MG) 0 .1 .01

S-A-V 2 T 500 1500 10

SAVE al-mg2si

MAP
```

A special type of ternary phase diagrams is liquidus surfaces. This is still not simple to calculate as a separate start point is needed for each separate line at each temperature.

However, you can easily calculate the monovariant lines where the liquid is stable together with two condensed phases:

```
SET-CONDITION T=800, P=1e5, N=1, X(MG)=0.01, X(SI)=.01
```

```
C-E
C-S P LIQ=FIX 0.3
S-C T=NONE
C-E
```

Now there should be an equilibrium where liquid is just stable. Set the axis to be the compositions.

```
S-A-V 1 X(MG) 0 1 .01
S-A-V 2 X(SI) 0 1 .01
SAVE almgsi-luni
MAP
```

TERNARY_DIAGRAM

The TERNARY_DIAGRAM module (short name, the TERN module) enables you to quickly calculate a simple ternary phase diagram.

To enter the module, at the SYS prompt type GOTO_MODULE TERNARY. There are no other commands for this module. Follow the prompts to plot a diagram.

Syntax	TERNARY_DIAGRAM
Prompts	`Database: /FEDEMO/`

	`First element:`
	`Second element:`
	`Third element:`

	`Phase diagram, Monovariants, or Liquidus Surface: /Phase_Diagram/`
	`Temperture (C) /1000/`
	`Global minimization on: /Y/`

About Quasi-Binary and Quasi-Ternary Phase Diagrams

Quasi-binary diagrams, as well as quasi-ternary diagrams and so forth, have often been misunderstood and misused. A real quasi-binary phase diagram is for a ternary system where one component has a fixed activity or chemical potential, and a real quasi-ternary phase diagram is for a quaternary system where one component has a fixed activity or chemical potential.

A typical example of quasi-ternary system is a quaternary system Fe-Cr-Ni-C calculated at fixed carbon activity. The condition can be set as follows:

```
SET-REF-STATE C GRAPH ,,,,
SET-CONDITION T=1273, P=1e5, N=1, X(CR)=.1, X(NI)=.1, ACR(C)=.002
```

In some cases, the activity may vary in a quasi-binary section if one has a phase fixed instead (and where the phase may vary in composition). The advantage with the quasi-binary section is that the tie-lines will be in the plane of the diagram and thus the lever rule etc is obeyed.

A quasi-binary section in Ca-Fe-O when the liquid oxide is in equilibrium with liquid Fe can be specified as follows:

```
DEFINE-COMPONENTS CAO FE FEO
SET-CONDITION T=1850, P=1e5, N=1, X(CAO)=.1
CHANGE-STATUS PHASE FE-LIQ=FIX 0
```

and the mapping can be done with the following axis

```
S-A-V 1 X(CAO) 0 1 .01
S-A-V 2 T 1500 2000 25
```

However, it is a problem as FE-LIQ is not the stable phase for pure iron below 1811. One will have to calculate separate sections depending on the stable modification of Fe.

Calculating a Quasi-Binary Phase Diagram

There are many ways to calculate phase diagrams in Thermo-Calc. The following is an example where a quasi-binary phase diagram is used for calculations on a ternary system in which one component has an activity or chemical potential that is fixed (although if you have fixed a phase and the phase composition varies, then the activity or chemical potential may also vary). The tie-lines in a quasi-binary diagram are in the diagram’s plane of the diagram. This means that the calculation follows the lever rule as well as other rules.

When calculating a quasi-binary phase diagram it is necessary to set a condition on either activity or chemical potential of the third component. To specify a meaningful value it is recommended that you first change the component’s reference state using SET_REFERENCE_STATE. For example, to calculate a phase diagram for a quasi-binary Fe-Cr-O system with fixed oxygen activity, you can enter the following:

```
SET_REFERENCE_STATE O GAS ,,
```

You must also use SET_CONDITION to set the activity of the component whose activity or chemical potential you have fixed. Do this by assigning a value to the ACR state variable. For example, if the component is oxygen, you might enter

```
SET_CONDITION ACR(O)=0.2
```

Alternative Way to Set the Component Activity

As an alternative to set the activity of the component, you can Use CHANGE_STATUS to set a phase to fixed. For example, suppose you want to compute the iron-saturated section in "FeO"-SiO2. You then enter:

```
CHANGE-STATUS FCC=FIX 0
```

Calculating a Quasi-Ternary Phase Diagram

There are many ways to calculate phase diagrams in Thermo-Calc. The following is an example of a quasi-ternary phase diagram used for calculations on a quaternary system where one component has a fixed activity or fixed chemical potential.

When calculating a quasi-ternary phase diagram it is necessary to set a condition on either activity or chemical potential of the fourth component. To specify a meaningful value it is recommended that you first change the component's reference state using SET_REFERENCE_STATE. For example, to calculate a phase diagram for a quasi-ternary Fe-Cr-Ni-C system with fixed carbon activity, you can enter the following:

```
SET_REFERENCE_STATE C GRAPH ,,
```

You must also use SET_CONDITION to set the activity of the component whose activity or chemical potential you have fixed. Do this by assigning a value to the ACR state variable. For example, if the component is carbon, you might enter

```
SET_CONDITION ACR(C)=0.002
```

T0 Temperature Simulations

In this section:

About T0 Temperature Simulations

The T0-temperature is the temperature at which two phases have the same Gibbs energy for a certain composition in a multicomponent system. The T_0-temperature is located within the two-phase field between the phases and it is the theoretical limit for a transformation without diffusion. T0 temperatures are often of interest if you want to understand how diffusionless transformations work. The T0 temperature in a multicomponent system with a fixed composition is temperature at which the tangent lines of the Gibbs energies of the two target phases are the same.

If the composition of one or two components varies, the common Gibbs energy for the two phases in partial equilibrium of a diffusionless transformation becomes a plane or surface, and the T0 temperature becomes a line or plane.

See Console Mode examples tcex 23 and tcex41.

Making a T0 Temperature Simulation

This describes how to perform a T0 temperature simulation and apply a stepping calculation to its initial result.

Before you perform a T0 temperature calculation, you must have defined your initial system and be in POLY. The initial overall composition must have appropriate settings for the desired T0 temperature calculation for the two target phases.

POLY Module Commands

1. Use SET_CONDITION to set the conditions of your calculation in the same way as when you calculate an ordinary equilibrium.
2. Use COMPUTE_EQUILIBRIUM to run the calculation. The calculation does not need to reach an equilibrium in which any of the target phases is stable.
3. When you have calculated your initial equilibrium, use ADVANCED_OPTIONS and choose `T-zero`.
4. When prompted, specify the names of the two target phases for which the T0 temperature (where the phases’ Gibbs energies are equal) is to be calculated.
5. If the T0 temperature between the two target phases is calculated, this temperature (in Kelvin) is shown in the Console window.
6. If you want to do a stepping calculation based on this initial T0 temperature calculation, then use SET_AXIS_VARIABLE to specify which state variable to use as the stepping variable. This is done the same way as when you calculate a normal property diagram.

When a T0 temperature simulation is run, you cannot set temperature as the stepping variable.

7. Use STEP_WITH_OPTIONS and choose `T-zero` to initiate the stepping calculation. You are prompted to specify the names of the target phases for which the T0 temperature is calculated.

   During the STEP T-ZERO calculation procedure, the calculated T0 values are presented next to the stepping variable.

   For example, part of the output might look like this:

```
Phase Region from   1.000000E-01 for:

BCC_A2

FCC_A1

1.000000E-01          940.24

9.250000E-02          941.20

2.500000E-03          977.61

7.500000E-09          979.34
```

   When the stepping calculation has finished, you can move to the POST module and plot the T0 line against the stepping composition variable or another varying axis value. Or you can impose the calculated T0 line onto a normal phase diagram.

Paraequilibrium

In this section:

About Paraequilibrium

A paraequilibrium is a partial equilibrium where one interstitial component (such as carbon C and nitrogen N) in a multicomponent alloy can diffuse much faster than the other components (the substitutional elements, including the matrix element and alloying elements). The chemical potential for the interstitial component in two partially equilibrated phases is equal in such a case, but this is not true for the other components. In such a paraequilibrium state, it is possible to have a transformation that is partly without partitions, where a new phase of the mobile component can form with different content but where the slowly diffusing components retain their compositions.

A paraequilibrium calculation is useful when, for example, you want to study phase transformations in systems with large differences in the diffusivities of different elements. Transformations occurring under paraequilibrium states can be much more rapid than if full local equilibrium holds at the phase interface.

? Calculating a Paraequilibrium

Calculating a Paraequilibrium

This topic describes both how to calculate an initial paraequilibrium with two target phases, and how to base a stepping calculation on this initial calculation.

Before you do any paraequilibrium calculations, you must have defined your initial alloy system and be in POLY. The initial overall composition must have appropriate settings for the desired paraequilibrium calculation for the two target phases.

1. Use SET_CONDITION to set the conditions of your calculation just like when you calculate an ordinary equilibrium.

2. Use CHANGE_STATUS to set the status of the chosen interstitial components to SPECIAL. For example, if C is an interstitial component, enter:

   ```
   CHANGE_STATUS COMPONENTS C=SPECIAL
   ```

   This gives you a clear picture on u-fractions of the substitutional and interstitial components, which are different from the overall composition in the system. The SPECIAL status means that the specified components are not included in summations for mole or mass fractions. Therefore, all the composition variables plotted from paraequilibrium calculations are u-fraction related quantities.

3. Use COMPUTE_EQUILIBRIUM to run the calculation.
4. When you have calculated your initial equilibrium, use ADVANCED_OPTIONS `Paraequilibrium` to perform the paraequilibrium calculation.

5. Specify the names of the target phases of the paraequilibrium state. For example, `FCC#1 BCC` and `FCC#2 M23C6`.

> Both phases must have similar interstitial/vacancy sublattices that the fast-diffusion interstitial components occupy. Both target phases should have phase constitution definitions that cover all the defined substitutional and interstitial components of the current alloy system.

6. Specify the names of one or more fast-diffusing components. These components must be located on the interstitial/vacancy sublattices in both of the chosen phases.

> Interstitial components (for instance C and N combined) may have significantly different behaviours depending on how they are partitioned in different structured phases.

If the paraequilibrium between the two specified phases is successfully calculated, then a message is displayed, for example:

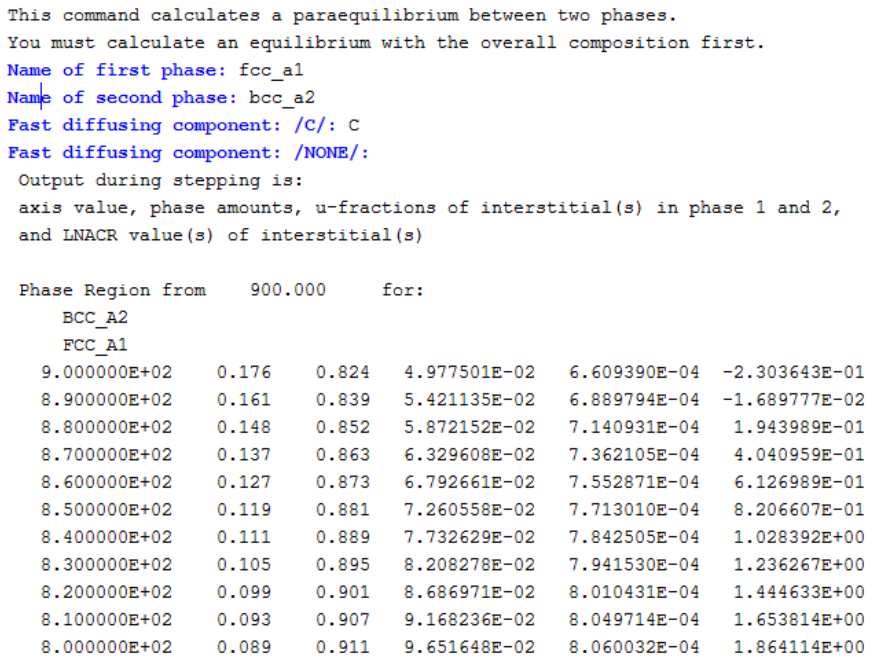
```
NP(FCC) = 0.3586 with U-fractions C = 2.71821E-02 N =
4.1548129E-03

NP(BCC) = 0.6414 with U-fractions C = 7.10061E-04 N =
2.3781027E-04

All other compositions are the same in both phases
```

The first two lines show the phase amounts expressed in mole-percent [NP(phase)] and the contents of the interstitial components C and N in each phase. These contents are expressed in u-fractions. The third line states that the compositions of the matrix component and all the remaining compositions (regarding substitutional components) are equal in the two target phases at the paraequilibrium state.

7. If you want to do a stepping calculation based on this initial paraequilibrium, then use SET_AXIS_VARIABLE to specify which state variable to use as the stepping variable. This is done exactly in the same way as when you calculate a normal property diagram.

8. Use STEP_WITH_OPTIONS → `Paraequilibrium` to initiate the stepping calculation. You are prompted to specify the names of the target phases of the paraequilibrium states as well as the fast-diffusing components.

The stepping calculation is performed, and the different phase regions are listed with columns for the value of the stepping variable, the amounts of the two target phases, the u-fractions of interstitial(s) in each of the two phases, and the LNACR value(s) of the interstitial component(s).



```
This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_a1
Name of second phase: bcc_a2
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
 Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
 and LNACR value(s) of interstitial(s)

 Phase Region from    900.000     for:
     BCC_A2
     FCC_A1
   9.000000E+02    0.176    0.824   4.977501E-02   6.609390E-04  -2.303643E-01
   8.900000E+02    0.161    0.839   5.421135E-02   6.889794E-04  -1.689777E-02
   8.800000E+02    0.148    0.852   5.872152E-02   7.140931E-04   1.943989E-01
   8.700000E+02    0.137    0.863   6.329608E-02   7.362105E-04   4.040959E-01
   8.600000E+02    0.127    0.873   6.792661E-02   7.552871E-04   6.126989E-01
   8.500000E+02    0.119    0.881   7.260558E-02   7.713010E-04   8.206607E-01
   8.400000E+02    0.111    0.889   7.732629E-02   7.842505E-04   1.028392E+00
   8.300000E+02    0.105    0.895   8.208278E-02   7.941530E-04   1.236267E+00
   8.200000E+02    0.099    0.901   8.686971E-02   8.010431E-04   1.444633E+00
   8.100000E+02    0.093    0.907   9.168236E-02   8.049714E-04   1.653814E+00
   8.000000E+02    0.089    0.911   9.651648E-02   8.060032E-04   1.864114E+00
```

It is possible to now move to the POST module and plot some of the results of the calculation. For an example of a paraequilibrium calculation and how it can be plotted, see Console Mode example tcex23.

Potential Diagrams

In this section:

About Potential Diagrams

If you have a metal-oxide/sulphide-gas interaction system, you might want to calculate a so-called potential phase diagram given certain temperature and pressure. A potential diagram uses the activities of two major species in the gaseous mixture phase as mapping variables. The activities (that is, the fugacities at 1 bar) of these two species are typically set as the X- and Y-axis when the diagram is plotted. The phase relations between the gaseous mixture and various metal forms, metal-oxides, metal-sulphides, or other metal-bearing solids, are represented by different fields controlled by these two potential quantities.

This topic describes how to calculate such potential diagrams with the POTENTIAL module, and how to later modify the pressure of such a calculation in POLY. The calculation done by the POTENTIAL module always assumes a pressure of 1 bar.

POTENTIAL_DIAGRAM

The POTENTIAL_DIAGRAM (POT or POTENTIAL) module is a potential phase diagram calculation module.

If you have a metal-oxide/sulphide-gas interaction system, you might want to calculate a so-called potential phase diagram given certain temperature and pressure. A potential diagram uses the activities of two major species in the gaseous mixture phase as mapping variables. The activities (that is, the fugacities at 1 bar) of these two species are typically set as the X- and Y-axis when the diagram is plotted. The phase relations between the gaseous mixture and various metal forms, metal-oxides, metal-sulphides, or other metal-bearing solids, are represented by different fields controlled by these two potential quantities.

To enter the module, at the SYS prompt type `GOTO_MODULE POTENTIAL`.

There are no commands for this module. Follow the prompts and see About Potential Diagrams for details about how to calculate using potential diagrams.

Syntax	POTENTIAL_DIAGRAM
Prompts	`Database: /POT/` Press <Enter> and the program lists the available databases. Type one of the database names and press <Enter> to select. The following default elements are then based on the chosen database.
	`Matrix element: /Fe/`
	`First potential species: /S1O2/`
	`Second potential species: /O2/`
	`Temperature: /1000/`

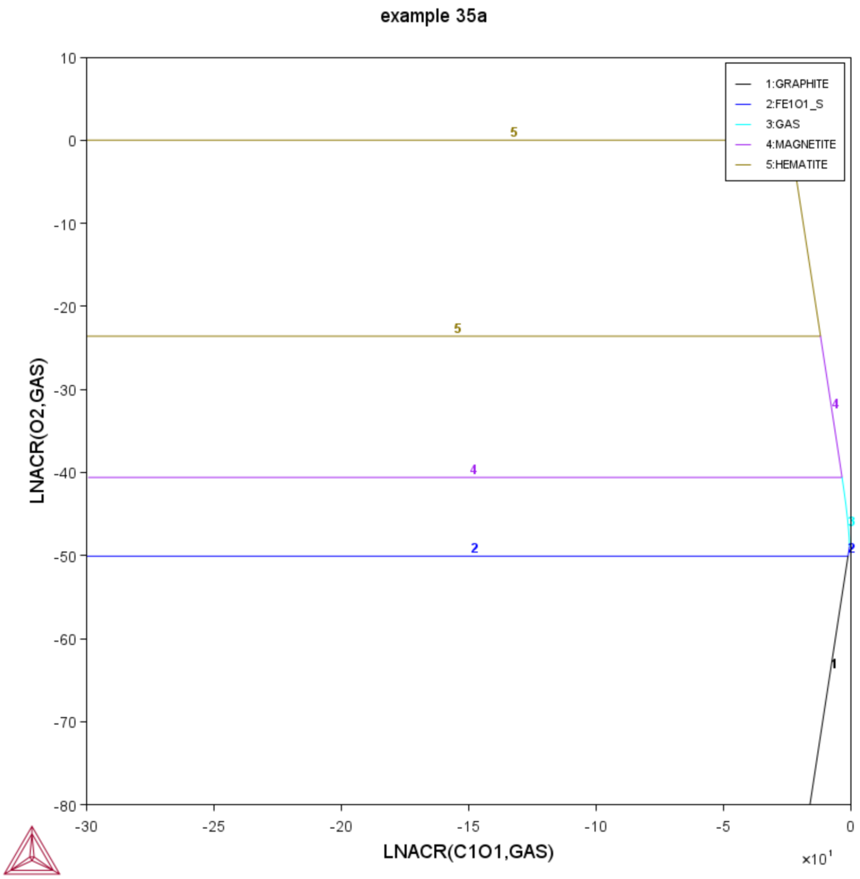
Calculating a Potential Diagram

You need access to a substance or solution database that contains a gaseous mixture phase, metals (or alloys), and solids such as metal-oxides, sulphides, sulphates, carbonates, silicates, nitrides or nitrates (stoichiometric or solution phases).

1. Use GOTO_MODULE and enter `POTENTIAL`.
2. Specify which substance or solution database to use. Any substance or solution database can be used that has a gaseous mixture phase, metals (or alloys), and solids such as metalxides, sulphides, sulphates, carbonates, silicates, nitrides, and nitrates (stoichiometric or solution phases).
3. Specify the matrix element (a metal) and the two gaseous species that define you metal-gas interaction system. The names of these components must be available in the database you are using.
4. Set the temperature (in Kelvin). (The pressure is always 1 bar.)

   A potential diagram with the activities of the two gaseous species as mapping variables is calculated. These mapping variables are also set as the axis variables in the plotted diagram.

   An example diagram (Console Mode example 35).



A POLY3 file is also automatically saved in the current working directory with the default name POT.POLY3.

5. When the diagram is plotted, it opens the POST module where you can modify the plotted diagram in any way you like.

Calculating a Potential Diagram with Different Pressure

It is possible to modify both the calculation and the plotted diagram that the POTENTIAL module generates in the POLY and POST modules. You can do this by opening a POLY3-file with the results from a POTENTIAL module calculation in either POLY or POST. You can modify the calculation in the same way that you can modify any ordinary mapping calculation or phase diagram. For example, this is useful for calculating a potential diagram at a pressure other than 1 bar.

POLY Module Commands

You must have calculated a potential diagram already, and have the saved POLY3-file available.

1. Use GOTO_MODULE and enter `POLY`.

2. Use READfollowed by the name of the POLY3 file that contains the results of the potential diagram calculation that you want to modify.

   A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

3. This opens the workspace file and loads the previous settings and results. The activities of the two gaseous species is now part of the conditions, and these conditions are set as the mapping variables.

4. Use SET_CONDITION to specify the pressure under which you want the potential diagram to be calculated. For example, to set the pressure to 1000 bar, enter:

   ```
   SET_CONDITION P=1e8
   ```

5. Use COMPUTE_EQUILIBRIUM to compute the initial equilibrium.

   You may also want to use ADD_INITIAL_EQUILIBRIUM to calculate some additional equilibria that the mapping calculations are based on.

6. Use MAP to perform the mapping calculations.
7. Use GOTO_MODULE and enter `POST` to set conditions for visualization and to plot the diagram.

Scheil Simulations

In this section:

About the Scheil-Gulliver Solidification Simulations

In Console Mode most of the set up for the Scheil module is via the START_WIZARD command where you are prompted to answer a series of questions. You can also perform Scheil calculations in Graphical Mode using the Scheil Calculator, which is recommended for most users. See Scheil in Graphical Mode vs Console Mode to compare.

Thermo-Calc is often used to perform equilibrium calculations, but some non-equilibrium transformations or partial-equilibrium transformations can also be simulated.

A well-known example of a non-equilibrium calculation is the *Scheil-Gulliver solidification simulation*. In Thermo-Calc, the available Scheil-Gulliver solidification simulations are *classic* Scheil, Scheil with *back diffusion* in the primary phase, or Scheil with *solute trapping*. There are also configuration options available with *fast diffusers* for the classic and back diffusion models.

Classic Scheil Simulation

This is a Scheil simulation based on the well-known *Scheil-Gulliver* model. If this model is used without "fast diffusers" it is *Classic Scheil* simulation with the following assumptions:

- Diffusion in the liquid phase is assumed to be very fast, that is, infinitely fast.
- Diffusion in the solid phases is so slow that it can be ignored, that is, diffusion is assumed to be zero.
- The liquid/solid interface is in thermodynamic equilibrium.

In this Classic Scheil simulation the temperature is decreased step-by-step. When the temperature drops below the liquidus temperature the equilibrium amount and composition of solid and liquid phase is calculated. The solid phase is removed from the system and only the amount and composition of the liquid phase is used for the next calculation step at a lower temperature. Again, the equilibrium amount and composition of solid and liquid phase is calculated and again the solid phase is removed from the system for the next step. This procedure is repeated until the last liquid disappears.

This calculation procedure is equivalent to assuming that there is no diffusion in the solid phase and infinitely fast diffusion of all elements in the liquid phase. It has been shown to be a good approximation of the solidification of most alloys such as Ni-superalloys, Cu alloys, Al alloys, Mg alloys, and others. However, in materials with interstitial elements, such as carbon, ignoring diffusion in the solid causes discrepancies with experimental results.

Interstitial elements have much faster diffusion rates. The assumption of no diffusion in the solid phase during solidification is thus not correct at most industrial or lab-scale solidification rates.

For this reason, a variant of the Scheil simulation was developed and implemented in Thermo-Calc, where one or more elements can be defined as *fast diffusers*. See Other Options: Fast Diffusers and Scheil Simulations.

Scheil Simulation with Back Diffusion in Primary Phase

The *Scheil simulation with back diffusion in primary phase* kinetic model quantitatively takes into account the real back diffusion of all elements in the primary solid phase (typically the FCC or BCC phase). This model requires the use of both a thermodynamic and mobility database. The calculation also requires the cooling rate to be specified; a fast cooling rate allows for less time for back diffusion and the simulation result is similar to the classic Scheil-Gulliver solidification simulation. A very slow cooling rate allows for almost complete back diffusion, the solidification simulation is then close to an equilibrium calculation. It also requires that the size of the solidification domain is specified. In most cases this domain size corresponds to the secondary arm spacing, as this is where typically the liquid is trapped during solidification.

> The secondary arm spacing also depends on the cooling rate. For this reason, a simple empirical relation between cooling rate and secondary arm spacing is predefined in Thermo-Calc.

For the *Scheil simulation with back diffusion in primary phase* model the following assumptions are made.

- Diffusion of all elements in the liquid phase is infinitely fast.
- Diffusion of all elements in the primary solid phase are quantitatively calculated using mobility data, a cooling rate and a domain size (typically this is the secondary arm spacing).
- The liquid/solid interface is in thermodynamic equilibrium.

Also see Other Options: Fast Diffusers and Scheil Simulations.

Scheil with Solute Trapping

The *Scheil with solute trapping* model simulates deviation from local equilibrium for the primary phase. It is useful for high solidification speeds, such as those seen in additive manufacturing applications.

For equilibrium- and classical Scheil-type solidification simulations thermodynamic equilibrium is established at the solid-liquid interface. This means that solutes are partitioned between the solid and liquid phases according to solidus and liquidus lines of the phase diagram. The assumption of thermodynamic equilibrium at the solid-liquid interface however, is invalid for very fast solidification rates, as encountered for example during additive manufacturing. The faster the solidification rate, the less the partitioning at the interface, which can be perceived as that solutes in the liquid are trapped in the advancing solid phase, hence the term *solute trapping*.

The *Scheil with solute trapping* model calculates the solute partitioning between liquid and primary solid that deviates from thermodynamic equilibrium due to solidification speed.

The following assumptions are made:

- Only one primary solid phase forms dendrite, NOT necessarily the first solid phase.
- Solute trapping in primary solid phase only. Other solid phases have equilibrium compositions following Scheil model.
- Dynamic liquidus for primary solid phases is dependent on solute trapping and solidification speed.
- Amounts of solid phases are dependent on solute trapping and solidification.

More theory details are in About Scheil with Solute Trapping.

Other Options: Fast Diffusers and Scheil Simulations

If a *Classic Scheil* or *Scheil simulation with back diffusion in primary phase* model is selected plus one or more *Fast diffuser* checkboxes selected, then Thermo-Calc takes into account the concept of the *fast diffuser*. Typically, C is defined as a fast diffuser, but also other elements such as N, O, or others can also be defined.

Fast diffuser does not quite define this since diffusion is not actually simulated. It is simply assumed that the “fast diffusers” distribute throughout the solid and liquid phase according to thermodynamic equilibrium. This corresponds to *infinitely fast diffusion* for the selected elements.

For a *Classic Scheil* model with the compositions defined with *Fast diffuser* the following assumptions are made.

- Diffusion of all elements in the liquid phase is infinitely fast.
- Diffusion of all elements in the solid phases, except the ones defined as “fast diffusers”, is zero.
- Diffusion of the elements defined as “fast diffusers” is infinitely fast in the solid phase.
- The liquid/solid interface is in thermodynamic equilibrium.

For a *Scheil simulation with back diffusion in primary phase* model with the compositions defined with *Fast diffuser* the following assumptions are made.

- Diffusion of all elements in the liquid phase is infinitely fast.
- Diffusion of all elements in the primary solid phase are quantitatively calculated using mobility data, a cooling rate and a domain size (typically this is the secondary arm spacing).
- Diffusion of the elements defined as “fast diffusers” is infinitely fast in the solid phase.
- The liquid/solid interface is in thermodynamic equilibrium.

The Classic Scheil simulation and Classic Scheil simulation with fast diffuser models can be considered *thermodynamic* models. There are clear limitations as a certain amount of back diffusion always takes place in the solid phase at real solidification.

You can also use the more sophisticated *Scheil simulation with back diffusion in primary phase* kinetic model. Adding the fast diffuser option to this can be useful, for example for interstitials like C in steels where these then equilibrate in all phases and not just the primary phase.

Homogenization, Segregation Profiles, and the Diffusion Module

Scheil calculations can be used in diffusion simulations with the Diffusion Module (DICTRA).

Homogenization is a process were you want to get rid of the composition segregation from solidification with a homogenization heat treatment. This composition segregation can be simulated with Scheil. Then with the Diffusion Module (DICTRA), you input the secondary dendrite arm spacing to get the right diffusion distances. With composition profile from file the idea is that you should be able to input for example a measured composition profile (from EDS/WDS, micro-probe etc). This could also be a segregation profile but also composition profiles over a weld, substrate/coating, diffusion couple, and so forth.

Summary

The available Scheil-Gulliver solidification simulations are *classic* Scheil, Scheil with *back diffusion* in the primary phase, or Scheil with *solute trapping*. There are also configuration options available with *fast diffusers* for the classic and back diffusion models.

There is also connectivity to the Diffusion Module (DICTRA) and *homogenization* where you collect data from a Scheil solidification calculation, which is then used as part of the kinetic homogenization simulation of segregated composition profiles.

Scheil in Graphical Mode vs Console Mode

The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. this model requires the use of a mobility database.

In Thermo-Calc, the Scheil calculation allows the calculation of:

- The solidification range of an alloy.
- Depression of the solidus temperature due to segregation.
- Composition of the last liquid to disappear in segregation pockets.
- Phases formed on final solidification in segregation pockets.
- The composition gradient in the primary solid phase(s) (segregation profile).
- Solute trapping to simulate deviation from local equilibrium for the primary phase
- Kinetic homogenization simulation of segregated composition profile (diffusion calculations)

Scheil in Graphical Mode vs Console Mode

Type of Calculation	*Console Mode*	*Graphical Mode*
Classic Scheil	Use the START_WIZARD command to answer prompts	Scheil Calculator > click the **Classic Scheil** button on the Configuration window. On the My Project Configuration window under Getting Started, click **Quick Start** and select **Scheil solidification simulation**.

Type of Calculation	***Console Mode***	***Graphical Mode***
Scheil with back diffusion in the primary phase	USE_BACK DIFFUSION command (turn on) then use the START_WIZARD command to answer prompts	Scheil Calculator > click the **Scheil with back diffusion in the primary phase** button on the Configuration window then enter the settings as needed. A mobility database is required.
Scheil with solute trapping	SOLUTE_TRAPPING command (turn on) then use the START_WIZARD command to answer prompts	Scheil Calculator > click the **Scheil with solute trapping** button on the Configuration window then enter the settings as needed.
Fast diffusers and Classic Scheil	Use the START_WIZARD command to answer the prompt`Fast diffusing components`where you enter the elements that diffuse fast in solid phases and can assume to be in equilibrium in the whole phase. E.g. C in a steel.	Scheil Calculator > click the **Classic Scheil** button plus one or more of the **Fast diffuser** checkboxes next to the composition(s) on the Configuration window then enter the settings as needed.
Fast diffusers and Scheil with back diffusion in the primary phase	USE_BACK DIFFUSION command (turn on) then use the START_WIZARD command to answer the prompt `Fast diffusing components`where you enter the elements that diffuse fast in solid phases and can assume to be in equilibrium in the whole phase. E.g. C in a steel.	Scheil Calculator > click the **Scheil with back diffusion in the primary phase** button plus one or more of the **Fast diffuser** checkboxes next to the composition(s) on the Configuration window then enter the settings as needed. A mobility database is required.
Homogenization	Use the EVALUATE_SEGREGATION_PROFILE command before START_WIZARD to generate the segregation profile to file. In DICTRA_MONITOR use INPUT_SCHEIL_PROFILE for use of segregated profile in simulation. An additional license to the Diffusion Module (DICTRA) is needed to work with more than three components.	Use the **Homogenization** template under **Non-Equilibrium** to automatically set up the project tree with the defaults needed to work with this. An additional license to the Diffusion Module (DICTRA) is needed to work with more than three components.

Scheil-Gulliver Examples

? About the Scheil-Gulliver Solidification Simulations

tcex15 - Simulating the Solidification of a Cr-Ni Alloy

This is an example of a solidification simulation of a Cr-Ni alloy. There is no back diffusion in the solid, i.e. this is a classic Scheil-Gulliver simulation. The FEDMO database is used and included with your installation.

These commands are of note and used in this example:

- START_WIZARD
- COMPUTE_TRANSITION
- ADD_INITIAL_EQUILIBRIUM
- ENTER_SYMBOL
- ADVANCED_OPTIONS
- STEP_WITH_OPTIONS
- MAKE_EXPERIMENTAL_DATAFILE
- CHANGE_STATUS

tcex30a and 30b - Scheil Calculation for an Al-4Mg-2Si-2Cu Alloy

The Equilibrium Calculation Module (POLY3) and About the Scheil-Gulliver Solidification Simulations

These examples show two ways to do a Scheil calculation for an Al-4Mg-2Si-2Cu alloy. In part A, you use the POLY3 module and the STEP_WITH_OPTIONS command with an EVALUATE option. Then in part B you use the SCHEIL module commands to do the same thing. Data from the COST2 database is used and included with the example in the file named *tcex30_cost2.TDB*.

tcex48 - Scheil Solidification with C Back Diffusion

The FEDEMO database is used and the example is available to all users.

This is an example of Scheil solidification with simulated back diffusion of carbon in solid phases. The results are compared between a simple Scheil and equilibrium calculation. First perform a Partial Equilibrium Scheil by assigning carbon as a fast diffusing element. Plot solidification curve and a microsegregation diagram and save to file (so called .exp files). The "back diffusion" of C in solid phases is not from any calculation involving kinetics, but comes from the equilibration of chemical potential of C at each step in temperature, thus allowing each already solidified part of the system to change its C concentration.

> See tcex54 for an example that calculates "real" back diffusion. This model requires a kinetic (mobility) database in addition to the thermodynamic one. Also see About the Scheil-Gulliver Solidification Simulations for details about the different Scheil options.

tcex54 - Scheil Solidification of an Al-2.1Cu-1Si Alloy including Back Diffusion

This is an example of a solidification simulation of a Al-2.1Cu-1Si alloy. The back diffusion option in the Scheil module is used, i.e. there is back diffusion in the primary phase. The example uses both the thermodynamic ALDEMO and mobility MALDEMO demo databases included with your installation.

tcex57 - Scheil Solidification with Solute Trapping

This is an example of a solidification simulation of a Al-7.5Si-0.2Cu system. The solute trapping option in the Scheil module is used. The example uses the thermodynamic ALDEMO demo database included with your installation.

See the Graphical Mode example T_13: Scheil Solidification with Solute Trapping for an additional comparison to Classic Scheil.

Simulating a Scheil Solidification Process

SCHEIL Module Commands

About the Scheil-Gulliver Solidification Simulations

Simulating a Scheil-Gulliver solidification process involves calculating the liquid composition of a higher-order multicomponent system at each step of a cooling process, and resetting the liquid composition as the composition of the entire system (after having removed all amount of solid phase).

The step-by-step instructions below are intended as a simple example of setting up a calculation using the wizard in Console Mode. You can also use the macros available and briefly described in Scheil-Gulliver Examples.

The following does not include any prompts related to using back diffusion or solute trapping. See START_WIZARD for additional details about when these options are enabled with the USE_BACK_DIFFUSION and SOLUTE_TRAPPING commands.

1. At the prompt type GOTO_MODULE SCHEIL.
2. Type START-WIZARD and press <Enter>.
3. Specify which `Database` to use. Type `?` for a list of available databases based on your license.
    - Type `FEDEMO` for this example.
4. Specify the `Major element or alloy` in your system. For example, enter `Fe` (steel/Fe-alloy), `Al` (Al-based alloy), or `Ni` (Ni-based super alloy).
    - Type `Fe` for this example.
5. Set whether to specify the `Composition input in mass (weight) percent` (the default) or in `Mole percent`. Press <Enter> to keep the default for mass (weight) percent or type `N` to use mole percent.
    - Keep the default for this example (press <Enter>).
6. Specify the name of the `1st alloying element`. You can directly specify mass or mole percent after the name. If this is not specified, then you are prompted to enter it separately.
    - Type `Cr 5` for this example.
7. Specify the other alloying elements in the same way as you specify the first.
    - Type `C 1` for this example.

8. After you have specified your last alloying element, press <Enter>. This ends the process of defining the bulk composition of the alloy system.

> You can also specify all the alloying elements and their corresponding compositions on the same line when you are prompted to specify your first alloying element. As a general example, you can enter `Cr 5 Ni 1 Mo 0.5 C 0.01 N 0.02`.

   - Press <Enter> for this example.

9. Specify the starting `Temperature (C)` in Celsius. The default is `2000`.

   This value should be sufficiently high so that the solidification simulation starts with the alloy system in the liquid single-phase region.

   - Keep the default for this example (press <Enter>).

10. At the `Reject phase(s)` prompt enter the name of the phases to reject or press <Enter> for the default `NONE`.
    - Keep the default s for this example (press <Enter>).

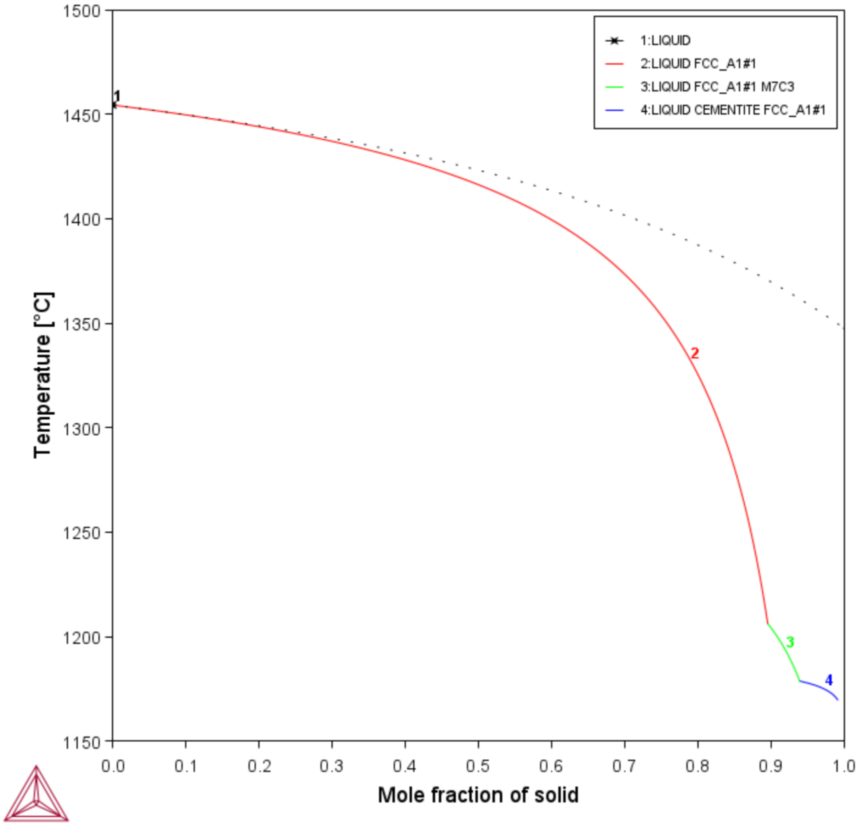
11. At the `Restore phase(s)` prompt you may want to restore a phase that you rejected when you ran the simulation earlier, or you may want to restore a phase that is rejected by default in your database. Enter the name of the phases to restore or press <Enter> for the default `NONE`.
    - Keep the default for this example (press <Enter>).

12. When prompted `OK?` type `N` to go back to reconsider which phases to reject or restore. Type `Y` to continue. The thermodynamic data about the alloy system you defined is retrieved from the database.
    - Keep the default for this example (press <Enter>).

13. At the `Should any phase have a miscibility gap check` prompt, press <Enter> for the default `N` or type `Y` then specify the `Phase with miscibility gap`.
    - For this example, type `Y` then enter `FCC` as the `Phase with miscibility gap`.

14. If you answer `Y` to the miscibility gap check, then next enter the following for `Major constituent(s) for sublattice 1` and `Major constituent(s) for sublattice 2`.
    - Enter `Cr` for sublattice 1 and `C` for sublattice 2 in this example. Then at the `Phase with miscibility gap` prompt press <Enter>. The system responds with `LIQUID PHASE NAME: LIQUID`.

15. Specify the names of any `Fast-diffusing components`. Press <Enter> for `NONE` or type all the names on the same line then press <Enter>. Keep the default for this example (press <Enter>).



After the Scheil-Gulliver solidification simulation runs, the diagram Temperature versus Mole Fraction of Solid is plotted in the Console Results window.

State Variables for Scheil

Post processing is done the same way as POLY-3: specific variables for plotting in the Scheil module are listed.

POLY Module Commands

For a comparable list in Graphical Mode, see Scheil Calculator Available Plot Variables.

The variables can be plotted along the X- and Y-axes. In the table, *ph* is an abbreviation of *phase*, and *el* is an abbreviation of *element*. An asterisk (*) can be used as a wild character for *el* and *ph*. Use the abbreviations of the variables when you specify what the X- and Y-axes represent in a diagram.

Abbreviation	***State Variable***
T	Temperature in Celsius
NL/BL/VL	Mole/mass fraction of liquid
NS/BS/VS	Mole/mass fraction of all solid phases
NS(ph)/BS(ph)	Mole/mass fraction of a solid phase
VS(ph)	Volume fraction of a solid phase
W(ph,el)	Weight fraction of an element in a phase
X(ph,el)	Mole fraction of an element in a phase
Y(ph,el)	Site fraction of an element in a phase
NN(ph,el)	Distribution of an element in a phase
NH/BH	Total heat per mole/gram (top curve) and Latent heat per mole/gram (bottom curve)
CP/BCP	Apparent heat capacity per mole/gram
NV/NV(ph)	Molar volume of the system or a phase
DS/DS(ph)	Average density of the system or a phase
BT	Apparent volumetric CTE of the system
DVIS(ph)	Dynamic viscosity of a phase
KVIS(ph)	Kinematic viscosity of a phase
SURF(ph)	Surface tension of a liquid phase
ELRS/ELRS(ph)	Electrical resistivity of the system or a phase
ELCD/ELCD(ph)	Electrical conductivity of the system or a phase

Abbreviation	*State Variable*
THCD/THCD(ph)	Thermal conductivity of the system or a phase
THRS/THRS(ph)	Thermal resistivity of the system or a phase
THDF/THDF(ph)	Thermal diffusivity of the system or a phase
DGV	Driving force for evaporation
DHV	Evaporation enthalpy
MMG	Molar mass of gas
XAVG(el)	Mole fraction of an element in solid phases
WAVG(el)	Mass fraction of an element in solid phases

Aqueous Solutions and Pourbaix Diagrams

In this section:

About Aqueous Solutions and the Pourbaix Diagram

This command or module is not available with GES6.

GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features. However, not all GES5 functionality is implemented in GES6. In such cases (except for the POURBAIX module), GES6 falls back silently and uses functionality from GES5 in the background.

Heterogeneous equilibrium calculations involving aqueous solutions are not different from other equilibrium calculations, but the setup of the equilibrium conditions and the reference states of the system is more complex. For example, the pH and Eh values of the aqueous solution phase are normally complex functions of bulk composition, temperature and pressure conditions.

For some simple systems, thermodynamic approximations of pH-Eh calculations can be used. But Thermo-Calc also has comprehensive thermodynamic models and databases for various non-ideal solution phases. These let you accurately calculate pH and Eh property diagrams (and many other types of property diagrams) in complex aqueous solutions in a variety of conditions.

A Pourbaix diagram is a kind of phase diagram that shows the stability boundaries for a metal-aqueous interaction system. The phase boundaries are shown as a function of pH (acidity) and Eh (standard hydrogen electronic potential). An aqueous solution phase is always present in such a system. At a given pH and Eh, a metal may lose its stability to a soluble or corrosive aqueous solution, or be in equilibrium with either the aqueous solution (insoluble/immune) or with a secondary-phase file that has formed (consisting of oxides, hydroxides, sulphides or other solids). In the latter case, further dissolution of the passive or protective metal is prevented.

A Pourbaix diagram is a pH-Eh phase diagram where the tie-lines are not in the plane. The chemical potentials or activities of two system components (H+ and EA) are used as mapping variables and the pH and Eh quantities are normally plotted on the X- and Y-axes of the diagram. You can use many other properties as axis variables in various property diagrams for the interaction system at a specific temperature and pressure. The phase relations between the aqueous solution and various metal forms, oxides, hydroxides, sulphides, sulphates, nitrates, silicates, carbonates and other solids, or gaseous mixtures, are represented as different fields defined by acidity and electric potential.

The POURBAIX module lets you construct Pourbaix diagrams and other types of property diagrams for heterogeneous interaction systems with aqueous solution phases. The compositional definition and variations and the basic solvent and electron components H2O, H+1 and ZE are automatically determined by the aqueous solution phase in the Pourbaix module.

See Console Mode examples tcex40 and tcex53.

Key Components

These key components are defined as follows:

Component	Component status	Reference state	Ref-T(K)	Ref-P(Pa)
H2O	ENTERED	AQUEOUS	*	100000
H+1	ENTERED	SER		
ZE	ENTERED	REFERENCE_ELECTRODE	*	100000

Besides the aqueous solution phase, your system may also contain a gaseous mixture phase. Other neutral and charged gaseous species may also be constituents. For multicomponent systems there are normally also some interacting solid phases (stoichiometric or solution) as the so-called secondary phases. These are typically the matrix and/or precipitate phases in the alloys of interest.

Some databases have been specially developed for the Pourbaix module’s diagram calculations. Such a database contains all necessary phases, i.e., an aqueous solution phase, a gaseous mixture phase, some alloy solid solution phases and some secondary solid phases. Databases developed for the Pourbaix module include *PAQ* (TCS Public Aqueous Solution Database) or *PAQS* (TGG Public Aqueous Solution Database).

If such a dedicated Pourbaix module is not used, then an aqueous solution database such as *TCAQ* (TC Aqueous Solution Database), *AQS* (TGG Aqueous Solution Database), or any user-specified aqueous databases can be used.

This database contains at least the AQUEOUS and REFERENCE_ELECTRODE phases. The aqueous solution database needs to be appended with additional required data and phases, such as interacting alloy (solid) solution phases and secondary (solid and liquid) phases. Additional data is from one or more databases, such as SSUB/SSOL/TCFE or other substances/solutions databases.

Calculating a Pourbaix Diagram

The POURBAIX module lets you construct Pourbaix diagrams and other types of property diagrams for heterogeneous interaction systems with aqueous solution phases.

When calculating a Pourbaix diagram, you need to have a database with an aqueous solution phase (that is, a phase with water as the dissolving solvent and with aqueous cation/anion and complex species as the dissolved solutes). Due to restrictions of aqueous solution models (SIT, HKF, Pitzer) used in the Thermo-Calc software, the aqueous solution database must be designed in the same Thermo-Calc database format as that used in the PAQ, PAQS, TCAQ and AQS databases for the aqueous solution phase.

Pourbaix diagram calculations are done in the advanced Pourbaix module.

How to Calcuate a Pourbaix Diagram

1. At the `SYS` prompt, enter GOTO_MODULE POURBAIX.
2. At the `Need any instruction on the POURBAIX module?` prompt, press <Enter> to skip or enter `Y` to learn more.
3. Press <Enter> at the prompt `Enforce a PAUSE after plotting when running a MACRO?`.
4. Press <Enter> to accept the default `1` to `Start a completely new POURBAIX diagram calculation` or enter `3` to `Open an old file and make another POURBAIX calculation`.

   To choose `3`, you must have already done a Pourbaix calculation and have it saved in a POLY3 file. The new calculation uses the same system definition as the previous calculation, but the other conditions, such as the bulk composition, temperature and pressure, can be modified in the next step.

5. Type `Y` or `N` to set whether to `Consider the GAS phase` (gaseous mixture phase) in the calculation.

   The gaseous mixture phase should at least contain H2O, O2 and H2. If a GAS phase is not considered, then only the interactions between the aqueous solution phase and various solid phases (alloy phases and secondary phases) are calculated. Such a calculation may not accurately present all the heterogeneous interactions. Some secondary phases are therefore usually needed. Such phases exist in the PAQ or PAQS Public Aqueous Solution Databases. They can also be appended from the SSUB/SSOL/TCFE or other appropriate substances/solutions databases.

6. Type `Y` or `N` to set whether to `Use single database` (`Y`) or a multiple database (`N`).

   If you choose to use a single database, at the `Combined Database: /PAQ2/` prompt specify a database that is specially developed for the Pourbaix module's diagram calculations.

   If you choose to use a multiple database, then you are prompted to specify an aqueous solution database and to append any additional required data and select necessary phases, such as various interacting alloy (solid) solution phases, and secondary (solid and liquid) phases, for example.

7. Specify all your solutes and the molality of each solute when prompted to do so. This can be done in terms of elements (such as Fe, Ni, Na, Cl, C or S) or arbitrary complex species (such as NaCl, CO2, CoCl3, Fe0.93S, NaSO4-1, or H2SO4). You can enter the element/species and the molarity on one line (for an example, NaCl 2.5).

   The definition of your system and its initial bulk composition is now presented.

   ❗ The first letter of the element abbreviation must always be upper case. Any second letters must be lower case. When you have finished your specification, press <Enter> when asked to specify `Next solute`.

8. Type `Y` to confirm the defined system and its bulk composition.

   The thermodynamic data for your system is now retrieved from the database(s) chosen.

9. Answer the questions that you are prompted regarding various parameters of your calculation. You are asked to do any of the following:
   - `Rejectphase(s)` or `Restore phases(s)`
   - Check for miscibility gaps on any phase (`Should any phase have a miscibility gap check?`)
   - `Enforce the Global Minimization Technique in calculations?`
   - Save all functions, variables and tables in POLY3 file?

- `Set numerical limits` on the calculation
- Confirm defined conditions?
- Accept the default settings for two mapping variables

10. The Pourbaix calculation starts. Answer the question `Any missing phase boundary you could possibly think of?` Type `Y` or `N` to set whether you want to add starting points to the calculation. If you suspect that the calculation has missed some phase boundaries, this may help the program to detect them.
11. Answer questions about how the diagram is plotted and how to save the results of your calculation. You are asked to do any of the following:
    - Change the pH/Eh steps for smoother curves?
    - `Zoom in` on a specific region of the diagram
    - `Change the curve-label option for the diagram`
    - `Add label-texts onto the Pourbaix diagram`
    - `Change the subtitle of the diagram`
    - `Change the axis-texts`
    - `Further refine the diagram in the POST Module`
    - Print the diagram (save a `Hard copy of the diagram`)
    - `Save the X-Y coordinates of curve on a text file`
    - `Modify the diagram`
    - Calculate and plot another Pourbaix diagram (`Any more diagram?`)

Plotting More Pourbaix Diagrams

When you have calculated a Pourbaix diagram, you can plot additional diagrams based on the results of the same calculation, but with different axis variables than Ph and Eh.

The variables can be plotted along the X- and Y-axes. Use the abbreviations of the variables when you specify what the X- and Y-axes represent in a diagram. In the table, *AQsp* refers to the name of a specific aqueous species. The asterisk (*) can be used as a wild card character for all such species. If neither *AQsp* nor * is entered in parenthesis, then all species are searched.

You must have plotted a Pourbaix diagram to plot a diagram with other variables than Ph and Eh on the Y-axis and the X-axis. You can either plot such additional diagrams directly after having finished the plotting and saving/printing of a Poubaix Ph-Eh diagram or by choosing option `2` (Open an old file and plot other property diagrams) when you enter the POURBAIX module and opening a POLY3 workspace file.

Abbreviations for Aqueous Solution Variables

Abbreviation	Variable
pH	Acidity
Eh	Electronic Potential (V)
Ah	Electronic Affinity (kJ)
Pe	Electronic Activity (log10ACRe)
IS	Ionic Strength
TM	Total Concentration
Aw	Activity of Water
Oc	Osmotic Coefficient
MF(AQsp)	Mole Fractions of Aqueous Species
ML(AQsp)	Molalities of Aqueous Species
AI(AQsp)	Activities of Aqueous Species
RC(AQsp)	Activity Coefficients of Aqueous Species

How to Plot an Aqueous Solution Diagram

1. Type `Y` when prompted whether to plot any more diagrams, or select option 2 when you enter the POURBAIX module.
2. Specify which variable you want the X-axis to represent. Use the abbreviation specified in the preceding table. When you specify the name of an aqueous species, you can use the asterisk (*) to select all species.
3. Specify which variable you want the Y-axis to represent. The diagram is then automatically plotted.

4. Answer questions about how the diagram is plotted and how to save it. You are asked to do any of the following:
    a. change the axis-type (linear, logarithmic or inverse) on the X-axis or Y-axis
    b. zoom in on a specific region of the diagram
    c. change the curve-label option for the diagram
    d. add label-texts onto the Pourbaix diagram
    e. change the subtitle of the diagram
    f. change the axis-texts
    g. refine the diagram in the POST Module
    h. print the diagram (save a hard copy)
    i. save the X-Y coordinates of curve on a text file
    j. modify the plotted diagram
    k. calculate and plot another aqueous solution diagram

Stepping Calculations in an Aqueous Solution

Performing the stepping calculation overwrites all the previous settings and stepping results on the POLY3-file. To avoid this, use SAVE_WORKSPACES to create a new workspace.

When you have calculated a Pourbaix diagram, you can use the saved results of the calculation (the POLY3 file), and make a property diagram based on stepping calculation.

Since the program normally sets the calculated initial equilibrium point as the starting point, the minimum value for the stepping variable must be specified as smaller or equal to the specific initial condition, and the maximum value as larger or equal to that condition. If pH is set as the stepping variable, the program automatically calculates the equilibrium constant in logarithmic (log10Ka) of the electrolysis reaction H2O (water) = H+ + OH- for the real aqueous solution under the current temperature-pressure-composition conditions, and thus this constant log10Ka value is considered as the highest pH in specifying the maximum value along stepping. Subsequently, confirm or modify an increment factor with a default value; for pressure and mole of a component, specify the step in logarithmic (log10P or log10N).

State Variable Abbreviations

You can use any of these state variables as a stepping variable.

State Variable	Abbreviation
Temperature (K)	T
Pressure (bar)	P
Acidity	pH
Electronic potential (V)	Eh
Mole number of a dissolving component (such as Fe, Na, Cl, or NaCl) in 1 kg of water.	N(Comp) (for example, `N(Fe)`)

How to Do a Stepping Calculation

You must have plotted a Pourbaix diagram before making a stepping calculation on an aqueous solution.

1. Use GOTO_MODULE POURBAIX to enter the POURBAIX module.
2. Type `4` to open an old file and make another STEPPING calculation.
3. Choose which POLY3 file to load.
4. Specify the conditions of the calculation by answering the questions that follows.

   The system definition is the same as in the previous Pourbaix calculation, but you can modify conditions such as bulk composition, temperature and pressure, and change some component definitions if necessary.

5. Specify which variable to use as the stepping variable (see the preceding table), its minimum and maximum value, and the length of each incremental step.

   The settings and stepping results are written to the opened POLY3 file, and a first default property diagram is plotted.

POURBAIX_DIAGRAM Module

This command or module is not available with GES6.

GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features. However, not all GES5 functionality is implemented in GES6. In such cases (except for the POURBAIX module), GES6 falls back silently and uses functionality from GES5 in the background.

Getting started with the Pourbaix module

After you enter the POURBAIX_DIAGRAM module, you are asked if you want to have step-by-step instuctions to help walk you through the module.

```
Need any instruction on the Pourbaix module? /N/: Y
```

If you answer `Y` a series of notes are displayed. The following is a more comprehensive summary of these same notes.

WHAT IS A POURBAIX DIAGRAM?

The Pourbaix diagram is a calculated equilibrium phase diagram mapped and plotted with the independently-varied electropotential (Eh, as defined with regard to the standard hydrogen electrode as its reference) and acidity (pH), that represents all the equilibrated phase boundaries among aqueous solution, gaseous mixture, and various primary and secondary solids (modeled as either complex solution or simple stoichiometric phases) in a certain multicomponent heterogeneous interaction system, under a defined T-P condition and a specific initial bulk composition (which is, by default, always set as 1 kg of water dissolving a specified amount of metals/alloys and other acids/alkalines/salts).

WHAT DATABASE SHOULD I USE?

At least one database is required that contains an aqueous solution phase (with thermodynamic data for water and various aqueous solutes), that shall be selected from TCAQ (PAQ) or AQS (PAQS) [which use the SIT Model or the Complete Revised HKF Model, respectively] within the Thermo-Calc databases.

CHOOSING A CUSTOM AQUEOUS SOLUTION DATABASE

You can also use a custom database but it must be in the Thermo-Calc TDB format. Due to the restrictions of aqueous solution models used within Thermo-Calc, such a database must be designed in the same format as in the default TCAQ (PAQ2) for aqueous solution phases. Among other things, keep the following requirements in mind:

The ELECTRON is defined as an special element (ZE) and as the only constituent in its reference phase REFERENCE_ELECTRODE (for determining the electro-potential that is defined as Eh with the standard hydrogen electrode as the reference), but it is not defined as an aqueous species;

The vacancy (VA) is unnecessary for AQUEOUS solution phase and it should be avoided in the definition of phase-constituents in the AQUEOUS phase;

The AQUEOUS solution phase should always be defined as a constitutional solution phase, implying that all the aqueous solution species must be included in a single site, rather than in two or multiple sublattices.

Beside the AQUEOUS solution phase, there shall exist a GAS mixture phase containing at least H2O1, O2 and H2; and for multicomponent systems, normally there shall also contain some solid (stoichiometric or solution) phases. Of course, if desired, you could also choose to calculate and generate a Pourbaix diagram without considering the GAS mixture phase entirely; however, such a plot is not really a complete Pourbaix diagram, due to the fact that thermodynamically-stable phase boundaries between the AQUEOUS solution phase and GAS mixture phase will then not be calculated at all!

All the required thermodynamic data for calculations of Pourbaix diagrams or other diagrams must be retrieved either from one (Single) database which consists of an AQUEOUS solution phase, a GASeous mixture phase, a REF_ELECTRODE phase, and some SOLID phases (being solutions and/or stoichiometric compounds; for primary metals/alloys and for secondary products formed from heterogeneous chemical/electrochemical interactions, or from several (Multiple) databases that respectively contain various solutions/compounds (as listed above).

Such databases suitable for calculations of aqueous-bearing heterogeneous interaction systems can be those default-prompted ones [i.e., in the Single-Database case, the PAQ or PAQS; and in the Multiple-Database case, the PAQ2 or as primarily-switched database, plus the SSUBx as firstly-appended one and the SSOLx as secondly-appended one if it is necessary; even more databases can be appended). Of course, you could also choose to append required data from other appropriate databases (such as TCFE, TCSLD, TCNI/TTNi, TCAL/TTAl, TCMG/TTMg, TTZr, TCMP, SLAG, etc.) for GASeous mixture phase and for varous solid solution and stoichiometric compound phases. Furthermore, an experienced user can also utilize his/her own USER-specified databases in various cases.

The advanced POURBAIX module is designed so that it requires you to just answer some necessary questions, rather than to go through the other Console Mode modules (i.e., TDB, GES5, POLY3 and POST) although you still enter commands at the prompts. Beside the default plotted Pourbaix diagram, it also allows the user to easily and quickly plot many different properties of the system, stable phases and aqueous species, varied along the calculated phase boundaries for the same defined heterogeneous interaction system. Moreover, it permits the user to directly change some plotting settings and manipulate all kinds of plotted diagrams.

The current advanced POURBAIX-Module has been extended so that it is additionally able to directly perform a normal STEPPING calculation (varied with a specified independent variable) and to easily generate various types of property diagrams, for the same heterogeneous interaction system that has been defined in a previous POURBAIX or TDB-GES5-POLY3-POST calculation.

COPY AND RENAME THE POLY3 FILE

At the end of a Pourbaix module calculation, a new POLY3 file is automatically saved.

A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

If you are using a POLY3 file more than once (as is done in the extended examples), it is recommended that you copy and rename the previously-generated POLY3 file. This is so that the required POLY3 file structure and Pourbaix results are not lost. Do this outside of Thermo-Calc i.e. do not save from within Thermo-Calc.

The reason you do not save from within Thermo-Calc is because of how the file is saved. When the command sequence (GO POLY3>SAVE <*FILE NAME*>.POLY3>Y) is used, the POLY3 workspace of the POURBAIX calculation results in the POLY3 module monitor and all the initial equilibrium points and the mapping/stepping calculation results are lost as well as parts of the POLY3 file structure (e.g., some definitions of the previously defined POURBAIX-type calculation system).

ENFORCE A PAUSE

After the initial set of information is displayed, you are asked:

```
Enforce a PAUSE after plotting when running a MACRO? /N/
```

- If you choose `Y` a pause is always enforced after each diagram is plotted;
- If you choose `N`, all the command-lines (answers) for the session continue without stopping or until the SET_INTERACTIVE_MODE line in the macro file is reached.

Whenever running a Thermo-Calc macro (TCM) file, you may want to pause after a specific diagram is plotted on screen. This gives you the flexibility to:

- Print it (of EMF/PS format) to a printer
- Convert it (of EMF format) to (PDF) graphical files;
- Save it as an EMF graphical file;
- Dump it as a PNG or BMP graphical file;
- Set background colour for the current diagram
- You can also set the default font/size and change plot layers for sequential plots.

Pourbaix Main Options

If you answer `Y` to the Pause prompt above, these options are displayed:

1. Start a completely new Pourbaix diagram calculation.
2. Open an old file and plot other property diagrams.
3. Open an old file and make another Pourbaix calculation.
4. Open an old file and make another stepping calculation.

POURBAIX_DIAGRAM Commands for Options 1 to 4

Tabulation Reactions

In this section:

About the Tabulation Reaction Module

The TABULATION_REACTION (TAB) module can be used to tabulate thermodynamic functions of any type of substance, stoichiometric phase or solution phase, or reaction. The module can tabulate thermodynamic functions of pure stoichiometric phases or solution phases at fixed composition, as well as various kinds of partial derivatives for a pure stoichiometric phase or solution phase at a given composition.

The TAB module begins by evaluating the most stable species of a substance in either a homogeneous state or in a reaction. Results are presented in a table or plotted as a graph.

? Tabulating a Reaction

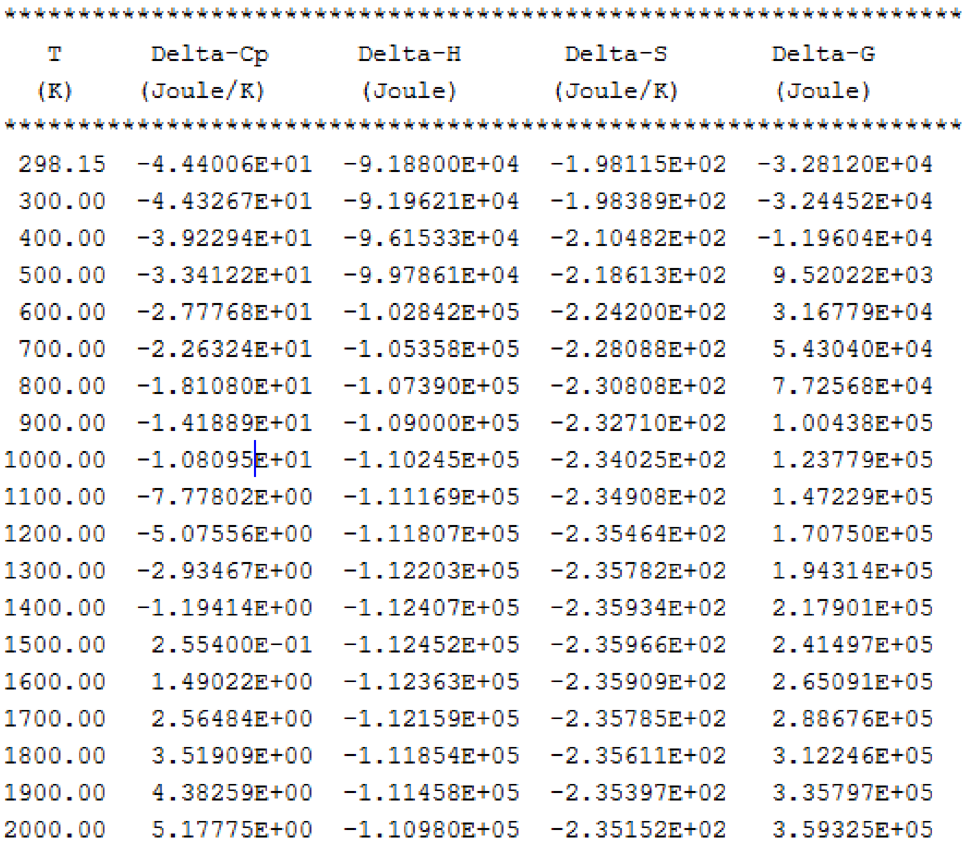
A reaction tabulation presents you with the following properties, on rows representing different temperature levels:

- Heat capacity change / Delta-Cp (Joule/K) in column 2.
- Enthalpy change / Delta-H (Joule) in column 3.
- Entropy change / Delta-S (Joule/K) in column 4.
- Gibbs energy change / Delta-G (Joule) in column 5.

In the case of a tabulation of a substance or solution phase at a fixed composition, the properties presented are the heat capacity, enthalpy, entropy and Gibbs energy, rather than the degree of change in those properties.

? Tabulating a Substance or Solution Phase at Fixed Composition

You can add a 6th column to the table that shows the values of a property or user-defined function of your choice.



```
*******************************************************************
  T       Delta-Cp       Delta-H        Delta-S        Delta-G
 (K)     (Joule/K)      (Joule)       (Joule/K)       (Joule)
*******************************************************************
 298.15  -4.44006E+01  -9.18800E+04  -1.98115E+02  -3.28120E+04
 300.00  -4.43267E+01  -9.19621E+04  -1.98389E+02  -3.24452E+04
 400.00  -3.92294E+01  -9.61533E+04  -2.10482E+02  -1.19604E+04
 500.00  -3.34122E+01  -9.97861E+04  -2.18613E+02   9.52022E+03
 600.00  -2.77768E+01  -1.02842E+05  -2.24200E+02   3.16779E+04
 700.00  -2.26324E+01  -1.05358E+05  -2.28088E+02   5.43040E+04
 800.00  -1.81080E+01  -1.07390E+05  -2.30808E+02   7.72568E+04
 900.00  -1.41889E+01  -1.09000E+05  -2.32710E+02   1.00438E+05
1000.00  -1.08095E+01  -1.10245E+05  -2.34025E+02   1.23779E+05
1100.00  -7.77802E+00  -1.11169E+05  -2.34908E+02   1.47229E+05
1200.00  -5.07556E+00  -1.11807E+05  -2.35464E+02   1.70750E+05
1300.00  -2.93467E+00  -1.12203E+05  -2.35782E+02   1.94314E+05
1400.00  -1.19414E+00  -1.12407E+05  -2.35934E+02   2.17901E+05
1500.00   2.55400E-01  -1.12452E+05  -2.35966E+02   2.41497E+05
1600.00   1.49022E+00  -1.12363E+05  -2.35909E+02   2.65091E+05
1700.00   2.56484E+00  -1.12159E+05  -2.35785E+02   2.88676E+05
1800.00   3.51909E+00  -1.11854E+05  -2.35611E+02   3.12246E+05
1900.00   4.38259E+00  -1.11458E+05  -2.35397E+02   3.35797E+05
2000.00   5.17775E+00  -1.10980E+05  -2.35152E+02   3.59325E+05
```

Tabulating a Reaction

A tabulation of a given chemical reaction provides you with data about the rate of change of the standard tabulation properties at various levels of temperature. You can also add a column for a property of your choice to the table.

1. Use GOTO_MODULE TAB to enter the TAB module.

2. If you want to add one thermodynamic functions to the tabulation calculation, which is present in a sixth column in the table, use ENTER_FUNCTION.

   You are prompted to enter the name of the column that is given at its head, and the function itself. The following state variables can be used to define the function: G, H, S, T, P, V and H298.

3. Use TABULATE_REACTION followed by a formula that specifies of the reacting species and products to perform the tabulation calculation. The name of the elements must be entered in upper case letters only. Terminate the chemical reaction with a semi-

colon. For example, you can enter:

```
TABULATE_REACTION 3H2+N2=2N1H3;
```

Elements that are designated with a single letter must be followed by a stoichiometry factor, even if this factor is 1. `CO` hence be interpreted as Cobalt rather than as carbon monoxide. Carbon monoxide is entered as `C1O1` or `O1C1`.

4. Set the pressure, the range of temperature that you want the tabulation to cover, and change in temperature between each row in the table. You can also specify if you want to output the calculation results to an EXP-file and whether you want any graphical output, and if so, which column you want to be plotted against temperature.

   The tabulation calculation is performed and you are given a table that shows the various properties at each temperature level within the range defined.

   If you have chosen to receive graphical output, then the Console Results window presents a graph that plots the column of you chose (on the Y-axis) against temperature (on the X-axis). When this graph is plotted, you are now in the POST module, where you can modify the graph in various ways.

Tabulating a Substance or Solution Phase at Fixed Composition

A tabulation of a substance or solution phase at fixed composition provides you with data about the standard tabulation properties at various levels of temperature for a given chemical reaction. You can also add one extra property column of your choice to the table.

> It is important to have already defined the system and retrieved thermodynamic data from a database before using the TAB command.

1. Use GOTO_MODULE TAB to enter the TAB module.
2. Use SWITCH_DATABASE to switch to a database that contains solution-based data, such as TCFE for example.

   > You cannot use the default SSUB database when tabulating solution phases at a fixed composition.

3. If you want to add one thermodynamic function to the tabulation calculation, which is present in a sixth column in the table, use ENTER_FUNCTION.

   You are prompted to specify the column header and the function itself. The following state variables can be used to define the function: G, H, S, T, P, V and H298.

4. Use TABULATE_SUBSTANCE followed by the name of the substance or solution phase to perform the tabulation calculation.
5. Set the pressure, the range of temperature that you want the tabulation to cover, and change in temperature between each row in the table. You can also specify if you want to output the calculation results to an EXP-file and whether you want any graphical output, and if so, which column you want to be plotted against temperature.

The tabulation calculation is performed and a table shows the various properties at each temperature level within the defined range.

If you have chosen to receive graphical output, then the Console Results window presents a graph that plots the column you chose (on the Y-axis) against temperature (on the X-axis).). When this graph is plotted, you end up in the POST module, where you can modify the graph in other ways.

Results

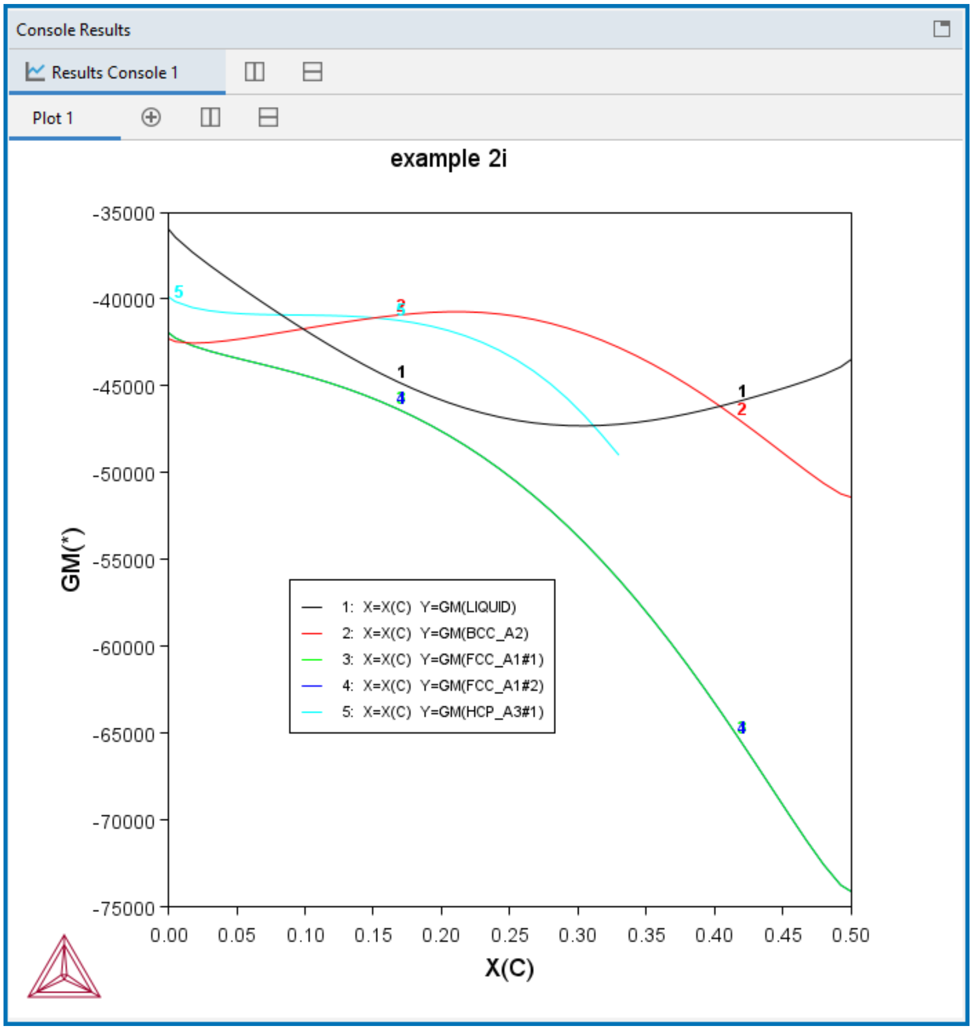
In this section:

Console Mode Results

The results of a calculation in Thermo-Calc can be plotted by the post-processor module, also called the POST module. The diagram is displayed in the **Console Results** window.

In the POST module, you can define and plot various kinds of diagrams based on a calculation. You can modify diagram type, which variables to plot on each axis and between which minimum and maximum values, append experimental data from an EXP-file, change labels and symbols in the diagram, zoom in on (and out from) a certain region in a diagram, etc.

If you calculate a property or phase diagram in POLY, then you have to open the POST module yourself. If your calculation was performed by a response-driven module such as SCHEIL or POURBAIX, then the plotting of a diagram based your calculation is part of the dialogue of questions and answers you have in that module (but under the hood, the response-driven module is actually utilizing the POST module to get the plotting done).



Example of output to the Console Results window.

Using the POST Module

Use the POST module after a STEP_WITH_OPTIONS or MAP calculation to generate *graphical* or *tabulated* presentations on screen or into files.

The graphical files are available in different formats (e.g. PS, EMF, PNG, BMP, PDF, JPG, TIF) or data forms (e.g. EXP, TAB and WRL). The graphical output can be phase diagrams, property diagrams, diffusion profiles and other types of plots. The tabulated presentation is into a basic text file (TXT) or a spreadsheet (e.g. an MS Excel file with an extension of .XLS).

> The POST module (post-processor) is a submodule to the POLY module and has its own set of commands. The TAB, BIN, TERN, POT, SCHEIL and POURBAIX modules use the POST module features as part of the automatic generation of the plots.

Within the POST module, you can choose any state variable, any derived variable, or any entered symbol (functions or variable) as the X/Y-axis.

Thermophysical Properties Data and Variables

When a diagram is plotted, appearance parameters for defining a high-standard graph can be further specified, e.g. curve labelling options, diagram titles and subtitles, plot size, axis length, axis types, axis-tic type, tie-line status, automatic or manual scaling and zooming, semi-automatic or manual labeling on phase boundaries and phase regions, graphic formats, text fonts, colors, raster plot, etc.

You can append experimental data onto a plotted diagram. You can also save the coordinates onto a textual file, which can be edited and used as an experimental data file to be merged onto another diagram or as a part of a setup file for PARROT-module assessment.

Phases can be suspended or restored in a plotted diagram. The reference states for components can also be modified for the resulted diagrams. Moreover, you can translate a plotted property diagram (after a stepping calculation) into a tabulated form, such as a simple list on screen or a textual file, and a spreadsheet .

Plotting Diagrams

Plotting a diagram is to graphically represent how several variables (typically two variables) co-vary. Each axis in a property diagram or a phase diagram represents the value of one variable. The default variables represented by the X- and Y-axes are the following:

- If you plot a diagram based on the results of a mapping operation (a phase diagram), then by default the X- and Y-axes represent the mapping axis variables 1 and 2 (set using SET_AXIS_VARIABLE in POLY).
- If you plot a diagram based on the results of a stepping operation (a property diagram), then by default, the X-axis represents the stepping variable (set using SET_AXIS_VARIABLE) and the Y-axis represents the sum of the mole fractions of all phases (that is, NP(*)).

? POLY Module Commands

How to Plot a Diagram

To plot a diagram, you must have already made a stepping or mapping operation in POLY (or in some cases, made a calculation as part of some opening a response-driven module), and you must have entered the POST module.

The POST command is available inside POLY. Use POST to enter the POST module

1. If you want to directly plot your diagram with the default variables represented by the X- and Y-axes, type `Plot` and press <Enter>. This plots a property or phase diagram with the default variables represented at each axis. If you do not want to plot your diagram with these default variables, go to the next step.
2. Use SET_DIAGRAM_AXIS to set which variables to plot on the X-axis and the Y-axis. For example, if you want to plot a phase diagram with pressure on the Y-axis and temperature on the X-axis, type:

   ```
   SET_DIAGRAM_AXIS X T

   SET_DIAGRAM_AXIS Y P
   ```
3. Use PLOT_DIAGRAM to plot your diagram.

Saving and Printing the Output in Console Mode

Global Settings: Graphical and Console Mode Plotting

Output can refer to results in the form of tabulated data in a table or a diagram.

The terms *diagram* and *plot* are interchangeable. The commands in Console Mode generally use the term diagram and in Graphical Mode it is also called a plot (e.g. the Plot Renderer).

Commands to Save and Print Diagrams

Use the following commands to create diagrams, which then display in the **Console Results** window. From this window, you can right-click the diagram and choose **Save as** or **Print**. You can also use the following commands for these actions.

PLOT_DIAGRAM

After you use the SET_PLOT_FORMAT command to define the default graphic device (the printer) you can use a PLOT_DIAGRAM command to either save the calculation output to a file or display the output in the **Console Results** window.

DUMP_DIAGRAM

DUMP_DIAGRAM is an alternative command used to create output. After a diagram is displayed to the **Console Results** window with the PLOT_DIAGRAM command, you can save (dump) it to a file using this command.

MAKE_EXPERIMENTAL_DATAFILE

Use MAKE_EXPERIMENTAL_DATAFILE to save all the data about the plotted diagram in an EXP-file. An EXP-file is a plain text file that describes the diagram in the DATAPLOT graphical language. Note that information about the underlying calculations that the diagram is based on is not saved in an EXP-file.

DATAPLOT User Guide included with this documentation set.

See the Tips and Tricks: How to Plot Experimental Data blog post on our website for useful guidance about this topic.

PRINT_DIAGRAM

First use PLOT_DIAGRAM to create output that displays in the **Console Results** window. Then after entering the PRINT_DIAGRAM command, the **Print** window opens where you can choose additional settings for a hard copy of the diagram.

Commands to Save Tables

Tables or tabulated data can be listed in the **Console** window. You then use commands to save the text to different file formats (txt, html, or xls) where you can then print the information.

- LIST_DATA_TABLE: Use this command to output to the screen or to file.
- TABULATE

Saving Diagrams

You can save the output in a variety of file formats. For JPG and PNG images you can also adjust the image quality.

In Console Mode, the diagram is output to the **Console Results** window after using the PLOT_DIAGRAM command.

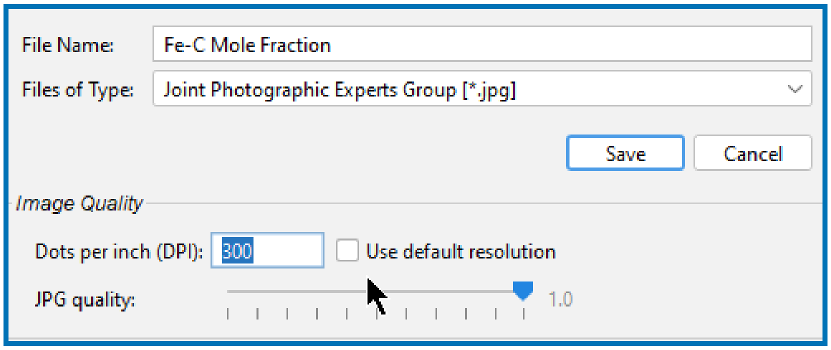
In Graphical Mode, the diagram is output to the **Visualizations** window after performing a tree that includes a Plot Renderer.

In the **Visualizations** window, right-click the diagram and select **Save as**.

In the Graphical Mode **Configuration** window you can also click the **Save Diagram** (or **Save table**) buttons to open the **Save** window.

Then in the **Save** window:

1. Navigate to where you want to save the diagram.
2. Enter a **File name**.
3. From the **Files of type** list choose **png** (the default), **jpg**, **ps**, **pdf**, **gif**, **svg**, or **emf**.
4. For PNG and JPG files only, under the **Image Quality** section, choose to improve the resolution of the image. For JPG files you can also adjust the file size.
    - To change the resolution of a PNG or JPG image, click to clear the **Use screen resolution** checkbox. Then enter a numerical value in the **Dots per inch (DPI)** field.
    - For JPEG files, you can also use the slider to choose a number between 0 and 1 for the **JPG quality**. The default is 0.9. The lower the number, the smaller the file.



File Name: Fe-C Mole Fraction

Files of Type: Joint Photographic Experts Group [*.jpg]

Dots per inch (DPI): 300 ☐ Use default resolution

JPG quality: 1.0

5. When you are ready, click **Save**.

Printing Diagrams

In the **Console Results** window, right-click the diagram and choose **Print**. Select additional settings as required on the **Print** window.

Use the LIST_DATA_TABLE command to save to file and then print the file.

Modifying Diagrams

Modifying a diagram amounts to changing the settings that determine how the POST module presents the calculated results and plots a new diagram. Suppose that you have already plotted a binary phase diagram with the mapping axis variables temperature and mole fraction of one of your components (the Fe component, say) on the X- and Y-axes. If you then want to modify your diagram so that the Y-axis instead represents, say, the mass fraction of Fe rather than the mole fraction, then you use SET_DIAGRAM_AXIS to set diagram axis `Y` to `w(Fe)`, and then use PLOT_DIAGRAM.

There are many ways in which you can modify your diagram and how it is presented. Any modification made in the plot settings is taken into account the next time you use PLOT.

Example Commands

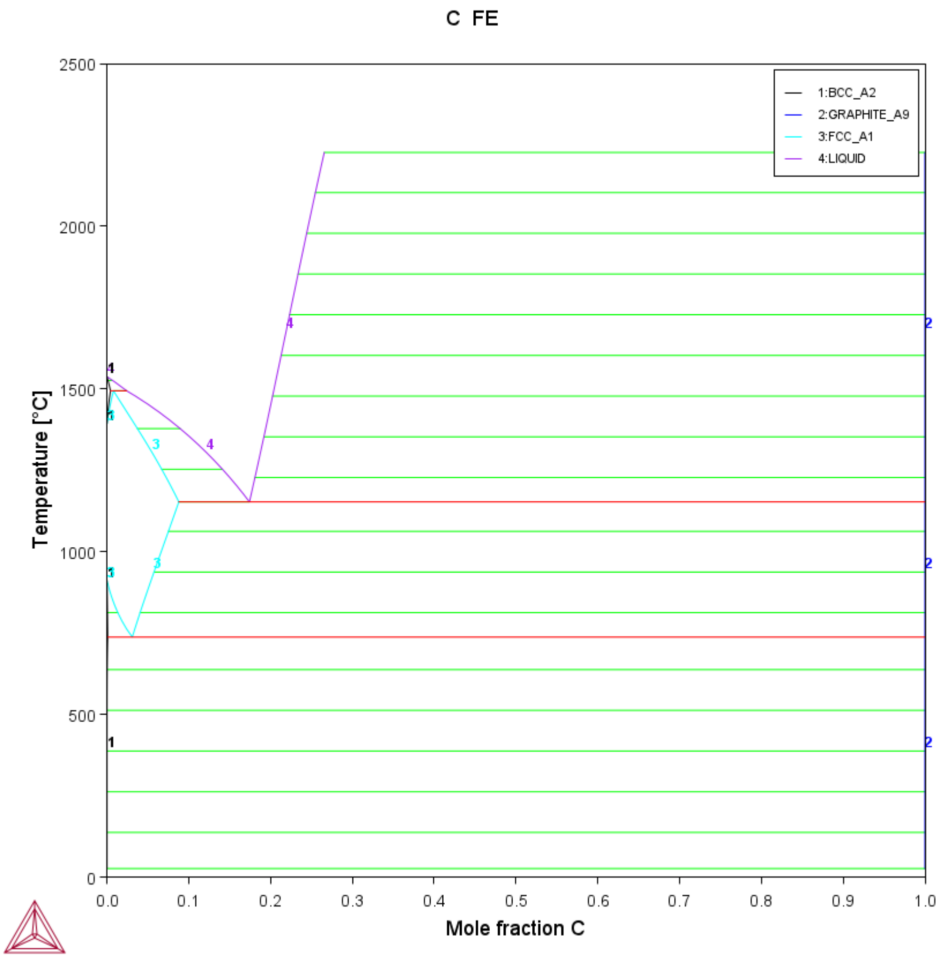
The following are some of the modifications you can make. Use:

- SET_TITLE to set add a title or to change an already existing title. The title is displayed above the plotted diagram in the Console Results window.
- ADD_LABEL_TEXT to add a label text that starts at a certain X- and Y-coordinate. If you have plotted a phase diagram, then you can let Thermo-Calc set the label text that specifies the names of the stable phases at that coordinate.
- SET_AXIS_TYPE to set whether the scale of an axis is linear, logarithmic or inverse.
- SET_DIAGRAM_TYPE to plot a triangular diagram with the X-axis on the triangle’s base and the Y-axis on the triangle’s left side. Such a diagram is often useful if you want to plot the fractions of two components in a ternary diagram.
- SET_SCALING_STATUS to modify the range of values that are displayed on an axis. In effect, you can use it to zoom in or out of the diagram. For example, to set the scale of the X-axis to range from 0 to 0 .3, type:

  ```
  SET_SCALING_STATUS X N 0 0.3
  ```

  The `X` specifies which axis to change the scaling on, the `N` turns off Thermo-Calc’s automatic scaling, and `0` and `0.3` specifies the minimum and maximum values on the scale. You can turn on automatic scaling again by setting the second parameter to `Y`.

- SET_LABEL_CURVE_OPTION to label each set of curves that have the same stable phases with a certain digit. A legend is also added, where you specify which phases each digit designates.


C FE
1:BCC_A2
2:GRAPHITE_A9
3:FCC_A1
4:LIQUID
Temperature [°C]
2500
2000
1500
1000
500
0
Mole fraction C
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1
2
3
4

Loading Saved Diagrams

If you have previously saved a diagram in an EXP-file, then you can load and superimpose the diagram on another diagram. Both the following command requires you to specify which prologue and dataset(s) that are loaded from an experimental data file.

Use APPEND_EXPERIMENTAL_DATA to plot selected data from an experimental data file (EXP-file). If you have set the axes of the diagram already, the labels on the diagram are not changed when you plot the additional data from the EXP-file, irrespectively of the data in that file.

Use QUICK_EXPERIMENTAL_PLOT to plot selected data from an experimental data file (EXP-file). If you have set the axes of the diagram already, these settings are overwritten with the axes settings from the EXP-file.

Working with the Console Mode Output

Pause, Resume or Stop Output to the Console Window

In response to a command or a lengthy calculation, Thermo-Calc may display a lot of text in the Console window. Use these keyboard shortcuts to pause, resume, or stop a process.

- To pause the text on printing press <Ctrl+S>.
- To resume the printing on screen, press <Ctrl+Q>.
- When Thermo-Calc is performing a stepping or mapping operation, the results are continuously printed in the Console window. To stop the calculation of the current region of the mapping and stop the output, press <Ctrl-A> (Windows) or <Ctrl-C> (Linux).

Controlling Console Output

In response to a command or a lengthy calculation, Thermo-Calc may display a lot of text in the Console window. Use these keyboard shortcuts to pause, resume or stop a process.

- To pause the text on printing press <Ctrl+S>.
- To resume the printing on screen, press <Ctrl+Q>.
- When Thermo-Calc is performing a stepping or mapping operation, the results are continuously printed in the Console window. To terminate the calculation of the current region of the mapping and stop the output, press <Ctrl-A> (Windows) or <Ctrl-C> (Linux).

In Console Mode, sometimes the output overflows the window text buffer. This is how to increase the buffer size.

1. In the Console window right-click the tab to edit. For example, if this is the first tab, it is labeled **Console 1**.
2. Select **Properties** and either enter a number in the field or use the arrows to increase or decrease the **Buffer size**.

Commands by Module

In this section:

System Utilities (SYS) Commands

In this section:

ABOUT

The ABOUT command lists basic information about the development history and ownership of the Thermo-Calc software as well as version information.

BACK

? GOTO_MODULE.

Use the BACK command to switch control back to the most recent module. Going from the POST module, BACK goes only to the TAB or POLY module (from where the POST module is entered).

CLOSE_FILE

Close an opened text file.

Syntax	CLOSE_FILE
Prompt	`Unit number: <Unit number>` A unit number given in an OPEN_FILE command must be specified.

DISPLAY_LICENSE_INFO

You can also access this same information from the top menu. Choose **Help → Show License Info**.

Use this command to launch a license diagnostics program implemented in the SYS module. It detects the license information for the Thermo-Calc installations on the current client computer (and on the connected license server), and lists the details, including the current status of available license file and all its included license features for the current installation (s), as well as the Safenet Environment Variables and detailed Local (Client) Information, on screen or into a textual file (*.TXT).

This is useful for a list of license details, and to obtain basic technical support by sending the *.TXT file to support@thermocalc.com. If you are running a network client installation of Thermo-Calc, you can see how many of the client example licenses that are currently checked out and how many of them are left. You can also see which clients computers it is that have checked these client example licenses out.

Syntax	DISPLAY_LICENSE_INFO
Prompt	`Output to screen or file /Screen/: <Mylicenseinfo.txt>` Press <Enter> to display a list of license information or into a *.TXT file under a specific file name which can later on be opened and edited by any basic text editor.

EXIT

Use the EXIT command to leave the program and return to the operating system. Use a SAVE command before exiting otherwise all data and results are lost (in either the GIBBS, POLY, PARROT or REACTOR module).

GOTO_MODULE

Switch between modules. The name of the module must be typed. To get a list of available modules, press the <Enter> key.

Syntax	GOTO_MODULE
Prompt	`Module name: <Module name>`
	If the <Enter> key is pressed without typing a unique module name (or typing a ? mark) it prompts for the `MODULE NAME` and lists the available modules.

HELP (? and ??)

Enter ? or ?? to get text help about the current prompt (whether this is the prompt of a module, or a prompt that requests you to specify the value of some parameter).

For some commands and prompts, more detailed help is given when two ?? are entered.

HELP

Lists the available commands or explains a specified command. Specifying a unique command displays an explanation on screen. Typing a command abbreviation that is not unique lists all matching commands. Get the command information by typing a unique abbreviation or the complete command name.

Syntax	HELP
Prompt	`Command: <Command name>` *Command name* is the name of the command (one of the-module commands) to get help. If the <Enter> key is pressed without typing a command name, then all the available commands are listed.

HP_CALCULATOR

The HP-CALCULATOR commend is the QBA simple interactive calculator using reverse Polish notations.

Available OPCODEs (HPC codes) are listed by entering the command HELP.

Use the BACK command to quit and go back to the SYS module.

Input are numbers, + - * / and ^ and OPCODEs. Several numbers an operations can be given on one line. The content of the X register is displayed after each operation.

For example, to compute 2*EXP(1.5**3-30000/(8*1273)), you should input the following:

```
30000 8/1273/chs 1.5 3 ^ + exp 2 *
```

INFORMATION

Get basic information about topics related to the module you are in.

Syntax	INFORMATION
Prompt	`Which subject /Purpose/: <Topic name>` Specify a subject (or its abbreviation as long as it is unique). Enter a question mark `?` for a list of topics.

MACRO_FILE_OPEN

Some of the information in this topic is related to the add-on Diffusion Module (DICTRA).

The macro file functionality is a way to predefine sequences of Thermo-Calc commands stored in a macro file (a basic text file usually with the default extension *.TCM or*.DCM for DICTRA) and then executing all of the sequences using this command (preceded by the macro file name). This command can be used within various modules (i.e. SYS, POLY, PARROT, TAB and DICTRA_Monitor).

Syntax	MACRO_FILE_OPEN
	`<Name of a macro file *.tcm>` An **Open** window displays to specify the filename of the macro file (*.TCM) with the macro command, so that the path (in the **Look in** field) and **File name** can be specified. The **Files of type** *.TCM for Thermo-Calc (Console Mode) calculations and *.DCM for DICTRA simulations, cannot be changed. Click **Open** or **Cancel** to continue. A window such as **Save**, **Open**, or **Print** opens if the macro file contains commands to: • set log files (these have a file extension .TCM) • save or read GIBBS, POLY or PARROT workspaces • switch user databases • compile experiments (from existing *.POP files) • create new *.PAR files • append *.EXP files • plot diagrams, etc. If required, opening these windows can be avoided by issuing the file names (preferably with file-type extensions; if the files are not in the current working area where the macro is located, the appropriate and complete paths of the files should also be specified) and sometimes with the required options after the corresponding commands or parameters/options. For details, see the related commands and modules. When using a macro file that intended to plot graphs on screen, but the command SET_PLOT_FORMAT is used to alter the plotting environment from the default value, it is important to first use the command SET_PLOT_FORMAT again to change back to the default value.

This is useful when the same or similar calculations are made frequently with small changes [in terms of system definitions, data manipulations, conditions (for single points, stepping or mapping calculations), plotting settings, etc.). For example, use this feature when calculating phase/property diagrams during an assessment of thermodynamic data.

A macro file can be automatically generated in Console Mode if in the SYS module the SET_LOG_FILE command is used and a log file name (with a file extension *.TCM) is given before any other SYS, DATA, TAB, GIBBS, POLY, POST, PARROT, or ED-EXP command or any special-module command (e.g. BIN, TERN, POTENTIAL, SCHEIL, POURBAIX, or REACTION). Such a log file generated in Console Mode is a text file. You can use a text editor (such as Notepad++) to remove unnecessary command lines, modify some commands, settings and definitions, add some pause points, add comment lines that start with `@@`, and so forth. Then save it as a macro file with the standard file extension TCM.

Experienced users can also write/edit an appropriate macro file for calculations/simulations, using any basic textual editor outside the Thermo-Calc program.

All commands can be used in a macro file.

The file can be terminated with EXIT or interrupted with SET_INTERACTIVE.

Within a macro file you can use comment-lines (for describing the problems and for explaining commands and inputs/outputs), which should always start with the @@ signs in the beginning of each comment-line. Such comment-lines help to document the macro file, while these are not considered as command lines and thus do not affect the proceeding of all the normal commands in modules when the file is called by Thermo-Calc.

You can put multiple-line comment-blocks in a macro file between the @ (” and “@)” signs. The former sign indicates where the comment begins and the latter sign indicates where the comment ends. A comment-block begins from a line started with the *begin comment* sign @ (and ends with the *finish comment* sign @); all the lines written in between are ignored, and the line started with @) is also ignored.

Another use for a macro file is to allow you to interact at some specific points, using the “@?” sign starting a text line (note that the text describing the expected user-specification/input should be written as a continuous string without any empty space), for user’s on-time specifications of arguments/parameters or inputs of parameter-values that are requested by a certain command. The macro temporally stops at the “@?” sign, prompt on screen the text given after “@?”, and waits for the specified argument/parameter/value. Thermo-Calc then uses specified argument/parameter/value as the input(s) for the associated command. For example, you can input the values of lower and higher temperature limits for the second axis-variable as follows:

```
GO POLY-3
SET-AXIS-VAR 2 T  @?Low-temperature-limit:
@?High-temperature-limit:
```

You can have macro-variables denoted by the signs of @#n (for definition) and ##n (for usage); and up to nine variables inside a single macro file. Such a macro-variable can be assigned with its desired value, as for example:

```
@#3First-element?
```

This writes the text (note that the text describing the expected user specification/input is written as a continuous string without any empty spaces) after the “@#3” sign as prompted on screen and then wait for a specification. The input is assigned to the macro-variable ##3, which is directly called in different parts within the current macro file.

For example, the content of the macro-variable `##3` is inserted in the command:

```
DEFINE-SYSTEM ##3
```

It is also useful in more complicated commands, such as:

```
SET AXIS VAR 1 x(##3) 0 1,,,
```

This command sets the mole fraction of macro variable 3 as axis 1.

A macro file can have any number of pauses at the `@&` signs, for the purpose of checking the details/results of executing certain commands when running the macro file. However, you can also prevent the software from temporarily stopping at any pause by typing any character (except for the `Y` character for confirming a Yes answer to a command prompt) after specifying the name of a macro file.

A macro file can have a maximum of five nested levels, i.e. a macro file can call another macro file, and if one sub-level macro is terminated by the command it resumes at the next command in the previous macro. If it is terminated by `end-of-file`, the Thermo-Calc (Console Mode) software stops.

This feature is especially useful for alloy design that requires many (hundreds) of calculations/simulations on similar material system/processes (specified in many different but appropriately-documented macro files that are organized in up to five levels) during a certain period of time (e.g. in an evening), you can run the main macro (on the top level) at a certain time (e.g. before leaving the office) and afterwards (e.g. next morning) you can systematically and efficiently check/compare/analyse the results (saved as graphical files, and/or EXP, TXT, XLS… files).

By adding the SYS command SET_ECHO at the beginning of a macro file (or in the primary macro file on the top level if any sub-level(s) of macro files are used), it is useful to automatically display the complete/detailed meaning of various commands in all the sequential operations in the software, all enforced according to the macro file(s).

OPEN_FILE

A text file is opened for use in other commands where a unit number is necessary. The program automatically assigns a unit number.

Syntax	OPEN_FILE
Prompt	`File name: <File name>` A legal file name must be specified.

SET_COMMAND_UNITS

This command is useful for reading inputs already prepared by a textual editor on a file. Such inputs can be a table of values or a large number of parameters. The file must be opened with OPEN_FILE.

The first two lines of an input file are skipped before any input is read.

Syntax	SET_COMMAND_UNIT
Prompt	`Input unit number /5/: <Input unit number>` Specify the input unit number returned from an OPEN_FILE command. The next command is taken from the file connected to this unit number. The last command on such a file must be EXIT or SET_INTERACTIVE when you are in POLY, POST or SYS module, in order to go back to read input from the keyboard. The default value is the current input unit.
	`Output unit number /6/: <Output unit name>` Specify the output unit number returned from an OPEN_FILE command.

SET_ECHO

> This command is only applicable to use with macro files, i.e. it does not work to enter this command directly into the Console.

Add the `SET_ECHO` command at the beginning of a macro *.TCM file (or to the primary macro file on the top level if any sub-level(s) of macro files are used).

Automatically displays on screen the complete details of various commands in all the sequential operations in the software, that are enforced according to the macro file(s).

SET_GES_VERSION

This command enables switching between the two versions of the Gibbs Energy System (GES) calculation engine. As of Thermo-Calc version 2019b, GES6 is the default. Also see About the Gibbs Energy System (GES) Module.

GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features. However, not all GES5 functionality is implemented in GES6. In such cases (except for the POURBAIX module), GES6 falls back silently and uses functionality from GES5 in the background.

Syntax	SET_GES_VERSION
Prompt	`USE GES VERSION 5 OR 6 /6/:` The default is version 6. If you change the version to GES5, it is set for the current session of Thermo-Calc only. If you launch a new Console window, the version resets to GES6.
	To globally set the default from GES6 back to GES5, go to the **Tools → Options →** Global General Settings tab and click **Version 5** for the *Preferred Gibbs Energy System* setting. This is useful if you are using the PARROT module (optimization) or if you have a custom database that is not compatible with GES6.

Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.

SET_INTERACTIVE

Use the SET_INTERACTIVE command to reset the input and output units to the initial values, i.e. keyboard and screen. Add this as the last command to the macro files.

SET_INTERACTIVE_MODE

Use the SET_INTERACTIVE_MODE command to reset the input and output units to the initial values, i.e. keyboard and screen.

Remember to add this as the last command to your macro files, in order to stop execution of the command file in the POST module. It has no meaning in interactive mode.

SET_LOG_FILE

Use it to save, in a basic text file, everything typed into Thermo-Calc. When having problems executing a command sequence, this command can be used to save the command typed onto a log file with the file extension *.TCM.

This command also makes the system echo the full command for all commands typed. This feature is useful when demonstrating the system since the abbreviated commands are often difficult.

The saved log file can then be edited as a macro file by using a basic text editor. This is useful to run the macro file(s) for similar calculations (the same system but slightly varied temperature-pressure-composition conditions), or run the example macro files.

? Macro Files

Syntax	SET_LOG_FILE
Prompt	A **Save** window opens to specify a file name for the *.TCM file, so that the path (in the **Save in** field) and **File name** can be specified. If a log file with the same name exists in the current working directory, it is overwritten. The **Files of type** (i.e. TCM) cannot be changed. Click **Save** or **Cancel** as applicable.

SET_PLOT_ENVIRONMENT

Use this command to set the plot devices to save or print plots to, which varies for by installation type.

> This command must be terminated with an empty line or two commas.

Syntax	SET_PLOT_ENVIRONMENT
Prompts	`Default plot device number /Default number/: <Device number>` The number given is unique for each type of graphical device. The default graphical device number should normally be selected. A question mark `?` gives you a list of all available graphical devices used.
	`Pseudo file name: <Pseudo-file name>` The name given here is a symbol which can be used to refer to a physical graphics device when asked for graphical output file.
	`Plot device number /1/: <Device number>` The number that specifies the type of graphical device.

	`Plot file name: <File name or printer name>`
	The name of the graphical device on system level (name of file or printer).
	Example
	`SET_PLOT_ENVIRONMENT 1 lasp 5 a0tr,,`
	This example sets the default plot device number to `1`, and defines an alias named `lasp` with plot device `5` and connected to a printer named `a0tr`.

SET_TC_OPTIONS

Predefine the default values of three general options for performing all the sequential single-points, stepping and mapping calculations.

Syntax	SET_TC_OPTIONS
Prompts	`Use_global_minimization /Y/:` By default it global minimization is used where possible (depending on the conditions setting). A global minimization test is performed when an equilibrium is reached. This costs more computer time but the calculations are more robust. Enter N to prevent global minimization being used to reach the equilibrium.
	`Global_test_interval /0/: <An integer value>` The integer number determines how often the global minimization should be used during calculations with STEP_WITH_OPTIONS and MAP. If it is set to 0 (zero), the recommended global test interval is used: i.e. every tenth step and at each phase change during step calculations, and only at node points during map calculations. Any other positive integer number, n, suggests it performs global minimization tests at every nth step during step and map calculations. Of course, the Global Minimization test is always carried out at a phase change or a node point. The software is initially configured with 0 (zero) as the default value, but such a configuration for the default value can be changed by this option.
	`Automatically_add_initial_equilibria /Y/:` When ADD_INITIAL_EQUILIBRIUM is not used before a map calculation, a mesh of INITIAL_EQUILIBRIUM is automatically added before the mapping procedure itself takes place. This mesh is only available when the two independent axis-variables have already been defined by the POLY command.
	`Set_axis_variable` If Y is entered, the POLY module always enforces the automatic procedures for adding initial equilibrium points during mapping. For N, no initial equilibrium points are then added during mapping.

STOP_ON_ERROR

Useful for batch jobs in order to prevent that an erroneous sequence of commands to the program causes waste of computer activity.

Syntax	STOP_ON_ERROR
	Give the preferred argument (`ON` or `OFF`) after the STOP command. If the default argument ON is given, the program terminates after an illegal or ambiguous command. It is possible to reset the effect of this command by giving the argument OFF.

Database (TDB) Module Commands

These commands are related to the DATABASE_RETRIEVAL module, which is also known as the TDB module.

Search the online help for step-by-step instructions to define a system.

In this section:

AMEND_SELECTION

This command is for the DATABASE_RETRIEVAL (TDB) module.

Use this command after defining the elements, species or the system (with the commands DEFINE_ELEMENTS, DEFINE_SPECIES, or DEFINE_SYSTEM). The prompts allow changes to the predefined system. By answering Y or N, each of the selected elements, species or phases can be accepted or rejected (although this is not the case for the constituents or the entire system).

Syntax	AMEND_SELECTION
Prompt	`Keep <Name1> No/Quit/Yes/` `Keep <Name2> No/Quit/Yes/`
Options	`Keyword-- Elements/Species/Phases name&` Names of the pre-defined or pre-selected elements/species/phases

APPEND_DATABASE

This command is for the DATABASE_RETRIEVAL (TDB) module.

Appends data to the current set of data already read from another database. The syntax is the same as for the SWITCH_DATABASE command.

This command enters all additional functions and parameters to already existing phases, e.g atomic mobilities, phase constituents, excess models, G0 and interaction parameters.

This command is most commonly used to read mobility data from stand-alone mobility databases.

This command should be used with some caution if thermodynamic data is appended and the application is run with Gibbs Energy System version 5 (see SET_GES_VERSION in the SYS module). It can change calculated values in an unexpected way. This can happen e.g. if the appended database has the same function name as a function in the data retrieved from a database opened with SWITCH_DATABASE.

Syntax	APPEND_DATABASE
Prompt	`New database name /XYZ/:` The name of either an existing database (e.g. FEDEMO) or USER.

DATABASE_INFORMATION

This command is for the DATABASE_RETRIEVAL (TDB) module.

Use the DATABASE_INFORMATION command to obtain a short description of the current database. This can include information on covered systems, used models, valid ranges for parameters in temperature and composition, major applications, and so on.

DEFINE_ELEMENTS

This command is for the DATABASE_RETRIEVAL (TDB) module.

Define the system in terms of elements. All possible species that can be formed by the given elements are retrieved from the database. The names of elements must be separated with a space or comma. It is possible to use a wildcard * after a common part of element names so that all the elements, which start with that common part and are available in the currently switched or appending database, are defined in the system. Up to 40 elements can be defined into a single system.

Also see Defining a System in Console Mode for step-by-step instructions to define a system with this command.

Syntax	DEFINE_ELEMENTS
Prompt	`Element& <Element1, Element2, …>` A list of elements to be defined into the system.
	When appending database(s), this command, or DEFINE_SPECIES or DEFINE_SYSTEM must be repeated with the same or similar elements as defined in the first switched database.

DEFINE_SPECIES

This command is for the DATABASE_RETRIEVAL (TDB) module.

Define the system in terms of species. Only those species given are retrieved. The different names of species must be separated with a space or comma. It is possible to use a wildcard * after a common part of species names so that all the species, which start with that common part and are available in the currently switched or appending database, are defined in the system. Up to 1000 species can be defined in a single system.

Defining a System in Console Mode

Syntax	DEFINE_SPECIES
Prompt	`Species& <Species1, Species2, …>` A list of species to be defined in the system.
	When appending database(s), this command, DEFINE_ELEMENTS or DEFINE_SYSTEM must be repeated with the same or similar elements as defined in the first switched database.

DEFINE_SYSTEM

This command is for the DATABASE_RETRIEVAL (TDB) module.

Define the system in terms of either elements (equivalent to DEFINE_ELEMENTS) or species (equivalent to DEFINE_SPECIES). Certain databases have a default value of the keyword (as either ELEMENTS or SPECIES) reflecting what is most appropriate when defining a system.

The different names of elements or species must be separated with a space or comma. It is possible to use a wildcard * after a common part of elements or species names so that all the elements or species, which start with that common part and are available in the currently switched or appending database, are defined in the system.

When appending database(s), this command (or DEFINE_ELEMENTS or DEFINE_SPECIES) must be repeated with the same or similar elements as defined in the first switched database. Different databases might contain different elements and have different species definitions: avoid defining elements/species that are missing in the appending database(s). Otherwise, the program indicates these missing elements/species, and ignores them in subsequent steps. But additional elements/species, and additional phases not available in the first switched database can be defined and retrieved from the appending database(s). Up to 40 elements and 1000 species can be defined in a single system.

Also see Defining a System in Console Mode for step-by-step instructions to define a system with this command.

Syntax	DEFINE_SYSTEM
Prompt	`Elements: <Element1, Element2, …>, or` `Species: <Species1, Species2, …>`
Options	**Description**
`Species or Elements`	Default keyword.
`Element&`	Specify a list of elements for the defining system.
`Species&`	Specify a list of species for the defining system.

GET_DATA

This command is for the DATABASE_RETRIEVAL (TDB) module.

Enter the defined system's elements, species, phases, and the connected parameters obtained from either the primary switched or additionally appending database(s) to the GIBBS and/or DICTRA workspace. Then use the GET_DATA command to get all information concerning a defined system from the databank.

Only after executing this command can you go to any of the application programs such as GES, POLY or DICTRA and use the retrieved data. When appending database(s), this command must be repeated in order to obtain the additional system definitions, parameters and functions.

LIST_DATABASE

This command is for the DATABASE_RETRIEVAL (TDB) module.

List all elements, species, phases or phase constituents in the database.

Syntax	LIST_DATABASE
Options	**Description**
`Keyword`	One of the keywords Elements, Species, Phases or Constituent must be used to indicate what to list
`Elements`	All available elements, the reference state, atomic mass, H298-H0 and S298. Some elements have spaces in the column for the reference state. This implies that there are no parameters stored for this element.
`Species`	All available species together with the stoichiometric factors.
`Phases`	All available phases together with the number of sublattices and the number of sites in each sublattice.
`Constituent`	All available phases, the number of sublattices, the number of sites in each sublattice and the species dissolved in each phase. Species in different sublattices are separated with a colon (:). It is important to realize, for example, a phase can consist of Fe, Mo, V, and Cr, and its thermodynamic parameters can come from the binary systems Fe-Mo, Fe-V, Fe-Cr, and Mo-Cr. These data can give a relatively good description of the corners of the Fe-Cr-Mo system, but would most certainly give a bad one for the system Mo-Cr-V, due to the fact that the interaction parameters are, by default, set to zero, which originates from binary systems not included in the database.

LIST_REFERENCES

This command is for the DATABASE_RETRIEVAL (TDB) module.

Use the LIST_REFERENCES command to list the relevant literature references for the assessed data for the present system. The command is used after the GET_DATA command.

Syntax	LIST_REFERNCES
`Prompt`	There is no prompt after entering the command. The list of references is shown in the Console Window.

You can highlight the list of references to copy to another program. Or if the reference list is very long, right-click the Console tab and select **Copy Command History to Clipboard** or **Copy All Text to Clipboard** (or use the keyboard shortcuts).

LIST_SYSTEM

This command is for the DATABASE_RETRIEVAL (TDB) module.

List all elements, species, phases or phase constituents in the defined system. It works only after a system is defined.

Syntax	LIST_SYSTEM
Keyword	One of the keywords `Elements`, `Species`, `Phases` or `Constituent` must be used to indicate what to list. ? LIST_DATABASE

REJECT

This command is for the DATABASE_RETRIEVAL (TDB) module.

Reject elements, species, phases or phase constituents that can form from the defined elements and species. Phases/species/constituents that are possible to form in the defined system are removed from the list of system phases/species/constituents (shown by the command LIST_SYSTEM). Phases/species/constituents that are not included in the list cannot be entered without first being restored. The different names must be separated with a space or comma. You can use a wildcard * after a common part of names so that all the elements/species/phases/constituents that start with that common part and are available in the currently switched or appending database, are rejected from the defined system.

This command can also reject a defined system, and thus reinitiate the entire DATA module memory and GES workspace.

Syntax	REJECT
Prompt 1	(Keyword = Elements or Species or Phases) `If keyword: <Name1, Name2, …>`

Prompt 2	(if keyword = Constituent)
	`Phase: <Phase name>`
	`Sublattice number: <Sublattice number in the phase>`
	`Constituent: <Constituent(s) in the sublattice of the phase>`

Prompt 3	If keyword = SYSTEM the DATA module is reset to its initial state; GIBBS is reinitiated and data already entered to GES is lost.
Options	**Description and additional information**
`Keyword`	One of the keywords `Elements`, `Species`, `Phases`, `Constituent` or `System` must be used to indicate what is rejected.
`Name&`	Names of the pre-defined elements/species/phases/constituents/system
`Elements`	The given elements are rejected.
`Species`	The given species are rejected, making it impossible to form them from the defined elements.
`Phases`	The given phases are rejected, making it impossible to form them from the defined elements or species.
`Constituent`	The given constituent in one phase are rejected. Add the following when prompted: `Phase`: The name of the phase containing the constituent to be rejected. `Sublattice number`: The sublattice where the constituent enters (the first sublattice is 1). The question is omitted if there exists only one possible sublattice. `Constituent`: The name(s) of the constituent(s) to be rejected.

RESTORE

This command is for the DATABASE_RETRIEVAL (TDB) module.

Restore already explicitly rejected elements, species, phases or constituents; it is the opposite of the command REJECT although it does not restore a completely rejected system.

Phases/species/constituents that are possible to form from the defined elements or species are entered to the list of system phases/species/constituents (shown by the command LIST_SYSTEM). Phases/species/constituents that are not included on the list can now be added to the list. The different names must be separated with a space or comma. It is possible to use a wildcard * after a common part of names so that all the elements/species/phases/constituents, which start with that common part and are available in the currently switched or appending database, are restored in the defined system.

Syntax	RESTORE
Prompt1	(if keyword = ELEMENTS or SPECIES or PHASES) `Keyword: <Name1, Name2, …>`

Prompt2	(if keyword = CONSTITUENT)
	`Phase: <Phase name>`
	`Sublattice number: <Sublattice number in the phase>`
	`Constituent: <Constituent(s) in the sublattice of the phase>`

Options	**Description and Information**
`Keyword`	One of the keywords `Elements`, `Species`, `Phases` or `Constituent` must be used to indicate what is rejected.
`Name&`	Names of the pre-defined elements, species, phases, and constituents
`Elements`	The given elements are restored.
`Species`	The given species are restored and thus possible to form from the defined elements.
`Phases`	The given phases are restored and thus possible to form from the defined elements or species.
`Constituent`	The given constituent in one phase are restored. Add the following when prompted: `Phase`: The name of the phase containing the constituent to be restored. `Sublattice number`: The sublattice where the constituent enters (the first sublattice is 1). `Constituent`: The name(s) of the constituent(s) to be restored.

SET_AUTO_APPEND_DATABASE

This command is for the DATABASE_RETRIEVAL (TDB) module.

Enforce an automatic action that appends thermodynamic data from a chosen database regarding the system to the data you already have about the system from the current database (that is, the default database or the database last chosen with SWITCH_DATABASE or APPEND_DATABASE).

This is useful to simultaneously retrieve both thermodynamic and mobility data for a defined system when performing a DICTRA module simulation.

This command should be used before defining a system (with the commands DEFINE_ELEMENTS, DEFINE_SPECIES, or DEFINE_SYSTEM) and retrieving the data with the GET_DATA command from the primary switched database.

Syntax	SET_AUTO_APPEND_DATABASE
Prompt	`Database name /XYZ/: <Additional database name>`
Option	`Additional database name` The name of an existing database or a User database that corresponds to the automatically-appending database.

It works in a way that is similar to the APPEND_DATABASE<DATABASE-NAME> command sequence, but only the phases that are also available in the primary switched database are appended. There is no possibility to manually list, reject and/or restore any phase that is available in the appending database. When retrieving data with GET_DATA afterwards, all the phases that exist in the appending database but not in the primary switched database are automatically rejected. The prompt is kept as for the primary switched database, `TDB_XYZ`: (where `XYZ` stands for the name of the primary switched database) until the execution of GET_DATA.

Therefore, to selectively append more phases from a secondary database to a system that is defined and retrieved from a primary switched database, then APPEND_DATABASE and sequential commands (such as DATABASE_INFORMATION, DEFINE_SYSTEM, DEFINE_ELEMENT, DEFINE_SPECIES, LIST_SYSTEM, REJECT, RESTORE and GET_DATA) should be used instead, before this command.

Although it is impossible to manually list, reject and restore any phase from the appending database, the DATA module automatically ignores all the phases that do not exist in both the primary switched database and the appending database, and append the data for the phases (that are also available in the primary switched database) from the appending database, as informed on screen when executing GET_DATA afterwards.

SWITCH_DATABASE

This command is for the DATABASE_RETRIEVAL (TDB) module.

Switch (or change) from the current database to a new one. It also reinitializes the entire module.

The database can be either a standard database (the ones in `tc_initd.tdb`) or a so-called user database. To open your own (user) database, type `USER` followed by the path to the user `.TDB` file or press <Enter> and select it in the window that opens.

Syntax	SWITCH_DATABASE
Prompt	`New database name /XYZ/:` The name of either an existing database (e.g. FEDEMO) or USER.

POLY Module Commands

In this section:

ADD_INITIAL_EQUILIBRIUM

This command is for the POLY module.

Add initial equilibrium points from which a phase diagram is calculated (through the MAP command).

For each initial equilibrium the first stage of the mapping varies the value of the given axis variable condition, changing it in the given direction. When a phase change is found it is saved as a start equilibrium, and if the symbol ">" was used, it continues the search until the end of the axis variable.

If no axis variable conditions differ between initial equilibria then the map results in several overlaid diagrams, in accordance with the selected conditions and the values.

The ADD_INITIAL_EQUILIBRIUM default command implicitly makes the MAP command search for phase changes according to settings set by ADVANCED_OPTIONS STEP_AND_MAP command. Default for STEP_AND_MAP are three initial equilibrium equidistantly along each axis variable, along the edge of the axis variable rectangle.

By default these default start points are used in MAP. If any ADD_INITIAL_EQUILIBRIUM is used these default start points are not used. They are again used if the command ADD default is used together with another ADD_INITIAL_EQUILIBRIUM command.

The ADD command with the default direction scans along the axis variables and generates start points each time the scan procedure crosses a phase boundary. In addition, it generates four start points, scanning cross the middle of each axis, if there is any solubility line that does not reach the axes. At the MAP command, a search for lines in the diagram is made along each direction of the axis variables in the diagram.

In this way, it should guarantee that all possible phase boundary lines in a phase diagram are found. It may take a little longer to execute than using the minimum number of start points, as some lines may be calculated more than once. But the POLY module remembers all node points and subsequently stops calculations along a line when it finds a known node point.

It is also possible to create a sequence of start points from one initial equilibria by appending a > after the direction at the ADD command. For example:

```
Direction /Default/: 2>
Direction /Default/: -2>
```

This generates one start point for each set of phase change in the positive direction of the axis 2 (or negative direction of the axis 2); this ensures finding all possible phase boundary lines (not just the first one) along such an axis direction.

This is particularly useful when you have a phase diagram with several lines with no intersection. It is thus possible to calculate e.g. an isopleth for a much more limited composition range. It is also useful for calculating CVD diagrams and Pourbaix diagrams.

Syntax	ADD_INITIAL_EQUILIBRIUM
Prompt	`Direction /Default/: <Direction code>` Direction code(s): - `1` or `2`for positive direction of axis 1 or 2, respectively. - `-1` or `-2`for negative direction of axis 1 or 2, respectively. - `Default` for MAP to start looking for phase changes from each corner of the axis variable rectangle. The direction is important when the initial equilibrium point is in a single-phase region or when the diagram is an isopleth (tie-lines not in the plane of calculation). In such cases, the program will search for a line in the diagram (i.e., a line where the amount of a phase is zero) in the given direction.

Normally, this command is not needed to calculate a property diagram (with the STEP_WITH_OPTIONS → `NORMAL` command-sequence), as the STEP procedure starts from the current equilibrium state already calculated. In many cases, the ADD_INITIAL_EQUILIBRIUM command is not required for MAP commands either.

In order to calculate a simple property diagram, set the equilibrium conditions and the stepping axis variable, and then give a STEP command. But if a phase diagram has disconnected lines, ADD_INITIAL_EQUILIBRIUM may still be needed to add two or more initial equilibria so that the MAP calculation starts from such initial equilibria at the specified directions to find all phase boundary lines.

This command becomes unnecessary in most cases, as the MAP routines that by default use the Global Minimization Technique handles all the initial equilibrium points in a robust and automatic way. Therefore, you do not need to have a good guess of the starting point and to add any initial equilibrium point prior to the calculations of various types of phase diagrams. However, if preferred, use this command to add any initial equilibrium points in certain directions, the POLY module uses the specified starting point(s) and corresponding user-added initial equilibrium point(s) for a mapping calculation; in such a case, the automatic procedure in the rewritten MAP routines are not enforced while the Global Minimization Technique can still be applied. Similar situations occur when a specific database, in which there are some definitions of initial-equilibrium adding direction(s) for accessed binary and/or ternary subsystems in its ACCESSED_SYSTEM section, is used in the BINARY or TERNARY module for calculating a binary or ternary phase diagram.

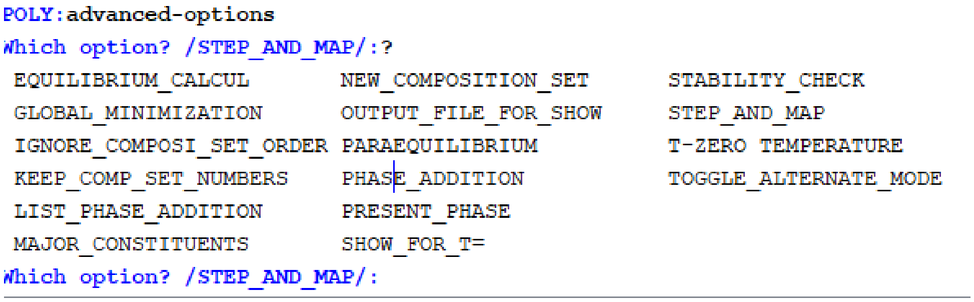
All the initial equilibrium points generated by ADD_INITIAL_EQUILIBRIUM (previously and presently; saved in the current POLY workspace) can be easily listed on screen with LIST_INITIAL_EQUILIBRIA. A certain initial equilibrium point (including its conditions and equilibrium results) can be loaded into the current equilibrium, if needed, with LOAD_INITIAL_EQUILIBRIUM. Any specific or all of the initial equilibrium points can be deleted from current POLY workspace, if desired, with DELETE_INITIAL_EQUILIBRIUM.

ADVANCED_OPTIONS

This command is available with the POLY and ED-EXP modules.

Syntax	ADVANCED_OPTIONS
Prompt	`Which option? /Step_and_Map/:  <Option>`

Several options are available after you enter this command at the prompt. The default is STEP_AND_MAP.



```
POLY:advanced-options
Which option? /STEP_AND_MAP/:?
 EQUILIBRIUM_CALCUL        NEW_COMPOSITION_SET      STABILITY_CHECK
 GLOBAL_MINIMIZATION       OUTPUT_FILE_FOR_SHOW     STEP_AND_MAP
 IGNORE_COMPOSI_SET_ORDER  PARAEQUILIBRIUM          T-ZERO TEMPERATURE
 KEEP_COMP_SET_NUMBERS     PHASE_ADDITION           TOGGLE_ALTERNATE_MODE
 LIST_PHASE_ADDITION       PRESENT_PHASE
 MAJOR_CONSTITUENTS        SHOW_FOR_T=
Which option? /STEP_AND_MAP/:
```

- EQUILIBRIUM_CALCUL
- GLOBAL_MINIMIZATION
- KEEP_COMP_SET_NUMBERS
- LIST_PHASE_ADDITION
- MAJOR_CONSTITUENTS
- NEW_COMPOSITION_SET
- OUTPUT_FILE_FOR_SHOW
- PARAEQUILIBRIUM
- PHASE_ADDITION
- PRESENT_PHASE
- SHOW_FOR_T=
- STABILITY_CHECK
- STEP_AND_MAP
- TOGGLE_ALTERNATE_MODE
- T-ZERO_TEMPERATURE

AMEND_STORED_EQUILIBRIA

This command is for the POLY module.

This command gives information about the calculated blocks (and phase regions included in blocks) after the STEP or MAP calculation(s). It allows you to list all or part of the calculation results, to suspend all or parts of the calculation results that are redundant or where metastable equilibria are calculated, and to restore all or parts of the calculation results (if having been suspended by another AMEND_STORED_EQUILIBRIA command).

The workspace for storing equilibria may overflow during stepping or mapping, and is then written to a file as blocks. Each block usually contains one or more ranges of equilibrium regions.

Use one these options:

- `L` to list the calculated equilibria (all or a specified block)
- `S` to suspend everything (all blocks and their regions)
- `Q` to suspend each set of equilibria individually (specified blocks and/or regions)
- `R` to restore everything (all blocks and their regions)

Syntax	AMEND_STORED_EQUILIBRIA
Prompts	`Name: <Name of a defined table>` List (`L`) the calculated equilibria, suspend everything (`S`) or suspend each set of equilibria individually (`Q`), or restore everything (`R`).
	`Block /*/: <Block number>` Specify a block number in the option `L`, `S`, `Q` or `R`. Or include all the blocks in the amending option, by accepting the wildcard * (press <Enter>). For `L`, a block (if a block number is specified) or all the blocks (if the wildcard * is accepted/used), with the regions and the equilibrium details, that are calculated during stepping or mapping is listed on screen or in a textual file. For `Q`, each ranger in a block (if a block number is specified) or in all blocks (if the wildcard * is accepted/used) then choose:

	`S(uspend) K(eep) /K/: <S or K>`
	For `S` or `R`, if a block is specified, you are asked what region in the block should be suspended or restored. However, if the wildcard * is accepted/used, you are asked the following:
	`Really suspend all /N/:`
	`Really restore all /N/:`
	In both cases the default is N and you are prompted for which block(s) and which region(s) in a certain block to execute the `S` or `R` action.
	`Really suspend all /N/:`

Syntax	AMEND_STORED_EQUILIBRIA
	Y suspends everything. `Really restore all /N/:` Y restores everything.
	`Range: <Range(s) of region>` Specify one or more ranges to be suspended (the `S` option) or restored (the `R` option). The wildcard * suspends or restores all ranges in the specified block. In order to know the ranges the LIST command must first be used.
	`S(uspend) K(eep) /K/: <S or K>` The Query suspend option (`Q`) asks for each region in a certain block if it should be suspended or kept. Suspended regions are not included on sequentially generated plots.
	`Output file: /Screen/: <File name>` This prompt is only for listing (the `L` option), and after it the command is terminated. The file name must be given here; or accept the default Screen (terminal) by pressing <Enter>. A list of stored equilibria as various blocks (with all their ranges) are shown out on screen or the file.

CHANGE_STATUS

This command is available with the POLY and ED-EXP modules.

In the POLY module, set the status for components, species and phases in the defined system for all the sequential calculations (single-point, stepping, and mapping) in equilibrium or local/partial equilibrium state. Each component, species and phase has a status. The default status is `ENTERED`.

The most important use is to calculate metastable equilibria and metastable phase diagrams by setting some phases (that would otherwise be stable) to the SUSPENDED or DORMANT phase-status. Another important applications is to calculate paraequilibria by setting some components to the SPECIAL component-status.

For a component and for a species, the status can be one of the following:

- `ENTERED`: the component(s) or species are included in the calculation. This is the default status.
- `SUSPENDED`: the component(s) or species are not considered in the calculation.
- `SPECIAL`: the specified component(s) are not included in summations for mole or mass fractions. It only works for component(s).

Only component(s) can have the status SPECIAL, which implies that these are not included in summations for mole or mass fractions.

For example, for the *u-fractions* or other normalized fractions, when one or more of the components are excluded from the summation, you must specify which component(s) should be excluded from the calculation of mole or mass fraction. This component status is particularly useful when calculating paraequilibrium states. Such component(s) are normally interstitial component, and must have the status SPECIAL. This is assigned by the CHANGE_STATUS command.

Syntax	CHANGE_STATUS
Prompts	`For phases, species or components? /Phases/: <Keyword>` *Keyword* = phase or species or components
	`Phase name(s): <Name(s) of the phase(s)>` For `phase` as the keyword, the names of the phases that have their status changed must be given (all on one line). A comma or space must be used as separator. The status to be assigned to the phases can also be given on the same line if preceded with an equal sign (=).

Syntax	CHANGE_STATUS
	An asterisk, *, can be used to denote all phases. The special notations `*S`, i.e. a wildcard * directly followed by an `S`, sign, means all suspended phases. In the same way, `*D` means all dormant phases, and `*E` means all entered phases.
	`Name(s): <Name(s) of the Species or Component(s)>` For species or components as the keyword, the names of the species or components that have their status changed must be given (all on one line). A comma or space must be used as separator. Similarly to the case of phase as the keyword, the status to be assigned to the species or components can also be given on the same line if preceded with an equal sign =. An asterisk, *, can be used to denote all species or components. The special notations `*S`, i.e. a wildcard * directly followed by an `S`, sign, means all suspended species or components. In the same way, `*E` means all entered species or components.
	`Status /Entered/: <New status>` The `new` status to be assigned must be given. For species, the values `ENTERED` or `SUSPENDED` can be used. For the POLY module, using the `Entered` or `Suspended` status here has the same result as using the commands MAKE_COMPONENT_ENTERED and MAKE_COMPONENT_SUSPENDED. The exception is that any existing conditions that depend on a suspended component are removed when using the MAKE_COMPONENT_SUSPENDED command. For components, the status `ENTERED`, `SUSPENDED` or `SPECIAL` can be given. SPECIAL means that this component is excluded from sums for mole fractions and mass fractions, which is useful when calculating the *ufractions* or other normalized fractions of system components. For phases, the status `ENTERED`, `SUSPENDED`, `DORMANT` or `FIXED` can be given. DORMANT means the same as suspended but the driving force is calculated. FIXED means that it is a condition that the phase is stable at a certain amount. For example, for the ufractions, when one or more of the components are excluded from the summation, you must specify which component should be excluded from the calculation of the mole fraction. This component must have the status SPECIAL. This is assigned by the CHANGE_STATUS command: `Change_Status comp C=special`.
	`Start value, number of mole formula units /0/: <Initial amount>` For ENTERED phases, an `initial amount` of the phase can be given. Normally, 0 is given if the phase is not likely to be stable, and 0.5 or 1 or any positive number if the phase could be stable, but such an initial amount is only used as the rough starting estimation in the equilibrium calculations.
	`Number of mole formula units /0/: <Equilibrium amount>`

Syntax	CHANGE_STATUS

For FIXED phases, the `equilibrium amount` of the phase [always using an initial estimation being the `NPF(phase)` value which it is the normalized mole number of components (per mole formula unit) of the specific status-fixed phase] must be given. If the equilibrium amount is zero, then the phase is at its stability limit.

NOTE WHEN SPECIFYING A FIXED PHASE STATUS

Special attention should be paid when specifying a FIXED phase status in equilibrium calculations (for single points, stepping or mapping calculations), as described below.

The phase amount variables, NP(phase), BP(phase) and VP(phase), as well as all their M/W/V-suffixed quantities, should not be used as conditions. Instead, use the CHANGE_STATUS command to set a relevant condition, e.g. `CHANGE_STATUS phase <phase>=fix <amount>` where the fixed <amount> is roughly the same as the F-suffixed quantity `NPF(phase)`.

The `NPF(phase)` quantity is the normalized mole number of components (per mole formula unit) of the specific phase in the defined system, which unlike other `F`-suffixed state variables [e.g. GF (phase), HF(phase) and DGF(phase)] cannot be directly applied in any POLY command, implying that it cannot be directly evaluated or listed/shown. If intended to shown such a normalized phase amount value in an equilibrium state, you should use a properly-entered symbol (function or variable), for example: `NPFabc = NP(abc)/NA` or `NPFabc = NPM(abc)/NA*N`. N is the total system size (in mole). The NA value is a quantity that is phase-dependent (and sometimes also equilibrium-dependent for ionic solution phases), and is the total atomic number in a mole-formula-unit of the specific phase abc (excluding interstitial component and, of course, vacancy). For example, the SIGMA, FCC, BCC and LIQUID phases (among others) in a defined Fe-Cr-Ni-C-N-O system (retrieved from a specific database) may be modeled by certain models, and their NA values must be evaluated in different ways, as described below:

```
LIQUID (C,Cr,CrO3/2,Fe,FeO,FEO3/2,N,Ni,NiO)1 NA = 1

FCC_A1 (Cr,Fe,Ni)1(Va,C,N,O)1 NA = 1

BCC_A2 (Cr,Fe,Ni)1(Va,C,N,O)3 NA = 1

SIGMA (Fe,Ni)8(Cr)4(Cr,Fe,Ni)18 NA = 30
```

If in the same Fe-Cr-Ni-C-N-O system the liquid solution phase is modeled by the Two-Sublattice Ionic Liquid Model, i.e.:

```
IONIC_LIQ  (Cr+3,Fe+2,Ni+2)p(VA,C,N,O-2,FEO3/2)q,7
```

then the evaluation of its NA value becomes even more complicated:

```
NA = p + q*yC2 + q*yN2 + q*yO2-2 + q*yFeO2 3/ 2
```

where the stoichiometric coefficients *p* and *q* are also dependent upon the real equilibrium state (rather than having fixed values in the system). Similar situations occur for other (solid) phases which are described by a multiple sublattice model with ionic constituents, such as SPINEL and HALITE phases in some databases.

There is no strange thing when using a zero value [i.e. `0`] in a FIXED phase-status, since it means the specified phase is stable in equilibrium state but has a zero-amount of mass in the equilibrium calculations; in other words, on a phase diagram, the specific phase is on a zero-fraction line (ZFL), i.e. it starts becoming stable on one side of a corresponding phase-boundary line or unstable on the other side of the same boundary. It is often and efficient to do so when calculating e.g. solidus equilibrium states.

However, when a non-zero value [it must always be positive; e.g. 1 or 0.5 or 0.3 or 1.5] is to be specified in a FIXED phase-status, it is unnecessarily the exactly same stable amount of the specific

Syntax	CHANGE_STATUS
	FIXED-status phase in a calculated equilibrium state any longer; instead, the <equilibrium amount> value is the NPF(phase) value that is only roughly used as the estimated starting-value of the FIXED-status phase in the equilibrium calculations. Therefore, a FIXED-status for a liquid phase being unity does not necessarily imply that it is a liquidus equilibrium state (where the liquid phase is in equilibrium with some solid phases but the liquid phase takes all the mass in the defined system). A unity value for setting the liquid phase status in calculating liquidus equilibrium state can only be used when the liquid mixture phase is predefined as a single-sublattice solution phase (such as metallic liquid phase in multicomponent alloy systems) and the total system size as one mole (i.e. N=1). When a phase is described by a solution model in which two or more sublattices are considered and these sublattice sites may also have different stoichiometric coefficients [meaning that the mixture phase could have more than one atom in formula [NA>1; see some examples above], the unity value should not be used when setting the FIXED status for the phase; instead, you should use an appropriate value that ranges from 0 to a NPF(phase) value that equals to or is smaller than 1/NA (if the total system size N=1) or 1/NA*N (if N differs from unity). For this reason, if a multicomponent system bears an IONIC_LIQUID phase that is described by the Two-Sublattice Ionic Liquid Model (or any other multiple-sublattice ionic solution phases), it is difficult to use a proper `NPF(ION_LIQ)` value in setting its FIXED phase-status, because that should be less than (or equal to) the complex value of $N/[p + q*^{y}C2 + q*^{y}{}_{N}2 + q^{*y}{}_{O}22 + q^{*}y_{FeO}2\ 3/\ 2\ ].$

Examples

For example, to obtain the metallic fraction in a system with carbon as an interstitial component, you can set the component status for carbon as `SPECIAL`:

```
Change_Status comp C=special
```

The `SUSPENDED` status for components and species does not always work as expected.

For a phase, it may have one of these statues:

- `ENTERED`: the phase(s) are included in the equilibrium calculations and these are stable if that minimizes the total Gibbs energy in the defined system. This is the default status for all phases already retrieved from the chosen database(s). An ENTERED phase-status is always associated with an initially-estimated amount [in mole number; normally, as 0 if the phase is not likely to be stable, and as 0.5 or 1 or any positive number if the phase could be stable] but it is only used as the rough starting value in the equilibrium calculations.

- `SUSPENDED`: the phase(s) are not considered in the equilibrium calculations.
- `DORMANT`: the phase(s) are not considered in the equilibrium calculations but their driving forces for precipitation are calculated.
- `FIXED`: it is an equilibrium condition that the status-fixed phase must be stable, and be in equilibrium at a specified amount [always using an initial estimation being the `NPF(phase)` value which it is the normalized mole number of components (per mole formula unit) of the specific status-fixed phase]. See more descriptions at the end of this command.

COMPUTE_EQUILIBRIUM

This command is for the POLY module.

The full equilibrium state is calculated for the given set of conditions. The Global Minimization Technique is by default enforced in this command (C_E), while it can be disabled temporarily (for the current single-point equilibrium calculation) if using C_E – or C_E * command-combination, or permanently (for all the sub sequential single-point calculations or stepping/mapping calculations within the current TCC run) if having decisively switched it off by a user (or possibly in some special modules) through changing the minimization option using the ADVANCED_OPTIONS → `MINIMIZATION_OPTION` command-sequence.

Syntax	COMPUTE_EQUILIBRIUM
Prompt	The C_E command can be used, in order to enforce the ordinary POLY minimization routines in an equilibrium calculation; this is because of that the ordinary C_E command is now associated with the Global Minimization Technique, and only after the Global Minimization If technique is permanently switched off the C_E command makes no difference from the C_E – command-combination. Only certain types of equilibrium conditions [e.g. `T`, `P`, `N`, `N`(`<component>`), `X`(`<component>`), `B`, `B`(`<component>`), and `W`(`<component>`)] are fully supported in the Global Minimization mode (called *Direct Global Minimization*); and when other types of equilibrium conditions are used, after the initial POLY, a Global Minimization test and corrections are performed until the lowest minimum is found (called *Indirect Global Minimization*). If there is any problem with convergence, you may try the C_E * command-combination. The character * enforces the command to use an advanced technique to obtain a complex equilibrium. However, after a successful C_E *calculation, you may repeat the C_E command and can check the status of phases, species or components (with LIST_STATUS → CPS command-sequence) and equilibrium conditions (with LIST_CONDITIONS) and list out the calculation results (with LIST_EQUILIBRIUM), because such actions may tell you how to further modify various settings for your current calculation. This command-combination is not that useful anymore, because the Global Minimization Technique that is always associated with the C_E command is even more powerful and more precise in finding the most-stable equilibrium state in a complex heterogeneous interaction system; therefore, the C_E * command-combination is functional and can be used only after the Global Minimization mode has already been disabled temporarily or permanently. Some phases that are not stable in the current equilibrium state may not have their most favorable composition after this command, and thus their driving forces may not be correct. You can force the program to correctly calculate the driving forces of metastable phases, by giving repeated C_E commands until the number of iterations (that is shown on screen after this command) is reduced to 2. Also see the POLY command SET_NUMERICAL_LIMITS which can set the approximate driving force for metastable phases option on or off in all the subsequent POLY calculations within the current TCC run.

Syntax	COMPUTE_EQUILIBRIUM
	If an equilibrium state for the defined system is not found, an error message is given. You can try repeating this command a few times, or change some of settings for the numerical limits, for starting variables and starting values, for starting constitutions of certain phases and for reference states of certain components, or to verify some of the defined conditions.

COMPUTE_TRANSITION

This command is for the POLY module.

This command is a combination of the CHANGE_STATUS, SET_CONDITION and COMPUTE_EQUILIBRIUM commands. It allows a direct calculation when a new phase may form by varying one of the already-set conditions. It can be used only after at least one equilibrium is calculated successfully; otherwise, you are informed on the necessity of first making an equilibrium calculation to find out the stable phases under the current conditions.

When this command is used, the program calls the command CHANGE_STATUS to temporarily change the phase status of a specified phase as FIXED at the *zero* amount, and at the same time to temporarily release one of the existing equilibrium conditions (which is chosen by you). The program calculates a new equilibrium in which that specific phase is stable but its equilibrium amount in the system is zero. The released condition is then assigned with a calculated value that ensures the calculated equilibrium. After wards, the program automatically changes the phase status of that specific phase back to ENTERED, and resets the temporarily released condition as one of the conditions and assigns it with the value that is calculated to ensure the zero-amount formation of that specific phase.

This command is useful to find melting temperature, boiling temperature, or solubility limits, and generally when you want to set the most optimal conditions for calculating an equilibrium where a specific phase becomes stable. It can also be used when you want to know exactly how far away the defined conditions are from the value that can ensure a zero-amount of a specific phase in the system when other conditions remain the same.

After a successful calculation, you can issue a COMPUTE_EQUILIBRIUM calculation to assure the calculated transitional equilibrium is a really stable one, and can also use LIST_EQUILIBRIUM to see the details of transitional equilibrium state.

Syntax	COMPUTE_TRANSITION

Prompts	`Phase to form: <Phase name>`
	A new `phase name`, e.g. `BCC` that is expected to form, is specified here. This changes the status of this new phase to be `FIXED` as `0` amount, and the program shows the information such as:
	`You must remove one of the these conditions`
	`P=100000, T=800, N=1, X(FE)=.5    DEGREE OF FREEDOM 0`
	If the key word `ANY` is used when prompted for `Phase to form` (instead of a specific phase name), it is possible to find out any new phase to be formed, in a given varying direction sign and at an estimated change of the released condition: a negative sign means at a lower value of the released condition any new phase is to be found, and a positive sign at a higher value; an estimated change of the released condition implies where any new phase is expected (but it is only estimated value, so any value within its reasonable scale would be enough). Such calculations can be repeated if required. This feature is useful to find out all possible phase transformations along a certain released condition.

Syntax	COMPUTE_TRANSITION

```
Give the state variable to be removed /T/: <One condition>
```

`One condition` must be removed, in order to calculate the transition equilibrium where the specified (or any) new phase to be formed at a calculated value of this released variable.

Therefore, the message may display (after a successful calculation) if, for example, `X(Fe)` is entered:

```
   To form BCC the condition is set to X(FE)=.48605791769
```

This calculated value is assigned as the parameter of that removed condition, in this case, the `X(FE)` variable. If the LIST_CONDITIONS command is typed this message displays:

```
   P=100000, T=800, N=1, X(FE)=4.86057918E-1
   DEGREES OF FREEDOM 0
```

If the key word `ANY` (instead of a specific phase) is given as the phase name when it is prompted for Phase to form, the line is prompted for a given varying direction sign and an estimated change of the released condition before the calculation of transition equilibrium:

```
 Estimated change (with sign) /1/: <+/-#>
```

A given varying direction sign and an estimated change of the released condition, in this case as `X (FE)`, must be given here: a negative sign means at a lower value of the released condition any new phase is to be found, and a positive sign at a higher value; an estimated change of the released condition implies where any new phase is expected (but it is only estimated value, so any value within its reasonable scale would be enough). For example, if a combination of -0.02 is input, this message may display (after a successful calculation):

```
   To form BCC_A2#1 the condition is set to X(FE)=.493708756187
```

This calculated value is then assigned as the parameter of that removed condition, in this case, the `X(FE)` variable. The message is shown if the LIST_CONDITIONS command is typed:

```
   P=100000, T=800, N=1, X(FE)=4.93708756E-1
   DEGREES OF FREEDOM 0
```

CREATE_NEW_EQUILIBRIUM

This command is available with the POLY and ED-EXP modules.

During data-assessments using the ED_EXP module (a submodule of PARROT), you can, in the POLY module, create several equilibria with different sets of conditions and phases (but normally with the same set of components). By default, there is one equilibrium. To keep the set of conditions and phase for this equilibrium, create another one using this command, and use another set of conditions for that. Two equilibria may be useful to calculate easily the enthalpy difference between two states. In the PARROT module, the experimental information is stored as a sequence of equilibria.

Syntax	CREATE_NEW_EQUILIBRIUM
Prompts	`Equilibrium number /2/: <A new equilibrium number>` Each equilibrium in the POLY workspace is identified by a unique integer number. Such an equilibrium number can be recalled with SELECT_EQUILIBRIUM.
	`Initiation code /2/:` When an equilibrium is created, you can choose to `ENTER` all components and phases (initiation code 2), `ENTER` the components only (initiation code 1) or `SUSPEND` everything (initiation code 0). No other values are legal. The entered components and phases can later be changed with CHANGE_STATUS.

DEFINE_COMPONENTS

This command is available with the POLY and ED-EXP modules.

Change the set of components. By default, the elements are used as components. The set of components can be important because some conditions are set using components, for example, the amounts, activities or chemical potentials.

For example, in the system Fe-Si-O, you can define FEO, FE2O3 and SIO2 as components, thus replacing the default FE, SI and O.

This implies a command REINITIATE_MODULE and it should be given as the first command in the POLY module.

Syntax	DEFINE_COMPONENTS
Prompt	`Give all new components / existing components/: <New components>` The `new components` must be specified all on one line. These replace the existing component definitions. The number of components cannot be changed with this command. Use CHANGE_STATUS instead.
	To keep some existing components, it is recommended that you also enter these on the line. Otherwise, the added new components may not be defined correctly. This is especially important if some components are built out of several elements. The new components do not have to be present as species.

DEFINE_DIAGRAM

This allows automatic calculation and plotting of a diagram with a single command. It is the same as the DEFINE_MATERIAL command up to when the first equilibrium is calculated. The alloy OPTION feature is also available in this command to specify alloying compositions for a special alloy predefined by the OPTION keyword in a selected database (e.g. the TCNI Ni-based Superalloys Database).

Use this command to calculate all types of phase diagrams after specifying all composition value and an initial temperature (if temperature is used as an axis). However, for binary and ternary diagrams, the special BIN and TERN modules may be preferred.

It then lists all the independent variables for the defined system (i.e. temperature and the components) and asks for a variable as the X-axis. You must also specify a maximum and minimum for the X-axis. The second axis (Y-axis) can be another composition (or the temperature if that is not on the X-axis) from the independent variable list. The program then calculates and plots a *phase diagram*, as there are two independent quantities on the axes.

Alternatively, select a dependent quantity as the Y-axis variable from the second list on screen (e.g. the amount of all phases, composition of a specific phase, or fractions of a component in all phases), and the program calculates and plots how this quantity depends on the condition on the X-axis. This is a *property diagram*.

This command ends up within the POST module monitor. You can refine the calculated phase diagram or property diagram.

Moreover, many more property diagrams with axes other than compositions can also be plotted (after the calculation), using SET_AXIS_VARIABLE in the sequent POST monitor.

Syntax	DEFINE_DIAGRAM
Prompts	These prompts are given:

```
Same elements as before /Y/?
Mole percent of <Element> /##/: <Value>
```

or

```
Mass percent of <Element> /##/: <Value>
 Database /ABCDE/: <Database name>
 Major element or alloy: <Element name>
 Composition in mass (weight) percent? /Y/:
1st alloying element:  <Element name>
Mass (weight) percent: <Amount of the above specified element>
2nd alloying element: <Element name>
Next alloying element: <Element name>
Mass (weight) percent: <Amount of the above specified element>
```

Syntax	DEFINE_DIAGRAM

	`Temperature (c) /1000/: <Temperature of interest in oc>`
	`Reject phase(s) /none/: <List of phase(s) to be rejected>`
	`Restore phase(s) /none/: <List of phase(s) to be restored>`
	`OK? /Y/: <Y or N>`
	`Should any phase have a miscibility gap check? /N/:`
	`Phase with miscibility gap: <phase name>`
	`Major constituent(s) for sublattice #: /aa/: <Constituent(s)>`
	`Phase with miscibility gap: <Phase name>`
	The first equilibrium is calculated, as with DEFINE_MATERIAL. Then a list of all independent conditions suitable to be chosen as X/Y-axis variables is given by the program.

	`Quit? /Y/: <Y or N>` This question is asked only when the axis variables are already defined, or if DEFINE_DIAGRAM is used. It then offers an opportunity to quit (Y) the calculation or to continue (N) the calculation but by defining other axes.
	`Give the number of the condition to vary /1/: <A condition index>` Select one of the independent conditions by giving its index on the condition list as the X-axis variable.
	`Minimum value /XXX/: <minimum value for X-axis>` Specify the minimum value of the chosen X-axis variable. A default value is shown automatically by the program; press <Enter> to accept it or input another value.
	`Maximum value /YYY/: <maximum value for X-axis>` Specify the maximum value of the chosen X-axis variable. A default value is shown automatically by the program; press <Enter> to accept it or input another value. Then another list with some dependent quantities is given by the program, which can be selected as the Y-axis variable.
	`Give the number of the quantity on the second axis /#/: <##>` Select one of the independent conditions or dependent quantities as the Y-axis variable, by giving its corresponding index given on the condition lists. It must be different from the X-axis variable already selected. If selecting one of dependent quantities (by giving the corresponding number from the second list) as the Y-axis, then a property diagram is to be automatically calculated (through a normal stepping procedure) and generated. For `composition of a phase` the phase name is asked for further specification subsequently. If selecting any of the other independent variables (conditions) on the first list as the Y-axis, then a phase diagram is automatically calculated (through a mapping procedure) and plotted.
	`Name of phase: /ABC/: <phase name>` This is prompted only in case of that the `composition of a phase` is selected as the Y-axis variable. The phase name for which the composition varied along with X-axis variable should be specified.

Syntax	DEFINE_DIAGRAM
	`Multiple start points? /Y/:` By default, the program automatically generates and uses multiple start points for mapping the defined phase diagram.
	`Save file /Result/: <File name>` The file name where the calculations are stored (saved as a *.POLY3 file) should be specified; the default file name is `RESULT.POLY3`. Linux and Mac are case sensitive so ensure you enter `.POLY3`.

DEFINE_MATERIAL

This command is for the POLY module.

Read data for a system from a database in the POLY module. It is convenient to use for alloys when there is a major component and the amount of the other elements is known in mass (weight) fraction. The command reads the system from the specified database, sets the composition and temperature (and pressure equal to 1 bar) and calculates the equilibrium state before the prompting for a new command. You can list the results with LIST_EQUILIBRIUM or set a new composition or set axis for a STEP or MAP command.

You cannot append data from different databases in this way. Use this command with data from a USER database.

Syntax	DEFINE_MATERIAL
Prompts	`Same elements as before /Y/?` This question is asked only if some data is already read from the database, or if the command DEFINE_MATERIAL or DEFINE_DIAGRAM is used. It then offers a convenient way to change the composition and temperature with one command. This command only works properly in cases where the composition of the material system is already defined as in the mole-percent or mass-percent unit.

	`Mole percent of <Element> /##/: <Value>`
	or
	`Mass percent of <Element> /##/: <Value>`
	If you have decided to use the same materials system (available in the current POLY3 workspace) by accepting the default (Y) to the previous prompt `Same elements as before /Y/?`, one of the alternative prompts display for each of the components in the defined system, depending on how the composition is defined (either in mole-percent, or in mass-percent).
	Prompts are repeated until all the defined components are completed. Then, the program prompts to specify the temperature condition.

	`Database /ABCDE/: <Database name>` The database with the description for the material must be given, or press <Enter> if using the current database. It is possible to give a USER database.
	`Major element or alloy: <Element name>` The material must have a major element, usually the element which is present in the largest amount. The fraction of this element is not set but is the rest.

Syntax	DEFINE_MATERIAL
	In some databases there are the alloys predefined. An alloy has a default major element and have limits of the amounts of the alloying elements. If you stay within these limits the calculation gives reasonable results.
	`Composition in mass (weight) percent? /Y/:` By default the input is taken as mass percent. Choose N to change to mole percent. ❗ Composition should be given in PERCENT not FRACTION, as it is required for the `w` and `x` state variables in the SET_CONDITION command.
	`1st alloying element: <Element name>` The first alloying element must be given. All alloying elements are asked for in a sequence. These can be given in any order. You must know if you are present as assessed systems in the database. There is no error or warning messages if data are missing. Check the documentation of the database selected. If an alloy is selected, a list of legal alloying elements and their maximum percent is listed on-line.
	`Mass (weight) percent: <Amount of the above specified element>` The amount of the alloying element in mass (weight) percent. Using DEFINE_MATERIAL you cannot use the normal flexibility for conditions, but all must be given in mass percent. However, you can after wards change the conditions using SET_CONDITION.
	`2nd alloying element: <Element name>` The second alloying element must be given. If only one, press <Enter>. If an element name is given then the program asks for its mass fraction.
	`Mass (weight) percent: <Amount of the above specified element>` The amount of the above specified alloying element in mass (weight) percent.
	`Next alloying element: <Element name>` Continue giving elements and mass (weight) fractions until all elements specified. When all alloying elements and their compositions (as in the above prompt) are specified, press <Enter> as answer to this question to finish the materials definition.
	`Temperature (C) /1000/: <Temperature of interest in oC>` POLY makes the first calculation after retrieving the data for this temperature. By pressing <Enter> to accept the default temperature. The value should be given in Celsius (°C). 📄 The pressure is set to 1 bar.
	`Reject phase(s) /None/: <List of phase(s) to be rejected>` This is a question generated by the database allowing you to select the phases. Normally, all phases should be included when you press <Enter>. If a phase is to be rejected, the name of the phase must be supplied. Several phase names can be specified in one line. It is possible to reject all phase

Syntax	DEFINE_MATERIAL
	by giving an asterisk *. If the number of phases to be included is much smaller than the total number of phases, it may be convenient to first reject all phases and then restore those that should be included. The question is repeated until you press <Enter> after rejecting all unwanted phases or an asterisk *.
	`Restore phase(s) /None/: <List of phase(s) to be restored>` You can restore phases that are accidentally or deliberately rejected. It may also be possible to restore some hidden phases. If phases are to be restored the name of the phases must be supplied. Several phase names can be specified in one line. It is possible to restore all phase by giving an asterisk *. The question is repeated until you press <Enter> after restoring all desired phases.
	`OK? /Y/:` By default, all phases to be selected from the database have the thermodynamic data retrieved and the references from the chosen database are listed. Enter N if there are any errors or you want to amend the selection then you are returned to the prompt about rejecting phase(s).
	`Should any phase have a miscibility gap check? /N/:` The database usually creates two or more composition sets for phases that can have miscibility gaps. However, for some phases this is not done automatically, for example the miscibility gap in the bcc phase in Fe-Cr is usually ignored. But if it is important to include a Cr-rich bcc phase, specify this here. It costs some computation time and may make the subsequent MAP or STEP more difficult to converge. If you do not want to have any phase with a miscibility gap in the calculation, press <Enter>. Then, DEFINE_MATERIAL starts calculating the equilibrium, and is terminated.
	To set such a phase with miscibility gaps in the calculation, answer Y. Then the software asks questions about the phase names and their constitutions, such as: `Phase with miscibility gap: <Phase name>` You must supply the phase name, which has a miscibility gap under the specified system and conditions.
	`Major constituent(s) for sublattice #: /AA/: <Constituent(s)>` The software shows a default constituent in the sublattice `#(1,2,3,…)`, according to the existing phase definition in the chosen database. You can specify one or more major constituents for the sublattice # in the phase. This question is repeated until all sublattices are specified.
	`Phase with miscibility gap: <Phase name>` You can supply another phase name with a miscibility gap under the specified system and conditions, and answer the questions concerning the major constituent(s) in associated sublattice (s). By pressing <Enter>, the command starts calculating the equilibrium, and then terminates.

Syntax	DEFINE_MATERIAL
	🗎 It is also possible to use this command to select an alloy from a specific database (e.g. the TCNI Ni-based superalloys database). Such alloys are predefined by the OPTION keyword inside the database, and have their default major elements and composition limits of their alloy elements. Such alloys available in the selected database (at the prompt `Database /ABCDE/` can be listed on the screen if typing a ? mark on the prompt `Major element or alloy`. When a specific predefined alloy (instead of a major element) is selected, the major element is staked from the alloy definition and shown on the screen (with a message like `Alloy found with major element NI`). You can only specify alloying elements and the compositions (weight percent or mole percent). Typing a ? at any of the prompts for the alloying element names, e.g. `1st alloying element`, `2nd alloying element`, lists all the alloying elements and the composition limits in the alloy. If the composition of an alloying element is outside of its limit, there is a message (such as `Amount above limit: 30.0000`) and a prompt `Override limit ? /N/`. If you decide to enforce the override by answering `Y` on this prompt (i.e. accepting the over-limit alloying composition), another warning message (such as `Amount of major element below limit: 70.0000`) and prompt `Override limit ? /N/`. Then further decide if enforcing the overriding: if Y then accepting the major element's composition below the limit; if N then using the predefined major element composition limit.

DELETE_INITIAL_EQUILIBRIUM

This command is for the POLY module.

Delete ONE specific initial equilibrium point or ALL of the initial equilibria. The initial equilibria are used as starting points for all the sub-sequential MAP and STEP calculations.

ADD_INITIAL_EQUILIBRIUM.

Syntax	DELETE_INITIAL_EQUILIBRIUM
Prompt	`Number /All/: <Number of an initial equilibrium>`
	Specify the number of an initial equilibrium (as a specific numerical value e.g. 3, or ALL) to be deleted from the POLY3 workspaces. It is recommended to use LIST_INITIAL_EQUILIBRIA to figure out the numbers for all the existing initial equilibrium points that have already been added (*manually* through ADD_INITIAL_EQUILIBRIUM, or *automatically* by some other POLY commands) and stored in the current POLY3 workspace. By default, ALL the initial equilibrium points are deleted.

DELETE_SYMBOL

This command is available with the POLY and ED-EXP modules.

Use the DELETE_SYMBOL command to remove symbols i.e. constants, variables, functions or tables.

Syntax	DELETE_SYMBOL
Prompt	`Name: <Name of a symbol>` Specify the name of the symbol to be deleted. Only one symbol can be deleted each time.

ENTER_SYMBOL

This command is for the POLY module.

There are also GES and POST module commands with the same name.

Symbols are a useful feature of the POLY and POST modules to define quantities that are convenient. Symbols can be constants, variables, functions or tables.

Functions or tables (with defined functions as values) can be entered in the POST module after a stepping or mapping calculation, for purposes of plotting such entered functions or tables as axis variables.

Within the POLY module, symbols are normally defined prior to an equilibrium calculation (enforced by a C_E command), stepping calculation (enforced by the command STEP_WITH_OPTIONS) or mapping calculation (enforced by MAP). These can be entered after an equilibrium calculation; however, for defined functions, variable or tables, it requires using EVALUATE_FUNCTIONS before showing the corresponding values in the calculated equilibrium state.

The symbols entered in the POST module are not saved in the currently-loaded POLY3 workspaces. Therefore, if you want to apply such symbols in other similar calculations for the same defined system, you must use the ENTER_SYMBOL command prior to the STEPPING or MAPPING calculation in the POLY module.

See example 44for an example of using variables and functions.

Symbols are a useful feature modules to define quantities that are convenient. Symbols can be constants, variables, functions, or tables.

Syntax	ENTER_SYMBOL
Prompt	`Constant, Variable, Function or Table? /Function/: <Keyword>` The `Keyword` can be specified as `CONSTANT`, `VARIABLE`, `FUNCTION`, or `TABLE`. • CONSTANTS can only be entered once and is a means of using a name for a numeric value. For example, the value of 1 atmosphere in Pascal can be denoted by `P0` after the command ENTER_CONSTANT `P0=101325`. Defined constants can be used as values in condition assignments, for example, `SET-COND P=P0`. • FUNCTIONS are expressions of state variables or other functions. These expressions are saved, and whenever a function value is requested all functions are evaluated. The reason for this is that they may depend on each other. • VARIABLES are similar to functions because they can also be expressions of state variables. However, contrary to functions, they are only evaluated when they are entered or if they are explicitly named in an EVALUATE_FUNCTIONS command. It is possible to enter a variable

Syntax	ENTER_SYMBOL
	with a new expression any time. This expression is evaluated directly and its value stored as the value of the variable. Defined variables can be used as values in the SET_CONDITION command. • TABLES are used for listing results from the STEP or MAP commands. A table consists of a list of any number of state variables, functions, or variables. Defined tables can also be used in the POST (post-processor) module. There is a special connection between tables and variables. If a variable is used in a table, it is evaluated for each line of the table in the TABULATE command or when the table is used in a plot.
	`Name: <Name of the symbol>` Each symbol has a unique name that must start with a letter and can have maximum 8 characters. Legal characters include letters (either UPPER or lower case), digits and underscore _. Any other special character, such as parentheses (and), plus +, minus -, slash / or \, full stop (.), are illegal for symbol names. You can enter the symbol name and the value or function on the same line; these must be separated with an equal sign =, for example, `TC=T-273.15` or `T_C=T273.15` which stands for a definition of temperature in Celsius. Otherwise, these questions are asked. For different types of symbols (constant, function, variable, or table), the questions have different prompts.

	`Function: <Definition for a function or variable>`
	Functions and *variables* are evaluated from an expression of state variables or other functions, constants, or variables. The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers).
	Unary functions like `LOG`, `LOG10`, `EXP`, `SIN`, `COS`, and `ERF` can also be used. An expression can be continued on more than one line. An expression should be terminated by a semicolon (;) or an empty line (press <Enter> at the next prompt).
	Examples of function expressions:
	• `GM(LIQUID)`: The Gibbs energy of liquid per mole component
	• `H.T/4.184`: The heat capacity of the system in calories
	• `ACR(CR)/X(FCC,CR)`: The activity coefficient for Cr in FCC
	• `T-273.15`: The temperature in Celsius
	`&: <Continuation of the definition for the symbol>`
	The ampersand & means that you can continue to write the function on the new line if one line is

<table>
<tr><th>Syntax</th><th>ENTER_SYMBOL</th></tr>
<tr><td></td><td>not enough for the function. If you finish the function press <Enter> again.</td></tr>
<tr><td></td><td><code>Value: <Value for a constant></code>

A constant can only be assigned a numeric value once.</td></tr>
<tr><td></td><td><code>Value or expression: <Value of expression for a variable></code>

A variable can be assigned a numeric value or an expression. An expression is evaluated immediately and discarded. Only the numeric value is kept. This gives a possibility to save a value between calculations with different conditions because all state variables and functions are evaluated for the new conditions.</td></tr>
<tr><td></td><td><code>Variable(s): <Variable(s) in a table></code>

A table consists of a list of state variables or functions. One way to obtain results from a STEP command is through a table.

Example:

<pre>   ENTER TABLE K=T,X(LIQ,C),X(LIQ,CR),ACR(C)</pre>
Which means that the table called K contains four columns, i.e. the temperature, the mole fractions of C and Cr in the LIQUID phase, and the activity of C.

To show the temperature in Celsius in a table, give the command ENTER_FUNCTION <code>TC=T-273</code>; and then use the symbol <code>TC</code> in the table.

<code>& <Continuation of the definition for the table></code>

The ampersand <code>&</code> means that you can continue to write the table on the new line if one line is not enough for the table. If you finish the table press <code><Enter></code> again.</td></tr>
</table>

EQUILIBRIUM_CALCUL

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

Use this command to decide how to perform the POLY minimization (i.e. the traditional Gibbs energy minimization). The *Global Minimization Technique* is used by default for various single point equilibrium calculations and for stepping or mapping calculations.

To permanently turn off the Global Minimization Technique (for all sequential calculations throughout the current run), use the GLOBAL_MINIMIZATION command and set the options to use only the local POLY minimization. You can also make other adjustments to control the steps in reaching Gibbs energy minima in an equilibrium state, for example.

When enforcing the Global Minimization Technique in the equilibrium calculations, you can further adjust how to assign grid points and to handle compositional set(s) for solution phases during stepping/mapping. In order to improve convergence, and because the Global Minimization Technique uses the normal POLY optimization routine for some calculations, you can also change how to control the steps in reaching Gibbs energy minima in an equilibrium state.

Settings for the Minimization of an Equilibria

The following prompts show how the POLY optimization does the local POLY minimization to reach the minimum of an equilibrium state.

```
Force positive definite phase Hessian /Y/:
```

Choose `Y` or `N` to determine how to reach the minimum of an equilibrium state in a normal POLY optimization procedure. This is related to the special quantity, the phase stability function `QF (phase)`, for all kinds of phases in an equilibrium state [a phase stability function for a phase is negative when the phase composition is inside a spinodal, and positive everywhere else].

If the composition of a solution phase is inside its spinodal, the enforcement of positive definite eigenvalues of a Hessian matrix (i.e. when `Y` is selected) makes the step be taken towards the minima rather than the local maxima. Furthermore, if an eigenvalue (for a phase) of the Hessian matrix is near `0.0`, the step size is large this sets a lower limit to this eigenvalue, reducing the step-size and improving the convergence.

The POLY command sequence SHOW_VALUE `QF(phase)` shows the size of the lowest eigenvalue of a phase in an equilibrium state.

If you answer:

- `Y` , it helps the local POLY minimization to converge (if there is a problem), especially if `QF(phase)=0` for phases.
- `N` the local POLY minimization routine is applied.

For each phase in a defined system, the molar Gibbs energy of the phase is a function of the temperature-pressure condition and its composition:

$$G_m(X) = G_m(T, P; y_1, y_2, \ldots, y_n)$$

Compute a Hessian matrix, which describes the curvature of the Gibbs energy curve of this phase at the defined composition X:

$$\partial^2 G_m / \partial y_i \partial y_j$$

Diagonalize this matrix and call the Eigenvalues as `e1,e2,...,en` . The `QF(phase)` quantity for this phase is the lowest of these eigenvalues divided by the same values for a corresponding ideal phase:

$$QF(ph) = \min(\{e_1, e_2, \ldots, e_n\}) / \min(\{se_1, se_2, \ldots, se_n\})$$

Here, `se1,se2,...,sen` are the Eigenvalues for the ideal phase. Therefore, for an ideal phase, the `QF(phase)` should always be `1.0`.

```
Control stepsize during minimization /Y/:
```

Choose `Y` or `N` to determine whether to introduce a control of step size while reaching the minimum of an equilibrium state in a normal POLY optimization procedure. If you choose `Y` it might help the POLY optimization to converge, especially if some site fractions are less than `1E-4`.

EVALUATE_FUNCTIONS

This command is available with the POLY and ED-EXP modules.

The value of one or more or all entered functions or variables are evaluated and listed.

Syntax	EVALUATE_FUNCTIONS
Prompt	`Name(s): <Name(s) of defined function(s)>` The names of one or more entered functions or variables must be specified. By typing a wildcard *, all functions and variables are evaluated. Variables are evaluated only if these are explicitly named.

GLOBAL_MINIMIZATION

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

Designed to decide how to perform the so-called Global Minimization in the POLY module. By default, the POLY module uses the Global Minimization technique for various single-point equilibrium calculations and for stepping or mapping calculations. You can use this to permanently (for all sequential calculations throughout the current software run) turn off the Global Minimization technique and consequently use only the Ordinary POLY Minimization, and additionally adjust the ways to proceed the normal minimization (mainly in terms of how to control the steps in reaching Gibbs energy minima in an equilibrium state). When enforcing the Global Minimization technique in the equilibrium calculations, you can adjust the manners for assigning grid-points and for handling new possible compositional set(s) for solution phases during stepping/mapping; since the Global Minimization technique also uses the normal POLY optimization routine for some calculations, it is also possible to change the ways on how to control the steps in reach Gibbs energy minima in an equilibrium state, in order to improve convergence.

The following prompts affect how the Global Minimization is done. Settings for global minimization:

```
Use global minimization as much as possible /Y/:
```

```
Use global minimization for test only? /N/:
```

```
Maximum number of gridpoints per phase /2000/: <Integer number>
```

```
Use global minimization as much as possible /Y/:
```

Choose Y or N to decide if using the Global Minimization Technique from start of calculation or not. The default value on start-up may be changed by SET_TC_OPTIONS in the SYS module.

If Y the calculation is done when possible (depending on the condition settings), and a Global Minimization test is always performed when an equilibrium is reached. This costs more computer time but the calculations are more accurate.

If N the calculation is not used to reach the equilibrium state. Use global minimization for test only? determines if the Global Minimization test is made against the calculated equilibrium states obtained by the Ordinary POLY Minimization calculation.

```
Use global minimization for test only? /N/:
```

If Y a calculated equilibrium state obtained by the Ordinary POLY Minimization calculation is tested against the Global Minimization Technique after it is reached; and if found it as unstable, there is an error message.

If N the Global Minimization Technique is never tested for or done for all sequential calculations throughout the current TCC run. This implies that Global Minimization Technique is permanently turned off, and that consequently only the Ordinary POLY Minimization routine is used.

```
Maximum number of gridpoints per phase /2000/: <Integer number>
```

Specify the maximum number of grid points that are computed for each of the phases in the currently defined system, during the calculations enforced by the global minimization. More grid points give a higher robustness and take more computation time. The total number of computed grid points in all phases is limited to 2E6.

KEEP_COMP_SET_NUMBERS

This is available with the ADVANCED_OPTIONS command in the POLY module.

ADVANCED_OPTIONS

COMPUTE_EQUILIBRIUM

This setting affects the COMPUTE_EQUILIBRIUM command and turns on/off the functionality to keep the composition set numbers from the previous equilibrium calculation. The setting is on by default.

To turn the setting on or off enter the ADVANCED_OPTIONS command in POLY, then enter this option and either press `<Enter>` to keep the default `Y` or enter `N` at the prompt:

```
Keep composition set numbers /Y/:
```

If this setting is on, performing the COMPUTE_EQUILIBRIUM command keeps the composition set number for any phases that were also present in the last result from COMPUTE_EQUILIBRIUM.

The composition set numbers are kept when the constitution of a phase in the new equilibrium result is similar to the constitution of one of the composition sets of that phase in the previous result. Making major changes to the conditions between calculations makes it therefore less likely that the composition set numbers are kept. The major constituents, given in the thermodynamic database, are used if no previous result exists.

LIST_AXIS_VARIABLE

This command is for the POLY module.

Syntax	LIST_AXIS_VARIABLE
	Lists all the axis variables for a stepping or mapping calculation that have already been set by SET_AXIS_VARIABLE.

LIST_CONDITIONS

This command is available with the POLY and ED-EXP modules.

All the conditions that are set by the SET_CONDITION command and the command-sequence CHANGE_STATUS PHASE `=FIXED <0 or 1 or alike>`, are listed. The current conditions are also listed by the LIST_EQUILIBRIUM command. The degree of freedom in the defined system is also shown.

- If this is zero, you can perform a COMPUTE_EQUILIBRIUM command.
- If it is larger than zero, some more conditions are required, and you must further set additional ones, using SET_CONDITION or CHANGE_STATUS.
- If it is negative, then too many conditions are defined and the unnecessary ones conditions need to be removed using the SET_CONDITION command (with a value of NONE for the to-be-deleted condition) or the CHANGE_STATUS command (i.e. changing a FIXED status of a phase to another type of phase status, ENTERED or DORMANT or SUSPENDED).

Syntax	LIST_CONDITIONS

Example

```
P=100000, T=800, N(NI)=1E-1, N=1

FIXED PHASES

FCC_A1=1 LIQUID=0   DEGREE OF
FREEDO 0
```

LIST_EQUILIBRIUM

This command is available with the POLY and ED-EXP modules.

The result (always in SI units) from the last calculated equilibrium is listed on screen or in a text file.

You can also execute this command if no calculation is made or if the calculation fails. Make sure to interpret the results accordingly.

Syntax	LIST_EQUILIBRIUM
Prompt	`Output to screen or file /Screen/: <File name>` The name of the text file where the calculation results shall be written.
	`Options /VWCS/: <Option(s)>` Select the output units and formats by optionally specifying a combination of these letters. • *Fraction order:*`V` means VALUE ORDER; `A` means ALPHABETICAL ORDER. • *Fraction type*: `W` means MASS FRACTION; `X` means MOLE FRACTION. • *Composition*: `C` means only COMPOSITION; `N` means CONSTITUTION and COMPOSITION. • *Phase*: `S` means including only STABLE PHASES; `P` means including ALL NON-SUSPENDED PHASES.
	Default options are `VWCS`. If the output fraction type should be in mole fraction (rather than mass fraction), then give `VXCS` or type `X` (implying that in this case the options V, C and S are accepted as the listing manners for fraction order, composition and phase). If accepting all the default options, or if accepting all the altered options that had already changed when using this command previously, you can type `L_E,,,` or `LIST_EQUILIBRIUM ,,,` LIST_EQUILIBRIUM displays ORD (ordered) or DISORD (disordered) (when available). See CHANGE_LEGEND for details.

LIST_INITIAL_EQUILIBRIA

This command is for the POLY module.

List all the equilibria added with ADD_INITIAL_EQUILIBRIUM.

Syntax	LIST_INITIAL EQUILIBRIA
	All the initial equilibria are used for the MAP (and STEP) calculations.

LIST_PHASE_ADDITION

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

The values set as additional contributions (given by PHASE_ADDITION) to Gibbs energy *G*m (J/mol formula unit) to all the phases (stoichiometric or solution) are listed at the current calculated equilibrium.

LIST_PHASE_ADDITION has no additional prompt.

LIST_STATUS

This command is for the POLY module.

There is also an ED-EXP module command with the same name.

List the status of components, species or phases.

Syntax	LIST_STATUS
Prompt	Specify what to list: `Option /CPS/:`*<keyword(s)>* keyword = C or P or S, or any combination - `C`: list component status - `P`: list phase status - `S`: list species status - `CS`: list both components and species Default is `CPS`.
	The results depend on the key word specified in the options for CHANGE_STATUS, a table with the current status of phases or species or components, or the combinations, is shown: - For components, the statuses and reference states are listed. - For species, only the status is listed. - For ENTERED and FIXED phases, the status, driving forces and equilibrium amounts are listed.
	The metastable phases are listed in descending order of stability. To avoid long outputs only 10 metastable phases (in ENTERED status) are listed by lines, while all other less stable phases are merged onto one line. For DORMANT phases, their phase names and driving forces are listed. For SUSPENDED phases, only the phase names are listed.

LIST_SYMBOLS

This command is for the POLY module.

There are also POST and ED-EXP module commands with the same name.

Use this command to list the definitions for all constants, functions, variables and tables. In order to find the value of a function or variable, use SHOW_VALUE or EVALUATE_FUNCTIONS. A table is tabulated with the TABULATE command.

Syntax	LIST_SYMBOLS
	The defined variables are listed up together with the defined functions, but variable names are followed by a percentage sign `%`.

LOAD_INITIAL_EQUILIBRIUM

This command is for the POLY module.

Copies all conditions and calculated results from a specific added initial equilibrium to the current equilibrium. The current conditions and calculation results are lost, and the newly loaded initial equilibrium point gets into the POLY workspace.

Syntax	LOAD_INITIAL_EQUILIBRIUM
Prompt	`Number: <Number of an initial equilibrium>` Specify the number of an initial equilibrium to be loaded as current. The number can be found with LIST_INITIAL_EQUILIBRIA.

MAKE_COMPONENT_ENTERED

This command is for the POLY module.

The MAKE_COMPONENT_ENTERED command sets the status for the components to be ENTERED in the defined system for all the sequential calculations (single-point, stepping, and mapping) in equilibrium or local/partial equilibrium states. ENTERED means that the component(s) are included in the calculation and these are stable if that minimizes the total energy.

This command has the same results as when using CHANGE_STATUS`Entered` option.

Syntax	MAKE_COMPONENT_ENTERED
Prompts	`Name(s) <Name(s) of the components>` The names of the components to set to ENTERED (all on one line). A comma or space must be used as separator. An asterisk, "*", can be used to denote all components.

MAKE_COMPONENT_SUSPENDED

This command is for the POLY module.

The MAKE_COMPONENT_SUSPENDED command sets the status for the components to be SUSPENDED in the defined system for all the sequential calculations (single-point, stepping, and mapping) in equilibrium or local/partial equilibrium states. SUSPENDED means that the component(s) are not considered in the calculation. Any conditions that depend on the suspended components are automatically removed.

Removing relevant conditions is unique to this command and does not occur when suspending components with the CHANGE_STATUS command and `Suspended` option.

Syntax	MAKE_COMPONENT_SUSPENDED
Prompts	`Name(s) <Name(s) of the components>` The names of the components to set to SUSPENDED (all on one line). A comma or space must be used as separator. An asterisk, "*", can be used to denote all components.

This command is useful when an element has a very low amount because you can now ignore it in the calculation instead of reading the entire system from the database. The command is also of use when working in an API with many calculations.

MAJOR_CONSTITUENTS

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

Use this to set the major constituent(s) of a composition sets in a miscibility gap of a solution phase. Normally, the major constituents are specified when a new composition set is created by the NEW_COMPOSITION_SET option; but for the first composition set, this option may be needed before using NEW_COMPOSITION_SET.

The following prompts are to specify the major constituent(s) on each of the sublattice sites for a composition set of a certain solution phase:

```
Phase name: <name of a phase>
```

Specify the name of the solution phase with a new set of major constituents.

```
Composition set number /1/: <#>
```

The default value for the composition set number (#) is usually /1/ as the other composition sets are given major constituents when creating them. Each phase has initially one composition set.

```
Major constituent(s) for sublattice 1: /XX/: <YY>
```

The major constituents (`YY`) on each sublattice of a solution phase can be given. This may simplify giving start values when calculating the equilibrium as phases with miscibility gaps should have different major constituents for each composition set.

This question is repeated for each sublattice in the phase.

MAP

This command is for the POLY module.

This command starts the mapping procedure for making a calculation of phase diagrams in a defined multicomponent heterogeneous system, from one or more initial equilibria. A phase diagram is usually mapped within a specific space that is constructed by two (or more) defined independent mapping axis-variables.

Syntax	MAP
	A phase diagram consists of mapped phase boundary lines/curves; on one side of each such phase-boundary line/curve, the amount of one specific stable phase is zero (i.e. the zero-fraction lines). From a single MAP calculation, many different types of phase diagrams in the defined multicomponent heterogeneous system can be plotted, with some desired properties (that vary along the calculated phase-region boundaries) plotted as X/Y-axis variables. All different types of phase diagrams are generated by the mapping calculations through this command.

Normally, you need to have calculated at least one initial equilibrium point and have also defined at least two independent varying variables (i.e. the controlling conditions in the system) that are set with SET_AXIS_VARIABLE. You can also have three, or four or maximum five independent varying variables that are defined by the SET_AXIS_VARIABLE command).

This lists the current values of each of the independent axis variables for each of the calculated equilibrium points along each of the mapped phase boundaries, and also lists the corresponding information when the set of stable phases changes.

The Global Minimization Technique is by default enforced in this command while it can be disabled if having decisively switched it off (or possibly in some special modules) through changing the minimization option using the ADVANCED_OPTIONS → MINIMIZATION_OPTION command-sequence. You can choose how often to do a Global Minimization test (via the Global Test Interval option) in the ADVANCED_OPTIONS STEP_AND_MAP command-sequence.

During a MAP calculation, the values of mapped axis-variables for presenting each phase boundary (lines/points) of the calculated phase-regions are listed, and the corresponding stable-phase sets are shown up.

You can terminate the mapping of a line by pressing a single <Ctrl-A> (Windows) or <Ctrl-C> (Linux). This can be useful in order to stop a longish calculation without losing what is already calculated.

If there is any convergence problem in finding a stable solution at a certain stage during a calculation procedure enforced by this command, these messages display on screen:

```
Convergence problems, increasing smallest site-fraction from 1.00E-30
to hardware precision 2.00E-14. You can restore using SET-NUMERICAL-
LIMITS
```

This implies that smallest site fraction in the current POLY3 workspace is automatically increased from the default value 1.00E-30 to the hardware-dependent precision (under Linux, as 2.00E-14). For other subsequent POLY-module calculation in the current TC run, you can use SET_NUMERICAL_LIMITS to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

In particular, for phase diagrams with tie-lines in the plane (i.e. most binary systems and ternary isotherms), there is a MAP procedure which checks for the best phase to use as axis variables in order to ensure reasonable increments between the tie-lines. This produces smoother curves and also gives a better stability in finding adjacent phase-regions.

Complex miscibility gaps of various solution phases are automatically detected during a mapping calculation, and two or more composition sets for each of such solution phases are automatically generated as well, through an automatic Global Minimization Test procedure (by specifying a Global Test Interval value and confirming the `Automatically add initial equilibria` in the ADVANCED_OPTION STEP_AND_MAP command-sequence). As a particular case, such an automatic Global Minimization Test ensures that you can start calculating from high temperatures in an austenitic steel (metallic FCC_A1 solution phase) where the MC carbides/nitrides/carbonitrides (i.e. the C-/N-rich sides of the FCC_A1 miscibility-gap, often (while not always) being referred to as `FCC_A1#2, FCC_A1#3`, etc.) are not stable, and during the MAP command the MC carbides/nitrides/carbonitrides may first become metastable with a composition different from the metallic FCC_A1 phase and later also stable. The advanced mapping procedure (enforced by the Global Minimization Technique) inside the Thermo-Calc software (both the Console Mode and Graphical Mode) can efficiently and effectively handle complex miscibility gaps in multicomponent heterogeneous systems.

To get a complete phase diagram, sometimes it may be necessary to have multiple starting equilibrium-points, and/or to have added multiple initial-equilibrium points (through ADD_INITIAL_EQUILIBRIUM) inside various phase-region boundaries under certain direction(s).

NEW_COMPOSITION_SET

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

A solution phase that can exist with two (or more) different compositions simultaneously must have two (or more) composition sets in its phase descriptions. Normally the database creates as many composition sets as is necessary but use this command to add or delete more composition sets. A complex solution phase in a defined multicomponent system can have up to 9 different composition sets for the purpose of appropriately handling its possible miscibility gap(s) under various temperature-pressure-composition conditions.

This option is unnecessary if the Global Minimization Technique is in use, as it can automatically detect all possible miscibility gap(s) for complex solution phases (normal or disordered/ordered phases) and then automatically add required composition sets for such phases in the defined system.

This option can automatically create composition sets also for disordered phase when it is executed for the ordered phase.

If you have your own data file, this option must be used to indicate that a solution phase can have a miscibility gap (or may exhibit some complex phase separations as to more than two composition sets), unless that the possibly-additional composition set(s) for the solution phase must have already been added inside the TDB file (through a TYPE_DEFINITION command to amend composition-set) or been manipulated through the GIBBS module (using the AMEND_PHASE_DESCRIPTION COMPOSITION_SET command-sequence). This option asks for default major constituents for the new sets and it is important that this is set correctly, otherwise the test for miscibility gaps may fail.

The following prompts are to specify the additional composition set(s) to handle possible miscibility gap(s) of a certain solution phase:

```
Phase with miscibility gap: <Name of a phase>
```

Specify the name of the phase with miscibility gap.

```
New highest composition set number /2/: <#>
```

The default value is usually one higher than the current value. Each phase has initially one composition set. If a lower value is given, composition sets are deleted. You cannot take away the first composition set.

A message displays to show that you need to specify the composition for the composition set # (2,3,…).

```
Major constituent(s) for sublattice 1: /XX/: <YY>
```

The major constituents (`YY`) in each sublattice can be given. This may simplify giving start values when calculating the equilibrium as phases with miscibility gaps should have different major constituents for each composition set.

This prompt is repeated for each sublattice in the phase, sometimes even for all sublattices in the first composition set if such major constituents have not been specified.

OUTPUT_FILE_FOR_SHOW

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

The name of a text file is asked for and all the results output from the command SHOW_VALUE is written to this file.

When you use this command, a window opens with a default name for the file `tc_show.dat`. Choose a location to save the file and click **Open**.

PARAEQUILIBRIUM

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

This calculates a paraequilibrium between two specific phases in an alloy system with one or more interstitial component(s) as fast diffusion species. Under the paraequilibrium state, two partially-equilibrated phases have the same chemical potential (but different contents) for one or more interstitial components (such as C, N, O, S, etc., as individual or combined)], along varied temperature or along a composition variable (of the matrix or one substitutional component) which has already set as the stepping variable with SET_AXIS_VARIABLE.

To ensure a successful point calculation of paraequilibrium state between two specific phases in a defined alloy system, it is important that you first have made a single-point equilibrium calculation with an initial overall composition in the current system before performing this advanced-option calculation; however, it is unnecessary to obtain an equilibrium in which either one or both of the target phases is stable. The initial overall composition must have a reasonable setting for the desired paraequilibrium calculation for the two target phases. This is especially true for cases where there are more than one interstitial components to be considered in the paraequilibrium state, because different interstitial components (for example C and N combined) may have significant different behaviors as partitioning into different structured phases; otherwise, for one chosen interstitial component the initial overall composition is OK for the paraequilibrium calculation between the specified two phases, but for other chosen interstitial component(s) it might be impossible to calculate the paraequilibrium state.

Note the following:

- Always check if the chosen phases A and B have the exactly same definition of elements and if the chosen interstitial components are all in the vacancy sublattice sites of the two phases; otherwise the program cannot find the paraequilibrium state (as it is impossible to correctly calculate u-fractions).
- Always have a comprehensive understanding of the normal phase diagram for the currently investigated system, so that you make the appropriate choice of the phase pair and staring bulk composition for the system.
- Always set the status of the chosen interstitial components as SPECIAL using the POLY command: CHANGE_STATUS`Component <interstitial component> = SPECIAL`. By doing this, you get a clear picture of u-fractions of various substitutional and interstitial components, which are different from the overall composition in the

system. The SPECIAL status means that specified component(s) are not included in summations for mole or mass fractions. Therefore, all the composition variables plotted from paraequilibrium calculations are u-fraction related quantities.

Settings

```
Name of first phase:  <Phase A>
```

```
Name of second phase: <Phase B>
```

The names of the two target phases A and B, between which the paraequilibrium state is to be calculated, must be entered subsequently or on the same (first) line at once then separated by an empty space, e.g. `FCC#1 BCC` or `FCC#2 M23C6`.

> You need to understand what you are dealing with in terms of calculating a paraequilibrium state between the two specified phases.

Specifically, there are four distinguished cases to understand: (1) both chosen phases must have similar interstitial/vacancy sublattices where the fast-diffusion interstitial component (s) occupy; (2) the choice on the target phase pair must be reasonable for the defined system and specified initial overall composition; (3) both target phases should have phase constitution definitions that cover all the defined substitutional and interstitial components of the current alloy system; or (4) it is impossible to calculate the paraequilibrium state between the target phase pairs with given interstitial component(s) in the currently defined system.

```
Fast diffusing component: /c/: <interstitial component(s)>
```

```
Fast diffusing component: /none/: <interstitial component(s)>
```

The name(s) of the fast-diffusing component(s) (C as the default single component) must be given at the above prompts subsequently or at the same (first) prompt. It is possible to specify more than one interstitial component as fast diffusion species.

Note the following:

Such specified interstitial component(s) must be appropriately defined according to the phase constitution definitions of the two selected phases: these must be located on the interstitial/vacancy sublattices in both chosen phases;

If there is only one fast-diffusing component which is carbon, press the <Enter> key to accept the default input at the first prompt; if the single fast-diffusing component is another element (e.g. N), type its name at the first prompt;

If there are two or more fast-diffusing components (e.g. `C` and `N`), type their names at the above prompts subsequently or at the same (first) prompt (separated by an empty space, such as `C N`);

To finish the input of fast-diffusing elements, accept NONE at a repeated prompt, i.e. by pressing <Enter> key to start the paraequilibrium point calculation;

If NONE or a non-existing component name is typed at the first prompt, it means no back diffusion is to be considered, and the para-equilibrium calculation is thus canceled entirely.

If the paraequilibrium state between the two specified phases is successfully calculated, the messages displays e.g.

```
 NP(FCC) = 0.3586 with U-fractions C = 2.71821E-02  N = 4.1548129E-03

 NP(BCC) = 0.6414 with U-fractions C = 7.10061E-04  N = 2.3781027E-04

 All other compositions the same in both phases

Note: LIST-EQUILIBRIUM is not relevant
```

The first and second lines list the phase amounts expressed in mole-percent [NP(phase)] and the contents of the interstitial components C and N in a specific phase expressed in the so-called u-fractions [u-f(phase,C) and u-f(phase,N)], for the phase A (in this case as FCC) and phase B (in this case as BCC), respectively. The third line states that the compositions of the matrix component and all the remaining compositions (regarding substitutional components) in both the target phase A and target phase B are the same at the current paraequilibrium state, while these are not shown on screen. The last line indicates that after this advanced-option calculation the LIST_EQUILIBRIUM command is irrelevant and does not list the paraequilibrium state for the system at the current condition.

However, if the single-point calculation of the paraequilibrium state between the two specified phases has failed, these messages display:

```
*** Error 4 in ns01ad

*** Numerical error
```

This implies that the chosen target phase pair may be unreasonable for the defined alloy system or for the defined initial overall composition, or one or both phases may have inappropriate phase constitution definitions regarding the specified interstitial component (s). Then, you must either modify the settings of initial overall composition or specify the reasonable target phase pair with an appropriate choice of the fast diffusion interstitials in the defined alloy system.

PHASE_ADDITION

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

Sometimes it is interesting to add a constant contribution to the Gibbs energy of a phase (stoichiometric or solution). This can be done in the Database module (DATA) or Gibbs Energy module (GIBBS), for a stoichiometric phase, or for a pure end-member in a solution phase. However, if the addition is related to the equilibrium state, for example, strain energies or surface energies, interfacial energies, or deformation energies, it may be more convenient to have this quantity related to the equilibrium state rather than the thermodynamic data.

Give a value of an addition to the Gibbs energy of a phase. The value should always be constant (implying that the addition is not a function of phase composition or temperature-pressure conditions in the equilibrium state) and always be given in the unit of J/mol formula unit of the phase.

The following prompts are to specify the additional energy term (always being a constant) of a given phase.

```
Phase name: <Name of a phase>
```

Specify the name of the (stoichiometric or solution) phase with the addition.

```
Addition to G per mole formula unit: <xxxxx>
```

The value (`xxxxx`) given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy, etc.

It is not composition-, temperature-, or pressure-dependent.

POST

The POST module (post-processor) is a submodule to the POLY module and has its own set of commands. The TAB, BIN, TERN, POT, SCHEIL and POURBAIX modules use the POST module features as part of the automatic generation of the plots.

POST Module Commands

Using the POST Module

Syntax	POST
	Switches to the POST module, which has its own command set.

PRESENT_PHASE

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

Specify the name of the present phase a the name of the phase that should be present at all calculated equilibria:

```
Present phase:
```

```
Phase name: <Name of a phase>
```

READ_WORKSPACES

This command is used in both the POLY and GES (GIBBS) modules.

Workspace Files

The POLY3 and GIBBS workspaces and the calculated results from the MAP and STEP commands can be READ from a file where they are saved with SAVE_WORKSPACES. Such a *.POLY3 file is not printable.

Syntax	READ_WORKSPACES
Options	`File name` is the name of a saved POLY3-file where the POLY3 and GIBBS workspaces shall be read from must be specified. You do not need to type the extension if it is the default *.POLY3, otherwise type the whole POLY-file name. A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters. A window opens so that the path (in the **Look in** field) and **File name** can be specified. The **Files of type** (i.e. POLY3) cannot be changed. Click **Open** to open the POLY3 and GIBBS workspaces from the saved *.POLY3 file.
	When reading back an original POLY3 workspace that has already been saved as an *.POLY3 file in the current Thermo-Calc (Console Mode) run or had been read from an existing POLY3 file under the current work area, while some additional changes in the settings may be made but do not need to be kept in further steps in the current Thermo-Calc (Console Mode) run or any diagram is plotted in the POST module, you can type `READ,,` or `READ_WORKSPACE ,,`

REINITIATE_MODULE

This command is for the POLY module.

This command makes sure that the whole POLY module (and thus the entire POLY workspace) is reinitiated to the state as it was when first entered.

Syntax	REINITIATE_MODULE
	All the defined components, defined conditions, changed status, entered symbols, defined independent axis-variables, calculated starting equilibrium-points, added initial equilibrium points, stepped/mapped equilibrium data, and so forth, are removed completely. The saved file name is restored to the default.

SAVE_WORKSPACES

This command is available for both the POLY and GES (GIBBS) modules.

Workspace Files

You can save the current status and workspaces, including thermodynamic data, conditions, options and results from a single, stepping or mapping calculation on a *.POLY3 file. The workspaces are saved to a file with this command. This is useful so you have access to the workspace for later use or when you need to terminate the current Console Mode session.

- In the Gibbs (GES) module workspace, all thermochemical data are stored.
- In the POLY module workspace, all the last set of conditions and equilibrium state, changed status, entered symbols, advanced options, defined stepping/mapping variables, added initial equilibria, stepped/mapped results, etc., are stored, so it also contain the GES workspace.
- When you are in a response-driven module such as POTENTIAL or SCHEIL for example, a workspace file is automatically opened. In the workspace file, system definitions, conditions for the calculation, calculation results, and plot settings are saved. The file is saved in the current working directory, and is named after the name of the module that created it. For example, the POTENTIAL module saves a workspace file called `POT.POLY3` ; the POURBAIX module saves a file called `POURBAIX.POLY3` and so forth.

After a SAVE_WORKSPACES command, you can always come back to exactly the state you had when you issued the command by giving a READ_WORKSPACE command. For example, after saving the POLY and GIBBS workspaces to a file, you can leave the program and at a later time READ the file and continue from the saved state.

Important Information About Map and Step Commands

A STEP or MAP command automatically saves the workspace with the most recently specified name. Do not use the SAVE_WORKSPACES command after a MAP or STEP command.

The results from the STEP or MAP commands are destroyed by the SAVE_WORKSPACE command. You can append several results obtained by sequential STEP or MAP calculations without destroying the previous results, whilst SAVE_WORKSPACE erases them all. Keeping this in mind is important and useful particularly for calculating various isothermal (or isoplethal) sections and plotting them on the same diagram in a single Thermo-Calc run.

To suspend some of the STEP or MAP results, use the AMEND_STORED_EQUILIBRIA command.

Syntax	SAVE_WORKSPACES
Options	A `file name` must be specified. The default extension of the POLY workspace file is *.POLY3 but you can have any other file extension. Linux and Mac are case sensitive so ensure you enter `.POLY3`. A **Save** window displays if a file name is not given after the command, so that the path (in the **Save in** field) and **File name** can be specified. The **Files of type** cannot be changed. If there is already a file with the same file name under the directory a warning message displays. Click **OK** to overwrite the current POLY or GIBBS workspace onto the existing file. Click **Cancel** to return to the module. You can use the SAVE command with an unspecified name (i.e. through `SAVE ,,,` command-sequence) to save the POLY or GIBBS workspace. When saving a POLY3 workspace under a name that already exists under the current work area, which is saved by default (after running a special module, e.g. BIN, TERN, POT, SCHEIL and POURBAIX) or in an earlier stage of the current Console Mode session or in a previous run (which is READ into the current POLY3 workspace), you can type `SAVE,,Y` or `SAVE_WORKSPACE ,,y`. However, this must also be avoided if some results from previous MAP or STEP calculations shall not be destroyed.

SELECT_EQUILIBRIUM

This command is available with the POLY and ED-EXP modules.

If you create more than one initial equilibrium (during data-assessments using the PARROT/ED_EXP modules), you can switch between them using this command.

Syntax	SELECT_EQUILIBRIUM
Prompt	`Number /Next/: <Choice on equilibrium>` Options: `FIRST`, `LAST`, `NEXT`, `PREVIOUS` or `PRESENT`. Most commands affect only the `PRESENT` equilibrium. However, the REINITIATE_MODULE and DEFINE_COMPONENTS commands remove all the stored equilibria.

SET_ALL_START_VALUES

This command is available for the POLY and ED-EXP modules.

Set start values, e.g. if the calculation fails or if you have a miscibility gap or ordering. If temperature and pressure are not conditions, you are asked for values of them. Then for each phase prompt on if it should be stable and on its constitution.

Syntax	SET_ALL_START_VALUES
	`T /XXXX/: <Temperature in K>` If the temperature is not a condition, supply a guess of its final value (in K).
	`P /100000/: <Pressure in Pa>` If the pressure is not a condition supply a guess of its final value (in Pa).
Prompts	`Automatic start values for phase constitutions? /N/: <Y, N or F>` • For N, enter an initial amount of each entered phase and the major constituents or site fraction of each constituent. • For Y, the program automatically sets the start values for phase constitutions in all possible phases. • `F` is for force. In some cases the calculation fails because impossible conditions are set, e.g. `W(C)=1.5 [W(C)` is mass fraction and must thus be less than unity. The program tries to fulfill this condition by putting maximum amount of carbon in all phases, but can fail anyway. When you detect the error and set `W(C) to 0.015`, the calculation may still fail because it could start from the previous values. To get back to 'fresh' start values, choose `F`.
	`Should <phase> be stable /N/: <Y/1 or N/2>` A guess if this phase should be stable or not is requested. All entered phases are prompted for this question and next two. You cannot have more phases stable than you have components, but at least one (which dissolves all constituents) must be set as stable. For backward compatibility, this question can be answered by 1 (for Yes) or 0 (for No). The `phase` name may have a hash sign # followed by a digit, e.g. `BCC_A2#2`. For phases with miscibility gaps, there should be two phases with the same name but with different numbers after the hash sign.
	`Major constituent(s): <Name of major constituent(s) in the phase>` The constituent with the largest fraction in the phase should be specified. If there are more than one constituent with a large fraction, give them all on the same line. If the default major constituents should be used answer with an asterisk (*). By giving $ the constitution is not changed. If there should be no major constituent give NONE and or if the major constituent(s) are improperly specified, you are asked for individual fractions in the phase.

Syntax	SET_ALL_START_VALUES
	`Y(<phase>,<constituent>) /.XXXXXXXXXX/: <.YYYYY>` The current value (`.xxxxxxxxxx`) is default. You can accept the default by pressing <Enter> or give a new value (`.YYYYY`). The phase name or constituent name may have a hash sign # followed by a digit, e.g. `Y(BCC_A2#2,FE), Y(BCC_A2#2,C#2)`. For phases with miscibility gaps, there should be two phases with the same name but with different numbers after the hash sign. For phases with sublattices, the constituents in sublattice 2 or higher is also be suffixed with a hash sign # followed by a digit.

SET_AXIS_VARIABLE

In order to calculate a diagram, set at least one axis variable in a stepping calculation, or at least two axis variables in a mapping calculation. For property diagrams, one axis is enough; for phase diagrams two or more are necessary. Any condition that can be set to calculate an equilibrium can be used as an axis variable (with its lower and upper limits and step length) by using SET_AXIS_VARIABLE, and the POLY program does, after a STEP or MAP command, vary the value of the condition between the limits set on its related axis variable. As an extraordinarily unique and powerful feature of the Thermo-Calc software, up to five independent axis variables can possibly be used in a mapping calculation of a multicomponent heterogeneous system; however, the axis numbers 3, 4 and 5 must have chemical potentials of components (or temperature or pressure) as conditions.

Syntax	SET_AXIS_VARIABLE
Prompts	`Axis number /#/: <An axis number>` Specify a number between 1 and 5. The axis numbers 3, 4 and 5 must have chemical potentials of components (or temperature or pressure) as conditions.
	`Condition /None/: <One condition>` Here the condition that should be varied along the axis must be given. The condition is specified as in SET_CONDITION, for example `W(C)` for mass fraction of carbon. By accepting `NONE`, the axis is removed.
	`Min value /0/: <Min value>` Specify the minimum value of the axis condition.
	`Max value /1/: <Max value>` Specify the maximum value of the axis condition.
	`Increment /.025/: <Step length>` Specify the maximum step length. By default, this is 1/40 of the total axis length.

You can give SET_AXIS_VARIABLE without having set a condition on the axis variable. Under such circumstances, the relevant condition is automatically created and the value set between the minimum and maximum axis limits; however, as a side effect, the POLY module creates two conditions, `P=1e5` and `N=1` (these have not been defined as a condition yet), in case you set an axis variable which is not already a condition.

You can use a logarithmic axis during calculations. This is useful for low fractions like in a gas phase where `1e-7` to `1e-2` might be an interesting range. The pressure is also suitable for logarithmic step. You specify the logarithmic axis by giving an asterisk * after the increment value.

The increment in this case is treated as a factor.

For example,

```
S-A-V 1 P 1E5 1E25 5*
```

This makes axis 1 a logarithmic axis where the difference between two calculated values makes a factor 5.

The factor must be larger than 1.0.

In some cases, such as when the DEFINE_DIAGRAM command is used or a special advanced module (e.g. BIN, TERN, POT, SCHEIL or POURBAIX) is called, some axis variables are automatically set by the program, not necessarily by this command.

SET_CONDITION

This command is available with the POLY and ED-EXP modules.

Specify the equilibrium conditions for the calculation. All kinds of state variables, as well as most of the `M/W/V/F`-suffixed state variables (for normalization) and `R`-suffixed state variables (with respect to chosen reference states), can be used as conditions. In addition to temperature and pressure conditions, a multicomponent system can have mixed types of conditions. You should repeat this command for a multicomponent system until the degree of freedom in the defined system becomes zero. When a FIXED phase status is used on a specific phase (use CHANGE_STATUS), it is equivalent to one condition (implying that particular phase is stable in the defined system).

Syntax	SET_CONDITION

	Each condition must be given explicitly, but can be given on the same line (separated by a comma (,) or an empty space) or on separate lines with each one started with the command.
	Example
	`SET_COND T=1273, P=1E5, W(C)=.0015, X(LIQ,CR)=.22, ACR(N)=.2`
	or
	`SET_COND T=1273, P=1E5`
	`SET_COND W(C)=.0015, X(LIQ,CR)=.22 ACR(N)=.2`
	In this example, the temperature is set to 1273 K, the pressure to 1 bar (1E5 Pascal), the mass (weight) fraction of C to 0.0015 and the mole fraction of Cr to 0.22 and the activity of N to 0.2.

Prompt	`State variable expression: <State variable name or linear expression> or a linear expression of state variables.` Some of the state variables that can be used in conditions are: • `T`: temperature in the system (in K) • `P`: pressure in the system (in Pascal) • `N`: system size (mole number in moles) • `B`: system size (mass in grams) • `N(<component>)`: mole number of a component in the system • `X(<component>)`: mole fraction of a component in the system • `W(<component>)`: weight fraction of a component in the system • For the SET_CONDITION command this is `ACR(<component>)`: activity of a component in the system. For the SET-ALTERNATIVE_CONDITION command, this is `ACR`(<`phase`>,<`component`>) (activity of a component in a phase) • For the SET_CONDITION command this is `MUR(<component>)`: chemical potential of a component in the system. For the SET-ALTERNATIVE_CONDITION command, this is `MUR` (<`phase`>,<`component`>) (chemical potential of a component in a phase)

Syntax	SET_CONDITION

- `X(<phase>,<component>)`: mole fraction of a component in a phase
- `W(<phase>,<component>)`: weight fraction of a component in a phase
- `ACR(<species>,<phase>)`: activity of a species referred to a phase
- `MUR(<species>,<phase>)`: chemical potential of a species referred to a phase
- `H`: enthalpy in the system (in J)
- `HM(<phase>)`: enthalpy of a phase (in J/mol)

There are many state variables that can be used in conditions. For more information, enter an `INFO STATE_VARIABLES` command. A condition is normally a value of a single state variable with its value.

Example

```
T=1273.15  P=1E5
X(C)=.002
W(CR)=0.5
ACR(CR)=0.85
X(FCC,C)=.001
H=-250000
 HM(BCC)=-225000
```

A condition can also be a value of a linear expression involving more than one state variable. For example,

```
X(LIQ,S)-X(PYRR,S)=0
```

This means that it is a condition that the mole fraction of `S` component should be the same in the LIQUID and PYRRHOTITE phases. In practice, that should be the congruent melting point.

After the equal sign only a numeric value is allowed in the expression.

`Factor: <A factor for the state variable, or a continuation>`

This question means you did not answer the previous question. The program is then expecting a single state variable or a complete state variable expression, or the numeric factor in an expression with only one state variable. In a state variable expression a state variable may be preceded by a constant factor. An example of this is:

```
2*MUR(FE)+3*MUR(O)=-35000
```

This means that it should be a condition that two times the chemical potential of `FE` plus three times the chemical potential of `O` should be -35000 J/mol.

`State variable: <A specified state variable, or a continuation>`

This question is prompted if a single state variable name has not given in either the prompt `State variable expression` or `Factor`, or a state variable expression is given but the expression is incomplete, for example, `T-` or `2*MUR(FE)+`, for which the program is then expecting a continuation of the unfinished expression. You need to specify a state variable or a complete state variable expression, or complete the unfinished state variable expression. If a numeric factor is given before

Syntax	SET_CONDITION
	this prompt, only one state variable can be specified; otherwise, the program only takes the first state variable to complete the expression (i.e. the factor times the state variable).
	`Value /X/: <A numeric value, a constant or a variable>` The value of the condition. This can be a numeric value, a constant or a variable. A suggestion is given as the default value. The special value `NONE` means that the condition is removed; for example `T=NONE` takes away the temperature condition.

SET_INPUT_AMOUNTS

Specify how a system is made up from mixing of various substances. It is useful with a substance database. In the C-H-O-N system, you can, for example, give:

```
S-I-A N(H2)=10, N(H2O)=25, N(C1O2)=5, N(N2)=100
```

The POLY module automatically converts this into conditions for the current set of components. In the case when the elements are defined as the components, the command above is equivalent to

```
SET-CONDITION N(H)=70, N(O)=35, N(C)=5, N(N)=200
```

Syntax	SET_INPUT_AMOUNTS
Prompts	`Quantity: <N(<specie>) or B(<specie>)>` You can give the amount also preceded with an equal sign `=` [e.g. `N(H2)=10` or `B(H2O)=1000`], or press <Enter> for the next prompt on the amount of the quantity.
	`Amount: <Value of the quantity>` Specify the numerical value of the quantity. You can give negative amounts in the SET-INPUT-AMOUNTS command.

SET_INTERACTIVE

In the POST module this is called SET_INTERACTIVE_MODE.

Use the SET_INTERACTIVE command to use it in demonstration or macro files to stop the execution of the command file and pass over input focus to the keyboard.

SET_NUMERICAL_LIMITS

This command is available for the POLY, Scheil, and ED-EXP modules.

Change the criteria for convergence. This is to speed up a calculation in a complex system.

If there is any convergence problem in finding a stable solution at any stage during a calculation procedure enforced by COMPUTE_EQUILIBRIUM, STEP_WITH_OPTIONS, MAP or ADVANCED_OPTIONS), this message displays:

```
Convergence problems, increasing smallest site-fraction from 1.00E-30
to hardware precision 2.00E-14. You can restore using SET-NUMERICAL-
LIMITS
```

This implies that smallest site fraction in the current POLY workspace is automatically increased from the default value 1.00E-30 to the hardware-dependent precision (under Linux, as 2.00E-14). For other subsequent POLY module calculations, you can use this command to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

Syntax	SET_NUMERICAL_LIMITS
Prompt	`Maximum number of iterations /500/:` By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.
	`Required accuracy /1E-6/:` This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.
	`Smallest fraction /1E-12/:` This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions. The default value for the smallest site-fractions is 1E-12 for all phases, except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as 1E-30 (unless you have used the SET_NUMERICAL_LIMITS command to reset an even-lower value (e.g. 1E-45, that is naturally enforced to all the phases in the system).
	`Approximate driving force for metastable phases /Y/:` `Y` is the default. Enter `N` to change the default as required and based on the options described below. This setting involves the convergence of metastable phases and affects their driving forces. It can also have an effect on when an equilibrium is considered successful. The default is to allow an equilibrium with metastable phases that have not converged, as long as the stable phases have converged. This is efficient but often causes approximate values of the

Syntax	SET_NUMERICAL_LIMITS
	driving forces for the metastable phases. If you change the default, it enforces metastable phases to converge. This gives accurate driving forces for metastable phases as well as stable phases. It can however take a slightly longer time, and if metastable phases do not converge it causes the equilibrium calculation to fail.

SET_REFERENCE_STATE

This command is available for the POLY, ED-EXP and POST modules.

The reference state for a component is important when calculating activities, chemical potentials, and enthalpies and is determined by the database being used. For each component the data must be referred to a selected phase, temperature, and pressure, i.e. the reference state.

All data in all phases where this component dissolves must use the same reference state. However, different databases can use different reference states for the same element/component. It is important to be careful when combining data obtained from different databases.

By default, activities, chemical potentials, and so forth are computed relative to the reference state used by the database. If the reference state in the database is not suitable for your purposes, use this command to set the reference state for a component using `SER`, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys dominated by the component). In such cases, the temperature and pressure for the reference state is not needed.

In order to specify conditions in the specific reference state, you can append an `R` to the state variables. Thus, `AC` is the activity (of a system component or of a species in a phase) with respect to the default reference state, and `ACR` is the activity with respect to the selected reference state; MU is the chemical potential of a system component with respect to the default reference state, and `MUR` stands for the chemical potential with respect to the selected reference state. The `AC` and `ACR` variables, for both components in a system and species in a phase, can be specified in natural logarithm, e.g. LNAC(Fe), LNACR(C), LNAC (O2,GAS), LNACR(O2,GAS).

For the POST module, and after calculating with the STEP_WITH_OPTIONS or MAP commands, the reference state for a component can also be changed to plot various properties of the component in the entire system or in a specific phase. Then you can set the diagram axes as the chemical potential or activity quantities with the `R` suffix, i.e. MUR(comp), MUR (comp,ph), ACR(comp), ACR(comp,ph) or the common logarithms [e.g. LNACR(comp,ph)].

Syntax	SET_REFERENCE_STATE
Prompts	`Component: <Name of the component>` The name of the component must be given.
	`Reference phase: <Name of a phase used as the new reference state>`

Syntax	SET_REFERENCE_STATE

Enter the `Name of a phase` for the system.

> For a phase to be usable as a reference for a component, the component needs to have the same composition as an end member of the phase. The reference state is an end member of a phase. The selection of the end member associated with the reference state is only performed once this command is executed.

If a component has the same composition as several end members of the chosen reference phase, then the end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy.

The following are example using temperature. Pressure is used in the same way:

- In the Fe-C system, BCC can be a reference state for Fe but not for C since BCC can exist as pure Fe but cannot exist as pure C.
- If GAS is chosen as the reference phase of component O at such a high temperature that O1 has the lowest energy, then O1 remains the reference state even at calculations performed at lower temperatures where O2 has a lower energy than O1.
- Setting the reference state for component O as gas (one sublattice) with constituents O1, O2 and O3 results in O2 being the reference state if, at the present temperature, pure O2 has the lowest energy of O1, O2 and O3. If the reference state is set above a critical higher temperature, then O1 has the lowest energy and consequently becomes the reference state.

`Temperature /*/: <Temperature for the reference state>`

Select the Temperature (in K) for the reference state. The wildcard value * means the current temperature is used at the time of evaluation of the reference energy for the calculation.

> The temperature set with this command does not affect the temperature used when evaluating the energy of the reference state during the end member selection process.

`Pressure /1E5/: <Pressure for the reference state>`

Select the Pressure (in Pa) for the reference state. The wildcard value * means the current pressure is used for evaluating the reference energy at the time of calculation.

Examples

```
S-R-S Fe SER
S-R-S Cr FCC * 100000
S-R-S H2O AQUEOUS * 100000
S-R-S ZE REF_ELECTRODE * 100000
```

SET_START_CONSTITUTION

This command is available with the POLY and ED-EXP modules.

This command is similar to SET_ALL_START_VALUES, but is used for an individual phase that may have a wrong constitution.

Syntax	SET_START_CONSTITUTION
Prompts	`Phase name: <Name of a phase, and possible major constituent(s)>` Specify the name of a phase for which the constitution shall be set. If there is a major constituent of the phase, you must specify this on the same line as the phase name. By giving an*, select the default major constituents. A $ means keeping the same constitution, and `NONE` means to give individual site-fractions.
	`Y(<Phase>#<Composition_set>,<Constituent>#<Sublattice>) /xxx/: <SF>` The site fraction (`SF`) of the constituent shall be given. The default value `xxx` is the last calculated one.

SET_START_VALUE

This command is available with the POLY and ED-EXP modules.

This command is not often required as the automatic start values can be handled for most problems.

Set a start value of an individual variable.

Syntax	SET_START_VALUE
Prompts	`State variable: <Name of a state variable>` The state variable must be given.
	`Value` Specify the value to be assigned the state variable as start value.

SHOW_FOR_T=

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

Display various thermodynamic properties (state variables, derived/partial variables or entered symbols) of the currently calculated (stable/meta-stable) equilibrium state but under a different temperature condition. This is useful for knowing, for example, a volume-related property of a frozen (stable/meta-stable) equilibrium state at a certain temperature, where the equilibrated phase assemblage and all the phase compositions are not adjusted while only the temperature condition is changed.

Use this option carefully. You must have successfully calculated a real equilibrium state under one temperature condition (normally the temperature for the last heat treatment). This can then be used to obtain the value(s) of any specified state variable(s) or derived/partial variable(s) or defined symbol(s) for thermodynamic properties of the entire system, of components, or of phases for the currently-defined system (being in a frozen state) under another temperature (normally at room temperature). No real equilibrium is re-calculated through this option, and thus the phase amounts and compositions in the system are the same as at the last real equilibrium calculation.

Settings

```
Temperature (K) /298.15/: <temperature_in_K>
```

Specify the new temperature condition (in K) under which the values of some specific state variable(s) or derived/partial variable(s) or defined symbol(s) for various thermodynamic properties of the entire system, of components, or of phases) in the currently-defined system (being in a *frozen* state) is shown on screen.

```
State Variable or symbol /VM/: <State variable or symbol name(s)>
```

Specify the name(s) of the desired state variable(s) or derived/partial variable(s) or defined symbol(s) for various thermodynamic properties of the entire system, of components, or of phases) in the currently-defined system. More than one state variable or symbol of interest can be simultaneously specified on the same line. For example, you can choose to show the values of VM or GM (i.e. molar volume or molar Gibbs energy of the entire system), or of VM(*) or HM(*).T (i.e. molar volumes or isobaric heat capacity of all phases), or of ACR(*), DGM(*) and LNACR(*,FCC) [i.e. activities of all system components, driving forces for all phases, and activities (in logarithm) of all system components in the FCC solution phase], under the new temperature condition (being in a frozen state).

SHOW_VALUE

This command is available for the POLY and ED-EXP modules.

Show the current value of any state variable, function or variable.

Syntax	SHOW_VALUE
Prompt	`State variable or symbol: <Name(s) of state variable(s) or symbol(s)>` A single or several state variables or symbols (entered functions or variables) can be specified.
	The wildcard * can be used to denote all phases or all components. You can use the dollar-sign `$` to denote all stable phases. Thus, the command SHOW W(*,*)lists the mass fraction of all phases, whereas `SHOW W($,*)` lists the mass fraction of all stable phases. If you `SHOW` a function, all functions are evaluated using the current values of the state variables. But if you `SHOW` a variable, it retains its value from the time it was `ENTERED` or last `EVALUATED`. Therefore to save a value from one calculation to another, `ENTER` it to a variable. This is frequently done in the PARROT module to transfer values between equilibria.

STABILITY_CHECK

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

In some composition ranges of a multicomponent system, it often happens that an unstable solution phase region locates inside a miscibility gap, and the stability limit (the *spinodal curve* or *spinodal*) may be not easy to find. A system inside a spinodal is thermodynamically unstable with respect to compositional fluctuations, and the system may experience the *spinodal decomposition* (i.e. decomposing to a mixture of regions with the two stable compositions, one on each side of the miscibility gap).

This option makes it possible to automatically check internal stability of both stable and unstable phases in all subsequent single-point equilibrium and MAP/STEP calculations. It can find out if any phase is subject to spinodal decomposition during the subsequent calculations. If there is an unstable phase located inside a miscibility gap in a calculation, it gives a warning so that you suspend the unstable phase, or use FORCED automatic start values for phase constituents (i.e. SET_ALL_START_VALUES → `FORCE` command-sequence), or create other composition sets; you can also ignore the warning message if you know that the unstable phase is not formed in the current calculations.

Settings

```
Stability check on? /Y/:
```

```
Check also for unstable phases? /Y/:
```

If the automatic stability-check option is switched on choose to also check the stability for unstable phases. The default is Y and if an unstable phase is found to be located in a miscibility gas during a subsequent single-point equilibrium or MAP/STEP calculation, a warning message informs you to selectively make adjustments in the calculation settings [e.g. suspending the unstable phase, or using FORCED automatic start values for phase constituents by the S_A_S_V F command-sequence, or creating other composition sets, etc.]. By answering N the stability check is enforced only to stable phases in the system.

STEP_AND_MAP

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

STEP_AND_MAP is the default ADVANCED_OPTIONS choice and is used to determine how to perform Global Minimization test and how to handle initial equilibrium points.

Settings for MAP and STEP:

```
Global test interval /0/: <Integer number>
```

Settings for MAP:

```
Automatically add initial equilibria /Y/:

Number of mesh along an axis /3/: <Integer number>

Use inside meshing points /N/:

Global test interval /0/: <Integer number>
```

The integer number determines how often the Global Minimization should be used during STEP_WITH_OPTIONS and MAP calculations. If it is set to 0 (zero), the recommended global test interval is used: i.e. every tenth step and at each phase change during STEP calculations, and only at node points during MAP calculations. Any other positive integer number, n, suggests it performs a Global Minimization test at every n-th step during STEP and MAP calculations. Of course, the Global Minimization test is always carried out at a phase change or a node point. The Thermo-Calc software is installed with 0 (zero) as the default value, but such a configuration for the default value can be changed by using SET_TC_OPTIONS in the SYS module.

```
Automatically add initial equilibria /Y/:
```

When ADD_INITIAL_EQUILIBRIUM is not used before MAP, a mesh of initial equilibrium points are added before the mapping itself takes place. This mesh is only available when two (2) axes are already defined. The default on start-up may be changed by SET_TC_OPTIONS in the SYS monitor.

```
Number of mesh along an axis /3/: <Integer number>
```

An integer for how many intervals of initial equilibrium points to be added along an edge in the diagram. For example, if set to 2 (two), initial equilibrium points are added at the beginning, center, and end of each axis-variable forming 2 intervals.

```
Use inside meshing points /N/:
```

If N the INITIAL_EQUILIBRIUM mesh consists of initial equilibrium points added only along the edge/border of the diagram defined by the axis-variables. If Y, the initial equilibrium points added are also added to the inside edge.

STEP_WITH_OPTIONS

This command is for the POLY module.

The STEP_WITH_OPTIONS (short name, STEP) command initiates the stepping procedure to make a calculation of property diagrams in a multicomponent heterogeneous system. A property diagram is usually stepped under one defined independent stepping axis-variable, and is often constructed by the defined independent mapping axis-variable against a chosen property (for the system, or for a specific phase, or for a certain species).

In the POLY module, it is possible to compute a series of equilibria with one condition as the stepping axis variable. This is achieved by first calculating a single equilibrium, and then selecting one of the conditions as the axis variable. The minimum and maximum value and the incremental step along the axis must also be given. By default, the global minimization technique is used .

A property diagram consists of property lines that change (normally) along with the stepping axis-variable. From a single STEP calculation, many different types of property diagrams in the defined multicomponent heterogeneous systems can be plotted. Various types of property diagrams are generated by the stepping calculations.

About Property Diagrams

Normally, before the command can be invoked, you need to have already calculated an initial equilibrium point and set one independent variable (i.e. the controlling condition in the system) . This is done using SET_AXIS_VARIABLE. You then list the current values of the axis variable for each calculated equilibrium, as well as the corresponding information when the set of stable phases changes.

By default, the global minimization technique is enabled, You can turn this off by using the command-sequence ADVANCED_OPTIONS → GLOBAL_MINIMIZATION.

You can choose how often to do a global minimization test using the command-sequence ADVANCED_OPTIONS → STEP_AND_MAP → GLOBAL TEST INTERVAL.

Syntax	STEP_WITH_OPTIONS
Prompt	`Option? /Normal/: <A chosen option, N, I, S, O, E, M, T, or P>`

Syntax	STEP_WITH_OPTIONS
	N = Normal, I = Initial equilibria, S = Separate phases, O = One phase at a time, E = Evaluate, M = Mixed Scheil, T= T0, and P Paraequilibrium

Normal (N)

When you accept the default, Normal (N), it allows a stepping calculation with the chosen independently-varying equilibrium condition (axis-variable). Only the step axis value is changed between each step.

When you repeat the STEP → NORMAL command-sequence, you can make several stepping calculations while still keep all the stepping-calculation results in the current POLY3 workspaces.

The calculation results are saved in the default `RESULT.POLY3` file or you can specify to save it in the `<MyName>.POLY3` file. This is as long as there is no SAVE_WORKSPACES command before the second set of command sequences (STEP → NORMAL). Repeated stepped results can be restored into the same current POLY3 workspaces/file.

Linux and Mac are case sensitive so ensure you enter `.POLY3`.

The addition of several steps enables you to generate special types of property diagrams and to calculate and plot special phase boundary lines on phase diagrams, such as:

- The missing part(s) of a specific property [that are calculated under another controlling condition inside the range of the stepping-variable] on the same property diagram.
- Two or more sets of a specific property [that are calculated under different controlling conditions and stepped over the same stepping-variable range] on the same property diagram for the same system.
- Calculate some special phase-boundary lines [especially for some defined secondary phase transformations or alike, e.g. the BCC_A1 <--> BCC_B2 phase-boundary, or equal-Gm for two specific phases, or equal-fraction or equal-activity for a certain species in two specific phases, that shall be calculated under different controlling-conditions and also be stepped over different stepping variable(s)], and then plot (or

impose) them onto a corresponding phase diagram (which can be resulted from several such STEP → NORMAL calculations or even from a separate MAP calculation) for the same system.

Initial_Equilibria (I)

An initial equilibria is added at each calculated point. This can be useful, for instance, to generate a set of isothermal calculations.

When you choose `I`, an initial equilibrium is stored at each calculated equilibria. It is intended to generate a matrix of calculated initial equilibria, first stepped under a STEP INITIAL_EQUILIBRIA command-sequence and then repeated by another STEP NORMAL command-sequence (or even continued by a MAP command).

For example, you can first use the temperature condition as the stepping axis-variable with this option, which calculates a number of initial equilibrium points and automatically adds each one as an initial equilibria for another STEP → NORMAL command-sequence (or even for a MAP command). Before the second STEP command (i.e. the STEP → NORMAL command-sequence), you can chose a compositional condition as the new stepping axis-variable; then the STEP → NORMAL command-sequence uses those created starting equilibrium points (at different temperatures) and steps in such a new compositional variable. As a result, these two STEP commands together give a matrix of values.

Separate_Phases (S)

In this way, you can calculate how the Gibbs energy for a number of phases varies for different compositions. This is particularly useful to calculate Gibbs energies for complex phases with miscibility gaps and for an ordered phase that is never disordered (e.g. SIMGMA-phase, G-phase, MU-phase, etc.).

One_Phase_at_Time (O)

This option is recommended for STEPPING heterogeneous systems with both ordered phases and the disordered pairs.

When you choose `O`, the stepping calculation is conducted individually for one phase at a time. That is, it is stepped over the whole stepping variable range, but the stepping is repeated for all the entered phases in the defined system. This is particularly useful to properly step in composition for an equilibrium heterogeneous system with both ordered phases and the disordered pairs. Thus, instead of calculating for the same composition for each of the phases at each composition step, it starts the stepping in each of the phases in the default most-stable compositions (the major constitutions).

Evaluate (E)

For Scheil-Gulliver simulations it is recommended you use the SCHEIL module.

Evaluate `E` is an advanced option and is useful when additional conditions (instead of the stepping variable) require changing during a stepping calculation. It allows a stepping calculation in a single axis with simultaneous evaluation of one or more variables after each step. As variables can be used as conditions, it means that you can change the conditions during the stepping. After a successful EVALUATE calculation, you can go to the POST module to manually define and plot property diagrams.

The variables given are evaluated after each step, which may change other conditions. This can be useful to perform the Ordinary ScheilGulliver Approach (non-equilibrium transformations) for simulating alloy solidification without back diffusion of fast-diffusing interstitial components in solid phases. However, it is recommended you use the SCHEIL module.

Specify the prompt:

```
Variable name(s): <Variable name>
```

The names of the variables that shall be evaluated after each step must be typed here.

The miscibility gap test is automatically used during stepping (see ADVANCED_ OPTIONS) if a phase has two or more composition sets.

The miscibility gap test means that you can start calculating from high temperatures in a steel where the MC carbide is not stable. During the calculation, the MC carbide first becomes metastable with a composition different from the metallic FCC phase and later also becomes stable.

See Console Mode example tcex30A.

Mixed_Scheil (M)

For Scheil-Gulliver simulations it is recommended you use the SCHEIL module.

This is an advanced stepping calculation designed for the Extended Scheil-Gulliver Approach (partial-equilibrium transformations) to simulate alloy solidifications with back diffusion of one or more fast-diffusing interstitial components (such as C, N, O, S, etc.) in solid phases is performed. It also will consider BCC-->FCC phase transformation (practically for steels) along the alloy solidification process.

To ensure a successful stepping calculation of mixed Scheil-Gulliver simulation of solidification process of a defined alloy system with a certain initial overall composition, it is important to note the following:

- For solution phases with possibility of miscibility gap existence, you have appropriately added the necessary composition set(s);
- You have already set the temperature condition as the stepping SET_AXIS_VARIABLE command, with minimum and maximum temperature points as well as an appropriate s temperature step for the cooling process).
- There must be a composition condition for each of the back diffusion components (i.e. fast-diffusing interstitial components, such as C, N and/or other elements) that are already defined in terms of mole-fraction or mass-fraction, e.g. `X(C)` and `W(N)`. Otherwise, a stepping calculation with this option can fail.
- An initial equilibrium in which the LIQUID mixture phase is the only stable must be calculated. This is why it is good to start with a relatively high temperature condition for the initial equilibrium calculation. It is always necessary to reject or suspend the GAS mixture phase (if it exists) before the C-E and STEP commands, to avoid its formation along with LIQUID.
- In cases where fast-diffusing interstitial components are specified as back diffusion components, you can choose to `allow BCC>FCC` phase transformation (practically for steels) during the alloy solidification process.

These are the prompts for this option:

```
Fast diffusing components: <Fast diffusion interstitial(s)>
```

Specify one or more interstitial component(s) as the back diffusion component(s).

- If there is only one fast-diffusing interstitial component (e.g. C or N), type its name;
- If there are two or more fast-diffusing interstitial components (e.g. C, N and S), always type the names on the same line at once (separated by an empty space in between, e.g. C N S);
- If there is no fast-diffusing interstitial component to be considered, type `NONE` to ignore back diffusion entirely, meaning a normal Scheil-Gulliver simulation is performed.

> Such specified back diffusion interstitial component(s) must be appropriately defined according to the phase constitution definitions of some major alloy solution phases (e.g. FCC, BCC, HCP, etc.). These are located on the interstitial/vacancy sublattices in such alloy solution phases; otherwise, such a Scheil-Gulliver simulation may not make sense at all.

```
Allow BCC -> FCC ? /Y/:
```

By default the BCC-->FCC phase transformation is allowed. This is usually a typical phenomenon along the cooling processes of steels/Fe-alloys.

During the calculation the simulated solidification path, including the locally-equilibrated phase assemblage (region), captured temperature condition (`T` in K), remaining liquid phase (`NL`, mole fraction), overall formed solid phases (`NS`, mole fraction) and latent heat formation (`NH`, J/mol) along the cooling process are shown after the information on starting temperature point of the alloy solidification process, e.g.

```
  Solidification starts at  1743.15 K

   Phase Region from   1.744150E+03 for:      LIQUID

   Phase Region from   1.742525E+03 for:

       LIQUID

       FCC_A1#1

         1742.5250         0.9960          0.0040         -1.1824

         1742.4000         0.9795          0.0205       -202.1585    . . . . . .

   Phase Region from   1.733150E+03 for:

       LIQUID

       BCC_A2

       FCC_A1#1

         1733.1500         0.3294          0.6707      -8032.6240

         1733.0250         0.3237          0.6763      -8095.1490    . . . . . .
```

After a successful calculation, you can go to the POST module to manually define and plot property diagrams for the alloy solidification process according to the chosen Scheil-Gulliver model, or to impose existing relevant experimental information or other types of calculated solidification results [e.g. Scheil-Gulliver simulation with or without considering fast-diffusing interstitial component(s), full-equilibrium approach, or Diffusion Module (DICTRA)-type simulation with moving-boundary conditions] onto the same plotted property diagrams. Normally, the solidus temperature (`T` in Celsius) is set as one of the axis variables (usually as Y-axis in most cases), while the other plotted quantity on the other axis can be the amount of overall formed solid alloy phases (`NS` in mole-fraction or `BS` in mass-fraction), the amount of remaining liquid phase (`NL` in mole-fraction or `BL` in mass fraction), the heat of latent along the solidification process (`NH` in J/mol or `BH` in J/gram), among many other properties in the solidified alloy phases or in the whole alloy system.

T-zero (T)

See Console Mode example 41.

This advanced option allows a stepping calculation of the so-called T0 (T-zero) line in a diffusionless transformation (where two specific partially-equilibrated phases have the same Gibbs energy) along a composition variable which has already set as the stepping variable with SET_AXIS_VARIABLE.

The temperature condition cannot be set as the stepping variable if you want to make a STEP T-ZERO calculation.

Prior to performing the step T0 command sequence, and to ensure a successful calculation of T0 line between two specific phases after an initial equilibrium calculation in the current system, it is sometimes recommended to make a single T0 point calculation using ADVANCED_OPTIONS → T-ZERO.

Specify these prompts:

```
Name of first phase:  <Phase A>
Name of second phase: <Phase B>
```

The names of the target phases, for which the Gibbs energies equal to each other at each point on the T0 line, must be entered.

During the calculation, the T0 values are shown after the corresponding scanned conditions (of the stepping composition variable), e.g.

```
 Phase Region from   1.000000E-01 for:
      BCC_A2
      FCC_A1
    1.000000E-01        940.24
    9.250000E-02        941.20
    . . . . . .
    2.500000E-03        977.61
    7.500000E-09        979.34
  Phase Region from   1.000000E-01 for:
      BCC_A2
      FCC_A1
    1.000000E-01        940.24
    1.075000E-01        939.62
    . . . . . .
    2.950000E-01       1084.87
 3.000000E-01       1080.99
```

After a successful calculation, you can go to the POST module to plot the T0 line against the stepping composition variable or another varying axis, or to impose the calculated T0 line onto a normal phase diagram [normally plotted as a `T-X` isopleth].

Paraequilibrium (P)

See Console Mode examples 42 and 43.

This is an advanced option. Select `P` to calculate the paraequilibrium state between two specific phases (the *paraequilibrium lines*). It allows a stepping calculation of paraequilibrium lines where the chemical potential for one or more interstitial components (that are considered as back diffusion elements, such as C and N) but not for the other (s) in two partially equilibrated phases are equal.

More than one interstitial component can be treated as fast-diffusion species (such as C, N, O, S, etc., as individual or combined) in a paraequilibrium stepping calculation.

The composition condition for the interstitial components cannot be set as the stepping variable if you want to make this calculation.

To ensure a successful stepping calculation of paraequilibrium states between two specific phases in a defined alloy system, it is important to first make a starting-point equilibrium calculation with an initial overall composition in the current system. However, it is unnecessary to obtain an equilibrium in which either one or both of the target phases is stable.

The initial overall composition must have a reasonable setting for the desired paraequilibrium calculation for the two target phases. This is especially true where there is more than one interstitial component to be considered in the paraequilibrium state, because different interstitial components (for example C and N combined) may have significant different behaviours as partitioning into different structured phases; otherwise, for one chosen interstitial component the initial overall composition is OK for the paraequilibrium calculation between the specified two phases, but for other chosen interstitial component(s) it might be impossible to calculate the paraequilibrium state.

Always check if the chosen `phaseA` and `phaseB` have the exact same definition of elements and if the chosen interstitial components are all in the vacancy sublattice sites of the two phases; otherwise the program cannot find the paraequilibrium state (as it is impossible to correctly calculate u-fractions).

Always have a comprehensive understanding of the normal phase diagram for the currently investigated system, so that you make the appropriate choice of the phase pair and staring bulk composition for the system.

Always set the status of the chosen interstitial components as SPECIAL using the command:

```
CHANGE_STATUS COMPONENT <interstitial component> = SPECIAL
```

By doing this, you get a clear picture on u-fractions of various substitutional and interstitial components, which are different from the overall composition in the system. The SPECIAL status means that specified component(s) are not included in summations for mole or mass fractions. Therefore, all the composition variables plotted from the paraequilibrium calculations are u-fraction related quantities.

Always make a single-point paraequilibrium calculation by the command-sequence of ADVANCED_OPTIONS → PARAEQUILIBRIUM, prior to performing this STEP → PARAEQUILIBRIUM command-sequence, although this might not be always necessary for some systems.

With this stepping calculation specify the following:

```
Name of first phase:  <Phase A>
```

```
Name of second phase: <Phase B>
```

The names of the two target phases `A` and `B`, between which the paraequilibrium states establish, must be typed at the above two prompts subsequently or on the same (first) line at once (separated by an empty space, e.g. `FCC BCC`, `FCC#2 M23C6`).

It is important to understand that this is the calculation of a paraequilibrium state between the two specified phases.

Particularly, there are these issues to consider:

1. Both chosen phases must have similar interstitial/vacancy sublattices where the fast-diffusion interstitial component(s) occupy.
2. The choice on the target phase pair must be reasonable for the defined system and specified initial overall composition.
3. Both target phases should have phase constitution definitions that cover all the defined substitutional and interstitial components of the current alloy system; or
4. It is impossible to calculate the paraequilibrium state between the target phase pairs with given interstitial component(s) in the currently defined system.

```
Fast diffusing component: /C/: <Interstitial component(s)>
Fast diffusing component: /None/: <Interstitial component(s)>
```

The name(s) of the fast-diffusing interstitial component(s) (`C` as the default single component) must be given either one by one at each of the above prompts subsequently or in a combination (separated by an empty space in between, e.g. `C N S`) at the same (first) prompt; otherwise, press <Enter> key to start the paraequilibrium line stepping-calculation.

Note the following:

Such specified fast-diffusing interstitial component(s) must be appropriately defined according to the phase constitution definitions of the two selected phases: These must be located on the interstitial/vacancy sublattices in both chosen phases.

If there is only one fast-diffusing component which is carbon, press <Enter> to accept the default value (`C`) at the first prompt; if the single fast-diffusing interstitial component is another element (e.g. N), appropriately type interstitial component the name at the first prompt;

If there are two or more fast-diffusing components (e.g. `C` and `N`), type their names at the above prompts subsequently or at the same (first) prompt (separated by an empty space, such as `C N`);

To finish the input of fast-diffusing elements, accept `NONE` at a repeated prompt;

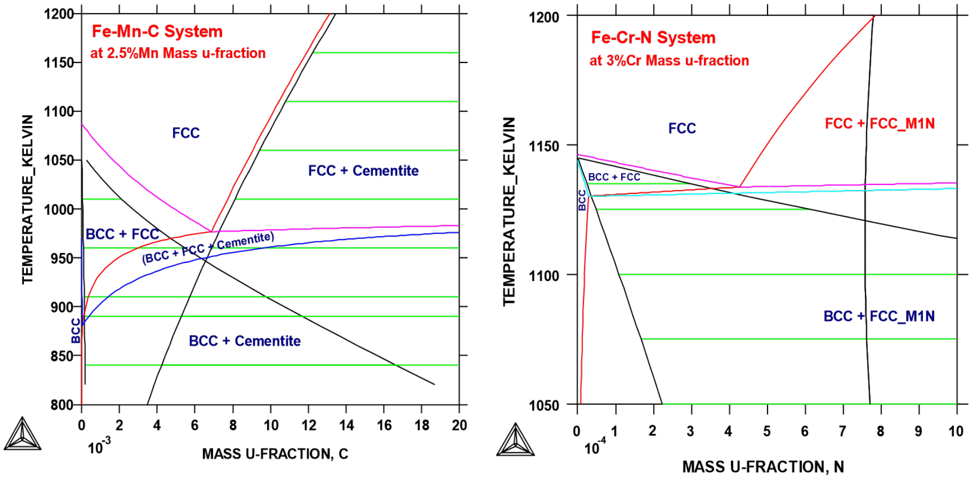
If NONE or a non-existing component name is typed at the first prompt, it means no back diffusion is to be considered, and the para-equilibrium calculation is thus cancelled entirely.

During the STEP → PARAEQUILIBRIUM calculation procedure, the calculated paraequilibrium states include the:

- corresponding stepping conditions (e.g. temperature in K, or the stepping composition variable of the matrix component or of one of substitutional components) which has already set as the stepping variable by the SET_AXIS_VAR command);
- amounts of the phase `A` in mole number [i.e. `NP(phaseA)`];
- amounts of the phase `B` in mole number [i.e. `NP(phaseB)`];
- contents of the interstitial component(s) in the phase `A` expressed in u-fractions [i.e. `u-f(phaseA,component(s))`];
- contents of the interstitial component(s) in the phase `B` expressed in u-fractions [i.e. `u-f(phaseB,component(s))`];
- `LNACR(component)` value(s) for the interstitial(s).

After a successful STEP → PARAEQUILIBRIUM calculation, you can go to the POST module to plot a paraequilibrium phase diagram, or to impose the calculated paraequilibrium states onto a normal phase diagram [normally plotted as a `T-X` isopleth with one of the considered interstitial component(s) as the x-axis variable].

However, the stepping calculation procedure for the currently specified paraequilibrium states between the two specified phases may find difficulties at some steps due to some possible numerical problems (normally regarding to the u-fractions of the interstitial components under some composition ranges), or it may completely fails. In the latter case, it implies that the chosen target phase pair may be unreasonable for the defined alloy system or for the defined initial overall composition, or one or both phases may have inappropriate phase constitution definitions regarding the specified interstitial component(s) and substitutional components. Then, you must either modify the settings of initial overall composition or specify the reasonable target phase pair with an appropriate choice of the fast diffusion interstitials in the defined alloy system.



The figure shows the plot of a paraequilibrium calculation of isopleths: Formation of para-pearlite in two Fe-based alloys, with equilibrium results appended.

The calculated paraequilibrium phase boundaries (black lines) are shown with tie-lines (in green-colour). In the Fe-2.5Mn-C alloy system, C is considered as fast diffusing interstitial component in the BCC+FCC and FCC+Cementite paraequilibrium stepping calculations; while in the Fe-3Cr-N alloy system, N is treated as fast diffusing interstitial components in the BCC+FCC and FCC+FCC_M1N (i.e. FCC#1+FCC#2) paraequilibrium stepping calculations.

During a STEP calculation, the value of the stepping axis variable for each calculated equilibrium is listed and also the set of stable phases.

You can terminate the mapping of a line by pressing a single <Ctrl-A> (Windows) or <Ctrl-C> (Linux). This can be useful in order to stop a longish calculation without losing what is already calculated.

If there is any convergence problem in finding a stable solution at any stage during a calculation procedure enforced by a STEP_WITH_OPTIONS command-sequence, this message displays:

```
Convergence problems, increasing smallest site-fraction from 1.00E-30   to
hardware precision 2.00E-14. You can restore using SET-NUMERICAL-LIMITS
```

This implies that smallest site fraction in the current POLY3 workspace is automatically increased from the default value `1.00E-30` to the hardware-dependent precision (under Linux, as `2.00E-14`). For other subsequent POLY-module calculation in the current TC run, you can use the POLY command SET_NUMERICAL_LIMITS to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

Complex miscibility gaps of various solution phases are automatically detected during a stepping calculation, and two or more composition sets for each of such solution phases are automatically generated as well, through an automatic Global Minimization Test procedure (by specifying a `Global Test Interval` value and confirming the `Automatically add initial equilibria` in the ADVANCED_OPTION STEP_AND_MAP command-sequence). As a particular case, such an automatic Global Minimization Test ensures that you can now start calculating from high temperatures in an austenitic steel (metallic FCC_A1 solution phase) where the MC carbides/nitrides/carbonitrides (i.e. the C-/N-rich sides of the FCC_A1 miscibility-gap, often (while not always) being referred to as `FCC_A1#2, FCC_A1#3`, etc.) are not stable, and during the MAP command the MC carbides/nitrides/carbonitrides may first become metastable with a composition different from the metallic FCC_A1 phase and later also stable.

Occasionally, it may be necessary to have a specified increment other than the default value for the defined stepping axis-variable, in order to calculate/plot a smoother property diagram.

To get a complete property diagram, sometimes (especially in some earlier Thermo-Calc versions) it may also be required to have more than one starting equilibrium-points (under another starting equilibrium condition), and repeat the stepping calculation over the same stepping axis-variable range (while without over-writing the same POLY3 workspaces via a SAVE_WORKSPACE command). However, using the current STEP procedure such a requirement become less necessary.

TABULATE

This command is available for a table entered in either the POLY or POST module.

For any entered table, this command gives a table of values from equilibria calculated with a STEP command.

Unlike the TAB module's command (also called TABULATE) it is not possible to plot columns from the tabulated tables. For this use normal POST commands.

Syntax	TABULATE
Prompts	`Name: <Name of a table entered in either POLY or POST>` Specify a table name that is entered in either the POLY or POST module.
	`Output on screen or file /Screen/:` Specify a file name if you want to save on a file the table values along the defined STEP calculation, or press <Enter> if want to see the table values displayed.

TOGGLE_ALTERNATE_MODE

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

Toggle the ALTERNATE mode for experimental equilibrium calculation between DEFAULT, ALWAYS and NEVER, during data-assessments using the PARROT optimization.

```
Set alternate toggle to DEFAULT, ALWAYS, or NEVER?
```

```
Set global toggle to DEFAULT, ALWAYS, or NEVER?
```

- `DEFAULT`: the experiment points are calculated according to the Alternate Technique depending on the SET_ALTERNATE command.
- `ALWAYS`: the experiment points are always calculated according to the Alternate Technique even if the Alternate Mode is switched off in the PARROT module.
- `NEVER`: the experiment points are calculated as normal equilibria even if you SET_ ALTERNATE in the PARROT module.

T-ZERO_TEMPERATURE

This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

ADVANCED_OPTIONS

This calculates the temperature when two specific phases have the same Gibbs energy, i.e. the so-called T0 temperature. You must calculate an equilibrium state at an estimated temperature before performing this advanced-option calculation; however, it is unnecessary to obtain an equilibrium state in which either one or both of the target phases is stable.

The following prompts are shown.

```
Name of first phase:  <Phase A>
```

```
Name of second phase: <Phase B>
```

The names of phases A and B must be given, for which the T0 temperature (where the Gibbs energies are equal) is to be calculated.

If the T0 temperature between the two specified phases is successfully calculated, a message displays, e.g.

```
The T0 temperature is 840.82 K. Note: LIST-EQUILIBRIUM is not relevant
```

The first message shows the calculated T0 temperature between the two specified phases.

The second message indicates that after this option calculation with LIST_EQUILIBRIUM is irrelevant and does not list the equilibrium for the system at the T0-temperature.

Gibbs Energy System (GES) Commands

In this section:

Solution Models in the GIBBS (GES) Module

AMEND_PHASE_DESCRIPTION

The AMEND_PHASE_DESCRIPTION command is used to specify/amend phase descriptions if a phase has a miscibility gap, uses a special excess energy model, or has a specific additional contribution to its Gibbs energy, for example.

This topic outlines the application of each option and includes important information about each command.

There are many solution models implemented in the GIBBS module (type `INFO MODELS` to see details about various thermodynamic models). However, these are switched on and handled differently via various GIBBS routines/commands:

- The first models the non-ideality as excess parts, i.e. by amending the phase's EXCESS_MODEL and/or TERNARY_EXTRAPOLAT models.
- The second models the non-ideality as ADDITIONAL parts, i.e. by amending the phase's other subjects in this command, e.g. MAGNETIC_ORDERING for the Magnetic Ordering Model, DISORDERED_PART for the CVM Approach in modeling chemical ordering/disordering phenomenon, QUASICHEM_IONIC for using a quasi-chemical entropy term for an ionic two-sublattice liquid solution phase, QUASICHEM_FACT00 or QUASICHEM_IRSID for describing a substitutional liquid solution phase, DEBYE_HUCKEL for the DHLL/SIT Model in describing a dilute aqueous solution phase, etc.
- The third implements the model entirely or partially into the GIBBS module and related database(s), such as for the electrostatic contribution in an AQUEOUS solution phase by the Complete Revised_HKF Model, the Murngham Model, Birch-Murngham Model or Generalized PVT Model for high-pressure/temperature volume contribution in a solid or liquid phase, the SUPERFLUID Model for the non-ideal EOS and non-ideal mixing in a gaseous mixture.

NEW_CONSTITUENT

Use this if you want to add a new constituent to a phase. It is illegal to add new constituents to an ionic two-sublattice liquid phase.

RENAME_PHASE

Use this to change the names of some specific phases. For example, a phase called *FE3O4_S* may be better named *Magnetite* to help identify it during the calculations and postprocessing. This is also a way to delete a phase by hiding it under a new name.

SITE_RATIOS

Use this to change the number of sites (i.e. the stoichiometric coefficients of various sublattices) in a sublattice phase.

COMPOSITION_SETS

Use this for solution phases that may have miscibility gap(s). However, this is less important today and often unnecessary to define additional composition set(s), since the implemented Global Minimization Technique can usually detect and add such composition set(s) in an automatic manner where it is really necessary during equilibrium calculations (of single-points, stepping or mapping).

MAJOR_CONSTITUENT

Use this to set major constituent(s) on each sublattice in each composition set for a solution phase. This is useful to make calculations converge faster because it may simplify giving start values when calculating the equilibrium as those phases with miscibility gaps should have different major constituents for each composition set. The databases often set major constituents for several phases automatically when data are retrieved.

FRACTION_LIMITS

Use this to limit the application range (in terms of mole-fractions of all the involved elements) of a particular solution phase. This is useful to avoid automatic creations (enforced by the Global Minimization Technique) of additional composition sets for some solution phases (such as AQUEOUS solutions or dilute Fe-based liquid mixtures) of which the used models [e.g. the `SIT Model` or the `Complete Revised_HKF Model` for AQUEOUS solution, or the modified dilute solution parameters (plus a quadratic term, according to Hillert (1986) based on the SigworthElliot Model [1974Sig] for Fe-rich liquid mixture] cannot be appropriately applied on a full scale.

Globally set the composition limits (in terms of mole fractions of various elements) in a specific solution phase, so that whenever the program finds a potential phase composition or a new composition set of possible miscibility gap(s) but that is out of this globally-set composition range, the program automatically ignores such a phase composition in an equilibrium calculation. This can be done either permanently inside a database (by enforcing this option for amending the phase-description of the solution phase) or temporarily within the GIBBS module (by using this phase-description amendment option).

This is important for solution phases for which the thermodynamic models and assessed data for the phases are for specific composition ranges, for example, the FE_LIQUID phase in the SLAG database is only applicable for Fe-rich liquid mixture, and the AQUEOUS phase in the TCAQ/PAQ and AQS/PAQS databases is only applicable for H2O-dominant aqueous solution phase.

Specify the low and high mole-fraction limits for each of the elements possibly available within the considered phase (in the currently defined system, or in a certain database). Do this for all the possible elements (defined in the phase) in a single AMEND_PHASE_DESCRIPTION FRACTION_LIMITS command-sequence, for example:

```
TYPE_DEFINITION R GES AM_PH_DES FE_LIQUID FRACTION_LIMITS Fe 0 0.6
      Ag 0 0.01  Al 0 0.05  Ca 0 0.05  Co 0 0.01  Cr 0 0.01
      Cu 0 0.02  Mg 0 0.05  Mn 0 0.05  Mo 0 0.05  Nb 0 0.05
      Ni 0 0.05  Pb 0 0.05  Si 0 0.10  Sn 0 0.02  Ti 0 0.05
U  0 0.01  V  0 0.02  W  0 0.02  Zr 0 0.03
      B  0 0.01  C  0 0.01  H  0 0.01  N  0 0.01  O  0 0.01
P  0 0.01  S  0 0.01  !
```

NEVER_DISORDER

The contribution from the disordered phase are added to the ordered phase. Use this to avoid entering several parameters to the ordered phase in the database. Instead it can be expressed as one parameter in the disordered phase.

The reference [2018Sun] section 2.3.4 has extensive details about this model. Original references from [1994Dup] and [2000Ans].

DISORDERED_PART

This command is needed for the special treatment of chemically-ordered phases where the contributions from the disordered state are described by a phase without ordering sublattices (the disordered phase name must be specified).

Several checks are made that the ordered and disordered phases are compatible (sublattices, sites and constituents). A link is then created between the phases, and the disordered phase is hidden from application programs. The Gibbs energy for the ordered phase also includes the Gibbs energy for the disordered phase.

Phases which can have an order/disorder transformation have parameters split on two phases and are referred to as the *two phase* description in the GIBBS module. One of them has sublattices for chemical ordering, the other one represents the disordered state. Normally, the ordered BCC and FCC or HCP phases may have either 2 or 4 substitutional sublattice (plus one additional interstitial site), that are handled by the Two Substitutional-Sublattice Ordering Model or Four Substitutional-Sublattice Ordering Model, respectively.

Two phase means that the *ordered* phase has parameters that describe the ordering. The *disordered* phase has all parameters for the reference state and those for describing the disordered phase. The ordered phase may occur only is some systems whereas the disordered phase may occur frequently, typical examples are the disordered FCC and BCC which may become ordered as L12 or B2 in certain systems. In order to treat multicomponent systems where some subsystems have ordering it would be necessary to transform all parameters of BCC into a B2 model.

The parameters describing the disordered phase are not changed but the Gibbs Energy system is informed that the Gibbs Energy for the two phases should be added.

The method used calculates the Gibbs Energy of a two phase model with two or four substitutional sublattices for ordering.

$$G_m = G_m^{ord}(y_i', y_i') + G_m^{dis}(x_i) - G_m^{ord}(y_i' = x_i, y_i'' = x_i)$$

The mole fractions *x*i are calculated from the site fractions *y*i. The last term means that the contribution from Gmord in a disordered state (same site fraction, equal to the mole fraction, on both sublattices) is subtracted. The effect of this is that the parameters in the ordered phase have no contribution to the disordered state.

MAGNETIC_ORDERING

Change the magnetic ordering parameter for a certain phase with magnetic ordering contribution, in terms of its anti-ferromagnetic factor. By default this is –1 for BCC phase and –3 for all other phases (FCC, HCP, etc.). The fraction value of the total enthalpy (due to short-range ordering above the magnetic transition temperature) is by default 0.40 for BCC phase and 0.28 for all other phases (FCC, HCP, etc.).

EXCESS_MODEL

See example tcex52.

Use this to change the default Excess Model (for interaction energies) from the default (REDLICH-KISTER_MUGGIANU). The model handles the excess interaction energies in a solution phase is chosen from:

- REDLICH-KISTER_MUGGIANU: for binary (R-K) & ternary (R-K-M) interactions
- REDLICH-KISTER_KOHLER: for binary (R-K) & ternary (R-K-K) interactions
- FLORY-HUGGINS POLYMER MODEL: for interactions in a polymer mixture phase (F-H)
- MIXED-EXCESS-MODELS: (R-K default) for mixed binary excess model (R-K, Legendre & Polynom) of a substitutional solution phase
- HKF: for interaction in an AQUEOUS solution phase (HKF)
- PITZER: for interaction in an AQUEOUS solution phase (PIT)
- CENTRAL_ATOM_MODEL: for interaction in a liquid slag solution phase (C-A-M)

For extrapolations of excess energies from related binary systems to ternary or higher-order systems, the Redlich-Kister binary excess interaction parameters may be extrapolated with either a Muggianu extension (i.e. the default REDLICH-KISTER_MUGGIANU model) and a Kohler extension (i.e. the alternative REDLICH-KISTER_KOHLER model), where there is no ternary, quaternary or higher-order interaction parameter.

The REDLICHKISTER_KOHLER model is implemented only for ternary systems.

The MIXED-EXCESS-MODELS option works only for a substitutional phase with no sublattice (such as the metallic LIQUID phase) and it can be used to invoke asymmetrical simple or Legendre polynomial as binary excess energy models in addition to the default symmetrical Redlich-Kister model for the chosen pair of constituents in a substitutional phase with no sublattice. Asymmetrical here means that the power series depend only on one of the constituents, for example with expansions based on the [1-2*X(B)] term rather than [X(A)X(B)].

Binary interaction parameters for such a pair of constituents must be entered prior to turning on the non-default Legendre or Polynom models.

TERNARY_EXTRAPOLAT

See example tcex52.

Use this to change the extrapolation method from the default REDLICH-KISTER_MUGGIANU to another extrapolation model. This method extrapolates from binary to ternary (and higher-order) excess interaction parameters in a solution phase and is chosen from:

- MUGGIANU for Muggianu Extrapolation from R-K parameters
- TOOP-KOHLER for Toop-Kohler Extrapolation Model
- KOHLER-ALL for Kohler Extrapolation Model
- MUGGIANU_RESTOR for Muggianu-Restor Extrapolation Model

> Only when all the relevant binary excess energies in the current solution phase are treated by the default Redlich-Kister Model (i.e. the Mixed-Excess-Model should have not been used), the MUGGIANU_RESTOR method for ternary extrapolations is equivalent to the Redlich-Kister_Muggianu Model, or the KOHLER-ALL method to the RedlichKister_Kohler Model.

The default ternary extrapolation method MUGGIANU_RESTOR applies to a solution phase as a whole, whatever the binary excess model(s) enforced to each of individual binary pairs in the phase. In case that all the binary pairs in the phase use the default binary excess model REDLICH-KISTER, then the ternary extrapolation method becomes the so-called Redlich-Kister_Muggianu Model (in short as R-K-M), for extrapolations from binary parameters to ternary (and higher-order) excess energy terms; when no ternary L parameter is entered for that, such a default R-K-M Model is always used.

The KOHLER-ALL ternary extrapolation method can be turned on also for a solution phase as a whole, whatever the binary excess model(s) enforced to each of individual binary pairs in the phase. In case that all the binary pairs in the phase use the default binary excess model.

REDLICH-KISTER, then the ternary extrapolation method becomes the so-called Redlich-Kister_Kohler Model (in short as R-K-K), for extrapolations from binary parameters to ternary (and higher-order) excess energy terms; when no ternary L parameter is entered for that, such an R-K-K Model is used.

The TOOP-KOHLER ternary extrapolation method is applied in a special way: for a specific ternary system (e.g. A-B-C) in a solution phase, specify which two constituents as the so-called Kohler constituents and the remaining constituent as the so-called Toop constituent on a given sublattice. If for the A-B-C ternary system you have specified A and B, or B and A, as the Kohler constituents (entered as the basis constituent and first interacting constituent) and C as the Toop constituent, only the A-B binary interaction parameters are used in accordance with the Kohler ternary extrapolation formula for A-B-C ternary interaction, while any other binary interaction parameters involving the Toop species C (i.e. of A-C and B-C binaries) are used in line with the Toop-Kohler ternary extrapolation formula (for the A-C-B and B-C-A ternary interactions).

DEBYE_HUCKEL

To use the DHLL (Debye-Hückel Limiting Law) model and SIT (Specific Ionic Interaction Theory) model for a dilute AQUEOUS solution phase, switch the DEBYE_HUCKEL part on, and it removes previously set (if any) ADDITIONAL part on the non-ideality for the chosen AQUEOUS phase.

HKF_ELECTROSTATIC

To use the hypothetical electrostatic contribution for the chosen phase (it must be an aqueous solution phase using the Complete Revised_HKF Model). It removes previously set (if any) ADDITIONAL part on the non-ideality for the chosen AQUEOUS solution phase.

QUASICHEM_IONIC

To use the Quasichemical-Ionic model for the chosen liquid phase, you must have already entered/retrieved a liquid phase as an ionic two-sublattice liquid solution phase (normally, that is the IONIC_LIQ phase), and then use this amending option to switch QUASICHEM_IONIC on. It creates a completely new liquid solution phase [namely the QUAS_IONIC phase which uses the Quasichemical Model for the entropy, according to Mats Hillert [2001Hil], while the original IONIC_LIQ phase remains in the system and is not changed by this option.

QUASICHEM_FACT00

See example tcex49.

To use the Quasichemical Model developed by Kongoli et al. [1998Kon], you must have entered/retrieved a liquid phase using a normal substitutional liquid model with specified associates or species (on a single lattice site), and then turn on the option QUASICHEM_FACT00. This removes the previously-set (if any) ADDITIONAL part on the non-ideality for the chosen liquid phase.

QUASICHEM_IRSID

To use the Kapoor-Frohberg-Gaye Quasichemical Cell Model (i.e. the Quasichemical Model developed by ISRID, France) for a liquid SLAG solution phase, you can use a normal liquid model with specified associates or species.

GLASS_TRANSITION

To use the special model for glass transition of a liquid phase. It removes previously set (if any) ADDITIONAL part on the non-ideality for the chosen liquid phase.

REMOVE_ADDITION

To remove all the selected ADDITIONAL part from the Gibbs energy description for the chosen phase. If preferred, set a specific phase-status bit for a phase, use the PHASE_BITS option as long you know the restrict meaning of each part of a phase- status bits.

DEFAULT_STABLE

Set phases as default-stable, which helps you to have a better guess of which phases that should be stable at the first calculation.

References

[1974Sig] G. K. Sigworth, J. F. Elliott, The Thermodynamics of Liquid Dilute Iron Alloys. Met. Sci. 8, 298–310 (1974).

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[1998Kon] F. Kongoli, A. D. Pelton, Y. Dessureault, Thermodynamic modeling of liquid Fe-Ni-Cu-Co-S mattes. Metall. Mater. Trans. B. 29, 591–601 (1998).

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[2001Hil] M. Hillert, The compound energy formalism (1). J. Alloys Compd. 320, 161–176 (2001).

About the ENTER_PHASE Command

ENTER_PHASE

With the command ENTER_PHASE, the phase name, phase-type, sublattice number, and constituents or constituent array(s) for the phase are entered into the GIBBS workspaces.

About Phase Names

A thermochemical system must have at least one phase (which is a homogeneous part of the system with a uniform composition and structure). In the GIBBS module, any number of phases can be entered for a system and for each phase there must be a description of how its Gibbs energy varies with temperature, pressure and composition. A phase has a large amount of data connected to it, e.g. it starts with a phase name:

- It may be treated as a special phase-type;
- It may have structural information about sublattice(s), etc.,
- There must be a list of constituents (for a substitutional phase with no sublattice) or of constituent arrays (for a sublattice phase);
- There may be basic information on what kind of EXCESS_MODEL (polynomial expression) is used to describe the binary, ternary and/or higher-order interactions between constituents;
- There may be so-called Additional contributions to the Gibbs energy of the phase from special physical phenomena, e.g. magnetic ordering, hypothetical electrostatic interaction, and so forth;
- There must exist all the parameters required for the descriptions of thermochemical properties (i.e. `G` terms for standard Gibbs energies, and `L` terms for binary, ternary or higher-order interaction excess energies) and of some special physical properties (e.g. the Curie temperature `TC` and Bohr magneton number `BMAGN` (or `BM`) for magnetic ordering, `V0-VA-VC-VK` parameters for volume contributions, Born functions for hypothetical electrostatic interaction in an aqueous solution phase) stored in connection with the phase.

About Phase Type Code

A G phase (gaseous mixture) or an A phase (aqueous solution) is usually treated as a substitutional phase without sublattice, and that an L phase (ordinary liquid solution) is normally (but not always) modeled as a substitutional phase without sublattice, too.

The F and B phase-types are useful for ordered FCC (or HCP) and BCC solution phases handled by the so-called Four Substitutional-Sublattice Ordering Model, which always requires that the solution phase must have four sublattices for substitutional ordering and can additionally have an interstitial sublattice.

For ordered FCC or HCP phases, these four substitutional sublattices represent four corners of the regular tetrahedron on these lattices all of which are the nearest neighbours. A *Normal 4-Sublattice Model* requires that all the G parameters for each of end-members with the same elements but distributed on different sites be given separately. However, as these corners are identical lattice points, the phase-type option F means that the G parameters need be given only once. The possible permutations are handled automatically. To be more clarified: An A-B binary solution phase (with the element A locates on one sublattice site and B on three sublattice sites) treated by the Normal 4-Sublattice Model has to have 4 G parameters for 4 end-members, i.e. G(phase,A:B:B:B), G(phase,B:A:B:B), G(phase,B:B:A:B) and G(phase,B:B:B:A), because of that in the general case these G parameters can be different from each other. But for the FCC and HCP orderings, these are identical and thus all G parameters of such end-members need be given only once, and the possible permutations are then automatically handled by the GIBBS module. This significantly simplifies the usage of this model (*Four Substitutional-Sublattice Ordering Model*) in multicomponent alloys.

There are restrictions on the excess parameters allowed with the phase-type option `F`. You can only have excess parameters of these types:

```
L(phase,A,B:*:*:*;0…9)
L(phase,A,B:C,D:*:*;0…9)
```

The asterisk * means that the interaction parameter is independent on the constituents on its corresponding sublattice. No ternary interaction parameters (i.e. with three elements on one sublattice site) are allowed. The reason for this restriction is that it would be too complicated to handle all possible permutations. In the current *Four Substitutional Sublattice Ordering Model*, the binary interaction between A and B atoms is thus independent of the constituents on the other sublattices, where there are many other parameters to model the composition-dependence of the Gibbs energy (both in the ordered and disordered parts of the phase). The model for these ordered phases are always partitioned in a disordered part (with a single substitutional sublattice) and an ordered part (with four substitutional sublattices for ordering).

For ordered BCC phases, the phase-type option B means the same thing but the situation is more complicated, as the 4-sublattice ordering phase represents an irregular tetrahedron with two pairs of sites that are next nearest neighbours. Thus, for an A-B binary solution phase (with the element A locates on two sublattice site and B on other two sublattice sites) treated by the Normal 4-Sublattice Model, the end-member described by the G (phase,A:A:B:B) term has four nearest neighbour bonds between A and B atoms, whereas the end-member described by the G(phase,A:B:A:B) term has two nearest neighbour bonds between A and B atoms and two next nearest neighbour bonds

For detailed reference visit the Crystal Lattice Structure web page https://www.nrl.navy.mil/mstd/6390.

The first end-member (described by the G(phase,A:A:B:B) term) represents B2- ordering and the second (described by the G(phase,A:B:A:B) term) stands for B32-ordering. There are two permutations of the G(phase,A:A:B:B) term and four permutations of the G(phase,A:B:A:B) term, automatically conducted in the Four Substitutional-Sublattice Ordering Model. And there are also two kinds of reciprocal interaction parameters, i.e.

```
L(phase,A,B:C,D:*:*;0…9) L(phase,A,B:*:C,D:*;0…9)
```

An advanced feature with the phase-type options F and B is that a composition set that represents the solution phase has a suffix (indicating that it is really as an ordered or disordered phase) that is automatically added to its phase name in some listings of equilibrium calculations (when performing either single-point or stepping or mapping calculations, and when plotting the calculated property diagrams or phase diagrams). Such suffix indications can be:

- `_L12` or `_L10` for ordered FCC
- `_A1` for disordered FCC
- `_B2`, `_B32`, `_D03` or `_L21` for ordered BCC
- `_A2` for disordered BCC
- `_D019` and `_B19` for ordered HCP
- `_A3` for disordered HCP

Solution Phase	Suffix for Disordered Phase	Suffix for Ordered Phase
FCC PHASE	PHASE_A1	PHASE_L12
		PHASE_L10
BCC PHASE	PHASE_A2	PHASE_B2
		PHASE_B32
		PHASE_D03
		PHASE_L21

Solution Phase	Suffix for Disordered Phase	Suffix for Ordered Phase
HCP PHASE	PHASE_A3	PHASE_D019
		PHASE_B19

ADD_COMMENT

This command is for the Gibbs Energy System (GES) module.

Use the ADD_COMMENT command to add a comment or make notes about parameters.

AMEND_ELEMENT_DATA

This command is for the Gibbs Energy System (GES) module.

The data for an element (in the SER, the Stable Element Reference, state) can be changed by this command. It should only be used for the elements that do not have any data in the database because the element data available in the database is set by the database-developer for the purpose of internal consistency. Except for the mass, the other values have no influence on the calculations.

Syntax	AMEND_ELEMENT_DATA
Prompts	`Element name: <Element name>` Specify the name of the element for which you want to change the data.
	`New stable element reference /ABCD/: <Name of ser>` Press <Enter> to accept the default `SER` or specify a new SER for the element. Important: The default name should not be changed if this data is retrieved from a database. This name is used when parameters for a phase are listed and the database assumes that the stable element reference is the same as in the database. Only if the element's data have not been fetched from a database, e.g. entered manually, can you enter a new SER.
	`New atomic mass /xx.xxxx/: <yyyyyy>` Press <Enter> to accept the default atomic mass or specify a new value for the element. The atomic mass of the element is given in g/mol.
	`New h(298.15)-h(0) /xxx.xxx/: <yyyyy>` Press <Enter> to accept the default H(298.15)-H(0) or specify a new value for the element. H (298.15)-H(0) is the enthalpy difference between 298.15 K and 0 K for the element in its SER state.
	`New s(298.15) /xx.xxxx/: <yyyyy>` Press <Enter> to accept the default S(298.15) or specify a new value for the element. S(298.15) is the absolute value of the entropy at 298.15 K for the element in its SER state.
	`Default element reference state symbol index /#/: <index>` The index only changes the symbol, not any value. Normally the index is set correctly by the database. Only when manually entering data, you must set the index to get the correct symbol. Specify an index for the default listing parameters (symbol), or press <Enter> to accept the pre-set index. 0 is for `G`, 1 is for `H298` and 2 is for `H0`. The index is to define the symbol printed in parameter listings. The symbol can be: • `G` the data are referred to Gibbs energy at a variable temperature (also called *lattice stability*).

Syntax	AMEND_ELEMENT_DATA
	- `H298` the data are referred to the enthalpy of the element at 298.15 K and 1 bar. - `H0` is the same as `H298` but at the temperature 0 K.

AMEND_PARAMETER

This command is for the Gibbs Energy System (GES) module.

There is also a PARROT module command with the same name.

Use this command to interactively change/amend the temperature-pressure function of a parameter. This is useful to correct typing errors because the old function is made available on the terminal for interactive editing.

About the ENTER_PARAMETER Command

Syntax	AMEND_PARAMETER

Prompts	`Parameter: <Parameter name>`
	Specify a correct parameter name. If a parameter name is not acceptable or you only press <Enter>, the error message displays:
	`Error, please re-enter each part separately`
	The program prompts for separate input for each part for a parameter name.

	`Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK>` Specify one of these legal identifiers as described for ENTER_PARAMETER.
	`Phase name (/ABCD/): <Phase name>` Specify the phase name.
	`Constituent (in sublattice # /ABC/): <Species name>` Specify the constituent name.
	`Interacting constituent (in sublattice # /xyz/): <Species name>` Specify the interacting constituent name: If there is no interacting constituent, press <Enter>.
	`Interacting constituent (in sublattice # /xyz/): <Species name>` If there are more than one interacting constituents, specify them; otherwise press <Enter>.
	`Degree /#/: <Degree>` Specify a numerical number as the degree of the phase parameter.
	After the parameter name is specified correctly, the program lists its current definition (either present in the database or defined by the ENTER_PARAMETER command), such as:

```
L(PHASE2,AL,MG;1)=
 298.15<T<2000.00: +5000
2000.00<T<4500.00: +4500
4500.00<T<6000.00: +4000
```

Then you are prompted to change the parameter definition, as shown below:

Syntax	AMEND_PARAMETER

```
Do you want to change the number of ranges /No/:
```

Enter Y if you want to change the number of ranges for the chosen function, or change some of the temperature limits in the definition. Then retype both the low/high temperature limits and functions.

If you do not want to change the number of ranges but want to change the function(s) in one or more ranges, press <Enter> to accept the default N, then the whole definition of the chosen parameter in all ranges (if any) is listed on screen, such as:

```
DIFFERENT FUNCTIONS IN THESE RANGES

298.15<T<2000.00

2000.00<T<4500.00

4500.00<T<6000.00
```

The prompt is given:

```
Do you want to change range limits /No/:
```

If there is more than one range, this question is prompted press <Enter>.

```
Range number (0 to exit) /0/: <Range number>
```

If the function of a parameter is different in two or more temperature ranges, you must specify the range of the function of which you want to amend. Or press <Enter> or type `0` to exit this command without making any changes.

```
Function:
```

The previous function is available for editing. The editing is performed within the general subroutine FOOLED, as described in AMEND_SYMBOL. This routine prompts as follows:

```
1:+:>
```

The prompt consists of the current position in the string and the character at that position between colons, (::).

Commands

These commands can be given:

- Help: `?`
- Move CP to last or first character: `<+/-> A`
- Delete characters from CP: `<+-#characters> D`
- Exit: `E`
- Find: `<#occurrences> F<string>@`
- Insert: `I<string>@`
- Move: `<+-#positions> M`
- Restore string: `R`
- Substitute: `S<OLD>@<NEW>@`
- Type string: `T`

Where CP denotes the current position in a string, # means number of, @ is a terminator of an

Syntax	AMEND_PARAMETER
	input or search string. When the string is typed the character at the current position is replaced by an underscore _. To finish the editing of the current function, type `E` at the prompt.

AMEND_PHASE_DESCRIPTION

This command is for the Gibbs Energy System (GES) module.

Also see Solution Models in the GIBBS (GES) Module for detailed information about this command and its options.

Specify/amend phase descriptions if a phase has a miscibility gap, uses a special excess energy model, or has a specific additional contribution to its Gibbs energy, for example.

Syntax	AMEND_PHASE_DESCRIPTION

Prompts	`Phase name: <Phase name>`
	Specify the name of the phase.
	`Amend what /Composition_Set/: <Subject>`
	Several subjects for the phase can be amended but most often this command is used to enter two or more composition sets for a phase. If a phase has a miscibility gap it is necessary to have two composition sets, one for each possible composition that can be stable simultaneously.
	Enter a question mark at the prompt to get a list of all possibly amended subjects for a phase.

	There are no additional prompts for DEBYE_HUCKEL, HKF_ELECTROSTATIC, GLASS_TRANSITION, QUASICHEM_FACT00, QUASICHEM_ISRID, REMOVE_ADDITION, and DEFAULT_STABLE.
`RENAME_PHASE`	`New phase name /ABCD/: <Phase name>` Give a new phase name for the chosen phase, or press <Enter> to keep the default shown.
`Site_ratios`	`Sites in first sublattice /XX/ : <YY> Sites in second sublattice /XX/ : <YY>` Specify the site numbers for each of the prompted sublattices for the current phase. Press <Enter> to accept the previous definitions.

`New_constituent`	`Sublattice /#/: <Sublattice number>`
	Specify the sublattice where the new constituents are located.
	`Species: <Species name>`
	Give a valid species name.

`Composition_sets`	`New highest set number /#/: <Set number n>` The default value (#) is usually one higher than the current value. All phases have initially one composition set. If a lower value (i.e. lower than the default one) is given, that specific composition sets are deleted.

Syntax	AMEND_PHASE_DESCRIPTION
	You cannot take away the first composition set. `Major constituent(s) for sublattice #: /AB/: <Major constituent(s)>` Specify the new major constituent(s) for the sublattice #, or press <Enter> to accept the default which was automatically set according to the specified composition set of the phase. This prompt is repeated for all available sublattices in the chosen phase. The major constituents in each sublattice can be given. This may simplify giving start values when calculating the equilibrium as phases with miscibility gaps should have different major constituents for each composition set.

`Major_constituent`	`Composition set /1/: <Composition set number>`
	Give the composition set (digit number) for the chosen phase, or press <Enter> if you want to set major constituents for the specified composition set.
	`Major constituent(s) for sublattice #: /AB/: <Major constituent(s)>`
	Specify the new major constituent(s) for the sublattice #, or press <Enter> to accept the default which is automatically set according to the specified composition set of the phase.
	This prompt is repeated for all available sublattices in the chosen phase for the specified composition set.
	The major constituents in each sublattice can be specified. This is useful in order to make calculations converge faster and more easily (because it may simplify giving start values when calculating the equilibrium as those phases with miscibility gaps should have different major constituents for each composition set). The databases often set major constituents for several phases automatically when data are retrieved.

`Fraction_limits`	`Element : <el1>`
	`Low fraction limit /0/ :  <Appropriate low limit>`
	`High fraction limit /1/ : <Appropriate high limit >`
	`Element : <el2>`
	`Low fraction limit /0/ :  <Appropriate low limit>`
	`High fraction limit /1/ : <Appropriate high limit>`
	`Element : <eln>`
	`Low fraction limit /0/ :  <Appropriate low limit>`
	`High fraction limit /1/ : <Appropriate high limit >`

`Magnetic_ordering`	`The antiferromagnetic factor /XX/: <YY>`
	Specify the anti-ferromagnetic factor for the chosen phase. This should be –1 for BCC phase and –3 for all other phases (FCC, HCP, etc.).
	`Short range order fraction of the enthalpy /XX/: <YY>`
	The magnetic ordering is a second-order transformation and part of the enthalpy due to this transformation is due to short-range order. This value is the fraction of the total enthalpy that is due to short-range ordering above the magnetic transition temperature.
	The default value (xx) is 0.40 for BCC phase, and 0.28 for all other phases (FCC, HCP, etc.).

`Never_disorder`	`Never disorder: <Phase name>`

Syntax	AMEND_PHASE_DESCRIPTION
	Give the phase name to never disorder. The contribution from the disordered phase are added to the ordered phase. Use this to avoid entering several parameters to the ordered phase in the database. Instead it can be expressed as one parameter in the disordered phase.
`Disordered_part`	`Disordered phase name: <Phase name>` Give the disordered phase name for which there is no ordering sublattice.

`Excess_model`	`Model name /ABCDEFG/: <Model name>`
	The default model is the pre-set model for the solution phase, normally the REDLICH-KISTER_MUGGIANU model, or choose another model for the phase to be amended:
	• REDLICH-KISTER_MUGGIANU
	• REDLICH-KISTER_KOHLER
	• FLORY-HUGGINS POLYMER MODEL
	• MIXED-EXCESS-MODELS (R-K default)
	• HKF
	• PITZER
	• CENTRAL_ATOM_MODEL
	The MIXED-EXCESS-MODELS option has sub-options:
	`First (the independent) constituent: <Constituent name>`
	`Second (the dependent) constituent: <Constituent name>`
	Specify the binary pair of constituents in the current substitutional solution phase (the first one as the so-called independent constituent, and the second one as the dependent constituent), for which you wish to change the binary excess model from the default REDLICH-KISTER model to another model (LEGENDRE or POLYNOM).
	You are prompted with the first sub-option (i.e. `First (the independent) constituent` after you have specified the desired binary Excess model type. To make further changes of binary excess model for other specific binary pairs in the current substitutional solution phase, press <Enter> (implying that there are no more changes of binary excess model for all other possibly-remaining binary pairs that shall still use the default REDLICH-KISTER model).
	`Excess model type: /Legendre/: <Desired binary excess model type>`
	For the currently-specified binary pair, choose one the legal binary excess models: LEGENDRE, POLYNOM or REDLICH-KISTER. If the default binary excess model REDLICH-KISTER is used for a certain binary pair, you can either specify the model name (or in short as R-K) or press <Enter>. After this sub-option, it returns to the first sub-option *First (the independent) constituent:* either for further change(s) of binary excess model of any other binary pair(s) or for termination (by pressing <Enter>) in the MIXED-EXCESS-MODELS option.

`Ternary_extrapolat`	`Extrapolation method: /Toop-Kohler/: <Ternary model>` Choose a ternary extrapolation model for the current solution phase:

Syntax	AMEND_PHASE_DESCRIPTION

	• TOOP-KOHLER for Toop-Kohler Extrapolation Model
	• KOHLER-ALL for Kohler Extrapolation Model
	• MUGGIANU_RESTOR for Muggianu-Restor Extrapolation Model
	The TOOP-KOHLER option further prompts:
	`Constituent in sublattice #: <Basis constituent name>`
	`First interaction constituent: <Interacting constituent name>`
	`Toop constituent: <Toop constituent name>`
	Specify the so-called Kohler constituents (entered as the basis constituent and first interacting constituent) and Toop constituent on a given sublattice in the current solution phase.

`Quasichem_ ionic`	To use the Quasichemical Model for the chosen liquid phase, you must first enter it as an ionic liquid phase, and then use this amending option. It creates a completely new phase, the original IONIC_LIQUID phase remains in the system and is not changed. `Number of bonds/atom /2/: <Number of bonds per atom>` Specify the Z value (number of bonds per atom).
`Status_bits`	Correct the phase status bits. It is important to fully understand this command before using it: `New status word (in hexadecimal) /04204000/: <New status bits>` LIST_STATUS Normally, these should never be changed in this way, because such phase status bits are automatically set on when all the phase descriptions (predefined in databases and amended in the GIBBS module) are defined properly. The only exceptions are for the Kapoor-Frohberg-Gaye cell model for liquid SLAG solution phase, which can be set only as 04208000; and for the complete Revised HKF AQUEOUS solution model, which can be set as `02084000`.

AMEND_SYMBOL

This command is for the Gibbs Energy System (GES) module.

The same command is also available for the PARROT module.

Interactively calculate the current values of a function or table (predefined by the switched database or previously entered with ENTER_SYMBOL) at the current temperature and pressure condition, and also possible to modify the definitions of variables or functions.

> The current values of the temperature and pressure used to calculate the functions or tables are the ones listed with LIST_STATUS. There is no way to change the current temperature and pressure values interactively.

To modify the definitions of entered symbols (variable, functions or parameters), the performance of this command is slightly different one from another, as described below:

- For variables, the values can be changed.
- For functions the low and high temperature limits in various ranges (if any), as well the expressions, can be changed.
- For parameters the low and high temperature limits in various ranges (if any), as well the expressions, can be changed.

Syntax	AMEND_SYMBOL

Prompts	`Name: <Symbol name>`
	Specify the name of an entered symbol.
	For tables and functions (or parameters which are treated as functions after these are entered by the ENTER_SYMBOL command with the `Parameter` keyword, but not by the ENTER_PARAMETER command), after the symbol name is specified here, the program automatically calculates the values under the current temperature and pressure conditions, and lists the current values, such as:
	`FUNCTION VALUE  2.52500000E+01`
	`TABLE VALUE  1.56000000E+02`
	For variables and functions (or parameters), there are additional prompts and depend on the symbol type.

	For a variable, its current value is displayed, and you can change it to a new value:
	`Value /Current value/: <New value>`
	For a function (or a parameter entered as a symbol):
	`Do you want to change the number of ranges /No/:`

Syntax	AMEND_SYMBOL

Enter Y to change the number of ranges for the function, or change some of the temperature limits in the definition, then retype both the low/high temperature limits and functions (see all the remaining details in the ENTER_SYMBOL command.

If you do not want to change it, press <Enter>. The definition of the chosen function in all ranges (if any) is listed, for example:

```
DIFFERENT FUNCTIONS IN THESE RANGES

298.15<T<2000.00

2000.00<T<4500.00

4500.00<T<6000.00
```

and this message displays:

```
Do you want to change range limits /No/:
```

If a function is different in two or more temperature ranges, you must specify the range of the function of which you want to amend. Or press <Enter> or type `0` to exit this command without making any change.

```
Range number (0 to exit) /0/: <Range number>

Function:
```

The previous function is available for editing. The editing is performed within the general subroutine FOOLED. This routine prompts as follows:

```
1:+:>
```

The prompt consists of the current position in the string and the character at that position between colons (::).

Commands

These commands can be given:

- Help: `?`
- Move CP to last or first character: `<+/-> A`
- Delete characters from CP: `<+-#characters> D`
- Exit: `E`
- Find: `<#occurrences> F<string>@`
- Insert: `I<string>@`
- Move: `<+-#positions> M`
- Restore string: `R`
- Substitute: `S<OLD>@<NEW>@`
- Type string: `T`

Where CP denotes the current position in a string, # means number of, @ is a terminator of an input or search string.

Syntax	AMEND_SYMBOL
	When the string is typed the character at the current position is replaced by an underscore _. To finish the editing of the current function, type `E` at the prompt.

CHANGE_STATUS

This command is for the Gibbs Energy System (GES) module.

The status of an element or species or phase can be either ENTERED or SUSPENDED. The suspended status can be either implicit or explicit. The implicitly suspended status can be set e.g. for a species if any of the elements in its chemical formula is explicitly suspended. A species that is implicitly suspended becomes entered automatically if all its elements are set entered. After this command, a message shows which elements/species/phases are suspended or restored (entered). Consequently, the status bits for the specified elements or species or phases are changed, as listed with LIST_STATUS.

Syntax	CHANGE_STATUS
Prompts	`For Element, Species or Phase /Species/: <Keyword>` Specify the keyword (element, species or phase).
	`Suspend /Y/:` By default the status is changed from ENTERED to SUSPENDED. If an element is suspended all species with this element become implicitly SUSPENDED too. A phase may become implicitly suspended if all its constituents or all constituents in a sublattice are suspended.
	`List of elements/species/phases: <Name of elements or species or phases>` Specify the names or indices of those elements or species or phases that shall become suspended or active. For names, these should be separated by a space and terminated with a semicolon (;) or an empty line. For indices it is possible to give a range by separating two numbers by a hyphen (-). The list should be terminated by a semicolon (;). Example: `5 1 7-12 FE;`

ENTER_ELEMENT

Specify a system interactively. The program searches the currently switched or preset database for data for the given elements. The data for the elements in the database are the:

- mass in g/mol
- name of the Selected Element Reference State (SER) which normally is the stable phase for the element at 298.15 K
- enthalpy difference for the element in the SER state at 298.15 K and zero K
- absolute entropy for the element in the SER state at 298.15 K.

The two predefined elements, i.e. electrons and vacancies, have the chemical symbols `/-` and `VA`, respectively. Initially, these are suspended but can be entered either by this command or CHANGE_STATUS.

If an aqueous solution phase is involved, in the GIBBS module you enter a special aqueous electron called, ZE. This is specially designed for appropriately calculating the standard electric potential in the aqueous solution system.

Syntax	ENTER_ELEMENT
Prompt	`Element name: <Element name>` Specify several elements on one line. The name of an element is its chemical symbol. The chemical symbols must be separated by spaces. Fictitious element names are legal but naturally no data are found in the database for them.
	An element name (maximum 2 characters) can either have its first letter in upper and the second (if any) in lower case (i.e. Lower Case Mode) or both letters can be in upper or lower case (i.e. Upper Case Mode). The Upper or Lower Case Mode is selected by the command REINITIATE, which removes all data, and should be executed before any other command.

ENTER_FUNCTION

This command is available with the GES and TAB modules.

Used to define a new thermodynamic function to be included in the sixth column of tabular output. The last entered function is listed in the 6th column of all tables, and can be plotted (if choosing the Plot Column value 6) in all graphs, for all subsequently tabulated substances or reactions.

Syntax	ENTER_FUNCTION
Prompt	`Name: <Name>` `Function: <Definition>`
	A limited number of state variables, G, H, S, T, P, V and H298 can be used in the function definition. For example, -(G-H)/T can be defined as a function which is identical to S for a substance or ΔS for a reaction, G+T*S-P*V can be defined as a function which is U (internal energy) for a substance or ΔU (internal energy change) for a reaction.
Options	`Name`of the function (maximum 8 characters) and `Definition` of the function. A long function can be typed over several lines. A function should be terminated by a semicolon (;) or an empty line.

Example

For the pure substance Fe (using the SSUB database), by entering a function as `G+T*S-P*V`, the following table is obtained by typing <Enter> in the prompt `Output file /Screen/:`, and the figure by typing `6` in the prompt `Plot column /2/:`

```
TAB: ENTER-FUNCTION

Name: InEnergy

Function: G+T*S-P*V;

TAB: TABULATE_SUBSTANCE

Substance (phase): Fe

Pressure /100000/: <Enter>

Low temperature limit /298.15/: <Enter>

High temperature limit /2000/: <Enter>

Step in temperature /100/: <Enter>

Output file /try1/: try2

Graphical output? /Y/: <Enter>

Plot column? /2/: 6
```

This gives the following output:

```
O U T P U T   F R O M   T H E R M O - C A L C
 Column 6: InEnergy G+T*S-P*V
 Phase : FE_S                       Pressure :      100000.00
 Specie: FE
***************************************************************
    T      Cp           H             S             G             InEnergy
   (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 ***************************************************************
  298.15   2.48446E+01   2.17972E-06   2.72800E+01  -8.13353E+03   2.17972E-06
  300.00   2.48905E+01   4.60049E+01   2.74338E+01  -8.18414E+03   4.60049E+01
  400.00   2.71299E+01   2.64957E+03   3.49085E+01  -1.13138E+04   2.64957E+03
  500.00   2.93561E+01   5.47211E+03   4.11976E+01  -1.51267E+04   5.47211E+03
  600.00   3.19293E+01   8.53245E+03   4.67701E+01  -1.95296E+04   8.53245E+03
  700.00   3.50985E+01   1.18777E+04   5.19207E+01  -2.44667E+04   1.18777E+04
  800.00   3.92042E+01   1.55830E+04   5.68623E+01  -2.99068E+04   1.55830E+04
  900.00   4.49645E+01   1.97726E+04   6.17903E+01  -3.58387E+04   1.97726E+04
 1000.00   5.42147E+01   2.46891E+04   6.69619E+01  -4.22728E+04   2.46891E+04
 1100.00   4.55851E+01   2.99025E+04   7.19412E+01  -4.92328E+04   2.99025E+04 $
Stable phase is FE_S2
 1200.00   3.40840E+01   3.51037E+04   7.64466E+01  -5.66322E+04   3.51037E+04
 1300.00   3.49398E+01   3.85549E+04   7.92086E+01  -6.44162E+04   3.85549E+04
1400.00   3.57994E+01   4.20918E+04   8.18293E+01  -7.24692E+04   4.20918E+04
 1500.00   3.66636E+01   4.57149E+04   8.43287E+01  -8.07780E+04   4.57149E+04
 1600.00   3.75330E+01   4.94247E+04   8.67226E+01  -8.93314E+04   4.94247E+04 $
Stable phase is FE_S3
 1700.00   4.05217E+01   5.41173E+04   8.95609E+01  -9.81363E+04   5.41173E+04
 1800.00   4.12595E+01   5.82055E+04   9.18975E+01  -1.07210E+05   5.82055E+04 $
Stable phase is FE_L
 1900.00   4.60000E+01   7.74165E+04   1.02377E+02  -1.17099E+05   7.74165E+04
2000.00   4.60000E+01   8.20165E+04   1.04736E+02  -1.27456E+05   8.20165E+04
```

ENTER_PARAMETER

This command is for the Gibbs Energy System (GES) module.

There is also a PARROT module command with the same name.

About the ENTER_PARAMETER Command

Use this command to enter TP-function(s) for a specific parameter for a phase interactively with this command. If there is already a parameter expression defined (for this parameter), that is deleted and replaced with newly entered one.

The entered TP-Function(s) for the parameter can be changed later with the command AMEND_PARAMETER.

Syntax	ENTER_PARAMETER

Prompts	`Parameter: <Parameter name>`
	As explained in About the ENTER_PARAMETER Command, specify a correct and complete `Parameter Name`, which should contain all the necessary parts of the general form:
	`<Identifier>(<Phase>,<Constituent array>;<Digit>)`
	If a parameter name is not acceptable or <Enter>, is pressed, a message displays:
	`*** Error, please re-enter each part separately`
	and you are prompted for input for each required part for a parameter name.

Options	**Description or Information**
`Identifier`	`Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK>` If this command is used one or more times, the previous value on this prompt is set as default. Press <Enter> for the same type identifier or specify a new type.
`Phase name`	`Phase name (/ABCD/): <Phase name>` Each parameter is valid for a specific phase only. The name of that phase must be supplied (maximum 24 characters). The name can be abbreviated.
`Constituent`	`Constituent (in sublattice # /ABC/): <Species name>` A parameter is identified by the constituents on a specified sublattice site of the given phase, the stoichiometric coefficients of which are multiplied with the parameter. The name of the constituent can be abbreviated. It is the species name, not the stoichiometric formula required here. If this command is used one or more times, the previous value on this prompt is set as default. Accept it by pressing <Enter> if the constituent is the same, or specify a new species name.

Syntax	ENTER_PARAMETER
`Interacting constituent`	For phases with several sublattices, the program asks for one constituent in each sublattice. `Interacting constituent (in sublattice # /XYZ/): <Species name>` If this command is used one or more times, the previous value on this prompt is set as default. Press <Enter> to accept it if the constituent is the same, or specify a new species name. To cancel the default value of the interacting constituent type `NONE` or the name of another constituent. This question is repeated until all the interested interacting constituent(s) on a specific sublattice in the phase are specified, and finally an <Enter> is enforced.
`Degree`	`Degree /#/: <Degree>` Degree is model-dependent. Specify an integer number (a value from 0 through 9) as the degree of composition-dependent interaction contribution for the phase parameter. This is valid for excess energy (`L`), Curie temperature (`TC`) and Bohr magneton number (`BMAGN`), as well as for volume-related parameters (`V0`, `VA`, `VC` or `VK`). For binary interaction parameters, the degree is usually the power in the Redlich-Kister expression. For ternary interaction parameters, it is usually the Hillert ternary index. For a standard `G` parameter for a pure component (end-member) its degree should be always 0 and this prompt should not display.

`Phase parameter`	After this prompt, the program echoes on the screen the full TP-Function of the phase parameter.
	`Low temperature limit /298.15/: <Lowest temperature limit in K>`
	Specify the lowest temperature limit (in Kelvin), or the lowest-pressure limit (in Pascal but entered as a negative number), for the current TP-Function.
	`Function: <Definition for a function>`
	A TP-Function consists of terms in T and P.
	`& <Continuation of the definition for the current function>`
	Continuation of a TP-Function definition.
	`High temperature limit /6000/: <High temperature limit in K>`
	Specify the high temperature limit (in Kelvin), or the high-pressure limit (in Pascal; only if the *lowest limit* is entered as a negative number) for the current TP-Function.
	`Any more ranges? /N/:`
	Enter Y for more function(s) or N to end this command.

ENTER_PHASE

See About the ENTER_PHASE Command for details about the phase-type and other prompts.

With this command, the phase name, phase-type, sublattice number, and constituents or constituent array(s) for the phase are entered into the GIBBS workspaces. However, for the remaining parts of thermodynamic descriptions (i.e. thermochemical and physical parameters, excess model, and possibly additional contribution term) for the phase, the GIBBS commands ENTER_PARAMETER and AMEND_PHASE_DESCRIPTION, should be used sequentially.

Normally, data for a system are retrieved from the preset database after the elements and species are specified. This is automatically done through GET_DATA. In some cases, specify a phase interactively.

Syntax	ENTER_PHASE
Options	**Description and Information**

`Phase name`	`Name of phase: <Phase name>`
	The phase name is any string starting with a letter and containing only letters, digits or the underscore character. The phase name must be unique.
	`Type code: <Phase-type code>`
	The `Phase-type code` must be specified for the phase if it is not an ordinary solution phase. Press <Enter> if the phase is ordinary.

`Phase-type`	
`G`	Gaseous mixture phase. There may only exist one gas phase in a system.
`A`	Aqueous solution phase.
`L`	Liquid solution phase but not `A` (aqueous) or `Y` (ionic liquid)
`Y`	Ionic liquid solution phase (that is specially treated by the Ionic Two Sublattice Liquid Model).
`I`	A phase with charged species but not `G` (gaseous), `A` (aqueous) or `Y` (ionic liquid).
`F`	An ordered FCC or HCP solution phase with four substitutional sublattices (additionally, such a phase can also have an interstitial sublattice).
`B`	An ordered BCC solution phase with four substitutional sublattices (additionally, such a phase

Syntax	ENTER_PHASE
	can also have an interstitial sublattice).

`Sublattice number`	`Number of sublattices /1/: <Sublattice number>`
	Phases with stoichiometric constraints usually have two or more sublattices. On each sublattice one or more species can be entered as constituents. The number of sublattices must not exceed 10. Substitutional phases with no sublattices are treated as phases with one sublattice.
	`Number of sites on sublattice  # /1/: <Site number>`
	For phases with sublattices, the ratio of the sites on each sublattice (donated with #) must be given. The program asks for values for all sublattices (by repeating this question for each sublattice), but these may have a common factor extracted. It is recommended to use integer numbers as sites if possible. For substitutional phases with no sublattices, this question does not show up.

`Constituents`	`Name of constituent: <Constituent name(s)>`
	For each sublattice specify at least one species as constituent. Several constituents can be given consequently (on the repeated prompt) or on the same line separated by a space. This question is repeated till pressing <Enter> or giving a semi-colon (;), meaning that the list of constituents is terminated by (;) or an empty line.
	`Will you add constituents later /N/:`
	For Y add other constituents to the phase by specifying new components in e.g. an ENTER_PARAMETER command.
	If illegal constituents are used, you get a message e.g. when parameters are entered.
	`Do you want a list of possible parameters /N/:`
	Enter Y for a list of all possible parameters up to the fifth interaction order for the entered phase.

ENTER_SPECIES

Specify a species from the already entered elements. The stoichiometry of the species is the chemical formula of the species. For each species, its name and chemical formula must be given.

All elements are automatically entered simultaneously as species. The constituents of a phase must be species, but there is no thermochemical data associated with the species except as constituents of a phase.

Syntax	ENTER_SPECIES

Prompt	`Species name: <Species name>`
	Enter a unique species name. This is usually its chemical formula but it can be any string which starts with a letter and contains only letters or digits. Parenthesis `()` and an underscore _ are permitted. The combination /- or /+ used to denote charge.
	Species Names Examples
	`NACL2, FE2O3, FEO3/2, FE1O1.5, CA.5MG.5SI1O3,`
	`AL1H1O1_Al(OH) , AL1H1O1_HAlO, C2H4O3_124TRIOXOLANE, NA+, SIO4-4, H1/+1, H1O1/-1, AGC2N2-1.`
	The species name can be used to separate isomers with the same stoichiometry, e.g. `C2H2Cl2, (CHCl)2_cis, (CHCl)2_trans, CH2_CCl2.`

	`Stoichiometry /Species name/: <Chemical formula>` The elements in the chemical formula are normally separated by stoichiometric numbers. Neither parenthesis () nor an underscore _ is allowed in the chemical formula, while the special combination /- or /+ can be used. In upper case mode (see REINITIATE), the stoichiometric number unity can be excluded only if the element symbol consists of two letters. In lower case mode, the element must be typed with the first letter in UPPER case and the second in lower, and it is thus possible to distinguish CO (carbon monoxide) from Co (cobalt) without any stoichiometry number. All elements in a species must be entered prior to entering the species.

ENTER_SYMBOL

This command is for the Gibbs Energy System (GES) module.

There are also a POLY and POST module commands with the same name. However, symbols entered in the GIBBS module are not the same symbols as defined in the POLY and POST modules.

In the GIBBS module, a symbol can be used to represent a numeric quantity (e.g. a *variable*), a *function*, or a *table*. The entered symbol (with a symbol name of maximum eight characters) can be used later when parameters are entered, and this is a flexible way to manipulate thermodynamic functions. Symbols are especially useful if the same function or table is used in several thermochemical parameters. A *parameter* symbol is used to assign the values of phase parameters (which are defined with the command ENTER_PARAMETER) to specific characterized symbols. If you want to define a constant quantity, enter it as a simple function with a constant value in all (temperature) ranges.

The symbols entered in the GIBBS module can also be listed and used in the PARROT module (for data optimization) where you can use the GIBBS-entered symbols (variables, functions or parameters) to define parameters that shall be optimized.

See example 44 for an example of using variables and functions.

Syntax	ENTER_SYMBOL

Prompt	`Variable, function, table or parameter? /Function/: <Keyword>`
	The keyword can be a variable, function, table or parameter.
	• `Variables` are similar to functions because these can also be expressions of state variables. It is possible to enter a variable with a new expression anytime.
	• `Functions` are expressions of state variables or other functions.
	• `Tables` are used for listing results. A table consists of a list of any number of state variables, functions or variables.
	• `Parameter` symbols are used to assign the values of phase parameters (which are defined by the command ENTER_PARAMETER) to specific characterized symbols. If the phase parameter is not defined yet, the parameter symbol is assigned zero or a symbol which is valued as zero. In this way it is easy to refer to entered phase parameters in further defining other phase parameters.
	`Name: <Name of the symbol>`
	Each symbol has a unique name that must start with a letter and can have maximum 8 characters.

Syntax	ENTER_SYMBOL
	The following prompts are based on the type of symbol.
`Variable` symbol	`Value: <Numeric value of a variable>` Only a constant numeric value, not an expression, is accepted.

`Function` symbol	Enter the lower-temperature limit, the expression, an upper-temperature limit and if there is another expression above this upper limit:
	`Low temperature limit /298.15/: <Lowest temperature limit in K>`
	Specify the lowest-temperature limit, below which its (first) expression is not applicable. The default lowest limit of all kinds of data is 298.15 K.
	If a negative number is given as the lowest-temperature limit, it is assumed that there are breakpoints in pressure for this function; in such a case, it is interpreted as the lowest-pressure limit (in Pascal), and the other limits in the current function are also taken as pressure limit values (in Pascal).
	The temperature/pressure limits for the functions are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit; and in such a case, an extrapolation is conducted using the TP-FUNCTIONS valid in the nearest temperature/pressure range.
	`Function: <Definition for a TP-function>`
	A TP-Function consists of terms in T and P. The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers). Unary-functions LN or LOG (both for natural logarithm) and EXP (for exponential) can also be used. An expression can be continued on more than one line. A PT-function must be terminated by a semicolon (;) or an empty line. No more than 78 characters can be written on a line. If this is not sufficient space on one line, press <Enter> and continue on the next line. The program prompts with an ampersand `&` when a continuation is expected.
	A function can have several temperature ranges, and a different expression (i.e. a TP-Function) for each region; if required, a single function can have up to ten different temperature ranges (and thus have up to ten different TP-Functions).
	This question is repeated if the current function has more than one expression (TPFunction) in various temperature ranges [or pressure ranges; only if the *lowest limit* is entered as a negative number)].
	`& <Continuation of the definition for the current TP-Function>`
	This is for a continuation of the definition for the current TP-Function. The ampersand & means that you can continue to write the function on the new line if one line is not enough for the current TP-Function. If you are finished the current TP-Function, press <Enter> again.
	`High temperature limit /6000/: <High temperature limit in K>`
	For a TP-Function, specify the high-temperature limit, above which its current expression is not applicable. The default high-temperature limit for all kinds of data is always 6000 K.
	This question is repeated if the function has more than one expression (TPFunction) in various temperature ranges.

Syntax	ENTER_SYMBOL
	All the temperature limits for the presently-be-entered TP-Function MUST be in an increasing order; otherwise the whole function is given a single value of zero. If a negative number is given as the lowest-temperature limit, it is interpreted as the low-pressure limit (in Pascal), and the high-temperature limit is also taken as the high-pressure limit (in Pascal) for the current TP-Function. The high-temperature/pressure limit for the current applicable expression (TPFunction) is the low temperature/pressure limit for the next range if several ranges are needed to describe the temperature/pressure-dependence of this function. The temperature/pressure limits for the functions are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit; and in such a case, an extrapolation is conducted using the TP-Function valid in the nearest temperature/pressure range. `Any more ranges /N/: <Y or N>` Answer `N` to finish the definition of the current function. If `Y` the program asks for a new function valid above the last high temperature limit and below a new high temperature limit. The maximum number of temperature ranges is 10. Important note: Make sure that the function and its first derivatives are continuous across break points.

`Table` symbol	Specify the low and high temperature limits, temperature step and tabled value at each specified temperature:
	`Low temperature limit /298.15/: <Low temperature limit in K>`
	The lowest temperature where the table has a value.
	`High temperature limit /6000/: <High temperature limit in K>`
	The highest temperature where the table has a value.
	`Step in temperature /100/: <Temperature step>`
	The step in temperature between each value in the table. This step must be constant for the whole table. If a table cannot be described with a single step it must be divided into several tables for different temperature ranges. The upper and lower limits are truncated to give reasonable values where the table values must be specified.
	`Table value at  XX /YY/: <Table value>`
	The value of the table at the specified temperature (`xx`) must be given. The default value (`yy`) is the last value.

`Parameter` symbol	Input the correct name of a phase parameter (including its identifier, phase name, constituent and interacting constituent(s) in various sublattices (if exist), and degree of the parameter. Most of the settings are the same as in the ENTER_PARAMETER command or the Function symbol prompts above. `Parameter: <Parameter name>` Specify a correct and complete parameter name, which should contain all the necessary parts of the general form:

Syntax	ENTER_SYMBOL

	`<Identifier>(<Phase>,<Constituent array>;<Digit>)`
	If a parameter name is not acceptable or <Enter> is pressed, this error message displays:
	`*** Error, please re-enter each part separately`
	The program prompts for separate input for each required part for a parameter name.
	`Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK>`
	Specify one of these types of legal identifiers.
	`Phase name (/abcd/): <Phase name>`
	Specify the phase name.
	`Constituent (in sublattice  # /abc/): <Species name>`
	Specify the constituent name on the specified sublattice site of the given phase.
	`Interacting constituent (in sublattice  # /XYZ/): <Species name>`
	Specify the interacting constituent name on the specified sublattice site of the given phase; if there is no interacting constituent, press <Enter>.
	`Interacting constituent (in sublattice  # /XYZ/): <Species name>`
	If there is more than one interacting constituent on the specified sublattice site of the given phase, specify them; otherwise press <Enter>.
	`Degree /#/: <Degree>`
	Specify an integer number (a value from 0 through 9) as the degree for the phase parameter.
	`Low temperature limit /298.15/: <Lowest temperature limit in K>`
	Specify the lowest-temperature limit (in Kelvin), or the lowest-pressure limit (in Pascal but entered as a negative number), for the current TP-Function.
	`Function: <Definition for a function>`
	Specify the desired TP-Function for the current temperature range (or current pressure range; only if the *lowest limit* is entered as a negative number).
	`& <Continuation of the definition for the current TP-function>`
	Specify the desired TP-Function continuation for the current temperature range (or current pressure range; only if the lowest limit is entered as a negative number).
	`High temperature limit /6000/: <High temperature limit in K>`
	Specify the high-temperature limit (in Kelvin), or the high-pressure limit (in Pascal; only if the lowest limit is entered as a negative number) for the current TP Function.
	`Any more ranges /N/:`

LIST_CONSTITUTION

This command is for the Gibbs Energy System (GES) module.

Syntax	LIST_CONSTITUTION
	List all the constitutions (as site-fractions) for all the phases in the defined system.
	This is mainly for software managers. There are no commands in the GIBBS monitor to set the constitution.

LIST_DATA

This command is for the Gibbs Energy System (GES) module.

Use the LIST_DATA command to retrieve and then list the data included with a database in the DATA module or directly entered in the GIBBS module. All data for the current system that is defined within the current GIBBS workspace is written in a readable manner in the output file. If no output file is specified, by default the data displays on screen. The behavior of this command differs slightly based on whether you are using GES6 (the default) or GES5.

> For encrypted commercial databases you may not be able to use this command to list any retrieved data. However, it can be used to list some basic definitions (such as phase models and phase-constituents) retrieved from an encrypted database, as well as all the references related to original assessments (but not thermodynamic parameters) for the currently-defined system.

Command Prompts

After entering the command in the console, the following prompt options are available.

<table>
<tr><th>Syntax</th><th>LIST_DATA</th></tr>
<tr><td>Prompts</td><td><code>Output to screen or file /Screen/: <File name></code>

Specify the name of a file in which the data shall be written in a readable manner. The default value is the screen (by pressing <Enter>).</td></tr>
<tr><td></td><td><code>Options?: <Option(s)></code>

Choose one or several of the following options for output.

See the section about the differences between GES5 and GES6 output for these options.

<code>N</code> the output is written as a user database format. For GES6, and only for an unencrypted database, this option has a subcommand that allows filtering of phase parameters with respect to the property type e.g., to include only volume parameters and/or viscosity parameters in the output.
The subprompt is <code>Property type /All/</code>. Choose <code>All</code> or enter the property type. The valid alternatives (when available) are: V0, VA, VB, VC, VK, TC, TN, BM, MQ, MF, DQ, DF, OQ, VS, G, L, THCD, ELRS, ESPD, VISC, GD, SIGM or XI
<code>P</code> the output is written as a macro file for future input. This is useful for creating <code>*SETUP</code> files for data assessments.</td></tr>
</table>

Syntax	LIST_DATA
	- `S` the symbols are suppressed. - `R` the references for the parameters are listed (only for some databases in which references are available) - `L` the output is written suitable for a LaTeX preprocessor.

Output Differences: GES5 vs GES6

GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features.

As required you can set Thermo-Calc to use GES5 instead of the default with the SET_GES_VERSION command. The application may also automatically and temporarily switch to GES5 when a database is being used that is not compatible with GES6.

For both GES5 and GES6 and when you enter `P`, `S`, `R`, or `L`, the output data consists of a list of all elements and the data followed by a list of all phases and the data associated with each phase. The thermochemical parameters listed for each phase are always in SI units.

For GES6, and only when option `N`, `P`, or nothing is entered, the output data consists of a list of all elements and the data followed by a list of all phase definitions and the data associated with the phases, sorted by system. In these modes, and only for unencrypted databases, there is a subcommand that allows filtering of phase parameters with respect to the property type e.g., to include only volume parameters and/or viscosity parameters in the output.

Other differences between the GES5 and GES6 output are related to the output as shown below.

Output	***GES5***	***GES6***
Parameters	Includes implicitly defined zero-valued thermodynamic parameters	Only contains parameters that are actually defined in the database
Automatically	Does not include	Includes

Output	*GES5*	*GES6*
suspended phases		
References	Contains references of functions and parameters with generic names, such as "REF123"	Retains the original reference names that are used in the database

LIST_PARAMETER

This command is for the Gibbs Energy System (GES) module.

There is also a PARROT module command with the same name.

List the TP-function(s) of a specific parameter for a phase. You must supply the name of the phase parameter:

`The parameter name: <Identifier>(<Phase>,<Constituent array>;<Digit>)`

For encrypted commercial databases, you may not be able to use this command to list any retrieved parameter.

Syntax	LIST_PARAMETER

Prompts	`Parameter: <Parameter name>`
	Specify a correct and complete parameter name, which should contain all the necessary parts of the general form: <identifier>(<phase>,<constituent array>;<digit>)
	See About the ENTER_PARAMETER Command to learn how to define the parameter name.
	If a parameter name is not acceptable or <Enter> is pressed, an error message displays:
	`*** Error, please re-enter each part separately`
	The program prompts for separate input for each required part for a parameter name.

	`Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK>` Specify one of these types of legal identifiers.
	`Phase name (/ABCD/): <Phase name>` Specify the phase name.
	`Constituent (in sublattice # /ABC/): <Species name>` Specify the constituent name on the specified sublattice site of the given phase.
	`Interacting constituent (in sublattice  # /XYZ/): <Species name>` Specify the interacting constituent name on the specified sublattice site of the given phase; if there is no interacting constituent, press <Enter>.
	`Interacting constituent (in sublattice # /XYZ/): <Species name>` If there is more than one interacting constituent on the specified sublattice site of the given phase, specify them; otherwise press <Enter>.
	`Degree /#/: <Degree>`

Syntax	LIST_PARAMETER
	Specify a numerical number as the degree for the phase parameter.

LIST_PHASE_DATA

This command is for the Gibbs Energy System (GES) module.

All data for a specific phase are written in a readable manner on screen. The thermochemical parameters listed for the phase are always in SI units.

For encrypted commercial databases you may not be able to use this command to list any phase data. However, this command can be used for listing some basic definitions (such as phase model and phase-constituents) for the specified phase, as well as all the references related to original assessments (but not thermodynamic parameters) for the currently-defined system.

Syntax	LIST_PHASE_DATA
Prompt	`Phase name: <Phase name>` Specify a phase name (if abbreviated, it should be unique).

Output Differences: GES5 vs GES6

GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features.

As required you can set Thermo-Calc to use GES5 instead of the default with the SET_GES_VERSION command. The application may also automatically and temporarily switch to GES5 when a database is being used that is not compatible with GES6.

For GES6 the output data consists of the phase definition and the data associated with the phase, sorted by system. In GES6, there is a subcommand that allows filtering of phase parameters with respect to the property type e.g., to include only volume parameters and/or viscosity parameters in the output.

LIST_STATUS

This command is for the Gibbs Energy System (GES) module.

Syntax	LIST_STATUS
	List the entered elements, phases and species with the status word. The command is included for system managers. Each element, species, phase and symbol has a set of status bits. The values of these bits are listed with this command. The bits are listed as hexadecimal, i.e. four bits are written as a hexadecimal number. Two hexadecimal numbers make a byte. In hexadecimal, 0 to 9 mean normal digits. A to F means values 10 to 15. The number `E4000000` has thus bit 1, 2, 3 and 6 equal to one. The bits are numbered starting with 1 for the most significant (leftmost) bit.

Element Status Word

Set the element status word (*Bit. Meaning*) if:

1. Element cannot be deleted (only vacancy and electron)
2. Suspended (inclusive OR of bit 3 and 4)
3. Explicitly suspended
4. Implicitly suspended (cannot occur for an element)

Species Status Word

Set species status word (*Bit. Meaning*) if:

1. Species record for an element (each element has a species record)
2. Suspended (inclusive OR of bit 3 and 4)
3. Explicitly suspended
4. Implicitly suspended (e.g. if a species element is suspended)
5. Charged (inclusive OR of bit 6 and 7)
6. Negative charge

7. Positive charge
8. Vacancy
9. Component (by default the elements are the components)

Phase Status Word

Set phase status word (*Bit. Meaning*) if:

1. Ideal (no sublattices and no excess parameters)
2. Suspended (inclusive OR of bit 3 and 4)
3. Explicitly suspended
4. Implicitly suspended (e.g. if all constituents suspended)
5. Gas phase
6. Liquid phase
7. Solution phase
8. Only one constituent (in each sublattice)
9. Ions (inclusive OR of bit 10 and 12)
10. New ionic liquid model (charge balance handled internally)
11. Constituents cannot be added
12. External charge balance needed
13. Aqueous model
14. Charged species (ions)
15. Dilute entropy
16. Last calculation exceeded temperature range for any parameter
17. Kapoor-Frohberg-Gaye cell model
18. Turbo calculation used
19. Turbo calculation impossible
20. Turbo calculation illegal
21. Phase is not ideal
22. Current site fractions saved
23. This phase is the ordered part
24. This phase is the disordered part (bit 2 and 3 also set)

25. Shadow phase with diffusion data
26. Error in ionic model
27. Sometimes
28. CVM-SRO (short-range ordering) entropy expression
29. CVM initialization is made
30. Used to test quasi-chemical ordering model
31. Major constituents check even if no miscibility gap (ordering)
32. Hoch-Arpshofen model

Symbol Status Word

Set symbol status word (*Bit meaning*) if:

1. Constant
2. Variable
3. Function
4. Table
5. Value must not be amended
6. Undefined

LIST_SYMBOL

This command is for the Gibbs Energy System (GES) module.

List the symbols available in the current GIBBS workspace, which are defined (retrieved from database in the DATA module, or directly entered in the GIBBS module) and used in TP-functions for the entered model parameters for various phases in the defined system.

> For encrypted commercial databases you may not be able to use this command to list any retrieved symbol.

Syntax	LIST_SYMBOL
Prompts	`Name: <Symbol name>` Specify a symbol name (either as the full name of a defined symbol, or as the first few common characters of several symbols which have names starting with such common characters). Only those symbols that match this name are listed. Or press <Enter> for a list of all the symbols defined (retrieved from database in the DATA module, or directly entered in the GIBBS module) for the current system, which are available in the current GIBBS workspace.
	`Output to screen or file /Screen/: <File name>` Specify the name of a simple-textual file in which the entered symbols shall be written in a readable manner (such a basic textual file can later on be opened and edited by any text editor). The default value is the screen (by pressing <Enter>).

READ_GES_WORKSPACE

This command is for the Gibbs Energy System (GES) module.

Workspace Files

The data saved into a `*.GES5` with SAVE_GES_WORKSPACE can be read back into the GIBBS workspace.

Syntax	READ_GES_WORKSPACE
	Enter a **File name** and specify the working directory where to save the file in the **Look in** field. Normally the default file-type in the **Files of type** field is the correct one for the GES workspace format. The saved *.GES5 files are unique for each CPU type, and therefore a file saved on one CPU type cannot be read and used on another CPU type.

READ_WORKSPACES

This command is used in both the POLY and GES (GIBBS) modules.

Workspace Files

The POLY3 and GIBBS workspaces and the calculated results from the MAP and STEP commands can be READ from a file where they are saved with SAVE_WORKSPACES. Such a *.POLY3 file is not printable.

Syntax	READ_WORKSPACES
Options	`File name` is the name of a saved POLY3-file where the POLY3 and GIBBS workspaces shall be read from must be specified. You do not need to type the extension if it is the default *.POLY3, otherwise type the whole POLY-file name. A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters. A window opens so that the path (in the **Look in** field) and **File name** can be specified. The **Files of type** (i.e. POLY3) cannot be changed. Click **Open** to open the POLY3 and GIBBS workspaces from the saved *.POLY3 file.
	When reading back an original POLY3 workspace that has already been saved as an *.POLY3 file in the current Thermo-Calc (Console Mode) run or had been read from an existing POLY3 file under the current work area, while some additional changes in the settings may be made but do not need to be kept in further steps in the current Thermo-Calc (Console Mode) run or any diagram is plotted in the POST module, you can type `READ,,` or `READ_WORKSPACE ,,`

REINITIATE

This command is for the Gibbs Energy System (GES) module.

All data in the stored GIBBS workspace are erased, and all variables are initiated to their default values.

Syntax	REINITIATE
Prompts	`Upper case only /Y/:` Press <Enter> to keep the default where the name of elements and species is in only UPPER case. Or choose N to have the elements with two letter names with the first letter in Upper case and the second in lower case. In upper case mode all input in lower case is automatically converted to upper case.
	`Lower temperature limit /298.15/: <Lowest T in K>` This value is used as the lower temperature limit when data are entered interactively.
	`Upper temperature limit /6000/: <Highest T in K>` This value is used as the upper temperature limit when data are entered interactively.
	`Default element reference state symbol index /1/: <1 or 2 or 3>` Specify a proper index for the default listing parameters (symbol), or press <Enter> to accept the preset index 1. The *index* is for defining the symbol printed in listings of parameters. The symbol can be: • `G`: the data are referred to Gibbs energy at a variable temperature (also called *Lattice Stability*). • `H298`: the data are referred to the enthalpy of the element at 298.15 K and 1 bar. • `H0` is the same as H298 but at the temperature 0 K. The index only changes the symbol, not any value. Normally the index is set correctly by the database. Only when manually entering data must you set the index to get the correct symbol. Set the index value to 0 to get the symbol `G`, to 1 to get the symbol `H298` and to 2 to get `H0`.

SAVE_GES_WORKSPACE

This command is for the Gibbs Energy System (GES) module.

Workspace Files

The data used by the GES workspace can be saved in a file with a default extension `*.GES5`. The default file name is `RESULT.GES5` or equal to the one used in a previous READ_GES_WORKSPACE command.

Syntax	SAVE_GES_WORKSPACE
	Enter a **File name** and specify the working directory where to save the file in the **Save in** field. Normally the default file-type in the **Files of type** field is the correct one for the GIBBS workspace format. The output is not formatted and cannot be printed.

SAVE_WORKSPACES

This command is available for both the POLY and GES (GIBBS) modules.

Workspace Files

You can save the current status and workspaces, including thermodynamic data, conditions, options and results from a single, stepping or mapping calculation on a *.POLY3 file. The workspaces are saved to a file with this command. This is useful so you have access to the workspace for later use or when you need to terminate the current Console Mode session.

- In the Gibbs (GES) module workspace, all thermochemical data are stored.
- In the POLY module workspace, all the last set of conditions and equilibrium state, changed status, entered symbols, advanced options, defined stepping/mapping variables, added initial equilibria, stepped/mapped results, etc., are stored, so it also contain the GES workspace.
- When you are in a response-driven module such as POTENTIAL or SCHEIL for example, a workspace file is automatically opened. In the workspace file, system definitions, conditions for the calculation, calculation results, and plot settings are saved. The file is saved in the current working directory, and is named after the name of the module that created it. For example, the POTENTIAL module saves a workspace file called `POT.POLY3` ; the POURBAIX module saves a file called `POURBAIX.POLY3` and so forth.

After a SAVE_WORKSPACES command, you can always come back to exactly the state you had when you issued the command by giving a READ_WORKSPACE command. For example, after saving the POLY and GIBBS workspaces to a file, you can leave the program and at a later time READ the file and continue from the saved state.

Important Information About Map and Step Commands

A STEP or MAP command automatically saves the workspace with the most recently specified name. Do not use the SAVE_WORKSPACES command after a MAP or STEP command.

The results from the STEP or MAP commands are destroyed by the SAVE_WORKSPACE command. You can append several results obtained by sequential STEP or MAP calculations without destroying the previous results, whilst SAVE_WORKSPACE erases them all. Keeping this in mind is important and useful particularly for calculating various isothermal (or isoplethal) sections and plotting them on the same diagram in a single Thermo-Calc run.

To suspend some of the STEP or MAP results, use the AMEND_STORED_EQUILIBRIA command.

Syntax	SAVE_WORKSPACES
Options	A `file name` must be specified. The default extension of the POLY workspace file is *.POLY3 but you can have any other file extension. Linux and Mac are case sensitive so ensure you enter `.POLY3`. A **Save** window displays if a file name is not given after the command, so that the path (in the **Save in** field) and **File name** can be specified. The **Files of type** cannot be changed. If there is already a file with the same file name under the directory a warning message displays. Click **OK** to overwrite the current POLY or GIBBS workspace onto the existing file. Click **Cancel** to return to the module. You can use the SAVE command with an unspecified name (i.e. through `SAVE ,,,` command-sequence) to save the POLY or GIBBS workspace. When saving a POLY3 workspace under a name that already exists under the current work area, which is saved by default (after running a special module, e.g. BIN, TERN, POT, SCHEIL and POURBAIX) or in an earlier stage of the current Console Mode session or in a previous run (which is READ into the current POLY3 workspace), you can type `SAVE,,Y` or `SAVE_WORKSPACE ,,y`. However, this must also be avoided if some results from previous MAP or STEP calculations shall not be destroyed.

SCHEIL Module Commands

In this section:

CALCULATE_BELOW_SOLIDUS

This command is for the SCHEIL module.

The CALCULATE_BELOW_SOLIDUS command enables or disables the calculation of solid state properties at temperatures below the solidus temperature, using the phase compositions and fractions from the Scheil calculation. By default this is disabled.

The calculation is performed at a set number of temperatures between the solidus temperature and a lower temperature, which is by default set to room temperature. The end temperature and the number of points can be changed.

Syntax	CALCULATE_BELOW_SOLIDUS

Prompts	`Calculate properties below solidus? /N/:`
	The default is `N`. Enter `Y` to calculate solid state properties below solidus .
	If `Y` is entered, then you are prompted:
	`Final temperature (C) /25/:?`
	Enter the final temperature in degrees Celsius. Must be 25 C or higher.
	`Number of points /50/:?`
	Enter the number of points where solid state properties are calculated.

CALCULATE_EVAPORATION_PROPERTIES

This command is for the SCHEIL module.

The CALCULATE_EVAPORATION_PROPERTIES command enables or disables the calculation of evaporation properties. By default this is disabled. The evaporation properties include driving force for evaporation, evaporation enthalpy, and molar mass of gas.

> To be able to calculate these properties the gas phase needs to be selected (in the START_WIZARD).

Syntax	CALCULATE_EVAPORATION_PROPERTIES
Prompts	`Calculate evaporation properties? /N/:` The default is `N`. Enter `Y` to calculate evaporation properties.

CALCULATE_FROM_START_TEMPERATURE

This command is for the SCHEIL module.

The CALCULATE_FROM_START_TEMPERATE command enables or disables the calculation of equilibria directly from the start temperature chosen in the START_WIZARD. By default this is disabled (set to `N`). Enable this (set to `Y`) if you want to obtain properties of the liquid phase (and gas phase if selected) before the solidification starts. Ordinarily the start temperature is only used as a start point in the search of the liquidus temperature, as the Scheil calculation starts from the liquidus temperature.

With this setting enabled single equilibrium calculations are performed at specific intervals above the liquidus temperature, and after that the Scheil solidification calculation proceeds as usual. The equilibrium calculations are performed at 50 Kelvin (K) intervals in the fully liquid region and at 5 K intervals in a possible two-phase (liquid/gas) region.

Syntax	CALCULATE_FROM_START_TEMPERATURE
Prompt	`Perform equilibrium calculations between start and liquidus temperatures? /N/:` The default is `N`. Enter `Y` to perform equilibrium calculations from the start temperature until liquidus temperature is reached (i.e. solidification starts). The calculations are performed at 5 Kelvin intervals in the two-phase gas/liquid region and at 50 Kelvin intervals in liquid.

CALCULATE_FROM_GAS

This command is for the SCHEIL module.

The CALCULATE_FROM_GAS command enables or disables the calculation of equilibria starting from the gas/liquid temperature, i.e. from the temperature above which the liquid phase is no longer stable. By default this is disabled (set to `N`). Enable this (set to `Y`) to perform single equilibrium calculations at 5 Kelvin (K) intervals in the two-phase region between the gas/liquid temperature and the liquid/gas temperature, which is the temperature below which the gas phase is no longer stable.

In the fully liquid region below the liquid/gas temperature single equilibrium calculations are performed at 50 K intervals until the liquidus temperature is reached. After that the Scheil solidification calculation proceeds as usual.

Syntax	CALCULATE_FROM_GAS

Prompts	`Calculate from gas/liquid temperature? /N/:`
	The default is `N`. Enter `Y` to perform equilibrium calculations from the gas/liquid temperature.
	`Gas phase name /GAS/:`
	Enter the name of the gas phase (default `GAS`).
	If you choose a phase that is not available in the system, Thermo-Calc checks if there is any phase present with the phase type code `G`.

DELTA_FERRITE_AUSTENITE_TRANSITION

This command is for the SCHEIL module.

The DELTA_FERRITE_AUSTENITE_TRANSITION command enables or disables BCC to FCC transition.

This feature should only be used for such steels for which it is reasonable to assume infinitely fast diffusion (equilibrium conditions) when delta ferrite is present. When the **Allow delta ferrite to austenite transition in steel** checkbox is selected in Graphical Mode or the DELTA_FERRITE_AUSTENITE_TRANSITION command used in Console Mode, this essentially assumes that diffusion can be considered (infinitely) fast when delta ferrite is present as a solid phase, i.e assumes an equilibrium condition. After delta ferrite is no longer stable, the usual Scheil assumptions for the selected calculation type are in effect. This setting is therefore not suitable for steels where you DO NOT have a complete BCC to FCC transition during solidification. This setting is also NOT available in combination with solute trapping.

Syntax	DELTA_FERRITE_AUSTENITE_TRANSITION
Prompt	`Allow delta-ferrite -> austenite ? /N/:` The default is `N`. Enter `Y`to enable BCC to FCC transition. This feature should only be used for such steels for which it is reasonable to assume infinitely fast diffusion (equilibrium conditions) when delta ferrite is present. See the above for details.

EVALUATE_SEGREGATION_PROFILE

This command is for the SCHEIL module.

This feature is not supported with fast diffusers.

Enable this feature before executing the START_WIZARD command.

Use this command in order to evaluate a segregation profile while performing the Scheil calculation. The Scheil calculation itself does not contain a spatial dimension. However, if it is assumed that the molar volume is constant and equal for all elements, and if a length is provided over which solidification occurs (for example the secondary dendrite arm spacing) then the generated profile corresponds to the segregation that would be obtained under the assumptions of a Scheil calculation. The grid is then equidistant and can be used as input for a DICTRA simulation.

The generated text file contains, on each line, the mole fractions of all elements in alphabetical order at a certain grid point. If the composition is the same on several consecutive lines it means that the composition of the then remaining liquid has reached a state in which there are no degrees of freedom.

Syntax	EVALUATE_SEGRATION_PROFILE
Prompt	`Evaluate segregation profile? /N/` If the answer is Y, a segregation profile will be evaluated and saved to disc. This feature is not supported with fast diffusers. You cannot select fast diffusers if evaluation of the segregation profile is enabled.
	`Number of grid points /100/` Enter the number of grid points for the segregation profile. An xf.txt file dialogue window opens and allows you to specify the name of the file in which the segregation profile is written. ***About the xf.txt File*** The file is started with this command, and available after the Scheil simulation is finished. The XF.txt file contains one line per grid point entered here. In a macro file it is possible to enter all arguments on a single line, e.g. `EVALUATE_SEGREGATION_PROFILE Y 100 XF.TXT`, meaning that the segregation profile is evaluated over 100 grid points and

Syntax	EVALUATE_SEGRATION_PROFILE
	saved to a file (XF.TXT) in the current working directory. The grid coordinate (actually fraction solid, but used later as distance) is not recorded in the XF.txt file. The file contains one column per element, listing the mole-fraction of each in alphabetical order, including the dependent element. As I understand it, it is the total concentration of each element in each point at the end point of the Scheil simulation. The XF.txt is then used with INPUT_SCHEIL_PROFILE command in the DICTRA module. Remember to use the same number of grid points in the DICTRA region as in this file.

GLOBAL_MINIMIZATION

This command is for the SCHEIL module.

Global minimization is enabled by default (i.e. set to `Y`) and global minimization is used throughout the simulation.

It is recommended to keep global minimization on as it makes the calculation more accurate. However, turn it off if you find that the calculation is taking too long for any particular system, and accuracy is not the highest priority.

For the GLOBAL_MINIMIZATION command, a global equilibrium test is performed when an equilibrium is reached, at selected intervals. By default it is at every 10th Scheil step but this can be changed using the command TEST_INTERVAL_FOR_GLOBAL. The global equilibrium test is also done every time the set of stable phases tries to change. This costs more computer time but the calculations are more robust.

Syntax	GLOBAL_MINIMIZATION
Prompt	`Use global minimization? /Y/` By default this is set to `Y`. This costs more computer time but the calculations are more robust.

LIQUID_PHASE_NAME

This command is for the SCHEIL module.

Use this command to use the liquid phase name from the database definitions or enter another phase name.

Syntax	LIQUID_PHASE_NAME
Prompt	`Liquid phase name /Default/` Default selects the liquid phase from the database definitions, otherwise enter a phase name.

SAVE_FILE_NAME

This command is for the SCHEIL module.

Use this command to save the file. The files get the console number added to this name, e.g. `005.->Scheil_006.POLY3 and Scheil_segregation_profile.txt`).

Syntax	SAVE_FILE_NAME
Prompt	Name of files to be saved, POLY and segregation profiles. Linux and Mac are case sensitive so ensure you enter `.POLY3`.

SET_MAX_GRID_POINTS_FOR_GLOBAL

This command is for the SCHEIL module.

Use the SET_MAX_GRID_POINTS_FOR_GLOBAL command to set the maximum number of gridpoints per phase for global minimization. The default is 2000.

Syntax	SET_MAX_GRID_POINTS_FOR_GLOBAL
Prompt	`Maximum number of gridpoints per phase /2000/:` Enter the maximum number of gridpoints per phase for global minimization

SET_NUMERICAL_LIMITS

This command is available for the POLY, Scheil, and ED-EXP modules.

Change the criteria for convergence. This is to speed up a calculation in a complex system.

If there is any convergence problem in finding a stable solution at any stage during a calculation procedure enforced by COMPUTE_EQUILIBRIUM, STEP_WITH_OPTIONS, MAP or ADVANCED_OPTIONS), this message displays:

```
Convergence problems, increasing smallest site-fraction from 1.00E-30
to hardware precision 2.00E-14. You can restore using SET-NUMERICAL-
LIMITS
```

This implies that smallest site fraction in the current POLY workspace is automatically increased from the default value 1.00E-30 to the hardware-dependent precision (under Linux, as 2.00E-14). For other subsequent POLY module calculations, you can use this command to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

Syntax	SET_NUMERICAL_LIMITS
Prompt	`Maximum number of iterations /500/:` By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.
	`Required accuracy /1E-6/:` This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.
	`Smallest fraction /1E-12/:` This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions. The default value for the smallest site-fractions is 1E-12 for all phases, except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as 1E-30 (unless you have used the SET_NUMERICAL_LIMITS command to reset an even-lower value (e.g. 1E-45, that is naturally enforced to all the phases in the system).
	`Approximate driving force for metastable phases /Y/:` `Y` is the default. Enter `N` to change the default as required and based on the options described below. This setting involves the convergence of metastable phases and affects their driving forces. It can also have an effect on when an equilibrium is considered successful. The default is to allow an equilibrium with metastable phases that have not converged, as long as the stable phases have converged. This is efficient but often causes approximate values of the

Syntax	SET_NUMERICAL_LIMITS
	driving forces for the metastable phases. If you change the default, it enforces metastable phases to converge. This gives accurate driving forces for metastable phases as well as stable phases. It can however take a slightly longer time, and if metastable phases do not converge it causes the equilibrium calculation to fail.

SKIP_STEP_CALCULATION

This command is for the SCHEIL module.

Use the SKIP_STEP_CALCULATION command to skip the step (also called *one axis*) calculation that is by default performed before the Scheil calculation in Thermo-Calc. The step calculation is used to plot the equilibrium solidification curve, which is shown for comparison if the default axis variables are used. This is sometimes referred to as the *equilibrium line*.

If a comparison to equilibrium is not necessary, change the default setting and then only a Scheil calculation is performed. This results in a much faster calculation, which for a complex system may be preferable.

Syntax	SKIP_STEP_CALCULATION
Prompt	`Skip the step calculation before Scheil (equilibrium curve)? /N/:` By default this is set to `N`. If a comparison to equilibrium is not necessary, enter `Y` and only a Scheil calculation is performed.

SOLUTE_TRAPPING

This command is for the SCHEIL module.

Details about the solute trapping model theory are in About Scheil with Solute Trapping.

The SOLUTE_TRAPPING command enables solute trapping. Once enabled, there are additional prompts and settings that are included and described with the START_WIZARD command.

Syntax	SOLUTE_TRAPPING
Prompt	`Consider solute trapping in primary phase? /N/` The default (`N`) does not use solute trapping. If you choose `Y`, then solute trapping is used. When the USE_BACK_DIFFUSION command is enabled, the SOLUTE TRAPPING command is automatically disabled (set to `N`).

START_WIZARD

This command is for the SCHEIL module.

About the Scheil-Gulliver Solidification Simulations

Use this command to use the START_WIZARD with step-by-step prompts to create a Scheil simulation.

You are prompted for settings including the major element or alloy, composition input in mass (weight) percent, the alloying elements, the temperature, fast diffusing components, and whether any phase should have a miscibility gap check. There are additional prompts included in the Start Wizard if USE BACK DIFFUSION or SOLUTE TRAPPING commands are set to `Yes` to enable back diffusion and solute trapping, respectively.

The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. this model requires the use of a mobility database.

Use the other commands to make changes to settings that are not included in this wizard.

- EVALUATE_SEGREGATION_PROFILE
- GLOBAL_MINIMIZATION
- LIQUID_PHASE_NAME
- SAVE_FILE_NAME
- STORED_COMPOSITION_TYPE
- TEMPERATURE_STEP
- TERMINATION_CRITERIA

If you also have a license for the Diffusion Module (DICTRA), you can import a previously calculated Scheil segregation profile into the software using the command INPUT_SCHEIL_PROFILE. Press F1 to search the online help.

Syntax	START_WIZARD
Prompt	The following is a list of the prompts. Press <Enter> to accept the defaults that are shown between the forward slashes (*/default/*). `Database /<Default>/:` The available thermodynamic database and its version are available to enter (based on license).

Syntax	START_WIZARD

Enter `?` for a list.

```
Major element or alloy:
```

The major element in the system, e.g. Fe for a steel.

```
Composition input in mass (weight) percent? /Y/:
```

Set whether to specify the `Composition input in mass (weight) percent` (the default) or in `Mole percent`. Enter `Y` for mass percent and `N` for mole percent.

```
1st alloying element:
```

> You can specify all the alloying elements and their corresponding compositions on the same line when you are prompted to specify your first alloying element. For example, you can enter `Cr 5 Ni 1 Mo 0.5 C 0.01 N 0.02`.

You can directly specify mass or mole percent after the name (for example, enter `Cr 5`). If this is not specified, then you are prompted to enter it separately.

```
Mass (weight) percent /1/
2nd alloying element:
```

Specify the other alloying elements in the same way as you specify the first (for example, `c 1`).

```
Mass (weight) percent /1/
Next alloying element:
```

After you have specified your last alloying element, press <Enter> when requested to specify the next element. This ends the process of defining the bulk composition of the alloy system.

```
Temperature (C) /2000/:
```

Enter a value for the temperature in degrees C (Celsius) . This value should be sufficiently high so that the solidification simulation starts with the alloy system in the liquid single-phase region.

Decide which phases (if any) to reject at the `Reject phase(s)` prompt. Enter the name of the phases to reject or press <Enter> for `NONE`.

Decide whether to `Restore phase(s)`. You may want to restore a phase that you rejected when you ran the simulation earlier, or you may want to restore a phase that is rejected by default in your database. Enter the name of the phases to restore or press <Enter> for `NONE`.

Then you are asked to confirm whether these phases should be retained in this system:

```
OK? /Y/:
```

Press <Enter> to accept the default `Y` or type `N` and press <Enter>. Thermodynamic data about the alloy system you defined is retrieved from the database.

```
Should any phase have a miscibility gap check? /N/:
```

If you answer `Y`, you are prompted to specify the `Phase with miscibility gap`. Answer with a solution phase name(s) (e.g. `FCC`) as well as the `Major constituents for sublattice`(for each sublattice site) (for this example, `Cr` is entered for sublattice 1 and `C` for sublattice 2).

Press Enter to specify another phase.

```
Fast diffusing components: /None/:
```

Syntax	START_WIZARD
	Enter the elements that diffuse fast in solid phases and can assume to be in equilibrium in the whole phase. E.g. C in a steel.

Back Diffusion and Solute Trapping Settings

The following prompts are included with the Start Wizard at various points in the set up if the:

- USE_BACK_DIFFUSION command is set to `Y` to enable back diffusion
- SOLUTE_TRAPPING command is set to `Y` to enable solute trapping

Syntax	START_WIZARD

Back Diffusion settings	`Mobility Database /<Default>/:`
	The available mobility database and its version are available to enter (based on license). Enter `?` for a list.
	You then are shown a list of what phases are available for the database and the defined system and have the opportunity to reject or restore phases at the next prompts.
	`Reject phase(s) /NONE/:`
	`Restore phase(s): /NONE/:`
	Then you are asked to confirm whether these phases should be retained in this system:
	`OK? /Y/:`
	Press <Enter> to accept the default `Y` or type `N` and press <Enter>.
	`Temperature time dependence /LINEAR/:`
	Specify the type of temperature time dependence. Press <Enter> to accept this default.
	An increased value moves the result from equilibrium toward a Scheil-Gulliver calculation.
	LINEAR is the only option and it corresponds to a constant cooling rate.
	`Cooling rate (K/s) /.1/:`
	Specify the cooling rate in Kelvin per second (K/s). An increased value moves the result from equilibrium toward a Scheil-Gulliver calculation.
	`Expression for secondary dendrite arm spacing /CONSTANT/:`
	Secondary dendrite arm spacing is the distance in meters (m) between two secondary dendrite arms. Specify the type of secondary dendrite arm spacing by entering `CONSTANT` (the default) or `POWER_LAW`.
	An increased value moves the result from equilibrium toward a Scheil-Gulliver calculation. Use
	• `CONSTANT` for a constant dendrite arm spacing. If you choose this, then enter a value for the `Secondary dendrite arm spacing (m) /5E-05/:` prompt.
	• `POWER_LAW` in the form `c*(cooling rate)^-n` where `c` and `n` are entered in the next prompts. If you choose this, then enter a value for the `Exponent n /.33/:` and `Scaling factor c /5E-05/:`

Syntax	START_WIZARD
	`Primary phase /AUTOMATIC/:` The primary phase is the phase where the back diffusion takes place. If `Automatic` is selected (or kept as the default), the program tries to find the phase which gives the most back diffusion. To override this setting, choose a specific primary phase from the list. For back diffusion, only phases with diffusion data can be used as primary phases.

Solute Trapping settings	`Expression for solidification speed /SCANNING_SPEED_AND_ANGLE/:`
	SCANNING_SPEED_AND_ANGLE is currently the only available option. It is calculated as scanning speed * cos(alpha) where scanning speed and the angle alpha are given by the user.
	Decreasing the value moves the result toward a Scheil-Gulliver calculation.
	`Scanning speed (m/s) /1/:`
	Enter the Scanning speed to calculate the solidification speed, Vs = $V_{scanning}$ * cos(α) m/s, where $V_{scanning}$ is the user specified scanning speed.
	`Alpha (degrees) /45/:`
	Enter an Alpha value in degrees, which is the alpha angle, α, between the solid/liquid boundary and scanning direction.
	`Primary phase /AUTOMATIC/:`
	If `Automatic` is selected (or kept as the default), the program tries to find the phase which gives the most solute trapping. To override this setting, choose a specific primary phase from the list. For solute trapping, only phases that dissolve all elements in the system can be used as primary phases.

TEMPERATURE_STEP

This command is for the SCHEIL module.

Use this command to define a temperature step.

Syntax	TEMPERATURE_STEP
Prompt	`Set temperature step (C) /1/`

TERMINATION_CRITERIA

This command is for the SCHEIL module.

Use this command to define the termination criteria for the fraction of liquid (unit = mole fraction) or temperature.

Syntax	TERMINATION_CRITERIA
Prompts	`Fraction of liquid or Temperature (F or T)? /F/`
	`Fraction of liquid /.01/`

TEST_INTERVAL_FOR_GLOBAL

This command is for the SCHEIL module.

By default, global minimization is enabled (i.e. set to `Y` with the command GLOBAL_MINIMIZATION).

Use the TEST_INTERVAL_FOR_GLOBAL command to change the interval at which a global equilibrium test is done, which by default is every 10th step as long as there are no changes in the set of stable phases. Every time the set of stable phases tries to change, a global equilibrium test is also done regardless of the test interval value chosen. A global equilibrium test means that the calculated equilibrium state obtained by the ordinary minimization calculation is tested against the Global Minimization Technique, and if the result is found unstable then the full global minimization calculation is performed instead.

Syntax	TEST_INTERVAL_FOR_GLOBAL
Prompt	`Global test interval /10/:` Global equilibrium test is done every Nth step, unless the set of stable phases changes. By default a test is done every 10th step. Enter a different number to change the interval.

USE_BACK_DIFFUSION

This command is for the SCHEIL module.

The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. this model requires the use of a mobility database.

About the Scheil-Gulliver Solidification Simulations

The USE_BACK_DIFFUSION command enables back diffusion in the solid primary phase. Once enabled, there are additional prompts and settings that are included and described with the START_WIZARD command.

Syntax	USE_BACK_DIFFUSION
Prompt	`Use back diffusion? /N/` The default (`N`) does not use back diffusion. If you choose `Y`, then back diffusion is used. When the SOLUTE TRAPPING command is enabled, the USE_BACK_DIFFUSIONcommand is automatically disabled (set to `N`).

PARROT Module Commands

The PARROT Module in the *Data Optimization User Guide*.

In this section:

About the ENTER_PARAMETER Command

For the PARROT Module, this command is the same and is described here. See ENTER_PARAMETER for the command details.

In the descriptions of the standard thermochemical properties and special physical properties for a phase, there are a number of parameters which may depend on the temperature and pressure. The expressions for these parameters can be given in a free form as a sum of terms with powers of T and P and may also include the natural logarithm and exponential function. This type of expression is called *TP-functions*. Identical parameters (in terms of parameter-names) are stored only once in the GIBBS workspaces.

The composition-dependence of the Gibbs energy is described in the GIBBS module by the internal data structure, which is created when the phase is entered. The Gibbs energy of a phase is always referred to one formula unit of the phase, i.e. the amount derived from the number of sites (i.e. the stoichiometric coefficient) for each sublattice. If vacancy is a constituent of a sublattice, the amount of matter per formula unit of the phase may vary with composition.

Gibbs Energy System (GES) Commands

How to Define a Parameter

A valid parameter should have the general form of:

```
<identifier>(<phase>, <constituent array>; <digit>) <xxx> <expression> <yyy>
<keyword Y or N> <zzz> !
```

The identifier must be followed by an opening parenthesis, a phase name, a comma and a constituent array. Optionally, the constituent array can be followed by a semicolon and a digit. The parameter name is terminated by a closing parenthesis. The parameter form is defined as:

- `<identifier>` is the parameter type;
- `<phase>` is the phase name (maximum 24 characters);
- `<constituent array>` is the specific constituent array in the phase;

- `<digit>` is the degree of composition-dependent interaction contribution (an integer number from 0 through 9), that is only for excess energy (L), Curie temperature (TC) and Bohr magneton number (BMAGN), as well as for volume-related parameters (V0 or VA or VC or VK); if it is valued as zero, or if it is for the standard Gibbs energy (G) for which the degree is always zero, it can be omitted;
- `<expression>` is the mathematical relation to describe the parameter;
- `<xxx>` and `<yyy>` are the low and high temperature limits respectively for the applicable temperature range of the parameter expression;
- `<keyword Y or N>` is the indicator on if there is continuation for the parameter expression or not;
- `<zzz>` is the reference index/number for the assessment of this parameter;
- The exclamation point `!` is used to indicate that the current parameter definition is ended.

Parameter Name

The GES parameter name has a general form of:

```
<identifier>(<phase>,<constituent array>;<digit>)
```

Examples of parameter names:

- `G(GAS,C1O2)`: The Gibbs energy of formation of a CO_2 molecule in gas.
- `G(FCC,FE:VA)`: The Gibbs energy of formation of fcc Fe with interstitials.
- `L(LIQ,Fe,Cr;0`: The regular solution parameter for Fe and Cr in liquid.
- `L(LIQ,Fe,Cr;1)`: The sub-regular solution parameter.
- `TC(BCC,Fe:Va)`: The Curie temperature of bcc Fe.
- `BMAGN(BCC,Fe:Va)`: The Bohr magneton number parameter of bcc Fe.

The parameter name consists of several parts. The first is a type-identifier and these can be used:

- `G`: Standard energy parameter (Gibbs energy of formation) or for interaction parameters;
- `L`: Excess energy parameter (Gibbs energy of interaction) always used for interaction parameters;
- `TC`: Curie temperature for magnetic ordering;

- `BMAGN` or `BM`: Bohr magneton number for magnetic ordering (or Born function ωPr,Tr for aqueous solute species).
- `VO`: Molar volume at 298.15 K and 1 bar (a numeric value only);
- `VA`: Integrated thermal expansivity; $\int_{298.15}^{T} \alpha(T)\mathrm{dT}$
- `VC`: High-pressure fitting parameter;
- `VK`: Isothermal compressibility.

For more information about the high pressure volume, see X.-G. Lu, M. Selleby, B. Sundman, "Implementation of a new model for pressure dependence of condensed phases in Thermo-Calc", Calphad. 29, 49–55 (2005).

When necessary quantities as `H` (enthalpy), `S` (entropy), `V` (Volume), `F` (Helmholtz energy), etc., can be calculated from the Gibbs energy.

Phase Name

Specifying the `PHASE NAME` in uppercase is recommended; however, if you prefer to write it as a mixture of uppercase and lowercase, it automatically converts all lowercase to uppercase, as the GIBBS module only recognizes uppercase phase names. It is important that if a phase bears a legal phase-type (among `G`, `A`, `Y`, `L`, `I`, `F` and `B`) in its phase definition (already by the `PHASE` keyword; such as GAS:G, LIQUID:L,SLAG:L, IONIC-LIQ:Y, SPINEL:I, FCC_L12:F, HCP_D021:F, BCC_B2:B, AQUEOUS:A), such a valid phase-type code should not be attached to the phase name when ENTER_PARAMETER is executed.

Constituent Array

The constituent array consists of a list of constituent names. Interaction parameters have two or more constituents from the same sublattice separated by a comma. If the phase has sublattices, at least one constituent in each sublattice must be specified. The constituents in different sublattices must be given in sublattice order and are separated by a colon.

After the component array, a sub-index digit can be specified after a semicolon. This digit must be in the range 0 to 9. The interpretation of the sub-index depends on the excess energy model used for the phase. If no semicolon and digit are given, the sub-index value is assumed to be as zero.

The excess energy parameters, e.g. the regular/subregular (binary) parameter or ternary parameters, are multiplied with two or more fractions of the constituents from the same sublattice of the solution phase. These additional constituents must be given as interacting constituents (as the following prompt).

> Solution phases with sublattices can have interacting constituents in each sublattice.

Interaction Parameter

An interaction parameter, which is used to describe the excess term of a quantity, must have two or more constituents that interact with each other on a specified sublattice site of the given phase. It is arbitrary which of these constituents is given as the first constituent and what is given as the interacting constituents. The software always sorts the constituents (in each sublattice) in alphabetical order when the parameter name is written as a prompt (for entering its parameter value) and when the parameter is listed (using the GIBBS commands LIST_PARAMETER or LIST_PHASE_DATA). This is important for all asymmetric interaction parameters where the sign of the interaction parameter must depend on the appearance order.

Use an asterisk* to denote that the excess interaction parameter is independent of the constituents of a specific sublattice. For example, `L(FCC_L12,AL,NI:*)` means that the interaction parameter is for the binary interaction between constituents AL and NI on the first sublattice in the `FCC_L12` solution phase, while it is independent of all constituents on the second sublattice. An interaction parameter in the list of constituents is always added to the Gibbs energy and the asterisk * is calculated with the term of [1∑y(specified constituents)], which implies that in an A-B binary system these `L` parameters are identical (but in higher-order systems, these are different):

- `L(phase,A,B)` is multiplied with X(A)*X(B)
- `L(phase,A,*)` is multiplied with X(A)*(1-X(A))
- `L(phase,B,*)` is multiplied with X(B)*(1-X(B))

If you press <Enter> when you are asked for a parameter name or if you have improperly input the entire parameter name, you are asked for each of these items in the name.

AMEND_PARAMETER

This command is for the PARROT module.

There is also a Gibbs (GES) module command with the same name.

Interactively modify the TP-function(s) for a specific parameter for a phase with this command. This is useful in order to correct typing errors because the old function is made available for interactive editing on the terminal.

Syntax	AMEND_PARAMETER

Prompts	`Parameter: <Parameter name>`
	Specify a correct parameter name. If a parameter name is not acceptable or <Enter> is pressed, the error message displays:
	`*** Error, please re-enter each part separately`
	The program prompts for separate input for each part for a parameter name.

	`Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK>` Specify one of these types of legal identifiers ENTER_PARAMETER
	`Phase name (ABCD/): <Phase name>` Specify the phase name.
	`Constituent (in sublattice # /ABC/): <Species name>` Specify the constituent name.
	`Interacting constituent (In sublattice # /XYZ/): <Species name>` Specify the interacting constituent name; if there is no interacting constituent, press <Enter>.
	`Interacting constituent (in sublattice # /XYZ/): <Species name>` If there is more than one interacting constituent, specify these; otherwise press <Enter>.
	`Degree /#/: <Degree>` Specify a numerical number as the degree of the phase parameter.

	After the parameter name is specified correctly, the program lists its current definition (either preset in database or defined by the ENTER_PARAMETER command), such as:
	`L(PHASE2,AL,MG;1)=`
	`298.15<T<2000.00: +5000`
	`2000.00<T<4500.00: +4500`
	`4500.00<T<6000.00: +4000`
	You are prompted to change the parameter definition:

Syntax	AMEND_PARAMETER

`Do you want to change the number of ranges /No/:`

Enter Y to change the number of ranges for the chosen function, or change some of the temperature limits in the definition, then retype both the low/high temperature limits and functions

If you do not want to change the number of ranges but want to change the function(s) in one or more ranges, press <Enter> and the whole definition of the chosen parameter in all ranges (if any) is listed such as:

```
DIFFERENT FUNCTIONS IN THESE RANGES
298.15<T<2000.00
2000.00<T<4500.00
4500.00<T<6000.00
```

This message prompts:

`Do you want to change range limits /No/:`

If there is more than one range, this question is prompted. Press <Enter>.

`Range number (0 to exit) /0/: <Range number>`

If the function of a parameter is different in two or more temperature ranges, you must specify the range of the function of which you want to amend. Or press <Enter> or type `0` to exit this command without making any change.

`Function`

The previous function is available for editing. The editing is performed within the general subroutine `FOOLED`, as described in AMEND_SYMBOL. This routine prompts as follows:

`1:+:>`

The prompt consists of the current position in the string and the character at that position between colons, (::).

Commands

These commands can be given:

- Help: `?`
- Move CP to last or first character: `<+/-> A`
- Delete characters from CP: `<+-#characters> D`
- Exit: `E`
- Find: `<#occurrences> F<string>@`
- Insert: `I<string>@`
- Move: `<+-#positions> M`
- Restore string: `R`
- Substitute: `S<OLD>@<NEW>@`
- Type string: `T`

Where CP denotes the current position in a string, # means number of, @ is a terminator of an

Syntax	AMEND_PARAMETER
	input or search string. When the string is typed the character at the current position is replaced by an underscore _. To finish the editing of the current function, type `E` at the prompt.
	`Range number (0 to exit) /0/: <Range number>` Give a range number to edit that function, or press <Enter> or type `0` to exit this command.

AMEND_SYMBOL

This command is for the PARROT module.

The same command is also available for the Gibbs (GES) module.

Interactively calculate the current values of a function or table (predefined by the switched database or previously entered with ENTER_SYMBOL) at the current temperature and pressure condition, and also possible to modify the definitions of variables or functions.

The current values of the temperature and pressure used to calculate the functions or tables are the ones listed with LIST_STATUS. There is no way to change the current temperature and pressure values interactively.

To modify the definitions of entered symbols (variable, functions or parameters), the performance of this command is slightly different one from another, as described below:

- For variables, the values can be changed.
- For functions the low and high temperature limits in various ranges (if any), as well the expressions, can be changed.
- For parameters the low and high temperature limits in various ranges (if any), as well the expressions, can be changed.

Syntax	AMEND_SYMBOL

Prompts	`Name: <Symbol name>`
	Specify the name of an entered symbol.
	For tables and functions (or parameters which are treated as functions after these are entered by the ENTER_SYMBOL command with the `Parameter` keyword, but not by the ENTER_PARAMETER command), after the symbol name is specified here, the program automatically calculates the values under the current temperature and pressure conditions, and lists the current values, such as:
	`FUNCTION VALUE 2.52500000E+01`
	`TABLE VALUE 1.56000000E+02`
	For variables and functions (or parameters), there are additional prompts and depend on the symbol type.

	For a variable, its current value is displayed, and you can change it to a new value:
	`Value /Current value/: <New value>`
	For a function (or a parameter entered as a symbol):
	`Do you want to change the number of ranges /No/:`

Syntax	AMEND_SYMBOL

Enter Y to change the number of ranges for the function, or change some of the temperature limits in the definition, then retype both the low/high temperature limits and functions (see all the remaining details in the ENTER_SYMBOL command.

If you do not want to change it, press <Enter>. The definition of the chosen function in all ranges (if any) is listed, for example:

```
DIFFERENT FUNCTIONS IN THESE RANGES
298.15<T<2000.00
2000.00<T<4500.00
4500.00<T<6000.00
```

and this message displays:

```
Do you want to change range limits /No/:
```

If a function is different in two or more temperature ranges, you must specify the range of the function of which you want to amend. Or press <Enter> or type `0` to exit this command without making any change.

```
Range number (0 to exit) /0/: <Range number>
Function:
```

The previous function is available for editing. The editing is performed within the general subroutine FOOLED. This routine prompts as follows:

```
1:+:>
```

The prompt consists of the current position in the string and the character at that position between colons (::).

Commands

These commands can be given:

- Help: `?`
- Move CP to last or first character: `<+/-> A`
- Delete characters from CP: `<+-#characters> D`
- Exit: `E`
- Find: `<#occurrences> F<string>@`
- Insert: `I<string>@`
- Move: `<+-#positions> M`
- Restore string: `R`
- Substitute: `S<OLD>@<NEW>@`
- Type string: `T`

Where CP denotes the current position in a string, # means number of, @ is a terminator of an input or search string.

Syntax	AMEND_SYMBOL
	When the string is typed the character at the current position is replaced by an underscore _. To finish the editing of the current function, type `E` at the prompt.

COMPILE_EXPERIMENTS

The descriptions of the experimental equilibria saved on a textual *.POP file, given as commands in the POLY and ED_EXP syntax, is compiled by this command into the PARROT structured data, i.e. stored into the current work *.PAR file which is created with CREATE_NEW_STORE_FILE, set by SET_STORE_FILE , or opened with READ_PARROT_WORKSPACES, all done before COMPILE_EXPERIMENTS.

This command also lists the compilation details on screen or onto a listing file (*.TXT).

> If a syntax error in the commands is detected, the compilation is terminated. You need to correct the error in the *.POP file (using a textual editor) and recompile it with the *.PAR work (store) file.

After a successful compilation, the program translates all the experimental data points in the *.POP file into a graphical experimental data file (*.EXP) in the DATAPLOT syntax, which can be further edited and used as a graphical experimental data file (*.EXP) for the purposes of imposing onto calculated/plotted phase diagrams and/or property diagrams for comparisons during the assessment process.

DATAPLOT User Guide included with this documentation set.

Syntax	COMPILE_EXPERIMENTS
	A window displays to open the original experimental data file (*.POP). Enter a *.POP **File name** box, and specify the working directory in the **Look in** box. Normally the default file-type in the **Files of type** field is the correct one for the experimental data format (i.e. *.POP file). Click **Open** or **Cancel** button as applicable.
Prompts	`Output to screen or file /Screen/: <*.pop file name>` A list of the source code in the *.POP file and error messages during compilation is written on screen (by pressing <Enter>) or on a list *.TXT file under a specific file name which can later on be opened and edited by any basic textual editor.
	`Initiate store file /Y/:` After a successful compilation, the data in the POLY workspace is stored as a new block of equilibria on the current work (store) file. By default the store file is initiated before compilation and only the compiled block is stored on the current work file (consequently, the *.PAR file is updated). A window displays to generate/store the graphical experimental data file (*.EXP) in the DATAPLOT syntax. Enter a *.EXP file name in the **File name** field and specify the working directory when opening the *.EXP file in the **Look in** field. Normally the default file type in the **Files of type** field is the correct one for the graphical experimental data format (i.e. *.EXP file). Click **Open** or **Cancel** as applicable. To keep the current work file, enter N.

CONTINUE_OPTIMIZATION

This command is for the PARROT module.

This command continues the optimization using the same Hessian matrix.

In some cases it is not possible to attempt continuation. For example, if the optimization has already converged or if the optimizing parameters or the set of experimental equilibria used in the current optimization runs are changed. The program gives a warning message if you try to continue when you make these changes.

Syntax	CONTINUE_OPTIMIZATION

Prompts	`Are you sure? /N/: <N or Y>`
	Prior to this question, a message displays to confirm if it is OK to continue:
	`It is safe to CONTINUE only after TOO MANY ITERATIONS  and no change in variables and experiments ...`
	You can accept the default (N) in order to cancel this special attempt.

	`Number of iterations /N/: <Integral number of iteration>` Specify an integral number for the optimization iteration. The specified iteration number is shown as the default number. The PARROT program tries this exact number of different sets of values of the optimizing variables without stopping the optimization even it would have converged earlier or should give up earlier.

CREATE_NEW_STORE_FILE

This file is hardware dependent and cannot be read by any text editor.

Create a binary file to be used as a *work file* (also called *store file*) before any optimization can be done. The workspace used by the GIBBS, POLY and PARROT modules is stored automatically on the work file but not any experimental information. The binary work file has a default extension of `PAR` under MS-Windows or `par` under Linux/UNIX.

A work file that is created at a previous run can be used in the PARROT module with the other command SET-STORE-FILE.

Syntax	CREATE_NEW_STORE_FILE
Prompt	<*.par file name> A **Save** window displays. Enter a **File name** and specify the working directory in the **Save in** field. Normally the default file-type in the **Files of type** field is the correct one for the PARROT workspace format (i.e. PAR file). Click **Save** or **Cancel** as applicable.

EDIT_EXPERIMENTS

Initialize and make available the sub-module for editing experimental equilibria, i.e. the ED_EXP module. All experimental equilibria compiled from the *.POP file can be accessed in the ED_EXP module.

The ED_EXP module is similar to the normal POLY module, but some commands are special and some POLY commands are not available. In the ED_EXP module, you can calculate each equilibrium separately or together, provide start values for equilibria which failed to converge, set weights, and modify the values of experiments or conditions.

Syntax	EDIT_EXPERIMENTS
	You are now in this submodule and can start using the commands.

- The first required command after entering the ED_EXP module for the first time (from the PARROT module GOTO MODULE ED-EXP) should always be READ_BLOCK in order to load the experimental data block from the current work *PAR-file for editing.
- The READ_BLOCK command must also be used prior to any other ED_EXP command if the module is reinitiated, or if no experimental data block is not previously read from a work file compiled with a proper experimental data .POP file, or if you want to change to another data block for editing.
- If any change is made in the ED_EXP module remember to use the command SAVE_WORKSPACE before going BACK to the PARROT module.

Although the TABLE_HEAD, COMMENT and FLUSH_BUFFER commands are visible in the ED_EXP module, these cannot be used here as these only work in a *.POP file (or *.DOP file for DICTRA).

ENTER_PARAMETER

This command is for the PARROT module.

There is also a Gibbs (GES) module command with the same name.

About the ENTER_PARAMETER Command

Use this command to enter TP-function(s) for a specific parameter for a phase interactively with this command. If there is already a parameter expression defined (for this parameter), that is deleted and replaced with newly entered one.

The entered TP-Function(s) for the parameter can be changed later with the command AMEND_PARAMETER.

Syntax	ENTER_PARAMETER

Prompts	`Parameter: <Parameter name>`
	As explained in About the ENTER_PARAMETER Command, specify a correct and complete `Parameter Name`, which should contain all the necessary parts of the general form:
	`<Identifier>(<Phase>,<Constituent array>;<Digit>)`
	If a parameter name is not acceptable or <Enter>, is pressed, a message displays:
	`*** Error, please re-enter each part separately`
	and you are prompted for input for each required part for a parameter name.

Options	**Description or Information**
`Identifier`	`Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK>` If this command is used one or more times, the previous value on this prompt is set as default. Press <Enter> for the same type identifier or specify a new type.
`Phase name`	`Phase name (/ABCD/): <Phase name>` Each parameter is valid for a specific phase only. The name of that phase must be supplied (maximum 24 characters). The name can be abbreviated.
`Constituent`	`Constituent (in sublattice # /ABC/): <Species name>` A parameter is identified by the constituents on a specified sublattice site of the given phase, the stoichiometric coefficients of which are multiplied with the parameter. The name of the constituent can be abbreviated. It is the species name, not the stoichiometric formula required here. If this command is used one or more times, the previous value on this prompt is set as default. Accept it by pressing <Enter> if the constituent is the same, or specify a new species name.

Syntax	ENTER_PARAMETER
`Interacting constituent`	For phases with several sublattices, the program asks for one constituent in each sublattice. `Interacting constituent (in sublattice # /XYZ/): <Species name>` If this command is used one or more times, the previous value on this prompt is set as default. Press <Enter> to accept it if the constituent is the same, or specify a new species name. To cancel the default value of the interacting constituent type `NONE` or the name of another constituent. This question is repeated until all the interested interacting constituent(s) on a specific sublattice in the phase are specified, and finally an <Enter> is enforced.
`Degree`	`Degree /#/: <Degree>` Degree is model-dependent. Specify an integer number (a value from 0 through 9) as the degree of composition-dependent interaction contribution for the phase parameter. This is valid for excess energy (`L`), Curie temperature (`TC`) and Bohr magneton number (`BMAGN`), as well as for volume-related parameters (`V0`, `VA`, `VC` or `VK`). For binary interaction parameters, the degree is usually the power in the Redlich-Kister expression. For ternary interaction parameters, it is usually the Hillert ternary index. For a standard `G` parameter for a pure component (end-member) its degree should be always 0 and this prompt should not display.

`Phase parameter`	After this prompt, the program echoes on the screen the full TP-Function of the phase parameter.
	`Low temperature limit /298.15/: <Lowest temperature limit in K>`
	Specify the lowest temperature limit (in Kelvin), or the lowest-pressure limit (in Pascal but entered as a negative number), for the current TP-Function.
	`Function: <Definition for a function>`
	A TP-Function consists of terms in T and P.
	`& <Continuation of the definition for the current function>`
	Continuation of a TP-Function definition.
	`High temperature limit /6000/: <High temperature limit in K>`
	Specify the high temperature limit (in Kelvin), or the high-pressure limit (in Pascal; only if the *lowest limit* is entered as a negative number) for the current TP-Function.
	`Any more ranges? /N/:`
	Enter Y for more function(s) or N to end this command.

LIST_ALL_VARIABLES

This command is for the PARROT module.

Create a list of the values and status of all variables in the PARROT workspace on screen or in a text file. After an optimization some statistical information is also written. The correlation matrix is written if that option is chosen.

SET_OUTPUT_LEVELS.

Syntax	LIST_ALL_VARIABLES
Prompt	`Output to screen or file /Screen/: <File name>` A list of the current values and status, as well statistical information (if after optimization) and the correlation matrix (optionally), for all variables is written on screen (by pressing <Enter>) or on the list file under a specific file name which can later on be opened and edited by basic text editor.

Example

The following is the listed variables for the example TCEX36, after the first optimization when having set all variables available for optimization.

```
== OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1   TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV

 V1      2.03729090E+04    2.03688352E+04    2.03688352E+04    3.41524152E+00

 V2     -2.94286372E+01   -2.94286372E+01   -2.94286372E+01    2.37944771E+00

 V11    -2.17373936E+04   -2.18095983E+04   -2.18095983E+04    3.97086303E-02

 V12     1.52107184E+01    1.51660547E+01    1.51660547E+01    5.84552327E-02

 V15     2.42082351E+04    2.45139169E+04    2.45139169E+04    5.00914471E+00

 V16    -8.38723972E+00   -8.83460472E+00   -8.83460472E+00    1.60961318E+01

 V17     3.08916533E+03    3.15802558E+03    3.15802558E+03    9.63738108E+00

 V19     2.20292586E+04    2.21385673E+04    2.21385673E+04    4.14274011E+01  V20    -
7.04217974E+00   -7.22424882E+00   -7.22424882E+00    1.00561540E+02

 NUMBER OF OPTIMIZING VARIABLES :    9

 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO

 THE SUM OF SQUARES HAS CHANGED FROM   8.00002729E+04 TO   8.00002719E+04

 DEGREES OF FREEDOM   45.  REDUCED SUM OF SQUARES   1.77778382E+03
```

LIST_CONDITIONS

This command is for the PARROT module.

Use this command to generate a list of the current values of optimization conditions, as well the current status of listing, either on screen or in a basic text file which can be opened and edited by a text editor.

Syntax	LIST_CONDITIONS
Prompt	`Output to screen or file /Screen/: <File name>` Press <Enter> to output to screen or on the list file under a specific file name.

LIST_PARAMETER

This command is for the PARROT module.

There is also a Gibbs (GES) module command with the same name.

List the TP-function(s) of a specific parameter for a phase. You must supply the name of the phase parameter:

```
The parameter name: <Identifier>(<Phase>,<Constituent array>;<Digit>)
```

For encrypted commercial databases, you may not be able to use this command to list any retrieved parameter.

Syntax	LIST_PARAMETER

Prompts	`Parameter: <Parameter name>`
	Specify a correct and complete parameter name, which should contain all the necessary parts of the general form: <identifier>(<phase>,<constituent array>;<digit>)
	See About the ENTER_PARAMETER Command to learn how to define the parameter name.
	If a parameter name is not acceptable or <Enter> is pressed, an error message displays:
	`*** Error, please re-enter each part separately`
	The program prompts for separate input for each required part for a parameter name.

	`Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK>` Specify one of these types of legal identifiers.
	`Phase name (/ABCD/): <Phase name>` Specify the phase name.
	`Constituent (in sublattice # /ABC/): <Species name>` Specify the constituent name on the specified sublattice site of the given phase.
	`Interacting constituent (in sublattice  # /XYZ/): <Species name>` Specify the interacting constituent name on the specified sublattice site of the given phase; if there is no interacting constituent, press <Enter>.
	`Interacting constituent (in sublattice # /XYZ/): <Species name>` If there is more than one interacting constituent on the specified sublattice site of the given phase, specify them; otherwise press <Enter>.
	`Degree /#/: <Degree>`

Syntax	LIST_PARAMETER
	Specify a numerical number as the degree for the phase parameter.

LIST_PHASE_DATA

This command is for the PARROT module.

List all the phase from the Gibbs (GES) module for a specific phase. These are displayed on screen. The thermochemical parameters listed for each phase are always in SI units.

Syntax	LIST_PHASE_DATA
Prompt	`Phase name: <Phase name>` Specify a phase name.

LIST_RESULT

This command is for the PARROT module.

List the result of the current optimization run on screen or in a specified file. The level of detail listed can be prescribed by the command SET_OUTPUT_LEVELS.

The LIST_RESULT command has an option `G` for creation of an experimental data file with two columns, one for the experimental value and the other for the calculated value. It allows plotting a diagram and visualizing the fitting results. The plot is automatically plotted and you can scale it giving commands in the POST module. The option `D` lists all experiments, including those with fulfilled inequalities which are suppressed with the default option `C`.

Syntax	LIST_RESULT
Prompt	`Full, Condensed, Detailed or Graphic format: /C/: <C or D or F or G>`
	Choose a format. • The `F` (full) format is obsolete but retained for backward compatibility. • `C` (condensed) is the default. • `D` (detailed) lists all experiments, including those with fulfilled inequalities (not included with the default condensed file). • The `G` (graphical) format creates an experimental data file containing two columns, one with the experimental value and the other with the calculated value. This allows plotting of a diagram where all symbols should be on the diagonal if the fit is perfect. The plot is automatically plotted and you can scale it giving commands in the POST module. `Output to screen or file /Screen/: <File name>` A list of the current optimization results are written on screen (by pressing <Enter>) or on the list file under a specific file name which can later on be opened and edited by basic text editor.
	The output normally consists of these parts: • A title showing the data of the action; • A message on successful optimization with the iteration number in the last optimization; • A paragraph describing the optimization condition; • A list of the latest set of optimized and fixed variables; • A paragraph describing the optimization quality (some statistical information); • A correlation matrix for all optimizing variables (optionally shown, pre-set by the SET_OUTPUT_LEVELS command); • A list of all parameters (including their symbol names, status and current values or function expressions), and all phase descriptions (including phase name, model names, constituents, and phase's `G/L/TC/BM` expressions) predefined for each phase in the system (optionally shown, pre-set by the SET_OUTPUT_LEVELS command); • A paragraph describing the alternate equilibria (and possible error during optimization);

Syntax	LIST_RESULT
	• A detailed list on all the equilibrium points used in the current optimization. If the alternate-mode is used in the optimization, only an error value is shown. For normal-mode calculations, a list is shown for the experimental equilibrium numbers (first column) and corresponding original experimental data (second column, in the form `quantity = value`) which are used in optimization (i.e. non-zero weighted points). Such experimental data are by each point compared by the calculated value (third column) after the last optimization. Also listed are the experimental error (column 4), the difference between the calculated value and original experimental data (column 5), and the contribution to the sum of least square (column 6).

Example

The following is the listed result after the first optimization based on the prescribed definitions in the TCEX36a.TCM and TCEX36b.TCM, but having set all variables available for optimization.

```
=====================================================

           OUTPUT FROM P A R R O T.

 *** SUCCESSFUL OPTIMIZATION. ***      NUMBER OF ITERATIONS:  10

 == OPTIMIZING CONDITIONS ==

   RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N

   MINIMUM SAVE ON FILE: Y

   ERROR FOR INEQUALITIES =  1.00000000E+00

   RELATIVE STEP FOR CALCULATION OF DERIVATIVES =  1.00000000E-04

 ARGUMENTS FOR SUBROUTINE VA05AD (HSL)

   MAXFUN =   1   DMAX =  1.00000000E+02   H =  1.00000000E-04    ACC = (INITIAL
SUM OF SQUARES) *  1.00000000E-03

 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV

 V1      2.03749463E+04    2.03729090E+04    2.03729090E+04    3.41455863E+00

 V2     -2.94286372E+01   -2.94286372E+01   -2.94286372E+01    2.37944774E+00

 V11    -2.17395673E+04   -2.17373936E+04   -2.17373936E+04    3.98405298E-02

 V12     1.52107184E+01    1.52107184E+01    1.52107184E+01    5.82861832E-02

 V15     2.42106560E+04    2.42082351E+04    2.42082351E+04    5.07239609E+00

 V16    -8.38723972E+00   -8.38723972E+00   -8.38723972E+00    1.69546796E+01

 V17     3.08947424E+03    3.08916533E+03    3.08916533E+03    9.85220694E+00
```

```
 V19     2.20314615E+04    2.20292586E+04    2.20292586E+04    4.16329629E+01
V20    -7.04217974E+00   -7.04217974E+00   -7.04217974E+00    1.03161466E+02

 NUMBER OF OPTIMIZING VARIABLES :   9

 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO

 THE SUM OF SQUARES HAS CHANGED FROM   8.00002719E+04 TO   8.00002709E+04

 DEGREES OF FREEDOM   45.  REDUCED SUM OF SQUARES   1.77778380E+03

Number of alternate equilibria           14

 SYMBOL        STATUS   VALUE/FUNCTION

R         80000000  8.3145100E+00

RTLNP     20000000 +R*T*LN(1E-05*P)

V1        48000000  2.0374946E+04

V2        48000000 -2.9428637E+01

V11       48000000 -2.1739567E+04

V12       48000000  1.5210718E+01

V15       48000000  2.4210656E+04

V16       48000000 -8.3872397E+00

V17       48000000  3.0894742E+03

  21 V19       48000000  2.2031462E+04   22 V20       48000000 -7.0421797E+00

 LIQUID

 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B

      G(LIQUID,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: +14000-10*T

      G(LIQUID,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +18000-12*T

      L(LIQUID,A,B;0) =    500.00<T< 2000.00: +V11+V12*T       L(LIQUID,A,B;1) =
500.00<T< 2000.00: +V13+V14*T

 A2B

  2 SUBLATTICES, SITES  2:  1     CONSTITUENTS: A : B

      G(A2B,A:B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =

             500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)

 BCC

 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B

      G(BCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: 0.0

      G(BCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: 0.0

      L(BCC,A,B;0) =    500.00<T< 2000.00: +V15+V16*T

      L(BCC,A,B;1) =    500.00<T< 2000.00: +V17+V18*T

 FCC
```

```
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B

      G(FCC,A;0)-G(BCC,A;0) =    500.00<T< 2000.00: 408

      G(FCC,B;0)-G(BCC,B;0) =    500.00<T< 2000.00: +3300-3*T

      L(FCC,A,B;0) =    500.00<T< 2000.00: +V19+V20*T

      L(FCC,A,B;1) =    500.00<T< 2000.00: +V21+V22*T

 ======  BLOCK NUMBER  1

 DEFINED CONSTANTS

    DX=2E-2, P0=101325, DH=500, DT=10

 DEFINED FUNCTIONS AND VARIABLES%

    HTR=HM(LIQUID)-HM(A2B)

Alternate equilibrium calculation                 0.4183

Alternate equilibrium calculation                 0.1932

Alternate equilibrium calculation                 0.1016

Alternate equilibrium calculation                 1.4354E-03

Alternate equilibrium calculation                 2.5063E-02

Alternate equilibrium calculation                 8.3929E-03

Alternate equilibrium calculation                  141.4

Alternate equilibrium calculation                  141.4

Alternate equilibrium calculation                  141.4

Alternate equilibrium calculation                  141.4

Alternate equilibrium calculation                 1.2532E-03

Alternate equilibrium calculation                 5.4781E-04

Alternate equilibrium calculation                 1.5404E-03

Alternate equilibrium calculation                 1.2702E-03

ACR(B)=9.4E-1              0.9397      2.85E-02 -2.7745E-04 -9.7472E-03

ACR(B)=8.4E-1              0.8395      2.82E-02 -4.9038E-04 -1.7396E-02

ACR(B)=7.4E-1              0.7407      2.81E-02  7.3804E-04  2.6305E-02

ACR(B)=6.4E-1              0.6424      2.81E-02  2.3935E-03  8.5272E-02

ACR(B)=5.4E-1              0.5434      2.82E-02  3.4449E-03  0.1220

ACR(B)=4.4E-1              0.4428      2.85E-02  2.8265E-03  9.9024E-02

ACR(B)=3.4E-1              0.3394      2.90E-02 -5.8174E-04 -2.0040E-02

ACR(B)=2.3E-1              0.2320      2.97E-02  2.0260E-03  6.8208E-02

ACR(B)=1.2E-1              0.1194      3.06E-02 -6.4192E-04 -2.0981E-02

HMR(LIQUID)=-1964          -1957.      5.00E+02   7.439      1.4878E-02

HMR(LIQUID)=-3500          -3478.      5.00E+02   21.67      4.3338E-02
```

```
HMR(LIQUID)=-4588              -4565.      5.00E+02   22.69      4.5382E-02

HMR(LIQUID)=-5239              -5217.      5.00E+02   21.50      4.3008E-02

HMR(LIQUID)=-5454              -5435.      5.00E+02   19.11      3.8216E-02

HMR(LIQUID)=-5233              -5217.      5.00E+02   15.50      3.1008E-02

HMR(LIQUID)=-4575              -4565.      5.00E+02   9.691      1.9382E-02

HMR(LIQUID)=-3481              -3478.      5.00E+02   2.669      5.3385E-03   118
HMR(LIQUID)=-1950              -1957.      5.00E+02  -6.561     -1.3122E-02
```

LIST_STORE_FILE

This command is for the PARROT module.

Use the LIST_STORE_FILE command to display the name of the store file and its full path.

LIST_SYMBOL_IN_GES

This command is for the PARROT module.

Lists TP-function(s) for the entered model parameters for phases in the system on screen. In many cases, the optimizing variables are parts of the TP-functions which in turn are entered in model parameters for various phases in the GIBBS workspace.

This command is a way to find out how the functions depend on the optimizing variables. In the PARROT module the list is only shown on screen, not written to any file (which the LIST_SYMBOL command in the GIBBS module does).

Syntax	LIST_SYMBOL_IN_GES
Prompt	`Name: <Symbol name>` Specify a symbol name. Only those symbols that match this name are listed. Or press <Enter> for a list of all available symbols entered in the system.

OPTIMIZE_VARIABLES

This command is for the PARROT module.

Perform variable optimization. All system-definition data needed for the optimization is read from the current work file (*.PAR). The result of the optimization is automatically stored in the current work file.

Syntax	OPTIMIZE_VARIABLES
Prompt	`Number of iteration /N/: <Integral number of iteration>` Specify an integral number for the optimization iteration. The specified iteration number is shown as the default number. The PARROT module tries this number of different sets of values of the optimizing variables unless it has converged earlier, or has given up earlier.
	It initially takes a small step in each variable to find the steepest slope. You can give zero iteration to calculate the error in all selected experiments, and then use LIST_RESULT to check how good (bad) the current fit is.

READ_PARROT_WORKSPACES

This command is for the PARROT module.

Workspace Files

Read the previous PARROT/GIBBS/POLY workspaces back to replace the current PARROT/GIBBS/POLY workspaces. It is useful if late changes made through various PARROT/GIBBS/POLY commands are not satisfactory.

Syntax	READ_PARROT_WORKSPACES
	The previous PARROT/GIBBS/POLY workspaces are always associated with the latest action to either open a work file by SET_STORE_FILE, or to create a work file by CREATE_NEW_STORE_FILE (either interactively in the PARROT module or through a MACRO_FILE_OPEN of an *SETUP.TCM file), or to update the work file by SAVE_PARROT_WORKSPACES.
	Unlike the READ commands in other modules (e.g. GIBBS or PLOY), this command in the PARROT module does not ask for the file name where to read a previously opened/created/updated PARROT/GIBBS/POLY workspaces, for the reason described above.
	You cannot use this command if there is no work file opened or created already.

RECOVER_VARIABLES

The RECOVER_VARIABLES command is used to set back the values of all variable to the start values.

REINITIATE

This command should not be used unless you want to destroy the current PARROT workspace. However, this PARROT command does not reinitiate the GIBBS/POLY3 workspaces.

This command is for the PARROT module.

The REINITIATE command is used to reinitiate the workspace used by PARROT. All output and optimizing conditions are given their default values. All variables are set fixed with their value equal to zero.

RESCALE_VARIABLES

When using the RESCALE_VARIABLES command, the current values of all the parameters are copied to their start values and the scaling factors for further optimization. Thus it should be done now and again, in particular if you think the optimization results are improved after the previous run(s), or if any variable changes more than a factor of 10.

SAVE_PARROT_WORKSPACES

This command is for the PARROT module.

If the latest changes made through various PARROT/GIBBS/POLY commands are as required, use this command to save the current workspace (i.e. data area) used by the PARROT program (also including the current GIBBS and POLY workspaces), onto the present work *.PAR file which has already been opened by SET_STORE_FILE or been created by CREATE_NEW_STORE_FILE (either interactively in the PARROT module or through a MACRO_FILE_OPEN of an *SETUP.TCM file).

> The PARROT/GIBBS/POLY workspaces are updated after each PARROT/GIBBS/POLY command. This means the current PARROT/GIBBS/POLY workspaces are always updated onto the latest work *.PAR file that is associated with the latest SET_STORE_FILE or CREATE_NEW_STORE_FILE command.

Workspace Files

Syntax	SAVE_PARROT_WORKSPACE
	Unlike the SAVE commands in other modules (e.g. GIBBS or PLOY), this command in the PARROT module does not ask for the file name where to save the current PARROT/GIBBS/POLY workspaces, for the reason described above. You cannot use this command if there is no work *.PAR file opened or created already.

SET_ALTERNATE_MODE

Turn the alternate mode on or off.

With the ALTERNATE mode is possible to include functions to be evaluated together with an alternate calculation and to select ALTERNATE mode for each experimental equilibrium.

The alternate mode is described in About Alternate Mode. It should be used only to optimize start values of the model parameters in the beginning of the assessment.

Syntax	SET_ALTERNATE_MODE
Prompt	`On /Y/:` By default alternate mode is ON.

SET_EXTERNAL_PARAMETER

This command is for the PARROT module.

Optimize model parameters of the so-called external models, which may not be as fully-implemented/integrated parts inside the GIBBS system and thus are independently defined within user-specified/written source codes. This command makes links between the PARROT optimizing variables and external model parameters.

In order to be able to build the specified external model and to use this SET_EXTERNAL_PARAMETER command, it requires you to first write codes for a preferred external model (as it is not within the standard GIBBS system of the Thermo-Calc software) and then provide it to a consultant at Thermo-Calc Software AB for the purpose of including the external model in a separate DLL that is interactively connected to the software. For more information, see theConsultancy page on our website.

Syntax	SET_EXTERNAL_PARAMETER
Prompt	`External name: <Parameter name in the external model>` Correctly specify the parameter name defined within a specified/written external model.
	`As optimizing variable number: <n>` Give the number of the PARROT optimizing variable, which should have a unique link to the specified parameter name of the external model. For example, @@ Link PARROT variables to CAM parameters:

```
SET-EXTER-PAR GT(SLAG_A,O-2,SI+4,CA+2) 1
SET-EXTER-PAR ET(SLAG_A,O-2,SI+4,CA+2) 2
SET-EXTER-PAR EXT(SLAG_A,O-2,SI+4,CA+2) 3
```

SET_FIX_VARIABLE

Prescribe a fixed value to a variable. The variable is considered as a constant at the optimization, usually after successful optimization runs for some specific variables (for some of the phases in the system). Such fixed variables can also be set back for further optimization run by using SET_OPTIMIZING_VARIABLE.

Syntax	SET_FIX_VARIABLE
Prompts	`Variable number: <Variable number(s)>` Specify the number of the variable. It is possible to give a range by giving two numbers with a hyphen in between (no spaces allowed), e.g. `1`. The parameters within the limits are set fixed to their current values (no question of values).
	`Start value /xxxx.xxxxx/: <A value to be fixed>` Specify a numerical value to be fixed for the selected variable (only when one variable number is specified at the previous prompt). The current value for the selected variable is shown as default. If a range of variable numbers is specified at the previous prompt, this question is not prompted, and the current values are used as fixed values.

SET_OPTIMIZING_CONDITION

This command is for the PARROT module.

Specify the conditions for the optimization. The default values are chosen automatically by the PARROT program, and in most cases these should not be changed.

> The optimization stops when the sum of errors decreases by this value, even though it might be possible to increase it further with a new OPTIMIZE command.

Syntax	SET_OPTIMIZING_CONDITION
Prompt	`Relative standard deviation for experiments? /N/:` By default the standard deviation of the experimental determinations are absolute values. Enter Y if these are used as relative weighting factors. The estimated standard deviations of the optimized variables might be different for the two cases.
	`Min save on file? /Y/:` Specify whether the program should minimize the transfer of data to and from the current work file during the optimization: • If the default (N) is kept, the workspaces are stored on the current work file after every iteration in the optimization procedure. • Enter Y to speed up the optimization. After optimization use the SAVE_PARROT_WORKSPACES command to update the progress onto the current work file.
	`Relative step for calculation of derivatives: /1e-04/: <xxx>` In the calculation of the correlation matrix for equilibria with inaccuracy in the independent state variables, some numerical derivatives might have to be calculated. Specify the relative step (`xxx`) for the calculation of these derivatives.
	`Maxfun (va05ad): /100/: <n>` The maximum number of iterations in the optimization. The same value set by the OPTIMIZE command.
	`Dmax (va05ad): /100/: <n>` An estimate of the maximum distance between the start and the final values of the variables. A smaller value makes the program vary the parameters with smaller factors.

Syntax	SET_OPTIMIZING_CONDITION
	`H (va05ad): /1e-04/: <xxx>` The step used in the scaled variables for calculating numerical derivatives during the optimization.
	`Acc/(initial sum of squares) (va05ad): /.001/: <xxx>` The break condition for the optimization. The accepted value is the difference between the true minimum and the calculated one.

SET_OPTIMIZING_VARIABLE

This command is for the PARROT module.

Specify which variable value should be estimated at the optimization. Such a variable can have a value of zero or another start value, or is fixed by SET_FIX_VARIABLE prior to the previous optimization run.

For a good reference prior to this command, a list of all variables (which are used to define various parameters for phases in the optimizing system, as pre-entered in the *SETUP.TCM file or interactively entered in the GIBBS module) are obtained by using LIST_ALL_VARIABLES.

Syntax	SET_OPTIMIZING_VARIABLE
Prompts	`Variable number: <Variable number(s)>` Specify the number(s) for the variable(s) to be set. Any non-zero parameter within the range is allowed to be optimized. A parameter with a current value equal to zero must be specified explicitly here in order to be optimized. Specify a range by giving two numbers connected by a hyphen (no space allowed!), e.g. `2-8`. Under this circumstance, no question of start values are asked.
	`Start value /xxxx.xxxxx/: <A guess value>` Specify a start guess of the optimum value (only when one variable number is specified at the previous prompt). The current numerical value for the selected variable is shown as default. This guess is critical as the initial guess of all parameters must make it possible to calculate the selected equilibria. If a range of variable numbers is specified at the previous prompt, this question is not prompted, and the current values (as start values) are not changed.

SET_OUTPUT_LEVELS

This command is for the PARROT module.

Choose the type of information the PARROT module gives during the optimization procedure and when listing results.

Syntax	SET_OUTPUT_LEVELS
Prompts	`List increment /1/: <Increment in iteration number>` Specify the increment in iteration number for which information is listed on screen during the optimization. By giving a larger number it shortens the list.
	`List sum of squares: /Y/:` Choose whether the sum of squares is listed on screen during the optimization procedure.
	`List scaled variables: /Y/:` Choose whether the scaled variable values are listed on the terminal during the optimization procedure.
	`List weighted residuals: /N/:` Choose whether the weighted residuals are listed on the terminal during the optimization procedure.
	`List all parameters: /N/:` Choose whether all parameters in the models are listed in LIST_RESULT.
	`List correlation matrix: /N/:` Choose whether the correlation matrix of the variables are listed with the commands LIST_RESULT and LIST_ALL_VARIABLES.

SET_SCALED_VARIABLE

This command is similar to SET_OPTIMIZING_VARIABLE in that it specifies start values for optimizing variables. The difference being it is functional for only one optimizing variable at one time. It also prescribes a minimum and maximum value for the variable. During the optimization runs, the variable value is limited within this min-max range.

Such a variable may have a value of zero or another start value, or may be fixed by SET_FIX_VARIABLE prior to the previous optimization run. For a good reference prior to using this command, a list of all variables (which are used to define various parameters for phases in the optimizing system, as entered in the *SETUP.TCM file or interactively entered in the GIBBS module) is obtained by using LIST_ALL_VARIABLES.

Syntax	SET_SCALED_VARIABLE
Prompts	`Variable number: <Variable number(s)>` Specify the number for an optimizing variable to be set. Any non-zero parameter is allowed to be optimized, and a parameter with a current value equal to zero must be specified explicitly here in order to be optimized.
	`Start value /xxxx.xxxxx/: <A guess value>` Specify a start guess of the optimum value. The current numerical value for the selected variable is shown as default. This guess is critical as the initial guess of all parameters must make it possible to calculate the selected equilibria.
	`Min value /xxxx.xxxxx/: <A guess value>` Specify a minimum guess of the optimum value. It should be smaller than, at least equal to, the current start value for the selected variable.
	`Max value /xxxx.xxxxx/: <A guess value>` Specify a maximum guess of the optimum value. It should be larger than, at least equal to, the current start value for the selected variable.

SET_STORE_FILE

This command is for the PARROT module.

Specify a store file (work file) to be used for compilation and optimization. The *.PAR work file must be created (CREATE_NEW_STORE_FILE) as a store file. The GIBBS, POLY and PARROT workspaces are read from the specified store file (with a default extension of PAR).

Syntax	SET_STORE_FILE
Prompt	Enter a `*.PAR file name` in the **File name** field and specify the working directory in the **Look in** field. Normally the default file-type in the **Files of type** field is the correct one for the PARROT workspace format (i.e. *.PAR file). Click **Open** or **Cancel** as applicable.

EDIT_EXPERIMENTS (ED_EXP) Submodule Commands

EDIT_EXPERIMENTS (ED-EXP) is a submodule of PARROT.

In this section:

ADVANCED_OPTIONS

This command is available with the POLY and ED-EXP modules.

ADVANCED_OPTIONS described for the POLY module.

Syntax	ADVANCED_OPTIONS
Prompt	`Which option? /Step_and_Map/:  <Option>`

CHANGE_STATUS

This command is available with the POLY and ED-EXP modules.

In the POLY module, set the status for components, species and phases in the defined system for all the sequential calculations (single-point, stepping, and mapping) in equilibrium or local/partial equilibrium state. Each component, species and phase has a status. The default status is `ENTERED`.

The most important use is to calculate metastable equilibria and metastable phase diagrams by setting some phases (that would otherwise be stable) to the SUSPENDED or DORMANT phase-status. Another important applications is to calculate paraequilibria by setting some components to the SPECIAL component-status.

For a component and for a species, the status can be one of the following:

- `ENTERED`: the component(s) or species are included in the calculation. This is the default status.
- `SUSPENDED`: the component(s) or species are not considered in the calculation.
- `SPECIAL`: the specified component(s) are not included in summations for mole or mass fractions. It only works for component(s).

> Only component(s) can have the status SPECIAL, which implies that these are not included in summations for mole or mass fractions.

For example, for the *u-fractions* or other normalized fractions, when one or more of the components are excluded from the summation, you must specify which component(s) should be excluded from the calculation of mole or mass fraction. This component status is particularly useful when calculating paraequilibrium states. Such component(s) are normally interstitial component, and must have the status SPECIAL. This is assigned by the CHANGE_STATUS command.

Syntax	CHANGE_STATUS
Prompts	`For phases, species or components? /Phases/: <Keyword>` *Keyword* = phase or species or components
	`Phase name(s): <Name(s) of the phase(s)>` For `phase` as the keyword, the names of the phases that have their status changed must be given (all on one line). A comma or space must be used as separator. The status to be assigned to the phases can also be given on the same line if preceded with an equal sign (=).

Syntax	CHANGE_STATUS
	An asterisk, *, can be used to denote all phases. The special notations `*S`, i.e. a wildcard * directly followed by an `S`, sign, means all suspended phases. In the same way, `*D` means all dormant phases, and `*E` means all entered phases.
	`Name(s): <Name(s) of the Species or Component(s)>` For species or components as the keyword, the names of the species or components that have their status changed must be given (all on one line). A comma or space must be used as separator. Similarly to the case of phase as the keyword, the status to be assigned to the species or components can also be given on the same line if preceded with an equal sign =. An asterisk, *, can be used to denote all species or components. The special notations `*S`, i.e. a wildcard * directly followed by an `S`, sign, means all suspended species or components. In the same way, `*E` means all entered species or components.
	`Status /Entered/: <New status>` The `new` status to be assigned must be given. For species, the values `ENTERED` or `SUSPENDED` can be used. For the POLY module, using the `Entered` or `Suspended` status here has the same result as using the commands MAKE_COMPONENT_ENTERED and MAKE_COMPONENT_SUSPENDED. The exception is that any existing conditions that depend on a suspended component are removed when using the MAKE_COMPONENT_SUSPENDED command. For components, the status `ENTERED`, `SUSPENDED` or `SPECIAL` can be given. SPECIAL means that this component is excluded from sums for mole fractions and mass fractions, which is useful when calculating the *ufractions* or other normalized fractions of system components. For phases, the status `ENTERED`, `SUSPENDED`, `DORMANT` or `FIXED` can be given. DORMANT means the same as suspended but the driving force is calculated. FIXED means that it is a condition that the phase is stable at a certain amount. For example, for the ufractions, when one or more of the components are excluded from the summation, you must specify which component should be excluded from the calculation of the mole fraction. This component must have the status SPECIAL. This is assigned by the CHANGE_STATUS command: `Change_Status comp C=special`.
	`Start value, number of mole formula units /0/: <Initial amount>` For ENTERED phases, an `initial amount` of the phase can be given. Normally, 0 is given if the phase is not likely to be stable, and 0.5 or 1 or any positive number if the phase could be stable, but such an initial amount is only used as the rough starting estimation in the equilibrium calculations.
	`Number of mole formula units /0/: <Equilibrium amount>`

Syntax	CHANGE_STATUS

For FIXED phases, the `equilibrium amount` of the phase [always using an initial estimation being the `NPF(phase)` value which it is the normalized mole number of components (per mole formula unit) of the specific status-fixed phase] must be given. If the equilibrium amount is zero, then the phase is at its stability limit.

NOTE WHEN SPECIFYING A FIXED PHASE STATUS

Special attention should be paid when specifying a FIXED phase status in equilibrium calculations (for single points, stepping or mapping calculations), as described below.

The phase amount variables, NP(phase), BP(phase) and VP(phase), as well as all their M/W/V-suffixed quantities, should not be used as conditions. Instead, use the CHANGE_STATUS command to set a relevant condition, e.g. `CHANGE_STATUS phase <phase>=fix <amount>` where the fixed <amount> is roughly the same as the F-suffixed quantity `NPF(phase)`.

The `NPF(phase)` quantity is the normalized mole number of components (per mole formula unit) of the specific phase in the defined system, which unlike other `F`-suffixed state variables [e.g. GF (phase), HF(phase) and DGF(phase)] cannot be directly applied in any POLY command, implying that it cannot be directly evaluated or listed/shown. If intended to shown such a normalized phase amount value in an equilibrium state, you should use a properly-entered symbol (function or variable), for example: `NPFabc = NP(abc)/NA` or `NPFabc = NPM(abc)/NA*N`. N is the total system size (in mole). The NA value is a quantity that is phase-dependent (and sometimes also equilibrium-dependent for ionic solution phases), and is the total atomic number in a mole-formula-unit of the specific phase abc (excluding interstitial component and, of course, vacancy). For example, the SIGMA, FCC, BCC and LIQUID phases (among others) in a defined Fe-Cr-Ni-C-N-O system (retrieved from a specific database) may be modeled by certain models, and their NA values must be evaluated in different ways, as described below:

```
LIQUID (C,Cr,CrO3/2,Fe,FeO,FEO3/2,N,Ni,NiO)1 NA = 1

FCC_A1 (Cr,Fe,Ni)1(Va,C,N,O)1 NA = 1

BCC_A2 (Cr,Fe,Ni)1(Va,C,N,O)3 NA = 1

SIGMA (Fe,Ni)8(Cr)4(Cr,Fe,Ni)18 NA = 30
```

If in the same Fe-Cr-Ni-C-N-O system the liquid solution phase is modeled by the Two-Sublattice Ionic Liquid Model, i.e.:

```
IONIC_LIQ  (Cr+3,Fe+2,Ni+2)p(VA,C,N,O-2,FEO3/2)q,7
```

then the evaluation of its NA value becomes even more complicated:

```
NA = p + q*yC2 + q*yN2 + q*yO2□2 + q*yFeO2 3/ 2
```

where the stoichiometric coefficients *p* and *q* are also dependent upon the real equilibrium state (rather than having fixed values in the system). Similar situations occur for other (solid) phases which are described by a multiple sublattice model with ionic constituents, such as SPINEL and HALITE phases in some databases.

There is no strange thing when using a zero value [i.e. `0`] in a FIXED phase-status, since it means the specified phase is stable in equilibrium state but has a zero-amount of mass in the equilibrium calculations; in other words, on a phase diagram, the specific phase is on a zero-fraction line (ZFL), i.e. it starts becoming stable on one side of a corresponding phase-boundary line or unstable on the other side of the same boundary. It is often and efficient to do so when calculating e.g. solidus equilibrium states.

However, when a non-zero value [it must always be positive; e.g. 1 or 0.5 or 0.3 or 1.5] is to be specified in a FIXED phase-status, it is unnecessarily the exactly same stable amount of the specific

Syntax	CHANGE_STATUS
	FIXED-status phase in a calculated equilibrium state any longer; instead, the <equilibrium amount> value is the NPF(phase) value that is only roughly used as the estimated starting-value of the FIXED-status phase in the equilibrium calculations. Therefore, a FIXED-status for a liquid phase being unity does not necessarily imply that it is a liquidus equilibrium state (where the liquid phase is in equilibrium with some solid phases but the liquid phase takes all the mass in the defined system). A unity value for setting the liquid phase status in calculating liquidus equilibrium state can only be used when the liquid mixture phase is predefined as a single-sublattice solution phase (such as metallic liquid phase in multicomponent alloy systems) and the total system size as one mole (i.e. N=1). When a phase is described by a solution model in which two or more sublattices are considered and these sublattice sites may also have different stoichiometric coefficients [meaning that the mixture phase could have more than one atom in formula [NA>1; see some examples above], the unity value should not be used when setting the FIXED status for the phase; instead, you should use an appropriate value that ranges from 0 to a NPF(phase) value that equals to or is smaller than 1/NA (if the total system size N=1) or 1/NA*N (if N differs from unity). For this reason, if a multicomponent system bears an IONIC_LIQUID phase that is described by the Two-Sublattice Ionic Liquid Model (or any other multiple-sublattice ionic solution phases), it is difficult to use a proper `NPF(ION_LIQ)` value in setting its FIXED phase-status, because that should be less than (or equal to) the complex value of $N/[p + q{*}^{y}C2 + q{*}^{y}{}_{N}2 + q^{*y}{}_{O}22 + q^{*}y_{FeO}2\ 3/\ 2\ ]$.

Examples

For example, to obtain the metallic fraction in a system with carbon as an interstitial component, you can set the component status for carbon as `SPECIAL`:

```
Change_Status comp C=special
```

The `SUSPENDED` status for components and species does not always work as expected.

For a phase, it may have one of these statues:

- `ENTERED`: the phase(s) are included in the equilibrium calculations and these are stable if that minimizes the total Gibbs energy in the defined system. This is the default status for all phases already retrieved from the chosen database(s). An ENTERED phase-status is always associated with an initially-estimated amount [in mole number; normally, as 0 if the phase is not likely to be stable, and as 0.5 or 1 or any positive number if the phase could be stable] but it is only used as the rough starting value in the equilibrium calculations.

- `SUSPENDED`: the phase(s) are not considered in the equilibrium calculations.
- `DORMANT`: the phase(s) are not considered in the equilibrium calculations but their driving forces for precipitation are calculated.
- `FIXED`: it is an equilibrium condition that the status-fixed phase must be stable, and be in equilibrium at a specified amount [always using an initial estimation being the `NPF(phase)` value which it is the normalized mole number of components (per mole formula unit) of the specific status-fixed phase]. See more descriptions at the end of this command.

COMMENT

This command is for the ED-EXP module.

The COMMENT command is only used in the *.POP/*.DOP files (so can be included with experimental data files) to write brief comments or descriptive information on a newly created equilibrium (experimental) data point or a set of points given in a table.

A comment can have a maximum of about 60 characters written on the same line.

COMPUTE_ALL_EQUILIBRIA

This command is for the ED-EXP module.

In ED_EXP and PARROT modules, each experiment is treated as an individual equilibrium with some measured values. These are created with CREATE_NEW_EQUILIBRIUM, and stored in an experimental data *.POP file and then compiled and saved in the POLY workspace of a PARROT work *.PAR file.

In the DICTRA module, you work with a .DOP file instead of a .POP file.

With COMPUTE-ALL-EQUILIBRIA, all equilibria from the current to the last experimental points are calculated. If an equilibrium calculation fails, the calculation is stopped at that equilibrium. Equilibria with weight zero is skipped.

A current or present experimental point means the latest selected or calculated one. Once used the current point turns to the last point in the data block; in such a case you first use SELECT_EQUILIBRIUM so that the current point is switched to a desired one.

For this command there is always a list output on screen, which consists of six columns for all experimental points available in the current data block:

- The first column is the *equilibrium identifier* (a number) assigned by this command,
- the second the *data label* assigned with LABEL_DATA,
- the third the *number of iterations*,
- the fourth the *current weight*, and
- the fifth the *current temperature*.
- In the sixth column the *fixed stable phases* are listed together with any *comment text* given after a COMMENT in the *.POP or *.DOP file.

If the weight is zero for an equilibrium columns 3-5 are replaced by the text *<unused>*. If the alternate mode is used for some experimental points, the listing is slightly different for such points. The 3-4 columns are displayed with *alt*, instead. If an alternate calculation is failed at one experimental point, the point is automatically assigned with a zero weight, and a warning message is shown above the data line (with all six columns).

CREATE_NEW_EQUILIBRIUM

This command is available with the POLY and ED-EXP modules.

During data-assessments using the ED_EXP module (a submodule of PARROT), you can, in the POLY module, create several equilibria with different sets of conditions and phases (but normally with the same set of components). By default, there is one equilibrium. To keep the set of conditions and phase for this equilibrium, create another one using this command, and use another set of conditions for that. Two equilibria may be useful to calculate easily the enthalpy difference between two states. In the PARROT module, the experimental information is stored as a sequence of equilibria.

Syntax	CREATE_NEW_EQUILIBRIUM
Prompts	`Equilibrium number /2/: <A new equilibrium number>` Each equilibrium in the POLY workspace is identified by a unique integer number. Such an equilibrium number can be recalled with SELECT_EQUILIBRIUM.
	`Initiation code /2/:` When an equilibrium is created, you can choose to `ENTER` all components and phases (initiation code 2), `ENTER` the components only (initiation code 1) or `SUSPEND` everything (initiation code 0). No other values are legal. The entered components and phases can later be changed with CHANGE_STATUS.

DEFINE_COMPONENTS

This command is available with the POLY and ED-EXP modules.

Change the set of components. By default, the elements are used as components. The set of components can be important because some conditions are set using components, for example, the amounts, activities or chemical potentials.

For example, in the system Fe-Si-O, you can define FEO, FE2O3 and SIO2 as components, thus replacing the default FE, SI and O.

> This implies a command REINITIATE_MODULE and it should be given as the first command in the POLY module.

Syntax	DEFINE_COMPONENTS
Prompt	`Give all new components / existing components/: <New components>` The `new components` must be specified all on one line. These replace the existing component definitions. The number of components cannot be changed with this command. Use CHANGE_STATUS instead.
	To keep some existing components, it is recommended that you also enter these on the line. Otherwise, the added new components may not be defined correctly. This is especially important if some components are built out of several elements. The new components do not have to be present as species.

DELETE_SYMBOL

This command is available with the POLY and ED-EXP modules.

Use the DELETE_SYMBOL command to remove symbols i.e. constants, variables, functions or tables.

Syntax	DELETE_SYMBOL
Prompt	`Name: <Name of a symbol>` Specify the name of the symbol to be deleted. Only one symbol can be deleted each time.

ENTER_SYMBOL

This command is for the ED-EXP module.

The GES, POLY and POST modules also have a command with the same name.

Symbols are a useful feature modules to define quantities that are convenient. Symbols can be constants, variables, functions, or tables.

Syntax	ENTER_SYMBOL
Prompt	`Constant, Variable, Function or Table? /Function/: <Keyword>` The `Keyword` can be specified as `CONSTANT`, `VARIABLE`, `FUNCTION`, or `TABLE`. • CONSTANTS can only be entered once and is a means of using a name for a numeric value. For example, the value of 1 atmosphere in Pascal can be denoted by `P0` after the command ENTER_CONSTANT `P0=101325`. Defined constants can be used as values in condition assignments, for example, `SET-COND P=P0`. • FUNCTIONS are expressions of state variables or other functions. These expressions are saved, and whenever a function value is requested all functions are evaluated. The reason for this is that they may depend on each other. • VARIABLES are similar to functions because they can also be expressions of state variables. However, contrary to functions, they are only evaluated when they are entered or if they are explicitly named in an EVALUATE_FUNCTIONS command. It is possible to enter a variable with a new expression any time. This expression is evaluated directly and its value stored as the value of the variable. Defined variables can be used as values in the SET_CONDITION command. • TABLES are used for listing results from the STEP or MAP commands. A table consists of a list of any number of state variables, functions, or variables. Defined tables can also be used in the POST (post-processor) module. There is a special connection between tables and variables. If a variable is used in a table, it is evaluated for each line of the table in the TABULATE command or when the table is used in a plot.
	`Name: <Name of the symbol>` Each symbol has a unique name that must start with a letter and can have maximum 8 characters. Legal characters include letters (either UPPER or lower case), digits and underscore _. Any other special character, such as parentheses (and), plus +, minus -, slash / or \, full stop (.), are illegal for symbol names. You can enter the symbol name and the value or function on the same line; these must be separated

Syntax	ENTER_SYMBOL

with an equal sign =, for example, `TC=T-273.15` or `T_C=T273.15` which stands for a definition of temperature in Celsius. Otherwise, these questions are asked.

> For different types of symbols (constant, function, variable, or table), the questions have different prompts.

`Function: <Definition for a function or variable>`

Functions and *variables* are evaluated from an expression of state variables or other functions, constants, or variables. The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers).

Unary functions like `LOG`, `LOG10`, `EXP`, `SIN`, `COS`, and `ERF` can also be used. An expression can be continued on more than one line. An expression should be terminated by a semicolon (;) or an empty line (press <Enter> at the next prompt).

Examples of function expressions:

- `GM(LIQUID)`: The Gibbs energy of liquid per mole component
- `H.T/4.184`: The heat capacity of the system in calories
- `ACR(CR)/X(FCC,CR)`: The activity coefficient for Cr in FCC
- `T-273.15`: The temperature in Celsius

`&: <Continuation of the definition for the symbol>`

The ampersand & means that you can continue to write the function on the new line if one line is not enough for the function. If you finish the function press <Enter> again.

`Value: <Value for a constant>`

A *constant* can only be assigned a numeric value once.

`Value or expression: <Value of expression for a variable>`

A *variable* can be assigned a numeric value or an expression. An expression is evaluated immediately and discarded. Only the numeric value is kept. This gives a possibility to save a value between calculations with different conditions because all state variables and functions are evaluated for the new conditions.

`Variable(s): <Variable(s) in a table>`

A *table* consists of a list of state variables or functions. One way to obtain results from a STEP command is through a table.

Example:

```
ENTER TABLE K=T,X(LIQ,C),X(LIQ,CR),ACR(C)
```

Which means that the table called K contains four columns, i.e. the temperature, the mole fractions of C and Cr in the LIQUID phase, and the activity of C.

To show the temperature in Celsius in a table, give the command ENTER_FUNCTION `TC=T-273`; and then use the symbol `TC` in the table.

`& <Continuation of the definition for the table>`

Syntax	ENTER_SYMBOL
	The ampersand `&` means that you can continue to write the table on the new line if one line is not enough for the table. If you finish the table press `<Enter>` again.

EVALUATE_FUNCTIONS

This command is available with the POLY and ED-EXP modules.

The value of one or more or all entered functions or variables are evaluated and listed.

Syntax	EVALUATE_FUNCTIONS
Prompt	`Name(s): <Name(s) of defined function(s)>` The names of one or more entered functions or variables must be specified. By typing a wildcard *, all functions and variables are evaluated. Variables are evaluated only if these are explicitly named.

EXPERIMENT

This command is for the ED-EXP module.

This command is used in original experimental data files (*.POP or *.DOP), but can also be given interactively inside the ED-EXP module, to change the value or uncertainty of an experiment or to add more experimental information.

In the DICTRA module, you work with a .DOP file instead of a .POP file.

An experiment usually consists of two parts with a colon (:) separating them:

- as a quantity relation, and
- as the uncertainty of the value for the quantity,

The quantity relation can be a normal POLY module condition or an inequality (which is similar to condition but the relation between the quantity and given value is not in equality, i.e. < or >). The uncertainty can be expressed as an absolute value or relative to the value (x%).

An experiment that uses an inequality gives zero contribution to the sum of errors in the optimization procedure of PARROT if the value is on the right side. If the value is on the wrong side, the value after the colon determines how steeply the error increases with the value.

Syntax	EXPERIMENT
	The experiment must be typed after the command. Several experiments can be given on the same line. The syntax of EXPERIMENT is similar to a CONDITION. Usually, a state variable set equal to a value with a given uncertainty is specified after the colon (:). For example, `T=1273.15:5`. An inequality, < or >, can also be used. For example: `ACR(C)<-0.01:0.001, W(BCC,AG)>0.05:10%`

Additional Information About the Experiment Command

A typical experiment added interactively specifies that a phase should not be stable in a certain experiment, because a phase may appear in a range of composition or of temperature where it has never been observed during the optimization. A phase is unstable if its driving force is negative, and you can add experimental information to enforce that. For example, you can suppress the HCP phase in an existing experimental point:

```
CHANGE-STATUS HCP=DORMANT

EXPERIMENT DGM(HCP)<-.001:.0001
```

DGM is the POLY variable for the driving force that is already divided by `RT`, and it is dimensionless. Only dormant phases can have driving forces larger than zero, as this indicates that these would be stable if allowed to form. The experiment in the above case tries to modify the model parameters to make the HCP phase unstable.

More general examples of experiment definitions:

```
EXPERIMENT X(LIQ,PB)=.10:.01 X(FCC,PB)=0.02:.01

EXPERIMENT ACR(PB)=0.8:5%

EXPERIMENT T=700:5
```

The first experiment above describes a tie-line where the experimentally measured mole fraction of Pb is 0.1 in the liquid phase and 0.02 in the FCC phase, and its uncertainty is 0.01 for both measurements. The second experiment is that the activity of Pb should be 0.8 with an uncertainty of 5 percent.

The reference state of the component Pb must be set with the command SET_REFERENCE_STATE. The final one is that the temperature should be 700 K with an uncertainty of 5 degrees.

Experiments that are functions of states variable(s) must be described as the defined functions. For example:

```
ENTER_FUNCTION HTR=HM(LIQUID)-HM(FCC);

EXPERIMENT HTR=7000:1000
```

EXPORT

This command is for the ED-EXP module.

Transfer/export a calculated value from an equilibrium to an optimizing variable in the PARROT workspace. Thus the value can be used, for example, in the Gibbs energy description of a phase. This variable should not be optimized (i.e. it should be set as a fixed variable in PARROT).

Syntax	EXPORT
Prompt	`Function name: <Function name>#<n>` Specify the name of the function, the value of which should be transferred to a `V` variable. The number (n) of the `V` variable must be given after the function name, separated by hash character #. The function name is UPPER/lowercase sensitive, and it should normally be given in UPPER case.

	Example
	`Enter_function strngy=gm(fcc).x(cu);`
	`Export strngy#6`
	This transfers the value of the partial derivative of the Gibbs energy of the FCC phase with respect to the mole fraction of Cu to the optimizing variable 6 (i.e. `V6`).

FLUSH_BUFFER

This command is for the ED-EXP module.

This command is only used in the *.POP file (i.e. it can also be used in the experimental data files). It is needed if the number of experiments require more space than can be fitted into one buffer.

In the DICTRA module, you work with a .DOP file instead of a .POP file.

When the PARROT program compiles experiments, it informs if any FLUSH commands are needed. FLUSH_BUFFER terminates the current block, saves it to the work file and starts a new block. With the READ command in the EDIT-EXP module, you can select the block to edit.

Syntax	FLUSH_BUFFER
	After a FLUSH_BUFFER command, the workspace is reinitiated and all functions or constants must be entered again in the *.POP file. You can take advantage of this; for example, you can use the FLUSH command to have blocks with different components in one *.POP file.

GRAPHICS_PLOT

This command is for the ED-EXP module.

This command can help create a experimental data file from the *.POP file. Several data sets and different symbols are allowed.

In the DICTRA module, you work with a .DOP file instead of a .POP file.

Syntax	GRAPHICS_PLOT
	`<Dataset#> <X value> <Y value> <Symbol index>`

IMPORT

This command is for the ED-EXP module.

Transfer/import the value of one of the optimizing variables to a constant. Normally, it is directly used inside an experimental data (*.POP) file. It is the opposite of the EXPORT command.

In the DICTRA module, you work with a .DOP file instead of a .POP file.

The IMPORT command is useful if several experiments are done at the same activity of a component, but this activity is not known. The activity should then be optimized and all equilibria with the same activity should use the same value. In this case the variable must be set as an optimizing variable, and an initial guess of the activity should be given. During the optimization, the PARROT program tries to find the activity that gives the best fit.

If an approximate value of the activity is known, it can be supplied as an experiment.

Syntax	IMPORT
Prompt	`Constant name: <Constant name>#<n>` The value of the `V` variable must be assigned a symbolic constant. The number (`n`) of the `V` variable must be given after the constant name, separated by hash character `#`. The constant name is UPPER/lowercase sensitive, and it should normally be given in UPPER case.

	Example
	`Enter_constant acu=0.1`
	`Import acu#2`
	This transfers the value of the optimizing variable 2 (i.e. `V2`) to the constant `ACU`.

LABEL_DATA

This command is for the ED-EXP module.

Add a label to the experimental equilibrium point, either as a single point or several points given individually or in a table. The label is maximum four characters and must start with the letter `A`. Normally, it is directly used inside an experimental data file (*.POP).

In the DICTRA module, you work with a .DOP file instead of a .POP file.

Several experimental equilibria can be given the same label, and the label can be used with SET_WEIGHT to assign the same weight to all equilibria with the same label.

Syntax	LABEL_DATA
Prompt	`Label? /A1/: a<bcd>` Specify a textual label (as maximum characters and must start with the letter `A`) for the current experimental equilibrium point(s).

LIST_ALL_EQUILIBRIA

This command is for the ED-EXP module.

Syntax	LIST_ALL_EQUILIBRIA
	List all the details (including equilibrium indicators, labels, iteration numbers, weight, and fixed phases or comments) of all equilibrium points from the current one to the last one on screen. You can always use SELECT_EQUILIBRIUM to select a specific point as the current equilibrium point for such a list.

LIST_CONDITIONS

This command is available with the POLY and ED-EXP modules.

All the conditions that are set by the SET_CONDITION command and the command-sequence CHANGE_STATUS PHASE `=FIXED <0 or 1 or alike>`, are listed. The current conditions are also listed by the LIST_EQUILIBRIUM command. The degree of freedom in the defined system is also shown.

- If this is zero, you can perform a COMPUTE_EQUILIBRIUM command.
- If it is larger than zero, some more conditions are required, and you must further set additional ones, using SET_CONDITION or CHANGE_STATUS.
- If it is negative, then too many conditions are defined and the unnecessary ones conditions need to be removed using the SET_CONDITION command (with a value of NONE for the to-be-deleted condition) or the CHANGE_STATUS command (i.e. changing a FIXED status of a phase to another type of phase status, ENTERED or DORMANT or SUSPENDED).

Syntax	LIST_CONDITIONS

Example	`P=100000, T=800, N(NI)=1E-1, N=1`
	`FIXED PHASES`
	`FCC_A1=1 LIQUID=0    DEGREE OF FREEDO 0`

LIST_EQUILIBRIUM

This command is available with the POLY and ED-EXP modules.

The result (always in SI units) from the last calculated equilibrium is listed on screen or in a text file.

You can also execute this command if no calculation is made or if the calculation fails. Make sure to interpret the results accordingly.

Syntax	LIST_EQUILIBRIUM
Prompt	`Output to screen or file /Screen/: <File name>` The name of the text file where the list of the calculation results shall be written.
	`Options /VWCS/: <Option(s)>` Select the output units and formats by optionally specifying a combination of these letters. - *Fraction order:*`V` means VALUE ORDER; `A` means ALPHABETICAL ORDER. - *Fraction type*: `W` means MASS FRACTION; `X` means MOLE FRACTION. - *Composition*: `C` means only COMPOSITION; `N` means CONSTITUTION and COMPOSITION. - *Phase*: `S` means including only STABLE PHASES; `P` means including ALL NON-SUSPENDED PHASES.
	Default options are `VWCS`. If the output fraction type should be in mole fraction (rather than mass fraction), then give `VXCS` or type `X` (implying that in this case the options V, C and S are accepted as the listing manners for fraction order, composition and phase). If accepting all the default options, or if accepting all the altered options that had already changed when using this command previously, you can type `L_E,,,` or `LIST_EQUILIBRIUM ,,,` LIST_EQUILIBRIUM displays ORD (ordered) or DISORD (disordered) (when available). See CHANGE_LEGEND for details.

LIST_STATUS

This command is for the ED-EXP module.

There is also a POLY module command with the same name.

List the status of components, species or phases.

Syntax	LIST_STATUS
Prompt	Specify what to list: `Option /CPS/:`*<keyword(s)>* keyword = C or P or S, or any combination - `C`: list component status - `P`: list phase status - `S`: list species status - `CS`: list both components and species Default is `CPS`.
	The results depend on the key word specified in the options for CHANGE_STATUS, a table with the current status of phases or species or components, or the combinations, is shown: - For components, the statuses and reference states are listed. - For species, only the status is listed. - For ENTERED and FIXED phases, the status, driving forces and equilibrium amounts are listed.
	The metastable phases are listed in descending order of stability. To avoid long outputs only 10 metastable phases (in ENTERED status) are listed by lines, while all other less stable phases are merged onto one line. For DORMANT phases, their phase names and driving forces are listed. For SUSPENDED phases, only the phase names are listed.

LIST_SYMBOLS

This command is for the ED-EXP module.

There are also POLY and POST module commands with the same name.

Use this command to list the definitions for all constants, functions, variables and tables. In order to find the value of a function or variable, use SHOW_VALUE or EVALUATE_FUNCTIONS. A table is tabulated with the TABULATE command.

Syntax	LIST_SYMBOLS
	The defined variables are listed up together with the defined functions, but variable names are followed by a percentage sign `%`.

MAKE_POP_FILE

This command is for the ED-EXP module.

In the DICTRA module, you work with a .DOP file instead of a .POP file.

Use this command to make interactive changes and additions to the original experimental data file (the *.POP or *.DOP file). For example, to document or transfer the current or final experimental data to a *.POP file, this command will write it to a new *.POP file or overwrite previous versions.

Check the output carefully for errors. Tables in original *.POP files are written as individual experimental points. The output can be shown on screen or be saved as a new *.POP file where to write or overwrite the edited experimental information in a simple text format.

Syntax	MAKE_POP_FILE
Prompt	`Output to screen or file /Screen/: <POP/DOP-file name>` Specify a name of the new *.POP file where to write or overwrite the edited experimental information in a simple text format. If an existing *.POP file name is specified, it is overwritten.

READ_WORKSPACES

This command must be given each time the ED_EXP module is entered, unless it is already given once in ED_EXP and does not use LIST_RESULT or OPTIMIZE_VARIABLES in PARROT in between.

Syntax	READ_WORKSPACES
Prompt	`Block number /#/: <n>` The number of a data block that should be edited must be given. If there is no FLUSH_BUFFER command in the original POP file, then there is only one data block with the number 1.
	READ_WORKSPACE = READ This command is equivalent to READ_WORKSPACES in the POLY module, but it only reads the POLY workspace from the work file set by SET_STORE_FILE in the PARROT module.

REINITIATE_MODULE

This command is for the ED-EXP module.

The REINITIATE_MODULE command makes sure that the entire ED-EXP module is reinitiated to the original state.

Syntax	REINITIATE_MODULE
	All the defined components, defined conditions, changed status, entered symbols, defined independent axis-variables, calculated starting equilibrium-points, added initial equilibrium points, stepped/mapped equilibrium data, and so forth, are removed completely. The saved file name is restored to the default.

RESTORE_ALL_WEIGHTS

This command is for the ED-EXP module.

Restore a specific weight-set (previously saved by STORE_ALL_WEIGHTS) and assign all the different experimental points in the current data block with the previously-set weights in the sequential assessments.

Syntax	RESTORE_ALL_WEIGHTS
Prompt	`Set number (0 for list) /0/: <weight-set number>` The default value 0 is for a list on screen.

SAVE_WORKSPACES

This command is for the ED-EXP module.

In the PARROT workspace this command saves the current status of the ED_EXP submodule before you switch back to the PARROT module. This is required when you want to save equilibria changes, including changes to conditions, experimental data, and/or computed equilibria results, as well as any newly added equilibria.

With this command all the changes made in the ED_EXP submodule are saved in the PARROT workspace. This means you do not need to execute SAVE_PARROT_WORKSPACES in the PARROT module.

However, when in the PARROT module, additional changes can only be saved with the SAVE_PARROT_WORKSPACES command even if they have been made prior to executing SAVE_WORKSPACES in ED_EXP.

When you exit the ED_EXP (or Thermo-Calc), the next time the file is opened it is in the same state as when you executed the SAVE_WORKSPACES command. However, if you use OPTIMIZE_VARIABLES the computed results are automatically updated.

Syntax	SAVE_WORKSPACES
Prompt	`<File name>` Sometimes good starting values (SET_START_VALUE) are required to successfully get or compute an equilibrium correctly. In this case, it is important to save the computed equilibrium in the PARROT workspace. It is important to remember that the computed results can be ruined by improper optimizations. For this reason, it is suggested you save the .PAR file with a different name to back up the PARROT workspace.

SELECT_EQUILIBRIUM

This command is available with the POLY and ED-EXP modules.

If you create more than one initial equilibrium (during data-assessments using the PARROT/ED_EXP modules), you can switch between them using this command.

Syntax	SELECT_EQUILIBRIUM
Prompt	`Number /Next/: <Choice on equilibrium>` Options: `FIRST`, `LAST`, `NEXT`, `PREVIOUS` or `PRESENT`. Most commands affect only the `PRESENT` equilibrium. However, the REINITIATE_MODULE and DEFINE_COMPONENTS commands remove all the stored equilibria.

SET_ALL_START_VALUES

This command is available for the POLY and ED-EXP modules.

Set start values, e.g. if the calculation fails or if you have a miscibility gap or ordering. If temperature and pressure are not conditions, you are asked for values of them. Then for each phase prompt on if it should be stable and on its constitution.

Syntax	SET_ALL_START_VALUES
Prompts	`T /XXXX/: <Temperature in K>` If the temperature is not a condition, supply a guess of its final value (in K).
	`P /100000/: <Pressure in Pa>` If the pressure is not a condition supply a guess of its final value (in Pa).
	`Automatic start values for phase constitutions? /N/: <Y, N or F>` • For N, enter an initial amount of each entered phase and the major constituents or site fraction of each constituent. • For Y, the program automatically sets the start values for phase constitutions in all possible phases. • `F` is for force. In some cases the calculation fails because impossible conditions are set, e.g. `W(C)=1.5 [W(C)` is mass fraction and must thus be less than unity. The program tries to fulfill this condition by putting maximum amount of carbon in all phases, but can fail anyway. When you detect the error and set `W(C) to 0.015`, the calculation may still fail because it could start from the previous values. To get back to 'fresh' start values, choose `F`.
	`Should <phase> be stable /N/: <Y/1 or N/2>` A guess if this phase should be stable or not is requested. All entered phases are prompted for this question and next two. You cannot have more phases stable than you have components, but at least one (which dissolves all constituents) must be set as stable. For backward compatibility, this question can be answered by 1 (for Yes) or 0 (for No). The `phase` name may have a hash sign # followed by a digit, e.g. `BCC_A2#2`. For phases with miscibility gaps, there should be two phases with the same name but with different numbers after the hash sign.
	`Major constituent(s): <Name of major constituent(s) in the phase>` The constituent with the largest fraction in the phase should be specified. If there are more than one constituent with a large fraction, give them all on the same line. If the default major constituents should be used answer with an asterisk (*). By giving $ the constitution is not changed. If there should be no major constituent give NONE and or if the major constituent(s) are improperly specified, you are asked for individual fractions in the phase.

Syntax	SET_ALL_START_VALUES
	`Y(<phase>,<constituent>) /.XXXXXXXXXX/: <.YYYYY>` The current value (`.XXXXXXXXXX`) is default. You can accept the default by pressing <Enter> or give a new value (`.YYYYY`). The phase name or constituent name may have a hash sign # followed by a digit, e.g. `Y(BCC_A2#2,FE), Y(BCC_A2#2,C#2)`. For phases with miscibility gaps, there should be two phases with the same name but with different numbers after the hash sign. For phases with sublattices, the constituents in sublattice 2 or higher is also be suffixed with a hash sign # followed by a digit.

SET_ALTERNATE_CONDITION

This command is for the ED-EXP module.

A special command used in the experimental data *.POP file but also possible in the ED_EXP module. It is used only when you have specified that the alternate mode is set in the PARROT module.

In the DICTRA module, you work with a .DOP file instead of a .POP file.

The command syntax is almost the same as for the POLY command SET_CONDITION while the uncertainty should also be specified.

The alternate condition (including the normally POLY module condition plus uncertainly; see below) must be given explicitly, but can be given on the same line or on separate lines with each one started with the command.

Syntax	SET_ALTERNATE_CONDITION
Prompt	`State variable expression: <State variable name or linear expression>` Give either a state variable or a linear expression of state variables.
Options	**Description and Information**
State variables	Some of the state variables that can be used in conditions are: • `T`: temperature in the system (in K) • `P`: pressure in the system (in Pascal) • `N`: system size (mole number in moles) • `B`: system size (mass in grams) • `N(<component>)`: mole number of a component in the system • `X(<component>)`: mole fraction of a component in the system • `W(<component>)`: weight fraction of a component in the system • For the SET_CONDITION command this is `ACR(<component>)`: activity of a component in the system. For the SET-ALTERNATIVE_CONDITION command, this is `ACR` (`<phase>`,`<component>`) (activity of a component in a phase) • For the SET_CONDITION command this is `MUR(<component>)`: chemical potential of a component in the system. For the SET-ALTERNATIVE_CONDITION command, this is `MUR` (`<phase>`,`<component>`) (chemical potential of a component in a phase)

Syntax	SET_ALTERNATE_CONDITION
	- `X(<phase>,<component>)`: mole fraction of a component in a phase - `W(<phase>,<component>)`: weight fraction of a component in a phase - `ACR(<species>,<phase>)`: activity of a species referred to a phase - `MUR(<species>,<phase>)`: chemical potential of a species referred to a phase - `H`: enthalpy in the system (in J) - `HM(<phase>)`: enthalpy of a phase (in J/mol)

Additional prompts	`Factor: <A factor for the state variable, or a continuation>`
	This question means that the previous question was not answered. The program is then expecting a single state variable or a complete state variable expression, or the numeric factor in an expression with only one state variable. In a state variable expression a state variable may be preceded by a constant factor. An example of this is:
	`2*MUR(FE)+3*MUR(O)=-35000`
	This means that it should be a condition that two times the chemical potential of FE plus three times the chemical potential of O should be -35000 J/mol.

	`State variable: <A specified state variable, or a continuation>` This question is prompted if a single state variable name has not given in either the prompt `State variable expression` or `Factor`, or a state variable expression is given but the expression is incomplete, for example, `T-` or `2*MUR(FE)+`, for which the program is then expecting a continuation of the unfinished expression. You need to specify a state variable or a complete state variable expression, or complete the unfinished state variable expression. If a numeric factor is given before this prompt, only one state variable can be specified; otherwise, the program only takes the first state variable to complete the expression (i.e. the factor times the state variable).
	`Value /X/:  <A numeric value, a constant or a variable>` The value of the condition. This can be a numeric value, a constant or a variable. A suggestion is given as the default value. The special value `NONE` means that the condition is removed.
	`Uncertainty /None/:  <Uncertainty of the condition>` The uncertainty of the condition. This can be a numeric value, a constant or a variable. The default value `NONE` means that the uncertainty for the value specified above is zero. The uncertainty can either be expressed as an absolute value or relative to the value of the condition in percent (`x%`).

Notes	There are more state variables that can be used in conditions. For more information, type an INFO STATE_VARIABLES command in the POLY module. A condition is normally a value of a single state variable with its value.
	Example
	`T=1273.15   P=1E5`
	`X(C)=.002`
	`W(CR)=1.5`
	`ACR(CR)=0.85`
	`X(FCC,C)=.001`
	`H=-250000`

<table>
<tr><th>Syntax</th><th>SET_ALTERNATE_CONDITION</th></tr>
<tr><td></td><td>

```
HM(BCC)=-225000
```

A condition can also be a value of a linear expression involving more than one state variable.

<i>Example</i>

```
X(LIQ,S)-X(PYRR,S)=0
```

This means that it is a condition that the mole fraction of `S` should be the same in the LIQUID and PYRRHOTITE phases. In practice that should be the congruent melting point.

After the equal sign only a numeric value is allowed.
</td></tr>
</table>

SET_CONDITION

This command is available with the POLY and ED-EXP modules.

Specify the equilibrium conditions for the calculation. All kinds of state variables, as well as most of the `M/W/V/F`-suffixed state variables (for normalization) and `R`-suffixed state variables (with respect to chosen reference states), can be used as conditions. In addition to temperature and pressure conditions, a multicomponent system can have mixed types of conditions. You should repeat this command for a multicomponent system until the degree of freedom in the defined system becomes zero. When a FIXED phase status is used on a specific phase (use CHANGE_STATUS), it is equivalent to one condition (implying that particular phase is stable in the defined system).

Syntax	SET_CONDITION
	Each condition must be given explicitly, but can be given on the same line (separated by a comma (,) or an empty space) or on separate lines with each one started with the command.

Example

```
SET_COND T=1273, P=1E5, W(C)=.0015, X(LIQ,CR)=.22, ACR(N)=.2
```

or

```
SET_COND T=1273, P=1E5
SET_COND W(C)=.0015, X(LIQ,CR)=.22 ACR(N)=.2
```

In this example, the temperature is set to 1273 K, the pressure to 1 bar (1E5 Pascal), the mass (weight) fraction of C to 0.0015 and the mole fraction of Cr to 0.22 and the activity of N to 0.2.

Prompt	`State variable expression: <State variable name or linear expression> or a linear expression of state variables.` Some of the state variables that can be used in conditions are: • `T`: temperature in the system (in K) • `P`: pressure in the system (in Pascal) • `N`: system size (mole number in moles) • `B`: system size (mass in grams) • `N(<component>)`: mole number of a component in the system • `X(<component>)`: mole fraction of a component in the system • `W(<component>)`: weight fraction of a component in the system • For the SET_CONDITION command this is `ACR(<component>)`: activity of a component in the system. For the SET-ALTERNATIVE_CONDITION command, this is `ACR`(<`phase`>,<`component`>) (activity of a component in a phase) • For the SET_CONDITION command this is `MUR(<component>)`: chemical potential of a component in the system. For the SET-ALTERNATIVE_CONDITION command, this is `MUR` (<`phase`>,<`component`>) (chemical potential of a component in a phase)

Syntax	SET_CONDITION

- `X(<phase>,<component>)`: mole fraction of a component in a phase
- `W(<phase>,<component>)`: weight fraction of a component in a phase
- `ACR(<species>,<phase>)`: activity of a species referred to a phase
- `MUR(<species>,<phase>)`: chemical potential of a species referred to a phase
- `H`: enthalpy in the system (in J)
- `HM(<phase>)`: enthalpy of a phase (in J/mol)

There are many state variables that can be used in conditions. For more information, enter an `INFO STATE_VARIABLES` command. A condition is normally a value of a single state variable with its value.

Example

```
T=1273.15  P=1E5
X(C)=.002
W(CR)=0.5
ACR(CR)=0.85
X(FCC,C)=.001
H=-250000
 HM(BCC)=-225000
```

A condition can also be a value of a linear expression involving more than one state variable. For example,

```
X(LIQ,S)-X(PYRR,S)=0
```

This means that it is a condition that the mole fraction of `S` component should be the same in the LIQUID and PYRRHOTITE phases. In practice, that should be the congruent melting point.

After the equal sign only a numeric value is allowed in the expression.

```
Factor: <A factor for the state variable, or a continuation>
```

This question means you did not answer the previous question. The program is then expecting a single state variable or a complete state variable expression, or the numeric factor in an expression with only one state variable. In a state variable expression a state variable may be preceded by a constant factor. An example of this is:

```
2*MUR(FE)+3*MUR(O)=-35000
```

This means that it should be a condition that two times the chemical potential of `FE` plus three times the chemical potential of `O` should be -35000 J/mol.

```
State variable: <A specified state variable, or a continuation>
```

This question is prompted if a single state variable name has not given in either the prompt `State variable expression` or `Factor`, or a state variable expression is given but the expression is incomplete, for example, `T-` or `2*MUR(FE)+`, for which the program is then expecting a continuation of the unfinished expression. You need to specify a state variable or a complete state variable expression, or complete the unfinished state variable expression. If a numeric factor is given before

Syntax	SET_CONDITION
	this prompt, only one state variable can be specified; otherwise, the program only takes the first state variable to complete the expression (i.e. the factor times the state variable).
	`Value /X/: <A numeric value, a constant or a variable>` The value of the condition. This can be a numeric value, a constant or a variable. A suggestion is given as the default value. The special value `NONE` means that the condition is removed; for example `T=NONE` takes away the temperature condition.

SET_NUMERICAL_LIMITS

This command is available for the POLY, Scheil, and ED-EXP modules.

Change the criteria for convergence. This is to speed up a calculation in a complex system.

If there is any convergence problem in finding a stable solution at any stage during a calculation procedure enforced by COMPUTE_EQUILIBRIUM, STEP_WITH_OPTIONS, MAP or ADVANCED_OPTIONS), this message displays:

```
Convergence problems, increasing smallest site-fraction from 1.00E-30
to hardware precision 2.00E-14. You can restore using SET-NUMERICAL-
LIMITS
```

This implies that smallest site fraction in the current POLY workspace is automatically increased from the default value 1.00E-30 to the hardware-dependent precision (under Linux, as 2.00E-14). For other subsequent POLY module calculations, you can use this command to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

Syntax	SET_NUMERICAL_LIMITS
Prompt	`Maximum number of iterations /500/:` By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.
	`Required accuracy /1E-6/:` This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.
	`Smallest fraction /1E-12/:` This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions. The default value for the smallest site-fractions is 1E-12 for all phases, except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as 1E-30 (unless you have used the SET_NUMERICAL_LIMITS command to reset an even-lower value (e.g. 1E-45, that is naturally enforced to all the phases in the system).
	`Approximate driving force for metastable phases /Y/:` `Y` is the default. Enter `N` to change the default as required and based on the options described below. This setting involves the convergence of metastable phases and affects their driving forces. It can also have an effect on when an equilibrium is considered successful. The default is to allow an equilibrium with metastable phases that have not converged, as long as the stable phases have converged. This is efficient but often causes approximate values of the

Syntax	SET_NUMERICAL_LIMITS
	driving forces for the metastable phases. If you change the default, it enforces metastable phases to converge. This gives accurate driving forces for metastable phases as well as stable phases. It can however take a slightly longer time, and if metastable phases do not converge it causes the equilibrium calculation to fail.

SET_REFERENCE_STATE

This command is available for the POLY, ED-EXP and POST modules.

The reference state for a component is important when calculating activities, chemical potentials, and enthalpies and is determined by the database being used. For each component the data must be referred to a selected phase, temperature, and pressure, i.e. the reference state.

All data in all phases where this component dissolves must use the same reference state. However, different databases can use different reference states for the same element/component. It is important to be careful when combining data obtained from different databases.

By default, activities, chemical potentials, and so forth are computed relative to the reference state used by the database. If the reference state in the database is not suitable for your purposes, use this command to set the reference state for a component using `SER`, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys dominated by the component). In such cases, the temperature and pressure for the reference state is not needed.

In order to specify conditions in the specific reference state, you can append an `R` to the state variables. Thus, `AC` is the activity (of a system component or of a species in a phase) with respect to the default reference state, and `ACR` is the activity with respect to the selected reference state; MU is the chemical potential of a system component with respect to the default reference state, and `MUR` stands for the chemical potential with respect to the selected reference state. The `AC` and `ACR` variables, for both components in a system and species in a phase, can be specified in natural logarithm, e.g. LNAC(Fe), LNACR(C), LNAC (O2,GAS), LNACR(O2,GAS).

For the POST module, and after calculating with the STEP_WITH_OPTIONS or MAP commands, the reference state for a component can also be changed to plot various properties of the component in the entire system or in a specific phase. Then you can set the diagram axes as the chemical potential or activity quantities with the `R` suffix, i.e. MUR(comp), MUR (comp,ph), ACR(comp), ACR(comp,ph) or the common logarithms [e.g. LNACR(comp,ph)].

Syntax	SET_REFERENCE_STATE
Prompts	`Component: <Name of the component>` The name of the component must be given.
	`Reference phase: <Name of a phase used as the new reference state>`

Syntax	SET_REFERENCE_STATE

Enter the `Name of a phase` for the system.

> For a phase to be usable as a reference for a component, the component needs to have the same composition as an end member of the phase. The reference state is an end member of a phase. The selection of the end member associated with the reference state is only performed once this command is executed.

If a component has the same composition as several end members of the chosen reference phase, then the end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy.

The following are example using temperature. Pressure is used in the same way:

- In the Fe-C system, BCC can be a reference state for Fe but not for C since BCC can exist as pure Fe but cannot exist as pure C.
- If GAS is chosen as the reference phase of component O at such a high temperature that O1 has the lowest energy, then O1 remains the reference state even at calculations performed at lower temperatures where O2 has a lower energy than O1.
- Setting the reference state for component O as gas (one sublattice) with constituents O1, O2 and O3 results in O2 being the reference state if, at the present temperature, pure O2 has the lowest energy of O1, O2 and O3. If the reference state is set above a critical higher temperature, then O1 has the lowest energy and consequently becomes the reference state.

`Temperature /*/: <Temperature for the reference state>`

Select the Temperature (in K) for the reference state. The wildcard value * means the current temperature is used at the time of evaluation of the reference energy for the calculation.

> The temperature set with this command does not affect the temperature used when evaluating the energy of the reference state during the end member selection process.

`Pressure /1E5/: <Pressure for the reference state>`

Select the Pressure (in Pa) for the reference state. The wildcard value * means the current pressure is used for evaluating the reference energy at the time of calculation.

Examples

```
S-R-S Fe SER

S-R-S Cr FCC * 100000

S-R-S H2O AQUEOUS * 100000

S-R-S ZE REF_ELECTRODE * 100000
```

SET_START_CONSTITUTION

This command is available with the POLY and ED-EXP modules.

This command is similar to SET_ALL_START_VALUES, but is used for an individual phase that may have a wrong constitution.

Syntax	SET_START_CONSTITUTION
Prompts	`Phase name: <Name of a phase, and possible major constituent(s)>` Specify the name of a phase for which the constitution shall be set. If there is a major constituent of the phase, you must specify this on the same line as the phase name. By giving an*, select the default major constituents. A $ means keeping the same constitution, and `NONE` means to give individual site-fractions.
	`Y(<Phase>#<Composition_set>,<Constituent>#<Sublattice>) /xxx/: <SF>` The site fraction (`SF`) of the constituent shall be given. The default value `xxx` is the last calculated one.

SET_START_VALUE

This command is available with the POLY and ED-EXP modules.

This command is not often required as the automatic start values can be handled for most problems.

Set a start value of an individual variable.

Syntax	SET_START_VALUE
Prompts	`State variable: <Name of a state variable>` The state variable must be given.
	`Value` Specify the value to be assigned the state variable as start value.

SET_WEIGHT

This command is for the ED-EXP module.

Each experimental value has an uncertainty associated with it, specified by the value after the colon (:) with the command EXPERIMENT. During an optimization the absolute difference between the experimental and calculated values gives a contribution to the sum of error.

With the SET_WEIGHT command, you can change the scale of such a contribution (the uncertainty) for a single experimental point, or the contributions (all uncertainties) for a set of equilibria. The default weight is always unity. A value smaller than one means that the experiments should have less weight. A value larger than one that these should have higher weight. The special value zero means that the set of equilibria should be ignored in editing in ED_EXP (as is given) and in OPTIMIZE_VARIABLES in PARROT.

The weight may be needed to obtain a balance between different kinds of experiments. For example, if there are only five experimental values of the composition of a phase diagram but 500 experimental values of activities or enthalpies, then the five composition points may have to be given higher weight than unity, otherwise these are not well described by the optimizing procedure.

Syntax	SET_WEIGHT
Prompts	`Value /1/: <Weight value>` Specify a weight of the experiments in the specified equilibria (asked in the next prompt). The contribution to the sum of errors of these experiments are multiplied by this weight. The weight is squared, thus use 0.7 to make the error half (0.49) as big, and 1.4 to make it twice (1.96) as large.
	`Equilibria (range) or label(s) /Present/:<Selection>` Define the equilibria. These are available in the read data block from the current work file and are given the above-defined weight. The selection may be given as a range but the equilibrium numbers must then be separated only by a minus sign.

Syntax	SET_WEIGHT
	The start and end equilibrium numbers must be available in the read data block read from the current work file. For example, `5-101`, means that all equilibria starting from the identifier 5 until the identifier `101`. Some of numbers between these two identifiers may not exist in the data block. The selection may also be given as one or more labels (which should be separated only by a space). All equilibria with the specified label(s) in the read data block are given the above-defined weight. By pressing <Enter> to accept the default value `present`, the above defined weight is only assigned to the current or present experimental point (which is selected by the POLY SELECT_EQUILIBRIUM command). If is used but no specific equilibrium point is selected afterwards, the last point in the read data block remains the `present` point.

SHOW_VALUE

This command is available for the POLY and ED-EXP modules.

Show the current value of any state variable, function or variable.

Syntax	SHOW_VALUE
Prompt	`State variable or symbol: <Name(s) of state variable(s) or symbol(s)>` A single or several state variables or symbols (entered functions or variables) can be specified.
	The wildcard * can be used to denote all phases or all components. You can use the dollar-sign `$` to denote all stable phases. Thus, the command SHOW W(*,*)lists the mass fraction of all phases, whereas `SHOW W($,*)` lists the mass fraction of all stable phases. If you `SHOW` a function, all functions are evaluated using the current values of the state variables. But if you `SHOW` a variable, it retains its value from the time it was `ENTERED` or last `EVALUATED`. Therefore to save a value from one calculation to another, `ENTER` it to a variable. This is frequently done in the PARROT module to transfer values between equilibria.

STORE_ALL_WEIGHTS

Store a new weight-set that is the current situation of specified weights for all the different experimental points read from the currently-selected experimental data block in an assessment. This is useful when you want to try various weight-settings for some experimental points or for all the points, and then compare the assessment results from different weight-sets. Such a saved weight-set can be recalled and restored for all experimental data point with RESTORE_ALL_WEIGHTS sequentially.

Syntax	STORE_ALL_WEIGHTS
Prompt	`Command line: <Weight-set name>` Give a weight-set name (comment line texts) for the current weight set for all experimental points.

TABLE_HEAD, TABLE_VALUES and TABLE_END

These commands are used only in the *.POP file. It represents a convenient way to enter many experimental measurements of the same type in a table format.

In the DICTRA module, you work with a .DOP file instead of a .POP file.

These commands should always be used together and in a sequence, meaning that a table should always start with the TABLE-HEAD command, then TABLE-VALUES, and finish with TABLE-END. Between TABLE_HEAD and TABLE-VALUES also add definition lines (e.g. on phase status, reference states, conditions, experiments, labels, etc.) for the experimental measurements of the current information type.

Syntax	TABLE_HEAD TABLE_VALUES TABLE_END
Prompt	
	After the TABLE-HEAD command, there must be an equilibrium description similar to a single experimental equilibrium but with some special notation. Then, there is always a TABLE-VALUES command, after which the actual data is given in columns. At the end of each table, there must be a TABLE-END command. The TABLE-HEAD command must be followed by a numeric value. This is used to generate unique numeric identifiers for all the equilibria in the table. The numeric identifier is incremented by one for each experimental (equilibrium) point in the table.

Example

An example of the use of a table for enthalpy measurements in the liquid is given here. Much more elaborate tables can be used

```
$ Enthalpies of mixing, Topor and Kleppa, Met Trans 1984 TABLE-HEAD 1

CREATE—NEW @@ 1

CHANGE-STATUS PHASE LIQ=FIX 1

SET-REFERENCE-STATE AU LIQ * 1E5

SET-REFERENCE-STATE CU LIQ * 1E5

SET-CONDITION P=1E5 T=1379 X(LIQ,AU)=@1

LABEL ALH

EXPER HMR=@2:5%

TABLE—VALUES

0.0115 -322
```

Syntax	TABLE_HEAD TABLE_VALUES TABLE_END

```
0.0563 -1520
0.8499 -2976
0.9002 -2114
TABLE—END
```

The equilibrium description between TABLE-HEAD and TABLE-VALUES is similar as for a single experiment, except for these details:

- `@@` Used to automatically generate a series of identifying numbers instead of creating only one with the command CREATE_NEW_EQUILIBRIUM. The program automatically generates the identifying numbers starting after the number given after the TABLE-HEAD command (in this case it is 1).
- `@1` values in the table are specified by an @ sign followed by a column number. In the above case, the mole fraction of Au in the liquid is in column 1 (see the line for SET_CONDITION). The columns may have other information than values, and you can use phase names or any text. If the text contains spaces or special characters, it must be surrounded by double quotes in the table, e.g. “`ABC DEF&ghi`”.
- For the *syntax checker* all commands describing the equilibrium must be in UPPER case after the TABLE_HEAD command.
- After the TABLE-VALUES command, there should be one line for each experimental measurement of the same type giving the values or texts that should be copied into the places of the condition or experiment defined by `@1`, `t`, etc. You can have columns that are not used but there must be exactly the same number of columns of each line, otherwise the syntax checker gives an error message in the PARROT module.

TRANSFER_START_VALUES

This command is for the ED-EXP module.

In the ED_EXP module it is time consuming to calculate all equilibria when the optimization is sensitive to start values of the composition of the phases. Usually in one data block there are several experimental points with the same kind of equilibrium and each must have its start value set. When you manage to calculate equilibriums of such experimental points, this command is useful to transfer the site fractions from a successfully-calculated equilibria to the present experimental point.

Syntax	TRANSFER_START_VALUES
Prompt	`From equilibrium /Previous/: <Equilibrium number>` The equilibrium number is the numeric identifier for the equilibrium from which the start values should be copied to the present experimental point. `Previous` is the default if you press <Enter>.

Tabulation Reaction (TAB) Commands

In this section:

ENTER_FUNCTION

This command is available with the GES and TAB modules.

Used to define a new thermodynamic function to be included in the sixth column of tabular output. The last entered function is listed in the 6th column of all tables, and can be plotted (if choosing the Plot Column value 6) in all graphs, for all subsequently tabulated substances or reactions.

Syntax	ENTER_FUNCTION
Prompt	`Name: <Name>` `Function: <Definition>`
	A limited number of state variables, G, H, S, T, P, V and H298 can be used in the function definition. For example, -(G-H)/T can be defined as a function which is identical to S for a substance or ΔS for a reaction, G+T*S-P*V can be defined as a function which is U (internal energy) for a substance or ΔU (internal energy change) for a reaction.
Options	`Name`of the function (maximum 8 characters) and `Definition` of the function. A long function can be typed over several lines. A function should be terminated by a semicolon (;) or an empty line.

Example

For the pure substance Fe (using the SSUB database), by entering a function as `G+T*S-P*V`, the following table is obtained by typing <Enter> in the prompt `Output file /Screen/:`, and the figure by typing `6` in the prompt `Plot column /2/:`

```
TAB: ENTER-FUNCTION

Name: InEnergy

Function: G+T*S-P*V;

TAB: TABULATE_SUBSTANCE

Substance (phase): Fe

Pressure /100000/: <Enter>

Low temperature limit /298.15/: <Enter>

High temperature limit /2000/: <Enter>

Step in temperature /100/: <Enter>

Output file /try1/: try2

Graphical output? /Y/: <Enter>

Plot column? /2/: 6
```

This gives the following output:

```
O U T P U T  F R O M  T H E R M O - C A L C
 Column 6: InEnergy G+T*S-P*V
 Phase : FE_S                     Pressure :     100000.00
 Specie: FE
**************************************************************
    T      Cp           H            S            G             InEnergy
   (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 **************************************************************
  298.15   2.48446E+01   2.17972E-06   2.72800E+01  -8.13353E+03   2.17972E-06
  300.00   2.48905E+01   4.60049E+01   2.74338E+01  -8.18414E+03   4.60049E+01
  400.00   2.71299E+01   2.64957E+03   3.49085E+01  -1.13138E+04   2.64957E+03
  500.00   2.93561E+01   5.47211E+03   4.11976E+01  -1.51267E+04   5.47211E+03
  600.00   3.19293E+01   8.53245E+03   4.67701E+01  -1.95296E+04   8.53245E+03
  700.00   3.50985E+01   1.18777E+04   5.19207E+01  -2.44667E+04   1.18777E+04
  800.00   3.92042E+01   1.55830E+04   5.68623E+01  -2.99068E+04   1.55830E+04
  900.00   4.49645E+01   1.97726E+04   6.17903E+01  -3.58387E+04   1.97726E+04
 1000.00   5.42147E+01   2.46891E+04   6.69619E+01  -4.22728E+04   2.46891E+04
 1100.00   4.55851E+01   2.99025E+04   7.19412E+01  -4.92328E+04   2.99025E+04 $
Stable phase is FE_S2
 1200.00   3.40840E+01   3.51037E+04   7.64466E+01  -5.66322E+04   3.51037E+04
 1300.00   3.49398E+01   3.85549E+04   7.92086E+01  -6.44162E+04   3.85549E+04
1400.00   3.57994E+01   4.20918E+04   8.18293E+01  -7.24692E+04   4.20918E+04
 1500.00   3.66636E+01   4.57149E+04   8.43287E+01  -8.07780E+04   4.57149E+04
 1600.00   3.75330E+01   4.94247E+04   8.67226E+01  -8.93314E+04   4.94247E+04 $
Stable phase is FE_S3
 1700.00   4.05217E+01   5.41173E+04   8.95609E+01  -9.81363E+04   5.41173E+04
 1800.00   4.12595E+01   5.82055E+04   9.18975E+01  -1.07210E+05   5.82055E+04 $
Stable phase is FE_L
 1900.00   4.60000E+01   7.74165E+04   1.02377E+02  -1.17099E+05   7.74165E+04
2000.00   4.60000E+01   8.20165E+04   1.04736E+02  -1.27456E+05   8.20165E+04
```

ENTER_REACTION

This command is for the TABULATE_REACTION (TAB) module.

This is the same as TABULATE_REACTION in that both the chemical reaction can be specified and the thermodynamic property changes for the reaction can be generated as a table, and plotted as a graph or saved as an experimental file (with an extension of .EXP). The thermodynamic data are automatically retrieved from the SSUB database (by default), or the current database set by SWITCH_DATABASE (thus there is no need to use the TDB module before this command). You can select any other database by using the SWITCH_DATABASE command in the TAB module. The rules to specify a reaction are the same as TABULATE_REACTION.

Syntax	ENTER_REACTION
Prompts	`Same reaction? /Y/:` This displays if there is at least one reaction already defined either by ENTER_REACTION or TABULATE_REACTION. For `Y` the next prompt for defining reaction is not asked.

	`Reaction: <Chemical reaction equation> & <RA+RB=PC+PD>`
	A long reaction can be typed over several lines. A reaction should be terminated by a semicolon (`;`) or an empty line. A list showing the used database, defined elements, getting-data sequence, references, etc.:
	`Pressure /100000/: <Pressure of interest, in pa>`
	`Low temperature limit /298.15/: <T-low, in K>`
	`High temperature limit /2000/: <T-high, in K> Step in temperature /100/: <T-step>`

	`Output file /Screen: <Return for screen, or type a file name>` If you type `Return for screen` a list of thermodynamic property changes for the defined/chosen reaction is shown up as a table (which is demonstrated in the example outputs given below), and the command is terminated. If typing a file name, the table is displayed and saved as an *.EXP or an *.TAB file. Then prompts:
	`Graphical output /Y/:` For `N` a table is output to the screen and this table is saved as a basic text file with the default extension .TAB under the current working directory. In this case, the graph cannot be plotted. By default a table is created with all thermodynamic functions as normal (which is displayed on screen) and generates a graph with temperature on the X-axis and a chosen property on a certain column in the table on the Y-axis (which is plotted on screen and saved as an *.EXP file). You are also prompted for the plot column.
	`Plot column? /2/: <1 or 2 or 3 or 4 or 5 or 6>` Specify which property (as column number) to be plotted as the Y-axis (versus temperature as X-axis) as a graph on the screen. Simultaneously, all tabulated properties and the Y-axis setting (i.e. the plotted column) for the graph is written into an *.EXP file using the DATAPLOT format. The default column 2 is heat capacity, 3 enthalpy, 4 entropy and 5 Gibbs energy, and the additional

Syntax	ENTER_REACTION
	column 6 is a user-entered function. The table displays on the screen. The plot then displays on the screen, followed by a `POST` prompt. The POST module (postprocessor) automatically opens, and all types of the POST-module commands to refine the plotted diagram may be used. Possibilities include scaling the X/Y-axis, changing the X/Y-axis texts, etc. The command BACK or EXIT at the `POST` prompt always takes you back to the TAB module.

LIST_SUBSTANCES

This command is for the TABULATE_REACTION (TAB) module.

List all species in the current database with a certain set of elements. This is useful to specify species as pure substances in the command TABULATE_SUBSTANCE.

Syntax	LIST_SUBSTANCES
Prompts	`With elements /*/ <* or a set of elements>` The elements building up various species must be specified. The wildcard * means all elements in the current database. If some elements are specified, it also prompts for how to list species with such elements.
	`Exclusively with those elements /Y/:` All species (not phases) in the current database are searched. Keep the default (Y) if you do not want other elements included in the search except for those specified. Enter N to list all species containing at least one of the specified elements.

Example

For the SSOL database, there are different lists, as shown below:

```
TAB: l-sub

With elements /*/: <Enter>

VA                      AG                      AL

AM                      AS                      AU

B                       BA                     BE BI   BR C

CA                      CD                      CE

CL                      CO                      CR

CS                      CU                      DY

ER                      EU                      F

FE                      GA                      GD

GE                      H                       HF

HG                      HO                      I

IN                      IR                      K

LA                      LI                      LU

MG                      MN                      MO

NA                      NB
```

```
ND                      NI                      NP
OS                      P
PA                      PB                      PD
PR                      PT                      PU
RB                      RE                      RH
RU                      S                       SB
SC                      SE                      SI
SM                      SN                      SR
TA                      TB                      TC
TE                      TH                      TI
TL                      TM                      U
V                       W                       Y
YB                      ZN                      ZR
C1                      C2                      C3
C4                      C5                      C6
C7                      N2                      O2
P1                      P2                      P4
NA/+1                   K/+1                    CL/-1
H2O                     H1/+                    LI1/+
CS1/+                   RB1/+                   O1H1/-
F1/-                    BR1/-                   I1/-
H1/+1                   H1O1/-1                 SI1O2 CA1O1 TAB:
TAB: l-sub
With elements /*/: fe cr ni c n o
Exclusively with those elements? /Y/: <Enter>
C               CR                    FE
N               NI                    O
C               C2                    C3
C          C5                    C6
C               N2                    O2
TAB:l-sub fe cr ni c n o
Exclusively with those elements? /Y/: n
C               CR                    FE N   NI O
C1              C2                    C3
C4              C5                    C6
C7              N2                    O2
```

```
H2O            O1H1/-              H1O1/-1 SI1O2 CA1O1 TAB:
```

SET_ENERGY_UNIT

Set the energy unit as calories or Joule, in all the subsequent outputs (tables, graphs, and files) in the current calculation operation.

Syntax	SET_ENERGY_UNIT
Prompt	`Energy unit (C=Cal, J=Joule) /J/: <Unit>`

SET_PLOT_FORMAT

This command is for the TABULATE_REACTION (TAB) module.

Set the plotting format while the result is plotted on screen or the file is saved as EXP file [using DATAPLOT graphical format] and TAB file (as a basic text file and as displayed on screen).

This command is different from SET_PLOT_FORMAT in the POST module, but is identical to SET_PLOT_ENVIRONMENT in the SYS (system utility) monitor.

Syntax	SET_PLOT_FORMAT
Options	The default set `Unit`is `1` (Windows) or `9` (Linux) for graphical presentation on screen, or all other units for outputs as *.EXP and *.TAB files. Also set the format of the graphical output to different graphical devices. The default unit 22 (1 for legacy Windows, and 9 for legacy Linux) may be altered with SET_PLOT_ENVIRONMENT in the SYS monitor or by the TC.INI file.

SWITCH_DATABASE

This command is for the TABULATE_REACTION (TAB) module.

By default, the TAB module always automatically retrieves thermodynamic data for substances or reactant/product substances in a defined reaction, or for pure phases or ideal solution phases, from the SSUB Substances database. However, you can select thermodynamic data for complex non-ideal solution phases from another database, which is possible with this command.

Syntax	SWITCH_DATABASE
Prompt	`Database /XYZ/: <new database name>` Specify a `New database name`. `XYZ` stands for the default SSUB database or the current database which is switched on. If an appropriate database name is not given and the `USER` option is not used, a list displays of available databases. Use one of these databases: • PURE = SGTE Pure Elements Database • SSUB = SGTE Substances Database • USER = user defined database

This command switches (or changes) from the current database to a new one, and reinitializes the entire TAB module for defining a substance or reaction and the GIBBS workspace for storing retrieved data. All the directly connected databases as predefined by the original database initiation file `tc_initd.tdb` are listed by pressing the <Enter> key without giving any argument. You can also supply your own database by giving the argument USER and then the database name and, if it is not located in the current working directory, its correct path.

This command (when required to use another database for subsequent tabulations) must be used before executing the TAB commands TABULATE_SUBSTANCE for substances, and ENTER_REACTION or TABULATE_REACTION for reactions.

When a predefined database or an appropriate USER database is switched on, the DATA command GET_DATA is automatically executed.

DATABASE NAME: The new database is specified by typing the abbreviation given in the front of one of the available predefined databases. For convenience when switching/appending databases you can add them to the predefined database list in the database initiation file `tc_initd.tdb` of your installed software.

When this command is used in a macro (*.TCM) file, if the `USER` option is selected, the database setup file name (*setup.TDB) containing the setup definitions of the user database, and its correct path, must be provided.

If a USER database name or its path is not given on the same line of the SWITCH_DATABASE command, or if it is incomplete or incorrect, an Open window displays to specify the filename of the database setup file name (*setup.TDB) of the to-be-switched USER database.

Unlike in the TDB module, if a user database is chosen, the Gibbs energy system is also reinitialized and only data from the user databases are retrieved for tabulations.

After this command, those commands to define systems (in terms of either elements or species), to reject/restore phases or species, retrieve data, as well as to append data from additional database(s), can be done.

TABULATE

This command is for the TABULATE_REACTION (TAB) module.

Gives the values of an already-defined table (with various properties varied with the stepping axis variable) from equilibria calculated with a STEP command. You can tabulate a table even if the table is entered after the step calculation.

Syntax	TABULATE
Prompts	`Name: <Name of a defined table>` The name of the table must be given. The table must be entered.
	`Output to Screen or file /Screen/: <File name>` The table can be listed on the screen (by pressing <Enter>), on a file (the file name must be specified here).

TABULATE_DERIVATIVES

This command is for the TABULATE_REACTION (TAB) module.

This command is mainly for system debugging purposes and for experienced users. It automatically calculates all partial derivatives for a pure phase or solution phase at a given composition.

This is not the same as the chemical potential.

Before using this command, the system must be defined and thermodynamic data retrieved from an appropriate solution database in the TDB module. The phase name can be given in either upper, lower or mixed cases, and can be abbreviated until it is unique, e.g. fcc, BCC, cem, Liq, etc. as the SSOL database is used for the tabulations, or GAS, FE-S, wustite, Fe2O3-hem, etc. as the SSUB database is used. The module then optionally goes through a specific sublattice or all the possible sublattices for the specified phase, as well as through the whole framework of a currently defined system (including all the defined elements/species, as well as the default defined vacancy and electron if necessary for the current database), when it prompts for inputs of site fractions for various species possibly occupying such sublattices. Therefore, thermodynamic properties can be tabulated for a pure phase, or for a solution phase as a pure end-member (with a composition definition for the corresponding non-interacting species on all necessary sublattices in the end-member), or for a solution phase as a real solution (with a composition definition for related interacting species on all necessary sublattices in the solution).

Syntax	TABULATE_DERIVATIVES
Prompts	`Phase name /XXXX/: <Name of the phase>` Specify the phase name of a pure phase or a solution phase. `XXXX` is the last phase the TAB module accounted for. It automatically prompts for other options and necessary inputs for the definition of the composition of the specified phase. For a pure phase (such as `Fe-S`, `Wustite`, and `Fe2O3-Hematite`), no further composition definition is needed. For a solution phase with one sublattice (such as `AQUEOUS` solution, `GAS` mixture and `SLAG` solution), it requests *n*-1 site-fraction inputs for the phase constituents (if there are *n* species in the defined phase within the whole framework of currently defined system, including all the defined elements/species, as well as the default defined vacancy and electron if necessary for the current database); the *n*th species is automatically assigned as the rest.

Syntax	TABULATE_DERIVATIVES

The sum of input site fractions must not exceed unity.

Example Prompts

For example, these prompts and inputs can be seen for a `LIQUID` solution phase (from the SSOL database) within the Fe-Cr-Ni-C-N-O framework (Note that by default, the unprompted `Ni` species are assigned as the rest):

```
FRACTION OF CONSTITUENT (RETURN FOR PROMPT): <RETURN> C /1/: .05
CR /1/: .1
FE /1/: < RETURN>
SUM OF FRACTIONS EXCEED UNITY, PLEASE REENTER
FE /1/: .8
N /1/: .005
```

For a solution phase with two or more sublattices (such as FCC alloy solution, and ION_LIQ ionic liquid solution), it first asks for which sublattice the site-fractions of constituents shall be specified: the default value 0 for all possible sublattices, and a given positive number for a specific sublattice (of course, this number must be reasonable for the currently specified phase, i.e. it must be smaller than the total sublattice number of the phase). Then, for the given sublattice or for all sublattices, it prompts for all the necessary inputs of site-fractions for the possible constituents on each sublattice n-1 times if there are n species on such a sublattice in the defined phase; the nth species on each of the sublattices is automatically assigned as the rest. For example, the following prompts and inputs can be seen for an FCC solution phase (from the SSOL database) within the Fe-Cr-Ni-C-N-O framework (Note that by default, the unprompted O species on its sublattice 1 and VA on its sublattice 2 are assigned as the rest):

```
SPECIFY SUBLATTICE (0 FOR ALL) /0/: <RETURN>
FRACTIONS IN SUBLATTICE 1
CR /1/: .1
FE /1/: .8
NI /1/: .0995
FRACTIONS IN SUBLATTICE 2
C /1/: .05
N /1/: .05
```

```
Temperature /2000/: <Temperature of interest, in K>
```

Specify the temperature of interest in K.

```
Pressure /100000/: <Pressure of interest, in pa>
```

Specify the pressure of interest in Pa.

Example Output

For the FCC phase in the Fe-Cr-Ni-C-N-O system (using the SSOL database), the following table is obtained at a specified composition:

```
TAB: TAB_DER

Phase name /BCC/: FCC

SPECIFY SUBLATTICE (0 FOR ALL) /0/: <Enter>

FRACTIONS IN SUBLATTICE 1

CR /1/: .1

FE /1/: .8

NI /1/: .3

SUM OF FRACTIONS EXCEED UNITY, PLEASE REENTER

NI /0/: .0995

FRACTIONS IN SUBLATTICE 2

C /1/: .05

N /1/: .05

Temperature /1800/: <Enter>

Pressure /100000/: <Enter>

Gibbs energy: .................... -1.27432533E+05

Helmholz energy: ................. -1.27433205E+05

Enthalpy: ........................  5.95773994E+04

Internal energy: .................  5.95767279E+04

Entropy: .........................  1.03894407E+02

Molar volume: ....................  6.71473258E-06

Thermal expansivity: .............  7.63886416E-05

Isothermal compressibility: .......  6.02925387E-12

Heat capacity at constant pressure:  4.33555074E+01

First partial derivative with respect to CR in sublattice  1     of Gibbs energy:
................ -1.26034739E+05     of enthalpy: ....................
4.63000206E+04     of entropy: .....................  9.57415334E+01     of
volume: .....................  6.87203263E-06

Second partial derivative of Gibbs energy with respect to also

  CR                       in  1:  1.54392858E+05

  FE                       in  1: -1.53353158E+04

  NI                       in  1: -1.71750366E+04

  O                        in  1:  0.00000000E+00
```

```
  C                        in  2: -1.82016870E+05

in  2: -3.73062665E+05

  VA                       in  2: -9.36260878E+04

 irst partial derivative with respect to FE in sublattice  1     of Gibbs energy:
................ -1.02869265E+05

    of enthalpy: ....................  6.11738912E+04     of entropy:
.....................  9.11350866E+01     of volume: .....................
7.53441165E-06

Second partial derivative of Gibbs energy with respect to also

 FE                       in  1:  1.82508696E+04

 NI                       in  1: -3.07043434E+03

in  1:  0.00000000E+00

 C                        in  2: -1.36027071E+05

in  2: -2.13007485E+05

VA                        in  2: -1.11741180E+05

First partial derivative with respect to NI in sublattice  1     of Gibbs energy:
................ -1.32427029E+05     of enthalpy: ....................
5.21563580E+04     of entropy: .....................  1.02546326E+02     of
volume: .....................  0.00000000E+00

    Second partial derivative of Gibbs energy with respect to also

  NI                       in  1:  1.48390257E+05

in  1:  0.00000000E+00

  C                        in  2: -7.70620431E+04

in  2: -1.61551726E+05

 VA                       in  2: -1.12772206E+05

First partial derivative with respect to O in sublattice  1     of Gibbs energy:
................ -2.62929308E+05     of enthalpy: ....................
5.02555370E+04     of entropy: .....................  1.73991581E+02     of
volume: .....................  0.00000000E+00

 Second partial derivative of Gibbs energy with respect to also

in  1:  2.99322360E+07

C                         in  2:  0.00000000E+00

N                         in  2:  0.00000000E+00

VA                        in  2: -1.82377137E+05

First partial derivative with respect to C in sublattice  2     of Gibbs energy:
................ -1.59508417E+05     of enthalpy: ....................
1.21269096E+05     of entropy: .....................  1.55987507E+02     of
volume: .....................  1.06885187E-05

Second partial derivative of Gibbs energy with respect to also

C                         in  2:  2.99322360E+05

N                         in  2: -1.90144000E+04
```

```
VA                       in  2: -2.78465070E+04

First partial derivative with respect to N in sublattice  2     of Gibbs energy:
................ -2.39671400E+05     of enthalpy: ....................
4.04456947E+04     of entropy: ....................  1.55620608E+02     of
volume: .....................  0.00000000E+00

Second partial derivative of Gibbs energy with respect to also

N                        in  2:  2.99322360E+05

VA                       in  2: -3.30383665E+04

First partial derivative with respect to VA in sublattice  2     of Gibbs energy:
................ -9.52042686E+04     of enthalpy: ....................
5.37142294E+04     of entropy: ....................  8.27324989E+01     of
volume: .....................  6.86700739E-06

Second partial derivative of Gibbs energy with respect to also

VA                       in  2:  1.66290200E+04
```

TABULATE_REACTION

This command is for the TABULATE_REACTION (TAB) module.

Tabulate thermodynamic property changes for a chemical reaction as a table, or variation of one chosen property can be plotted against temperature as a graph, or saved as an experimental file (with an extension of .EXP). The thermodynamic data are automatically retrieved from the SSUB5 database (by default), or the current database set by the SWITCH_DATABASE command (thus there is no need to use the DATA module before this command). You can select any other database by using SWITCH_DATABASE.

It is important to remember the rules to specify a reaction:

- The reaction is specified, by giving the reactants and products, such as `Ga+S=GaS`, `5Al+2Fe=Al5Fe2`.
- Under Linux environments, the notation for a chemical formula treats upper and lower cases as the same (such as `ga+s=GaS, 5Al+2Fe=al5fe2`); but under Windows, the TAB module only accepts upper cases, e.g. `GA+S=GAS, 5AL+2FE=AL5FE2`.
- Elements with a single letter symbol must be followed by a stoichiometry factor, even if it is 1; thus, the symbol `CO` is taken as cobalt, carbon monoxide must be given as `C1O1` (or `O1C1`).
- All the reactants and products must be defined as species-stoichiometries in the currently-used database; in other words, the reaction definition only accepts already-defined species-stoichiometries as reactants and products. For example, if a database does not have a species defined with a stoichiometry of Al5Fe2 {e.g. the Al and Fe (but not Al5Fe2) may be defined as species, and the Al5Fe2 phase may be defined as a two-sublattice stoichiometric phase [Al]5[Fe]2, rather than a single sublattice stoichiometric phase [Al5Fe2]}, then the reaction 5Al+2Fe=Al5Fe2 cannot be tabulated.
- Make sure that the Gibbs free energy expression for a stoichiometric phase is really corresponding to the species-stoichiometry. For example, if a database has a definition of Function GAL5FE2 for 1/7 of the AL5FE2 formula, then the relation G (Al5Fe2)=7*GAL5FE2 must be defined; otherwise, the tabulated thermodynamic properties for the reaction 5Al+2Fe=Al5Fe2 is wrong.

Syntax	TABULATE_REACTION
Prompts	`Same reaction? /Y/:` This prompt displays if there is at least one reaction already defined either with the commands ENTER_REACTION or TABULATE_REACTION. The following prompts only display if `N` is entered.
	`Reaction: <Chemical reaction equation> & <RA+RB=PC+PD>`

Syntax	TABULATE_REACTION

	A long reaction can be typed over several lines. A reaction should be terminated by a semicolon (`;`) or an empty line. A list showing the used database, defined elements, getting-data sequence, references, etc.
	`Pressure /100000/: <pressure of interest, in pa>`
	`Low temperature limit /298.15/: <T-low, in K> Specify the starting temperature K.`
	`High temperature limit /298.15/: <T-high, in K> Specify the ending temperature K. Step in temperature /100/: <T-step> Specify the temperature step for the tabulation.`

	`Output file /Screen/: <Return for screen, or type a file name>` If you type `Return for screen`, a list of thermodynamic property changes for the defined/chosen reaction is shown as a table (which is demonstrated in the example outputs given below), and the command is terminated. If typing a file name, the table is both displayed on screen and saved as an *.EXP or a *.TAB file, and the program prompts:
	`Graphical output /Y/:` • For N a table is output to the screen, and the same table is saved as a basic text file with the default extension .TAB under the current working directory. In this case, the graph cannot be plotted. • For Y a table is created with all thermodynamic functions as normal (which is displayed on screen) and generates a graph with temperature on the X-axis and a chosen property on a certain column in the table on the Y-axis (which is plotted on screen and saved as an *.EXP file), and it also asks which column is to be plotted on the resulting graph:
	`Plot column? /2/: <1 or 2 or 3 or 4 or 5 or 6>` Specify which property (as column number) to be plotted as the Y-axis (versus temperature as X-axis) as a graph on the screen. Simultaneously, all tabulated properties and the Y-axis setting (i.e. the plotted column) for the graph is written into an *.EXP file using the DATAPLOT format. The default column 2 is heat capacity, 3 enthalpy, 4 entropy and 5 Gibbs energy, and the additional column 6 is a user-entered function. The table displays on the screen. The plot then displays on the screen, followed by a POST: prompt. The POST module automatically opens, and all types of the POST module commands to refine the plotted diagram may be used. Possibilities include scaling the X/Y-axis, changing the X/Y-axis texts, etc. The command BACK or EXIT at the `POST:` prompt always takes you back to the TAB module.

Example

For the reaction Ga+S=GaS (using the SSUB database), the following table is obtained by typing <Enter> in the prompt Output file /SCREEN/, and the figure by typing `2` in the prompt `Plot column /2/`:

```
     O U T P U T   F R O M   T H E R M O - C A L C

      Reaction:   S+GA=GA1S1

  stable as S_S

  GA stable as GA_S
```

```
GA1S1 stable as GA1S1_S
Delta-Cp      Delta-H       Delta-S       Delta-G
(K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)
 ***************************************************************
298.15  -2.79489E+00  -2.09200E+05  -1.50580E+01  -2.04710E+05
300.00  -2.87516E+00  -2.09205E+05  -1.50755E+01  -2.04683E+05
302.   ---- GA becomes GA_L ,delta-H =   5589.80
367.   ---- S becomes S_S2 ,delta-H =    401.00
389.   ---- S becomes S_L ,delta-H =   1721.00
400.00  -1.22278E+01  -2.17521E+05  -4.07488E+01  -2.01222E+05
500.00  -1.57686E+01  -2.19323E+05  -4.47280E+01  -1.96959E+05
600.00  -1.02518E+01  -2.20583E+05  -4.70410E+01  -1.92359E+05
700.00  -6.58954E+00  -2.21430E+05  -4.83534E+01  -1.87583E+05
800.00  -4.46246E+00  -2.21963E+05  -4.90686E+01  -1.82709E+05
900.00  -2.82671E+00  -2.22328E+05  -4.94995E+01  -1.77778E+05
1000.00  -1.21787E+00  -2.22530E+05  -4.97138E+01  -1.72816E+05
1100.00   3.71702E-01  -2.22572E+05  -4.97552E+01  -1.67841E+05
```

TABULATE_SUBSTANCE

This command is for the TABULATE_REACTION (TAB) module.

Tabulate thermodynamic properties of a substance (with a given chemical formula but it is not certain in which phase/state it may form) or a pure stoichiometric phase (getting data from a specific substance database such as SSUB, or from a specific solution database such as SSOL and TCFE), or of a solution phase with a fixed composition (getting data from a specific solution database such as SSOL and TCFE), under a constant pressure and various temperatures.

In case of a pure stoichiometric phase or a solution phase with a fixed composition, you must already define the system and get thermodynamic data from an appropriate solution database in the TDB module before using this TAB command. The phase name can be given either upper or lower or mixed cases, and can be abbreviated until it is unique, e.g. `fcc`, `BCC`, `Liq`, `cem`, `Al5Fe2`, etc. as the SSOL database is used for the tabulations, or `GAS`, `FE-S`, `wustite`, `Fe2O3-hem`, etc. as the SSUB database is used. The module then optionally goes through a specific sublattice or all the possible sublattices for the specified phase, as well as through the whole framework of a currently defined system (including all the defined elements/species, as well as the default defined vacancy and electron if necessary for the current database), when it prompts for inputs of site fractions for various species possibly occupying such sublattices. Therefore, you can tabulate thermodynamic properties for a pure phase, or for a solution phase as a pure end-member (with a composition definition for the corresponding non-interacting species on all necessary sublattices in the end-member), or for a solution phase as a real solution (with a composition definition for related interacting species on all necessary sublattices in the solution).

Moreover, the variation for one of the tabulated properties for a substance, a pure stoichiometric phase, or a solution phase with a fixed composition can be plotted against temperature as a graph or saved as an experimental file (with an extension of .EXP).

Syntax	TABULATE_SUBSTANCE
Prompt	`Substance (phase): <Name of the species or phase>` In case of a substance, give its chemical formula, e.g. Fe, H2, C1H6, FeC1, CaC1O3, MgSiO3, etc. When the TABULATE_SUBSTANCE <SUBSTANCE> command sequence is used for the first time in the TAB module, it always uses the SSUB Substances database as the default. If SSUB is not available and a specific database has not been switched on yet, it may prompt to specify an appropriate substance or solution database (e.g. typing `SSUB<version number>`; `SSOL<version number>`; `TCFE<version number>` etc.). Prior to this command, you can also use SWITCH_DATABASEto set the current database. If a solution database is set as the current database, only the neutral species that are valid substance standing by themselves as phases can be tabulated.

Syntax	TABULATE_SUBSTANCE

Before other prompts, a list of the used database, defined elements, getting-data sequence, references, etc. is displayed on screen. From such information, you know what the TAB module is performing.

In case of a pure stoichiometric phase or a solution phase, give its phase name, e.g. FCC, CEMENTITE, LIQUID, SLAG, AQUEOUS, GAS, Al5Fe2, Fe-S, Wustite, Fe2O3-Hematite, etc.

REMEMBER: It is important that you have already defined the system and gotten thermodynamic data from an appropriate solution database in the TDB module before using this TAB_SUB command. It automatically prompts for other options and necessary inputs for the definition of the composition of the specified phase.

For a pure stoichiometric phase defined with one single sublattice (such as Fe-S, Wustite, and Fe2O3-Hematite), no further composition definition is needed.

For a solution phase defined with one sublattice (such as AQUEOUS solution, GAS mixture and SLAG solution), it requests n-1 site-fraction inputs for the phase constituents (if there are *n* species in the defined phase within the whole framework of currently defined system, including all the defined elements/species, as well as the default defined vacancy and electron if necessary for the current database); the *n*th species is automatically assigned as the rest.

The sum of input site fractions must not exceed unity. For example, the following prompts and inputs can be seen for a LIQUID solution phase (from the SSOL database) within the Fe-Cr-Ni-C-N-O framework (Note that by default, the unprompted Ni species is assigned as the rest):

```
Fraction of constituent (return for prompt): <Return>
   C /1/: .05
   CR /1/: .1
   FE /1/: <RETURN>
```

```
Sum of fractions exceed unity, please reenter
   FE /1/: .8
   N /1/: .005
```

For a pure stoichiometric phase defined with two or more sublattices (such as Al5Fe2 inter-metallic stoichiometric phase) and for a solution phase defined with two or more sublattices (such as FCC alloy solution, and ION_LIQ ionic liquid solution, Al5Fe4 inter-metallic solution phase), it first asks for which sublattice the site-fractions of constituents shall be specified: the default value 0 for all possible sublattices, and a given positive number for a specific sublattice (this number must be reasonable for the currently specified phase, i.e. it must be smaller than the total sublattice number of the phase). Then, for the given sublattice or for all sublattices, it prompts for all the necessary inputs of site-fractions for the possible constituents on each sublattice *n*-1 times if there are n species on such a sublattice in the defined phase; the *n*th species on each of the sublattices are automatically assigned as the rest. For example, these prompts and inputs can be seen for an FCC

Syntax	TABULATE_SUBSTANCE

solution phase (from the SSOL database) within the Fe-Cr-Ni-C-N-O framework (Note that by default, the unprompted `O` species on its sublattice `1` and `VA` on its sublattice `2` is assigned as the rest):

```
Specify sublattice (0 for all) /0/:
   FRACTIONS IN SUBLATTICE            1
   CR /1/: .1
   FE /1/: .8
   NI /1/: .0995
   FRACTIONS IN SUBLATTICE            2
   C /1/: .05
   N /1/: .05
```

```
Pressure /100000/: <Pressure of interest, in pa>
```

Specify the constant pressure condition in Pa.

```
Low temperature limit /298.15/: <T-low, in K>
```

Specify the starting temperature K.

```
High temperature limit /298.15/: <T-high, in K>
```

Specify the ending temperature K.

```
Step in temperature /100/: <T-step> Specify the temperature step for the tabulation.
```

```
Output file /Screen/: <Return for screen, or type a file name>
```

If you type `Return for screen` a list of basic thermodynamic functions for the chosen substance or for the specified pure or solution phase with the fixed composition is shown up as a table (which is demonstrated in the example outputs given below), and the command is terminated.

If typing a file name, the table is both displayed on screen and saved as an *.EXP or a *.TAB file, and the program further prompts:

```
Graphical output /Y/:
```

- For N a table is output to the screen, and the same table is saved as a basic text file with the default extension .TAB under the current working directory. In this case, the graph cannot be plotted.
- For Y a table is created with all the thermodynamic functions as normal (which is displayed on screen) as well as generates a graph with temperature on the X-axis and a chosen property on a certain column in the table on the Y-axis (which is plotted on screen and saved as an *.EXP file), and it also ask which column is to be plotted on the resulting graph:

```
Plot column ? /2/: <1 or 2 or 3 or 4 or 5 or 6>
```

Specify which property (as column number) to be plotted as the Y-axis (versus temperature as X-axis) as a graph on the screen. Simultaneously, all tabulated properties and the Y-axis setting (i.e. the plotted column) for the graph is written into an *.EXP file using the DATAPLOT format. The default column 2 is heat capacity, 3 enthalpy, 4 entropy and 5 Gibbs energy, and the additional column 6 is a user-entered function. The table displays on the screen. The plot then displays on the screen, followed by a POST: prompt. The POST module (postprocessor) automatically opens, and all types of the POST-module commands to refine the plotted diagram may be used. Possibilities include scaling the X/Y-axis, changing the X/Y-axis texts, etc. The command BACK or EXIT at the POST: prompt always takes you back to the TAB module.

Example 1

For the `FCC` alloy phase as a non-ideal solution with a fixed composition

```
[Fe0.80,Cr0.10,Ni0.0995,O0.005][C0.05,N0.05,VA0.90]
```

The following table is obtained by typing `Return for screen` at the prompt `Output file /SCREEN/`:

```
O U T P U T   F R O M   T H E R M O - C A L C

Phase : FCC                       Pressure :      100000.00

 Specie: CR1/--2

 ***************************************************************

   T      Cp            H             S             G

  (K)    (Joule/K)      (Joule)      (Joule/K)      (Joule)

 ***************************************************************

298.15   2.70517E+01   6.23824E+03   4.40241E+01  -6.88755E+03
300.00   2.70889E+01   6.28832E+03   4.41916E+01  -6.96915E+03
400.00   2.87304E+01   9.08420E+03   5.22235E+01  -1.18052E+04
500.00   2.99904E+01   1.20222E+04   5.87742E+01  -1.73649E+04
600.00   3.10889E+01   1.50770E+04   6.43408E+01  -2.35275E+04
700.00   3.21116E+01   1.82375E+04   6.92106E+01  -3.02100E+04
800.00   3.30994E+01   2.14982E+04   7.35633E+01  -3.73524E+04
900.00   3.40742E+01   2.48569E+04   7.75182E+01  -4.49094E+04
1000.00   3.50483E+01   2.83130E+04   8.11586E+01  -5.28456E+04
1100.00   3.60268E+01   3.18667E+04   8.45449E+01  -6.11327E+04
1200.00   3.70143E+01   3.55187E+04   8.77219E+01  -6.97476E+04
1300.00   3.80149E+01   3.92700E+04   9.07241E+01  -7.86713E+04
1400.00   3.90311E+01   4.31222E+04   9.35784E+01  -8.78875E+04
1500.00   4.00649E+01   4.70768E+04   9.63064E+01  -9.73827E+04
1600.00   4.11174E+01   5.11358E+04   9.89256E+01  -1.07145E+05
1700.00   4.21896E+01   5.53010E+04   1.01450E+02  -1.17165E+05
1800.00   4.33555E+01   5.95774E+04   1.03894E+02  -1.27433E+05
1900.00   4.58528E+01   6.40379E+04   1.06306E+02  -1.37943E+05
2000.00   4.75402E+01   6.87138E+04   1.08704E+02  -1.48694E+05
```

Example 2

For a phase, as either an end-member or real solution, the listed species name is irrelevant.

For the H2 species as a pure substance (using the SSUB5 database), the following table is obtained by typing `Return for screen`at the prompt `Output file /SCREEN/`, whilst the figure is generated by typing 5 at the prompt Plot column /2/:

```
           O U T P U T F R O M T H E R M O - C A L C

      Phase : GAS                           Pressure :      100000.00

     Specie: H2

    ****************************************************************    T       Cp
    H             S             G

       (K)     (Joule/K)       (Joule)       (Joule/K)       (Joule)

    ****************************************************************  298.15
    2.88369E+01   3.17684E-06   1.30680E+02  -3.89622E+04

    300.00   2.88473E+01   5.33580E+01   1.30858E+02  -3.92042E+04

    400.00   2.91591E+01   2.95686E+03   1.39209E+02  -5.27268E+04

    500.00   2.92650E+01   5.87874E+03   1.45729E+02  -6.69856E+04

    600.00   2.93441E+01   8.80908E+03   1.51071E+02  -8.18336E+04

    700.00   2.94579E+01   1.17488E+04   1.55602E+02  -9.71730E+04

    800.00   2.96320E+01   1.47027E+04   1.59547E+02  -1.12935E+05

    900.00   2.98786E+01   1.76776E+04   1.63050E+02  -1.29068E+05

    1000.00   3.02043E+01   2.06810E+04   1.66214E+02  -1.45533E+05

    1100.00   3.05319E+01   2.37171E+04   1.69108E+02  -1.62302E+05

    1200.00   3.09281E+01   2.67897E+04   1.71781E+02  -1.79348E+05

    1300.00   3.13615E+01   2.99040E+04   1.74274E+02  -1.96652E+05

    1400.00   3.18115E+01   3.30625E+04   1.76614E+02  -2.14197E+05

    1500.00   3.22641E+01   3.62664E+04   1.78824E+02  -2.31970E+05

    1600.00   3.27094E+01   3.95151E+04   1.80921E+02  -2.49958E+05

    1700.00   3.31406E+01   4.28078E+04   1.82917E+02  -2.68151E+05

    1800.00   3.35526E+01   4.61426E+04   1.84823E+02  -2.86539E+05

    1900.00   3.39415E+01   4.95175E+04   1.86648E+02  -3.05113E+05

    2000.00   3.43045E+01   5.29300E+04   1.88398E+02  -3.23866E+05
```

REACTOR (REACTOR_SIMULATOR) Commands

In this section:

CREATE_DIVIDERS

This command is for the REACTOR_SIMULATOR (REACTOR) module.

Define the segment boundaries and the ways on how to distribute phases between various segments and to split the feeds of heat and mass.

Syntax	CREATE_DIVIDERS
Prompts	`Number of dividers /4/: <The number of dividers>` Specify the number of dividers (boundaries between various segments) in the reactor. It is normally the segment number plus one: for example, if the stage box number is defined as 4, the divider number should be defined as 5.
	`Number of outputs for divider # /3/: <The number of outputs>` Specify the number of outputs for a specific divider #.
	`Percent of input to output 1 /100/: <Percent of input>` Define the percentage of input to the output 1 in the current divider #.
	`Percent of input to output ## /100/: <Percent(s) of input(s)>` Define the percentages of inputs to the outputs ## in the current divider #. It is repeated till the last output is specified.

CREATE_PIPES

This command is for the REACTOR_SIMULATOR (REACTOR) module.

Define the pipes between various segments and the ways on how the mass and heat transport between the surroundings (with the record number as 0) and the reactor, among various segments in the reactor, and along various dividers (segment boundaries in the reactor).

Syntax	CREATE_PIPES
Prompts	`From record: <A record number>` Specify a record number. If there are four segments in the reactor, these records are available: • `0` surroundings • `1-4` stage boxes (segments) • `5-9` dividers (segment boundaries)
	`Pipe to record: <Another record number>` Specify another record number to which the mass or heat flows from the current record (specified above). Before this prompt, a message shown on the screen indicates what kind of mass or heat flow (according to the definitions of stage boxes and dividers, which have already been created prior to this command) should be specified in the pipe. This is repeated for all inputs and/or outputs for mass and/or heat in current record.

CREATE_STAGE_BOXES

This command is for the REACTOR_SIMULATOR (REACTOR) module.

Create several reaction stages as boxes (segments), where the you define the feed in either mass input and initial temperature or heat input from surroundings, as well as the mass out and initial temperature in each of the segments.

Syntax	CREATE_STAGE_BOXES
Prompts	`Number of stage boxes /4/: <The number of stage boxes>` Specify the number of stage boxes in the reactor. Then define the feed of mass and/or energy (from surroundings to) the rector.
	`Give feed to system: <Feed>` One feed (of mass or heat) to the reactor must be specified here. Two types of feeds can be used: - As input amount of heat (enthalpy): `H=Value`. - As input amount of specific species or element and its initial temperature: `N (SPECIES)=Value, Input temperature` (in one line, or the input temperature in the next prompt).
	`Input temperature /298.15/: <Input temperature>`

	`Give feed to system: <Feed>`
	Specify other feeds (mass or energy) to the reactor. Press <Enter> to finish the feed inputs, and then:
	`Give for stage box #`
	Now start to define the type of stage box (segment is specifically numbered as #), and to specify a guess of initial temperature and an output for each phase in the segment.

	`Type of box/Equilibrium/: <Type of box>` Only the `EQUILIBRIUM` type is allowed. Press <Enter> to accept it.
	`Is the stage heat controlled? /Y/: <Yes or No>` Y means the current segment is heat controlled.
	`Initial guess of temperature? /1000/: <Initial temperature>` Give a guess of initial temperature (in K) for the current segment; press <Enter> to accept the default.
	`Give initial amount: <Initial amount of mass or heat>` The initial amount of mass and/or heat in the current segment can be specified here. Two types of initial amount can be used: - As initial amount of heat (enthalpy): `H=Value`. - As initial amount of specific species or element and its initial temperature: `N (SPECIES)=Value, Input temperature` (in one line, or the input temperature in the next

Syntax	CREATE_STAGE_BOXES
	prompt).
	`Input temperature /298.15/: <Input temperature>`

	`Give initial amount: <Initial amount of mass or heat>`
	Specify initial amount (mass or energy) in the current segment. Press <Enter> to finish the initial amount inputs, and then this message displays:
	`Each phase may have a separate output, give these`
	Now start to define the output for each phase.

	`Phase name /Rest/: <Name of phase>` Specify a phase that has a separate output, e.g. `GAS`; by pressing <Enter> to accept that all `REST` phases do not have separate outputs. Then the program asks for further definitions of all the other segments (one by one), repeating some of the above questions, till the last segment in the reactor is defined.

EXECUTE_POLY3_COMMAND

This command is for the REACTOR_SIMULATOR (REACTOR) module.

Syntax	EXECUTE_POLY3_COMMAND
	To directly use all kinds of POLY commands inside the REACTOR module. Any legal POLY commands can be entered. POLY Module Commands

LIST_RECORDS

This command is for the REACTOR_SIMULATOR (REACTOR) module.

Syntax	LIST_RECORDS
	Lists all the already-created records for the reactor (including stage boxes, dividers, pipes, etc.).

READ_WORKSPACE

This command is for the REACTOR_SIMULATOR (REACTOR) module.

The REACTOR workspace (along with the related POLY and GIBBS workspaces) and the simulated results from the SIMULATE command can be read by this command from a binary file where they must be saved with SAVE_WORKSPACE. The *.RCT file is not printable.

Syntax	READ_WORKSPACE
Options	`File name`: The name of a saved *.RCT file where the REACTOR and POLY/GIBBS workspaces shall be read from must be specified. You do not need to type the extension if it is the default .RCT, otherwise type the whole *.RCT file name. An **Open** window displays if a file name is not given after the command or its path is incorrect, so that the path (in the **Look in** field) and **File name** can be specified. The **Files of type** (i.e. RCT) cannot be changed.

SAVE_WORKSPACES

This command is for the REACTOR_SIMULATOR (REACTOR) module.

The POLY module and Gibbs (GES) module also have a command with the same name.

The workspaces are saved to a file with this command. In the REACTOR workspace, all definitions of multi-stage steady-state rector and its distribution coefficients are saved, together with the GIBBS and POLY workspaces.

After using this command, you can always return to the state when you issued the command by giving a READ command.

After saving the workspaces to a file, you can exit the software and at a later time READ the file and continue from the saved state.

START_SIMULATION automatically saves on the work file with the most lately specified name. To avoid destroying the simulated results, do not SAVE after a START_SIMULATE command is enforced, similar to that you should not use SAVE after a STEP or MAP command. You may append several results by START_SIMULATE without destroying the previous results but SAVE erases them all.

Syntax	SAVE_WORKSPACES
	`File name` A file name must be specified. The default extension of the RCT file is .RCT, while or any other extension as required.
	A **Save** window displays if a file name is not given after the command, so that the path (in the **Save in** field) and **File name** can be specified. The **Files of type** (i.e. RCT) cannot be changed. If there is already a file with the same file name under the directory a warming message displays. Click **OK** to overwrite the current REACTOR (and POLY3/GIBBS) workspaces onto the existing *.RCT file. Click **Cancel** to return to the REACTOR module. You can use the SAVE command with an unspecified name (i.e. through `SAVE ,,,` command-sequence) to save the REACTOR (and POLY3/GIBBS) workspaces.

START_SIMULATION

This command is for the REACTOR_SIMULATOR (REACTOR) module.

Start the reactor simulation, and list the results for all iterations. The output for each iteration consists of the conditions set in each segment, and you can also select some state variables to list. After each loop, the temperatures in all segments are listed.

Syntax	START_SIMULATION
Prompts	`Max number of loops /10/: <The max number of loops>` Give the max number of loops. The reactor simulation repeats until this loop number is reached.
	`Output to screen or file /Screen/: <File name or return>` Decide on either listing simulation results on the screen (by pressing <Enter>) or saving them on an experimental file (with the default extension .EXP). The conditions in each segment are not saved in the file, only on the screen.
	`Output variables /T BP($)/: <Variable name(s)>` Specify the variable name(s) that is also listed on the screen together with the conditions in each segment, or in the output experimental file.

Example

For a four-stage reactor, the output at a certain iteration may look like this:

```
H=-991745.1, P=100000, N(C)=2.8468936, N(N)=6.78399966E-4, N(O)=3.8171615,
N(SI)=1.77031
DEGREE OF FREEDOM 0
BP(GAS)=43.464341, BP(C1SI1_BETA)=25.175981, BP(C_S)=8.1588099,
BP(QUARTZ_S3)=68.193896
1.78803E+03
BP(GAS)=61.971213, BP(C1SI1_BETA)=38.144346, BP(QUARTZ_L)=66.230717 2.06569E+03
BP(GAS)=67.66262, BP(C1SI1_BETA)=35.480983, BP(QUARTZ_L)=58.219292
2.08691E+03
BP(GAS)=71.23129, BP(SI_L)=22.471787
2.20831E+03
H=-924751,87, P=100000, N(C)=2.0594558, N(N)=5.17999978E-4, N(O)=4.0142358,
```

```
N(SI)=2.7551438
DEGREE OF FREEDOM 0
BP(GAS)=43.464341, BP(C1SI1_BETA)=25.175981, BP(C_S)=8.1588098,
BP(QUARTZ_S3)=68.193896
1.78803E+03
BP(GAS)=61.971213, BP(C1SI1_BETA)=38.144346, BP(QUARTZ_L)=66.230717 2.06569E+03
BP(GAS)=67.66262, BP(C1SI1_BETA)=35.480983, BP(QUARTZ_L)=58.219292
2.08691E+03
BP(GAS)=71.23129, BP(SI_L)=22.471787
2.20831E+03
H=-813239., P=100000, N(C)=1.6592668, N(N)=3.59999988E-4, N(O)=3.7549293,
N(SI)=2.896635
DEGREE OF FREEDOM 0
BP(GAS)=43.464341, BP(C1SI1_BETA)=25.175981, BP(C_S)=8.1588098,
BP(QUARTZ_S3)=68.193896
1.78803E+03
BP(GAS)=61.971213, BP(C1SI1_BETA)=38.144346, BP(QUARTZ_L)=66.230717 2.06569E+03
BP(GAS)=67.66262, BP(C1SI1_BETA)=35.480983, BP(QUARTZ_L)=58.219292
2.08691E+03
BP(GAS)=71.23129, BP(SI_L)=22.471787
2.20831E+03
H=7374.6403, P=100000, N(C)=8.84911857E-1, N(N)=1.99999996E-4, N(O)=1.9379203,N
(SI)=1.853872
DEGREE OF FREEDOM 0
BP(GAS)=43.464341, BP(C1SI1_BETA)=25.175982, BP(C_S)=8.1588097,
BP(QUARTZ_S3)=68.193896
1.78803E+03
BP(GAS)=61.971213, BP(C1SI1_BETA)=38.144346, BP(QUARTZ_L)=66.230717 2.06569E+03
BP(GAS)=67.66262, BP(C1SI1_BETA)=35.480983, BP(QUARTZ_L)=58.219292
2.08691E+03
BP(GAS)=71.23129, BP(SI_L)=22.471787
2.20831E+03
10  1788.03  2065.69  2086.91  2208.31     0.00     0.00     0.00
```

POST Module Commands

The POST module (post-processor) is available from the these modules: POLY, TAB, BIN, TERN, POT, SCHEIL and POURBAIX.

? Using the POST Module

In this section:

ADD_LABEL_TEXT

Add a text to an area in a phase diagram or a property diagram. The label is written starting from the specified coordinates. Optionally, you can also let the program automatically add the text by first calculating an equilibrium state at the specified coordinates and then making a label out of the stable phase names.

The label texts and coordinates, either added by this command or modified with MODIFY_LABEL_TEXT (or manually edited in the **Console Results** window), are stored in the workspace, and these may later be saved onto an *.EXP file (with MAKE_EXPERIMENTAL_DATAFILE).

In some cases such an optional calculation for automatic phase region labeling may not work. It is not possible to automatically add labels for certain sets of axes, like entropy, enthalpy, pH, Eh, etc.

Plot Labels

Syntax	ADD_LABEL_TEXT
Prompts	`Give X coordinate in axis units: <Value of the X coordinate>` Specify the value of the X coordinate where the label is to start.
	`Give Y coordinate in axis units: <Value of the X coordinate>` The labels disappear if any axis is changed after wards. Specify the value of the Y coordinate where the label is to start.
	`Automatic phase labels? /Y/:` By default the program automatically calculates the equilibrium at the given coordinates and generates a label with the names of the stable phases. However, the automatic calculation works only for phase diagrams that are mapped with two axes in the POLY module, and sometimes it may not work correctly especially for complex heterogeneous interaction systems; in such cases, a message displays.

	`Text: <Text for the label>`
	If you answer N enter text at the prompt. You can enter simple text, use LaTeX, rotate the text, as well as adjust the font size.
	LaTeX: You can use LaTeX commands to enter text and symbols. First enter the command followed by the expression or string, for example to display `Al2O3` with subscripts:
	`\latex Mole-fraction Al_2O_3`

Syntax	ADD_LABEL_TEXT

By default when using the LaTeX command, you are in math mode and Thermo-Calc automatically interprets the entered text as math. The above link uses the dollar sign ($) in all the examples but this is NOT required. For example, if you enter `$E=mc^2$` this is displayed including the $ instead of the equation.

To add a mixture of plain text and equation text, you can exit math mode using the string \textsf followed by the text to display enclosed in curly brackets.

For example `\latex \textsf{Mole-fraction }Al_2O_3` displays this sans serif label

Mole-fraction Al_2O_3

White space has to be entered in the text context and not outside in math mode.

Rotate the text: If you want to rotate the label, start a text string with the rotation command (which is case sensitive and must be in lower case letters) then enter the number of degrees to rotate the label. For example, to rotate the label 45 degrees enter:

```
\rotation 45
```

To rotate the text and use LaTeX, the rotation command must be used first. For example:

```
\rotation 45 \latex Mole-fraction Al_2O_3
```

Rotates the text 45° and includes subscripts in the title Mole-fraction Al_2O_3.

```
Text size: /.35/: <Size for the label>
```

A smaller size of the text may be necessary to fit the label text into the diagram. A default size is given using the latest size in adding label texts, or .35 if the command is called for the first time. A recommended size is e.g. 0.25.

These changes to plot labels can also be manually edited in the **Console Results** window.

Examples

To produce a label with the unit Celsius:

```
\textsf{Temperature [}^\circ C\textsf{]}
```

Text with white space, suitable for an axis label:

```
\textsf{Text with space} Al_2O_3
```

APPEND_EXPERIMENTAL_DATA

Add experimental data and text onto a calculated diagram. This is done by placing the experimental data and text on a formatted textual file (always having an extension of EXP) that is prepared outside of Thermo-Calc software (Console Mode and Graphical Mode), according to the syntax of the DATAPLOT Graphical Language.

The picture generated from the data is superimposed on the ordinary graphical output from the postprocessor. Such an experimental data file (*.EXP) may be created by an ordinary textual editor.

Another important usage of this command is to superimpose plots from several independent calculations. For this purpose, there is a command MAKE_EXPERIMENTAL_DATAFILE, which dumps a calculated diagram on an EXP file according to the DATAPLOT syntax. With the aid of a normal text editor, many such files may be merged together. Remember that you can only have one prologue section on each such EXP file.

DATAPLOT User Guide included with this documentation set.

Syntax	APPEND_EXPERIMENTAL_DATA
Prompts	`Use experimental data (Y or N) /N/:` By default, no experimental data are plotted. Enter Y to use the data from an experimental data file in the next plot. An **Open** window displays to specify the name of the file with the experimental data.
	`Prologue number: /0/: <Prologue number>` Select which prologue to use. In a prologue, you can, for example, give the scaling of an axis, the axis texts, and so on. By answering -1, a list of all prologues on the file is given; and by 0, no experimental data are appended.
	`Dataset number(s) /-1/: <Dataset number(s)>` Select from which dataset(s) data should be read. Several datasets may be given separated with commas or spaces. By answering -1, a list of all datasets on the file is given; and by 0, no experimental data are appended.

CHANGE_LEGEND

When there is a legend in the diagram you can append constitution and/or ordering descriptions to the phase name.

LIST_EQUILIBRIUM also displays `ORD` (ordered) or `DISORD` (disordered) (when available).

In some cases the legend only shows the phase name for a line when SET_LABEL_CURVE_OPTION is set to `F`.

Syntax	CHANGE_LEGEND
Prompt	`Set suffix for phase names in legend? (All, None, Constitution, Ordering)/None/:` • `None`: the legend includes the standard information about the phases. • `All`: the Constitution description and the Ordering description (when there is ordering) are also included. • `Constitution`: it is added to the standard description. • `Ordering` (when applicable): it is added to the standard description.
	For examples and more details about what these options show, see About Legend Styles and Legend and Label Styles where it is described for Graphical Mode.

DUMP_DIAGRAM

This is an alternative command used to create output. First use the PLOT_DIAGRAM command to send output to the Console Results window. Then you can save it to a file either using this command or right-click the diagram in the Console Results window and select Save as.

Similar to PRINT_DIAGRAM, it does not matter what graphic device/printer is set up. The command can convert the diagram shown in the Console Results window to the selected format.

Syntax	DUMP_DIAGRAM
Prompt	`Output format/: (jpg,ps,pdf,svg,emf,gif,png) /png/`
	Enter a format or press <Enter> to accept the default (png). If you choose to enter the parameters and file name in one line (i.e. when you are entering the command), the **Save** window does not open as described below. For example, if you enter `dump_diagram png test` at the prompt, an image file called **test.png** is output to the same folder where the macro file is stored. If a file with the specified name already exists, you are prompted to overwrite the old file. You can alternatively add `Y` or `N` to the command string to specify whether to overwrite the file or not e.g. `dump_diagram png test y`. A **Save** window opens if you have not specified a file name. Select a directory path and enter a **File name**. If a file with the specified name already exists, then you are prompted whether to overwrite the old file or not. The third argument of the command (Y) allows you to specify whether to overwrite the old file or not (N).

After the output is done, the temporarily set graphic device for conversion and printing is switched back to the one set by the command SET_PLOT_FORMAT, so that you can save the graph in file(s) using PLOT_DIAGRAM.

ENTER_SYMBOL

This command is for the POST module.

There are also a GES and POLY module commands with the same name.

Symbols are a useful feature of the POLY and POST modules to define quantities that are convenient. Symbols can be constants, variables, functions or tables.

Functions or tables (with defined functions as values) can be entered in the POST module after a stepping or mapping calculation, for purposes of plotting such entered functions or tables as axis variables.

Within the POLY module, symbols are normally defined prior to an equilibrium calculation (enforced by a C_E command), stepping calculation (enforced by the command STEP_WITH_OPTIONS) or mapping calculation (enforced by MAP). These can be entered after an equilibrium calculation; however, for defined functions, variable or tables, it requires using EVALUATE_FUNCTIONS before showing the corresponding values in the calculated equilibrium state.

The symbols entered in the POST module are not saved in the currently-loaded POLY3 workspaces. Therefore, if you want to apply such symbols in other similar calculations for the same defined system, you must use the ENTER_SYMBOL command prior to the STEPPING or MAPPING calculation in the POLY module.

See example 44for an example of using variables and functions.

Symbols are a useful feature modules to define quantities that are convenient. Symbols can be constants, variables, functions, or tables.

Syntax	ENTER_SYMBOL
Prompt	`Constant, Variable, Function or Table? /Function/: <Keyword>` The `Keyword` can be specified as `CONSTANT`, `VARIABLE`, `FUNCTION`, or `TABLE`. • CONSTANTS can only be entered once and is a means of using a name for a numeric value. For example, the value of 1 atmosphere in Pascal can be denoted by `P0` after the command ENTER_CONSTANT `P0=101325`. Defined constants can be used as values in condition assignments, for example, `SET-COND P=P0`. • FUNCTIONS are expressions of state variables or other functions. These expressions are saved, and whenever a function value is requested all functions are evaluated. The reason for this is that they may depend on each other. • VARIABLES are similar to functions because they can also be expressions of state variables. However, contrary to functions, they are only evaluated when they are entered or if they are explicitly named in an EVALUATE_FUNCTIONS command. It is possible to enter a variable

Syntax	ENTER_SYMBOL

with a new expression any time. This expression is evaluated directly and its value stored as the value of the variable. Defined variables can be used as values in the SET_CONDITION command.

- TABLES are used for listing results from the STEP or MAP commands. A table consists of a list of any number of state variables, functions, or variables. Defined tables can also be used in the POST (post-processor) module.

There is a special connection between tables and variables. If a variable is used in a table, it is evaluated for each line of the table in the TABULATE command or when the table is used in a plot.

`Name: <Name of the symbol>`

Each symbol has a unique name that must start with a letter and can have maximum 8 characters. Legal characters include letters (either UPPER or lower case), digits and underscore _. Any other special character, such as parentheses (and), plus +, minus -, slash / or \, full stop (.), are illegal for symbol names.

You can enter the symbol name and the value or function on the same line; these must be separated with an equal sign =, for example, `TC=T-273.15` or `T_C=T273.15` which stands for a definition of temperature in Celsius. Otherwise, these questions are asked.

For different types of symbols (constant, function, variable, or table), the questions have different prompts.

`Function: <Definition for a function or variable>`

Functions and *variables* are evaluated from an expression of state variables or other functions, constants, or variables. The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers).

Unary functions like `LOG`, `LOG10`, `EXP`, `SIN`, `COS`, and `ERF` can also be used. An expression can be continued on more than one line. An expression should be terminated by a semicolon (;) or an empty line (press <Enter> at the next prompt).

Examples of function expressions:

- `GM(LIQUID)`: The Gibbs energy of liquid per mole component
- `H.T/4.184`: The heat capacity of the system in calories
- `ACR(CR)/X(FCC,CR)`: The activity coefficient for Cr in FCC
- `T-273.15`: The temperature in Celsius

`&: <Continuation of the definition for the symbol>`

The ampersand & means that you can continue to write the function on the new line if one line is

Syntax	ENTER_SYMBOL
	not enough for the function. If you finish the function press <Enter> again.
	`Value: <Value for a constant>` A *constant* can only be assigned a numeric value once.
	`Value or expression: <Value of expression for a variable>` A *variable* can be assigned a numeric value or an expression. An expression is evaluated immediately and discarded. Only the numeric value is kept. This gives a possibility to save a value between calculations with different conditions because all state variables and functions are evaluated for the new conditions.

	`Variable(s): <Variable(s) in a table>`
	A *table* consists of a list of state variables or functions. One way to obtain results from a STEP command is through a table.
	Example:
	`ENTER TABLE K=T,X(LIQ,C),X(LIQ,CR),ACR(C)`
	Which means that the table called K contains four columns, i.e. the temperature, the mole fractions of C and Cr in the LIQUID phase, and the activity of C.
	To show the temperature in Celsius in a table, give the command ENTER_FUNCTION `TC=T-273`; and then use the symbol `TC` in the table.
	`& <Continuation of the definition for the table>`
	The ampersand `&` means that you can continue to write the table on the new line if one line is not enough for the table. If you finish the table press `<Enter>` again.

FIND_LINE

Identifies various property curves on a plotted property diagram (after a stepping calculation); it also works well in find stable phase regions on a phase diagram (after a mapping calculation).

Syntax	FIND_LINE
Prompts	`X coordinate /.484623611/: <Value of the X coordinate>` Specify the `value of the X coordinate` where you want to find the details of property curve (or phase region).
	`Y coordinate /.5153737962/: <Value of the Y coordinate>` Specify the `value of the Y coordinate` where you want to find the details of property curve (or phase region). The POST module displays the identified property (for a property curve on a property diagram), or the identified stable phase-assemblage (for a phase region on a phase diagram).

LIST_DATA_TABLE

This is a POST module command.

This command is used for listing various properties (i.e. the Y-axis variable on a property diagram) that change with an independent variable (i.e. the X-axis variable on a property diagram), which have already been defined in the POST module (and often are plotted on the **Console Results** window), but only after a STEP calculation.

The listing output can be either on screen or in a spreadsheet file in the MS Excel format (under specified file name with the default file extension of XLS), which can be further edited or used for graphical handling by opening the file (using the MS-Excel program) outside of the Thermo-Calc software system.

Syntax	LIST_DATA_TABLE
Prompt	`Output to screen or file /Screen/: <File name or return >` Specify a file name if you want to save on a spreadsheet file (in the MS Excel format, with the default extension of `XLS`) on which the already-defined properties on a property diagram (after a STEP calculation) is saved, or press <Enter> if want to see a simple textual table on screen (for the already-defined properties that change alone with an independent variable). This command only works for a property diagram after a stepping calculation but not for any phase diagram after a mapping calculation.

LIST_PLOT_SETTINGS

This is a POST module command.

Syntax	LIST_PLOT_SETTINGS
	Lists the present values of most parameters specifying the type of diagram to be plotted.

LIST_SYMBOLS

This command is for the POST module.

There is also a POLY module command with the same name.

Use this command to list the definitions for all constants, functions, variables and tables. In order to find the value of a function or variable, use SHOW_VALUE or EVALUATE_FUNCTIONS. A table is tabulated with the TABULATE command.

Syntax	LIST_SYMBOLS
	The defined variables are listed up together with the defined functions, but variable names are followed by a percentage sign `%`.

LIST_TIME_STEPS

This for the POST PROCESSOR module.

Use the LIST_TIME_STEPS command to list all integration time steps.

MAKE_EXPERIMENTAL_DATAFILE

Write the graphical information onto screen or a formatted text file (always having an extension of `.EXP`) using the DATAPLOT graphical format. In order to merge two or more diagrams from separate calculations, you can write them out on files with this command, and then add/edit them together with a normal text editor.

There is another type of experimental data file that is generated in Thermo-Calc when working with the PARROT module. For more information seeExperimental Data Files (*.POP, *.DOP).

Syntax	MAKE_EXPERIMENTAL_DATAFILE
Prompt	`Output to screen or file /Screen/: <Name of a file or return>` Specify the name of the desired file. Press <Enter> for a list. Otherwise enter a file name where the graphical information is written. The default file extension is `EXP` (for Windows) or `exp` (for Linux).

MODIFY_LABEL_TEXT

Move a label created with the command ADD_LABEL_TEXT to another position, or replace its text with another one.

The label texts and the coordinates, either added by ADD_LABEL_TEXT command or modified by this command or manually edited on the Console Results window, are stored in the workspace, and can be saved onto an *.EXP file (through MAKE_EXPERIMENTAL_DATAFILE).

Syntax	MODIFY_LABEL_TEXT
Prompts	`Which label to modify? /#/: <Number of the label>` Before this prompt, all the labels created by the ADD_LABEL_TEXT command is listed with an identifying number. Specify the `Number of the label` you want to modify. The default one (#) is the last added label.
	`New X coordinate: /xxx/: <New X position>` Specify the `New X position`. The previous X coordinate is displayed. Press <Enter> to accept.
	`New Y coordinate: /yyy/: <New Y position>` Specify the `New Y position`. The previous Y coordinate is displayed. Press <Enter> to accept.
	`New text /ABCDEFGH.../: <New labeling text>` Specify the `New labeling text`. The previous text is displayed. Press <Enter> to accept. ❗ The new label text must not be longer than the previous text.

PLOT_DIAGRAM

After you use the SET_PLOT_FORMAT command to define the default graphic device (the printer) you can use a PLOT_DIAGRAM command to either save the calculation output to a file or display the output in the Console Results window.

> ❗ The diagram axes must be set first.

The functionality of this command is shared in two ways:

- in PLOT_DIAGRAM for normal screen display and file saving and
- *Windows OS*: If the device is not defined, you can alternatively use PRINT_DIAGRAM for a hard copy.

Syntax	PLOT_DIAGRAM
Prompt	`Output to screen or file /Screen/: <Name of a file or return for screen>` `Specify the name of the file`
	For Linux users, the prompt is `PLOTFILE /SCREEN/`). A file with a proper extension for the selected graphic format (set by SET_PLOT_FORMAT) is saved under the current working directory. If no extension is given in the file name, the default extension e.g. ps for Postscript portrait/landscape modes, P7 or p7 for HPGL landscape, P8 or p8 for HPGL portrait, etc.) is automatically given to the file name. If the default device is set (SET_PLOT_FORMAT), press <Enter> to plot the diagram on the screen in the Console Results window or give a file name to save it.

PRINT_DIAGRAM

Saving and Printing the Output in Console Mode

First use PLOT_DIAGRAM to create a diagram that displays in the **Console Results** window. Then after entering the PRINT_DIAGRAM command, the **Print** window opens where you can choose additional settings for a hard copy of the diagram.

PRINT_DIAGRAM functions in the same way as in the **Console Results** window where you can right-click a diagram and choose **Print**.

QUICK_EXPERIMENTAL_PLOT

This is similar to APPEND_EXPERIMENTAL_DATA but can be used when there is no graphical information to be plotted in the POLY3 workspace. It defines a pair of axes, sets the axis labels to X and Y, and scales both X- and Y-axes between 0.0 and 1.0 unless a prologue is read from the DATAPLOT (*.EXP) data file.

Plotting Experimental Data Files in the *DATPLOT User Guide* included with this documentation set.

Syntax	QUICK_EXPERIMENTAL_PLOT
Prompts	`Prologue number: /0/: <Prologue number>` An **Open** window displays. Select the prologue to use. In a prologue, you can, for example, give the scaling of an axis, the axis texts, and so on. By answering -1, a list of all prologues on the file is given; and with 0, no experimental data are appended.
	`Dataset number(s) /-1/: <Dataset number(s)>` Select from which dataset(s) data should be read. Several datasets may be given separated with commas or spaces. By answering `-1`, a list of all datasets on the file is given; and with `0`, no experimental data are appended.

REDUCE_TIMESTEPS_TO_PLOT

The REDUCE_TIMESTEPS_TO_PLOT command reduces the number of timesteps used in a plot. The command requires a fraction of the total number of stored timesteps, where `1` is to use all timesteps and `0` is to use no timesteps.

If post-processing a large store file with too many timesteps, this factor may be automatically reduced.

Syntax	REDUCE_TIMESTEPS_TO_PLOT
Prompt	`Fraction of Timesteps to Use /1/:` The fraction of the total number of stored timesteps to be used in the post-processing, where `1` is to use all timesteps and `0` is to use no timesteps.

REINITIATE_PLOT_SETTINGS

The REINITIATE_PLOT_SETTINGS command gives default values to all parameters describing the diagram. All plot settings made in the POST module are deleted, and it returns to the initial settings when the POST module is entered.

RESTORE_PHASE_IN_PLOT

Restores a phase previously suspended from the plot with SUSPEND_PHASE_IN_PLOT. It works only after at least one phase is suspended.

Syntax	RESTORE_PHASE_IN_PLOT
Prompt	`Phase name: <Name of a phase>` Give the name of the phase to be restored.

SELECT_CELL

Select the cell data to be processed. You can only plot data from one cell at a time. Type `?` to get a list of valid cell numbers. This command is for the POST PROCESSOR.

Also see the DICTRA module prompt of the same name.

> The current cell number is displayed as a part of the POST PROCESSOR prompt.

Syntax	SELECT_CELL
Prompt	`Number` Number of the cell to be selected. Specify cell number by giving an integer or one of the key words NEXT or PREVIOUS.
	`Tabulate` Tabulate a named table. The independent variable is always printed in the first column.
	`Name` Give the symbolic name of the table.
	`Output file /Screen/` Select output device/file. Press Enter to get output on the screen.

SELECT_PLOT

Select a plot (diagram) within the current **Results** tab in the **Console Results** window.

Syntax	SELECT_PLOT
Prompt	`Plot <N/New>` Where `N` is a positive integer. Enter the number of the plot that is selected in the **Console Results** window (in the currently selected **Results** tab). If a plot with that number does not exist, it is created. The default parameter value is `NEW`. If this is entered, then a new plot is created. Create a new plot can also be done by pressing <Ctrl+Shift+T>.

SET_AXIS_LENGTH

Change the real length of an axis in inches. The default number of tic-marks on an axis is 10 when the relative length is 1. The number and units per tic-mark must be a multiple of 1, 2 or 5 to obtain a reasonable scaling of an axis.

Syntax	SET_AXIS_LENGTH
Prompts	`Axis (X, Y or Z): <Name of an axis>` Specify which axis to set the length.
	`Axis length /11.5/: <New relative axis length>` Specify the new real axis length in inches. The relative length 1 corresponds to 10 tic-marks on the axis.

SET_AXIS_PLOT_STATUS

Specify whether the axis title texts and axis label texts are to be plotted or not on a diagram. It does not work for the axis lines and tic-marks. If you want to plot a diagram without tic-marks, use SET_TIC_TYPE first.

This can be used to merge different diagrams on a pen-plotter or to obtain the diagram faster. The default status is that all the set axes are to be plotted.

Syntax	SET_AXIS_PLOT_STATUS
Prompt	`Axis plot (Y or N) /Y/: (Y or N)`

SET_AXIS_TEXT_STATUS

Change the axis text from the automatic text given by the axis specification to a text.

ADD_LABEL_TEXT

Syntax	SET_AXIS_TEXT_STATUS
Prompts	`Axis (X, Y or Z): <Name of an axis>` Specify which axis text status to change.
	`Automatic axis text (Y or N) /N/:` Specify if automatic axis text is to be used.
	`Axis text: <Enter axis text>` You can enter simple text, use LaTeX, rotate the text, as well as adjust the font size.

SET_AXIS_TYPE

Change the axis type among linear, logarithmic and inverse axis.

Syntax	SET_AXIS_TYPE
Prompts	`Axis (X, Y or Z): <Name of an axis>` Specify which axis to change the axis type.
	`Axis type /Linear/: <New axis type>` Specify which new axis type to set. Select `LIN`ear (default), `LOG`arithmic or `INV`erse. Only the three first characters are relevant.

SET_COLOR

Some devices support colours or line thickness. With this command, select different colors or line types on some types of information on a diagram.

This command can fail if a chosen device does not support colors or line thickness.

This command gives four sequential prompts (i.e. text and axis, invariant equilibria, tie-lines, and all other lines), with the keyword and default option (both listed below). Depending on if the switched-on graphic device (by SET_PLOT_FORMAT) supports colors or line types, the POST automatically switches on the appropriate Keyword.

Syntax	SET_COLOR

Prompt	`Text and axis keyword /Default option/`
	`<Return or new option>`
	`Invariant equilibria keyword /Default option/: <Return or new option>`
	`Tie-lines color keyword /Default option/: <Return or new option>`
	`Keyword of all other lines /Default option/: <Return or new option>`
	This is usually for the solubility lines.

	The `Keyword` is either `Color` or `LineType`, depending on if color or line type is supported by the switched-on graphic device (by SET_PLOT_FORMAT); the POST module *automatically* switches on the appropriate `Keyword` .

Color Options

The options for `Color` are:

BACKGROUND	BLUE	PURPLE	GRAY
FOREGROUND (default)	YELLOW	GOLD4	ORANGERED3
RED (default for invariant equilibria)	MAGENTA	TURQUOISE4	MAROON
GREEN (default for tie lines)	CYAN	PINK	PLUM

	SIENNA	OLIVEDRAB	SEAGREEN
	ORANGE1	CORAL1	USERDEF

LineType Options

The options for `LineType` are:

INVISIBLE	VERY_THICK (default for invariant equilibria)
NORMAL (default)	THIN (default for tie lines)
THICK	VERY_THIN
DASHED	DOTTED

SET_CORNER_TEXT

Adds text to the corners on a plotted diagram. Normally, you can write such texts as a subtitle.

The primary database (not the appended ones) used in calculations and the calculated conditions are automatically plotted at the upper-left corner as a part of the header on all plotted diagram. Unless the plotting option WRITE CONDITIONS is switched off by the command SET_PLOT_OPTIONS, the calculated conditions are always written on plotted diagrams; and only when the plotting option PLOT HEADER is switched off by the command SET_PLOT_OPTIONS, the used database also always appear. Under such circumstance, avoid writing texts at the UPPER_LEFT corners.

Syntax	SET_CORNER_TEXT
Prompt	`Corner/Lower_Left/: <Return or new option>` Choose an option: • LOWER_LEFT • UPPER_LEFT • UPPER_RIGHT • LOWER_RIGHT • TOP_OF_TRIANGLE
	`Text: <Texts as a subtitle or a note>` Write the texts that are to be written on the specified diagram corner.

SET_DIAGRAM_AXIS

Specify an axis variable for a plot or a listing. To be able to plot a diagram, at least two axis variables (X and Y) must be specified. In Console Mode, three axes (X, Y, and Z) can be specified for a diagram.

The axis variables in the plot can be different from the number of axis used for the mapping.

If you want to plot a phase diagram with tie-lines in the plane after a MAP calculation, then the composition axis must be `mole-fraction` or `weight-fraction`, or `mole-percent` or `weight-percent` of one specific component. You must not use the stable variable `x(comp)` or `w(comp)` even if that is what you used when calculating the diagram, because that only gives one side of the two-phase region. It may be sufficient to indicate that mole-fraction is the same as the stable variable `x(*,comp)`, and weight-fraction is the same as the stable variable `w(*,comp)`.

If you plot a phase diagram where the tie-lines are not in the plane after a MAP calculation, then `mole-fraction` and `x(comp)` are identical.

When you plot a property diagram after a STEP calculation and want a composition axis variable, you should normally use x(comp) and not mole-fraction.

The axis must have exactly the same number of columns, or one axis must have one column. In the first case the columns are plotted matching them one by one; in the latter all columns on one axis is plotted against the single column. For example, you can have the temperature on one axis and the amount of each phase on the other. The amount of each phase is the state variable `NP(*)` in mole fraction or `BPW(*)` for mass fractions of phases.

Automatic diagram axis: The POST module can set automatic diagram axis identical to those used in the MAP command.

If the state variable `x(comp)` is used in a MAP calculation, then mole-fraction of the component is used as diagram axis; if a potential or some other state variables are used, then that is used as a diagram axis.

After a STEP calculation, automatic diagram axis is not set as there is only one axis used in the calculation.

Syntax	SET_DIAGRAM_AXIS
	`Axis (X, Y or Z): <Axis name>` Specify which axis (X or Y or Z) to set with a variable.

Syntax	SET_DIAGRAM_AXIS
Prompts	`Variable type: <Variable name>` Specify a variable for the chosen axis here. The valid variables are: • TEMPERATURE-CELSIUS as temperature in °C • TEMPERATURE as temperature in K • PRESSURE as pressure in Pa • ACTIVITY for a component • LNACTIVITY for a component [ln(ACR(component)] • MOLE-FRACTION for a component • MOLE-PERCENT for a component • WEIGHT-FRACTION for a component • WEIGHT-PERCENT for a component • ENTHALPY as enthalpy in J/mol • ENTROPY as entropy in J/mol/K • NONE to clear the axis • Any valid state variable including those with wildcards, e.g. NP(*) or x(*,component). Due to the use of wildcard * in such a state variable, the program asks for a column number. • Any entered function or variable. • Any entered table.
	If you specify an entered table as the variable, then you are given these prompts: `For component: <Component name>` When an activity, mole or weight fraction or percent of a component shall be plotted, the component name must be supplied here.
	`Column number: <Column number(s)>` Specify the column number(s) in the chosen table that are to be plotted onto the earlier specified axis. For example: • `1` for column 1 • `2,3` for columns 2 and 3 • `2,3 >5` for column 2,3 and all columns above column 5 • `*` for all columns

SET_DIAGRAM_TYPE

Choose the diagram type as perpendicular plot or triangular plot (Gibbs triangle, especially for ternary systems). The default is with a perpendicular axes.

For phase diagrams of ternary or pseudo-ternary systems, it is usually need to plot isothermal sections as triangular grams. If desired, all lines outside the region limited by a line joining the end points of the X- and Y-axis is removed.

Syntax	SET_DIAGRAM_TYPE

Prompts	`Triangular diagram (Y or N) /N/:`
	The default is to set a perpendicular axis. Perpendicular diagrams have (almost) the same scaling on both axes.
	`Create tetrahedron WRML file (Y or N) /N/:`
	The 3D plotting in Console Mode does not work. Enter Y to specify a triangular plot instead.

	`Plot 3rd axis (Y or N) /N/:` If a triangular plot is selected, enter Y to specify a 3rd axis and to connect (and plot) the end points of the X- and Y-axes.
	`Clip along 3rd axis (Y or N) /N/:` If a triangular plot is selected, enter Y so that all lines outside the region limited by a line joining the end points of the X- and Y-axis are removed.

SET_FONT

Select the font to use for labels and numbers when plotting the diagram under the currently selected graphic device (SET_PLOT_FORMAT). For some devices there may be other fonts available and these are selected by SET_PLOT_FORMAT.

Syntax	SET_FONT
Prompts	`Select font number /1/: <#>` Specify an available font number # as the default font for the current graphic device, or accept the font number 1 by pressing <Enter>. By typing a question mark `?` here, the program lists the available fonts under the currently selected graphic device.
	`Font size /.34/: <##>` The size of the chosen font is specified. A value around 0.34 is recommended.

SET_INTERACTIVE_MODE

In the POLY module this is called SET_INTERACTIVE.

Use the SET_INTERACTIVE_MODE command to use it in demonstration or macro files to stop the execution of the command file and pass over input focus to the keyboard.

SET_LABEL_CURVE_OPTION

Identify the curves drawn in the post-processor by marking each curve with a digit and then list the meaning of these digits beside the plot.

> The number of digits can be quite large in some cases. If so, use SET_FONT and reduce the font size; usually, 0.2 is sufficient.

<table>
<tr><th>Syntax</th><th>SET_LABEL_CURVE_OPTION</th></tr>
<tr><td>Prompt</td><td><code>Curve label option (A, B, C, D, E, F OR N) /A/: <Option></code></td></tr>
<tr><td></td><td>
<p>The options:</p>

<code>A</code>: List stable phases along line
<code>B</code>: As A but curves with same fixed phase have same number
<code>C</code>: List axis quantities
<code>D</code>: As <code>C</code> but curves with same quantities have same number
<code>E</code>: As <code>B</code> with changing colors
<code>F</code>: As <code>D</code> with changing colors
<code>N</code>: No labels

<p>This question is rather cryptic but usually the option B or E is good for phase diagrams (after a MAP command) and option D or F for property diagrams (after a STEP command). Those interested can try out the option A and C by themselves.</p>
<blockquote>Option B or E lists the fixed phases along each curve, whereas option D or F gives the axis variables used along each curve. E provides varied colors for different stable-phase curves on phase diagrams (after a MAP command); F provides varied colors for different property curves on property diagrams (after a STEP command). The option <code>N</code> (NONE) disables all curve labels and lists.</blockquote>
<p>If, for example, you use <code>T</code> (temperature in K) as the variable axis in a STEP command and then plot the amount of stable phases (with SET_DIAGRAM_AXIS <code>Y NP(*)</code>) on the Y-axis versus <code>T-C</code> on the X-axis, then the list may have lines like:</p>
<pre>1: T-273.15, NP(LIQUID)
2: T-273.15, NP(FCC_A1)</pre>
<p>This means that for curve <code>1</code> the X-axis is <code>T-273.15</code> (the same for all curves, of course) and <code>NP (LIQUID)</code> on the Y-axis. Curve <code>2</code> has the same X-axis but <code>NP(FCC_A1)</code> on the Y-axis.</p>
</td></tr>
</table>

SET_PLOT_FORMAT

Adjust the format of the graphical output to another graphical device. This default can be changed with the SET_PLOT_ENVIRONMENT command in the SYSTEM MONITOR.

Syntax	SET_PLOT_FORMAT
Prompt	`Graphic device number /#/: <Number of the device>` Specify a graphic device number. Depending on the hardware, different plot formats (graphic devices) may be available. These are listed online by giving a question mark `?`. For some formats there can be additional sub-prompts (Y or N) about the available fonts being used for the chosen format. Also enter Y for further specifications, e.g. font type and size.

SET_PLOT_OPTIONS

You are prompted for and can toggle on (`Y`) or off (`N`) the plotting of some options on all subsequently generated diagrams.

For the `Always initiate POST on re-entering` prompt, the default is Y which implies that the POST module automatically reinitiates whenever the POLY3 workspace is changed upon re-entering. If answered N the same diagram axis variables are kept even if the workspaces in the POLY module are read from or written to a *.POLY3 file. The N answer is useful when there are several sets of *.POLY3 files with the same calculation but for different sets of model parameters.

For the `Always solid line` prompt, the default answer is `N` which means that the POST module plots solid lines for stable phases but dashed lines for metastable phases. This is normally for plotting property diagram after a STEPPING calculation; however, when there is a metastable extrapolation in a phase region on a phase diagram after a MAPPING calculation, this is also enforced. When the alternative answer Y is chosen, all the lines are always plotted in solid lines.

Syntax	SET_PLOT_OPTIONS
Prompts	`Plot header /Y/:` Toggle the plotting of the header text above a diagram.
	`Plot logo /Y/:` Toggle the plotting of the Thermo-Calc logo at the lower-left corner of a diagram.
	`Plot footer /Y/:` Toggle the plotting of the footer identifier text at the right margin of a diagram.
	`White-Contoured-PS-CHARS /Y/:` By default, the PostScript characters are written as a white contoured status.
	`Plot remote exponent(s) /Y/:` By default the remote exponent on the axis is plotted.
	`Plot symbols at node points /0/: <#>` This makes it possible to plot symbols at the node points on plotted lines on a diagram.
	`Symbol size /.1/: <.#>` Set the size of symbols which are plotted at the node points.
	`Write condition? /Y/:` By default, the initial equilibrium conditions for the current calculations are automatically plotted at the upper-left corner as a part of the header. If you enter N, the calculated conditions are not included on a plotted diagram.
	`Write database name? /Y/:`

Syntax	SET_PLOT_OPTIONS
	By default, the primary database (not appended ones) used in the current calculations are plotted at the upper-left corner as a part of the header. If you enter N, the database name is not included on a plotted diagram.
	`Always initiate POST on re-entering: /Y/:` By default the POST module automatically reinitiates whenever the POLY3 workspaces are changed upon re-entering. If you enter N, the same diagram axis variables are kept even if the workspaces in the POLY module is read from or written to a *.POLY3 file. This can be useful when there are several sets of *.POLY3 files with the same calculation but for different set of model parameters.
	`Always solid line: /N/:` By default the POST module plots solid lines for stable phases and dashed lines for metastable phases. This is normally for plotting property diagrams after a STEPPING calculation. However, when there is a metastable extrapolation in a phase region on a phase diagram after a MAPPING calculation, this is also enforced. Enter Y to always plot solid lines in this case, for example.

SET_PLOT_SIZE

Change the size of the diagram by specifying a global plot size (as a relative scaling factor). The default value of the relative scaling factor is 1, while the real size of the plotted diagram depends on what output device is chosen with SET_PLOT_FORMAT. The default plot size (corresponding to the default global plot size 1) is adjusted to the chosen device.

Syntax	SET_PLOT_SIZE
Prompt	`Global plot size /1/: <Relative scaling factor>` Enter the relative scaling factor as a numerical number (e.g. `0.5`, `0.8`, `1.0`, `1.5`, etc.). By pressing <Enter>, the default relative scaling factor (`1`) is accepted.

SET_PREFIX_SCALING

Specify on which axis is to have a prefix scaling then set the scaling of remote exponents with certain powers.

Syntax	SET_PREFIX_SCALING
Prompt	`Axis (X, Y or Z): <Name of an axis>` Specify which axis is to have a prefix scaling.
	`Use prefix scaling /Y/: (Y or N or #)` • `NO` switches off its action. • `YES` arranges the prefix scaling so that the axis scaling is done with the remote exponents being powers of three, i.e. `...,-6,-3,0,3,6,...`. The default is 3. • # is an integer number that sets the remote exponents as being powers of # (as the powers for the remote exponents).

SET_RASTER_STATUS

Plot a raster (i.e. with gridlines on both axis directions) in the diagram.

Syntax	SET_RASTER_STATUS
Prompt	`Raster plot (Y or N) /N/:` By default no raster is plotted. Enter Y to plot using a raster plot.

SET_REFERENCE_STATE

This command is available for the POLY, ED-EXP and POST modules.

The reference state for a component is important when calculating activities, chemical potentials, and enthalpies and is determined by the database being used. For each component the data must be referred to a selected phase, temperature, and pressure, i.e. the reference state.

All data in all phases where this component dissolves must use the same reference state. However, different databases can use different reference states for the same element/component. It is important to be careful when combining data obtained from different databases.

By default, activities, chemical potentials, and so forth are computed relative to the reference state used by the database. If the reference state in the database is not suitable for your purposes, use this command to set the reference state for a component using `SER`, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys dominated by the component). In such cases, the temperature and pressure for the reference state is not needed.

In order to specify conditions in the specific reference state, you can append an `R` to the state variables. Thus, `AC` is the activity (of a system component or of a species in a phase) with respect to the default reference state, and `ACR` is the activity with respect to the selected reference state; MU is the chemical potential of a system component with respect to the default reference state, and `MUR` stands for the chemical potential with respect to the selected reference state. The `AC` and `ACR` variables, for both components in a system and species in a phase, can be specified in natural logarithm, e.g. LNAC(Fe), LNACR(C), LNAC (O2,GAS), LNACR(O2,GAS).

For the POST module, and after calculating with the STEP_WITH_OPTIONS or MAP commands, the reference state for a component can also be changed to plot various properties of the component in the entire system or in a specific phase. Then you can set the diagram axes as the chemical potential or activity quantities with the `R` suffix, i.e. MUR(comp), MUR (comp,ph), ACR(comp), ACR(comp,ph) or the common logarithms [e.g. LNACR(comp,ph)].

Syntax	SET_REFERENCE_STATE
Prompts	`Component: <Name of the component>` The name of the component must be given.
	`Reference phase: <Name of a phase used as the new reference state>`

Syntax	SET_REFERENCE_STATE

Enter the `Name of a phase` for the system.

> For a phase to be usable as a reference for a component, the component needs to have the same composition as an end member of the phase. The reference state is an end member of a phase. The selection of the end member associated with the reference state is only performed once this command is executed.

If a component has the same composition as several end members of the chosen reference phase, then the end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy.

The following are example using temperature. Pressure is used in the same way:

- In the Fe-C system, BCC can be a reference state for Fe but not for C since BCC can exist as pure Fe but cannot exist as pure C.
- If GAS is chosen as the reference phase of component O at such a high temperature that O1 has the lowest energy, then O1 remains the reference state even at calculations performed at lower temperatures where O2 has a lower energy than O1.
- Setting the reference state for component O as gas (one sublattice) with constituents O1, O2 and O3 results in O2 being the reference state if, at the present temperature, pure O2 has the lowest energy of O1, O2 and O3. If the reference state is set above a critical higher temperature, then O1 has the lowest energy and consequently becomes the reference state.

`Temperature /*/: <Temperature for the reference state>`

Select the Temperature (in K) for the reference state. The wildcard value * means the current temperature is used at the time of evaluation of the reference energy for the calculation.

> The temperature set with this command does not affect the temperature used when evaluating the energy of the reference state during the end member selection process.

`Pressure /1E5/: <Pressure for the reference state>`

Select the Pressure (in Pa) for the reference state. The wildcard value * means the current pressure is used for evaluating the reference energy at the time of calculation.

Examples

```
S-R-S Fe SER
S-R-S Cr FCC * 100000
S-R-S H2O AQUEOUS * 100000
S-R-S ZE REF_ELECTRODE * 100000
```

SET_SCALING_STATUS

When an axis variable is selected by SET_DIAGRAM_AXIS, the scaling status for the axis is always set to automatic scaling. By this command, choose between manual or automatic scaling on a specified axis. If manual scaling is chosen, specify a minimum and a maximum value. Manual scaling can be used to magnify interesting parts of a diagram.

Syntax	SET_SCALING_STATUS
Prompts	`Axis (X, Y or Z): <Name of an axis>` Specify which axis that you want to set the scaling status.
	`Automatic scaling (Y or N) /N/:` The default is manual scaling. Enter Y for automatic scaling (N). For manual scaling specify the Min and Max values.
	`Min value: <Minimum value>` The minimum value at the start point of the specified axis.
	`Max value: <Maximum value>` The maximum value at the end point of the specified axis.

SET_TIC_TYPE

Change the drawing of the axis tics. You may alter the placement of tic marks on the axis, e.g. inside or outside or no tic marks. The size of tic marks cannot be altered by this command, but these are adjusted based on the selected graphic device and the defined relative scaling factor (global plot size).

Syntax	SET_TIC_TYPE
Prompt	`TIC Type /1/: <1 or -1 or 0>` The tic type 1 is default, i.e. the tics are drawn outside the diagram. -1 means that the tics are inside the diagram and 0 means no tics.

SET_TIELINE_STATUS

If the tie-lines are in the plane of the calculation, you can select to plot the tie-lines in two-phase fields with this command.

Syntax	SET_TIELINE_STATUS
Prompt	`Plotting every tie-line no. /0/: <Number of tie-lines>` The tie-lines plotted are not equally spaced by the graphics software. Instead, you can select to plot a subset of the calculated tie-lines, i.e. every one (1), every second (2), every three (3), etc. By accepting the default value 0, no tie-line is plotted.

SET_TITLE

Specify a title that displays on all listed tables and plotted diagrams from the POST module.

ADD_LABEL_TEXT

Syntax	SET_TITLE
Prompt	`Title` Enter the title you want to appear on all tabulation or graphic outputs. There is a maximum length of about 60 characters for the title. You can enter simple text, use LaTeX, rotate the text, as well as adjust the font size.

SET_TRUE_MANUAL_SCALING

The tic-marks on the axes are normally placed in even intervals using the whole axis length. The scaling routine adjusts the given minimum and maximum values slightly to accomplish this. If such an automatic adjustment behaviour is unwanted, it can be avoided by using this command (followed by a message showing the TRUE MANUAL SCALING set for a specific axis).

The command works like a toggle. To reset the automatic scaling behaviour, repeat the command a second time for that specific axis (followed by a message saying the SEMI_ MANUAL SCALING set for the specific axis.

Syntax	SET_TRUE_MANUAL_SCALING
Prompt	`Axis (X, Y or Z): <Name of an axis>` Specify which axis (X or Y or Z) you want to toggle between automatic adjustments or avoid the adjustment of the given maximum and minimum values.

SUSPEND_PHASE_IN_PLOT

Specify that lines originating from the presence of a certain phase shall not be plotted on a diagram. If you want to bring the suspended phase back to the diagram, use RESTORE_PHASE_IN_PLOT.

Syntax	SUSPEND_PHASE_IN_PLOT
Prompt	`Phase name: <Name of a phase>` Specify the name of the phase to be suspended from the diagram.

TABULATE

This command is available for a table entered in either the POLY or POST module.

For any entered table, this command gives a table of values from equilibria calculated with a STEP command.

Unlike the TAB module's command (also called TABULATE) it is not possible to plot columns from the tabulated tables. For this use normal POST commands.

Syntax	TABULATE
Prompts	`Name: <Name of a table entered in either POLY or POST>` Specify a table name that is entered in either the POLY or POST module.
	`Output on screen or file /Screen/:` Specify a file name if you want to save on a file the table values along the defined STEP calculation, or press <Enter> if want to see the table values displayed.

Technical Notes

In this section:

Technical Note: Pipe or Redirect Output Data from Console Mode

Audience:	Advanced Programmers and Users
OS:	Windows, Linux, or macOS
Application:	For users who want to pipe or redirect data from Thermo-Calc running a macro in Console Mode. For example, you can start the application with the Thermo-Calc.bat file and the entire application closes when you enter the EXIT command in the Console prompt.
Command examples:	See below
Command line definitions	
>	Redirection command. The arrow indicates the flow of data. For example in `./Thermo-Calc.sh macro.tcm > output.log`, the contents of macro.tcm is used as input to the Thermo-Calc.sh script file and the resulting output (standard out) is then written to `output.log` instead of to the screen.

Command examples:

WINDOWS

```
Thermo-Calc.bat macro.tcm > output.log
```

LINUX

```
./Thermo-Calc.sh batch macro.tcm > output.log
```

MACOS

```
./Thermo-Calc.command batch macro.tcm > output.log
```

Console Mode Examples

In this section:

Console Mode Examples

There are many examples to examine and to help you learn Thermo-Calc in Console Mode (CM). Some of the examples in the table below are included with specific sections, whereas some of the general examples are included (repeated) in more than one section.

Opening Console Mode Macro Files

Thermo-Calc and DICTRA Console Mode Example Macros PDF

All the macro files and the outputs are also combined into one file that you can search and read. This is included with your installation as a PDF (go to **Help > Manuals folder > All Thermo-Calc Documentation** and open *Thermo-Calc Console Mode Example Macros*.

All the macro files and the outputs are also combined into one file that you can search and read. This is included with your installation as a PDF (go to **Help → Manuals folder → Diffusion Module (DICTRA)** and open *Diffusion Module Console Mode Example Macros*.

Thermo-Calc CM Examples

Each topic has a brief description of the example and includes some or all of the commands used in the macros.

Topic	*TCEX Examples included*
Binary Phase Diagram Examples	1, 4, 13, 16, 17, 26, 31, 34, 50
Property Diagram Examples	2, 8, 9, 11, 12, 22, 23, 28, 29, 32, 41, 49, 50
Ternary Phase Diagram Examples	3, 5, 14, 17, 19A, 19B, 21, 33, 37, 42, 43
Multicomponent Phase Diagram Examples	6, 10, 23, 27
Thermodynamic and Related Quantities Examples	2, 13, 14, 18, 22, 26, 34, 39, 51
Single Equilibrium Calculation Examples	7, 18, 20
Potential Diagram Example	35

Topic	***TCEX Examples included***
Scheil-Gulliver Examples	15, 30A, 30B, 48, 54, 57
Chemical Ordering Example	16
Gibbs Energy System (GES) Examples	31, 38, 39, 49, 52
T0 Temperature Example	23
Paraequilibrium Examples	23, 42, 43
Functions and Variables Examples	44
PARROT and EDIT_EXPERIMENT Examples	36A (consists of various parts).
Pourbaix Diagram Examples	40, 40A, B, C, and E, 53
Tabulate Reaction (TAB) Example	12
REACTOR Module Example	24
Thermophysical Properties Examples	55 - Viscosity 56 - Surface Tension 58 and 59 - Molar Volume 60 - Electrical Resistivity and Thermal Conductivity
Application Examples	9 - Dew Point 10 - Continuous casting, preventing Cr_2O_3 clogging 11 - Gas oxidation of Cu_2S 20 - Adiabatic decompression in Geological system 24 - Silicon arc furnace 27 - Chemical Vapour Deposition 28 - Materials design of a stainless steel 29 - Gas speciation 41 - Solubility product 44 - Proof strength calculated from empirical functions

Binary Phase Diagram Examples

tcex01 - Calculating the Binary Fe-C Phase Diagram

This example calculates the binary Fe-C phase diagram using the Binary module. The TCBIN database is used and included with your installation.

Some of the main commands used:

- LIST_EQUILIBRIUM
- LIST_STATUS
- LIST_CONDITIONS
- CHANGE_STATUS
- COMPUTE_EQUILIBRIUM
- SET_DIAGRAM_AXIS
- SET_TIELINE_STATUS
- PLOT_DIAGRAM
- SET_SCALING_STATUS
- SET_LABEL_CURVE_OPTION
- ADD_LABEL_TEXT
- MODIFY_LABEL_TEXT

tcex04 - Calculating the Fe-Cr Miscibility Gap

This example calculates the miscibility gap in the Fe-Cr system. The FEDEMO database is used and included with your installation.

These commands are used:

- SWITCH_DATABASE
- GET_DATA
- LIST_EQUILIBRIUM
- SET_AXIS_VARIABLE
- DEFINE_SYSTEM
- AMEND_PHASE_DESCRIPTION

- SET_CONDITION
- SAVE_WORKSPACES
- REJECT
- LIST_STATUS
- COMPUTE_EQUILIBRIUM
- SET_TIELINE_STATUS

tcex13 - Calculating the Binary Al-Ti Phase Diagram and its G Curve

This example calculates an Al-Ti binary phase diagram and G curve using the BINARY module. The TCBIN database is used and included with your installation.

tcex16 - Second Order Transition of the Al-Fe System

This example calculates the second order transition line in the BCC field of the Al-Fe system.

This uses the SSOL database. A license is required to run the example.

These commands are of note and used in this example:

- REJECT
- RESTORE
- ADVANCED_OPTIONS
- SET_SCALING_STATUS
- DEFINE_SYSTEM
- MAKE_EXPERIMENTAL_DATAFILE
- LIST_EQUILIBRIUM
- APPEND_EXPERIMENTAL_DATA
- STEP_WITH_OPTIONS

tcex17 - The Pseudo-binary System - CaO-SiO2

This example calculates the pseudo-binary system CaO-SiO_2 using the OXDEMO database, which is included with your installation.

The oxide demo (OXDEMO) database can be used both for pseudo-binary systems like the one in this case, CaO-SiO_2, or for full ternary systems like Ca-Fe-O.

For a more advanced example in Graphical Mode using the TCS Metal Oxide Solutions Database (TCOX), see T_17: Al2O3-MgO Phase Diagram.

These commands are of note and used in this example:

- LIST_SYSTEM
- REJECT and RESTORE
- AMEND_PHASE_DESCRIPTION
- LIST_STATUS
- DEFINE_COMPONENTS
- SET_CONDITION
- COMPUTE_EQUILIBRIUM and LIST_EQUILIBRIUM

tcex26 - The As-Ga Phase Diagram: Plotting the Partial Pressures of a Gas Species

This is an example of plotting the partial pressures of a gas species along the solubility lines in the As-Ga phase diagram. The calculation makes it possible to monitor the input gases to a process of depositing solid As-Ga. The data is taken from the PG35 Binary Semi-Conductors database.

These commands are of note and used in this example:

- REJECT
- RESTORE
- SET_DIAGRAM_AXIS
- SET_SCALING_STATUS
- SET_AXIS_TEXT_STATUS
- SET_LABEL_CURVE_OPTION

tcex31 - Using GES to Calculate CVM

Using the Gibbs Energy System (GES) module, this example calculates the CVM and compares it with the sublattices of a fictitious A B system. You also learn how to overlay diagrams from two calculations.

> This example uses some GES commands that are not yet supported by GES6. Therefore, we enforce the use of GES5.

These GES commands are of note and used in this example:

- ENTER_ELEMENT
- ENTER_SPECIES
- ENTER_SYMBOL
- ENTER_PHASE
- ENTER_PARAMETER
- LIST_PHASE_DATA

tcex34 - The Al-Zn Phase Diagram and its G Curve

This example uses the BINARY module to calculate the phase diagram and G curves in the Al-Zn system. It uses the TCBIN database included with your installation.

Property Diagram Examples

tcex02 - Plotting Thermodynamic Functions

This example shows how to plot thermodynamic functions in unary, binary, and ternary systems. It also involves working with partial derivatives and partial quantities.

This uses the SSOL database. A license is required to run the example.

These commands are used and may be of interest:

GOTO_MODULE	GET_DATA	SET_CONDITION
SWITCH_DATABASE	AMEND_PHASE_DESCRIPTION	LIST_EQUILIBRIUM
DEFINE_SYSTEM	COMPUTE_EQUILIBRIUM	SET_AXIS_VARIABLE
SAVE_WORKSPACES	STEP_WITH_OPTIONS	SET_DIAGRAM_AXIS
ENTER_SYMBOL	PLOT_DIAGRAM	SET_LABEL_CURVE_OPTION
REJECT	RESTORE	LIST_SYSTEM
LIST_STATUS	CHANGE_STATUS	SHOW_VALUE
SET_INTERACTIVE		

tcex08 - Property Diagrams for a High Speed Steel

This example shows how to calculate property diagrams for a high speed steel i.e. phase fraction plots, activity vs temperature, and so forth.

This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- DEFINE_DIAGRAM
- DEFINE_ELEMENTS
- AMEND_PHASE_DESCRIPTION
- REINITIATE_PLOT_SETTINGS

tcex09 - Calculating a Dew Point with POLY3

This is an example calculating the dew point in the POLY3 module. The SUBDEMO database is used and included with your installation.

The STEP_WITH_OPTIONS and MAP commands are of note and used in this example.

tcex11 - Oxidation of Cu2S with an H2O/O2 Gas Mixture

This example demonstrates the oxidation of Cu_2S with an H_2O/O_2 gas mixture. Thermo-Calc is used to find the optimum O/H ratio (i.e. oxygen potential) as certain oxygen potential values can desulphurize Cu_2S without forming copper oxides.

In Thermo-Calc, the problem reduces to perform equilibria calculations in a Cu-S-H-O system. The amounts of the components should be kept to correct ratio corresponding to Cu_2S and H_2O using a command SET_INPUT_AMOUNTS in POLY3. Initially, O/H = 0.5 is given. Optimum O/H ratio is calculated with the desired calculation conditions. For example, to simulate one phase disappearing, you can FIX the phase with zero amount.

The *tcex11.TDB* file is used to access data and this is included with your installation.

These commands are of also of note and used in this example:

- SET_NUMERICAL_LIMITS
- SET_REFERENCE_STATE
- SHOW_VALUE

tcex12 - Tabulation of Thermodynamic Data for Reactions

This example shows a number of independent cases using the TABULATE_REACTION (TAB) module to tabulate thermodynamic data for reactions.

This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- TABULATE_REACTION
- DEFINE_SPECIES
- ENTER_FUNCTION
- QUICK_EXPERIMENTAL_PLOT
- SET_SCALING_STATUS
- LIST_SUBSTANCES
- TABULATE_SUBSTANCE

tcex22 - Calculating an Adiabatic Flame Temperature

This example examines a heat balance when C_3H_8 is burned in oxygen by calculating the adiabatic flame temperature.

This uses the SSUB database. A license is required to run the example.

tcex23 - Calculating a Paraequilibrium and the T0 Temperature in a Low Alloyed Steel

This example calculates a paraequilibrium and the T0 temperature in a low alloyed steel.

This uses the TCFE database. A license is required to run the example.

tcex28 - Pitting Resistance Equivalence (PRE) for a Duplex Stainless Steel

This example calculates the Pitting Resistance Equivalence (PRE) for a duplex stainless steel.

This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- REJECT
- RESTORE
- DEFINE_ELEMENTS
- AMEND_PHASE_DESCRIPTION
- EVALUATE_FUNCTIONS
- SET_START_CONSTITUTION

tcex29 - Calculating the Speciation of a Gas

This example shows how to calculate the speciation of a gas.

This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- SET_INPUT_AMOUNTS
- LIST_CONDITIONS
- SET_CONDITION

tcex32 - Calculating Oxide Layers on Steel

This example calculates oxide layers on a steel.

This uses the TCOX database. A license is required to run the example.

These commands are of note and used in this example:

- SET_START_CONSTITUTION
- SET_REFERENCE_STATE
- APPEND_DATABASE

tcex41 - Calculating a Solubility Product

Calculation of a solubility product.

This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- DEFINE_ELEMENTS
- REINITIATE_PLOT_SETTINGS
- SET_DIAGRAM_AXIS

tcex49 - Quasichemical Model Using GES

This example shows how to enter parameters for a FACT quasichemical liquid model and how to calculate the sulfur activity using the GIBBS_ENERGY_SYSTEM (GES) module commands.

This example uses some GES commands that are not yet supported by GES6. Therefore, the example uses GES5.

These commands are of note and used in this example:

- ENTER_ELEMENT
- ENTER_SYMBOL
- AMEND_ELEMENT_DATA
- ENTER_PARAMETER
- ENTER_SPECIES
- SET_REFERENCE_STATE
- SHOW_VALUE

Ternary Phase Diagram Examples

tcex03 - Calculating an Isothermal Section

This example calculates an isothermal section using the Ternary module. The FEDEMO database is used and included with your installation.

These commands are used:

- AMEND_PHASE_DESCRIPTION
- ADD_LABEL_TEXT
- PLOT_DIAGRAM
- SET_DIAGRAM_AXIS; SET_DIAGRAM_TYPE; and SET_AXIS_TYPE
- SET_REFERENCE_STATE
- CHANGE_STATUS
- SET_SCALING_STATUS

tcex05 - Calculating a Vertical Section in the Al-Cu-Si System

This example calculates a vertical section in the Al-Cu-Si system and of a vertical section from Al to 10% Cu_2Si. The ALDEMO database is used and included with your installation.

tcex14 - Variations in Solidification of an Al-Mg-Si Alloy

This example calculates the heat and heat capacity variations during solidification of an Al-Mg-Si alloy. The ALDEMO database is used and included with your installation.

These commands are of note and used in this example:

- LIST_SYSTEM
- LIST_CONDITIONS
- SET_AXIS_TEXT_STATUS

tcex17 - The Pseudo-binary System - CaO-SiO2

This example calculates the pseudo-binary system CaO-SiO_2 using the OXDEMO database, which is included with your installation.

The oxide demo (OXDEMO) database can be used both for pseudo-binary systems like the one in this case, $CaO\text{-}SiO_2$, or for full ternary systems like Ca-Fe-O.

For a more advanced example in Graphical Mode using the TCS Metal Oxide Solutions Database (TCOX), see T_17: Al2O3-MgO Phase Diagram.

These commands are of note and used in this example:

- LIST_SYSTEM
- REJECT and RESTORE
- AMEND_PHASE_DESCRIPTION
- LIST_STATUS
- DEFINE_COMPONENTS
- SET_CONDITION
- COMPUTE_EQUILIBRIUM and LIST_EQUILIBRIUM

tcex19a and tcex19b - Mapping of Univariant Equilibria with the Liquid in Al-Cu-Si

- Part A. Step-by-step calculation using the POLY3 module.
- Part B. Using the TERNARY module, you can get the information on invariant reactions, such as temperature and compositions.

The database used with this example is included with the file named tcex19_cost2.TDB. It is in the same folder as this example.

These commands are of note and used in these examples:

- DEFINE_SYSTEM
- GET_DATA
- AMEND_PHASE_DESCRIPTION
- SET_CONDITIONand LIST_CONDITIONS
- ADVANCED_OPTIONS
- SAVE_WORKSPACES and READ_WORKSPACES
- APPEND_EXPERIMENTAL_DATA
- MAKE_EXPERIMENTAL_DATAFILE

tcex21 - Calculating a Ternary Isotherm in Fe-Cr-Ni

This example calculates a ternary isotherm in Fe-Cr-Ni with a user-defined database included with the example in the file named *tcex21.TDB*.

These commands are of note and used in this example:

- DEFINE_SYSTEM
- GET_DATA
- SET_CONDITION
- SET_DIAGRAM_TYPE

tcex33 - An Fe-Cr-C Isopleth

This example is a benchmark calculation of an isopleth in the Fe-Cr-C system. The FEDEMO database is used and included with your installation.

tcex37 - Calculating an Isothermal Section

This example shows how to use command lines to enter and calculate an isothermal section using the POLY3 module. The FEDEMO database is used and included with your installation.

tcex42 - Paraequilibrium Calculation - Formation of Para-pearlite - Isopleth

This uses the TCFE database. A license is required to run the example.

This example uses an Fe-Mn-C system at 2.5%Mn Mass u-fraction to show a paraequilibrium calculation where there is formation of para-pearlite. It is an isopleth calculation and shows the STEP_WITH_OPTIONS command using the Paraequilibrium option.

tcex43 - Paraequilibrium Calculation - Formation of Para-pearlite - Isothermal

This uses the TCFE database. A license is required to run the example.

This example uses an Fe-Mn-C system at 700 °C to show a paraequilibrium calculation where there is formation of para-pearlite. It is an isothermal calculation and shows the STEP_WITH_OPTIONS command using the Paraequilibrium option.

Multicomponent Phase Diagram Examples

tcex06 - An Isopleth in Low Alloyed Fe-Mn-Si-Cr-Ni-C Steel

This example calculates a multicomponent phase diagram using the DEFINE_MATERIAL command in POLY and the TCFE steel database. The material contains 1.5 %Cr + 0.4 %Mn + 3.5 %Ni + 0.3 %Si and 1 %C (by weight). These conditions and the temperature are set by the DEFINE_MATERIAL command.

After the first equilibrium results, a phase diagram is calculated with one axis variable as temperature and the other as the carbon content.

This uses the TCFE database. A license is required to run the example.

tcex10 - Preventing Cr2O3 Clogging in a Continuous Casting Process

The example calculates an equilibrium with suspended or dormant phases and shows how to avoid Cr-oxide clogging in a continuous casting process.

This uses the TCOX database. A license is required to run the example.

The background of this example is that a manufacturer wanted to increase the Cr content of a material from 18 to 25 weight percent. They then had trouble in the continuous casting of this material because solid Cr_2O_3 was formed.

Using Thermo-Calc to calculate the equilibria in the steel/slag system, a simple correction was found: modify the Mn or Si content to decrease the oxygen potential.

In Thermo-Calc, you can FIX a phase with zero amount to simulate how to avoid forming this phase. You then release one of the conditions, usually one of the compositions, and this composition is determined by the equilibrium calculation.

These commands are of note and used in this example:

- DEFINE_SYSTEM
- CHANGE_STATUS
- COMPUTE_EQUILIBRIUM
- DEFINE_SYSTEM

- DEFINE_SYSTEM
- LIST_CONDITIONS
- LIST_EQUILIBRIUM
- LIST_STATUS
- SET_CONDITION
- SET_NUMERICAL_LIMITS
- SET_REFERENCE_STATE
- SHOW_VALUE

tcex23 - Calculating a Paraequilibrium and the T0 Temperature in a Low Alloyed Steel

This example calculates a paraequilibrium and the T0 temperature in a low alloyed steel.

> This uses the TCFE database. A license is required to run the example.

tcex27 - Calculating Chemical Vapor Depositions (CVD)

This example calculates the chemical vapor deposition (CVD).

> This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- DEFINE_COMPONENTS
- SET_CONDITION
- ADD_INITIAL_EQUILIBRIUM
- LIST_AXIS_VARIABLE
- LIST_INITIAL_EQUILIBRIA

Thermodynamic and Related Quantities Examples

tcex02 - Plotting Thermodynamic Functions

This example shows how to plot thermodynamic functions in unary, binary, and ternary systems. It also involves working with partial derivatives and partial quantities.

This uses the SSOL database. A license is required to run the example.

These commands are used and may be of interest:

GOTO_MODULE	GET_DATA	SET_CONDITION
SWITCH_DATABASE	AMEND_PHASE_DESCRIPTION	LIST_EQUILIBRIUM
DEFINE_SYSTEM	COMPUTE_EQUILIBRIUM	SET_AXIS_VARIABLE
SAVE_WORKSPACES	STEP_WITH_OPTIONS	SET_DIAGRAM_AXIS
ENTER_SYMBOL	PLOT_DIAGRAM	SET_LABEL_CURVE_OPTION
REJECT	RESTORE	LIST_SYSTEM
LIST_STATUS	CHANGE_STATUS	SHOW_VALUE
SET_INTERACTIVE		

tcex13 - Calculating the Binary Al-Ti Phase Diagram and its G Curve

This example calculates an Al-Ti binary phase diagram and G curve using the BINARY module. The TCBIN database is used and included with your installation.

tcex14 - Variations in Solidification of an Al-Mg-Si Alloy

This example calculates the heat and heat capacity variations during solidification of an Al-Mg-Si alloy. The ALDEMO database is used and included with your installation.

These commands are of note and used in this example:

- LIST_SYSTEM
- LIST_CONDITIONS
- SET_AXIS_TEXT_STATUS

tcex18 - A3 Temperature of a Steel

This example calculates the A3 temperature of a steel and examines the influence of each alloying element on this temperature.

A3 temperature is the temperature where ferrite starts to form from austenite. You can easily read A3 from an Fe-C phase diagram. However, for complex multicomponent steels no simple diagram can be used. Using POLY, it is easy to find out the influence of each alloying element on the A3 temperature. This information is useful if you want to modify the compositions of a steel but keep A3 unchanged.

This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- DEFINE_ELEMENTS
- AMEND_PHASE_DESCRIPTION
- COMPUTE_TRANSITION
- DEFINE_MATERIAL
- ENTER_SYMBOL
- SHOW_VALUE

tcex22 - Calculating an Adiabatic Flame Temperature

This example examines a heat balance when C_3H_8 is burned in oxygen by calculating the adiabatic flame temperature.

This uses the SSUB database. A license is required to run the example.

tcex26 - The As-Ga Phase Diagram: Plotting the Partial Pressures of a Gas Species

This is an example of plotting the partial pressures of a gas species along the solubility lines in the As-Ga phase diagram. The calculation makes it possible to monitor the input gases to a process of depositing solid As-Ga. The data is taken from the PG35 Binary Semi-Conductors database.

These commands are of note and used in this example:

- REJECT
- RESTORE
- SET_DIAGRAM_AXIS
- SET_SCALING_STATUS
- SET_AXIS_TEXT_STATUS
- SET_LABEL_CURVE_OPTION

tcex34 - The Al-Zn Phase Diagram and its G Curve

This example uses the BINARY module to calculate the phase diagram and G curves in the Al-Zn system. It uses the TCBIN database included with your installation.

tcex39 - Calculating Reversible Carnot Cycles of a Heat Engine

This example shows how to calculate the reversible Carnot cycle of a heat engine using one mole of an ideal gas with two fictitious species A and A2. The GES, POLY3, and POST modules are used, as well as the SUBDEMO database, which is included with your installation.

One application of the Second Law is to the efficiencies of heat engines, pumps and refrigerators. Whenever there is a difference of temperature, work can be produced - the principle of heat engines. The Gibbs energy also enables the prediction of the maximum work that a process may achieve. The goal of this example is to help relate the results to different thermodynamic quantities.

These commands are of note and used in this example:

- REINITIATE
- ENTER_PARAMETER

- ENTER_SPECIES
- SET_PLOT_FORMAT
- ENTER_PHASE

tcex51 - Calculation of Molar Volume, Thermal Expansivity, and Density

This example uses the POLY3 module to calculate the molar volume, thermal expansivity and density of the FCC_A1, BCC_A2 LIQUID, and liquid phases of C-Fe. The FEDMO database is used and this example is available to all users.

Single Equilibrium Calculation Examples

tcex07 - Single Equilibria in Low Alloyed Fe-Mn-Si-Cr-Ni-C Steel

This example shows how to calculate a single equilibria in a low alloyed Fe-Mn-Si-Cr-Ni-C steel. There are two common ways to perform a single equilibrium calculation:

- Get data from a database, then in POLY use SET_CONDITION and COMPUTE_EQUILIBRIUM.
- Go directly to POLY and use DEFINE_MATERIAL.

The COMPUTE_TRANSITION command is also used to determine the temperature or composition where one phase forms or disappears. It is the same as the CHANGE_STATUS → SET_CONDITION→ COMPUTE_EQUILIBRIUM sequence of commands.

A STEP_WITH_OPTIONS command using the option *normal* is also used in addition to the other commands that should be becoming more familiar as you work through the examples.

This uses the TCFE database. A license is required to run the example.

tcex18 - A3 Temperature of a Steel

This example calculates the A3 temperature of a steel and examines the influence of each alloying element on this temperature.

A3 temperature is the temperature where ferrite starts to form from austenite. You can easily read A3 from an Fe-C phase diagram. However, for complex multicomponent steels no simple diagram can be used. Using POLY, it is easy to find out the influence of each alloying element on the A3 temperature. This information is useful if you want to modify the compositions of a steel but keep A3 unchanged.

This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- DEFINE_ELEMENTS
- AMEND_PHASE_DESCRIPTION
- COMPUTE_TRANSITION
- DEFINE_MATERIAL
- ENTER_SYMBOL
- SHOW_VALUE

tcex20 - Adiabatic Decompression in a Geological System

This example calculates the adiabatic decompression in a geological system using the geochemical database. The database is included with the file named PGEO.TDB, which is in the same folder as this example.

These commands are of note and used in this example:

- DEFINE_SYSTEM
- DEFINE_COMPONENTS
- SET_INPUT_AMOUNTS
- LIST_CONDITIONS
- SET_CONDITION
- SHOW_VALUE

Potential Diagram Example

tcex35 - Calculating a Potential Diagram

This example uses the POTENTIAL module to calculate a potential diagram. Note that there are no commands for this module, you just follow the prompts. The SUBDEMO database is used and included with your installation.

Scheil-Gulliver Examples

? About the Scheil-Gulliver Solidification Simulations

tcex15 - Simulating the Solidification of a Cr-Ni Alloy

This is an example of a solidification simulation of a Cr-Ni alloy. There is no back diffusion in the solid, i.e. this is a classic Scheil-Gulliver simulation. The FEDMO database is used and included with your installation.

These commands are of note and used in this example:

- START_WIZARD
- COMPUTE_TRANSITION
- ADD_INITIAL_EQUILIBRIUM
- ENTER_SYMBOL
- ADVANCED_OPTIONS
- STEP_WITH_OPTIONS
- MAKE_EXPERIMENTAL_DATAFILE
- CHANGE_STATUS

tcex30a and 30b - Scheil Calculation for an Al-4Mg-2Si-2Cu Alloy

? The Equilibrium Calculation Module (POLY3) and About the Scheil-Gulliver Solidification Simulations

These examples show two ways to do a Scheil calculation for an Al-4Mg-2Si-2Cu alloy. In part A, you use the POLY3 module and the STEP_WITH_OPTIONS command with an EVALUATE option. Then in part B you use the SCHEIL module commands to do the same thing. Data from the COST2 database is used and included with the example in the file named *tcex30_cost2.TDB*.

tcex48 - Scheil Solidification with C Back Diffusion

The FEDEMO database is used and the example is available to all users.

This is an example of Scheil solidification with simulated back diffusion of carbon in solid phases. The results are compared between a simple Scheil and equilibrium calculation. First perform a Partial Equilibrium Scheil by assigning carbon as a fast diffusing element. Plot solidification curve and a microsegregation diagram and save to file (so called .exp files). The "back diffusion" of C in solid phases is not from any calculation involving kinetics, but comes from the equilibration of chemical potential of C at each step in temperature, thus allowing each already solidified part of the system to change its C concentration.

See tcex54 for an example that calculates "real" back diffusion. This model requires a kinetic (mobility) database in addition to the thermodynamic one. Also see About the Scheil-Gulliver Solidification Simulations for details about the different Scheil options.

tcex54 - Scheil Solidification of an Al-2.1Cu-1Si Alloy including Back Diffusion

This is an example of a solidification simulation of a Al-2.1Cu-1Si alloy. The back diffusion option in the Scheil module is used, i.e. there is back diffusion in the primary phase. The example uses both the thermodynamic ALDEMO and mobility MALDEMO demo databases included with your installation.

tcex57 - Scheil Solidification with Solute Trapping

This is an example of a solidification simulation of a Al-7.5Si-0.2Cu system. The solute trapping option in the Scheil module is used. The example uses the thermodynamic ALDEMO demo database included with your installation.

See the Graphical Mode example T_13: Scheil Solidification with Solute Trapping for an additional comparison to Classic Scheil.

Chemical Ordering Example

tcex16 - Second Order Transition of the Al-Fe System

This example calculates the second order transition line in the BCC field of the Al-Fe system.

This uses the SSOL database. A license is required to run the example.

These commands are of note and used in this example:

- REJECT
- RESTORE
- ADVANCED_OPTIONS
- SET_SCALING_STATUS
- DEFINE_SYSTEM
- MAKE_EXPERIMENTAL_DATAFILE
- LIST_EQUILIBRIUM
- APPEND_EXPERIMENTAL_DATA
- STEP_WITH_OPTIONS

Gibbs Energy System (GES) Examples

tcex31 - Using GES to Calculate CVM

Using the Gibbs Energy System (GES) module, this example calculates the CVM and compares it with the sublattices of a fictitious A B system. You also learn how to overlay diagrams from two calculations.

> This example uses some GES commands that are not yet supported by GES6. Therefore, we enforce the use of GES5.

These GES commands are of note and used in this example:

- ENTER_ELEMENT
- ENTER_SPECIES
- ENTER_SYMBOL
- ENTER_PHASE
- ENTER_PARAMETER
- LIST_PHASE_DATA

tcex38 - Calculating the Morral “Rose”

This example uses the Gibbs energy system (GES) module to calculate the Morral rose, which are miscibility gaps.

These commands are of note and used in this example:

- REINITIATE
- ENTER_ELEMENT
- AMEND_ELEMENT_DATA
- ENTER_PARAMETER
- ENTER_PHASE

tcex39 - Calculating Reversible Carnot Cycles of a Heat Engine

This example shows how to calculate the reversible Carnot cycle of a heat engine using one mole of an ideal gas with two fictitious species A and A2. The GES, POLY3, and POST modules are used, as well as the SUBDEMO database, which is included with your installation.

One application of the Second Law is to the efficiencies of heat engines, pumps and refrigerators. Whenever there is a difference of temperature, work can be produced - the principle of heat engines. The Gibbs energy also enables the prediction of the maximum work that a process may achieve. The goal of this example is to help relate the results to different thermodynamic quantities.

These commands are of note and used in this example:

- REINITIATE
- ENTER_PARAMETER
- ENTER_SPECIES
- SET_PLOT_FORMAT
- ENTER_PHASE

tcex49 - Quasichemical Model Using GES

This example shows how to enter parameters for a FACT quasichemical liquid model and how to calculate the sulfur activity using the GIBBS_ENERGY_SYSTEM (GES) module commands.

This example uses some GES commands that are not yet supported by GES6. Therefore, the example uses GES5.

These commands are of note and used in this example:

- ENTER_ELEMENT
- ENTER_SYMBOL
- AMEND_ELEMENT_DATA
- ENTER_PARAMETER

- ENTER_SPECIES
- SET_REFERENCE_STATE
- SHOW_VALUE

tcex52 - Changing the Excess Models for Interaction Parameters in a Solution Phase

Solution Models in the GIBBS (GES) Module

This example uses some GES commands that are not yet supported by GES6. Therefore, the example uses GES5.

This example shows how to change the excess models for binary and ternary interactions in a solution phase, either

- through direct interactive amendments of phase descriptions within the GIBBS_ ENERGY_SYSTEM (GES) module, or
- enforced by specific type-definitions given in a database file retrieved by the DATABASE_RETRIEVAL module (also called the TDB module).

For binary excess models, the example changes it from the default *R-K model* to a *Mixed-Excess-Model*. The phase has to be a substitutional phase in this case.

For ternary extrapolation models, the example changes it from the default *R-K-M model* to a *Toop_Kohler model*.

Notes Related to the Example

The following is included in the macro file as part of the instructions but may be of use to new users:

AMENDING THE BINARY EXCESS MODEL

The default binary excess model is the Redlich-Kister Model for all the three associated binary interaction pairs (A-B, A-C and B-C) in the substitutional LIQUID solution phase (without sublattice) that consists of three elements (A, B and C).

Before changing this default binary excess model for the ternary LIQUID solution phase, one must have already entered the G parameters (for standard Gibbs energies of all pure end-members) and L parameters (for binary R-K excess interaction energies), as shown in the example.

In this particular example, we want to change from the default R-K binary excess model to the Mixed-Excess-Model (with three different binary excess models, namely Legendre, Polynom and Redlich-Kister models, applied to the A-B, A-C and B-C binaries, respectively), as demonstrated below:

For the A-B interaction, the Legendre binary excess model should be used (rather than the default Redlich-Kister Model), with the first species (i.e. A) as the independent constituent and the second species (i.e. B) as the dependent constituent, while the L parameters for the A-B interaction shall remain the same as those handled by the R-K model.

For the A-C interaction, the Polynom binary excess model should be used (rather than the default Redlich-Kister Model), with the second species (i.e. C) as the independent constituent and the first species (i.e. A) as the dependent constituent, while the L parameters for the A-C interaction shall remain the same as those handled by the R-K model.

AMENDING THE TERNARY EXTRAPOLATION MODEL

The default ternary excess model is the Redlich-Kister_Muggianu Model (i.e., the MUGGIANU_RESTOR method for ternary extrapolation based on binary parameters) for the associated ternary interaction terms; when no ternary L parameter is entered for that, such a default Redlich-Kister_Muggianu Model is thus to be used for extrapolation from binary excess energies to ternary interactions in the substitutional LIQUID solution phase (without sublattice) that consists of three elements (A, B and C).

However, in this particular example as illustrated in the following, we shall change from this default R-K-M ternary excess model to the TOOP-KOHLER method for the ternary extrapolation method, with the species C as the Toop constituent, while the species A and B as the Kohler constituents (entering A and B, or B and A, as the basis constituent and first interacting constituent). This will implicitly enforce that, during the ternary extrapolation, only the A-B binary interaction parameters are utilized in accordance with the Kohler ternary extrapolation formula for A-B-C ternary interaction, while any other binary interaction parameters used in line with the Toop-Kohler ternary extrapolation formula (for the A-C-B and B-C-A ternary interactions). This makes the extrapolated ternary excess interaction terms different from those handled either by the default MUGGIANU_RESTOR method or by the alternative KOHLER-ALL method.

Note that only when all the relevant binary excess energies in a ternary system are treated by the default Redlich-Kister Model (i.e., the Mixed-Excess-Model should have not been used), the MUGGIANU_RESTOR method for ternary extrapolations is equivalent to the Redlich-Kister_Muggianu Model, or the KOHLER-ALL method to the Redlich-Kister_Kohler Model.

T0 Temperature Example

tcex23 - Calculating a Paraequilibrium and the T0 Temperature in a Low Alloyed Steel

This example calculates a paraequilibrium and the T0 temperature in a low alloyed steel.

This uses the TCFE database. A license is required to run the example.

Paraequilibrium Examples

tcex23 - Calculating a Paraequilibrium and the T0 Temperature in a Low Alloyed Steel

This example calculates a paraequilibrium and the T0 temperature in a low alloyed steel.

This uses the TCFE database. A license is required to run the example.

tcex42 - Paraequilibrium Calculation - Formation of Para-pearlite - Isopleth

This uses the TCFE database. A license is required to run the example.

This example uses an Fe-Mn-C system at 2.5%Mn Mass u-fraction to show a paraequilibrium calculation where there is formation of para-pearlite. It is an isopleth calculation and shows the STEP_WITH_OPTIONS command using the Paraequilibrium option.

tcex43 - Paraequilibrium Calculation - Formation of Para-pearlite - Isothermal

This uses the TCFE database. A license is required to run the example.

This example uses an Fe-Mn-C system at 700 °C to show a paraequilibrium calculation where there is formation of para-pearlite. It is an isothermal calculation and shows the STEP_WITH_OPTIONS command using the Paraequilibrium option.

Functions and Variables Examples

tcex44 - Exploring Variables and Functions

This example uses variables and functions to predict properties e.g. proof strength for an austenitic stainless steel at elevated temperatures (20-550 °C). The example was created using an expression from [2000Eli].

This uses the TCFE database. A license is required to run the example.

In Graphical Mode there is a Yield Strength Property Model that does not require user input of empirical functions. See About the Yield Strength Property Model.

REFERENCE

[2000Eli] J. Eliasson, R. Sandström, Proof strength values for austenitic stainless steels at elevated temperatures. Steel Res. 71, 249–254 (2000).

PARROT and EDIT_EXPERIMENT Examples

tcex36a - Using PARROT and EDIT EXPERIMENTS

The example is divided into parts corresponding to the files in the **tcex36a** folder. It is recommended you open *tcex.36.readme* before continuing with this advanced exercise.

Also see the *Data Optimization User Guide*.

Each problem has "selected" experimental data. The example uses a fictitious binary A-B system where element A is BCC until it melts. Element B is BCC up to 1100 K and FCC above. There is a compound A2B stable in a limited temperature range.

- The creation of the "setup" file is described (*tcex36a.TCM*) where you enter the elements and phases into the Gibbs Energy System (GES) module
- The creation of the experimental data file is described (*tcex 36b.TCM*). When you run the TCEX36a macro, the contents of this macro file is automatically launched and the experimental data file created.
- The actual run in the PARROT module in order to obtain the result (*tcex 36cpd.TCM*)

There are many commands used in this advanced example (listed in alphabetical order):

ADVANCED_OPTIONS	AMEND_ELEMENT_DATA	AMEND_PHASE_DESCRIPTION
APPEND_EXPERIMENTAL_DATA	COMPILE_EXPERIMENTS	
CONTINUE_OPTIMIZATION	CREATE_NEW_EQUILIBRIUM	CREATE_NEW_STORE_FILE
DEFINE_COMPONENTS	EDIT_EXPERIMENTS	ENTER_PARAMETER
ENTER_PHASE	LABEL_DATA	LIST_ALL_VARIABLES
LIST_PHASE_DATA	LIST_RESULT	MACRO_FILE_OPEN
OPTIMIZE_VARIABLES	QUICK_EXPERIMENTAL_PLOT	READ_WORKSPACES
RESCALE_VARIABLES	SAVE_PARROT_WORKSPACES	SAVE_WORKSPACES

SELECT_EQUILIBRIUM	SET_ALL_START_VALUES	SET_ALTERNATE_CONDITION
SET_ALTERNATE_MODE	SET_FIX_VARIABLE	SET_OPTIMIZING_VARIABLE
SET_STORE_FILE	SET_WEIGHT	

Pourbaix Diagram Examples

tcex40

This is the first in a series of examples to demonstrate the advanced POURBAIX module calculations and plotting. This example automatically calculates and plots a Pourbaix diagram for 0.001 m Fe in a 0.1 m NaCl aqueous solution at 25 °C and 1 bar. Other diagrams, along various phase boundaries for the same interactions resulted from the same Pourbaix module calculation, are also plotted.

It is recommended you read the text file *TCEX40-README.txt*, which is located in the **Extended** subfolder.

Also see the *Pourbaix Diagrams Educational Material Guide.*

A so-called Pourbaix diagram is actually a phase diagram with independently-varied acidity (pH) and electropotential (Eh), for a heterogeneous interaction system at a certain bulk composition (that is by default always set as 1 kg of water dissolving a specified amount of metals and other solutes), under a defined temperature and pressure condition.

The PAQ2 Database

The example uses the PAQ2 (TCS Public Aqueous Solution Database using the SIT aqueous solution model) included with your installation. The database contains an AQUEOUS solution phase and REF_ELECTRODE phase (as a reference for electron in aqueous electrolyte systems), as well as some data for various solid phases (solution or stoichiometric) and gaseous mixture phase. The PAQ2 is specially designed for these example calculations of the so-called Pourbaix diagrams (i.e., pH-Eh plots) and other types of phase diagrams or property diagrams in some aqueous-bearing multicomponent heterogeneous interaction systems within the limited chemical framework of Fe-Co-Cr-Ni-C-N-S-H2O-NaCl, via the Single-Database Option in the advanced POURBAIX module or through the normal TDB-GES-POLY-POST routine.

Additional Examples in this Series

Additional examples (TCEX40A, TCEX40B, TCEX40C, and TCEX40E) are provided to demonstrate options and features in the Pourbaix module and to show more advanced applications of the TCAQ and AQS aqueous solution databases [in the Multiple-Database

Option, i.e., with appended data from the SSOL and SSUB databases]. See Pourbaix Examples TCEX40A, 40B, 40C, and 40E.

Example TCEX40D is deprecated as of version 2022a.

tcex53 - Pourbaix Diagram Calculations for a Heterogeneous Interaction System

Also see the *Pourbaix Diagrams Educational Material Guide.*

This example uses the PAQ2 database to calculate some Pourbaix diagrams. The DATABASE_ RETRIEVAL (TDB), GIBBS_ENERGY_SYSTEM (GES), POLY3, and POST modules are used for the Fe-X-H2O-NaCl heterogeneous interaction system, where X = Cr-Ni-Co.

The initial bulk composition of Fe-based alloy in this calculation is just preliminarily assigned, in which the BCC_A2 and/or FCC_A1 solution phase(s) are considered as of primarily interest. For practical calculations, one shall have more precise inputs for the initial bulk compositions of alloys.

Step 1: Single-Point Calculations for H2O-NaCl system

To demonstrate how to define the molality of NaCl in an aqueous-bearing heterogeneous interaction system.

Step 2: Single-Point Calculations for Fe-X (X = Cr-Ni-Co) system

To demonstrate how to define the initial amount of alloy in an aqueous-bearing heterogeneous interaction system. In this example, we are interested in only the BCC_A2 and FCC_A1 phases in the Fe-based alloy.

Step 3: Single-Point Calculations for Fe-Cr-Ni-Co + H2O-NaCl system

Step 4: Pourbaix Diagram Mapping for Fe-Cr-Ni-Co + H2O-NaCl system - define the variables

From the same mapping calculations you arrive at by the end of the example, you can plot more diagrams using a variety of X-Y axis variables.

> For a list of pre-defined symbols, go to the end of the tcex53.TCM macro file (open it in a text editor).

Pourbaix Examples TCEX40A, 40B, 40C, and 40E

These are the extended examples that are described in Pourbaix Diagram Examples.

TCEX 40A

This example shows you how to use Option 1 where you **start a completely new calculation**. It uses a single database. The Pourbaix diagram for 0.001 m Fe in a 0.1 m NaCl solution at 25 °C and 1 bar is automatically calculated and plotted.

A more advanced version of 40A can be found in TCEX40E, which also uses Option 1 but with multiple databases. However, licenses are required for three commercial Thermo-Calc databases.

See POURBAIX_DIAGRAM Commands for Options 1 to 4.

A so-called Pourbaix diagram is actually a phase diagram with independently-varied electropotential (Eh) and acidity (pH), for an heterogeneous interaction system at a certain bulk composition (that is by default always set as 1 kg of water solving a specified amount of metals and other solutes), under defined temperature and pressure conditions. Some property diagrams, along various phase boundaries for the same interactions resulting from the same Pourbaix module calculation, are also plotted, without leaving Option 1.

At the end of this example, a new POLY3 file called *POURBAIX.POLY3* is automatically saved. The following examples (TCEX40B and TCEX40C) use this same POLY3 file for the calculations. Therefore it is important to make copies of this file and rename these to TCEX40A.POLY3, TCEX40B.POLY3, and TCEX40C.POLY3. This must be done outside of the Thermo-Calc software and after the TCEX40A calculation and plotting is complete. This is so that the required POLY3 file structure is not lost.

The reason you do not save from within Thermo-Calc is because of how the file is saved. When the command sequence (GO POLY3>SAVE TCEX40A.POLY3>Y) is used, the POLY3 workspace of the POURBAIX calculation results in the POLY3 module monitor and all the initial equilibrium points and the mapping/stepping calculation results are lost as well as parts of the POLY3 file structure (e.g., some definitions of the previously defined POURBAIX-type calculation system).

A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

TCEX 40B

This example shows you how to use Option 2 where you **Open an old (existing) file and plot other property diagrams**.

Example 40A calculated and plotted the Pourbaix diagram for 0.001 m Fe in a 0.1 m NaCl solution at 25 °C and 1 bar. Example 40B reads the original POURBAIX.POLY3 file , and uses the calculated results to plot property diagrams for the same heterogeneous interaction system.

For example 40B, the POLY3 file is not modified. However, it is still recommended that a copy of the original POLY3 file is used so you do not lose the file structure and calculated results.

If you have a POLY3 file generated after choosing Option 4, that file can also be used for Option 2, and vice versa.

TCEX 40C

This example shows you how to use Option 3 where you **Open an old file and make another Pourbaix calculation**. The previously calculated (and copied) POURBAIX.POLY3 file from TCEX40A is edited to make another Pourbaix calculation and plot.

The same chemical system is used (Fe-H_2O-NaCl) but with different P-T-X (pressure-temperature-composition) conditions and without the GASeous mixture phase. The new conditions are 0.01 m Fe in a 1 m NaCl solution at 200 °C and 1 kbar.

In this example, the GASeous mixture phase for the Pourbaix diagram is not considered.

The POLY3 file is modified and rewritten with the new conditions. As previously recommended, make a copy of the original POLY3 file and rename it (e.g.TCEX40C.POLY3) so you do not lose the file structure and new calculated results.

A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

After the default Pourbaix diagram is generated and refined, you can also use Option 3 to plot property diagrams along different phase boundaries for the same system. These settings are possible from within Option 3 and you do not need to go back to Option 2.

TCEX 40E

This example shows you how to use Option 1 where you **start a completely new calculation**. It uses multiple databases (TCAQ, SSUB, and SSOL). The Pourbaix diagram for 0.001 m $Fe_{90}Co_5Ni_5$ alloy (9E-3 m Fe + 5E-4 m Co + 5E-4 m Ni) in an aqueous solution with 2E-2 m H_2S and 3 m NaCl at 25 °C and 1 bar is automatically calculated and plotted.

You need licenses for three Thermo-Calc databases, i.e.

- A: AQS (TGG Aqueous Solution Database; HKF model) or TCAQ (TCS Aqueous Solution Database; SIT model);
- B: SSUB (SGTE Pure Substances Database)
- C: SSOL (SGTE Alloy Solutions Database) or TCFE (TCS Steels/Fe-Alloys Database) or similar.

The TCAQ database contains only an AQUEOUS solution phase (using the SIT model) and REF_ELECTRODE phase (as a reference state for electron in aqueous electrolyte systems). The SSUB database is appended for the GASeous mixture phase and some pure solid phases (so-called secondary phases formed during aqueous-involving interaction processes), and the SSOL database is appended for various solid solution phases.

The Pourbaix module inside the software also accepts the AQS2 aqueous solution database (using the complete Revised HKF model) in the Multiple Database Option, in addition to the TCAQ2 aqueous solution database (using the SIT model).

POURBAIX_DIAGRAM Commands for Options 1 to 4

Option 1: Start a Completely New Pourbaix Diagram Calculation

Option 1 is used to make a completely new Pourbaix diagram calculation and automatically plot a pH-Eh diagram. i.e., define a new chemical system; specify the T-P-X conditions; calculate the initial equilibria; perform the pH-Eh mapping calculation; plot pH-Eh and various property diagrams.

Many of the commands in Option 1 are also repeated for Options 2 to 4. The details for each command are included with this section unless it is specific to one of the other option choices. The order that the commands display on screen is also different and based on what is entered at the prompts. These prompts are also available in other commands and when applicable a link to that command is included.

```
Consider the GAS phase in calculating a Pourbaix diagram? /Y/
```

You can choose to ignore the GAS mixture phase on a calculated/plotted Pourbaix diagram. However, such a plot is actually not a complete Pourbaix diagram because the thermodynamically-stable phase boundaries between the AQUEOUS solution phase and GAS mixture phase will not be calculated.

- If you enter `Y` (the default), GAS mixture phase is always considered.
- If you enter `N` the GAS mixture phase is completely ignored.

```
Use single database? /Y/
```

If you keep the default you are prompted for a database.

```
Combined database: /PAQ2/
```

The default is PAQ2, a database included with all installations.

The following information is provided on screen if you chose Y at the first prompt, `Need any instruction on the POURBAIX module? /N/`.

Define a Chemical System and its Initial Bulk Composition

Normally a Pourbaix diagram and its related equilibrium property in a heterogeneous interaction system are calculated under a certain bulk composition, which is usually 1 kg of water with defined amounts of dissolving solute substances. The solutes may either be completely dissolved into the aqueous solution, or be partially dissolved and simultaneously form some solid phases.

CHEMICAL SYSTEM (ELEMENTS)

- Default defined elements (solvent H2O): H and O and specially assigned ZE (electron) and VA(vacancy).
- Prompt specified elements (solutes ELEM): Fe Ni Co Cr C N S Na Cl

INITIAL BULK COMPOSITION

- Default defined composition (solvent): 1.0 kg of H2O
- Prompt specified composition (solutes): x mole of ELEM
- Mass of Water (weight) = 1 kg

When entering solutes in chemical formulas, the first element's letter must be in UPPER case, and second in lower case, for example `NaCl`, `CO2`, `CoCl3`, `Fe0.93S`, `NaSO4-1`, and `H2SO4`.

`First solute`

Enter a solute, e.g. `Fe`.

`Molality of <first solute> [mol/kg] /.001/`

Enter a molality for the first solute, e.g. Fe.

`Second solute`

Enter a second solute and its molality on the same line, e.g. `NaCl .1`.

`Next solute`

You can continue to enter solutes. Press <Enter> to skip to the next prompt.

The following information is provided on screen if you chose Y at the first prompt, `Need any instruction on the POURBAIX module? /N/`.

Defined Chemical System and Initial Bulk Composition

Solutes have been split up into chemical elements and their mole numbers. If confirmed, the Pourbaix module will, in further steps, count the initial bulk composition in terms of chemical elements.

```
Confirm defined system and initial bulk composition? /Y/
```

If you keep the default (`Y`) thermodynamic data is retrieved from the database. Then it lists the database's phases for the defined system.

You can then reject or restore phases as required with the next prompts.

```
Reject phase(s) /NONE/
```

```
Restore phase(s): /NONE/
```

Then the program lists the phases retained in the system and you prompted whether this is OK or not.

```
OK? /Y/
```

If you answer `Y`, then a list of references for the assessed data is displayed on the screen. The next prompt is related to miscibility gap checks, global minimization, saving the information to a POLY3 file, and setting numerical limits.

```
Should any phase have a miscibility gap check? /N/
```

The database usually creates two or more "composition sets" for phases that can have miscibility gaps. However, for some phases this is not done automatically, for example the miscibility gap in the bcc phase in Fe-Cr is usually ignored. But if it is important to include a Cr-rich bcc phase specify this here. It costs some computation time and may make subsequent MAP or STEP processes more difficult to converge. To keep the default (not to have any such phase) press <Enter>. Otherwise answer Y and follow the additional prompts.

```
Enforce Global Minimization Technique in calculations? /N/
```

If you choose `Y`, the Global Minimization is done when possible (depending on the conditions setting), and a Global Minimization test is performed when an equilibrium is reached. This costs more computer time but the calculations are more robust.

```
Save all functions, variables and tables in POLY3 file? /Y/
```

Choose `Y` if you want to save all the defined symbols (functions, variables and tables) into the POURBAIX.POLY3 file, for further normal POLY3 calculations or normal POST post-processing. Choosing yes may result in a large POLY3 file.

```
Set numerical limits? /N/
```

? SET_NUMERICAL_LIMITS

The Pourbaix module has a default setting for numerical limits.

- Maximum number of iterations: 20000
- Required accuracy: 1E-6
- Smallest fraction: 1E-15
- Approximate driving force for metastable phases: Y

If you kept the defaults for the above prompts, the program lists the default and pre-defined calculation conditions and you are prompted to confirm.

```
Confirm defined conditions? /Y/
```

Now Thermo-Calc calculates the start points. This can take a few moments. Near the end of the calculation there is a list of the default axis variables. The maximum pH limit is calculated precisely and determined automatically by the Pourbaix module as a function of the temperature-pressure conditions and initial bulk compositions of the current defined interaction system. You are prompted to accept these settings.

```
Accept the default settings for two mapping variables? /Y/
```

The program now lists the initial equilibria for mapping and continues to calculate the mapping. Then it sets the automatic diagram axes and starts to plot the diagram. But first there are several prompts to guide you.

```
Any missing phase boundary you could possibly think of? /N/
```

Sometimes the Pourbaix module may miss some phase boundaries during the mapping process. If you answer `Y` you can add additional starting point(s) into the calculation. You are now prompted to specify a pH-Eh coordinate pair, for instance (4.0, -0.15), which is close to the expected phase boundary. However, such additional pH-Eh point should not outside the AQUEOUS/GAS(O2) or AQUEOUS/GAS(H2) boundaries; otherwise, the module will fail in finding any new starting point.

The next set of prompts relate to plotting.

```
Change the pH/Eh steps for smoother curves? /N/
```

You can modify the mapping steps of X/Y axes for smoother curves; sometimes it may help finding missing phase boundaries by decreasing the pH and Eh increments.

```
Zoom in? /N/
```

Change the scaling status for both X and Y axes. The program then asks for minimum and maximum values for the axes. In some cases values are suggested.

```
Change Curve-Label Option for the diagram? /N/
```

Change the Curve-Label option to one of the following:

- A: List stable phases along phase boundaries
- B: As A, but curves with same fix phase have same number
- C: List axis quantities
- D: As C, but curves with same quantities have same number
- E: As B, but curves with changing colours
- F: As D, but curves with changing colours
- N: No labels

Usually, Option E or B is good for phase diagrams such as pH-Eh plots, and F or D is good for property diagrams like pH-RC(Fe+2).

? SET_LABEL_CURVE_OPTION

`Add Label-Texts onto the Pourbaix diagram? /N/`

Add label text to an area in the diagram. The label is written starting from the specified coordinates. Optionally, let the program automatically add the text by calculating an equilibrium at some specific coordinates and also make a label as the stable phase names in the area. However, such an automatic calculation may fail, especially for a Pourbaix diagram where either pH or Eh is not an intensive variables.

In most cases, the program is able to write the label if the coordinates and texts are specified.

`Change the Subtitle of the diagram? /N/`

This is the same as the POST module commandSET_CORNER_TEXT→ UPPER_RIGHT <SUBTITLE>. The default subtitle is automatically assigned by the POURBAIX module and is based on the defined conditions in the system (temperature, pressure and initial bulk compositions).

If you choose `Y` then the existing subtitle is displayed and you are prompted to enter a new subtitle or to have None.

`New Subtitle /NONE/`

You can change the subtitle for all the diagrams in the same POURBAIX run (i.e., within the same Option). The new subtitle that can be altered later at the same option, when further modifying the present graph or when refining any sequentially defined plot. By entering text (empty space at any position is allowed), the new subtitle is defined. By typing OLD, the existing subtitle is kept.

By pressing <Enter> (i.e., accepting None), the subtitle is deleted from all sequential plots, which can be set back later at the same option, too.

`Change Axis-Texts? /N/`

Change the axis text for both X and Y axes.

```
Further Refine the diagram in POST Module? /N/
```

With this option, you can further change the appearance the plot and use any command in the normal POST Module.

POST Module Commands

```
Hard copy of the diagram? /N/
```

Recommended Responses

- Hard copy of the diagram? /N/: Y
- CURRENT DEVICE: MS-Windows
- GRAPHIC DEVICE NUMBER /1/: 5
- NEW DEVICE: Postscript portrait mode
- USE POSTSCRIPT FONTS /YES/: Y
- SELECT FONTNUMBER /9/: 27
- NEW FONT: Times-Bold
- FONT SIZE /.35833/: .32
- PLOTFILE : /defaultname/: yourfilename

```
Save X-Y coordinates of curve on text file? /N/
```

Write all the current graphic information (generated and modified in the above procedure) on a text file using the DATAPLOT format (see the *DATAPLOT User Guide* or search the online help). This also makes it possible to merge two or more diagrams from separate but similar calculations, or put some experimental data points onto a calculated diagram. You do this by first writing them onto text files with this option and then edit them together (using a general text editor). The program asks for a file name. Accept the default (usually POURBAIX) or use another name. If an extension is not given, the written file is given an extension of *.EXP.

```
Modify the diagram? /N/
```

Further modify the appearance of the created plot. This brings you back to the above prompts for changing various features.

```
Any more diagram? /N/
```

Make many other plots using the same POURBAIX module calculation file.

Option 2: Open an Existing File and Plot Other Property Diagrams

Copy and Rename the POLY3 file

At the end of a Pourbaix module calculation, a new POLY3 file is automatically saved.

A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

If you are using a POLY3 file more than once (as is done in the extended examples), it is recommended that you copy and rename the previously-generated POLY3 file. This is so that the required POLY3 file structure and Pourbaix results are not lost. Do this outside of Thermo-Calc i.e. do not save from within Thermo-Calc.

The reason you do not save from within Thermo-Calc is because of how the file is saved. When the command sequence (GO POLY3>SAVE <*FILE NAME*>.POLY3>Y) is used, the POLY3 workspace of the POURBAIX calculation results in the POLY3 module monitor and all the initial equilibrium points and the mapping/stepping calculation results are lost as well as parts of the POLY3 file structure (e.g., some definitions of the previously defined POURBAIX-type calculation system).

Open an existing POLY3 file created by the Pourbaix module (from a previous Pourbaix calculation Option 1 or 3 or a previous Stepping calculation Option 4), and selectively plotting other property diagrams. i.e., open the old GES and POLY3 workspaces; plot pH-Eh or various property diagrams.

```
File name /ABCDEF/
```

The name of a previously saved POLY3 file where the POLY3 and GES5 workspaces is to be read must be specified. You do not need to enter the file extension if it is the default .POLY3 name. The default file name (e.g. ABCDEF) is the most recent specified POLY3-file name or RESULT if there is no workspace already saved in the run. You can press <Enter> or type a specific file name to read the POLY3 and GES5 workspaces from the file.

For Windows, and at the prompt, an **Open file** window displays if a file name is not given or the file path is incorrect. The file type (i.e. POLY3) cannot be changed. Click **Open** or **Cancel** to continue with the selected file.

When the file opens, it confirms on screen what kind of calculation is contained in the POLY3 file. For example: *The loaded POLY3 file is of POURBAIX-MAPPING Calculation*.

On screen it also lists the system components and the default and predefined calculation conditions to enable you to review these.

Next you are given a set of properties that are available to be selected as axis variables for making other diagrams from the same calculation.

Abbreviation	Definition
pH	Acidity
Eh	Electronic potential (V)
Ah	Electronic affinity (kJ)
pe	Electronic activity [log10ACRe)
IS	Ionic strength
TM	Total concentration
Aw	Activity of water
Oc	Osmotic coefficient
MF (AQsp)	Mole fractions of aqueous species
ML (AQsp)	Molalities of aqueous species
AI (AQsp)	Activities of aqueous species
RC (AQsp)	Activity coefficients of Aq species
Where AQsp is the name of a specific aqueous species, and "*" can be used as a wild sign for all AQSp. It is not necessary to give a complete aqueous species name. However, the entered AQsp name must be unique. If neither AQsp nor * is given, all species are searched.	

The rest of the prompts are the same as with Option 1 and relate to plotting. Enter `?` at any prompt for details.

Option 3: Open an Existing File and Make Another Pourbaix Calculation

Copy and Rename the POLY3 file

At the end of a Pourbaix module calculation, a new POLY3 file is automatically saved.

A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

If you are using a POLY3 file more than once (as is done in the extended examples), it is recommended that you copy and rename the previously-generated POLY3 file. This is so that the required POLY3 file structure and Pourbaix results are not lost. Do this outside of Thermo-Calc i.e. do not save from within Thermo-Calc.

The reason you do not save from within Thermo-Calc is because of how the file is saved. When the command sequence (GO POLY3>SAVE <*FILE NAME*>.POLY3>Y) is used, the POLY3 workspace of the POURBAIX calculation results in the POLY3 module monitor and all the initial equilibrium points and the mapping/stepping calculation results are lost as well as parts of the POLY3 file structure (e.g., some definitions of the previously defined POURBAIX-type calculation system).

Open an existing POLY3 file created by the Pourbaix module and make another Pourbaix diagram calculation i.e. open the old GES and POLY3 workspaces, adopt the defined chemical system, modify the T-P-X conditions, calculate the initial equilibria, perform the pH-Eh mapping calculation and plot pH-Eh or other property diagrams.

The rest of the prompts are the same as with Option 1 or Option 2. Enter `?` at any prompt for details.

```
Modify Label-Texts on the Pourbaix diagram? /N/
```

Once some labels are written by the Add-Label-Text command onto the diagram, you can also modify the labels (changing their positions and text contents). The text-size cannot be changed. The program asks which label and you enter its new X/Y coordinates with the new text. The new text must not be longer than the old one.

```
Modify Label-Curve-Option on the Pourbaix diagram? /N/
```

Because some phase-region labels have been written onto the diagram, the Label-Curve-Option might need to be modified, normally to the Option N.

Important Information About Option 3

The default definitions of the Eh and pH quantities in the advanced Pourbaix module (and in the ordinary TDB-GES-POLY calculation routines) should ALWAYS be as below:

```
Eh = MUR(ZE)/RNF

pH = -log10[AI(H+1,AQUEOUS)]

= -log10[ACR(H+1,AQUEOUS)*AH2O]
```

where RNF is the Faraday constant (96485.309 C/mol), and AH2O is the molecular weight of H2O (55.508435 g). MUR(ZE) is the electrochemical potential (ECP; in the unit of J/mol; w.r.t. the standard hydrogen electrode). ACR(H+1,AQUEOUS) is the site-fraction-based activity of the H+1 aqueous species in AQUEOUS solution phase, but AI(H+1,AQUEOUS) [that equals ACR(H+1,AQUEOUS)*AH2O] is the molality-based activity of the H+1 aqueous species that should be used for defining the pH quantity.

Within an aqueous-bearing heterogeneous interaction system, the fundamental system-components must be H2O, H+1 and ZE, which are corresponding to the basic elements O & H and the hypothetical electron (ZE) in the aqueous solution phase. For the additional chemical elements in the system, their corresponding system-components shall be defined as in their element forms (such as Fe, Cr, Mn, Ni, Na, Cl, S) or (for some) in their molecular forms (e.g., NaCl, H2S). The reference state for the H2O component must always be defined as the solvent species H2O in the AQUEOUS solution phase under the current temperature (*) and 100000 Pascal (i.e., 1 bar). The reference states for the H+1 and ZE components are by default set as their SER.

Various conventional properties of aqueous solute species I are converted in the following manners:

```
ML = Y(AQUEOUS,I)*AH2O/YH2O

RC = ACR(I,AQUEOUS)*YH2O/Y(AQUEOUS,I)

AI = RC*ML

= ACR(I,AQUEOUS)*AH2O
```

where YH2O [i.e., Y(AQUEOUS,H2O)] and Y(AQUEOUS,I) are the site-fractions of solvent H2O and solute species I.

LIST THE DEFINED AXIS-VARIABLES:

```
Axis No 1: LNACR(H+1)Min: -34.532525Max: 2.3025851 Inc: 0.8

Axis No 2: MUR(ZE)   Min: -150000   Max: 200000    Inc: 7718.85
```

The default settings (listed above) for two mapping variables [in terms of lnACR (H+1) and MUR(ZE), and their minimum/maximum values and increment steps] are covering the following pH-Eh ranges/steps:

```
pH:  0.00 -> 14.00, at a step of 0.35
Eh: -1.55 ->  2.07, at a step of 0.08 (V)
```

The maximum pH limit has been calculated precisely and determined automatically by the Pourbaix module, as a function of the temperature-pressure conditions and initial bulk compositions of the current defined interaction system.

Option 4: Open an Existing File and Make another Stepping Calculation

Open an existing POLY3 file created by POURBAIX Module (from a previous POURBAIX calculation Option 1 or 3 or a previous STEPPING calculation Option 4), and make a normal STEPPING calculation. i.e., open the old GES and POLY3 workspaces; adopt the defined chemical system; specify one of the T-P-X conditions as the stepping variable; calculate the initial equilibria; perform the stepping calculation; plot various property diagrams.

Many prompts are the same as with Option 1 or Option 2. Enter `?` at any prompt for details.

Copy and Rename the POLY3 file

At the end of a Pourbaix module calculation, a new POLY3 file is automatically saved.

A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

If you are using a POLY3 file more than once (as is done in the extended examples), it is recommended that you copy and rename the previously-generated POLY3 file. This is so that the required POLY3 file structure and Pourbaix results are not lost. Do this outside of Thermo-Calc i.e. do not save from within Thermo-Calc.

The reason you do not save from within Thermo-Calc is because of how the file is saved. When the command sequence (GO POLY3>SAVE *<FILE NAME>*.POLY3>Y) is used, the POLY3 workspace of the POURBAIX calculation results in the POLY3 module monitor and all the initial equilibrium points and the mapping/stepping calculation results are lost as well as parts of the POLY3 file structure (e.g., some definitions of the previously defined POURBAIX-type calculation system).

The stepping calculation modifies the POLY3 file but this can be used for other Stepping calculations inside the Pourbaix module (e.g. repeating Option 4) or in normal POLY3 module.

Stepping Parameters

The following parameters are suitable for a STEPPING calculation for the defined aqueous-bearing system. Choose one of them as the stepping variable:

```
T Temperature (C)

P Pressure (bar)

pH Acidity

Eh Electronic Potential (V)

N(Comp) Mole of One Component
```

where "Comp" is the name of a specific component as listed below. One should not use any key component (H2O or H+1 or ZE) as such a stepping variable, because of that their compositional definitions and variations are determined by the AQUEOUS solution phase in the POURBAIX Module.

An interacting component defined as an element (such as Fe or Na or Cl) can be selected as a stepping variable.

However, if you want to make a stepping calculation with a non-element chemical formula (such as NaCl or CaS2) as the stepping variable, one must have made some necessary modifications in the POLY3 Module, before reaching this point, by conducting some POLY3 commands as given below (as an example for the system Fe-Na-Cl-H-O):

```
POLY_3: def-component H2O H+1 ZE Fe NaCl Cl

POLY_3: set-ref-state H2O AQUEOUS * 1E5

POLY_3: set-ref-state ZE REF_ELEC * 1E5

POLY_3: change-status phase REF-ELEC=SUSPEND

POLY_3: set-cond b(H2O)=1000 n(H+1)=0 n(ZE)=0

POLY_3: set-cond P=1E5 T=298.15**
```

```
  POLY_3: set-cond n(Fe)=1E-3 n(Cl)=0 n(NaCl)=3 **
```

** Here the P-T-n(Fe) conditions can be set as what you wanted, while the initial n(NaCl) value must be set as between its minimum and maximum values that you are interested in. Later on, it will be prompted for specifying the n(NaCl) Min-Max-Step values of the stepping calculation.

```
Stepping variable: /T/
```

The chosen stepping variable must be one of the suitable parameters listed above.

```
Minimum temperature (C) /15/

Maximum temperature (C) /35/

Increment in temperature (C) /1/
```

The AQUEOUS solution phase under the defined bulk composition and pressure condition is stable only between 0 and 99° C. However, you can make a stepping calculation outside this temperature range, where the AQUEOUS solution phase become metastable. In this case, the resulting POLY3 file is possibly able to be opened by any other option within the Pourbaix module.

Tabulate Reaction (TAB) Example

tcex12 - Tabulation of Thermodynamic Data for Reactions

This example shows a number of independent cases using the TABULATE_REACTION (TAB) module to tabulate thermodynamic data for reactions.

> This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- TABULATE_REACTION
- DEFINE_SPECIES
- ENTER_FUNCTION
- QUICK_EXPERIMENTAL_PLOT
- SET_SCALING_STATUS
- LIST_SUBSTANCES
- TABULATE_SUBSTANCE

REACTOR Module Example

tcex24 - Simulation of the Silicon Arc Furnace

This is a simple reactor model with output of gases at the top and output of condensed phases at the bottom. The gas phase from one segment flows to higher segments, 80% reacts in the first above, 15% in the second above and 5% in the third above.

The condensed phases flow downwards and all of it goes to the next lowest segment. Heat can be added at any module. The only way to specify the initial state of the reactants added to the reactor is to specify the heat content.

This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- DEFINE_SPECIES
- CREATE_STAGE_BOXES
- CREATE_DIVIDERS
- CREATE_PIPES
- START_SIMULATION

Thermophysical Properties Examples

tcex55 - Plotting Viscosity of Cr-Ni at 1873 K

This is an example of including viscosity in the calculations.

Using the FEDEMO database, which is the free demonstration version of the TCS Steel and Fe-alloys Database (TCFE), the viscosity of metallic liquids is plotted at 1873 K for Cu-Ni and compared to experimental data from [2005Sat].

Reference

[2005Sat] Y. Sato, K. Sugisawa, D. Aoki, T. Yamamura, Viscosities of Fe–Ni, Fe–Co and Ni–Co binary melts, Meas. Sci. Technol. 16, 363–371 (2005).

The example includes an experimental data (`*.exp`) file called `Cr-Ni_1873K.exp`.

The same example is also provided in Graphical Mode as **T_12_Viscosity_in_Cr-Ni.tcu**.

tcex56 - Plotting Surface Tension of Cu-Zr at 1373 K

This is an example of including surface tension in the calculations.

Using the ALDEMO database, which is the free demonstration version of the TCS Al-based Alloy Database (TCAL), the surface tension of liquid metallic is plotted at 1373 K for Cu-Zr and compared to experimental data from [2005Kra].

Reference

[2005Kra] V. P. Krasovskyy, Y. V. Naidich, N. A. Krasovskaya, Surface tension and density of copper–Zirconium alloys in contact with fluoride refractories, J. Mater. Sci. 40, 2367–2369 (2005).

The example includes an experimental data (`*.exp`) file called `Cr-Zr_ALDEMO.exp`.

The same example is also provided in Graphical Mode as **T_11_Surface_tension_in_Cu-Zr.tcu**.

tcex58 and tcex59 - Molar Volume

There are two examples that include molar volume in the calculations and use the ALDEMO database, which is the free demonstration version of the TCS Al-based Alloy Database (TCAL).

The examples calculate volumetric thermal expansion coefficients of the L12-type Al3Sc (tcex58) and the L12-type Al3Zr (tcex59), respectively. Both Al3Zr and Al3Sc are modeled as the same phase (named as AL3SC, since Al3Sc is stable while Al3Zr is metastable).

The examples include an experimental data (`.exp`) file called Al3X.exp, which is the same for both examples to read the data from [2015Sah].

The same example, combining both tcex58 and tcex59 is also provided in Graphical Mode as **T_15_Molar_Volume_for_Al3Sc-Al3Zr.tcu**.

REFERENCE

[2015Sah] S. Saha, T. Z. Todorova, J. W. Zwanziger, Temperature dependent lattice misfit and coherency of Al3X (X=Sc, Zr, Ti and Nb) particles in an Al matrix. Acta Mater. 89, 109–115 (2015).

tcex60 - Electrical Resistivity and Thermal Conductivity

This example calculates the electrical resistivity (ELRS) and thermal conductivity (THCD) or pure Cu. It makes a step calculation over a wide temperature range, covering both the FCC_A1 state and the liquid state. It plots thermal conductivity of the system (both FCC_A1 and liquid) and that of a single phase (taking FCC_A1 as an example), respectively. Also plots electrical resistivity of the system and that of FCC_A1.

The example is available to all users as it uses the ALDEMO database, which is the free demonstration version of the TCS Al-based Alloy Database (TCAL).

The example includes two experimental data (`*.exp`) files called 1972Ho_cu_thcd.exp and 1981Ho_cu_elrs.exp.

The same example is also provided in Graphical Mode as **T_16_Electrical_Resistivity_Thermal_Conductivity_Cu.tcu**

REFERENCES

[1972Ho] C. Y. Ho, R. W. Powell, P. E. Liley, Thermal Conductivity of the Elements. J. Phys. Chem. Ref. Data. 1, 279–421 (1972).

[1981Ho] C. Y. Ho, M. W. Ackerman, K. Y. Wu, T. N. Havill, R. H. Bogaard, R. A. Matula, S. G. Oh, and H. M. James. Electrical resistivity of ten selected binary alloy systems. CINDAS report 59, for Office of standard reference data National Bureau of Standards, Department of Commerce (1981).

More Information about the Thermophysical Properties

The thermophysical properties are progressively being added to the Thermo-Calc databases starting with Thermo-Calc software version 2020a.

You can learn more about the models by searching the help (press F1 when in Thermo-Calc).

You can find information on our website about the properties that can be calculated with Thermo-Calc and the Add-on Modules.

Application Examples

tcex09 - Calculating a Dew Point with POLY3

This is an example calculating the dew point in the POLY3 module. The SUBDEMO database is used and included with your installation.

The STEP_WITH_OPTIONS and MAP commands are of note and used in this example.

tcex10 - Preventing Cr2O3 Clogging in a Continuous Casting Process

The example calculates an equilibrium with suspended or dormant phases and shows how to avoid Cr-oxide clogging in a continuous casting process.

This uses the TCOX database. A license is required to run the example.

The background of this example is that a manufacturer wanted to increase the Cr content of a material from 18 to 25 weight percent. They then had trouble in the continuous casting of this material because solid Cr_2O_3 was formed.

Using Thermo-Calc to calculate the equilibria in the steel/slag system, a simple correction was found: modify the Mn or Si content to decrease the oxygen potential.

In Thermo-Calc, you can FIX a phase with zero amount to simulate how to avoid forming this phase. You then release one of the conditions, usually one of the compositions, and this composition is determined by the equilibrium calculation.

These commands are of note and used in this example:

- DEFINE_SYSTEM
- CHANGE_STATUS
- COMPUTE_EQUILIBRIUM
- DEFINE_SYSTEM
- DEFINE_SYSTEM
- LIST_CONDITIONS
- LIST_EQUILIBRIUM
- LIST_STATUS
- SET_CONDITION

- SET_NUMERICAL_LIMITS
- SET_REFERENCE_STATE
- SHOW_VALUE

tcex11 - Oxidation of Cu2S with an H2O/O2 Gas Mixture

This example demonstrates the oxidation of Cu_2S with an H_2O/O_2 gas mixture. Thermo-Calc is used to find the optimum O/H ratio (i.e. oxygen potential) as certain oxygen potential values can desulphurize Cu_2S without forming copper oxides.

In Thermo-Calc, the problem reduces to perform equilibria calculations in a Cu-S-H-O system. The amounts of the components should be kept to correct ratio corresponding to Cu_2S and H_2O using a command SET_INPUT_AMOUNTS in POLY3. Initially, O/H = 0.5 is given. Optimum O/H ratio is calculated with the desired calculation conditions. For example, to simulate one phase disappearing, you can FIX the phase with zero amount.

The *tcex11.TDB* file is used to access data and this is included with your installation.

These commands are of also of note and used in this example:

- SET_NUMERICAL_LIMITS
- SET_REFERENCE_STATE
- SHOW_VALUE

tcex20 - Adiabatic Decompression in a Geological System

This example calculates the adiabatic decompression in a geological system using the geochemical database. The database is included with the file named PGEO.TDB, which is in the same folder as this example.

These commands are of note and used in this example:

- DEFINE_SYSTEM
- DEFINE_COMPONENTS
- SET_INPUT_AMOUNTS
- LIST_CONDITIONS
- SET_CONDITION
- SHOW_VALUE

tcex24 - Simulation of the Silicon Arc Furnace

This is a simple reactor model with output of gases at the top and output of condensed phases at the bottom. The gas phase from one segment flows to higher segments, 80% reacts in the first above, 15% in the second above and 5% in the third above.

The condensed phases flow downwards and all of it goes to the next lowest segment. Heat can be added at any module. The only way to specify the initial state of the reactants added to the reactor is to specify the heat content.

This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- DEFINE_SPECIES
- CREATE_STAGE_BOXES
- CREATE_DIVIDERS
- CREATE_PIPES
- START_SIMULATION

tcex27 - Calculating Chemical Vapor Depositions (CVD)

This example calculates the chemical vapor deposition (CVD).

This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- DEFINE_COMPONENTS
- SET_CONDITION
- ADD_INITIAL_EQUILIBRIUM
- LIST_AXIS_VARIABLE
- LIST_INITIAL_EQUILIBRIA

tcex28 - Pitting Resistance Equivalence (PRE) for a Duplex Stainless Steel

This example calculates the Pitting Resistance Equivalence (PRE) for a duplex stainless steel.

> This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- REJECT
- RESTORE
- DEFINE_ELEMENTS
- AMEND_PHASE_DESCRIPTION
- EVALUATE_FUNCTIONS
- SET_START_CONSTITUTION

tcex29 - Calculating the Speciation of a Gas

This example shows how to calculate the speciation of a gas.

> This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- SET_INPUT_AMOUNTS
- LIST_CONDITIONS
- SET_CONDITION

Data Optimization User Guide

Thermo-Calc Version 2025b

Introduction

In this section:

Introduction to Data Optimization

This guide describes the basic idea behind data optimization, contains brief descriptions of the modules and file types that you work with while doing your optimization, as well as rough outline of overarching workflow that you typically follow when working with optimization.

This guide assumes that you are familiar with using Thermo-Calc Console Mode. It also assumes that you understand the principles of thermodynamics and are familiar with the theoretical foundations of computational thermodynamics.

Press F1 to search the help for information about all the commands available in the Thermo-Calc Console Mode, including PARROT and ED_EXP. Note that the commands listed under PARROT and ED_EXP are only commands that are specific to PARROT and/or ED_EXP. These modules also contain some commands that are also available in POLY.

Thermo-Calc Console Mode example tcex36 is a detailed example of assessment and optimization in Thermo-Calc.

More about data optimization and PARROT, including a video about how to use PARROT, is available on the Thermo-Calc Software website. The video is also available on our YouTube playlist.

Data Optimization

In a thermodynamic database, each phase in a system is characterized using a mathematical model of its Gibbs energy. The Gibbs energy of a phase depends on various state variables. It can be defined individually even in a heterogeneous system with many stable phases since the properties of one phase are completely independent of the properties of the other phases in the system. In most alloy systems, the thermodynamic properties of a phase can be modeled by expressing how the Gibbs energy depends on temperature and composition. State variables such as pressure, volume or entropy can also serve as parameters in the Gibbs energy expression. The Gibbs energy of the whole system is the sum of the products of the Gibbs energy of each phase multiplied by the amount of that phase.

How the Gibbs energy of the phase varies with various state variables is determined by a mathematical model and how various adjustable parameters of the model is set. By optimizing these parameters, you can calculate the thermodynamic properties of a system under various conditions (by calculating phase diagrams for example). The thermodynamic properties themselves are functions of temperature, pressure or composition. They include, among other properties, standard enthalpy of formation, entropy, heat capacity, molar volume, thermal expansivity, compressibility and Curie temperature for magnetic transformations.

Data optimization is about adjusting the model parameters so that calculated equilibria fit well with experimental data. An important part of a data optimization is therefore collecting and assessing available experimental and theoretical information about phase equilibria and thermochemical properties of a system.

When you optimize the parameters of the model of a phase, you put what is called optimizing variables into the Gibbs energy expressions of those parameters. During the optimization, the values of these variables are varied in order to find a fit between the calculated equilibria and the experimental data that you base the optimization on. Once you have settled on a Gibbs energy expression for a certain parameter of a phase of the element, then you must stick to this expression in all future optimizations involving the element. If you do not do this, then you must re-optimize all previous systems that involve this element when the expression is changed.

The Thermo-Calc software allows you to optimize parameters that characterize not only binary systems, but also ternary system and systems of even higher orders. You can even optimize parameters that characterize systems of different orders at the same time.

More about data optimization and PARROT, including a video about how to use PARROT, is available on the Thermo-Calc Software website. The video is also available on our YouTube playlist.

The Least-Squares Method

Data optimization in Thermo-Calc is based on the least-squares method for fitting values calculated on the basis of a model with observed quantities. The software is accordingly trying to find the optimizing variable values that lead the minimized sum of the squares of the differences between the calculated values and the observed quantities (that is, of the errors or residuals).

The least-squares method works best under the following conditions:

- The observed quantities have a Gaussian probability distribution.
- The observed quantities are only subject to random errors.
- The different observations (experiments) are uncorrelated
- The standard deviation of each observation can be estimated.
- The number of observations is large.
- The models used give precise predictions.

Of course, these conditions are usually not all met in a normal thermodynamic assessment. But even in non-ideal conditions, there is no known method that works better than the least-squares method.

The CALPHAD Approach

CALPHAD is originally an abbreviation for *CALculation of PHAse Diagrams*, but was later expanded to refer to *computer coupling of phase diagrams and thermochemistry*. More about the CALPHAD methodology, including some of its history, is available on the Thermo-Calc Software website.

The data optimization functionality in Thermo-Calc works according to the CALPHAD approach to computational thermodynamics. This approach builds on the development of models that accurately represent thermodynamic properties for various phases. These models enable you to predict the thermodynamic properties of multicomponent systems-based data concerning binary and ternary subsystems. The predictions can take many factors into accounts, such as, for example, crystallography, type of bonding, order-disorder transitions and magnetic properties.

References

For in-depth information about CALPHAD as well as data optimization, see *Computational Thermodynamics – The Calphad Method* by Hans Leo Lukas, Suzana G. Fries and Bo Sundman (Cambridge University Press, 2007). CALPHAD was given its first general description in *Computer Calculations of Phase Diagrams* by Larry Kaufman and Harold Bernstein (Academic Press, 1970). The book contains some case studies of optimizations using Thermo-Calc.

Information about the concept of ‘lattice stability’ (which is important for the development of multicomponent thermodynamic databases) can also be found in the paper *Hume-Rothery and Calphad Thermodynamics* by Larry Kaufman, published in *Calphad and Alloy Thermodynamics*, edited by Patrice E.A. Turchi, Antonios Gonis, Robert Shull (The Minerals, Metals & Materials Society, 2002), pp. 3-19.

Working with Data Optimization in Thermo-Calc

In this section:

Data Optimization in Thermo-Calc

More about data optimization and PARROT, including a video about how to use PARROT, is available on the Thermo-Calc Software website. The video is also available on our YouTube playlist.

The actual performance of the optimization of a system is primarily done in the PARROT module, and in its sub-module ED_EXP. The POLY and POST modules are used to calculate and plot property or phase diagrams based on the optimized variables. This allows you to visually assess how good a fit you have achieved between your calculated results and your experimental data.

The end result of a successful optimization is typically an updated Thermo-Calc database file (with filename extension *.TDB) or a new database file.

Data Optimization Workflow

When you carry out an optimization using Thermo-Calc, you typically follow a workflow as outlined below.

1. Collect experimental data about your system from various sources such as journal articles and reports.
2. Create a POP file in which you enter the experimental data you have collected.
3. Create a setup macro file in which you define your system and the variables you want to optimize. A useful general procedure is to first find a minimum set of variables that allows you to calculate most of the experiments.
4. Run the setup macro file.
5. Compile your POP file. This file often contains errors, which need to be corrected, and the file recompiled several times before the compilation is completed without errors.
6. In the ED_EXP module, check that the experiments in your POP file reach equilibrium with reasonable results. If any experiments do not reach equilibrium with reasonable results, then try changing the starting values on equilibrium conditions (such as composition) to see whether the equilibrium can be computed after all. If this does not work, then you can temporarily exclude the experiment from the optimization. At a later stage in the optimization, when the optimizing variables have different values, you can check whether the experiments can be computed with reasonable results.
7. Back in the PARROT module, run the first optimization cycle and evaluate the feedback in the console. You can also plot diagrams in the POLY module that allow you to visually inspect the fit between calculated optimization results and the experimental data. If you are not satisfied with the fit, then enter the ED_EXP module again and adjust the weights of the experiments in a way that is likely to improve the fit and run another optimization cycle. Reiterate until you are satisfied with the fit.
8. Once you get the optimization stable and smooth with the minimum set of variables chosen in step 3 above, try using different sets of variables to see whether improvements are possible.
9. When you are satisfied with the fit between calculated results and experimental data with your final set of optimizing variables, update your setup file and POP file. In the setup file, enter the calculated optimizing variable values as the variables’ start values. In the POP file, enter the final weights of the experiments. With these files updated, you can easily regenerate the parameter values of your optimized system. Having the files updated also makes it easier to optimize the system again in light of

new data or new theoretical models.

10. Finally, update the database with your calculated results or create a new database with information about the system that you have optimized.

The PARROT Module

More about data optimization and PARROT, including a video about how to use PARROT, is available on the Thermo-Calc Software website. The video is also available on our YouTube playlist.

The PARROT module consists of a comprehensive subroutine package for data evaluation of thermodynamic model parameters from experimental data. The module has 99 variables that you can use for optimization and the module can handle a thousand experimental measurements in an optimization. However, there are limits on the simultaneous numbers of variables and experiments. These limits are listed at each optimization.

The PARROT module is part of the Thermo-Calc software. The module is not included in the software development kits (SDKs).

The experimental data is entered and edited in a sub-module of PARROT: The EDIT_ EXPERIMENTS Module.

The EDIT_EXPERIMENTS Module

The EDIT_EXPERIMENTS module, or ED_EXP for short, is used for entering, evaluating, and editing experimental data. To enter the module, go to The PARROT Module and then issue the command EDIT_EXPERIMENTS.

Since ED_EXP uses the POLY module for doing equilibrium calculations of experimental data points, many POLY commands are also available in the ED_EXP module. However, the commands may work somewhat differently in the two modules. There are also unique ED_ EXP commands which are not found in POLY.

When you execute ED_EXP commands, the PARROT workspace is modified. However, note that you must always first use READ_WORKSPACES in ED_EXP before doing anything in the module. The command loads the experimental data that you are going to work with during the optimization. Furthermore, before leaving ED_EXP you must use SAVE_WORKSPACES or the results of your work in the ED_EXP module is lost.

Data Optimization in Other Modules

All kinds of thermodynamic data, calculated equilibrium states or dynamic parameters are transferred back and forth between the PARROT and the GIBBS module as well between these and the POLY module. Whenever an optimization run is performed, PARROT calls the GIBBS module for stored system definition data and model parameters.

In Thermo-Calc, the GIBBS module (the Gibbs Energy System) handles the models of the various phases that can form in a multicomponent system. It stores thermodynamic data and performs various Gibbs energy equilibrium calculations. It contains subroutines to analytically calculate the first and second partial derivatives of integral Gibbs energy with respect to any set of variables. Many thermodynamic models for various types of substances are implemented in the module. Some commands that are available in the PARROT module are also available in the GIBBS module.

In the GIBBS module, parameters of the Gibbs energy models are referred to as *TP-functions*.

PARROT calls the POLY module for equilibrium calculations. The POLY module is used for calculating and storing complex heterogeneous equilibria.

Optimization File Types

These are the important files you work with when optimizing.

File type	***Description***
POP file	The POP file (Parrot OPtimization file) is the file that contains all the experimental data that you use for optimizing Gibbs energy values for your system. The POP file is a plain text file that contains ED_EXP commands. By default, the file has the filename extension *.POP in Thermo-Calc.
Setup file	The setup file is a Thermo-Calc macro file (*.TCM). This file typically contains commands that define your system, opens the PARROT workspace (and associated GIBBS and POLY workspaces) and sets optimizing variables.
Other macro files	It is often useful to have other macro files than the setup file at hand while you are doing your optimization. For example, it is convenient to have a macro file that automatically plots phase diagrams or other diagrams based on the latest values of your optimizing variables. An optimization process typically involves many optimization cycles, so this operation needs to be done many times during a typical optimization.
Workspace files	The PARROT module has its own workspace with dynamic memories, similar to the workspaces of POLY and GIBBS. It is stored and updated in a PARROT workspace file with the filename extension *.PAR. The workspace file is a binary file whose format is hardware dependent. This means that the format is unique for each type of CPU. Hence, a workspace file saved on a computer with one type of CPU cannot be used on a computer with another type of CPU.
EXP-file	The EXP-file is a plain text file with information in the form of DATAPLOT Graphical Language commands. These commands can specify some or all of the data points in your POP file. This allows you to plot these data points on top of your plotted optimization results (with the POST commands APPEND_EXPERIMENTAL_DATA or QUICK_EXPERIMENTAL_PLOT). You can then visually assess the fit between these results and the experimental data. The PARROT workspace is not influenced in any way by the creation or use of EXP-files. *DATPLOT User Guide* included with this documentation set.

Optimization Workspaces

When writing the setup file, you enter a CREATE_NEW_STORE_FILE command which creates a PARROT workspace file. Alternatively, select an existing PARROT workspace file with SET_STORE_FILE. The workspace file is automatically updated and saved with the latest optimization results (after each use of the OPTIMIZE_VARIABLES command). You can also explicitly instruct Thermo-Calc to save the workspace using SAVE_PARROT_WORKSPACES. If you want to get rid of your latest changes and return to the state of your workspace when it was last saved, use READ_PARROT_WORKSPACES.

When the PARROT workspace is saved, parts of the POLY and GIBBS workspaces are also saved to the PARROT workspace file, along with the PARROT workspace itself. Using the POLY command SAVE_WORKSPACES creates a new POLY3 file, nothing is saved to the PARROT workspace file.

If you do any POLY calculations based on data in the current workspace file, then a *.POLY3 file is created, which contains a copy of the current set of parameters. If you continue on your optimization and read the old *.POLY3 file, then the new set of parameters is overwritten with the old set. It is therefore recommended that you never read a *.POLY3 or *.GES5 file while you are doing an optimization.

Method for Optimization and Simulation

The PARROT module typically uses ordinary POLY minimization for equilibrium calculations. The global minimization technique that is used in POLY cannot be used because it automatically creates new composition sets which corrupt the PARROT workspace. Furthermore, the equilibrium definitions that you use as input for your optimization must each be attributed to a specific phase. Some of these definitions may specify some local or partial equilibrium state rather than a global minimum. However, it is possible to use the global minimization technique for some equilibrium calculations by using the ED_EXP command ADVANCED_OPTIONS with the `Toggle_Alternate` option.

Optimization in PARROT is performed on the basis of a ‘maximum likelihood’ principle. According to this principle, the best fit between various calculated results and all the input of experimental data is found where the sum of the square of the weighted residuals is at its minimum.

Typically, the results of an optimization is considered to be better the fewer optimizing variables that are needed to get the same level of fit between computed results and experimental data. If you can get almost the same fit using eight instead of twelve parameters, then this should be considered to be a significant improvement. When more parameters are used, the values of the individual parameters tend to become unrealistic. This is particularly true when it comes to temperature-dependent parameters. However, relatively small differences in the number of parameters are often insignificant. For example, it does not typically matter whether you used 24 or 25 parameters to reach a certain degree of fit.

It is often difficult to compare the quality of different optimizations based on the number of optimizing variables that have been optimized. Since you may rely more or less heavily on different pieces of available experimental data (and do so with good reason), it is possible that two different users could end up with very different numbers of parameters for the same system. For example, suppose you optimize the Fe-Al system to incorporate it into an Al database, while someone else optimizes the same system to incorporate it into an Fe database. In this situation, the two of you would probably make different judgements about which experimental information your calculated results must have a good fit with.

Creating the POP File

Before starting an optimization in Thermo-Calc, you must collect relevant experimental data about your system that is available in the research literature. This data is then entered in the POP file. The experimental data points and measurements are entered in this plain text file in the form of ED_EXP commands.

The syntax of the POP file is in principle independent of the models used for describing the phases in the system.

In this section:

Experimental Information

An optimization of thermodynamic model parameters should be based on a range of reliable experimental results that is as wide as possible, as well as on empirical or semi-empirical correlations and theoretical considerations. During an optimization in Thermo-Calc, many kinds of thermochemical and thermophysical data can be mixed and used together.

The information needed for an optimization represent measurements of thermodynamic parameters in the system at equilibrium. These can be measurements of any of the thermodynamic quantities that can be set as conditions in Thermo-Calc. The information may represent measurements of activities or enthalpies in single-phase regions for example, or solubilities or transformation temperatures in a multi-phase region.

For each equilibrium that is used in the optimization, at least one quantity must have been measured and you also need to know the conditions that must be set to compute the system's equilibrium state. For example, consider a binary system in a single-phase region. Suppose that you have measured the temperature, pressure, composition and the chemical potential. Three of these quantities are necessary to specify the equilibrium state and the forth can be used as experimental information to model the phase.

If you have a two-phase region and know the temperature and pressure conditions, as well as which the stable phases are, then you could use the compositions of one or both phases as experimental data. The former information about the conditions is sufficient to determine the equilibrium. The experimental information can then be used to optimize the parameters that are used to characterise and model the system.

For examples how to enter various kinds of experimental data in the POP file, see Experiments and Experimental Data.

Conflicting or Missing Information

You are likely to sometimes have inconsistent or conflicting experimental information. In principle, all available experimental data should still be entered into the POP file, unless you have good reasons to exclude some information. For example, if you have reason to believe that the samples used in some experiments were not pure, then these experiments could be excluded from the POP file.

For some systems, you have very little experimental data to go on. When this is the case, do not try to fit the available data uncritically with high accuracy without considering possible errors. You can look for data in systems with similar elements to get an idea about what the reasonable estimates of data that is lacking could be. Or you can use calculations from first principles or semi-empirical methods to get reasonable estimates that can be used as experimental data.

Invariant Equilibria Information

The most valuable experimental information for an optimization is information about stable invariant equilibria. An invariant equilibrium is such that neither pressure, temperature nor composition can be changed without there being a change in the set of phases present in the system. It is recommended that all information about invariant equilibria for a system is included in the POP file. These equilibria need not all be based on explicit experimental measurements of thermodynamic properties.

Reasonable estimates from available experimental data are often useful to include in the POP file. Such estimates, which should be based on the available experimental data, helps Thermo-Calc find a good set of start values on the optimization variables. However, at the end of the assessment, these estimated equilibria should be excluded and you should complete the optimization based only on the experimental information that is based on measurements.

With some experience from phase diagram evaluation, it is possible to make reasonable estimates of metastable invariant equilibria. Such estimates helps reduce the number of phases that are assessed simultaneously during the optimization. For example, you may assume that a certain intermediate phase does not form in a system. Then extrapolate the liquidus curves below the stable three-phase equilibria and finally, estimate temperatures and compositions of metastable three-phase equilibria between two other phases and the liquid.

Another useful technique is to extrapolate a liquidus line from a peritectic equilibrium to estimate the congruent melting temperature of a compound. This estimate may be more useful than the information about the peritectic equilibrium itself as the equilibrium involves only two phases.

Equilibria in Higher-Order Systems Information

When you optimize a binary system, the available experimental information can often be described equally well by very different sets of parameters. Information about ternary and higher order systems that include the components of the binary system are then often useful for optimizing the binary system (the same is true of information about quaternary system with respect to optimizing ternary systems). Often, it is only when you extrapolate the optimized parameters to a higher-order system that you can judge which of the sets of model parameters that is best. Sometimes information from several ternary systems is required to make a reliable judgement about which set of parameters best describes a particular binary system.

Heat Capacity Information

If you want to optimize your system based on data about heat capacities, then the corresponding parameters should first be optimized separately before you perform the general optimization of your system. The parameters should be kept fixed during the general optimization. This is because it is normally not possible to optimize heat capacity data together with other data in a meaningful way. If you do this, then it is very likely that the parameters related to the heat capacity are badly determined.

POP File Syntax

It is recommended that you specify an experimental equilibrium as close as possible to actual experimental conditions. Ideally, there is information about the set of stable phases, temperature, pressure and some or all compositions for the equilibrium.

In addition, it is recommended that you keep the POP file well-organised and extensively commented. This is especially important if someone else reassesses the system when new experimental information is available.

If you have too many equilibria defined in your file, or if you define equilibria with different sets of components in the same file, then you must divide the POP file in *blocks* (using the FLUSH_BUFFER command). You know whether you have defined too many equilibria for one block when you compile the file. A too large number of equilibria leads to an error message when the file is compiled.

If you use the DEFINE_COMPONENTS command, then it must be the first command in the POP file (or if you have several blocks, DEFINE_COMPONENTS can also be put as the first command after FLUSH_BUFFER). This is because the command automatically reinitiates the current workspace, so the effect of any commands placed before it are not saved.

The last command in the POP file should always be SAVE_WORKSPACES .

Legal Commands in a POP File

The following commands can be used in a POP file.

- ADVANCED_OPTIONS
- CHANGE_STATUS
- COMMENT
- CREATE_NEW_EQUILIBRIUM
- DEFINE_COMPONENTS
- ENTER_SYMBOL
- EVALUATE_FUNCTIONS
- EXPERIMENT
- EXPORT
- FLUSH_BUFFER

- IMPORT
- LABEL_DATA
- SAVE_WORKSPACES
- SET_ALL_START_VALUES
- SET_ALTERNATE_CONDITION
- SET_CONDITION
- SET_NUMERICAL_LIMITS
- SET_REFERENCE_STATE
- SET_START_VALUE
- SET_WEIGHT
- TABLE_HEAD, TABLE_VALUES and TABLE_END

Entering Experimental Information

A POP file in Thermo-Calc (*.POP) mainly consists of descriptions of equilibria, each equilibrium describing a data point that is based on an experiment from the existing literature on your system. An equilibrium is specified using ED_EXP commands.

The following is an example of a specification of an equilibrium with a single stable phase in the Au-Cu system. Equilibria with a single stable phase are often from experiments where enthalpies of mixing or chemical potentials have been measured.

```
CREATE_NEW_EQUILIBRIUM 1 1

CHANGE_STATUS PHASE LIQUID=FIX 1

SET_CONDITION T=1379 P=1E5 X(LIQUID,AU)=0.0563

SET_REFERENCE_STATE AU LIQ * 1E5

SET_REFERENCE_STATE CU LIQ * 1E5

EXPERIMENT HMR=-1520:200

COMMENT Measurement by Topor and Kleppa, Met trans 1984
```

Creating a New Equilibrium

The first command in an equilibrium specification is always CREATE_NEW_EQUILIBRIUM. This command takes two integers as arguments. The first integer should specify a unique identifier that can be used later to refer to the equilibrium in question. The second integer is an initialisation code 0, 1 or 2:

- Code 1: This means that all components are entered but all phases are suspended. This code is appropriate in most cases.
- Code 0: This means that all components and phases in the equilibrium are suspended initially. This code is needed if you are using experimental data about systems of different orders simultaneously, such as data about both binary and ternary systems for example.
- Code 2: This means that all components and phases are initially entered.

For example, the first command in the example above creates an equilibrium data point with the unique identifier 1. All components of the system are entered but all phases are suspended:

```
CREATE_NEW_EQUILIBRIUM 1 1
```

Setting Equilibrium Conditions and Uncertainty

All the equilibrium-related commands that are placed in between two CREATE_NEW_EQUILIBRIUM commands are interpreted as specifying the conditions of the equilibrium created by the first command. The values of these conditions should be based on the conditions specified in the experiment that you base the equilibrium definition on.

In the example, the CHANGE_STATUS command specifies that the equilibrium is a single-phase equilibrium with the liquid phase.

```
CHANGE_STATUS PHASE LIQUID=FIX 1
```

Furthermore, the temperature is 1379 K, the pressure is 1 bar (1E5 Pa) and the mole fraction of Au is 0.0563.

```
SET_CONDITION T=1379 P=1E5 X(LIQUID,AU)=0.0563
```

Sometimes you have reason to think that some information about an equilibrium condition may not be accurate. If this is the case, then you specify the degree of uncertainty for a condition with a colon after the condition quantity, directly followed by either an absolute value or a percentage. For example, if you have reason to doubt the reliability of the Au mole fraction measurement, then you could write:

```
SET_CONDITION T=1379 P=1E5 X(LIQUID,AU)=0.0563:10%
```

This indicates that you think the Au mole fraction is between 0.0507 and 0.0619. PARROT calculates the equilibrium twice, once for 0.0507 and once for 0.0619, and then computes the change of each experimental value between these two equilibria. This change is used to modify the uncertainty specified for the experimental value.

? Entering the Experimental Value and its Uncertainty

The possibility of specifying uncertainties on conditions may be useful when you have experimental data about a ternary system. In a binary system, a tie-line is determined by the two phases, the temperature and the pressure. Measurements of the compositions of both phases can then be used as experimental data. To specify the tie-line in a ternary two-phase equilibrium one of the four compositions must also be set as a condition. If the measurement of this composition has the same uncertainty as the other compositions, then you can assign this same degree of uncertainty both to the composition selected as a condition and the compositions selected as experimental data. Alternatively, the sample (overall) composition could be used as a condition and all four phase compositions could be used as experiment values. These phases must have the status *entered* (not fixed) since the relative amount of each is unknown.

Setting Reference States

If you want to specify a non-default reference state for one or several of your system components, then you do this with the SET_REFERENCE_STATE command. In the following example, the reference states for Au and Cu are set to the liquid phase at current temperature (*) and a pressure of 1E5 Pa.

```
SET_REFERENCE_STATE AU LIQ * 1E5
SET_REFERENCE_STATE CU LIQ * 1E5
```

> In order for these reference states to be taken into account, the `R` suffix must be used when the measurement of the enthalpy per mole of the system is entered for an experiment.

The Reference State Suffix R

Suffixes

You can use the reference state suffix `R` for some thermodynamic variables to calculate their value with respect to a reference state that you have previously set for a system component with the SET_REFERENCE_STATE command in POLY (or in response-driven modules such as the POURBAIX module). The value of energy-related variables that are used with the `R` suffix depends on the reference states of all the components in the defined system.

> It is possible to use an `R` suffix on all compositional extensive state variables as well, but the value of the state variable is always the same, with or without the suffix.

If the reference state for a system component is the default reference state (the stable reference state (SER) which is defined in a Thermo-Calc database), then MUR(comp)= MU (comp), ACR(comp)= AC(comp) and LNACR(comp)= LNAC(comp).

In the case of some thermodynamic variables, you can also use the `R` suffix to express chemical potentials and activities of species relative to some single-substitutional-lattice solution phases (such as aqueous solution, gaseous mixture, metallic liquid solution, slag mixture or MO solid solution). These state variables are MU(sp,ph), MUR(sp,ph), AC(sp,ph), ACR(sp,ph), LNAC(sp,ph) and LNACR(sp,ph).

The reference states and standard states of various solution species are pre-defined for some solution phases in some databases. For all solution species in any solution model in any database, it is always the case that MUR(sp,ph)= MU(sp,ph), ACR(sp,ph)= AC(sp,ph) and LNACR(sp,ph)= LNAC(sp,ph).

Entering the Experimental Value and its Uncertainty

The EXPERIMENT command is used to specify the quantity that the calculated results should be fitted to. When specifying this quantity, you both specify the measured quantity itself and your estimation of the uncertainty of this value.

In the example, the EXPERIMENT command specifies the enthalpy per mole of the system, where this value is specified with respect to non-default reference states that you have set in the equilibrium specification:

```
EXPERIMENT HMR=-1520:200
```

The value before the colon is the quantity of the variable. The value after the colon is an assessment of the uncertainty of this quantity. A higher value means a greater uncertainty. In the example, the uncertainty has been specified with an absolute value but it could also be specified in percent of the quantity:

```
EXPERIMENT HMR=-1520:13%
```

Several experiments can be specified after the experiment command. Besides assigning values to conditions, it is also possible to specify that a certain quantity is greater than or less than a certain value. For instance, the following command would specify that the activity of the C-component is less than 0.01 and the mass fraction of the BCC phase of Ag is greater than 0.05:

```
EXPERIMENT ACR(C)<0.01:0.001 W(BCC,AG)>0.05:10%
```

Note that an experimental quantity can typically also be treated as an equilibrium condition, and vice versa. Which measured quantities that you treat as conditions and which quantities you treat as experimental data should be based on the accuracy of the different measurements. In most cases, the quantity that is based on the experimental technique with the lowest accuracy should be used as the experimental value.

Entering Many Equilibria as a Table

When one thermodynamic variable (e.g. heat capacity) has been measured as a function of another (e.g. temperature), then experimental data is often presented as a table. By using the TABLE_HEAD, TABLE_VALUES and TABLE_END commands, you can enter such experimental information into the POP file in the form of a table. These three commands should always be used together and must be entered in the right order. See TABLE_HEAD, TABLE_VALUES and TABLE_END.

The TABLE_HEAD command is followed by a number. This number identifies the table as a whole, but also uniquely identifies the first equilibrium that is included in the table. This numeric identifier is incremented by one for each additional equilibrium in the table. Each row in the table represents one equilibrium. Thus, the equilibrium defined by the first row in the table above (on the line immediately below TABLE_VALUE) is uniquely identified with the number 1, the equilibrium defined by the second row by number 2, and so on until the last equilibrium on the sixth row, which is identified by the number 6.

Since the unique identifiers of the equilibria in the table are automatically generated from the unique numerical identifier that you give to the table, the unique numerical identifier that is normally given to the CREATE_NEW_EQUILIBRIUM command is replaced by two at signs (@@).

At least one of the equilibria conditions specified with the SET_CONDITION command must be a condition whose value is set by the numbers in one of the table columns. To assign the numbers in a column to a condition, use the syntax SET_CONDITION `<condition>=@<column number>`. For instance, in the example above, the mole fraction of X(ALO3/2) is for each equilibrium given by the number in the first column of the table.

At least one of the measured variables that are entered with the experiment command must be a variable whose value is set by the numbers in a table column. To assign the numbers in a column to a measured variable, use the syntax EXPERIMENT `<variable>=@<column number>`. In the example above, the measured temperature for each equilibrium is given by the number in the second table column.

The actual table should be entered between TABLE_VALUES and TABLE_END. Separate the columns with tabs or any number of spaces. The columns do not have to contain numbers, but can also contain other types of values, such as phase names for example. If a column contains text with spaces or special characters, then the text must be surrounded by double quotes (`“ABC DEF&ghi”`, for example). The table may have columns that are not used, but each row must have exactly the same number of columns.

The following block of commands exemplifies how a table can be entered into a POP file:

```
TABLE_HEAD 1

CREATE_NEW_EQUILIBRIUM @@ 1

CHANGE_STATUS PHASE TETR=FIX 0

CHANGE_STATUS PHASE ION=ENT 1

SET_CONDITION P=101325 N=1 ACR(O2,GAS)=.21 X(ALO3/2)=@1

EXPERIMENT T=@2:5

TABLE_VALUE

0.4608 2476

0.5714 2380

0.6682 2276
```

```
0.7496 2176
0.5038 2426
0.6313 2249
TABLE_END
```

Setting Site Fraction Start Values

In some systems, you have to set non-default composition start values on some experiments in order to get them to converge properly during optimization. This may be important if your system has a miscibility gap for example, in which case several equilibria with different compositions exist at certain temperatures. In such cases, you have to make sure it is specified in the POP file which side of the miscibility gap the equilibrium is on. The calculated equilibrium could otherwise end up on the wrong side, resulting in a large error.

In the POP file, you can set the site fraction of a constituent on an equilibrium with SET_START_VALUE.

For example, the following command sets the composition start value of VA constituent of the FCC_A1 phase to 0.99:

```
SET_START_VALUE Y(FCC_A1,VA#2)=0.99
```

Setting the mole fraction for a component in a phase is not as reliable as setting the site fraction.

Additional equilibria entered after the last SET_START_VALUE command are automatically given a similar start value if the following command appears previously in the POP file:

```
SET_ALL_START_VALUES Y
```

If start values are not set automatically for phase constituents, then you may have to set the composition start value for each equilibrium (or table of equilibria) separately.

Commenting About an Equilibrium

The COMMENT command inserts a comment about the equilibrium that is saved to the PARROT workspace file when the POP file is compiled. The comment must be entered on one line.

Comments can also be entered immediately after a dollar sign (`$`), but these are not saved to the PARROT workspace. Instead, these comments are ignored by Thermo-Calc when the POP file is compiled.

Simultaneous Use of Binary and Ternary Experiments

You can use experimental information about binary and ternary systems (as well as systems of even higher order) in the same POP file and optimization. To do this, you must inform the PARROT module that not all components of the ternary system (or system of even higher order) should be considered. This allows you, for example, to use experimental information about a binary equilibrium that exists within a ternary system.

Use CHANGE_STATUS with the keyword component and which components that should be entered. You should also give the initialization code 0 (rather than 1) to the CREATE_NEW_EQUILIBRIUM command. This code indicates that all components must be entered.

For example, the following set of ED_EXP commands characterises a binary (A-B) three-phase equilibrium (FCC-BCC-LIQ) in a ternary system (A-B-C). It can be used in a POP file that otherwise only contain experimental information about the ternary system (A-B-C):

```
CREATE_NEW_EQUILIBRIUM 1 0

CHANGE_STATUS COMPONENT A B = ENTERED

CHANGE_STATUS PHASE FCC BCC LIQ=FIX 1

SET_CONDITION P=1E5

EXPERIMENT T=1177:10

COMMENT from A-B
```

Using Stability Conditions

Early in the optimization when parameter values are not so good it is often useful to set the driving force for precipitation of a phase (per mole of components) to make sure that it appears where it should. The DGM condition is very useful for making sure that phases appear where they should. It can be removed when the optimization becomes stable.

The DGM condition is also useful for suppressing phases that appear where they should not appear. Do this by setting the value and the uncertainty to something reasonable. For example, the driving force for precipitation of the BCC phase could be set as follows:

```
DGM(BCC)<-0.1:0.1
```

This produces an error even before BCC becomes stable and the weight of the experiment in question can be adjusted as needed. If you specify that the driving force for the BCC phase should be below 0 (DGM(BCC)<0:1E-4 for example), then the optimization converges extremely slowly (if at all). With such a sharp error condition, calculating the equilibrium is like finding the minimum point on a lawn that gently slopes towards a rock wall. The optimization keeps bouncing into the wall.

Another useful stability condition is the phase stability function, abbreviated QF. This can be used to specify that a phase is outside the miscibility gap for a solution phase. If QF(phase) is negative, then the phase is inside the miscibility gap; if QF(phase) is positive, then it is outside the miscibility gap.

Grouping Equilibria with Labels

If you have several equilibria describing experiments that you want to be able to treat collectively, you can give all of the equilibria one and the same label.

Use LABEL to give an equilibrium a label. The label must start with the letter A and can only be up to four characters long. For example, you can insert the following command in several equilibria specifications:

```
LABEL ALH
```

During the optimization, you could use this label to, for example, set all the equilibria that have it to the same weight in the ED_EXP module.

Dividing the POP File into Several Blocks

For two different reasons, you may have to divide your POP file into different blocks:

- PARROT uses a buffer for storing compiled experimental data. If there is not enough memory in this buffer for storing all the experiments from the POP file, then the POP file can be divided into several blocks. When PARROT encounters the end of a POP file block, it saves the experimental data that has been compiled to PARROT workspace, clears out the memory buffer and then proceeds to read the next block in the POP file. This goes on until the experimental data from all the blocks have been saved to the PARROT workspace.
- If you want to put equilibria with different sets of components in one and the same POP file, then you must divide the file up into blocks. Each block should only contain equilibria that all have the same set of components.

To divide the equilibria in the POP file into different blocks, enter the FLUSH_BUFFER command between two equilibria. This command marks the beginning of new block. When the command is encountered during the compilation of the POP file, the compilation of the current block is terminated, the equilibria saved to the PARROT workspace file and a new block is initiated. That the buffer is reinitiated means that all functions and constants that were entered in the previous block must be entered again in new block in order to be used.

When editing your experimental data in the ED_EXP module, you can select which block to load and edit using READ_WORKSPACES `<block number>`. The block before the first instance of FLUSH_BUFFER is block number 1, the block after the first instance and before the second instance is block number 2, and so on.

The Setup File

In this section:

Creating the Setup File

The second step is to create the setup file. This is an ordinary Thermo-Calc macro file (*.TCM). Typically, your setup file should contain the following:

- A system definition.
- A section where you enter model parameters and optimizing variables.
- A GO PARROT command.
- A section where initial values are assigned to the optimizing variables for the first optimization cycle.
- A CREATE_NEW_STORE_FILE `<filename.par>` which creates the PARROT workspace file onto which the results of your optimization are continuously saved and updated. By default this workspace file has the same filename as the setup file, but with the *.PAR filename extension.
- A COMPILE_EXPERIMENTS `<filename.pop>` command. Since you often encounter syntax errors when you first try to compile a POP file, it may be useful to execute this command from the console rather than as part of the setup macro file.
- Normally, you also have a SET_INTERACTIVE at the end of the setup file. This command returns control over Thermo-Calc to the console.

It is possible to interactively execute all these commands one at a time in the console. It may be instructive to enter the commands that would normally go into the setup file interactively while using the on-line help while you are learning to use the PARROT module.

Defining the System

If you have an existing database with information about your system, then you can write the system definition part of your setup file in two different ways.

- If you have an unencrypted user database, then you can define your system by entering DATA module commands directly in the setup file. Use the DATA commands that you normally use to define a system when doing equilibrium calculations in Thermo-Calc Console Mode.
- Define your system by entering DATA module commands directly in the console, then generate a macro file with the GIBBS command LIST_DATA `<name of setup file>.tcm p` . This command saves all the data that has been loaded in the GIBBS workspace as a macro file. This file can then be modified as required into an optimization setup file.

Creating Additional Composition Sets of a Phase

If you need several composition sets of a phase, then these should be created with the GIBBS command AMEND_PHASE_DESCRIPTION `<phase name> composition_sets <composition set number>` in the setup file.

> If you add composition sets of a phase after the POP file has been compiled, the data structure in the workspace is corrupted and you have to recompile the POP file.

Entering the Optimizing Variables

When you have retrieved the data about your system for the setup file, you must manually enter the model parameters that you want to optimize. This is done using the GIBBS command ENTER_PARAMETER, but when you specify the Gibbs energy expression for the parameter, you enter variables that can be given various values into the expression. It is the values of these variables (and thus, the Gibbs energy of the parameter) that you are optimizing.

How you in detail specify the optimizing variables in your set up file depends on which phase you are trying to optimize and what thermodynamic model that is used in the optimization.

Thermodynamic Models

Entering Optimizing Variables in Parameter Specifications

There are ninety-nine predefined variables in the PARROT module which you can use in your optimization. These variables are referred to as `V1`, `V2`, `V3`, … `V98` and `V 99`. When the GIBBS workspace is initialized, all optimizing variables are set to a fixed numerical value of zero. When you do an optimization, there is always some variable for which you want to evaluate the best value, but you can assign fixed values to optimizing variables too. It is often useful to enter all the variables that you can conceivably want to optimize, and then you can interactively select and change which variable to focus at various stages of the optimization.

The setup file excerpts that follow show how optimizing variables are entered. However, before the optimizing variables are introduced in this example, the following command enters an ionic liquid solution phase (a phase for which you have some experimental information):

```
ENTER_PHASE IONIC_LIQ  Y,
AL+3,ZR+4 ; ALO2-1,O-2 ; N N
```

This ENTER_PHASE command enters a phase called IONIC_LIQ into the GIBBS workspace. This phase is of the type ionic liquid solution, which is specified by type code `Y`. Such a phase is modeled by the *Ionic Two Sublattice Liquid Model*. The next two arguments specify the two sublattices, in this case the cations AL+3,ZR+4 and the anions ALO2-1,O-2. Components that interact in a sublattice are separated by a comma. The first `N` at the end means that no additional constituents are added to the phase. The second `N` means that a list of possible parameters for the phase should not be shown in the console.

There are model parameters that describe the phase which you do not want to optimize, in which case the Gibbs energy expression of the parameter does not contain any optimizing variables.

Example 1

For example, the following parameters of the IONIC_LIQ phase do not contain any optimizing variables:

```
ENTER_PARAMETER G(IONIC_LIQ,AL+3:ALO2-1;0) 298.15 +2*GAL2O3_L; 6000 N
```

```
ENTER_PARAMETER G(IONIC_LIQ,AL+3:O-2;0) 298.15 +GAL2O3_L+400000; 6000
N
```

```
ENTER_PARAMETER G(IONIC_LIQ,ZR+4:O-2;0) 298.15 +2*GZRO2L; 6000 N
```

These parameters define the Gibbs energy expressions for three constituents in the constituent array, namely AL+3:ALO2-1, AL+3:O-2 and ZR+4:O-2. The names that occur in these expressions—that is, GAL2O3_L and GZRO2L—are the names of complex functions of temperature that are entered in the GIBBS workspace with the ENTER_SYMBOL command.

The numbers that frame the Gibbs energy expressions specify the temperature range within which the expression should be applied. In the above, the expressions are applied in a temperature range from 298.15 K to 6000 K.

Example 2

In this example, suppose that you want to optimize the model parameter for the ZR+4:ALO2-1 combination, then you could enter the variables V1 and V2 in the Gibbs energy expression for that parameter in the following way:

```
ENTER_PARAMETER G(IONIC_LIQ,ZR+4:ALO2-1;0) 298.15 +GZRO2L +2*GAL2O3_L
+V1+V2*T; 6000 N
```

You normally have different optimizing variables in different parameters, but in some cases you may want several parameters to vary together, in which case you can use the same variable in the Gibbs energy expressions of several parameters.

Entering Interaction Parameters

For some systems, you have to consider interaction parameters in order to take excess Gibbs energy into account and correctly model the phase. By default, the software uses a Redlich-Kister expression for the excess Gibbs energy. The coefficient is entered after the constituent array when you use the ENTER_PARAMETER command. In the last section, all the parameters were entered with a coefficient of zero (`0`).

To take account of the excess Gibbs energy, you might enter the following:

```
ENTER_PARAMETER L(IONIC_LIQ,ZR+4:ALO2-1,O-2;0) 298.15  +V11+V12*T;
6000 N
```

```
ENTER_PARAMETER L(IONIC_LIQ,ZR+4:ALO2-1,O-2;1) 298.15  +V13+V14*T;
6000 N
```

```
ENTER_PARAMETER L(IONIC_LIQ,ZR+4:ALO2-1,O-2;2) 298.15  +V15+V16*T;
6000 N
```

Parameters with interaction coefficients are referred to as *interaction parameters*. The regular parameter has a coefficient of 0. The subregular parameter has a coefficient of 1. It is possible to interaction coefficients up to a value of 9, but you are advised not to use more than three coefficients (that is, with coefficient values of 0, 1 and 2).

Initializing Optimizing Variables in PARROT

Variables that have been entered into Gibbs energy expressions for model parameters in the setup file have to be initialized and given start values before they are optimized.

You have to estimate what start values to give to the optimizing variables based on your knowledge of the system or of relevantly similar systems. There are no general rules for what start values your optimizing variables should have. If you are not able to make any informed estimation about what start values to use, then you may not be able to find a good fit between your experimental data and your calculated results. In this case, it is often best to start the optimization in the so-called alternate mode. In alternate mode, the PARROT module helps you find some reasonable start values for your optimizing variables.

? About Alternate Mode

Even if you are starting your optimization in alternate mode, you still have to initialize the optimizing variables though (you can all give them a start value of 0).

To initialize an optimizing variable and to give it a start value, use either SET_OPTIMIZING_VARIABLE or SET_SCALED_VARIABLE. Using SET-OPTIMZING_VARIABLE results in a scaling factor equal to the current value of the parameter unless the current value is zero, in which case the scaling factor is 1000. This is typically appropriate for enthalpic parameters, but not necessarily for other parameters. The scaling factor is the factor by which the optimizing variable value is varied during the optimization.

For example, if you want to optimize the variables V1, V2, V11, V13 and V17, then you could enter the following in the setup file:

```
SET_OPTIMIZING_VARIABLE 1 +43000

SET_OPTIMIZING_VARIABLE 2 -35.2

SET_OPTIMIZING_VARIABLE 11 +72000

SET_OPTIMIZING_VARIABLE 13 +27000

SET_OPTIMIZING_VARIABLE 17 -100000
```

The value given to each optimizing variable (+43000 for variable V1 for example) is also that variable's initial scaling factor. If you want to set the initial scaling factor of a variable to a value that is lower or higher than its start value, then use SET-SCALED_VARIABLE `<start value><scaling factor><min value><max value>`.

Creating the Workspace File

In the setup file, after the system definition and the entered optimizing variables, use the PARROT command CREATE_NEW_STORE_FILE to create and save a PARROT workspace file for the system defined in the setup file. For example, the following command saves all current data on system definitions (elements, species, components, phases), symbol definitions (constants, variables, functions, tables) and parameters that are stored in the workspace used by GIBBS, POLY and PARROT into a file called AL2O3-ZRO2.PAR:

```
CREATE_NEW_STORE_FILE AL2O3-ZRO2
```

> The experimental information in the POP file is not saved to this PARROT workspace file.

Compiling the POP File

At the end of the setup file, use the command COMPILE_EXPERIMENTS followed by the name of your POP file to compile the data in that file and save it to the current PARROT workspace file. Note that you must first have opened or created a new PARROT workspace file before you compile your POP file. The other argument to the command can typically be given default values with comma signs (,):

```
COMPILE_EXPERIMENTS AL2O3-ZRO2.POP,,,
```

If Thermo-Calc encounters errors in the syntax of the POP file, then error messages are displayed in the console. Normally, the compilation also stops when syntax errors are encountered. If this happens, then you must correct the errors and recompile the file. It is useful to have two console windows open when you do this. That way, you can use one console for editing the experimental data and another console for compiling and reading any further error messages.

Returning Control to the Console

Put the command SET_INTERACTIVE at the end of the setup file if you want to return control to the console when the commands in the setup file have all been executed.

Optimizing in PARROT

In this section:

Optimizing the System in PARROT

When you have created a POP file, a setup macro file, and (optionally) EXP files, you should start doing optimization runs interactively in the console. This process can be divided into a number of steps (such as running optimization, evaluating optimization results, modifying weights and models and adding new information), but usually, you have to go through many optimization cycles before achieving a satisfactory fit between calculation results and experimental data.

Typically, it is not obvious when an optimization is finished. You must exercise your judgment about when the fit you have achieved is good enough.

It is possible to interactively change almost everything in the initial setup macro file and in the POP file. For example, you can add more parameters to be optimized and modify or add more experimental information.

Changes that Require POP File Recompilation

Some changes that you do interactively in the PARROT module or the ED_EXP sub-module destroys the data structure in the workspace. For example, if you add more composition sets to a phase, then the number of phases actually change and the links break between the experimental data and the thermodynamic models. Note that if the global minimization technique is used in POLY, then new composition sets that corrupts the PARROT workspace may be created automatically. If this happens, then you have to compile the POP file again.

If you recompile the POP file, then the experimental equilibria are calculated with the default start values.

Optimization Workflow

Normally, the workflow during an optimization is the following:

1. In the PARROT module, run the setup macro file using MACRO_FILE_OPEN.
2. Go to ED_EXP with EDIT_EXPERIMENTS, use READ_WORKSPACES to load your experimental data and then execute .
3. If an equilibrium cannot be computed, then this either means that the start values (site fractions, for example) were inappropriate or that the equilibrium cannot be calculated with the current set of parameters. If the latter, then the equilibrium may have to be excluded from the optimization. However, you should make an effort to exclude the possibility that the reason is just that you do not have the appropriate start values for the equilibrium.
4. When each equilibrium is either successfully computed or excluded from the calculation, go back to the PARROT module and run the OPTIMIZE_VARIABLES command. Give the number of optimization iterations you want the Thermo-Calc program to carry out as an argument to the command. This number specifies how many different sets of values for the optimizing variables that PARROT tries to fit with the experimental data. It is recommended that you run `0` iterations first to see the discrepancy between the experimental data and the initial calculated results. The current workspace file is automatically updated with the last set of optimized variables and calculated results.
5. List and evaluate the result of the optimization using LIST_RESULT. Typically, what is of interest in the results are the relative standard deviation of the optimizing variables and the error values in the list of calculated experimental data results. If the relative standard deviation for an optimizing variable is very large, this means that the variable doesn’t have any effect on the computed results and that the variable should not be used (you can make PARROT ignore the variable by setting its value to `0` with SET_FIX_VARIABLE). If the relative standard deviation is close to zero for a variable, then this might indicate that you need to use more variables. When it comes to errors in the calculated equilibrium results, these can be decreased by lowering the weight that PARROT gives the experiment in the calculation (the more weight, the more the experiment affects the calculated results).
6. Use OPTIMIZE_VARIABLES or CONTINUE_OPTIMIZATION to carry out a new optimization cycle. Go back to step 5 above and continue to do optimization cycles until you judge that there is a good enough fit between your calculated results and your experimental data. It is recommended that you do not only rely on feedback from LIST_RESULT but also frequently plot various diagrams and compare them visually to some of your experimental data.

Ensuring Computation of all Equilibria

When you have run the setup macro file, you should start by trying to compute all the equilibria that were created when your POP file was compiled. To do this, you must first go to the ED_EXP submodule, and load the experimental data from the current PARROT workspace file with the READ_WORKSPACES `<block #>` command (normally, the block number is `1`).

When you have loaded all equilibria, you should try to compute them all using the ED_EXP command . A list of calculated equilibrium results are shown in the console, but the software is not able to reach an equilibrium for an experiment, then the program cancels the calculations and displays an error message.

The following list shows an example output where the first two experiments in the POP file have been successfully computed, but an equilibrium is not reached for the third experiment. No other equilibria are computed, since the calculations are aborted when the error occurs.

```
Eq  Lab  Iter Weight Temp   Exp  Fix phases or comments
  1 A1    22   1.    2575.3      IONIC_ FLUORI TETR
  2 A1    18   1.    2156.9      IONIC_ CORUND TETR
 *** ERROR  1614 IN QTHISS
 *** CONDITIONS CAN NOT BE FULLFILLED
```

When this happens, try to find out why the equilibrium calculation fail. Are the condition start values that you have given the equilibrium inappropriate for example? If you have a similar equilibrium that has already been successfully computed, then you can select the equilibrium that does not work, use the ED_EXP command SET_ALL_START_VALUES and accept all the suggestions for the site fractions. Alternatively, use TRANSFER_START_VALUE `<equilibrium number>` to make the currently selected equilibrium inherit the start values of the indicated equilibrium. Run COMPUTE_EQUILIBRIUM again to see if the equilibrium can be computed with the inherited start value.

If you cannot find an explanation of why the equilibrium cannot be computed, then it may be that the experiment is faulty. If so, then this experiment should be excluded from the optimization by being given a weight of 0. You should then run COMPUTE_EQUILIBRIUM again to make sure that all equilibria can be computed. However, experiments that fail to reach equilibria could succeed in doing so if the optimizing variables have other values. It is therefore sometimes worth trying to include experiments later in the optimization process (when the optimizing variables are relatively close to their final values), even if they had to be excluded at its start. In some cases, it might also be appropriate to change the error tolerance for in an experiment (using the ED_EXP command EXPERIMENT).

❗ You must save the PARROT workspace with SAVE_WORKSPACES before you exit the ED_EXP module.

Setting Weights

To change the weight of an experiment, first enter the ED_EXP module from PARROT using EDIT_EXPERIMENTS. Then use the SET_WEIGHT command to set the weight for a specific equilibrium (equilibrium number `3` for example), for a range of equilibria (the equilibria `10-19`) or all the equilibria that have a certain label (such as all the equilibria with the label `A1`). To save the new weight(s), use SAVE_WORKSPACES .

By default, all the experimental information in your POP file is treated equally: each experiment has a weight of `1`. However, experiments that you excluded because they did not reach equilibrium now have a weight of `0`. The higher the weight of an experiment is, the more Thermo-Calc tries to ensure that the computed result fits the condition measured in that experiment.

The contribution of an experiment's error to the sum of errors is multiplied by the square of the weight set for that experiment. In other words, if you want to cut the error of an experiment with weight 1.0 by half, then you should use a weight of 0.7. This makes the experiment's error 0.49. Setting the weight to 1.4 instead makes the error twice as large (1.96).

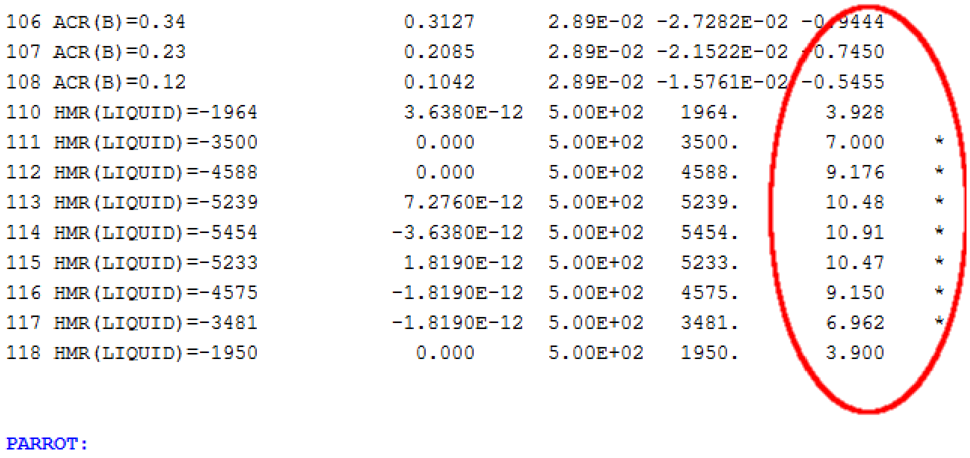
Note that if you use READ_WORKSPACES after you have changed weights on the experiments, your changes are lost unless you have saved those changes. In the ED_EXP module, you can get a list of all the experiments in the console if you first read the experimental data from the workspace file (with READ_WORKSPACES) and then use LIST_ALL_EQUILIBRIA.

Optimizing and Evaluating Results

When you have ensured that all the experimental data points can reach equilibrium, go back to the PARROT module and use OPTIMIZE_VARIABLES `<number of iterations>` with `0` iterations. Present the result of this initial optimization by using LIST_RESULT.

When evaluating the optimization results, the most important information is found in the list of experiments at the end of the listed results. The rightmost column shows the difference between the value of the experimental data and the value computed by Thermo-Calc in the last optimization cycle.

The following shows part of list of experiments in the output of a LIST_RESULT command:



```
106 ACR(B)=0.34                0.3127      2.89E-02 -2.7282E-02 -0.9444
107 ACR(B)=0.23                0.2085      2.89E-02 -2.1522E-02 -0.7450
108 ACR(B)=0.12                0.1042      2.89E-02 -1.5761E-02 -0.5455
110 HMR(LIQUID)=-1964          3.6380E-12  5.00E+02   1964.       3.928
111 HMR(LIQUID)=-3500           0.000      5.00E+02   3500.       7.000    *
112 HMR(LIQUID)=-4588           0.000      5.00E+02   4588.       9.176    *
113 HMR(LIQUID)=-5239          7.2760E-12  5.00E+02   5239.       10.48    *
114 HMR(LIQUID)=-5454         -3.6380E-12  5.00E+02   5454.       10.91    *
115 HMR(LIQUID)=-5233          1.8190E-12  5.00E+02   5233.       10.47    *
116 HMR(LIQUID)=-4575         -1.8190E-12  5.00E+02   4575.       9.150    *
117 HMR(LIQUID)=-3481         -1.8190E-12  5.00E+02   3481.       6.962    *
118 HMR(LIQUID)=-1950           0.000      5.00E+02   1950.       3.900


PARROT:
```

The experiments for which the optimization has not found a good fit are marked with an asterisk (*) or a hash sign (#) in the rightmost column. An asterisk in this column indicates that the experiment has an error that is larger than the error tolerance and a hash sign indicates that the error is much larger. The error tolerance depends on the degree of accuracy set for that particular piece of experimental information. The error values are presented in the next to rightmost column.

Note that if you are optimizing in *alternate mode*, then you usually do not need to change the weights for the experiments. Instead, you can simply run OPTIMIZE_VARIABLES again, specifying, say, thirty iterations, evaluate the results again, and continue in that way until you are satisfied with the results.

About Alternate Mode

The Critical Set of Experiments

The set of weighted experiments that you end up with as a result of your optimization is referred to as the *critical set* of experiments. When you work to determine this set and the weights of the experiments, the following factors should be reflected in both the selection of experiments and the weights of those experiments:

- The reliability of the experimental technique.
- The extent of agreement/disagreement between independent measurements of the same quantity.
- The extent of agreement/disagreement between data obtained with different experimental methods.

Continuing the Optimization and Resetting Variables

To continue the optimization after you have used OPTIMIZE_VARIABLES, you can either use this command and enter `<Number of iterations>` again or CONTINUE_OPTIMIZATION `<Number of iterations>`.

If you use CONTINUE_OPTIMIZATION, then PARROT continues the optimization using the same Hessian matrix. If the optimization is going well but you run out of iterations, then continuing with the same Hessian matrix may be useful.

As before, use LIST_RESULT to inspect the fit between the calculated and the experimental values for your experiments. If necessary, adjust the weights of the experiments again in the ED_EXP module. You may even discover that you have to exclude additional experiments from the optimization.

Besides looking at the rightmost column in the list of experiments (that is produced when you use LIST_RESULT), it is also useful to look at the *sum of squares* of the errors of all the variables. This is shown in the output of OPTIMIZE_VARIABLES and CONTINUE_ OPTIMIZATION. This sum should be as low as possible.

The following shows part of the output that you get when using LIST_RESULT:

```
 == OPTIMIZING VARIABLES ==

 AVAILABLE VARIABLES ARE V1  TO V00

 VAR.   VALUE            START VALUE      SCALING FACTOR    REL.STAND.DEV
 V1      6.94641846E+05   4.30000000E+04   4.30000000E+04   1.42299558E+00
 V2     -3.32619842E+02  -3.52000000E+01  -3.52000000E+01   7.91369573E-01
 V11     8.37422071E+04   7.20000000E+04   7.20000000E+04   2.02212692E-01
 V13     2.65253341E+04   2.70000000E+04   2.70000000E+04   1.45201828E-01
 V17    -3.66637428E+05  -1.00000000E+05  -1.00000000E+05   8.04279315E-01

 NUMBER OF OPTIMIZING VARIABLES :   5
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
 THE SUM OF SQUARES HAS CHANGED FROM   3.50196879E+05 TO   3.49096720E+05
 DEGREES OF FREEDOM   14.  REDUCED SUM OF SQUARES   2.49354800E+04
```

In the example you can see that the sum of squares have decreased slightly. (The final sum of squares that you get after an optimization run is also presented directly in the output from OPTIMIZE_VARIABLES and CONTINUE_OPTIMIZATION.) As long as the sum of squares figure is decreasing, the optimization is working as it should.

When your calculated results have been improving for a while, that is, when the sum of squares has been decreasing, and you are confident that you are making definitive progress, then you should use the PARROT command RESCALE_VARIABLES to reset the starting values of the optimizing variables to their current values. When you do this, the start values and scaling factors of the optimizing variables (shown in the table’s third column in the preceding screen shot), are all set to the current values (shown in the table’s second column).

If your optimization is not going well, then you may want to reset the values of your optimization variables to their current start values. To do this, use RECOVER_VARIABLES.

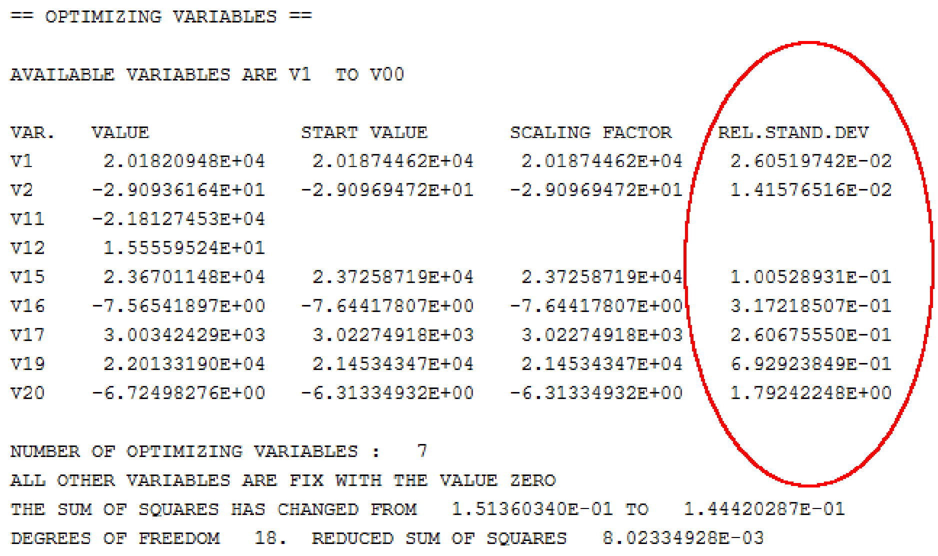
After rescaling the variables, continue the optimization using OPTIMIZE_VARIABLES again. Cycle through calls of the commands OPTIMIZE_VARIABLES/CONTINUE_OPTIMIZATION, CONTINUE_OPTIMIZATION, RESCALE_VARIABLES and OPTIMIZE_VARIABLES again until your set of optimizing variables does not seem to improve anymore. Even when it seems to you that you have reached this point, it is recommended that you use OPTIMIZE_VARIABLES/CONTINUE_OPTIMIZATION a few extra times to make sure that the variable values cannot be further improved, that is, that the sum of squares of the errors of all the variables cannot be reduced further. If the final solution is repeatedly calculated after the same number of iterations and reaching the same result, then it is generally reasonable to accept the current variable values.

Updating the Set of Optimizing Variables

Besides evaluating the fit between the calculated results and the experimental data, you should also ensure that you have the right number of optimizing variables. If you have too many or too few optimizing variables, then you may not be able to use your model to accurately extrapolate thermodynamic properties in a wide range of temperature, pressure and composition conditions.

With more optimization parameters, the sum of errors usually decrease, but the parameters also tend to become less precisely determined. A measure of this precision is the Relative Standard Deviation (RSD) of each optimizing variable. However, the RSD is only significant if you have used RESCALE_VARIABLES followed by an optimization which converges and the values of the variables do not change much. The RSD tells you how much the parameter can be changed in either a positive or in a negative direction without changing the reduced sum of errors with more than one unit.

A large RSD value thus means that the parameter has not been determined well.



```
== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1  TO V00

VAR.   VALUE             START VALUE       SCALING FACTOR    REL.STAND.DEV
V1      2.01820948E+04    2.01874462E+04    2.01874462E+04    2.60519742E-02
V2     -2.90936164E+01   -2.90969472E+01   -2.90969472E+01    1.41576516E-02
V11    -2.18127453E+04
V12     1.55559524E+01
V15     2.36701148E+04    2.37258719E+04    2.37258719E+04    1.00528931E-01
V16    -7.56541897E+00   -7.64417807E+00   -7.64417807E+00    3.17218507E-01
V17     3.00342429E+03    3.02274918E+03    3.02274918E+03    2.60675550E-01
V19     2.20133190E+04    2.14534347E+04    2.14534347E+04    6.92923849E-01
V20    -6.72498276E+00   -6.31334932E+00   -6.31334932E+00    1.79242248E+00

NUMBER OF OPTIMIZING VARIABLES :    7
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM   1.51360340E-01 TO   1.44420287E-01
DEGREES OF FREEDOM   18.  REDUCED SUM OF SQUARES   8.02334928E-03
```

If such a significant RSD has a value larger than 1, then this typically means that you are using too many optimizing variables. However, the RSD values also depend on the weighting of the experiments, so it is sometimes possible to reduce the RSD by changing weights.

The RSD should not be too low either. If one or more of them is very close to 0, then this suggests that you are trying to optimize the system with too few optimizing variables. You can add optimizing variables interactively using ENTER_PARAMETER in GIBBS. However, it is recommended that you add a sufficient number of variables in the setup file from the start so that do not need to do this. You can fix variables to a value of 0 until you discover that they are needed.

Besides the RSD, you should also keep an eye on the variable values themselves (shown in the VALUE column, next to the leftmost column in the table shown in the preceding screenshot). If the value of a variable is in the order of 1E5 or higher and this variable has been put in the temperature-independent part of an interaction parameter’s Gibbs energy expression, then you may not have the right weights on your experiments or you are using too many optimizing variables. This is also typically the case if a variable with a value in the order of 10 or more (per mole atoms) is in the temperature-dependent part of the Gibbs energy expression of an interaction parameter. Such a high parameter value may lead to inverted miscibility gaps or re-stabilisation of a phase at high temperature. It is important to keep an eye on this since the temperature-independent and the temperature-dependent interaction parameter often varies together. If the temperature-dependent interaction parameter cannot be reliably determined, you may have to fix its value.

Note that even if you have found a good enough fit between calculated and experimental values after an optimization run, a parameter value may suddenly start to change by several orders of magnitude when you use OPTIMIZE_VARIABLES is used again. If this happens, then careful reconsideration of the weighting of the experiments of the set of optimizing variables is required. However, when the optimization has converged and the parameter values remain stable after repeated use of OPTIMZE_VARIALBES, this should usually not happen.

Reducing the Number of Optimizing Variables

If you have one or more optimizing variables with RSD larger than 1, then you should remove one or more of the variables by setting them to a value of 0, or alternately, set them to a reliably estimated value (estimated based on, for example, semi-empirical methods).

To fix an optimizing variable to certain value, use the PARROT command SET_FIX_VARIABLE `<variable number> <value>`.

Plotting Intermediate Results

It is typically not sufficient to look at the plain text output of LIST_RESULT to reliably judge how the optimization is progressing. Plotting a phase or property diagram of the system you are optimizing using the POLY and POST modules is often very useful.

It is recommended that you create a macro file for plotting the diagram since you probably want to repeatedly plot the diagram as you progress with the optimization. This macro file can then be called directly from the PARROT module with the MACRO_FILE_OPEN command.

Superimposing Experimental Data from EXP Files

If you create one or several EXP files based on the experiments in your POP file, you can visually compare the fit your plot and the experimental data you are optimizing the system against. An EXP-file contains data points specified in the DATAPLOT format. You could make an EXP-file for each type of data that you are using in the optimization.

Use the POST command APPEND_EXPERIMENTAL_DATA to superimpose the data points in an EXP-file on a phase or property diagram that you have plotted. For example, to put the experimental data points from a file entitled DP.EXP onto a plotted diagram, you could enter the following:

```
APPEND_EXPERIMENTAL_DATA Y DP.EXP 0 1
```

Such a command call tells Thermo-Calc to superimpose the data points in dataset 1 of DP.EXP onto the plot in the Console Results window, but not to impose any information about axis scaling, labels and other information which is normally found in the prologue of the DP.EXP file.

The POST command QUICK_EXPERIMENTAL_PLOT can also be used to superimpose data points on a plotted phase or property diagram.

? *DATPLOT User Guide* included with this documentation set.

Finalizing the Optimization

In this section:

Finishing the Optimization

When to stop optimizing is a matter of judgment. It is rarely the case that you finish optimizing a system with the feeling that it cannot be improved.

The final step is to update your files with the final results. Besides updating your database file (or alternatively, creating a new database file), it is advised that you also update your setup and POP files with the final weights and optimizing variable values.

Rounding off Optimizing Variable Values

When you save the optimizing variable values, it is important that you round off the values correctly. When you have a metallic system, it is usually best to keep whatever number of decimal digits that you need to make less than one J/mol difference at 1000 K. When you have an aqueous system or a system that you are optimizing based on data from very different temperature ranges, then this is not always the only appropriate guideline. However, rounding off the values in such a way that it gives a difference that is larger than one J/mol may lead to differences in the phase diagram.

Another approach you can take when rounding off variable values is by progressively fixing the value of more and more of the variables. This allows you to round-off all but one of the variables values so that each only has a few significant digits. Variables whose values have been rounded off in this way are easier to handle compared with those that that are rounded off so that they continue to have many significant (non-zero) digits.

To round off the variable values according to this second approach, first use SET_FIX_VARIABLE to set the variable(s) with the highest RSD to a rounded off value (such as, say, 0.4). When you then re-optimize using OPTIMIZE_VARIABLES, the sum or errors changes. However, you should get almost exactly the same sum of errors as before after you rescale the variable values using RESCALE_VARIABLES. (If the sum of errors is different, then this means that the variable with the highest RSD was not rounded off in a good way.) If you successfully round off the first variable value, then continue to round of the optimizing variable which now has the highest RSD. Continue doing this until you have fixed all but one of the optimizing variables to their rounded-off values. The final sum of errors that you get after having fixed the variable values should not deviate significantly from the initial sum of errors you had before starting to round-off the variable values.

Updating the Database File

About the Database Files

To update the database file (with filename extension TDB) open it in a text editor and enter or update each of the parameters that you have optimized.

For example, suppose you have the following command in your setup file:

```
ENTER_PARAMETER L(IONIC_LIQ,AL+3,ZR+4:O-2;0) 298.15  +V17; 6000 N
```

If you then end up with a value for optimizing variable V17 of -100000, then you should enter the following under the IONIC_LIQ phase in the database file:

```
PARAM L(IONIC_LIQ,AL+3,ZR+4:O-2;0) 298.15 -100000; 6000 N REF !
```

If you often need to round-off the optimizing variable value in some way, see Rounding off Optimizing Variable Values.

When you have updated or entered the parameters that you optimized, save the database file.

Creating a Database File

In some circumstances you may want to save all the information about your system into a new database file. To do this, go to the GIBBS module and use LIST_DATA `<Filename> N`. This creates a new user database file that contains all the information about the system that is in the workspace.

The N-argument tells the LIST_DATA command to save the output into database file rather than some other type of file, such as a macro file for example. Note that the output database file that you get from LIST_DATA have to undergo some manual editing before it can be used as proper database file.

Updating the Setup File and the POP file

It may be useful for you to be able to recreate your optimization from scratch. It is therefore recommended that you do the following when you are done with the optimization:

- Update your POP file so that it contains the weights of your critical set of experiments. Use SET_WEIGHT to set the weights directly in the POP file. You may also have to use SET_START_VALUE for some conditions in the POP file. Otherwise, you may not be able to compute the equilibria with .
- Copy the final values of your optimizing variables and set them as start values of the variables in the setup macro file (with SET_FIX_VARIABLE).

It is important that you round off the values of the optimizing variables correctly. See Rounding off Optimizing Variable Values. When you have done this, you can run the setup macro file to recreate the final result of the optimization.

Alternate Mode

In this section:

About Alternate Mode

To turn Alternate Mode ON or OFF, use the PARROT command SET_ALTERNATE_MODE.

When you have one or more multi-phase equilibria (that is, with the fixed phase-status) in your POP file and the optimizing values lack appropriate starting values (such as the default value of 0 for example), then Thermo-Calc may not be able to compute the equilibria for the experiments. In these cases, a common tangent cannot be found, that is, a state where the chemical potentials for all components are the same in all phases cannot be found. A common tangent may not exist or it be found at the wrong composition or temperature given the initial set of model parameters.

If you are not able to estimate reasonable starting values for the optimizing variables, then this problem can be overcome by initially running your optimization in alternate mode. The alternate mode in PARROT module should help you find reasonable starting values for the optimizing variables. Note that you are only supposed to use alternate mode in the beginning of the optimization. Once you have achieved a reasonable fit between calculated results and experimental data, turn off alternate mode and calculate all equilibria again in the normal mode.

In alternate mode, PARROT modifies multi-phase equilibria so that the chemical potentials for each stable phases is calculated separately. For example, consider the following experimental equilibrium:

```
CREATE_NEW_EQUILIBRIUM 1 1

CHANGE_STATUS PHASE LIQ FCC=FIX 1

SET_CONDITION T=1000 P=1E5

EXPERIMENT X(LIQ,B)=.2:.01 X(FCC,B)=.1
```

When PARROT optimizes in alternate mode, the computation of this equilibrium is done by way of the following two calculations:

```
CHANGE_STATUS PHASE LIQ=FIX 1

SET_CONDITION T=1000 P=1E5 X(LIQ,B)=.2

CHANGE_STATUS PHASE FCC=FIX 1

SET_CONDITION T=1000 P=1E5 X(FCC,B)=.1
```

The difference between the chemical potentials in every pair of phases is calculated and PARROT tries to adjust the parameters of the phases so that these differences are minimized. In other words, PARROT tries to make the chemical potentials equal in all phases. For PARROT to be able to do this, some additional information about the experimental multi-phase equilibria is required, at least for all invariant equilibria.

Optimizing in Alternate Mode

When you are optimizing in the alternate mode, you usually do not need to enter the ED_ EXP module and manually change the weights of experiments that the computed results have not been fitted well with. Instead, after using OPTIMIZE_VARIABLES initially with no iterations, and listing the result with LIST_RESULT, simply run OPTIMIZE_VARIABLES again specifying, say, thirty iterations. Continue to optimize until your optimization seems to be going in the right direction, then set the optimizing variables’ starting values to their current values use RESCALE_VARIABLES before you turn alternate mode off by answering N at the SET_ALTERNATE_MODEprompt.

Preparing the POP File for Alternate Mode

Information in your POP file that concerns equilibria with ENTERED or DORMANT phases is ignored when you optimize in alternate mode.

To use the alternate mode, ensure that there is enough information about each phase in a given equilibrium. In addition to the temperature and pressure of the system, you should specify the composition of all phases in a given equilibrium. This is done with, SET_CONDITION, EXPERIMENT, or SET_ALTERNATE_CONDITION.

If both compositions of a binary tie-line have been measured, then you could specify this in the POP file in the following way:

```
CREATE_NEW_EQUILIBRIUM 1 1

CHANGE_STATUS PHASE FCC BCC=FIX 1

SET_CONDITION P=1E5 T=1000

EXPERIMENT X(BCC,B)=.2:.01 X(FCC,B)=.3:.01
```

This equilibrium could be calculated with alternate mode without any modification. The compositions specified with the experiment command is used as condition when the thermodynamic properties of each phase are calculated.

Examples of SET_ALTERNATE_CONDITION

The following topics demonstrate how SET_ALTERNATE_CONDITION is used to prepare different kinds of equilibria for optimization in alternate mode.

Specify the Composition of One Side of a Binary Tie-Line

If only one side of the tie-line has been measured, then you must provide an estimate of the composition of the other phase. You can make such an estimate with SET_ALTERNATE_CONDITION. This command has no effect unless alternate mode is turned on. The equilibrium described could thus be specified in the following way:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE FCC BCC=FIX 1
SET_CONDITION P=1E5 T=1000
EXPERIMENT X(BCC,B)=.2:.01
SET_ALTERNATE_CONDITION X(FCC,B)=.3
```

When the alternate mode is turned on, the composition given by the SET_ALTERNATE_CONDITION command is used for the FCC phase. The properties of the BCC phase is calculated using the composition specified by experiment as a condition.

Specify the Compositions of a Three-Phase Equilibrium

If you have a three-phase equilibrium in your POP file, then one of its compositions can be specified as experimentally determined, while two can be provided as alternate conditions:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE FCC BCC LIQ=FIX 1
SET_CONDITION P=1E5
EXPERIMENT T=912:5 X(LIQ,B)=0.2:.02
SET_ALTERNATE_CONDITION X(FCC,B)=0.1 X(BCC,B)=.4
```

Specify the Composition of a Stoichiometric Phase

When you specify the composition of stoichiometric phase with SET_ALTERNATE_CONDITION, the value must be given with at least seven decimal digits, as in the following example:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE LIQ A2B=FIX 1
```

```
SET_CONDITION P=1E5 X(LIQ,B)=0.2
EXPERIMENT T=992:5
SET_ALTERNATE_CONDITION X(A2B,B)=.6666667
```

Entering Other Experiments in the POP with Alternate Mode

The following table shows some additional examples of how to enter different kinds of experiments in the POP file when you are using the alternate mode.

Example	ED_EXP commands
Two-phase equilibrium: The melting temperature of an Au-Cu alloy	`CHANGE_STATUS PHASE LIQUID FCC=FIX 1 SET_CONDITION X(FCC,CU)=0.14 P=1E5 EXPERIMENT T=970:2 SET_ALTERNATE_CONDITION X(LIQUID,CU)=0.16`
Invariant equilibrium experiment: A three-phase equilibrium in a binary system	`CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC BCC LIQUID=FIX 1 SET_CONDITION P=1E5` `EXPERIMENT T=912:5 SET_ALTERNATE_CONDITION X(FCC,B)=0.1SET_ALTERNATE_CONDITION X(BCC,B)=0.4SET_ALTERNATE_CONDITION X(LIQ,B)=0.2`
Ternary system, with two compositions measured (both with uncertainty 0.02)	`CREATE_NEW_EQUILIBRUM 1 1 CHANGE_STATUS PHASE FCC BCC=FIX 1 SET_CONDITION T=1273 P=1E5 SET_CONDITION X(FCC,B)=0.1:0.02 EXPERIMENT X(FCC,C)=0.12:.02 SET_ALTERNATE_CONDITION X(BCC,B)=0.17 SET_ALTERNATE_CONDITION X(BCC,C)=0.07`

Troubleshooting

During an optimization, you are likely to run into many different problems and challenges. This topic gives some general guidelines that can help avoid common mistakes and problems.

In this section:

Useful Guidelines

The following rules of thumb are generally good to adhere to when you are planning and executing an optimization:

- Do not use data from thermochemical tables of unknown origin.
- Use experimentally determined properties; avoid converted quantities.
- Carefully estimate the accuracy of the experiments.
- Correct systematic errors (by adjusting a temperature scale for example).
- Use negative information such as, for example, the information that a phase should not be stable in a composition or temperature region.
- With a hundred activity measurements in a system but only ten composition points from the phase diagram, it is often appropriate to decrease the weights on the activity experiments.
- If you initially exclude any intermediate phases to only optimize the liquid and the terminal or end-member phases for the pure components, then it is often useful to compute a metastable phase diagram with just these phases. In the metastable phase diagram, the metastable solubility lines should not have any strange kinks or turns. Such a diagram is often also useful to compute at later stages in the optimization.
- When you have fitted the liquid phase and some solution phases reasonably well, then you can fix the optimizing variables that characterise these phases. You can then go on and optimize the variables for the intermediate phases.
- Phases with miscibility gaps are always difficult to optimize. Try to keep control of the miscibility gaps by using real or estimated experimental information. (Note that it is not possible to calculate the top of a miscibility gap as a single equilibrium.)
- Phases with order/disorder transformation are often difficult to optimize. It may be difficult to find the right start values on the optimizing variables. The TABULATION module can be useful sometimes. Properties for specified site fractions can be calculated in the TABULATION module. This is not possible in the POLY module since this module only calculates for equilibrium site fractions. The ordered state may also disappear during the optimization of these phases. If this happens, you may be able to add an experiment that controls the state of order.
- Only use the alternate mode to find an initial set of model parameters that can then be make it possible to calculate the experimental equilibria in the normal mode.
- When you have achieved a satisfactory fit between calculated results and experimental data with an appropriate number of optimization variables, perform a couple of final optimization runs to make sure that your results are stable.

- Make sure that the values of the optimizing variables keep within a reasonable range. If a variable starts to change several orders of magnitudes, then you must consider whether you have the right weights on the experiments and whether you are using too many optimizing variables.

Excluding and Including the Correct Equilibria

Use as few experiments as possible initially to get a reasonable overall fit. It is generally best to first focus on the invariant equilibria, as well as metastable states that can be estimated by excluding some phases. Crucially, any experiments for which the computed results are clearly faulty should be excluded from the final critical set, while all important invariant equilibria are calculated and included in this critical set.

If you cannot compute some invariant equilibria with intermediate phases, then it may be best to first exclude those phases from the optimization and only optimize the liquid and the most important solution phases. After you have obtained reasonable results for these phases, you can enter the intermediate phases back in again. With the variables for the optimized liquid and solid phases set fixed, you can finally optimize the intermediate phases.

Conflicting Data

It is important that you do not include conflicting sets of data at the same time during an optimization. After all, if they are genuinely conflicting, then at least one of the sets must be incorrect. If you have conflicting sets of data, then only use one of these sets at a time together with the rest of the data. Often, the optimization makes it clear which dataset coheres best with the other information that is available about the system.

Sometimes, conflicting data cannot be detected directly. For example, you may have activity data which is inconsistent with solubility data from the phase diagram. This would be indicated by large errors in the fit when both the activity data and the solubility data are included. To find these inconsistencies, let alone correct the errors, you may thus have to optimize with some datasets excluded.

Experiments and Experimental Data

These topics contain examples of different kinds of equilibria in different kinds of systems. They are intended to help you figure out how to use various kinds of experimental data when creating POP files. The topics that follow contain examples how to enter various kinds of experimental data into a POP file.

In this section:

Phase Diagram Data

P-T-X phase diagram data for binary and ternary systems, or systems of even higher order can be used in the POP file. This includes data of the following types:

- Data about the temperature- and composition-dependence of various properties (obtained from differential thermal analysis (DTA) measurements for example), including enthalpy, lattice parameter, dilatometric length, electronic conductivity and magnetic susceptibility;
- Data about reaction types (invariant/monovariant) and phase relations obtained from qualitative or quantitative metallographic studies;
- Data about phase amounts or compositions obtained from microprobe measurements (using X-ray spectroscopy or transmission electron microscopy (TEM));
- Data about the positions or directions of two-phase tie-lines and three-phase equilibria for ternary systems.

The following table shows a POP file excerpt that demonstrates how some kinds of phase diagram data can be entered.

Example	ED_EXP commands

Solidus (melting temperature) of an Au-Cu alloy	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE LIQUID FCC=FIX 1`
	`SET_CONDITION X(FCC,CU)=0.14 P=1E5`
	`EXPERIMENT T=970:2`

Three-phase equilibrium in a binary A-B system	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE FCC BCC LIQUID=FIX 1`
	`SET_CONDITION P=1E5`
	`EXPERIMENT T=912:5`

Congruent transformation in a binary A-B system	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE BCC LIQUID=FIX 1`
	`SET_CONDITION P=1E5 X(BCC,B)-X(LIQ,B)=0`
	`EXPERIMENT T=1213:10`

Tie-line in a ternary A-B-C system	An uncertainty factor is set not only for the experimental measurement, but also for the X(FCC,B) condition. The factor is 0.02.
	`CREATE_NEW_EQUILIBRUM 1 1`
	`CHANGE_STATUS PHASE FCC BCC=FIX 1`
	`SET_CONDITION T=1273 P=1E5 X(FCC,B)=0.1:0.02`
	`EXPERIMENT X(FCC,C)=0.12:.02`

Data for Individual Compounds

You can use data about individual components in the POP file. Such data includes activity, heat capacity, heat content, entropy, Gibbs energy of phase transformations, heat of transition, and heat of melting.

Example	ED_EXP commands
Carbon activity data in the fcc phase	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC_A1=FIX 1 CHANGE_STATUS PHASE GRAPHITE=D SET_REFERENCE_STATE C GRAPHITE,,,, SET_CONDITION P=101325 T=1273 X(MN)=0.03 SET_CONDITION X(C)=0.03 EXPERIMENT ACR(C)=0.29:5%
Ln(activity coefficient for O)	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE IONIC_LIQ=FIX 1 CHANGE_STATUS PHASE GAS=D SET_CONDITION X(O)=0.02 T=1523 P=101325 SET_REFERENCE_STATE O GAS,,,, ENTER_SYMBOL FUNCTION LNFO=LOG(ACR(O)/X(O)); EXPERIMENT LNFO=-1.5:0.01
Entropy at 298.15 K of Cu_2O	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE CU2O=FIX 1 CHANGE_STATUS PHASE CUO=FIX 0 SET_CONDITION P=101325 T=298.15 EXPERIMENT S=92.36:1
Gibbs energy of formation of $NiAl_2O_4$	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE SPINEL=ENT 1 CHANGE_STATUS PHASE FCC O2GAS=DORM SET_REFERENCE_STATE NI FCC,,,, SET_REFERENCE_STATE AL FCC,,,, SET_REFERENCE_STATE O O2GAS,,,, SET_CONDITION P=101325 T=1000 N(NI)=1 N(AL)=2 SET_CONDITION N(O)=4 EXPERIMENT GM=-298911:5%
Heat capacity of $MgFe_2O_4$	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE SPINEL=ENT 1 SET_CONDITION P=101325 N(FE)=2 N(MG)=1 N(O)=4 SET_CONDITION T=800

Example	ED_EXP commands
	`ENTER_SYMBOL FUNCTION CP=H.T;` `EXPERIMENT CP=207:5%`

Heat content (H-H_{298}) for $MnFe_2O_4$	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE SPINEL=ENT 1`
	`SET_CONDITION P=101325 T=298.15 N(MN)=1 N(FE)=2`
	`SET_CONDITION N(O)=4`
	`ENTER_SYMBOL VAR H298=H;`
	`ENTER_SYMBOL FUN HMNFE2O4=H-H298;`
	`CREATE_NEW_EQUILIBRIUM 2 1`
	`CHANGE_STATUS PHASE SPINEL=ENT 1`
	`SET_CONDITION P=101325 N(MN)=1 N(FE)=2 N(O)=4`
	`SET_CONDITION T=400`
	`EXPERIMENT HMNFE2O4=16610:5%`

Single Phase Mixing Enthalpies or Partial Enthalpies

You can use calorimetric data for mixing in the POP file. This data could be the result of, for example, drop calorimetry or scanning calorimetry. This includes data about, for example, enthalpy of mixing of liquids, series of mixing-enthalpy and about partial enthalpy. Information about enthalpies of mixing can also be derived from theoretical principles using special quasi-random structures (SQSs).

Example	ED_EXP commands

Enthalpy of mixing in the liquid state of an Au-Cu alloy	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE LIQUID=FIX 1`
	`SET_CONDITION T=1379 P=1E5`
	`SET_CONDITION X(LIQUID,AU)=0.0563`
	`SET_REFERENCE_STATE AU LIQ * 1E5`
	`SET_REFERENCE_STATE CU LIQ * 1E5`
	`EXPERIMENT HMR=-1520:200`

Enthalpies of Formation and Enthalpies of Reactions

You can use calorimetric data for phase transformations in the POP file. This data could be the result of, for example, direct-reaction calorimetry, solution calorimetry or combustion calorimetry. Information about enthalpies of formation can also be derived from theoretical principles.

Example	ED_EXP commands

Enthalpy of melting of the eutectic in the Al2O3-ZrO2 binary (J/g)	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE CORUNDUM ZRO2_TETR=FIX 0`
	`CHANGE_STATUS PHASE IONIC_LIQ=ENT 1`
	`SET_CONDITION P=101325 N=1 LNAC(O)=-80`
	`SET_REFERENCE_STATE ZRO2 TETR,,,,,,`
	`SET_REFERENCE_STATE AL2O3 CORUND,,,,,,`
	`EXPERIMENT HWR=1080:90`

Enthalpy of formation of o-CaZrO3 from the component oxides	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE ZRO2_MONO HALITE CAZRO3_O=ENT 1`
	`SET_CONDITION T=298.15 P=101325 N(CAO)=.5`
	`SET_CONDITION N(ZRO2)=.5 LNAC(O)=-20`
	`SET_REFERENCE_STATE CAO HALITE,,,,`
	`SET_REFERENCE_STATE ZRO2 ZRO2_MONO,,,,`
	`EXPERIMENT HMR(CAZRO3_O)=-15960:5%`

Chemical Potentials via EMF Measurements

You can use chemical potentials and activities/activity coefficients from electromagnetic field (EMF) measurements in the POP file.

Example	**ED_EXP commands**

Emf data on Cu(s)/Cu2O(s)	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE FCC CU2O=FIX 1`
	`CHANGE_STATUS PHASE O2GAS=DORM`
	`SET_CONDITION P=101325 T=1000`
	`SET_REFERENCE_STATE O O2GAS,, 100000`
	`EXPERIMENT MUR(O)=-95387:1000`

Driving Force for Metastable Phases

You can use chemical driving forces for metastable phases in the POP file.

Example	ED_EXP commands

To prevent BCC_A2 to be stable	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE FCC_A1 M7C3 M23C6=FIX 1`
	`CHANGE_STATUS PHASE BCC_A2=D`
	`SET_CONDITION P=101325 T=1473`
	`EXPERIMENT DGM(BCC)<-0.1:0.1`

To promote CEMENTITE to be stable	`CHANGE_STATUS PHASE BCC M7C3 GRAPHITE=FIX 1`
	`CHANGE_STATUS PHASE CEMENTITE=DORMANT`
	`SET_CONDITION P=P0 T=973`
	`EXPERIMENT DGM(CEM)>0.1:0.01`

Pressure-Temperature-Volume EOS Data

You can use Pressure-Temperature-Volume Equation of State (EOS) data in the POP file. Such data includes, for example, molar volume, density, thermal expansion and bulk modulus/compressibility.

Example	ED_EXP commands

Volume of liquid Pt	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE LIQUID=ENT 1`
	`SET_CONDITION P=101325 N=1 T=1873`
	`EXPERIMENT VM=1.00758E-5:5%`

Thermal expansion	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE FCC_A1=ENT 1`
	`SET_CONDITION P=101325 N=1 T=400`
	`ENTER_SYMBOL FUNCTION ALPHA=VM.T/VM/3;`
	`EXPERIMENT ALPHA=2.35E-5:5%`

Crystal Structure, Lattice Parameters, and Site-Occupancy

You use information about defects, ordering or site occupancy, as well as information about crystal structures in the form of lattice parameter values. This information may come from measurements made by X-ray, neutron diffraction, Mössbauer spectroscopy or perturbed angular-correlation.

Example	ED_EXP commands

Lattice parameter for fcc	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE FCC_A1=ENT 1`
	`SET_CONDITION P=101325 N=1 T=298.15`
	`SET_CONDITION X(CR)=0.05`
	`ENTER_SYMBOL FUNCTION LPFCC=((4*VM/6.02214179E23)**(1/3))*1E10;`
	`EXPERIMENT LPFCC=4.02:5%`

Lattice parameter for bcc	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE BCC_A2=ENT 1`
	`SET_CONDITION P=101325 N=1 T=298.15`
	`SET_CONDITION X(AL)=0.08`
	`ENTER_SYMBOL FUNCTION LPBCC=((2*VM/6.02214179E23)**(1/3))*1E10;`
	`EXPERIMENT LPBCC=2.90:5%`

Site-occupancy, degree of inversion for spinel	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE SPINEL=ENT 1`
	`SET_CONDITION P=101325 N(MG)=1 N(AL)=2 N(O)=4`
	`SET_CONDITION T=1073`
	`EXPERIMENT Y(SPINEL,AL+3#1)=0.31:5%`

Magnetism and Other Atomistic Properties

You can use data about atomistic properties such as magnetism and Curie temperatures in the POP file.

Example	ED_EXP commands

Curie temperature of MnxFe3-xO4, x=1.26	`CREATE_NEW_EQUILIBRIUM 1 1`
	`CHANGE_STATUS PHASE SPINEL=ENT 1`
	`SET_CONDITION  T=520 P=101325 N(O)=4`
	`SET_CONDITION N(FE)+N(MN)=3 N(MN)=1.26`
	`EXPERIMENT TC(SPINEL)=520:5`

Data About Systems of Different Orders

You might want to use data about systems of different orders in the same optimization, such as data about a binary equilibrium with components A and B in a ternary system with components A, B and C, together with data about equilibria in the binary system with components A and B. To do this, you must first suspend all components in the ternary system (A, B and C), and then set the two components you want binary information on (A and B) to status `ENTERED`.

Suspending all components is done by giving the initialization code 0 to the CREATE_NEW_ EQUILIBRIUM command. The components about which you want to use binary information must then be entered again using the CHANGE_STATUS command.

Example	ED_EXP commands

A binary (A-B) three-phase equilibrium (FCC-BCC-LIQ) in a ternary system (A-B-C)	`CREATE_NEW_EQUILIBRIUM 1 0`
	`CHANGE_STATUS COMPONENT A B = ENTERED`
	`CHANGE_STATUS PHASE FCC BCC LIQ=FIX 1`
	`SET_CONDITION P=1E5`
	`EXPERIMENT T=1177:10`

Thermodynamic Models

The most common models used in assessments are described briefly in these topics. Examples of how to write the phase definitions in the setup-file are also given for each of these models. In addition to the models described here, a large number of thermodynamic models for various phases in different states have been implemented.

In this section:

Gas

The gaseous mixture phase is usually treated as a substitutional phase without sublattice. In the gaseous mixture phase, there are usually molecules formed, and the number of constituents of the gas phase is often much larger than the number of elements. These complex constituents have to be defined as species. The ideal gas model may handle a gas phase under low pressures (and low temperatures). This implies that the P-V-T relations and thermodynamic properties of pure gaseous species are calculated as for ideal gas, and that there is interaction between gaseous species in the mixture. In a defined system, there may only exist one gaseous mixture phase. Type code `G` is used for the gas phase:

```
ENTER_PHASE GAS G, 1 H,H1O1,H1O2,H2,H2O1,H2O2,O,O2,O3; N N
```

Compound Energy Formalism (CEF)

If the atoms are sufficiently different in size, electronegativity or charge, they may prefer different types of sites in the lattice of crystalline solids. In some cases, a solute atom may even occupy interstitial sites between the normal lattice sites. All such phenomena are treated in Thermo-Calc by the sublattice concept. The Compound Energy Formalism (CEF) has proved to be the most general formalism for many different types of solution phases. It is therefore by default applied to various solid solution phases in the Thermo-Calc software package. CEF can also take ionic constraints (charged cation/anion species) into account. For a comprehensive description on the CEF, please see Hillert (2001), Frisk and Selleby (2001), Sundman and Ågren (1981).

Since the CEF is used by default, no special notation is needed in the phase definition, except for ionic phases, where type code `I` is given.

Examples of phase definitions in a setup-file using the CEF:

```
ENTER_PHASE SPINEL I, 4 1 2 2 4

     FE+2,FE+3; FE+2,FE+3,VA; FE+2,VA; O-2; N N

ENTER_PHASE SIGMA, 3 10 4 16

     AL,CO,CR,FE,NB; AL,CO,CR,FE,NB; AL,CO,CR,FE,NB; N N

ENTER_PHASE FCC_A1, 2 1 1

     CR,FE,MN; C,N,VA; N N

ENTER_PHASE BCC_A2, 2 1 3

     CR,FE,MN,VA; C,N,VA; N N
```

Substitutional Liquid

The liquid phase is normally (but not always) modeled as a substitutional phase with no sublattice, which is occupied by two or more constituents. The constituents are normally the elements, but molecules or associates can also be used. Type code `L` is used for the liquid phase.

```
ENTER_PHASE LIQUID L, 1

     AL,C,CR,FE,MO,NI,SI ;  N N

ENTER_PHASE LIQUID L, 1

     C,FE,FEO,FEO3/2,NI,NIO ;  N N
```

Ionic Two-Sublattice Liquid Model

Within the framework of the CEF, the ionic two-sublattice liquid (I2SL) model was developed to be used when there is a tendency for ionization in the liquid, which happens in liquid oxides and sulphides for example. The same model can be used both for metallic and oxide melts. At low levels of oxygen, the model becomes equivalent to a substitutional solution model between metallic atoms. Two sublattices are assumed, one containing charged cations and one containing charged anions, neutrals and vacancies. The complication for an ionic liquid is that the numbers of sites on the cation sublattice and anion sublattice vary with the composition to preserve electroneutrality. For a comprehensive description on the I2SL model, see [1985Hil; 1991Sun]. In these references, the possible excess parameters are also discussed. Type code `Y` is used for the I2SL model.

Examples of phase definitions in a setup-file:

```
ENTER_PHASE LIQUID Y,
     AL+3,CR+2,FE+2,NI+2; VA; N N
ENTER_PHASE IONIC_LIQ Y,
     CA+2,MG+2; O-2; N N
ENTER_PHASE IONIC_LIQ Y,
     AL+3,CA+2,FE+2,MG+2,SI+4;
     ALO2-1,O-2,SIO4-4,VA,FEO3/2,SIO2; N N
```

References

[1985Hil] M. Hillert, B. Jansson, B. Sundman, J. Ågren, A two-sublattice model for molten solutions with different tendency for ionization. Metall. Trans. A. 16, 261–266 (1985).

[1991Sun] B. Sundman, Modification of the two-sublattice model for liquids. Calphad. 15, 109–119 (1991).

Models for Ordered Phases

Some solution phases have chemical order-disorder transformations: for example, the disordered FCC_A1 phase can transform to the ordered $L1_2$ or $L1_0$ structure where the atoms of different kinds occupy different sublattices. In some cases, it may be advantageous and easy to describe such ordered structures as completely different phases; but in some other cases, like the B2-ordered BCC structure in Al-Fe, the disordered and ordered structures must be described as one singe phase because the transformation is of second order along a line in temperature and composition.

The ordering can easily be described by the CEF. For instance, an ordered FCC phase with only $L1_2$ or $L1_0$ ordering can be efficiently handled by the so-called Two Substitutional-Sublattice Ordering Model (2SL model), while an ordered FCC with both $L1_2$ and $L1_0$ ordering must be described with four sublattices using the so-called Four Substitutional-Sublattice Ordering Model (4SL model). Please note that in both these models, all the substitutional constituents must enter into these sublattices. In addition, you may also have one sublattice for interstitials.

Thermo-Calc supports a feature of splitting the parameters of a chemically ordered phase onto two different phase descriptions. This is very convenient. In this way, you can have one phase for all parameters describing the disordered state (the configuration independent state) and in the other phase only those parameters needed to describe the remaining part (the configuration dependent part), that is, the Gibbs energy contribution due to the ordering transformation. This has been implemented in such a way that the contribution from the configuration dependent part is zero when the solution phase is disordered. The optimization of the disordered phase is independent of the order-disorder transformation; the ordering energy is an add-on to the disordered part. This is particularly useful in higher order systems, as an ordered phase can dissolve several elements that have no particular contribution to the actual ordering. The phases Gibbs energy add together by giving this command in the setup-file: AMEND_PHASE_DESCRIPTION `<ordered phase> disordered_part <disordered phase>`

Since PARROT does not automatically create new composition sets, it is necessary to create composition sets for both the ordered and disordered phases in the setup-file: `Amend_phase_description <phase> composition_sets <new highest set number>,,,,`

Example of phase definitions for the corresponding disordered and ordered parts in a setup-file:

```
ENTER_PHASE FCC_A1, 2 1 1

     AL,CR,FE,NI; VA; N N

ENTER_PHASE FCC_L12, 3 .75 .25 1

     AL,CR,FE,NI ; AL,CR,FE,NI; VA; N N

AMEND_PHASE_DESCRIPTION FCC_L12 DIS_PART FCC_A1
```

4SL Model for FCC, HCP, and BCC

Ordered FCC, HCP and BCC solution phases handled by the 4SL model requires four sublattices for substitutional ordering and can additionally have an interstitial sublattice. A 4SL model is especially useful for modelling different kinds of ordered phases that are based on the same disordered phase, such as $L1_0$ and $L1_2$ based on FCC_A1, and B2, $D0_3$, $L2_1$ and B32 based on BCC_A2 etc.

For ordered FCC or HCP phases, these four substitutional sublattices represent four corners of the regular tetrahedron on these lattices, all of which are the nearest neighbours. These corners are equivalent lattice points, thus all G parameters for each end-member with the same elements, but distributed on different sites, must be identical. It should be emphasized that the end-member energy here represents the ordering energy rather than the formation energy of the compound.

The constraints on the parameters in the 4SL model can be derived based on the symmetry of the lattice:

$G_{A:B:B:B}=G_{B:A:B:B}=G_{B:B:A:B}=G_{B:B:B:A}$

$G_{A:A:B:B}=G_{A:B:A:B}=G_{A:B:B:A}=G_{B:A:A:B}=G_{B:A:B:A}=G_{B:B:A:A}$

$G_{B:A:A:A}=G_{A:B:A:A}=G_{A:A:B:A}=G_{A:A:A:B}$

$L_{A,B:*:*:*}=L_{*:A,B:*:*}=L_{*:*:A,B:*}=L_{*:*:*:A,B}$

The asterisk * means that the interaction parameter is independent of the occupation of that sublattice. For the disordered phase to be completely disordered, i.e. that all site fractions are equal on all four sublattices, all constraints must be correct.

For ordered BCC phases, the situation is a bit more complicated, as the four sublattice ordering phase represents an irregular tetrahedron with two pairs of sites that are next nearest neighbors. Thus, for an A-B binary solution phase, with A located on two sublattice sites and B on the other two, the end-member described by $G_{A:A:B:B}$ has four nearest neighbour bonds between A and B atoms, whereas the end-member described by $G_{A:B:A:B}$ has two nearest neighbour bonds between A and B atoms and two next nearest neighbour bonds. Many parameters thus have a relation:

$G_{A:B:B:B}=G_{B:A:B:B}=G_{B:B:A:B}=G_{B:B:B:A}$

$G_{B:A:A:A}=G_{A:B:A:A}=G_{A:A:B:A}=G_{A:A:A:B}$

$G_{A:A:B:B}=G_{B:B:A:A}$

$G_{A:B:A:B}=G_{A:B:B:A}=G_{B:A:A:B}=G_{B:A:B:A}$

$L_{A,B:*:*:*}=L_{*:A,B:*:*}=L_{*:*:A,B:*}=L_{*:*:*:A,B}$

The $G_{A:B:B:B}$ term represents $D0_3$, $G_{A:A:B:B}$ B2 and the $G_{A:B:A:B}$ B32 ordering. There are also two kinds of reciprocal interaction parameters:

$L_{A,B:A,B:*:*;0…9}$

$L_{A,B:*:A,B:*;0…9}$

Kusoffsky et al. (2001) have shown the influence of different parameters available in the 4SL model applied to fcc ordering. The possibility to use the 4SL model to BCC ordering has been studied by Sundman et al. (2009) in the Al-Fe system.

2SL Model for FCC, HCP, and BCC

The reason for using a 2SL model instead of a 4SL model is that the calculations are faster, but on the other hand it can only model one kind of ordered phase(s). For instance, it is not possible to model FCC with both $L1_0$ and $L2_1$, or BCC with $D0_3$ and B2, etc.

In order to get the fully disordered phase to form, constraints are needed as for the 4SL model. For the symmetric phases, e.g. B2 and $L1_0$, the relation between parameters are:

$G_{A:B}=G_{B:A}$

$L_{A,B:*}=L_{*:A,B}$

For a 2SL asymmetric model including, but not limited to, $L1_2$, more constraints are needed. This model has many complicated relations between the parameters. The relation between the parameters for the 2SL $L1_2$ model can be derived from a 4SL model. The conversion from 4SL model parameters to 2SL parameters for $L1_2$ can be found in Dupin et al. (2001) and for $L1_0$ in Yuan et al. (2012). Higher-order systems with an $L1_2$ phase modeled with two sublattices require a lot of ternary and some quaternary interaction parameters in order to make the disordered state stable. These parameters have been derived by e.g. Dupin (1995), also found in Kusoffsky et al. (2001).

Many publications exist on how to model order/disorder transformations using a two-sublattice model, see e.g. Dupin, Ansara (1999), De Keyzer et al. (2009).

Magnetic Ordering

The magnetic contribution to the Gibbs energy is given by a model proposed by Inden (1975) and adapted by Hillert and Jarl (1978), and is described by:

```
G=RTln(b+1)f(t)
```

where $t=T/T_C$.

The values of the Curie temperature, T_C, and Bohr magneton number, b, at a certain composition are then used in an optimization procedure to calculate the contribution to Gibbs energy due to magnetic ordering. Curie temperature and Bohr magneton number are given in the command ENTER_PARAMETER for phases that undergo a magnetic transition:

```
AMEND_PHASE_DESCRIPTION BCC_A2 MAGNETIC -1.0 0.4

ENTER_PARAMETER TC(BCC_A2,FE:VA;0) 298.15 +V1; 6000 N

ENTER_PARAMETER BMAGN(BCC_A2,FE:VA;0) 298.15 +V2; 6000 N
```

The arguments -1 and 0.4 specify the values of parameters in the magnetic model: -1 is the antiferromagnetic factor and 0.4 is the structure factor. Usually the antiferromagnetic factor =-1 for bcc and =-3 for fcc (and other non-bcc phases). The structure factor corresponds to the short range order fraction of the enthalpy. This factor is 0.4 for bcc and 0.28 for non-bcc phases.

Molar Volumes and High Pressure

Including volumes in a thermodynamic database enable calculations of volume changes, volume fraction, lattice mismatch in cubic structures and phase diagrams at increased pressure. Pressure independent volumes can be used up to about 1 GPa. At pressures above 1 GPa the pressure dependence of the volumes must be included by using a proper equation of state (EOS). An EOS has been developed by Lu et al. (2005), based on the EOS from Jacobs and Oonk (2000). Four parameters are used in the implementation of the model in Thermo-Calc:

- `V0`: Volume at 1 bar and at reference temperature T_0
- `VA`: Integrated thermal expansivity
- `VK`: Isothermal compressibility at 1 bar
- `VC`: Parameter to fit high pressure data

All parameters can be composition dependent in the same way as all other model parameters in Thermo-Calc. Experimental information about the temperature, pressure and composition dependence of the volume can be assessed using these model parameters. To evaluate V0, VA and VK experimental data at 1 bar only are needed.

Examples on modeling molar volume in a setup-file:

```
ENTER_PARAMETER V0(BCC_A2,FE:VA;0) 298.15 +V1; 6000 N

ENTER_PARAMETER VA(BCC_A2,FE:VA;0) 298.15 +V2*T+V3*T**2; 6000 N

ENTER_PARAMETER VC(BCC_A2,FE:VA;0) 298.15 +V4+V5*T; 6000 N

ENTER_PARAMETER VK(BCC_A2,FE:VA;0) 298.15 +V6+V7*T; 6000 N

ENTER_PARAMETER V0(FCC_A1,CR,FE:VA;0) 298.15 +V8; 6000 N

ENTER_PARAMETER VA(FCC_A1,CR,FE:VA;0) 298.15 +V9*(T-298.15); 6000 N
```

Excess Models

Unless specifically amended, the excess Gibbs energy terms are modeled by the Redlich-Kister-Muggianu Model. Other excess models for the Gibbs energy are also implemented in Thermo-Calc, such as e.g. Kohler and Toop-Kohler extrapolation models.

Thermo-Calc is not restricted to binary interaction parameters. Ternary, quaternary and higher-order interaction parameters can also be used if there is enough information to evaluate these from experimental data. The ternary interaction parameters are identified by the degrees of the so-called ternary L parameter (i.e. 0, 1 and 2) in the command ENTER_PARAMETER. If the parameter is composition-independent, you only need a single interaction parameter with a degree of zero, i.e. only the ^0L term. If there is a ternary composition-dependent interaction parameter, you must enter all three parameters (0,1 and 2). If such a ternary interaction parameter should be zero, then assign it a function which is zero. If the three interaction parameters have the same value, then that is identical to having a composition-independent ternary parameter.

```
ENTER_PARAMETER L(LIQUID,A,B,C;0) 298.15 +1000; 6000 N

ENTER_PARAMETER L(LIQUID,A,B,C;1) 298.15 +1000; 6000 N

ENTER_PARAMETER L(LIQUID,A,B,C;2) 298.15 +1000; 6000 N
```

is identical to

```
ENTER_PARAMETER L(LIQUID,A,B,C;0) 298.15 +1000; 6000 N
```

This also means that

```
ENTER_PARAMETER L(LIQUID,A,B,C;0) 298.15 +1000; 6000 N

ENTER_PARAMETER L(LIQUID,A,B,C;1) 298.15 +ZERO#; 6000 N

ENTER_PARAMETER L(LIQUID,A,B,C;2) 298.15 +ZERO#; 6000 N
```

is NOT identical to

```
ENTER_PARAMETER L(LIQUID,A,B,C;0) 298.15 +1000; 6000 N
```

General Einstein Model

An Einstein model implemented in a general way with multiple Einstein temperatures and accompanying weight functions.

The LNTHETA and THETAF parameters are only available with GES6.

It describes the vibrational contribution to Cp at low and intermediate temperatures.

The model is implemented as:

$$G_{Einstein} = f \times n \times R \times (\frac{3}{2}\Theta + 3T \times \ln(1 - e^{-\frac{\Theta}{T}}))$$

Where

- Θ is the Einstein temperature. $ln(\Theta)$ is entered as the database parameters `LNTHETA1`, `LNTHETA2`, `LNTHETA3`, `LNTHETA4`, and `LNTHETA5`.
- f is a weight function, entered as the database parameters `THETAF1`, `THETAF2`, `THETAF3`, `THETAF4`, and `THETAF5`.
- n is the number of atoms per mole formula unit
- R is the universal gas constant
- T is the temperature

Examples of parameters for this model:

```
PARAMETER LNTHETA1(GRAPHITE,C;0) 298.15 +LN(1953); 6000 N REF0 !
PARAMETER THETAF1(GRAPHITE,C;0) 298.15 +0.484786; 6000 N REF0 !
PARAMETER LNTHETA2(GRAPHITE,C;0) 298.15 +LN(947); 6000 N REF0 !
PARAMETER THETAF2(GRAPHITE,C;0) 298.15 +0.349135; 6000 N REF0 !
PARAMETER LNTHETA3(GRAPHITE,C;0) 298.15 +LN(448); 6000 N REF0 !
PARAMETER THETAF3(GRAPHITE,C;0) 298.15 +0.121463; 6000 N REF0 !
PARAMETER LNTHETA4(GRAPHITE,C;0) 298.15 +LN(193); 6000 N REF0 !
PARAMETER THETAF4(GRAPHITE,C;0) 298.15 +0.0387523; 6000 N REF0 !
PARAMETER LNTHETA5(GRAPHITE,C;0) 298.15 +LN(65); 6000 N REF0 !
PARAMETER THETAF5(GRAPHITE,C;0) 298.15 +0.0058637; 6000 N REF0 !
```

The Einstein function also can used with the GEIN(THETA) function.

For more information about this see FUNCTION and PARAMETER in the *Database Manager User Guide*.

References

[2001Che] Q. Chen, B. Sundman, Modeling of thermodynamic properties for BCC, FCC, liquid, and amorphous iron. J. Phase Equilibria. 22, 631–644 (2001).

[2018Big] S. Bigdeli, Q. Chen, M. Selleby, A New Description of Pure C in Developing the Third Generation of Calphad Databases. J. Phase Equilibria Diffus. 39, 832–840 (2018).

Database Manager User Guide

Thermo-Calc Version 2025b

Introduction to the Database Manager Guide

In this section:

Thermodynamic and Kinetic/Mobility Databases

This guide describes how to define and construct a thermodynamic or kinetic database. It includes details about the data structures and formats of the Thermo-Calc databases as well as the Diffusion Module (DICTRA) database-extensions.

The Thermo-Calc databases are created and maintained in the Thermo-Calc Database Format (TDB) which is an international standard for the CALPHAD-type thermodynamic calculations and kinetic simulations. This document gives a full description of the TDB format (with the Diffusion Module (DICTRA) database extension) and is a comprehensive guide about how to create and manage a Thermo-Calc (and Diffusion Module (DICTRA)) database.

Usually, a Thermo-Calc or Diffusion Module (DICTRA) database is constructed as a single text file with an extension of TDB, for example, `PAQ2setup.TDB`. For some databases (especially large databases used with older versions of Thermo-Calc or Diffusion Module (DICTRA)) a database may consist of one primary-definition file (`***setup.TDB`) and several additional-definition TDB files (such as `***param.TDB`, `***funct.TDB`, `***refer.TDB`, etc. These are built for a variety of defined parameters, functions, references and so forth, and are linked to the `***setup.TDB` file through the correct use of the TYPE_DEFINITION and/or FTP_FILE commands inside the `***setup.TDB` file.

> With Thermo-Calc, the Add-on Modules and Thermo-Calc Software Development Kits (SDKs), you can code everything into a single *****setup.TDB** file for a database at any scale.

Initialization of the TDB Module

The following explains how a database initialization file is constructed to work with the so-called TDB (database) module. When you start, the TDB module looks for a file that has information about the available standard databases. The database initialization file is called `tc_initd.tdb`. By default it is located in the data subdirectory of the Thermo-Calc installation directory.

See Database Installation Folder in the *Thermo-Calc User Guide*.

The location can be overridden by:

- A command line parameter `-t` followed by the path to the directory containing the `tc_initd.tdb` file.
- The environment variable `TC_DATABASE_DIRECTORY` pointing to the directory containing the `tc_initd.tdb` file. This overrides both the default value and a directory given with the `-t` command line argument.

Each database defined in `tc_initd.tdb` represents a database that can be used within Thermo-Calc. Each entry has three parts:

1. The database short-name (e.g. `FEDEMO`, maximum seven characters, no white space, no commas).
2. The path to the database setup file (max 78 characters, no commas, can contain white space if it is a quoted absolute path).
3. A short description of the database (max 60 characters, can contain white space). The entry must end with an exclamation mark (`!`).

The paths can be relative to the `tc_initd.tdb` file or absolute. For platform independence, the recommendation is to always use forward slashes (`/`) in the paths, but on Windows backslash (`\`) also works.

You can add comment lines in the database initialization file. Comments must start with a `$` sign.

Examples

The following are examples of an initialization file defining two databases:

```
SSOL8 SSOL8\SSOL8SETUP.TDC  SGTE Solutions Database version 8.0 !
MYDB1 ../../../MYDATABASES/ABC.TDB My database 1.0 !
```

In the initialization file you can also add databases with absolute file names with white space, if the path is surrounded by quotation marks (`"`):

```
TEST "G:\My Drive\My Folder\Test.TDB" My test database v0.1!
```

The use of absolute paths should be used with caution as these are not portable.

The Database Definition File and Keywords

In this section:

Database Definition File Syntax

The database definition (*.TDB) file (normally named `***setup.TDB`) consists of a set of keyword codes each followed by one or several parameters (arguments).

- A complete keyword entry must end with an exclamation mark (!).
- A single keyword entry can be up to 2000 characters long. However, the maximum length of a line in an *.TDB file is 78 characters--it may be necessary to continue the keyword parameter (arguments) on several lines. The ! must be at the end of the last line.
- It is recommended to always have at least one empty space at the beginning of each continuation line for the keyword parameters (arguments); otherwise, the DATA module can misunderstand the parameters (or arguments), or issue an error message.
- The keyword and its various parameters (arguments) are separated by a space or a comma.
- A dollar sign ($) in the first position of the line indicates that the line is a comment line, which is ignored by the DATA module.

When the database is selected the DATA module only reads the database definition file (***setup.TDB) once, from beginning to end. The DATA module checks continuously when reading the definition file. This implies that (nearly) everything must be declared or defined before it is used in any other way.

For example, if the GRAPHITE phase is to be included in the database definition, the element C (carbon) and the phase GRAPHITE must be defined before declaring that carbon dissolves in graphite. This definition order is necessary to build the internal data structure acceptable by the DATA module (during its consistency checking).

This topic gives a description of the available keywords and the appropriate arguments. A basic knowledge of the Gibbs Energy System (GIBBS) module is assumed.

This syntax is used:

```
KEYWORD [arg.1]*# [arg.2]*## {optional arg.3}!
```

The keywords are written in full length but can be abbreviated as long as the abbreviation is unique. A keyword may have syntax consisting of several arguments and optional arguments. The number, # or ##, in the notation, [...]*# or [...]*##, indicates an argument with a maximum length of # ASCII characters.

Arguments within square brackets `[...]` must always be given, but are optional when enclosed in curly brackets `{...}`.

ELEMENT

```
ELEMENT [element name]*2 [ref. state]*24 [mass] [H298] [S298] !
```

The *element name* (maximum two characters) is the one found in the periodic chart but there are no naming restrictions. However, the GIBBS module only recognizes UPPER-case element names (if the `Upper Case Mode` is selected by the GIBBS command REINITIATE), which means that lower-case (if defined in a database) is automatically converted to UPPER-case by the DATA/GIBBS module.

The elements are automatically entered as species using the same names of the elements. If, for example, the species corresponding to FE needs to be named FE1, you can define the species as FE1, which results in an element named FE and a species named FE1. Vacancies (VA) and electrons (denoted either as /- in gaseous, liquid or solid phases, or ZE in an aqueous solution phase), need to be entered as special elements for correct handling by the DATA module.

The *reference (ref.) state* (maximum 24 characters) is the stable phase (at 298.15 K and 1 bar) that should contain this element and be used as the reference state for all element thermodynamic data. The *mass*, given in gram per mole, is used in various calculation programs and should always be given the correct value. *H298* and *S298* denote the enthalpy and entropy difference between 0 and 298.15 K for the element in SI units. If these are unknown, the values can be set to zero. All this information (reference state, H298 and S298) define the SER (Stable Element Reference state).

Examples

```
ELEMENT /- ELECTRON_GAS      0.0   0.0   0.0 !
ELEMENT VA VACUUM            0.0   0.0   0.0 !
ELEMENT ZE UNIT_CHARGE       0.0000000001  0.0  0.0 !
ELEMENT AL FCC_A1            26.98154 4577.296 28.3215 !
ELEMENT C  GRAPHITE          12.011  1054.0    5.74 !
ELEMENT FE BCC_A2            55.847  4489     27.28 !
ELEMENT O  1/2_MOLE_O2(G)    15.9994 4341    102.5158 !
ELEMENT TI HCP_A3            47.88   4810     30.648 !
ELEMENT ZR HCP_A3            91.224  5566.27  39.181 !
ELEMENT ZY DUMMY              1         1         1 !
```

SPECIES

```
SPECIES [species name]*24 [stoichiometric formula] !
```

This keyword defines species in the data structure. Every *species name* (maximum 24 characters) must be unique. The species are built from the predefined set of elements in the stoichiometric formula. If an undefined element is referenced, DATA displays an error message and the data structure is probably damaged.

The species names do not have to be the same as the stoichiometry formula, although in general this is recommended. The elements are automatically entered as species using the same names of the elements.

You can define a species name as a mixture of UPPER-case and lower-case letters in a database, but the DATA module automatically converts all lower-case to UPPER-case because the GIBBS module only recognizes UPPER-case species names.

When naming the species in a database, use special characters (such as +, -, _, / and .) in species names. Avoid using other special characters (such as `(` and `)`).

The *stoichiometric formula* is written with a simplified chemical notation, in which the chemical elements should always be given in UPPER-case and in any preferred order, and the stoichiometric coefficients are written in either real numerical factors or integer digits.

It is important that the numerical factor of `1` is not left out. Subgroups are not allowed in a stoichiometry formula; however, while specifying the stoichiometry formula for a specific species in a database, you can specify it in a way that some elements (always together with the corresponding partial stoichiometric coefficients) are repeated (as in the examples below).

Examples

```
SPECIES AL2O3      AL2O3 !

SPECIES Silica     SI1O2 !

SPECIES NaSb_6OH   NA1SB1O6H6 !

SPECIES FE+2        FE/+2 !
```

```
SPECIES SB-3        SB/-3 !
SPECIES AlCl2/3            AL.33333CL.666667 !
SPECIES AL1CL1H2O2         AL1CL1H2O2 !
SPECIES AlCl3_3H2O         AL1CL3H6O3 !
SPECIES AlO2H2Cl.H6O3      AL1O2H2CL1H6O3 !
SPECIES AlCl2-OH.3H2O      AL1CL2O1H1H6O3 !
SPECIES AlCl2OH.3Water     AL1O1H1CL2H6O3 !
```

PHASE

```
PHASE [phase name]*24 [data-type code]*8 [numb. subl.] [sites in
subl. 1] [sites in subl. 2] etc... {auxiliary text string} !
```

This keyword defines a phase and its properties (except for what species are allowed to enter it and for its parameters).

The *phase name* (maximum 24 characters) must be unique; otherwise the DATA module sees it as an attempt to redefine a previously defined phase. This causes DATA to display an error message and ignore the rest of the line. A phase name can be suffixed by an underscore (_and letters to identify the physical state(s) or structure type(s) of the phase.

Examples of Recommended Suffixes

Suffix	*Definition*
`ABC_S`	The ABC phase in solid state.
`ABC_S2`	The ABC phase in solid state 2.
`ABC_S3`	The ABC phase in solid state 3.
`ABC_LT`	The ABC phase in solid state at low temperatures.
`ABC_HT`	The ABC phase in solid state at high temperatures.
`ABC_L`	The ABC phase in liquid state.
`ABC_LIQ`	The ABC phase in liquid state.
`FCC_A1`	The FCC phase in disordered structure type A1.
`FCC_L12`	The FCC phase in ordered structure type L12.

The *phase name* can also be attached with a colon sign (`:`) and a letter for a legal GIBBS phase-type code (e.g. `IONIC_LIQ:Y` and `GAS:G`).

GIBBS Phase-type Codes

Code	*Definition*
`G`	Bit set for a gaseous mixture phase.

Code	***Definition***
`A`	Bit set for an aqueous solution phase.
`Y`	Bit set for an ionic liquid solution phase (specially treated by the Ionic Two-Sublattice Liquid Model).
`L`	Bit set for a liquid solution phase (but not A (aqueous) or Y (ionic liquid)).
`I`	Bit set for a phase with charged species (but not G (gaseous), A (aqueous) or Y (ionic liquid)).
`F`	Bit set for an ordered FCC or HCP solution phase using the *Four Substitutional-Sublattice Ordering Model*(additionally, such a phase can also have interstitial sublattices).
`B`	Bit set for an ordered BCC solution phase using the *Four Substitutional-Sublattice Ordering Model* (additionally, such a phase can also have interstitial sublattices).

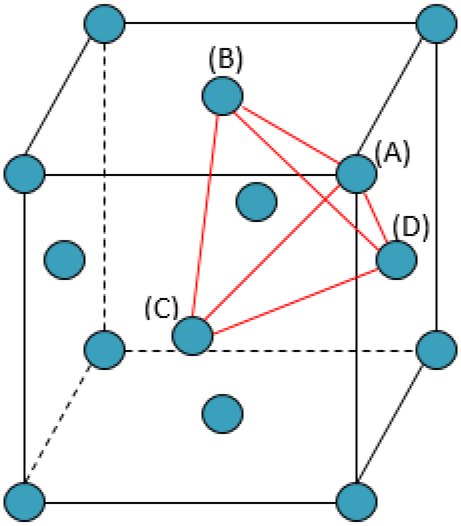
Other invalid characters (e.g. `M` or `P`) are eventually treated, together with the colon (:) as a part of a phase name.

A `G` phase (gaseous mixture) or an `A` phase (aqueous solution) is usually treated as a substitutional phase without sublattice, and an `L` phase (ordinary liquid solution) is normally (but not always) modeled as a substitutional phase without sublattice, too.

For ordered FCC or HCP phases, these four substitutional sublattices represent four corners of the regular tetrahedron on these lattices, all of which are the nearest neighbours, as shown.

FCC Unit Cell Example

An FCC unit cell with the lattice positions indicated that correspond to the G (FCC,A:B:C:D) end member. All lattice positions are equivalent for a four substitutional-sublattice ordering model.



A *Normal 4-Sublattice Model* requires that all the `G` parameters for each of the end-members with the same elements but distributed on different sites be given separately. However, as these corners are identical lattice points, the phase-type option `F` means that the `G` parameters need be given only once. The possible permutations are handled automatically.

Additional Clarification

An `A-B` binary solution phase (with the element A located on one sublattice site and `B` on the other three sublattice sites) treated by the Normal 4-Sublattice Model has to have four `G` parameters for four end-members, i.e.

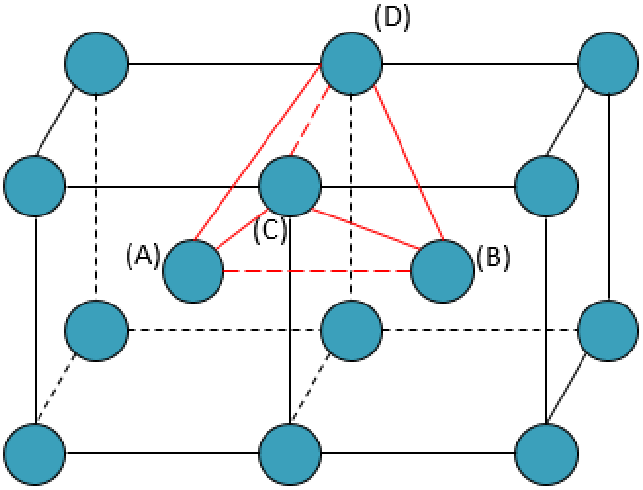
- G(phase,A:B:B:B)
- G(phase,B:A:B:B)
- G(phase,B:B:A:B, and
- G(phase,B:B:B:A)

This is because in the general case these `G` parameters can be different from each other. But for the FCC and HCP orderings, they are identical and thus all `G` parameters of such end-members need to be given only once, and the possible permutations are then automatically handled by the GIBBS module. Also, only one of the identical permutations is listed; in this example, `G(phase,A:B:B:B)` where it is alphabetically the first in the list of permutations. This significantly simplifies the usage of this model (*Four Substitutional-Sublattice Ordering Model*) in multicomponent alloys.

For ordered BCC phases, the phase-type option `B` means the same thing but it is more complicated since the 4-substitutional-sublattice ordering phase represents an irregular tetrahedron with two pairs of sites that are next nearest neighbours as shown:

BCC Unit Cell Example

Two BCC unit cells with the lattice positions indicated that correspond to the G (BCC,A:B:C:D,0) end member. Lattice positions (A) and (B) are equivalent, as are lattice positions (C) and (B) for a four substitutional-sublattice ordering model.



For an end member described by the parameter `G (phase,A:B:C:D)` A and B are next nearest neighbours, as are C and D. And the nearest neighbours of A (or B) are C and D. Thus, for an `A-B` binary solution phase (with the element A located on two sublattice sites and `B` on two sublattice sites) treated by the Normal 4-Sublattice Model, the end-member described by the `G(phase,A:A:B:B)` term has four nearest neighbour bonds between A and B atoms, whereas the end-member described by the `G(phase,A:B:A:B)` term has two nearest neighbour bonds between A and B atoms and three next nearest neighbour bonds.

The first end-member (described by the `G(phase,A:A:B:B)` term) represents B2-ordering and the second (described by the `G(phase,A:B:A:B)` term) stands for B32-ordering. There are two permutations of the `G(phase,A:A:B:B)` term and four permutations of the `G (phase,A:B:A:B)` term, automatically conducted in the *Four Substitutional-Sublattice Ordering Model*. If you enter the unary, binary, ternary and quaternary parameters you are dealing with 1, 6, 21, 55 parameters for BCC:B, 1, 5, 15, 35 parameters for FCC:F and 1, 16, 81, 256 parameters for phases without F/B.

An additional feature with the phase-type options `F` and `B` is that a composition set that represents the solution phase has a suffix (indicating what ordering the phase has) that is automatically added to its phase name in some listings of equilibrium calculations (when performing either single-point or stepping or mapping calculations, and when plotting the calculated property diagrams or phase diagrams).

Such suffix indications can be:

Solution Phase	***Suffix for Disordered Phase***	***Suffix for Ordered Phase***
`FCC PHASE`	`FCC_A1`	`FCC_L12`
		`FCC_L10`
`BCC PHASE`	`BCC_A2`	`BCC_B2`
		`BCC_B32`
		`BCC_D03`
		`BCC_L21`
`HCP PHASE`	`HCP_A3`	`HCP_D019`
		`HCP_B19`

> If you want to convert an existing database TDB file to use the F/B feature, add the phase-type code to the corresponding phase name in the PHASE and CONSTITUENT commands in the TDB-file, then when running the LIST_DATA command in the Gibbs (GES) module. The created database file is in this less verbose format.

The *data-type code* consists of 1 to 8 characters where each character must stand for an action, which is to be coupled to this phase. The keyword TYPE_DEFINITION, described below, must be used in the current database to specify what action should be taken by DATA for each character code.

The data entries `[numb. subl.] [sites in subl. 1] [sites in subl. 2]` etc., specify the total number of sublattices (always as an integer digit) and the sites (i.e. stoichiometric coefficients) of each of the sublattices (given in either integer digits or real numerical factors) for the phase.

Optionally, an *auxiliary text string* (maximum 10,000 characters) can be given after the last [sites in sublattice #] but before the exclamation mark `!`. This string displays in connection with the phase name in some listings within the DATA module.

Examples

```
PHASE GAS:G  % 1 1.0 !
```

```
PHASE LIQUID:L %ZCDQ  2  1.0  1.0
> Metallic liquid solution, modeled by CEF Model. !
PHASE IONIC-LIQ:Y %ZCDQ  2  1.0  1.0
> Ionic liquid solution, modeled by Ionic Two-Sublattice Model. !
PHASE SPINEL:I    %ZA   4   1  2  2  4
> Complex Spinel Solution, by CEF model with ionic constraints. !
PHASE M23C6  % 3 20.0 3.0 6.0 !
PHASE FCC_A1    %&A  2  1 1
> Disordered FCC phase; also as MX carbides/nitrides. !
PHASE FCC_L10   %&AX  3  0.75 0.25 1
> Ordered FCC phase, modeled by 2-Sublattice Model for Ordering. !
PHASE FCC_L12:F %&AX  5  0.25 0.25 0.25 0.25 1.0
> Ordered FCC phase, modeled by 4-Sublattice Model for Ordering. !
PHASE AQUEOUS:A %HIJMR 1 1.0
> Aqueous Solution: using the Complete Revised HKF Model. !
```

CONSTITUENT

```
CONSTITUENT [phase name]*24 [constituent description]*2000 !
```

This keyword (and the ADD_CONSTITUENT keyword for large solution phase) defines the phase-constitution as a list of constituents (for a substitutional phase with no sublattice) or of constituent arrays (for a sublattice phase).

The *phase name* (maximum 24 characters) must be a predefined phase (i.e. already through the PHASE keyword).

> ❗ It is important that if a phase bears a legal phase-type (among G, A, Y, L, I, F and B) in its phase definition (already by the PHASE keyword; such as GAS:G, SLAG:L, LIQUID:L, IONIC_LIQ:Y, SPINEL:I, FCC_L12:F, HCP_D021:F, BCC_B2:B, AQUEOUS:A), such a valid phase-type code must also always be attached to the phase name in the CONSTITUENT keyword (and the ADD_CONSTITUENT keyword).

> Specifying the phase name in UPPER-case is recommended. You can define a phase name as a mixture of UPPER-case and lower-case letters in a database, but the DATA module automatically converts all lower-case to UPPER-case because the GIBBS module only recognizes UPPER-case phase names.

The *constituent description* (maximum 2000 characters) is a list of the species that enter a phase. The list starts with a colon (`:`), indicating the start of the sub-list of species for the first sublattice, and different sublattices are separated by colons. The complete sequence ends with a final colon.

Optionally, each sublattice may specify which species are considered to be major constituents. This is done by adding a percent sign (`%`) directly to the species name. The start values on the site fractions of the major constituents should sum to 0.99 on a specific sublattice. Thus, the minor constituents (i.e. those without a `%`) add up to 0.01. A maximum of 2000 characters can be coded in the constituent description, continuing in sequent lines. If the phase has a constituent description longer than 2000 characters, the rest can be coded in one or several ADD_CONSTITUENT keywords.

Examples

```
CONSTITUENT BCC_A2 :FE
```

```
CONSTITUENT IONIC-LIQ:Y :FE+2 : SB-3: !

CONSTITUENT M23C6 :CR FE :FE CR W MO : C: !

CONSTITUENT AQUEOUS:A :H2O% AG+1 AGF AGCL AGCL2-1 AGI3-2 AGSO4-1
AGC2H4+1

   AGN2H6+1 AGC2N2-1 AGC2H4NO2 AL+3 ALF3 ALO2-1, ... : !

CONSTITUENT SPINEL:I  : AL+3% CR+3 FE+2% FE+3 MG+2% NI+2

                     : AL+3% CA+2 CR+3 FE+2 FE+3 MG+2% NI+2 VA

                     : FE+2 MG+2 VA%

                     : N-3 O-2% :!
```

ADD_CONSTITUENT

```
ADD_CONSTITUENT [phase name]*24 [constituent description]*2000 !
```

This keyword adds more constituents to a phase that already has some constituents. Its syntax is the same as for the CONSTITUENT keyword. This keyword can be used several times, if the phase is very large, e.g. a gaseous mixture or a complex aqueous solution. This is useful when there are so many constituents in a phase that the 2000 characters available for the constituent description list is not enough.

> Constituents are not necessary on all sublattices. In the second example below, no addition is made to the first sublattice.

Examples

```
ADD_CONSTITUENT GAS :S1 S2 S3 ... : !

ADD_CONSTITUENT IM-PHASE : :CR:W ... : !

ADD_CONSTITUENT AQUEOUS:A :CUCL+1 CUCL2 CUCL2-1 CUCL3-2 CUOH+1 CUO2H2
CUO3H3-1

    CUO4H4-2 CU2OH+3 CU2O2H2+2 CU3O4H4+2 NIO2H2 NIO3H3-1 NIO4H4-2
NI2OH+3

    NI4O4H4+4 ZNOH+1 ZNO2H2 ZNO3H3-1 ZNO4H4-2 ... : !
```

COMPOUND_PHASE

```
COMPOUND_PHASE [phase name]*24 [data-type code]*8 [constituent] !
```

The keyword is a compact way to simultaneously define a species, a *compound phase* (maximum 24 characters) and its phase-constituent. It is useful for stoichiometric phases with constant compositions. The species name and stoichiometric formula must be identical, i.e. being the given *constituent*. The phase has this species as its only constituent. This keyword allows the database definition file for a large substance database to be more compact; it is a combination of the SPECIES, PHASE and CONSTITUENT keywords.

Examples

```
COMPOUND_PHASE AL2O3 % AL2O3 !
```

```
COMPOUND_PHASE MAGNETITE %MF FE3O4 !
```

```
COMPOUND_PHASE QUARTZ % SIO2 !
```

ALLOTROPIC_PHASE

```
ALLOTROPIC_PHASE [phase name]*24 [data-type code]*8 [constituent] !
```

This keyword does the same as the COMPOUND_PHASE keyword for entering an allotropic phase (maximum 24 characters), but does not enter the constituent as a species to the data structure. Use this if the species is already defined.

Examples

```
ALLOTROPIC_PHASE BETHA-AL2O3 % AL2O3 !

ALLOTROPIC_PHASE CRISTOBALITE % SIO2 !

ALLOTROPIC_PHASE TRIDYMITE % SIO2 !
```

TEMPERATURE_LIMITS

```
TEMPERATURE_LIMITS [lower limit] [upper limit] !
```

This keyword sets the default upper and lower temperature limits used by the GIBBS module for Gibbs energy parameters and functions. It can be used only once in one database definition file and all its sequential files.

Example

```
TEMPERATURE_LIMITS 500.0 1800.0 !
```

DEFINE_SYSTEM_DEFAULT

```
DEFINE_SYSTEM_DEFAULT [keyword] {G-ref. type index} !
```

This keyword sets the default value to ELEMENT or SPECIES in the DATA command DEFINE_SYSTEM.

For a substance database, it can be appropriate to have ELEMENT as a default value whereas a large solution database can benefit from having SPECIES as a default value. A proper default value is useful for beginners. An advanced user is more likely to use the DATA commands DEFINE_ELEMENT and DEFINE_SPECIES to override the default value.

{G-ref. type index} is an integer indicating the reference state type for an element when entering and listing data in the GIBBS module. The following lists legal numbers and the corresponding meaning (the reference state type for an element):

Number	*Definition*
1	symbol: G
2	symbol: H298
3	symbol: H0

For example:

```
DEFINE_SYSTEM_DEFAULT element 2 !
```

DEFAULT_COMMAND

```
DEFAULT_COMMAND [secondary keyword and parameters] !
```

This keyword specifies commands to be executed by the DATA module at database initialization. The syntax of the available command is currently not the same as the user available DATA commands but the actions are similar. The available *secondary keyword and parameters* in syntax are:

```
DEFINE_SYSTEM_ELEMENT [element names]

DEFINE_SYSTEM_SPECIES [species names]

DEFINE_SYSTEM_CONSTITUENT [phase] [sublattice] [species]

REJECT_SYSTEM_ELEMENT [element names]

REJECT_SYSTEM_SPECIES [species names]

REJECT_SYSTEM_CONSTITUENT [phase] [sublattice] [species]

REJECT_PHASE [phase names]

RESTORE_PHASE [phase names]
```

Examples

```
DEFAULT_COMMAND DEFINE_SYSTEM_ELEMENT FE VA !

DEFAULT_COMMAND REJECT_SYSTEM_CONSTITUENT LIQUID 2 C !

DEFAULT_COMMAND REJECT_PHASE LIQUID !

DEFAULT_COMMAND RESTOR_PHASE GAS !
```

DATABASE_INFORMATION

```
DATABASE_INFORMATION [text]*10000 !
```

This keyword defines a text for the detailed description of the current database. The text can be listed with the DATA command DATBASE_INFORMATION. An apostrophe (`'`) can be used in the text to indicate a new line; and two apostrophes, (`''`) can be used in the text to indicate a new line plus an empty line.

> The continuous *text* length (each line with max 78 characters) is 10,000 characters.

Example

```
DATABASE_INFORMATION This is the XXX-Alloy Solution Database '
      in the A-B-C-D-...... System. '
   Developed by TCS, released in May 2001. ''
... more ... !
```

TYPE_DEFINITION

```
TYPE_DEFINITION [data-type code]*1 [secondary keyword with
parameters] !
```

This keyword couples phases to an action performed by the DATA module when the DATA command GET_DATA is executed.

Secondary Keywords

The secondary keywords and associated parameters in syntax are:

```
SEQ [filename]

RND# [filename]

GES [valid GIBBS command with parameters]

POLY3 [valid POLY command with parameters]

TDB [valid DATA command with parameters]

IF [conditional statement] THEN [keyword with parameters]

AFTER [valid GIBBS command with parameters]
```

The secondary keyword `SEQ` specifies a sequential file that stores parameters belonging to the phases using the associated data type code (which is defined by this keyword). A special case where the filename is given as an asterisk (`*`) implies that the database definition file also acts as a sequential data storage file. This case makes it possible to have a single file for a small database, which is especially suited for personal databases.

The secondary keyword `RND` should be concatenated with a positive integer `#` to indicate the type of the random file. Currently, there are these types of random files:

- `RND0`, the default, is used for complete Gibbs energy expressions (G0 parameters), where the search field is the unabbreviated parameter name.
- `RND1` is designated for functions, where the function name is used as the search field.
- `RND2` is reserved for binary interaction parameters, where its search field is also the unabbreviated parameter name without any interaction order notation.

Ternary and higher order interaction parameters must be specified on a sequential file. Moreover, the internal structures of these random files are subject to changes with different versions of DATA, and with implementations of DATA on various computer systems. For more information, see the FORTRAN program TDBSORT, which is available from Thermo-Calc Software AB.

The secondary keywords `GES`, `POLY3`, or `TDB` specifies a modification of, or addition to, phases having the associated data type code, such as magnetic contribution, another excess model, or any other valid GIBBS/POLY/DATA command that applies to a certain phase. By implementing this as a call to the interactive GIBBS/POLY/DATA module, flexibility is achieved. If a new type of addition is implemented in a GIBBS/POLY/DATA module, it can be immediately used in the database definition file without reprogramming the DATA module.

In several examples below, the use of the at (`@`) sign indicates any phase to which the relevant type definition (e.g. `A`, `B`, `4`, or `E`) applies.

The secondary keywords `IF` and `THEN` allow specification of a conditional statement structured with respect to the phase constitution that controls the execution of a following type-definition (keyword with parameters) string. See the last four examples.

The secondary keyword `AFTER` is similar to the GES keyword except the defined GIBBS command is executed after all parameters are entered. The reason for this is that the command has no effect unless there is a parameter. Following the `AFTER` keyword, a GIBBS command must be given and it is executed after entering the parameters of the phase.

The data-type code (always as one string) can be any normal or special character, e.g. `0`, `5`, `A`, `F`, `M`, `%`, `&`, and so forth, and is referred in the definition keywords PHASE, COMPOUND_PHASE and ALLOTROPIC_PHASE for various phases.

A phase can have several ADDITIONAL parts of different types (that are enforced by certain TYPE_DEFINITIONS which call the GIBBS command AMEND_PHASE_DESCRIPTION for describing various contributions to Gibbs energy). However, the DATA/GIBBS module automatically deletes any early-defined ADDITIONAL part(s) of the same type.

The DATA module can selectively retrieve functions that are necessary for a defined system from a database that has functions stored in its `setup` file or `SEQ` sequential function file, while all other functions irrelevant for the defined system are ignored and are not saved in associated GIBBS and POLY workspaces.

Examples

```
TYPE_DEF % SEQ  TCPATH\DATA\[DATABASE]\PARAMETERS.TDB !
TYPE_DEF I SEQ  TCPATH\DATA\[DATABASE]\INTERACTION-PARAMS.TDB !
TYPE_DEF G RND0 TCPATH\DATA\[DATABASE]\GZERO-PARAMS.TDB !
TYPE_DEF F RND1 TCPATH\DATA\[DATABASE]\FUNCTIONS.TDB !
TYPE_DEF & RND2 TCPATH\DATA\[DATABASE]\BINARY-INTERACTIONS.TDB !
TYPE_DEF A GES AM_PH_DES @ MAGNETIC -1 0.40 !
TYPE_DEF B GES AM_PH_DES @ MAGNETIC -3 0.28 !
TYPE_DEF 4 GES AM_PH_DES @ EXCESS_MODEL REDLICH-KISTER_KOHLER !
TYPE_DEF 5 GES AM_PH_DES AQUEOUS EXCESS_MODEL HKF !
TYPE_DEF 6 GES AM_PH_DES AQUEOUS HKF_ELECTROSTATIC !
TYPE_DEF 7 GES AM_PH_DES AQUEOUS STATUS 02084000,,, !
TYPE_DEF 8 GES AM_PH_DES AQUEOUS MAJOR_CONST 1 H2O !
TYPE_DEF E AFTER AM_PH_DES LIQUID EXCESS MIXED-EXCESS
                         A B LEGENDRE   C A POLYNOM ,,,, !
TYPE_DEF T AFTER AM_PH_DES LIQUID TERN-EXT TOOP-KOHLER  B A C ,,,, !
TYPE_DEF Q AFTER AM_PH_DES LIQUID TERN-EXT KOHLER FE CR NI !
TYPE_DEF C IF (PD AND PT AND SN)  THEN TDB RESTORE_PHASE BCT_A5 !
TYPE_DEF D IF (PD AND (PT OR SN)) THEN TDB REJECT_PHASE BCC_A2 !
TYPE_DEF E IF ((NB OR TI OR V) AND (C OR N)) THEN
          GES AM_PH_DES @ COMP_SET ,, CR NB TI V: C N: !
TYPE_DEF F IF (ALO3/2 OR CRO3/2 OR FEO OR MNO OR SIO2) THEN
          GES AM_PH_DES LIQUID COMP_SET ,, ALN%,ALO3/2%,CRO3/2%,
             FEO%,FEO3/2,MNO3/2%,MNS%,SIO2%,TIO2% : !
TYPE_DEF R GES AM_PH_DES FE_LIQUID FRACTION_LIMITS  Fe 0 0.6
         Ag 0 0.01  Al 0 0.05  Ca 0 0.05  Co 0 0.01  Cr 0 0.01
         Cu 0 0.02  Mg 0 0.05  Mn 0 0.05  Mo 0 0.05  Nb 0 0.05
         Ni 0 0.05  Pb 0 0.05  Si 0 0.10  Sn 0 0.02  Ti 0 0.05
         U  0 0.01  V  0 0.02  W  0 0.02  Zr 0 0.03
         B  0 0.01  C  0 0.01  H  0 0.01  N  0 0.01  O  0 0.01
         P  0 0.01  S  0 0.01  !
```

Ordered Phase Restores Disorder Contribution

When an ordered phase with disordered contribution is restored, the disordered contribution is automatically restored as well. You can also restore the disordered phase *without* restoring the ordered phase.

However the DIS_PART TYPE_DEFINITION must always be set on the ordered phase. It is important that the disordered phase is declared *before* the ordered phase. Otherwise it causes an error when DIS_PART TYPE_DEFINITION is executed and then either the ordered or disordered phase is rejected.

Example

```
TYPE_DEFINITION & GES A_P_D FCC_A1 MAGNETIC  -3.0    2.80000E-01 !
PHASE FCC_A1  %&  2 1   1 !
    CONSTITUENT FCC_A1  :CR,NI% : C%,VA :  !
$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM FCC_A1
TYPE_DEFINITION ' GES AMEND_PHASE_DESCRIPTION FCC_L12 DIS_PART FCC_
A1,,,!
TYPE_DEFINITION ( GES A_P_D FCC_L12 MAGNETIC  -3.0    2.80000E-01 !
PHASE FCC_L12  %'(  3 .75   .25   1 !
    CONSTITUENT FCC_L12  :CR,NI% : CR,NI% : C,VA% :  !
```

For example a GES command such as the following only affects phases defined above or at the phase with this TYPE_DEFINITION in the TDB file:

```
TYPE_DEFINITION ( GES A_P_D FCC_L12 DIS_PART FCC_A1,,, !
```

For example a TDB command such as the following only affects phases defined *below* the phase with this TYPE_DEFINITION in the TDB file:

```
TYPE_DEFINITION ( TDB RESTORE_PHASE FCC_A1 !
```

FTP_FILE

```
FTP_FILE [filename] !
```

FTP_FILE is a special function random file and the function names correspond to the record numbers where these record names and the functions are stored. The FTP_FILE decreases search time for the associated database in the DATA module. The file is used for large substance databases along with a SEQ sequential or RND0 random file for storage of G0 parameters referring the functions named `FxxxxT` that are stored in the FTP file. The integer number `xxxx` is a search code used by DATA when such files are processed.

No modification of this file type is allowed.

Example

```
FTP_FILE TCPATH\DATA\[DATABASE]\FTP-FILE.DATA !
```

FUNCTION

```
FUNCTION [function name]*8 [lowest temp. limit]
[expression 2]; [upper temp. limit 2] Y
[expression 1]; [upper temp. limit 1] Y
[expression 3]; [upper temp. limit 2] Y
   .......... ; ..... Y
[expression n-1]; [upper temp. limit n-1] Y
[expression n]; [upper temp. limit n] N {Ref. Index} !
```

GIBBS can use predefined functions in the expression (TP-Function) of a Gibbs energy parameter or in other functions. This is often used when several parameters (or functions) have a common sub-expression, such as for metastable modifications of elements. This keyword can appear in both files for database definition and sequential storage, but not in FTP files. A valid *function name* can have up to 8 characters.

A function always starts with a lowest temperature limit of its applicability, followed by one or more (up to 10) expressions (TP-Functions) that are coded as mathematical relations of constants, functions of stable variables (T and P) and other entered functions (normally with a # suffix, e.g. +3*GHSERAL#).

ENTER_PARAMETER

The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers). Unary-functions LN or LOG (both for natural logarithm) and EXP (for exponential) can also be used. There is also the GEIN function available for the Einstein Model.

```
GEIN(THETA) = 1.5*R*THETA + 3*R*T*LN(1-EXP(-THETA/T))
```

General Einstein Model

Each expression (TP-Function) should end with a semicolon (;), and be followed by its upper applicable temperature limit and a continuation indicator (Y to continue with the next expression or N to end the function's expression). If there is no continuation after a specific expression (TP-Function), the reference index can optionally be given after the N indicator.

A complete/valid function entry can be written in several continuation lines if the function's expression (TP-Function) is too long or if there is more than one applicable expression (TP-Function), as the maximum length of each line is 78 characters.

It is recommended to always have at least one empty space at the beginning of each continuation line. Otherwise, the DATA module may misunderstand the expression or issue some error messages when reading the function entry. Avoid entering functions like the one below.

```
FUNCTION GHSERXY  298.15
-1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```

Such a function is read by the DATA module as

```
1000+1058*T-38.9*T*LOG(T)+GFUNXY#
```

rather than

```
-1000+1058*T-38.9*T*LOG(T)+GFUNXY#
```

This is because the DATA module concatenates all lines and removes extra spaces before trying to enter the function in the GIBBS workspace. Thus, the - sign is taken as a delimiter between 298.15 and 1000, and the function incorrectly becomes:

```
FUNCTION GHSERXY 298.15 1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```

Avoid this mistake by giving at least one empty space as the first character of a new line, such as

```
FUNCTION GHSERXY  298.15
-1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```

which is read correctly as

```
FUNCTION GHSERXY  298.15 -1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```

The lowest-temperature limit (in Kelvin) for the applicability of the (first) TP-Function in a function is normally set by default as 298.15 K, in most cases. However, you can set another limit when it is applicable (according to experimental data and assessments).

An upper-temperature limit (in Kelvin; followed by a Y or N sign) for the applicability of each TP-Function in a function must be given after the semicolon (;) immediately following the specific TP-Function. The highest-temperature limit (in Kelvin) for the applicability of the current function is always followed by the N sign. If a negative number is given as the lowest-temperature limit, it assumes there are breakpoints in pressure for this function. In these cases, it is interpreted as the lowest-pressure limit (in Pascal), and the other limits in the current function is also taken as pressure limit values (in Pascal).

The temperature/pressure limits for the functions are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit. In these cases, an extrapolation is done using the TP-Function valid in the nearest temperature/pressure range.

The optional reference index *{Ref. Index}* is an integer number indicating where to find the particular function in a special reference file. The references are listed when doing the GET_DATA command in the DATA module. They can also be listed in the GIBBS module with the command LIST_DATA with the option R.

For accounting for the reference indices, also see the keyword REFERENCE_FILE.

The reference index field can also be an abbreviation (such as REF:250, REF_002, or REF-SGTE) which denotes the original reference. In this case, the reference cannot be obtained when issuing the DATA command GET_DATA or the GIBBS command LIST_DATA (with the option R).

However, the references directly coded in the database definition file (***setup.TDB) starting with a letter can be shown when issuing the DATA command GET_DATA or the GIBBS command LIST_DATA (with the option N or R). Normally, such references must be located after the LIST_OF_REFERENCE keyword. It is recommended to use reference code names such as REF001, REF018, etc. The reference list, which is generated by the GIBBS command LIST_DATA <file> with the N or R option, is also possible to be directly read by the DATA module.

The DATA module can selectively retrieve functions which are necessary for a defined system from a database that has functions stored in its setup file or SEQ sequential function file, while all other functions irrelevant for the defined system are ignored and are not saved in associated GIBBS and POLY workspaces. Previously, this can only be done for large databases that have functions stored in RND1 random or FTP function files.

Examples

```
FUNCTION GFREE  298.15  1000+GFUNXY#; 6000 N !

FUNCTION GFUNXY 298.15 -1000+200*T+30*T*LOG(T); 6000 N 505 !

FUNCTION G0_CAO 298.15 -663538.11+352.67749*T-57.7533*T*LN(T)

        +5.3895E-03*T**2-8.879385E-07*T**3+575530*T**(-1);

     1400.00 Y -625196.99+78.896993*T-20.40145*T*LN(T)

        -1.112923E-02*T**2+5.1896733E-07*T**3-6917350*T**(-1);

     2900.00 Y -499226.55-490.37695*T+51.95912*T*LN(T)

       -2.961051E-02*T**2+1.4033905E-06*T**3-48114685*T**(-1);
```

```
3172.00 Y -587711.89+375.04117-62.76*T*LN(T);
6000.00 N REF020 !
```

PARAMETER

```
PARAMETER <parameter name> [lowest temp. limit]
[expression 1]; [upper temp. limit 1] Y
[expression 2]; [upper temp. limit 2] Y
[expression 3]; [upper temp. limit 2] Y
   .......... ; ..... Y
[expression n-1]; [upper temp. limit n-1] Y
[expression n]; [upper temp. limit n] N {Ref. Index} !
```

This keyword can appear in both files for database definition and sequential storage, but not in FTP files. After the keyword, a valid < *parameter name*> in some cases should be given.

It is used to define standard Gibbs energies (i.e. the G parameters for Gibbs energy of formations) of all valid end-members of various stoichiometric and solution phases, and excess Gibbs energies (i.e. the L parameters for Gibbs energy of interactions) of all binary, ternary, quaternary or higher-order interactions in various solution phases; both standard Gibbs energies and excess energies can also have parameters for contributions from PT-depended volume variations (i.e. the V0, VA, VC and VK parameters for molar volume, thermal expansivity, bulk modulus, isothermal compressibility and high-pressure fitting parameter), magnetic ordering (i.e. the TC and BM parameters for Curie temperature and Bohr magneton number) and hypothetical electrostatic interactions (i.e. BM parameter for Born functions ωPr,Tr of aqueous solute species).

The general form of a parameter is:

```
<identifier>(<phase>, <constituent array>; <digit>) <xxx>
<expression> <yyy> <keyword Y or N> <zzz> !
```

General Form

Name	***Description***
identifier	The parameter type.
phase	The phase name (maximum 24 characters).
constituent array	The specific constituent array in the phase.

Name	***Description***
digit	The degree of composition-dependent interaction contribution (an integer number from 0 to 9), that is only for excess energy (L), Curie temperature (TC) and Bohr magneton number (BMAGN), as well as for volume-related parameters (V0 or VA or VB or VC or VK); if it is valued as zero, or if it is for the standard Gibbs energy (G) for which the degree is always zero, it can be omitted.
expression	The mathematical relation to describe the parameter.
xxx and yyy	The low and high temperature limits respectively for the applicable temperature range of the parameter expression
keyword Y or N	The indicator on if there is continuation for the parameter expression or not
zzz	The reference index/number for the assessment of this parameter;
!	The exclamation mark is used to indicate that the current parameter definition is ended

GIBBS Parameter Name

The GIBBS parameter name has a general form of:

```
<identifier>(<phase>,<constituent array>;<digit>)
```

Type-Identifier and Definition

The GIBBS parameter name consists of several parts. The first is a *type-identifier*. The following type-identifiers are legal:

Type-Identifier	***Definition***
G	Standard energy parameter (Gibbs energy of formation)
L	Excess energy parameter (Gibbs energy of interaction)
TC	Curie temperature for magnetic ordering
BMAGN or BM	Bohr magneton number for magnetic ordering (or Born function ω Pr,Tr for aqueous solute species).
LNTHETA1, LNTHETA2, LNTHETA3, LNTHETA4, and LNTHETA5	$ln(\Theta)$ where Θ is the Einstein temperature. Used by the general Einstein model and together with a corresponding THETAF parameter with the same number. See General Einstein Model in the *Database Optimization User Guide*.

Type-Identifier	***Definition***
	This parameter is only available with GES6.
THETAF1, THETAF2, THETAF3, THETAF4, and THETAF5	A weight function used together with a corresponding LNTHETA parameter with the same number. Used by the general Einstein model. See General Einstein Model in the *Database Optimization User Guide*. This parameter is only available with GES6.
V0	Molar volume at 298.15 K and 1 bar (a numeric value only)
VA	Integrated thermal expansivity $\int_{298.15}^{T} \alpha(T)dT$
VC	High-pressure fitting parameter
VK	Isothermal compressibility
VISC	RT*ln(η) where η is the dynamic viscosity
ELRS	Electric resistivity
THCD	Thermal conductivity
SIGM	Surface tension of a liquid end-member
XI	Surface tension dampening factor/interaction for one constituent in a two-constituent combination. See the examples for how to use these parameters
ECij	Elastic constant parameter
ECijMAG	Scaling factor for magnetic contribution to elastic constants

Examples

Parameter	Definition
`G(GAS,C1O2)`	The Gibbs energy of formation of a CO2 molecule in gas.
`G(FCC,FE:VA)`	The Gibbs energy of formation of fcc Fe with interstitials.
`L(LIQ,Fe,Cr;0)`	The regular solution parameter for Fe and Cr in liquid.
`L(LIQ,Fe,Cr;1)`	The sub-regular solution parameter.
`TC(BCC,Fe:Va)`	The Curie temperature of bcc Fe.
`BMAGN(BCC,Fe:Va)`	The Bohr magneton number parameter of bcc Fe.
`SIGM(LIQUID,AL;0)`	Surface tension of Al in LIQUID. Constant value or linear temperature dependence.
`XI(LIQUID,AL,CU;0)`	Surface tension dampening factor for Al in the Al-Cu combination in LIQUID. Constant value.
`XI(LIQUID,AL,CU;1)`	Surface tension dampening factor for Cu in the Al-Cu combination in LIQUID. Constant value.
`EC11(HCP_A3, TI:VA;0)`	The regular solution parameter for elastic constant C11 of HCP Ti with interstitials.
`EC11MAG(BCC_A2, FE:VA; 0)`	The scaling factor for the magnetic contribution to elastic constant C11 for BCC Fe with interstitials.

You can also use G for interaction parameters; and on output list (performed by the GIBBS command LIST_PARAMETER or LIST_PHASE_DATA) the type-identifier L is always used for interaction parameters. Note that the type-identifier BM is also used for Born functions ωPr,Tr of aqueous solute species.

The identifier must be followed by an opening parenthesis, a phase name, a comma and a constituent array. Optionally, the constituent array can be followed by a semicolon and a digit. The parameter name is terminated by a closing parenthesis.

It is important that if a phase bears a legal phase-type (among G, A, Y, L, I, F and B) in its phase definition (already by the PHASE keyword; such as GAS:G, LIQUID:L, SLAG:L, IONIC_LIQ:Y, SPINEL:I, FCC_L12:F, HCP_D021:F, BCC_B2:B, AQUEOUS:A), such a valid phase-type code should not be attached to the phase name in the PARAMETER keyword.

Specifying the phase name in UPPER-case is recommended. You can define a phase name as a mixture of UPPER-case and lower-case letters in a database, but the DATA module automatically converts all lower-case to UPPER-case because the GIBBS module only recognizes UPPER-case phase names.

The *constituent array* consists of a list of constituent names. Interaction parameters have two or more constituents from the same sublattice separated by a comma. If the phase has sublattices, at least one constituent in each sublattice must be specified. The exception is if the phase is ionic liquid (specified with the "phase bit" :Y), then neutral endmember and interaction parameters are written as if the first sublattice does not exist, e.g. PARAM G (IONIC_LIQ,FEO3/2;0), i.e. the constituent array does not contain any constituents from the first (cation) sublattice.

For more ionic liquid specific parameters, see Parameters for the Two Sublattice Ionic Liquid Model.

The constituents in different sublattices must be given in sublattice order and are separated by a colon.

After the component array, a sub-index digit can be specified after a semicolon. This digit must be in the range 0 to 9. The interpretation of the sub-index depends on the excess energy model used for the phase. If no semicolon and digit are given, the sub-index value is assumed to be as zero.

The excess energy parameters, e.g. the regular/subregular (binary) parameter or ternary parameters, are multiplied with two or more fractions of the constituents from the same sublattice of the solution phase. These additional constituents must be given as interacting constituents.

Be careful about the sign of odd terms, for example, L(BCC, B, A:VA;1) is treated as L(BCC,A,B:VA;1), i.e. it is always put into alphabetical order.

Solution phases with sublattices may have interacting constituents in each sublattice.

You can use an asterisk (*) to denote that the excess interaction parameter is independent of the constituents of a specific sublattice. For example, L(FCC_L12,AL,NI:*) means that the interaction parameter is for the binary interaction between constituents AL and NI on the first sublattice in the FCC_L12 solution phase, while it is independent of all constituents on the second sublattice. A interaction parameter in the list of constituents is always added to the Gibbs energy and the asterisk (*) is calculated with the term of [1-∑y(specified constituents)], which implies that in an A-B binary system the following three L parameters are identical (but in higher-order systems, they are different):

- `L(phase,A,B)`is multiplied with`X(A)*X(B)`
- `L(phase,A,*)`is multiplied with`X(A)*(1-X(A))`
- `L(phase,B,*)`is multiplied with`X(B)*(1-X(B))`

A parameter always starts with a lowest temperature limit of its applicability, followed by one or more (up to 10) expressions (TP-Functions) coded as mathematical relations of constants, functions of stable variables (T and P) and entered functions (normally with a # suffix, e.g. +3*GSERAL#).

The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers). Unary-functions LN or LOG (both for natural logarithm) and EXP (for exponential) can also be used.

There is also the Einstein function GEIN available:

```
GEIN(THETA) = 1.5*R*THETA + 3*R*T*LN(1-EXP(-THETA/T))
```

General Einstein Model

Each expression (TP-Function) should ends with a semicolon (;) and be followed by its upper applicable temperature limit and a continuation indicator (Y to continue with the next expression, or N to end the parameter’s expression). If there is no continuation after a specific expression (TP-Function), the reference index can be optionally given after the N indicator.

A complete/valid parameter entry can be written in several continuation lines if the parameter’s expression (TP-Function) is too long or if there is more than one applicable expression (TP-Function), as the maximum length of each line is 78 characters.

It is recommended to always have at least one empty space at the beginning of each continuation line. Avoid entering parameters such as:

```
PARAMETER G(LIQUID,A,B) 298.15
-2000+4568*T+2*GFUNAB#; 6000 N !
```

Such a parameter is read by the DATA module as 2000+4568*T+2*GFUNAB#, rather than as -2000 +4568*T+2*GFUNAB#.

Avoid this mistake by giving at least one empty space as the first character of a new line, such as

```
PARAMETER G(LIQUID,A,B) 298.15
-2000+4568*T+2*GFUNAB#; 6000 N !
```

The lowest-temperature limit (in Kelvin) for the applicability of the (first) TP-Function in a parameter is normally set by default as 298.15 K, in most cases; however, you can set another limit when it is applicable (according to experimental data and assessments). An upper-temperature limit (in Kelvin; followed by a Y or N sign) for the applicability of each TP-Function in a parameter must be given after the semicolon (;) immediately following the specific TP-Function; and the highest-temperature limit (in Kelvin) for the applicability of the current parameter is always followed by the N sign. If a negative number is given as the lowest-temperature limit, it is assumed that there are breakpoints in pressure for this parameter. In such cases, it is interpreted as the lowest-pressure limit (in Pascal), and the other limits in the current parameter are also taken as pressure limit values (in Pascal).

The temperature/pressure limits for the parameters are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit. In these cases, an extrapolation is done using the TP-Function valid in the nearest temperature/pressure range.

The optional reference index *{Ref. Index}* is an integer number indicating where to find the particular parameter in a special reference file. The references are listed when doing the GET_DATA command in the DATA module. These can also be listed in the GIBBS module with the command LIST_DATA and the option R or N.

For accounting the reference indices, also see the keyword REFERENCE_FILE.

The reference index field can also be an abbreviation (such as REF:250, REF_002, or REF-SGTE) denoting the original reference. In this case, the reference cannot be obtained when issuing the DATA command GET_DATA or the GIBBS command LIST_DATA (with the option R or N).

However, the references directly coded in the database definition file (***setup.TDB) that starts with a letter can be shown when issuing the DATA command GET_DATA or the GIBBS command LIST_DATA (with the option R or N). Normally, such references must be located after the LIST_OF_REFERENCE keyword. It is recommended to use reference code names such as REF001, REF018, etc. The reference list, which is generated by the GIBBS command LIST_DATA <file> with the N option, is thus also possible to be directly read by the DATA module.

Examples

```
PARAMETER G(BCC,FE:VA) 298.15 1000+200*T+...; 6000 N 91DIN !
PARAMETER TC(BCC,FE:VA)    298.15 +1043; 6000 N 91DIN !
PARAMETER BMAGN(BCC,FE:VA) 298.15 +2.22; 6000 N 91DIN !
PARAMETER G(SIGMA,FE:CR:CR;0) 298.15 1000+200*T+...; 6000 N 101 !
PARAMETER G(LIQUID,AL;0)  298.15  +11005.553-11.840873*T
        +7.9401E-20*T**7+GHSERAL#;
933.60 Y +10481.974-11.252014*T+1.234264E+28*T**(-9)+GHSERAL#;
   2900.00 N  REF:283 !
PARAMETER G(BCC_A2,PB:C)   298.15 UN_ASS#; 300 N REF:0 !
PARAMETER G(BCC_A2,NI:C;0) 298.15 +GHSERNI#+3*GHSERCC#
                                    +400000-100*T; 6000 N REF071 !
PARAMETER G(BCC_A2,MN:VA)  298.15 +GMNBCC#; 6000 N REF285 !
PARAMETER G(PHASE,A:B) 298.15 +3*GEIN(800); 6000 N 101 !
PARAMETER BM(AQUEOUS,OH-1) 298.15 +Z0002PW0#; 1600 N 155 !
PARAMETER L(BCC,FE,CO:VA;0) 298.15 1000+200*T+...; 6000 N !
PARAMETER L(BCC,FE,CO:VA;1) 298.15 1000+200*T+...; 6000 N !
PARAMETER L(BCC,FE,CO:VA;2) 298.15 1000+200*T+...; 6000 N !
PARAM    TC(BCC_A2,CO,MO:VA;0) 298.15  -3700;    6000 N R454 !
PARAM    TC(BCC_A2,CO,MO:VA;1) 298.15  +2300;    6000 N R454 !
PARAM BMAGN(BCC_A2,CO,MO:VA;0) 298.15 -3.445;    6000 N R454 !
PARAM V0(BCC_A2,CR,FE:VA;0) 298.15 +ZERO#; 6000 N REF06V !
PARAM V0(BCC_A2,CR,FE:VA;1) 298.15 -1.10524097E-7; 6000 N REF06V !
```

```
PARAM V0(BCC_A2,CR,FE:VA;2) 298.15 +1.40024130E-7; 6000 N REF06V !
```

```
PARAM VA(BCC_A2,CR,FE:VA;0) 298.15 -6.49444634E-6*DELTAT#; 6000 N
REF06V !
```

```
PARAM VA(BCC_A2,CR,FE:VA;1) 298.15 +2.91269321E-5*DELTAT#; 6000 N
REF06V !
```

Parameters for the Two Sublattice Ionic Liquid Model

For the two sublattice ionic liquid model (specified with the "phase bit" :Y in the phase declaration), there are some additional requirements on the allowed parameters. While in the regular case all combinations of a phase's constituents are allowed as end-members, there are some constraints on the allowed parameters for ionic liquid.

In the ionic liquid model, the vacancy has been given an "induced" charge -Q, where Q is the average charge of the first (cation) sublattice.

All allowed parameters are listed below. The following notations are used:

- `C`= Cation
- `C1`= Cation 1 if more than one. Similar for anions and neutrals.
- `A`= Anion
- `VA`= Vacancy
- `N`= Neutral
- `D`= Anion or vacancy or neutral (i.e. anything on the second sublattice)

The phase description is:

```
(C1,C2…Ci)P(A1,A2...Ai,VA,N1, N2...Ni)Q
```

In the ionic liquid model,the Vacancy has been given an "induced" charge -Q, where Q is the average charge of the first (cation) sublattice.

Allowed end-members, assuming the phase name is IONIC_LIQ:

```
G(IONIC_LIQ,C:A;0)
```

```
G(IONIC_LIQ,C:VA;0)
```

```
G(IONIC_LIQ,N;0)
```

(The last line is an exception to the case that the constituent array must contain constituents from all sublattices)

This leaves one not allowed end-member:

```
G(IONIC_LIQ,C:N;0)
```

Allowed binary interaction parameters, where i is the interaction order in a Redlich-Kister expansion.

```
G(IONIC_LIQ,C1,C2:A;i)
G(IONIC_LIQ,C1,C2:VA;i)
G(IONIC_LIQ,C:VA,N;i)
G(IONIC_LIQ,N1,N2;i)
G(IONIC_LIQ,C:A1,A2;i)
G(IONIC_LIQ,C:A,VA;i)
G(IONIC_LIQ,C:A,N;i)
```

No other binary interactions are allowed.

Allowed ternary interaction parameters. The interaction is composition independent if there is one parameter with i = 0. It is composition dependent if there are three parameters with i = 0, 1 and 2. There can only be one or three parameters for one combination of constituents

```
G(IONIC_LIQ,C1,C2,C3:A;i)
G(IONIC_LIQ,C1,C2,C3:VA;i)
G(IONIC_LIQ,N1,N2,N3;i)
G(IONIC_LIQ,C1,C2:VA,N;i)
G(IONIC_LIQ,C:VA,N1,N2;i)
G(IONIC_LIQ,C:A,D1,D2;i)
G(IONIC_LIQ,C1,C2:A,D;i)
```

No other ternary interactions are allowed.

OPTIONS

```
OPTIONS /[alloy name]([composition limitations for all alloying
elements]) !
```

This keyword defines an alloy in a database. An alloy has a name, a major component and a number of alloying elements. The purpose for defining an alloy is to be able to tell you about applicable composition limits of the current database in applications to that particular type of alloy. It is possible to have several alloys in the same database. The alloys are given after the keyword in the database.

The alloy name must be proceeded by a slash (`/`) and terminated by the opening parenthesis, with no spaces are allowed in between.

- The alloy name is maximum 8 characters.
- After the parenthesis, follows the major element and a parenthesis with its minimum mass and minimum mole percent given inside.
- Then, the alloying element names, each with its maximum mass and mole percent are given within parenthesis.
- There must a space between definitions for each alloying element.
- The alloy definition is terminated by a closing parenthesis, and the whole OPTIONS keyword by the exclamation mark (`!`).

Example

```
OPTIONS /SSteel(Fe(60,60) CR(30,30) NI(15,15) SI(1,1) N(.1,1)) !
```

TABLE

❗ It is recommended to always have at least one empty space at the beginning of each continuation line. Otherwise, the DATA module may issue some error messages when reading the table entry.

```
TABLE [name]*8 [start temp] [end temp] [delta temp] [table values] !
```

This keyword can appear in both files for database definition and sequential storage, but not in FTP files. It makes a table of Gibbs energy as a function of temperature where the values are given from the start temperature to the end temperature, at a step of the delta temperature.

Example

```
TABLE DEMTAB 1000.0 1500.0 100.0 -2912.9008 -2834.2416 -2755.5824
              -2677.7600 -2600.7744 -2524.2072 !
```

ASSESSED_SYSTEMS

```
ASSESSED_SYSTEM [descriptions on special treatments for specific
assessed systems]*8000 !
```

This keyword can be included in the database definition file (the `***setup.TDB` file). A maximum of 8000 characters after the keyword (to describe some special options when the DATA, GIBBS and POLY models deal with the existing systems with assessed data) is allowed until the exclamation mark (`!`).

Several ASSESSED_SYSTEMS keywords can be used in the same TDB file in order to have more lists of assessed systems. There is no limit to the number of the entries in the same TDB file.

The assessed systems in the database, and the special treatment options, are typed after the keyword. The elements (always in UPPER CASE) in each assessed system must be in alphabetical order and be separated by a hyphen, such as `C-FE` for the Fe-C binary system, and `C-CR-FE` for the Fe-Cr-C ternary system. A space must be between each assessed system. Information on assessed binary, ternary or higher-order systems may also be given in this way.

A ternary system like C-CR-FE does not imply that the binary C-CR, C-FE and CR-FE are assessed. There is no way to indicate partially assessed systems.

- There is a field to give some descriptive information for a specific system, with various options about how to:
- Reject or restore phase(s) from the current database in the DATA module;
- Set major constituent(s) in the first composition set and to set a second composition set for a specific phase available in the current database in the GIBBS module; *and*
- Calculate this specific system in the POLY module.
- This is the facility used by the BIN (binary phase diagrams) and TERN (ternary phase diagrams) modules in the Thermo-Calc software/database package.

The descriptive information must immediately follow the specific system name, and must be enclosed within parenthesis `(` and `)`, and the left parenthesis must follow directly after the system, such as :

```
AL-NI(TDB +L12 ;G5 C—S:L12/NI:AL:VA ;P3 STP:.8/1200/1 STP:.2/600/1)
```

The syntax TDB means that the commands to the DATA module proceed, and +L12 in the example means that the phase called L12 should be restored (it has been rejected by default).

The directive `;G5` means that the following are commands to the GIBBS module. `C_S:` means creating a second composition set, after the colon follows the phase name and after the slash the major constituents.

After the directive `;P3` follows commands to the POLY module. `STP:` means setting a start point with the value of the X-axis first (composition for the second element in a binary system), the slash separates the Y-axis value (temperature), and possibly one or more directions (`-1`, `1`, `-2` or `2`).

A summary of the allowed syntax is:

TDB accepts

- `+phase` and `-phase` for restore/reject.
- `;G5` accepts
- `MAJ:phase/constituent-array` for major constituents of the first composition set.
- `C_S:phase/constituent-array` for a second composition set.
- `;P3` accepts
- `TMM:lt/ht` for the low-/high-temperature limits (`lt` and `ht`; for instance `TMM:500/4000`) suitable for calculating phase diagrams and property diagrams of a binary system.
- `*` for a default start point which is set as:
- for a binary system: at the composition X(2nd element)=.1234, temperature `T=1100 K` and with the default directions; or
- for a ternary system: at the compositions X(2nd element)=.1234 and X(3rd element)=.1234 and with the default directions.
- `STP:x/t/d1/d2/d3` for a specific start point in a binary system which is set as at the composition X(2nd element)=x and temperature `T=t` (in K), and with the directions `d1`, `d2` and/or `d3`.
- `STP:x1/x2/d1/d2/d3` for a specific start point in a ternary system which is set as at the compositions X(2nd element)=x1 and X(3rd element)=x2 and with the directions `d1`, `d2` and/or `d3`.
- The direction(s) can be defined as `-1`, `1`, `-2` or `2`. If no direction is specified, all default directions are used (meaning no `ADD` command is enforced in the POLY module).

- If only one start point is specified, the direction(s) may be omitted; if more than one start points are specified, at least one direction for each start point must be given for all start points.

Each entry for a specific binary or ternary sub-system can be written in one or several lines (each line with 78 characters).

Other Examples

```
ASSESSED_SYSTEMS
AL-NI(TDB +L12 +BCC_B2 ;G5 C_S:L12/NI:AL:VA
       ;P3 STP:.8/1000/1 STP:.45/700/1 STP:.7/700/1)
AL-PB(TDB -HCP -BCC
       ;G5 MAJ:LIQ/AL MAJ:FCC/AL:VA C—S:LIQ/PB C—S:FCC/PB:VA ;P3 *)
CR-FE(;G5 C—S:BCC/CR:VA ;P3 STP:.6/1200/1/-2/2)
AG-CU(;G5 MAJ:FCC/AG:VA C_S:FCC/CU:VA ;P3 STP:.3/1000)
C-NB(;P3 STP:.9/1100/1)
C-SI(;P3 *)
CO-CR(;G5 MAJ:FCC/CO:VA C_S:FCC/CR:VA ;P3 STP:.1/1100)
CR-FE(TDB -HCP ;G5 C_S:BCC/CR:VA ;P3 STP:.6/1200/1/-2/2)
CR-NI(;P3 *)
CR-W(;G5 MAJ:BCC/W:VA C_S:BCC/CR:VA
       ;P3 TMM:500/4000 STP:.3/700/1 STP:.3/1800/2 )
CU-FE(TDB -HCP ;G5 MAJ:LIQ/CU MAJ:FCC/FE:VA C_S:FCC/CU:VA
       ;P3 STP:.9/1400)
FE-N(TDB +FE4N ;P3 *)
FE-O(TDB -LIQUID +IONIC ;G5 C_S:ION_LIQ/FE+2:O-2 MAJ:ION_LIQ/FE+2:VA
      ;P3 STP:.2/2000/1 )
FE-S(TDB -LIQUID +IONIC ;G5 C_S:ION_LIQ/FE+2:S MAJ:ION_LIQ/FE+2:S-2
;P3 *)
AL-MG-SI(;P3 *)
C-CR-FE ;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA ;P3 *) !
```

The semicolon (`;`) is a part of the `;G5` and `;P3` directives. A long descriptive information can be written in more than one line, such as for the `AL-NI`, `AL-PB` , `CU-FE` and `FE-O` systems shown above.

The directive `;P3 *` is needed if the default start point should be used. If there is no `P3` directive, the BIN or TERN module generates some 20 different start points in order to cover all possible compositions and temperatures (for a binary system) or all possible compositions (for a ternary system under any specific temperature).

REFERENCE_FILE

```
REFERENCE_FILE [file name] !
```

This keyword takes a reference file name as its argument. This reference file (that must be edited in a restrictive way and be saved as a blocked file with a fixed line-length for each line in the file, as described below) contains a complete list of the references for the various parameters (and sometimes functions) in the database. The file must have a fixed record structure: each reference entry with one or several records, and each record with exactly 78 characters written in one single blocked line; and no empty space is allowed at the beginning of all lines in the file. If there are more than one record entered for a reference entry, all the continuation lines must start with an ampersand (`&`). The line number of the first record for a specific reference entry is then accounted as the unique integer for that specific reference, which is referred when a parameter or function calls this integer as the optional *{Ref. Index}*.

Keywords PARAMETER or FUNCTION have information about specifying a reference index.

Example

```
/-1<G>            T.C.R.A.S. Class 1

AG1.64TE1         THERMODATA 01/93

&28/01/93

&SILVER 1.64-TELLURIDE. Solid Standard State.

AG1               HULTGREN SELECTED VAL.        SGTE **

&AT.WEIGHT 107.870,STANDARD STATE:CODATA KEY VALUE.MPT=1234.93K. &--
U.D. 30/10/85.

AG1<G>            T.C.R.A.S  Class: 1

AG1/+1<G>         T.C.R.A.S  Class: 1

AG1BR1            N.P.L.                        SGTE **

&Tfusion uncertain and heat vaporization estimated.

AG1BR1<G>         THERMODATA 01/93

&28/01/93

&Gaseous Standard State.

AG1BR1O3          BARIN & KNACKE.SUPPL.REF:62,* SGTE **

&AGO3BR   SILVER OXYTRIBROMIDE
```

In the example, the unique integers of related references (for assessed elements, species, phases, interactions, etc.) are:

```
1/-1<G>
2AG1.64TE1
5 AG1
8AG1<G>
9AG1/+1<G>
10AG1BR1
12AG1BR1<G>
15AG1BR1O3
```

LIST_OF_REFERENCE

```
LIST_OF_REFERENCE
NUMBER SOURCE
  [REFxxx]  '[Detailed reference]'
..........
.......... !
```

This keyword starts a reference list that is directly coded in the database definition file (`***setup.TDB`). Its argument begins on the following line, and normally has an explanation line (NUMBER SOURCE) that is followed by various reference codes. Each reference code may occupy one or more lines (each line with maximum 78 characters), but must have a reference code name (that starts with a letter) and the detailed reference information (that is written within two single-quotation marks, `''`). It is recommended to use reference code names such as `REF001`, `REF018`, etc. A maximum of 400,000 characters after the keyword is allowed until the exclamation mark (`!`).

Such a reference list can be shown when issuing the DATA command GET_DATA or the GIBBS command LIST_DATA (with the `R` option). The reference list, which is generated by the GIBBS command LIST_DATA `<file>` with the `N` option, has this structure, and is thus possible to be directly read by the DATA module.

Example

```
LIST_OF_REFERENCES
 NUMBER  SOURCE
 REF283 'Alan Dinsdale, SGTE Data for Pure Elements,
          Calphad Vol 15(1991) p 317-425,
          also in NPL Report DMA(A)195 Rev. August 1990'
 REF224 'P-Y Chevalier, Thermochimica Acta, 130 (1988) p 33-41; AG-
SI'
 !
```

ADD_REFERENCE

```
ADD_REFERENCE
  [REFxxx]  '[Detailed reference]'
..........
.......... !
```

Use this keyword to have an unlimited number of references. The use of this is the same as that of LIST_OF_REFERENCE, and is used after it. Several `ADD_REFERENCES` sections can be used in a single database if there are too many references.

It is recommended to always start with a so-called *empty reference* (such as the `DUMP0` reference in the following example) as the first entry in each of the `ADD_REFERENCE` sections to make sure that all references are listed appropriately as retrieving data by issuing the GET_DATA command.

Example

```
ADD_REFERENCE
   DUMP0  'Empty reference 0'
   REF4 'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92
          TRITA 0270 (1986); CR-FE'
   REF5 'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636
          TRITA 0207 (1986); C-CR-FE'
   REFS 'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys
Database,
          v1.2; Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters
          at high temperatures.'
   ... ...
 !
ADD_REFERENCE
   DUMP1  'Empty reference 1'
   REF275 'A. Fernandez Guillermet, Z. Metallkde. Vol 79(1988) p.524-
536,
          TRITA-MAC 362 (1988); C-CO-NI AND C-CO-FE-NI'
   REF393   'K. Frisk, Metall. Trans. Vol 21A (1990) p 2477-2488,
          TRITA 0409 (1989); CR-FE-N'
   REF1096  'P. Gustafson, Metall. Trans. 19A(1988) p 2547-2554,
```

```
         TRITA-MAC 348, (1987); C-CR-FE-W'
  ... ...
!
```

CASE and ENDCASE

```
CASE [ELEMENT/SPECIE/PHASE] !
  IF (boolean algebra on element, species or phase names) THEN
       [GIBBS/POLY/DATA command] !
ENDCASE !
```

This keyword takes as its argument, a definition on which type of the following Boolean algebra operates. A simple Boolean algebra using `AND` and `OR` with a maximum of four levels of parentheses works. The `CASE` construction must end with the `ENDCASE` keyword. This makes it possible to have additional GIBBS or POLY commands executed depending on the user selection of elements, species or phases. The DATA commands that can be given as secondary keyword to DEFAULT_COMMAND can also be executed.

Example 1

```
CASE ELEMENT !
   IF((CR OR TI OR V) AND N)
   THEN GES AM_PH_DES @ C_S ,, CR MO TI V:C N: !
 ENDCASE !
```

Example 2

```
CASE ELEMENT !
   IF(O) THEN TDB DEFINE_SYSTEM_ELEMENT /- !
 ENDCASE !
```

Example 3

```
CASE ELEMENT !
   IF(AL AND FE)
   THEN TDB DEF_SYS_ELEMENT VA !
 ENDCASE !
```

VERSION_DATA

```
VERSION_DATE [string]*78 !
```

The string is denoted as the version/revision date and database manager of the database. Nowadays, this directive is used mainly for the purpose of keeping the development and revision history mostly updated.

Example

```
VERSION_DATE Last update and adjustment: Database Manager, 2015-09-25
!
```

Working with the Mobility Databases

In this section:

Extensions to Database Definition File Syntax

Software packages for simulation of diffusional phase transformations, such as the Diffusion Module (DICTRA) and Precipitation Module (TC-PRISMA), need both thermodynamic data and kinetic data (i.e. diffusivities or mobilities). Naturally, the handling and storage of kinetic data also benefits from the use of some kind of database management. Thus, the TDB database definition file syntax has been extended to incorporate some keywords needed for storing kinetic data - PARAMETER, DIFFUSION, and ZEROVOLUME_SPECIES .

PARAMETER

```
PARAMETER [special GIBBS parameter name] [low temp. limit]
[expression 1]; [upper temp. limit 1] Y
[expression 2]; [upper temp. limit 2] Y
[expression 3]; [upper temp. limit 2] Y
   .......... ; ..... Y
[expression n-1]; [upper temp. limit n-1] Y
[expression n]; [upper temp. limit n] N {Ref. Index} !
```

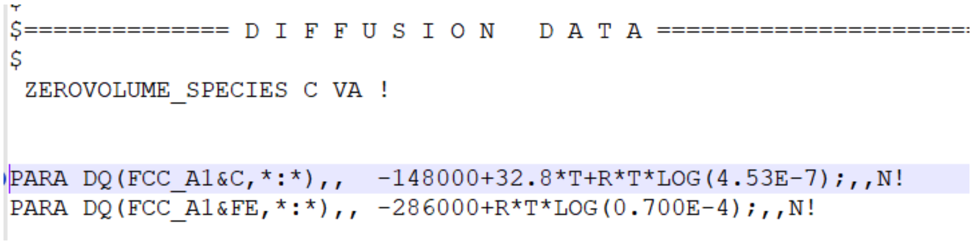
This keyword allows you to enter all types of normal GIBBS parameters for thermodynamic data as well as five special extensions suitable for kinetic data used in the Diffusion Module (DICTRA).

Valid extensions to special GIBBS parameter names are:

- `MQ`: Activation enthalpy for mobility equation.
- `MF`: Pre-exponential factor for mobility equation.
- `DQ`: Activation enthalpy for diffusivity equation.
- `DF`: Pre-exponential factor for diffusivity equation.
- `VS`: Volume counted per mole of volume carrying species.

Example

See the TDB file for DICTRA example *exa4: Carburization of binary Fe-C alloy: Comparison to an analytical erf solution*. Press F1 in Thermo-Calc to search the help for more information.



```
$============== D I F F U S I O N   D A T A =====================
$
 ZEROVOLUME_SPECIES C VA !


PARA DQ(FCC_A1&C,*:*),,  -148000+32.8*T+R*T*LOG(4.53E-7);,,N!
PARA DQ(FCC_A1&FE,*:*),, -286000+R*T*LOG(0.700E-4);,,N!
```

DIFFUSION

```
DIFFUSION [model keyword] [phase name] [additional parameter(s)] !
```

This keyword specifies the type of diffusion model to use for a phase if the default model is not desired. The default model calculates the full diffusion matrix. A diffusivity is calculated from the different mobilities and the thermodynamic factors. The former ones are calculated as:

```
M = exp (∑MF/RT) exp (∑MQ/RT) / RT
```

where ∑ stands for a weighted summation of the different MF’s and MQ’s plus possibly a Redlich-Kister term.

Valid Model Keywords

Keyword	*Description*
NONE	No diffusion in this phase
DILUTE	Constitution list of dependent species in each sublattice must be given as an additional parameter. Only the diagonal terms in the diffusion matrix are calculated. D = exp (∑ DF/RT) exp (∑DQ/RT).
SIMPLE	Constitution list of dependent species in each sublattice must be given as additional parameter. Only the diagonal terms in the diffusion matrix are calculated. D = ∑ DF + ∑ DQ.
MAGNETIC	The so-called ALPHA and ALPHA2 parameters must be given as additional parameters. ALPHA is for the substitutional magnetic model and ALPHA2 for the interstitial one. By appending an `&` sign and a species name after the alpha keyword one can supply individual values for the different species. The full diffusion matrix is calculated.

Examples

```
DIFFUSION NONE SIGMA !

DIFFUSION DILUTE CEMENTITE : FE : C : !

DIFFUSION MAGNETIC BCC_A2 ALPHA=0.3 ALPHA2&C=1.8 ALPHA2&N=0.6 !
```

ZEROVOLUME_SPECIES

```
ZEROVOLUME_SPECIES [list of species] !
```

In the Diffusion Module (DICTRA), the assumption that the volume is carried by the substitutional elements only is applied. The interstitial elements are assumed to have zero molar volumes. This keyword uses a list of which species are to be considered as zero volume ones for an argument.

There is no underscore (_) between *Zero* and *Volume*.

Example

```
ZEROVOLUME_SPECIES VA C N !
```

Database Definition File Examples

In this section:

Example 1: A Steel Database

```
TEMP-LIM 500.0 2000.0 !
$
$ELEMENT, NAME, REF.STATE, ATOMIC-MASS, H0, S0 !
 ELEMENT VA VACUUM             0.0    0.0 0.0 !
 ELEMENT C  GRAPHITE          12.011  0.0 0.0 !
 ELEMENT V  BCC               50.9415 0.0 0.0 !
 ELEMENT CR BCC-PARAMAGNETIC 51.996  0.0 0.0 !
 ELEMENT FE FCC-PARAMAGNETIC 55.847  0.0 0.0 !
 ELEMENT NI FCC-PARAMAGNETIC 58.69   0.0 0.0 !
 ELEMENT MO BCC               95.94   0.0 0.0 !
 ELEMENT W  BCC              183.85   0.0 0.0 !
$
$PHASE, NAME, TYPE, NR-OF-SUBL, SITES-IN-EACH-SUBL. !
 PHASE BCC       B1M  2 1.0 3.0 !
 PHASE FCC       F2M  2 1.0 1.0 !
 PHASE HCP       0    2 2.0 1.0 !
 PHASE LIQUID    3    2 1.0 1.0 !
 PHASE CEMENTITE 4    2 3.0 1.0 !
 PHASE M23C6     4    2 23.0 6.0 !
 PHASE M7C3      4    2 7.0 3.0 !
 PHASE M6C       4    4 2.0 2.0 2.0 1.0 !
 PHASE SIGMA     0    3 10.0 4.0 16.0 !
 PHASE MU-PHASE  0    3 7.0 2.0 4.0 !
 PHASE R-PHASE   0    3 27.0 14.0 12.0 !
 PHASE GRAPHITE  4    1 1.0 !
$
$CONSTITUENT, PHASE-NAME : CONSTITUENTS !
 CONSTITUENT BCC :V CR FE NI MO W:VA C: !
 CONSTITUENT FCC :V CR FE NI MO W:VA C: !
 CONSTITUENT HCP :CR FE NI:VA C N: !
 CONSTITUENT LIQUID :C V CR FE NI MO W VA:VA C: !
 CONSTITUENT CEMENTITE :CR FE:C: !
 CONSTITUENT M23C6 :CR FE:C: !
 CONSTITUENT M7C3 :CR FE:C: !
```

```
 CONSTITUENT M6C :FE:W:FE W:C: !
 CONSTITUENT SIGMA :FE:V CR MO:FE V CR MO: !
 CONSTITUENT MU-PHASE :FE:MO W:FE MO W: !
 CONSTITUENT R-PHASE :FE:MO :FE MO: !
 CONSTITUENT GRAPHITE :C: !
$
$TYPE_DEFINITIIONS:
 TYPE-DEFINITION 0 SEQ TCPATH\DATA\METDATA\TC-THEREST.TDB !
 TYPE-DEFINITION 1 SEQ TCPATH\DATA\METDATA\TC-BCC.TDB !
 TYPE-DEFINITION 2 SEQ TCPATH\DATA\METDATA\TC-FCC.TDB !
 TYPE-DEFINITION 3 SEQ TCPATH\DATA\METDATA\TC-LIQUID.TDB !
 TYPE-DEFINITION 4 SEQ TCPATH\DATA\METDATA\TC-CARBIDES.TDB !
 TYPE-DEFINITION M SEQ TCPATH\DATA\METDATA\TC-CURIE-BOHR.TDB !
 TYPE-DEFINITION B GES AM-PH BCC MAGNETIC -1 .4 !
 TYPE-DEFINITION F GES AM-PH FCC MAGNETIC -3 .28 !
$
$DEFAULT_COMMANDS:
 DEFAULT-COMMAND DEF_ELEMENT VA !
 DEFAULT-COMMAND REJ_SYS-CONST LIQUID 1 VA !
$DATABASE_INFORMATION:
 DATABASE-INFO The following binary and ternary systems are available: '
  FE-CR-NI by Hertzman'
  FE-MO       Fernandez'
  FE-CR-C     Andersson'
  FE-W-C      Gustafson'
  FE-W        Andersson & Gustafson' !
```

Example 2: A Custom Database for the Sb-Sn Binary System

```
$
$ELEMENT, NAME, REF.STATE, ATOMIC-MASS, H0, S0 !
 ELEM VA VACUUM             0.0    0.0 0.0 !
 ELEM MG HCP(A3)           24.305 0.0 0.0 !
 ELEM SB RHOMBOHEDRAL(A7) 121.75   0.0 0.0 !
 ELEM SN BCT(A5)          118.69   0.0 0.0 !
 ELEM /- ELECTRON-GAS       0      0   0 !
$
$SPECIES, NAME, STOICHIOMETRIC-FORMULA !
 SPECIE MG1 MG1!
 SPECIE MG2 MG2!
 SPECIE MG2+ MG/+2!
 SPECIE SB1 SB1!
 SPECIE SB2 SB2!
 SPECIE SB4 SB4!
 SPECIE SB3- SB/-3!
 SPECIE SB5- SB/-5!
 SPECIE SN1 SN1!
 SPECIE SN4- SN/-4!
$
$PHASE, NAME, TYPE, NR-OF-SUBL, SITES-IN-EACH-SUBL. !
 PHASE BCT        Z 1 1.0!
 PHASE HCP        Z 1 1.0!
 PHASE RHOMBO     Z 1 1.0!
 PHASE GAS:G      Z 1 1.0!
 PHASE LIQUID:L   Z 1 1.0!
 PHASE IONICLIQ:Y Z 2 1 1!
 PHASE SPLIQ:Y    Z 2 1 1!
 PHASE BMG3SB2:I  Z 2 3 2!
 PHASE AMG3SB2:I  Z 2 3 2!
 PHASE MG2SN:I    Z 2 2 1!
 PHASE SBSN       Z 2 1 1!
 PHASE SB2SN3     Z 2 2 3!
$
```

```
$CONSTITUENT, PHASE-NAME : CONSTITUENTS !
 CONSTITUENT RHOMBO :SB SN:!
 CONSTITUENT HCP :MG SN:!
 CONSTITUENT BCT :SB SN:!
 CONSTITUENT GAS:G :MG1 MG2 SB1 SB2 SB4 SN1:
  > Gas phase, using the Ideal EOS and Mixing Model. !
 CONSTITUENT LIQUID:L :SB SN:!
 CONSTITUENT IONICLIQ:Y :MG2+:SB SB3- SN SN4- VA:
  > This is the Ionic Liquid Solution Phase. !
 CONSTITUENT SPLIQ:Y :MG2+:SB SB3- SN SN4- VA:!
 CONSTITUENT BMG3SB2:I :MG2+:SB3- SB5- VA SN4-:!
 CONSTITUENT AMG3SB2:I :MG2+:SB3- VA SN4-:!
 CONSTITUENT MG2SN:I :MG2+ VA:SB3- SN4-:!
 CONSTITUENT SBSN :SB SN:SB SN:!
 CONSTITUENT SB2SN3 :SB:SN:!
$
$DEFAULT_COMMANDS:
 DEFAULT-COM DEF-ELEM VA /-!
 DEFAULT-COM REJ-PHASE LIQUID!
 DEFAULT-COM REJ-PHASE SPLIQ!
$
$TYPE_DEFINITIIONS:
 TYPE-DEFINITION Z SEQ * !
$
$DATABASE_INFORMATION:
 DATABASE_INFO The Sb-Sn system with isentropic temperatures!
$
$VERSION_DATE:
 VERSION_DATE Last update 1986-05-18 11:39:49 !
$
$
$ HERE COMES THE THERMODYNAMIC DATA (expressed in functions &
parameters):
$
 FUNCTION MGLIQUID 298.15 -4630.90976+192.994374*T-34.0888057*T*LOG(T)
   -36544605.6*T**(-2); 6000 N!
$
```

```
 FUNCTION MGSOLID 298.15 -8367.34+143.677876*T-26.1849785*T*LOG(T)
   +4.858E-4*T**2-1.393669E-6*T**3+78950*T**(-1);
    923.00 Y -13804.4772 +202.909445*T-34.0888057*T*LOG(T)
   -3.65446056E7*T**(-2) +1.06753982E28*T**(-9); 6000 N!
$
 FUNCTION SBLIQUID 298.15 9071.98+146.800*T-31.38*T*LOG(T)
   -2.441646E8*T**(-2); 6000 N!
$
 .....
 ..... <more>
$
 FUNCTION LFCT 298.15 -17325.6+5.03600*T; 6000 N!
 FUNCTION GFCTSBSN 298.15 LFCT+SBSOLID+SNSOLID+2948.291+3721.286;
   6000 N!
 FUNCTION ISB 298.15 15000; 6000 N!
 FUNCTION ISN 298.15 47199.9-95.6270*T; 6000 N!
$
 .....
 ..... <more>
$
 PARAMETER G(RHOMBO,SB;0) 298.15 SBSOLID; 6000 N!
 PARAMETER G(RHOMBO,SN;0) 298.15 2035+SNSOLID; 6000 N!
$
 PARAMETER G(HCP,MG;0) 298.15 MGSOLID; 6000 N!
 PARAMETER G(HCP,SN;0) 298.15 32000+SNSOLID; 6000 N!
 PARAMETER G(HCP,MG,SN;0) 298.15 -69566-9.23183*T; 6000 N!
$
 PARAMETER G(BCT,SN;0) 298.15 SNSOLID; 6000 N!
 PARAMETER G(BCT,SB;0) 298.15 1000+SBSOLID; 6000 N!
 PARAMETER G(BCT,SB,SN;0) 298.15 0.5*ISB+0.5*ISN; 6000 N!
 PARAMETER G(BCT,SB,SN;1) 298.15 0.5*ISB-0.5*ISN; 6000 N!
$
 PARAMETER G(IONICLIQ,MG2+:SB3-;0) 298.15 -204389-4.98506*T
   -2.75637E9*T**(-2)+3*MGLIQUID+2*SBLIQUID; 6000 N!
 PARAMETER G(IONICLIQ,MG2+:SN4-;0) 298.15 -98639.5+881.073*T
   -174.523*T*LOG(T)-1.79808E9*T**(-2); 6000 N!
 PARAMETER G(IONICLIQ,MG2+:SB;0) 298.15 SBLIQUID; 6000 N!
```

```
$
 ......
 ...... <more>
$
```

Example 3: A Public Database for the Fe-Cr-C Ternary System

```
$
$   Revision history:
$       Created as PDEMO  by Pingfang Shi  on 2004-10-05
$       Renamed to DFeCrC by Pingfang Shi  on 2006-10-25
$
$ FURTHER MODIFICATIONS:
$ ======================
$ pfs: /20041005 (PDEMO)
$       * Retrieved all definitions from PTERN for the Fe-Cr-C ternary !
$
$ pfs: /20061025 (DFeCrC)
$       * Ignore ELEMENT /- definition.
$       * Modify the L(BCC_A2,FE:C,VA;0) [and L(BCC_A2,CR:C,VA;0)]
$         parameters, in order to avoid BCC-appearance (Fe-C)
$         at temperatures higher than 3900 K.
$           $L(BCC_A2,CR:C,VA;0) 298.15 -190*T;           6000 N REF1 !
$            L(BCC_A2,CR:C,VA;0) 298.15 -190*T; 3000 Y 0; 6000 N REF1 !
$           $L(BCC_A2,FE:C,VA;0) 298.15 -190*T;           6000 N REF3 !
$            L(BCC_A2,FE:C,VA;0) 298.15 -190*T; 3900 Y 0; 6000 N REF3 !
$       * Add Cr into HCP_A3 phase, and
$         add all necessary G0/L parameters (according to SSOL2/TCFE3):
$           G(HCP_A3,CR:VA;0)
$           TC(HCP_A3,CR:VA;0)
$           BMAGN(HCP_A3,CR:VA;0)
$           G(HCP_A3,FE:C;0)
$           G(HCP_A3,CR:C;0)
$           L(HCP_A3,CR:C,VA;0)
$           L(HCP_A3,CR,FE:VA;0)
$       * Add "TMM:300/3000" limits to all three binary joins in the
$           ASSESSED_SYSTEM section.
$       * Change the reference indices, e.g., 101 to REF1, in order to
$           always get the reference list correctly.
$       * Re-arrange database format slightly.
```

```
$       * Updated the DATABASE_INFO section.
$-------------------------------------------------------------------------
$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ DATABASE INFORMATION:
$*************************************************************************
$
 DATABASE_INFO                                   DFeCrC '
               TCS Demo Fe-Cr-C Alloy Solutions Database'
        (only for demonstration purposes in TCC-Demo/TCW-Demo)'
      ******************************************************** '
                          (Version 1.2, Oct. 2006) ''
         Copyright @ 2004-2012: Thermo-Calc Software AB, Sweden ''
The DFeCrC database (previously called PDEMO) is the TCS Demo Fe-Cr-C '
Alloy Solutions Database, which is especially designed for primarily '
demonstrating the uses of: '
  * TCC-Demo software: BIN, TERN, SCHEIL and some other modules; '
  * TCW-Demo software: '
     "Binary" module calculations of phase diagrams and property
diagrams'
                in available binary systems; '
     "Ternary" module calculations of phase diagrams (e.g., isothermal'
                sections, monovariant lines involving liquid, liquidus'
                surface projections) and property diagrams in available'
                ternary systems; '
     "Scheil" module simulations of alloy solidifications; and/or '
     "Equilibrium" calculation routines for phase diagrams and property'
                diagrams in available binary or ternary systems. '
It can also be used for other types of calculations/simulations in both'
TCC and TCW software, and in their application programming interfaces.''
It includes critically-assessed data for all possible three binary joins'
(i.e. Cr-C, Fe-Cr and Fe-Cr) and one complete ternary alloy solutions '
within the Fe-Cr-C system. However, due to the fact that experimental'
data for the Fe-C and Cr-C binary joins and Fe-Cr-C ternary system at '
extremely-high temperatures are not sufficient, the available assessed'
data can not be applied to temperature conditions higher than 4000 K.''
Included thermodynamic data are available for various stoichiometric '
```

```
and solution phases, e.g. liquid mixture, various alloy solutions and '
intermetallic phases. But the gaseous mixture phase is excluded in this'
DEMO version.''
The DFeCrC database can be used not only in calculating various types '
of phase diagrams (binary phase diagrams, ternary isothermal sections,'
ternary monovariant lines involving liquid, ternary liquidus surface '
projections, ternary isopleth sections, etc.) and property diagrams '
(the easiest ways are through the BIN and TERN modules), but also in '
simulating alloy solidification processes (with the SCHEIL module) of'
Fe-based or Cr-based alloys (but limited within the Fe-Cr-C ternary '
system in this DEMO version). Many unique features of the TCC/TCW '
software can be demonstrated using this and other specially-designed '
DEMO databases. ''
However, this DFeCrC database (similar to other DEMO and/or PUBLIC TC '
databases) is provided within the TCC-Demo/TCW-Demo software only for '
the purposes of demonstration, testing and evaluation. For R&D projects'
and teaching activities, you are highly encouraged to only use the FULL'
versions of the TCC and/or TCW software together with some commercial '
databases that are appropriate for your specific applications. Please '
contact us for all kinds of details. ''
Release History: Version 1.1 with minor improvements,  Oct. 2004 '
                 Version 1.2 with minor modifications, Oct. 2006 ''
Edited by: Dr. Pingfang Shi (Thermo-Calc Software, Oct. 2006). ''
 !

$ -----------------------------------------------------------------------
$VERSION_DATE Last update and adjustment: Pingfang Shi, 2004-10-05 !
 VERSION_DATE Last update and adjustment: Pingfang Shi, 2006-10-25 !

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ Definition of Elements in the Database System:
$------------------------------------------------------------------------
$ELEM NAME STABLE_ELEMENT_REF         ATOMIC MASS  H298-H0     S298 !
$------------------------------------------------------------------------
$ELEMENT /-   ELECTRON_GAS            0.0000E+00  0.0000E+00  0.0000E+00!
 ELEMENT VA   VACUUM                  0.0000E+00  0.0000E+00  0.0000E+00!
```

```
 ELEMENT C    GRAPHITE                1.2011E+01  1.0540E+03  5.7400E+00!
 ELEMENT CR   BCC_A2                  5.1996E+01  4.0500E+03  2.3560E+01!
 ELEMENT FE   BCC_A2                  5.5847E+01  4.4890E+03  2.7280E+01!

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ TYPE_DEFINITIONS for data inclusions:
$------------------------------------------------------------------------
 TYPE_DEFINITION % SEQ *!

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$  TYPE_DEFINITIONS for phase descriptions:
$------------------------------------------------------------------------
$... For magnetic contributions:
 TYPE_DEFINITION A GES AMEND_PHASE_DES @ MAGNETIC  -1.0  4.00000E-01 !
 TYPE_DEFINITION B GES AMEND_PHASE_DES @ MAGNETIC  -3.0  2.80000E-01 !

$... For Cr/Fe-C in FCC phase and Cr/Fe-C in HCP phase:
 TYPE_DEFINITION C IF(C) THEN GES AMEND_PHASE_DES @ C_S ,, :C: !

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ Default Commands:
$------------------------------------------------------------------------
$DEFINE_SYSTEM_DEFAULT SPECIES 2 !
 DEFINE_SYSTEM_DEFAULT ELEMENT 2 !

 DEFAULT_COMMAND DEF_SYS_ELEMENT VA !

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ FUNCTIONS for various phases:
$------------------------------------------------------------------------
$
 FUNCT GHSERCC  298.15 -17368.441+170.73*T-24.3*T*LN(T)
     -4.723E-04*T**2+2562600*T**(-1)-2.643E+08*T**(-2)
```

```
    +1.2E+10*T**(-3); 6000 N!
FUNCT GHSERCR  298.15 -8856.94+157.48*T-26.908*T*LN(T)
    +.00189435*T**2-1.47721E-06*T**3+139250*T**(-1);  2180 Y
     -34869.344+344.18*T-50*T*LN(T)-2.88526E+32*T**(-9); 6000 N!
FUNCT GHSERFE  298.15 +1225.7+124.134*T-23.5143*T*LN(T)
    -.00439752*T**2-5.8927E-08*T**3+77359*T**(-1);  1811.00 Y
    -25383.581+299.31255*T-46*T*LN(T)+2.29603E+31*T**(-9); 6000 N!

FUNCT GFELIQ   298.15 +GHSERFE#+12040.17-6.55843*T
    -3.6751551E-21*T**7;  1811 Y
     -10839.7+291.302*T-46*T*LN(T);  6000 N!
FUNCT GFEFCC   298.15 +GHSERFE#-1462.4+8.282*T
    -1.15*T*LN(T)+6.4E-04*T**2;  1811 Y
     -27098.266+300.25256*T-46*T*LN(T)+2.78854E+31*T**(-9);  6000 N!
FUNCT GFECEM   298.15 +GPCEM1#-10745+706.04*T-120.6*T*LN(T); 6000 N!
FUNCT GFEM23C6  298.15 +7.666667*GFECEM#-1.666667*GHSERCC#
    +66920-40*T; 6000 N!

FUNCT GCRFCC   298.15 +GHSERCR#+7284+.163*T;  6000 N!
FUNCT GCRM23C6 298.15 -521983+3622.24*T-620.965*T*LN(T)
    -.126431*T**2;   6000 N!
FUNCT GCRM3C2  298.15 -100823.8+530.66989*T-89.6694*T*LN(T)
    -.0301188*T**2;  6000 N!
FUNCT GCRM7C3  298.15 -201690+1103.128*T-190.177*T*LN(T)
    -.0578207*T**2;  6000 N!

FUNCT GPCLIQ   298.15 +YCLIQ#*EXP(ZCLIQ#);    6000 N!
FUNCT ACLIQ    298.15 +2.32E-05*T+2.85E-09*T**2;  6000 N!
FUNCT BCLIQ    298.15 +1+3.2E-10*P;               6000 N!
FUNCT CCLIQ    298.15 1.6E-10;                    6000 N!
FUNCT DCLIQ    298.15 +1*LN(BCLIQ#);              6000 N!
FUNCT ECLIQ    298.15 +1*LN(CCLIQ#);              6000 N!
FUNCT VCLIQ    298.15 +7.626E-06*EXP(ACLIQ#);     6000 N!
FUNCT XCLIQ    298.15 +1*EXP(.5*DCLIQ#)-1;        6000 N!
FUNCT YCLIQ    298.15 +VCLIQ#*EXP(-ECLIQ#);       6000 N!
FUNCT ZCLIQ    298.15 +1*LN(XCLIQ#);              6000 N!
```

```
FUNCT GPCGRA   298.15 +YCGRA#*EXP(ZCGRA#);    6000 N!
FUNCT ACGRA    298.15 +2.32E-05*T+2.85E-09*T**2;  6000 N!
FUNCT BCGRA    298.15 +1+3.6E-10*P;               6000 N!
FUNCT CCGRA    298.15 3.3E-10;                    6000 N!
FUNCT DCGRA    298.15 +1*LN(BCGRA#);              6000 N!
FUNCT ECGRA    298.15 +1*LN(CCGRA#);              6000 N!
FUNCT VCGRA    298.15 +5.259E-06*EXP(ACGRA#);     6000 N!
FUNCT XCGRA    298.15 +1*EXP(.9166667*DCGRA#)-1;  6000 N!
FUNCT YCGRA    298.15 +VCGRA#*EXP(-ECGRA#);       6000 N!
FUNCT ZCGRA    298.15 +1*LN(XCGRA#);              6000 N!

FUNCT GPCFCC   298.15 +YCFCC#*EXP(ZFEFCC#);   6000 N!
FUNCT ACFCC    298.15 +1.44E-04*T;              6000 N!
FUNCT VCFCC    298.15 +1.031E-05*EXP(ACFCC#);   6000 N!
FUNCT YCFCC    298.15 +VCFCC#*EXP(-EFEFCC#);    6000 N!

FUNCT GPCRLIQ  298.15 +YCRLIQ#*EXP(ZCRLIQ#);    6000 N!
FUNCT ACRLIQ   298.15 +1.7E-05*T+9.2E-09*T**2;  6000 N!
FUNCT BCRLIQ   298.15 +1+4.65E-11*P;            6000 N!
FUNCT CCRLIQ   298.15 3.72E-11;                 6000 N!
FUNCT DCRLIQ   298.15 +1*LN(BCRLIQ#);           6000 N!
FUNCT ECRLIQ   298.15 +1*LN(CCRLIQ#);           6000 N!
FUNCT VCRLIQ   298.15 +7.653E-06*EXP(ACRLIQ#);  6000 N!
FUNCT XCRLIQ   298.15 +1*EXP(.8*DCRLIQ#)-1;     6000 N!
FUNCT YCRLIQ   298.15 +VCRLIQ#*EXP(-ECRLIQ#);   6000 N!
FUNCT ZCRLIQ   298.15 +1*LN(XCRLIQ#);           6000 N!

FUNCT GPCRBCC  298.15 +YCRBCC#*EXP(ZCRBCC#);  6000 N!
FUNCT ACRBCC   298.15 +1.7E-05*T+9.2E-09*T**2;  6000 N!
FUNCT BCRBCC   298.15 +1+2.6E-11*P;             6000 N!
FUNCT CCRBCC   298.15 2.08E-11;                 6000 N!
FUNCT DCRBCC   298.15 +1*LN(BCRBCC#);           6000 N!
FUNCT ECRBCC   298.15 +1*LN(CCRBCC#);           6000 N!
FUNCT VCRBCC   298.15 +7.188E-06*EXP(ACRBCC#);  6000 N!
FUNCT XCRBCC   298.15 +1*EXP(.8*DCRBCC#)-1;     6000 N!
FUNCT YCRBCC   298.15 +VCRBCC#*EXP(-ECRBCC#);   6000 N!
FUNCT ZCRBCC   298.15 +1*LN(XCRBCC#);           6000 N!
```

```
FUNCT GPFELIQ  298.15 +YFELIQ#*EXP(ZFELIQ#);  6000 N!
FUNCT AFELIQ   298.15 +1.135E-04*T;                           6000 N!
FUNCT BFELIQ   298.15 +1+4.98009787E-12*P+3.20078924E-14*T*P; 6000 N!
FUNCT CFELIQ   298.15 +4.22534787E-12+2.71569924E-14*T;       6000 N!
FUNCT DFELIQ   298.15 +1*LN(BFELIQ#);                         6000 N!
FUNCT EFELIQ   298.15 +1*LN(CFELIQ#);                         6000 N!
FUNCT VFELIQ   298.15 +6.46677E-06*EXP(AFELIQ#);              6000 N!
FUNCT XFELIQ   298.15 +1*EXP(.8484467*DFELIQ#)-1;             6000 N!
FUNCT YFELIQ   298.15 +VFELIQ#*EXP(-EFELIQ#);                 6000 N!
FUNCT ZFELIQ   298.15 +1*LN(XFELIQ#);                         6000 N!

FUNCT GPFEFCC  298.15 +YFEFCC#*EXP(ZFEFCC#);  6000 N!
FUNCT AFEFCC   298.15 +7.3097E-05*T;                          6000 N!
FUNCT BFEFCC   298.15 +1+3.25236341E-11*P+3.36607808E-16*T*P; 6000 N!
FUNCT CFEFCC   298.15 +2.62285341E-11+2.71455808E-16*T;       6000 N!
FUNCT DFEFCC   298.15 +1*LN(BFEFCC#);                         6000 N!
FUNCT EFEFCC   298.15 +1*LN(CFEFCC#);                         6000 N!
FUNCT VFEFCC   298.15 +6.688726E-06*EXP(AFEFCC#);             6000 N!
FUNCT XFEFCC   298.15 +1*EXP(.8064454*DFEFCC#)-1;             6000 N!
FUNCT YFEFCC   298.15 +VFEFCC#*EXP(-EFEFCC#);                 6000 N!
FUNCT ZFEFCC   298.15 +1*LN(XFEFCC#);                         6000 N!

FUNCT GPFEBCC  298.15 +YFEBCC#*EXP(ZFEBCC#);  6000 N!
FUNCT AFEBCC   298.15 +2.3987E-05*T+1.2845E-08*T**2;          6000 N!
FUNCT BFEBCC   298.15 +1+2.80599565E-11*P+3.06481523E-16*T*P; 6000 N!
FUNCT CFEBCC   298.15 +2.20949565E-11+2.41329523E-16*T;       6000 N!
FUNCT DFEBCC   298.15 +1*LN(BFEBCC#);                         6000 N!
FUNCT EFEBCC   298.15 +1*LN(CFEBCC#);                         6000 N!
FUNCT VFEBCC   298.15 +7.042095E-06*EXP(AFEBCC#);             6000 N!
FUNCT XFEBCC   298.15 +1*EXP(.7874195*DFEBCC#)-1;             6000 N!
FUNCT YFEBCC   298.15 +VFEBCC#*EXP(-EFEBCC#);                 6000 N!
FUNCT ZFEBCC   298.15 +1*LN(XFEBCC#);                         6000 N!

FUNCT GPFEHCP  298.15 +YFEHCP#*EXP(ZFEHCP#);  6000 N!
FUNCT AFEHCP 298.15 +7.3646E-5*T;                           6000 N!
FUNCT BFEHCP 298.15 +1+32.5236341E-12*P+3.36607808E-16*P*T; 6000 N!
```

```
 FUNCT CFEHCP 298.15 +26.2285341E-12+2.71455808E-16*T;       6000 N!
 FUNCT DFEHCP 298.15 +LOG(BFEHCP#);                          6000 N!
 FUNCT EFEHCP 298.15 +LOG(CFEHCP#);                          6000 N!
 FUNCT VFEHCP 298.15 +6.59121E-6*EXP(AFEHCP#);               6000 N!
 FUNCT XFEHCP 298.15 +EXP(0.8064454*DFEHCP#)-1;              6000 N!
 FUNCT YFEHCP 298.15 +VFEHCP#*EXP(-1*EFEHCP#);               6000 N!
 FUNCT ZFEHCP 298.15 +LOG(XFEHCP#);                          6000 N!

 FUNCT GPCEM1   298.15 +VCEM1#*P;     6000 N!
 FUNCT ACEM1    298.15 -1.36E-05*T+4E-08*T**2;    6000 N!
 FUNCT VCEM1    298.15 +2.339E-05*EXP(ACEM1#);    6000 N!

 FUNCT GPSIG1   298.15 +1.09E-04*P;        6000 N!
 FUNCT GPSIG2   298.15 +1.117E-04*P;       6000 N!

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ Define the various Phase and their Constituents, and
$ Assign parameters to phases:
$------------------------------------------------------------------------
$PHASE  NAME:TYPE  MARKCODE  #SUBL  SITES_IN_EACH_SUBL. !
$------------------------------------------------------------------------

$***** LIQUID (Solution) ************************************************
 PHASE LIQUID:L %  1  1.0
  > This is metallic liquid solution phase, with C species !
 CONST LIQUID:L  : C,CR,FE :  !

 PARAM G(LIQUID,C;0)  298.15 +GHSERCC#+GPCLIQ#
                               +117369-24.63*T; 6000 N REF0 !
 PARAM G(LIQUID,CR;0)  298.15 +GHSERCR#+GPCRLIQ#
                  +24339.955-11.420225*T+2.37615E-21*T**7;  2180 Y
                              +GHSERCR#+GPCRLIQ#
                  +18409.36-8.563683*T+2.88526E+32*T**(-9); 6000 N REF0 !
 PARAM G(LIQUID,FE;0)  298.15 +GFELIQ#+GPFELIQ#;  6000 N REF0 !

 PARAM L(LIQUID,C,CR;0)  298.15 -90526-25.9116*T; 6000 N REF1 !
```

```
 PARAM L(LIQUID,C,CR;1)  298.15 +80000;           6000 N REF1 !
 PARAM L(LIQUID,C,CR;2)  298.15 +80000;           6000 N REF1 !
 PARAM L(LIQUID,C,FE;0)  298.15 -124320+28.5*T;  6000 N REF3 !
 PARAM L(LIQUID,C,FE;1)  298.15  +19300;         6000 N REF3 !
 PARAM L(LIQUID,C,FE;2)  298.15  +49260-19*T;    6000 N REF3 !
 PARAM L(LIQUID,CR,FE;0)  298.15 -14550+6.65*T;   6000 N REF4 !
 PARAM L(LIQUID,C,CR,FE;0)  298.15 -496063;  6000 N REF2 !
 PARAM L(LIQUID,C,CR,FE;1)  298.15  +57990;  6000 N REF2 !
 PARAM L(LIQUID,C,CR,FE;2)  298.15  +61404;  6000 N REF2 !

$***** FCC_A1 (Solution) ************************************************
$PHASE FCC_A1  %BC  2 1   1 !
$ Note the C TYPE_DEF for 2nd FCC composition-set (MC) is not necessary
$    for the (Fe,Cr)-C system.
 PHASE FCC_A1  %B   2 1   1 !
 CONST FCC_A1  : CR,FE%
               : C,VA% :  !

 PARAM G(FCC_A1,CR:VA;0)  298.15 +GCRFCC#+GPCRBCC#;  6000 N REF0 !
 PARAM TC(FCC_A1,CR:VA;0)     298.15 -1109;  6000 N REF0 !
 PARAM BMAGN(FCC_A1,CR:VA;0)  298.15 -2.46;  6000 N REF0 !
 PARAM G(FCC_A1,FE:VA;0)  298.15 +GFEFCC#+GPFEFCC#;  6000 N REF0 !
 PARAM TC(FCC_A1,FE:VA;0)     298.15 -201;  6000 N REF0 !
 PARAM BMAGN(FCC_A1,FE:VA;0)  298.15 -2.1;  6000 N REF0 !

 PARAM G(FCC_A1,CR:C;0)  298.15 +GHSERCR#+GHSERCC#
                                 +1200-1.94*T;     6000 N REF2 !
 PARAM G(FCC_A1,FE:C;0)  298.15 +GFEFCC#+GHSERCC#+GPCFCC#
                                 +77207-15.877*T;  6000 N REF3 !
 PARAM TC(FCC_A1,FE:C;0)     298.15 -201;  6000 N REF3 !
 PARAM BMAGN(FCC_A1,FE:C;0)  298.15 -2.1;  6000 N REF3 !

 PARAM L(FCC_A1,CR:C,VA;0)  298.15 -11977+6.8194*T; 6000 N REF2 !
 PARAM L(FCC_A1,FE:C,VA;0)  298.15 -34671;          6000 N REF3 !
 PARAM L(FCC_A1,CR,FE:VA;0) 298.15 +10833-7.477*T;  6000 N REF4 !
 PARAM L(FCC_A1,CR,FE:VA;1) 298.15  +1410;          6000 N REF4 !
 PARAM L(FCC_A1,CR,FE:C;0)  298.15 -74319+3.2353*T; 6000 N REF2 !
```

```
$***** BCC_A2 (Solution) ************************************************
 PHASE BCC_A2  %A  2 1   3 !
 CONST BCC_A2  : CR%,FE%
               : C,VA% :  !

 PARAM G(BCC_A2,CR:VA;0)  298.15 +GHSERCR#+GPCRBCC#;  6000 N REF0 !
 PARAM TC(BCC_A2,CR:VA;0)     298.15 -311.5;  6000 N REF0 !
 PARAM BMAGN(BCC_A2,CR:VA;0)  298.15   -.01;  6000 N REF0 !
 PARAM G(BCC_A2,FE:VA;0)  298.15 +GHSERFE#+GPFEBCC#;  6000 N REF0 !
 PARAM TC(BCC_A2,FE:VA;0)     298.15 1043;  6000 N REF0 !
 PARAM BMAGN(BCC_A2,FE:VA;0)  298.15 2.22;  6000 N REF0 !

 PARAM G(BCC_A2,CR:C;0)  298.15 +GHSERCR#+3*GHSERCC#+GPCRBCC#+3*GPCGRA#
                                  +416000;            6000 N REF1 !
 PARAM TC(BCC_A2,CR:C;0)     298.15 -311.5;  6000 N REF1 !
 PARAM BMAGN(BCC_A2,CR:C;0)  298.15  -.008;  6000 N REF1 !
 PARAM G(BCC_A2,FE:C;0)  298.15 +GHSERFE#+3*GHSERCC#+GPFEBCC#+3*GPCGRA#
                                  +322050+75.667*T;   6000 N REF3 !
 PARAM TC(BCC_A2,FE:C;0)     298.15 1043;  6000 N REF3 !
 PARAM BMAGN(BCC_A2,FE:C;0)  298.15 2.22;  6000 N REF3 !

$ PF-20061025: Modify the L(BCC_A2,FE:C,VA;0) [and L(BCC_A2,CR:C,VA;0)]
$         parametera, in order to avoid BCC-appearance (Fe-C)
$         at temperatures higher than 3900 K.
$PARAM L(BCC_A2,CR:C,VA;0) 298.15 -190*T;           6000 N REF1 !
 PARAM L(BCC_A2,CR:C,VA;0) 298.15 -190*T; 3000 Y 0; 6000 N REFS !
$PARAM L(BCC_A2,FE:C,VA;0) 298.15 -190*T;           6000 N REF3 !
 PARAM L(BCC_A2,FE:C,VA;0) 298.15 -190*T; 3900 Y 0; 6000 N REFS !
$
 PARAM L(BCC_A2,CR,FE:VA;0) 298.15 +20500-9.68*T;   6000 N REF4 !
 PARAM TC(BCC_A2,CR,FE:VA;0)     298.15 1650;  6000 N REF4 !
 PARAM TC(BCC_A2,CR,FE:VA;1)     298.15  550;  6000 N REF4 !
 PARAM BMAGN(BCC_A2,CR,FE:VA;0)  298.15 -.85;  6000 N REF4 !

 PARAM L(BCC_A2,CR,FE:C;0)  298.15 -1250000+667.7*T; 6000 N REF2 !
```

```
 PARAM TC(BCC_A2,CR,FE:C;0)    298.15 1650;  6000 N REF5 !
 PARAM TC(BCC_A2,CR,FE:C;1)    298.15  550;  6000 N REF5 !
 PARAM BMAGN(BCC_A2,CR,FE:C;0) 298.15 -.85;  6000 N REF5 !

$***** HCP_A3 (Solution) *************************************************
$PHASE HCP_A3  %BC  2 1   .5 !
$ Note the C TYPE_DEF for 2nd HCP composition-set (M2C) is not necessary
$    for the (Fe,Cr)-C system.
 PHASE HCP_A3  %B   2 1   .5 !
 CONST HCP_A3  : CR,FE,
               : VA%,C :  !

 PARAM G(HCP_A3,CR:VA;0) 298.15 +GHSERCR#+4438;           6000 N REF1 !
 PARAM TC(HCP_A3,CR:VA;0)    298.15 -1109;  6000 N REF1 !
 PARAM BMAGN(HCP_A3,CR:VA;0) 298.15 -2.46;  6000 N REF1 !
 PARAM G(HCP_A3,FE:VA;0) 298.15 +GHSERFE#+GPFEHCP#
               -3705.78+12.591*T-1.15*T*LN(T)+6.4E-04*T**2; 1811 Y
                                +GHSERFE#+GPFEHCP#
               -3957.199+5.24951*T+4.9251E+30*T**(-9);      6000 N REF0 !
 PARAM G(HCP_A3,CR:C;0) 298.15 +GHSERCR#+.5*GHSERCC#
               -18504+9.4173*T-2.4997*T*LN(T)+.001386*T**2; 6000 N REF1 !
 PARAM G(HCP_A3,FE:C;0) 298.15 +GFEFCC#+.5*GHSERCC#+GPCFCC#
                                 +52905-11.9075*T;          6000 N REF3 !

 PARAM L(HCP_A3,CR:C,VA;0)  298.15  +4165;  6000 N REF1 !
 PARAM L(HCP_A3,FE:C,VA;0)  298.15 -22126;  6000 N REF3 !
$PARAM L(HCP_A3,FE:C,VA;0)  298.15 -17335;  6000 N TCFE3 !
 PARAM L(HCP_A3,CR,FE:VA;0) 298.15 +10833-7.477*T; 6000 N REF4 !

$***** SIGMA (Solution) **************************************************
 PHASE SIGMA  %  3 8   4   18 !
 CONST SIGMA  : FE
              : CR
              : CR,FE :  !

 PARAM G(SIGMA,FE:CR:CR;0)  298.15 +8*GFEFCC#+22*GHSERCR#
                                +92300-95.96*T+GPSIG1#;   6000 N REF4 !
```

```
 PARAM G(SIGMA,FE:CR:FE;0)  298.15 +8*GFEFCC#+4*GHSERCR#+18*GHSERFE#
                                +117300-95.96*T+GPSIG2#;  6000 N REF4 !

$***** CEMENTITE (Solution) *********************************************
 PHASE CEMENTITE  %  2 3   1 !
 CONST CEMENTITE  : CR,FE%
                  : C :  !

 PARAM G(CEMENTITE,CR:C;0)  298.15 +3*GHSERCR#+GHSERCC#
                                     -48000-9.2888*T; 6000 N REF2 !
 PARAM G(CEMENTITE,FE:C;0)  298.15 +GFECEM#;          6000 N REF3 !

 PARAM L(CEMENTITE,CR,FE:C;0)  298.15 +25278-17.5*T;  6000 N REF2 !

$***** M3C2 (Compound) **************************************************
 PHASE M3C2  %  2 3   2 !
 CONST M3C2  : CR
             : C :  !

 PARAM G(M3C2,CR:C;0)  298.15 +GCRM3C2#;  6000 N REF2 !

$***** M7C3 (Solution) **************************************************
 PHASE M7C3  %  2 7   3 !
 CONST M7C3  : CR%,FE
             : C :  !

 PARAM G(M7C3,CR:C;0)  298.15 +GCRM7C3#;          6000 N REF2 !
 PARAM G(M7C3,FE:C;0)  298.15 +7*GHSERFE#+3*GHSERCC#
                                +75000-48.2168*T; 6000 N REF2 !

 PARAM L(M7C3,CR,FE:C;0)  298.15 -4520-10*T;  6000 N REF2 !

$***** M23C6 (Solution) *************************************************
 PHASE M23C6  %  3 20   3   6 !
 CONST M23C6  : CR%,FE%
              : CR%,FE%
              : C :  !
```

```
 PARAM G(M23C6,CR:CR:C;0)  298.15 +GCRM23C6#;           6000 N REF5 !
 PARAM G(M23C6,FE:CR:C;0)  298.15 +.1304348*GCRM23C6#
                                   +.8695652*GFEM23C6#; 6000 N REF5 !
 PARAM G(M23C6,CR:FE:C;0)  298.15 +.8695652*GCRM23C6#
                                   +.1304348*GFEM23C6#; 6000 N REF5 !
 PARAM G(M23C6,FE:FE:C;0)  298.15 +GFEM23C6#;           6000 N REF5 !

 PARAM L(M23C6,CR,FE:CR:C;0) 298.15 -205342+141.6667*T; 6000 N REF2 !
 PARAM L(M23C6,CR,FE:FE:C;0) 298.15 -205342+141.6667*T; 6000 N REF2 !

$***** GRAPHITE (Compound) ***********************************************
 PHASE GRAPHITE  %  1  1.0  !
 CONST GRAPHITE  : C :  !

 PARAM G(GRAPHITE,C;0)  298.15 +GHSERCC#+GPCGRA#; 6000 N REF0 !

$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ ASSESSED_SYSTEMS information:
$    *  necessary for the BIN and TERN modules in TCC
$                      the Binary Phase Diagram module in TCW
$                  and the Equilibrium calculation routine in TCW
$-------------------------------------------------------------------------
 ASSESSED_SYSTEM
$... Binary ...
  C-FE(;P3 TMM:300/4000 *)
  C-CR(;P3 TMM:300/4000 *)
  CR-FE(;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA
        ;P3 TMM:300/3000 STP:.6/1200/1/-2/2)
$ CR-FE(TDB -HCP ;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA
$       ;P3 TMM:300/3000 STP:.6/1200/1/-2/2)
$
$... Ternary ...
  C-CR-FE(;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA
          ;P3 STP:.4/.5/1 STP:0.1/0.5/1)
 !
```

```
$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$
$ LIST OF REFERENCE:
$
$--------------------------------------------------------------------------
 LIST_OF_REFERENCES
 NUMBER  SOURCE
 REF0 'Alan Dinsdale, SGTE Data for Pure Elements, Calphad Vol 15(1991)
       p 317-425, also in NPL Report DMA(A)195 Rev. August 1990'
 REF1 'J-O Andersson, Calphad Vol 11 (1987) p 271-276, TRITA 0314; C-CR'
 REF2 'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
 REF3 'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267
       TRITA 0237 (1984); C-FE'
 REF4 'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92
       TRITA 0270 (1986); CR-FE'
 REF5 'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636
       TRITA 0207 (1986); C-CR-FE'
 REFS 'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys Database,
       v1.2; Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters
       at high temperatures.'
 !
```

Database Checker

In this section:

About the Database Checker

The Thermo-Calc software package includes a program to check that the syntax of unencrypted database files is correct. The program applies the syntax rules set out in the *Database Manager User Guide* and reports errors and issues warnings. This program is intended for advanced users who develop and manage databases.

> Thermo-Calc accepts some deviations from these syntax rules. Although warnings can be ignored, errors must be corrected. Reported errors must be corrected in the TDB file before the database can be loaded by the application. Sometimes the warnings can also reveal the need for additional corrections as shown in the example below.

For example, a warning is generated if a phase name is detected that is also an abbreviation of another phase name in the database. Although allowed, it is not recommended as this can (in some cases) lead to unexpected results because abbreviations are also used when entering commands in the Console and included in macro files. The following shows why in this case an abbreviation is not recommended.

Imagine that a macro file uses the abbreviation `ABC` to refer to a phase in a database that is named `ABCDE`. As long as there is no other phase in the database with the same exact name or initial abbreviation, it works. But if a new phase is added to the database and is actually named `ABC` then the macro can in error refer to the wrong phase. The macro still runs but now refers to the phase `ABC` instead of `ABCDE` because `ABC` is an exact match, *which takes precedence over abbreviations*. The Database Checker displays a warning because this situation can only occur when one phase name is an abbreviation of another.

With respect to using this tool, the executable `DatabaseChecker` file is found in the Thermo-Calc home directory.

The program can also be launched by selecting **Tools** → **Database Checker**from the main menu in Thermo-Calc.

> Large amounts of RAM can be required when checking large databases.

The Database Checker application is standalone and available as indicated from the **Tools** menu in Thermo-Calc. However, as required, you can run the `DatabaseChecker.exe` file as a stand-alone program from the file Thermo-Calc installation directory.

Installation Default Directory: Windows, Installation Default Directory: macOS, or Installation Default Directory: Linux

Using the Database Checker

Custom Databases: GES5 and GES6 Calculation Engine Version

As of Thermo-Calc version 2019b, the default calculation engine is set to GES6. For custom database users, you may sometimes see messages in the log indicating that additional preparation is being done by Thermo-Calc prior to a calculation. The preparation is carried out automatically; it is usually fast and only needed the first time a custom database is used after a modification. While databases with warnings are tolerated, databases that contain errors can only be loaded by GES6 after the errors are corrected.

The Database Checker tool uses the same parser as GES6 and can be used to verify the consistency and correctness of databases during development, before the databases are actually used.

Database Checker

To globally set the default from GES6 back to GES5, go to the **Options**window Global General Settings tab and click **Version 5** for the *Preferred Gibbs Energy System* setting. The SET_GES_VERSION Console Mode command is used to change GES versions for a single Thermo-Calc session.

Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.

Using the Database Checker

[About the Database Checker](#)

Once you have installed the Thermo-Calc and are familiar with the TDB database file concept you can start working with the file to ensure it does not contain errors that prevent it from working with Thermo-Calc.

Example of Working with the Database Checker

The following shows a couple of the features available when using an unencrypted TDB database file included with Thermo-Calc Console Mode example *tcex11 - Oxidation of* Cu_2S *with an* H_2O/O_2 *Gas Mixture*.

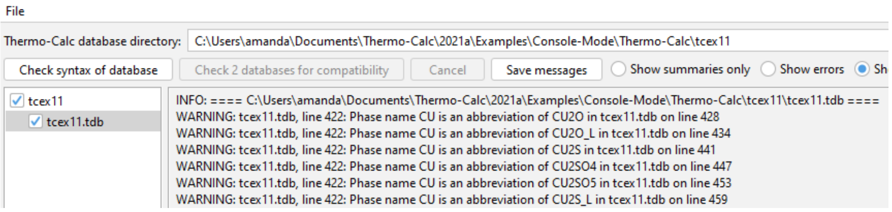
[Console Mode Examples](#)

Open a TDB file. This example uses `tcex11.TDB`, which is the user-defined database referred to from the Thermo-Calc macro file `tcex11.TCM`.

1. In Thermo-Calc, from the menu select **Tools→Database Checker**.
2. In the Thermo-Calc Database Checker window, click the **File** button and navigate to a directory with TDB files or a file with a `.TDB` extension.

> If two databases are selected at the same time, these can be tested for compatibility i.e., whether the databases can be appended. The tool generates error messages for database entities e.g., phases, that are not compatible but this does not necessarily mean that the databases cannot be appended, only that the erroneous phases cannot be appended and must be rejected from the system.

3. Click **Select directory or file**.With the file loaded, click **Check syntax of database**. Choose how to show the information: **Show summaries only**, **Show errors**, **Show errors and warnings**, or **Show all messages**. The Database Checker lists the information in the window.



Thermo-Calc database directory: C:\Users\amanda\Documents\Thermo-Calc\2021a\Examples\Console-Mode\Thermo-Calc\tcex11

```
INFO: ==== C:\Users\amanda\Documents\Thermo-Calc\2021a\Examples\Console-Mode\Thermo-Calc\tcex11\tcex11.tdb ====
WARNING: tcex11.tdb, line 422: Phase name CU is an abbreviation of CU2O in tcex11.tdb on line 428
WARNING: tcex11.tdb, line 422: Phase name CU is an abbreviation of CU2O_L in tcex11.tdb on line 434
WARNING: tcex11.tdb, line 422: Phase name CU is an abbreviation of CU2S in tcex11.tdb on line 441
WARNING: tcex11.tdb, line 422: Phase name CU is an abbreviation of CU2SO4 in tcex11.tdb on line 447
WARNING: tcex11.tdb, line 422: Phase name CU is an abbreviation of CU2SO5 in tcex11.tdb on line 453
WARNING: tcex11.tdb, line 422: Phase name CU is an abbreviation of CU2S_L in tcex11.tdb on line 459
```

4. Click **Save messages** as needed to save a `.txt` file and use this to help improve your database.

TDB Editor

In this section:

About the TDB Editor

❗ In order to use this tool, it is important to understand how to work with the standard TDB database format. For example, see Thermodynamic and Kinetic/Mobility Databases in the *Database Manager User Guide*, which is part of the *Thermo-Calc Documentation Set*, or press F1 in Thermo-Calc and search for *TDB file* in the help.

The TDB Editor is an editing tool for those who develop their own custom databases for use with Thermo-Calc or other applications. The tool speeds up the database editing process by providing immediate feedback through syntax coloring, syntax checking, and by allowing formatting and easy navigation to items of interest in the TDB file.

The advantage to using the TDB Editor compared to a basic text editor includes features such as syntax coloring and checking, formatting of TDB files, and generally easier navigation.

The TDB Editor has two components (see Installing the Code Editor and the TDB Editor for details):

1. As an installed extension to a code editor, which provides the user interface for the TDB Editor. Currently, these code editors are supported:
    - Microsoft Visual Studio Code (VSCode): VSCode is open source and available for free.
    - JetBrains IntelliJ: The full version of IntelliJ is a commercial product but there are also free limited editions available.
    - JetBrains PyCharm: The full version of PyCharm is a commercial product but there are also free limited editions available.
2. A server application that runs invisibly in the background and provides the code editor extension with services specific to the TDB format, such as syntax checking, formatting and the location within the document of various items, such as functions and references.

The syntax checker uses the same text parsing engine as the Database Checker tool and the Thermo-Calc application itself. This means that an edited TDB file (with no errors shown in the TDB Editor) is also accepted by the Thermo-Calc application. For more information see About the Database Checker.

Installing the Code Editor and the TDB Editor

About the TDB Editor

To use the TDB Editor, you install the Code Editor (Visual Studio Code (VSCode), JetBrains IntelliJ, or JetBrains PyCharm) and then in the editor you install the TDB Editor extension, which is included with your Thermo-Calc installation.

> In order to access the most-up-to-date version of the TDB editing functionality, it must be reinstalled every time a *new* version of Thermo-Calc is installed.

System Requirements

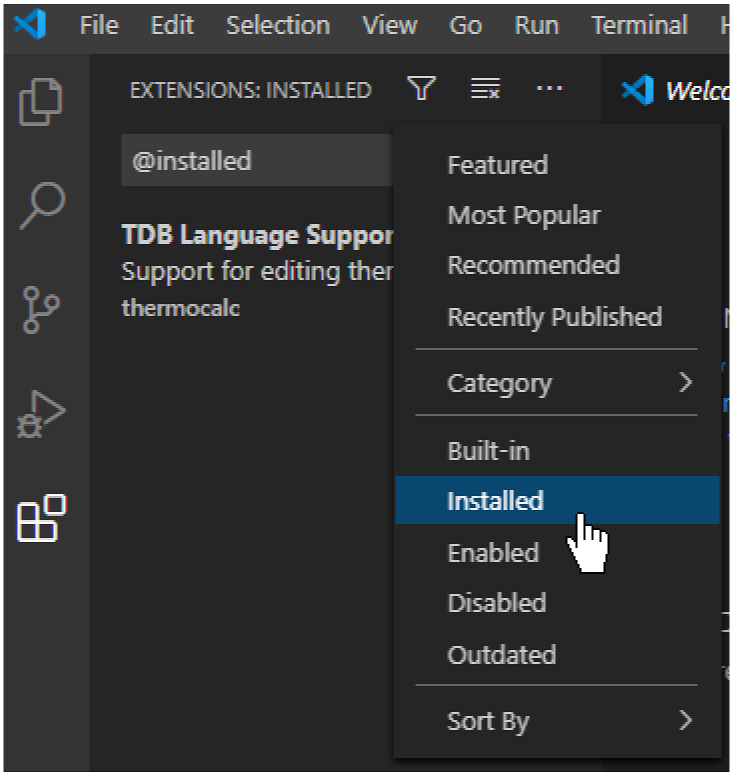
The same system requirements apply to the TDB Editor as to the Thermo-Calc installation.

A full list of system requirements and program availability is found on the Thermo-Calc website. You can also see the roadmap for platform support to use for planning purposes.

How to Install the TDB Editor Extension in VSCode

1. Navigate to the Thermo-Calc distribution directory based on your operating system. Locate the file `tdb-language-support.vsix`.
    a. On Windows, the file is typically located under `C:\Program Files\Thermo-Calc-<version>`.
    b. On Linux, the file is typically located under `<user>/Thermo-Calc/<version>`.
    c. On macOS, the file is typically located under `/Applications/Thermo-Calc-<version>/Contents/Resources`.
2. Copy the `tdb-language-support.vsix` file to your desktop.
3. Install VSCode for your platform from https://code.visualstudio.com/download.
4. In VSCode, press Ctrl+Shift+X (or from the menu, select **View→Extensions**). The **Extensions** panel opens.
5. In the upper right corner of the **Extensions** panel, click the three dots (...) **Views and More Actions** button. Select **Install from VSIX** and select the `tdb-language-support.vsix` file on your desktop.

6. Locate **TDB Language Support** in the Extensions panel. For example, click **Filter Extensions → Installed** and the file displays in the panel.



7. Click **TDB Language Support** to see the README file, which includes current version information, known bugs, and limitations.

How to Install the TDB Editor Extension in JetBrains IntelliJ and PyCharm

1. Open the **File → Settings** window (Ctrl+Alt+S). All the following settings are done in panels of this window:
2. Open the Editor panel and select **TextMate Bundles**.
3. Click **+** to add a new bundle. Select the bundle by navigating to the **TDBLanguage.tmBundle** located in the Thermo-Calc software distribution directory:
    - On Windows, the distribution directory is typically `C:\Program Files\Thermo-Calc-<version>`.
    - On Linux, the distribution directory is typically `<user>/Thermo-Calc/<version>`.

  - On macOS, the distribution directory is typically `/Applications/Thermo-Calc-<version>/Contents/Resources`. You might need to copy the bundle from the installation directory to the desktop before being able to select it.

   The editor supports syntax coloring of TDB files.

4. Open the **Plugins** panel and download and install the **LSP4IJ plugin**. Restart the IDE if required.
5. Open the **Languages & Frameworks** panel and select **Language Servers**. Click **+** to add a new server and set the following:
   - Name: **TDB Language Server**
   - Server / Command: `<Thermo-Calc’s distribution directory>TDBLanguageServer.`*`<file extension>`* where file extension is:
     - Windows: `.exe`
     - Linux: `.sh`
     - macOS: `.command`
   - Mappings / File name patterns:
     - `*.tdb`
     - `Language id: tdb`
6. The editor supports syntax checking, clickable items with jumping and formatting of TDB files. Click the **Language Servers** icon in the left margin of the output pane at the bottom of the screen.

   The TDB Language Server should now be listed.

7. If you want to see details about the communication between the editor and the language server (which might require a restart of the editor), click the entry to configure verbose tracing in the **Debug** tab.
8. Expand the **TDB Language Server** entry to show the server status. If a TDB file is loaded in the editor, the status should display the text *started pid:<number>*.

Notes about the TDB Editor Extension

- The syntax checker cannot resolve references to TDB files with partial database information and gives errors in such cases. Only databases contained in single files can be handled. For syntax checking of multi-file databases, use the stand-alone Database Checker tool. See About the Database Checker.

- If you encounter warning messages that do not match the content in the TDB Editor, a possible solution is to save the file to disk (press Ctrl+S on the keyboard), which reloads the file and restarts the syntax checker.
- Very large files can sometimes cause issues with the language support functionality although the actual editing should be unaffected by this.
  - In VSCode, the default maximum file size can be changed in **Preferences → Settings → Text Editor → Diff Editor → Max File Size**.
  - In IntelliJ and PyCharm, the default maximum size of 2.5 MB can be changed by setting the following custom property under **Help**: `idea.max.intellisense.filesize=<the filesize in kB>`.
    - For example enter `2500` for 2.5 MB, `idea.max.intellisense.filesize=2500`.

Using the TDB Editor

About the TDB Editor

Once you have installed the TDB Editor and are familiar with the TDB database file concept you can start working with it to edit an existing file or create a new TDB file.

How to Create a TDB File

To create a new TDB file, save an empty text file with a `.TDB` extension.

How to Open a TDB File

In the code editor, from the menu select **File→Open** and navigate to a file with a `.TDB` extension.

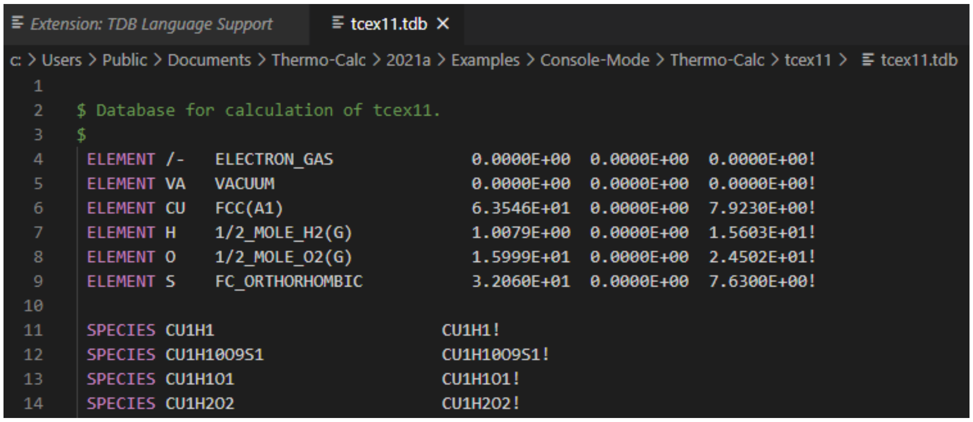
Example of Working with the TDB Editor

The following shows a couple of the features available when using an unencrypted TDB database file included with Thermo-Calc Console Mode example *tcex11 - Oxidation of* Cu_2S *with an* H_2O/O_2 *Gas Mixture*.

Console Mode Examples

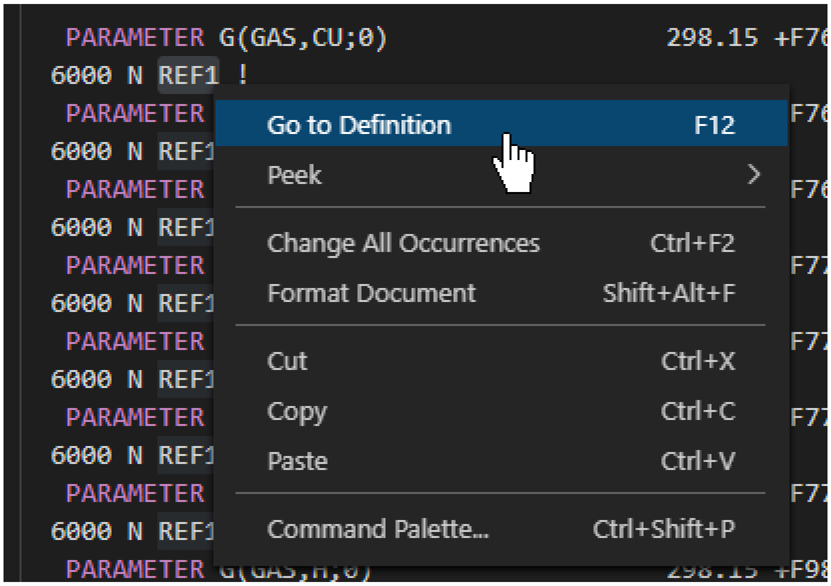
Open a TDB file. This example uses `tcex11.TDB`, which is the user-defined database referred to from the Thermo-Calc macro file `tcex11.TCM`.

The unencrypted database opens in the TDB Editor where you can quickly see the color syntax of the commands making it easy to navigate. The images below show VSCode but the appearance in IntelliJ and PyCharm is similar.



```

$ Database for calculation of tcex11.
$
 ELEMENT /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00!
 ELEMENT VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00!
 ELEMENT CU   FCC(A1)                   6.3546E+01  0.0000E+00  7.9230E+00!
 ELEMENT H    1/2_MOLE_H2(G)            1.0079E+00  0.0000E+00  1.5603E+01!
 ELEMENT O    1/2_MOLE_O2(G)            1.5999E+01  0.0000E+00  2.4502E+01!
 ELEMENT S    FC_ORTHORHOMBIC           3.2060E+01  0.0000E+00  7.6300E+00!

 SPECIES CU1H1                       CU1H1!
 SPECIES CU1H10O9S1                  CU1H10O9S1!
 SPECIES CU1H1O1                     CU1H1O1!
 SPECIES CU1H2O2                     CU1H2O2!
```

Where there are definitions or references included with the file, you can also navigate quickly to these using **Go To Definition** (ctrl-click or right-click to select from the menu).



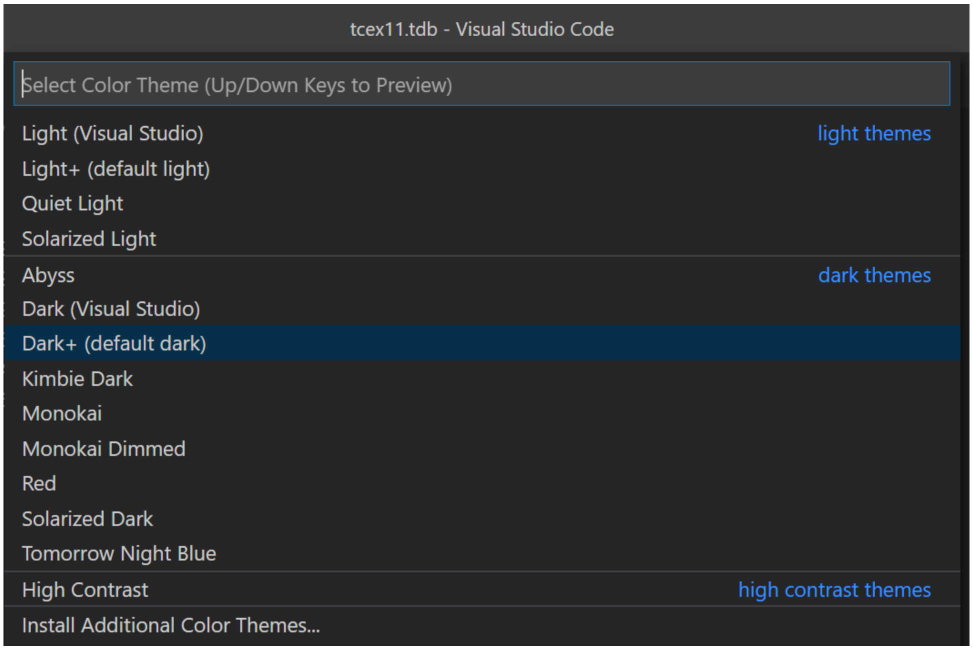
```
 PARAMETER G(GAS,CU;0)                298.15 +F76
6000 N REF1 !
```

There are many other editor features available that you can learn more about from the respective Help menus. One such item of particular use is to be able to customize the color scheme.

Customize the Color

The code editors come with a number of pre-defined color themes and additional themes can be downloaded as extensions.

To select a color theme, in VSCode press `Ctrl+K` then `Ctrl+T`. In IntelliJ and PyCharm open the Settings by pressing Ctrl-Alt-S and then select Appearance & Behavior and Appearance.



tcex11.tdb - Visual Studio Code

Select Color Theme (Up/Down Keys to Preview)

Light (Visual Studio)	light themes
Light+ (default light)	
Quiet Light	
Solarized Light	
Abyss	dark themes
Dark (Visual Studio)	
Dark+ (default dark)	
Kimbie Dark	
Monokai	
Monokai Dimmed	
Red	
Solarized Dark	
Tomorrow Night Blue	
High Contrast	high contrast themes
Install Additional Color Themes...	

A preview of each theme is shown. Use the arrow keys to try each and select the theme that best suits your preferences.

DATAPLOT User Guide

Thermo-Calc Version 2025b

Thermo-Calc Software

Introduction to the DATAPLOT User Guide

In this section:

Using this Guide

The *DATAPLOT User Guide* gives all the details on the graphical language DATAPLOT that a phase diagram or property diagram calculated by Thermo-Calc or a kinetic profile simulated by the Diffusion Module (DICTRA) can be defined.

This guide

- Discusses the important features of the DATAPLOT language.
- Describes the commands to define PROLOGUE and DATASET.
- Several examples and the standard codes for formatting are provided.

One topic introduces the method of formatting DIGLIB symbols in LaTeX documents, for the purpose of necessarily/appropriately referring to the corresponding LaTeX symbols (closest to those DIGLIB symbols which have been plotted on a diagram using the DATAPLOT Graphical Language) in the texts of LaTeX documents for publications/reports.

About the DATAPLOT Graphical Language

In order to obtain graphical output of any numerical data and informative strings, a graphical language called DATAPLOT was developed in connection with the graphical software DIGLIB. Using this graphical language, you can store information in a normal text file (*.EXP), which can be plotted as graphical symbols, lines, texts or Greek letters on any plot device support by DIGLIB.

You can generate and plot DATAPLOT (*.EXP) files together with various calculation and/or experimental results from, for example, phase and property diagrams calculated with the Thermo-Calc software composition profiles or other diagrams simulated by the Diffusion Module (DICTRA).

An EXP file automatically generated by the POST-processor (using the MAKE_ EXPERIMENTAL_DATAFILE command) in the Thermo-Calc software is a DATAPLOT (*.EXP) file and may contain all types of legal DATAPLOT commands and parameters. With a text editor, you can modify or add some DATAPLOT commands and related parameters in an existing EXP file. This is useful when appending experimental information to calculated/simulated plots, and when specifying user-defined texts, symbols, colors, fonts, filled patterns, diagram types, diagram sizes, symbol/character sizes, titles, special characters, etc.

There is another type of experimental data file that is generated in Thermo-Calc when working with the PARROT module. For more information seeExperimental Data Files (*.POP, *.DOP).

See the Tips and Tricks: How to Plot Experimental Data blog post on our website for useful guidance about this topic.

DATAPLOT Examples

To help you prepare your EXP (experimental) files to use for your plotted diagrams generated by Thermo-Calc simulations, there are examples of EXP files using the DATAPLOT graphical language standard, which are normally independent of software versions.

Installed Examples, Manuals, and Materials Folders

Plotting Experimental Data Files

You can read and plot experimental data files in both Console Mode and Graphical Mode.

> See the Tips and Tricks: How to Plot Experimental Data blog post on our website for useful guidance about this topic.

Graphical Mode

In Graphical Mode, the Experimental File Reader activity can only be created from the top My Project node. This activity allows you to read an experimental data file (*.EXP). This type of file has information specifying a plotted diagram, written in the DATAPLOT graphical language. From this activity node you can plot the EXP file or save a copy of the file to another location.

How to Plot an EXP file in Experimental File Reader

1. Right-click **My Project** and from the **Create New Activity** submenu choose **Experimental File Reader**.
2. In the **Configuration** window in the *EXP file* field, enter the name of the EXP file to plot. Or click the **Select Exp file** button to navigate to a location on the computer to add the dataset.
3. Once the .EXP file is added, under **Dataset Selection** you can choose to include or exclude specific datasets. Use the **Select/Deslect all datasets** checkbox as required.
4. Right-click the **Experimental File Reader** node and from the **Create New Successor** submenu choose **Plot Renderer**.

   If the source EXP file is changed, you can also click the **Reload the selected EXP file from disk** button to refresh the data. If you want to save or export the loaded file, click the **Save EXP file** button, then navigate to where you want to save it and give it a file name.

5. In the **Configuration** window click **Perform** or right-click the **Plot Renderer** node and select **Perform**.

Console Mode

In Console Mode you use the QUICK EXPERIMENTAL PLOT command found in the POLY-3 POST module (as well as in the Diffusion Module (DICTRA) POST module) to plot the .EXP files. This command can be used when there is no graphical information to be plotted in the POLY3 workspace. It defines a pair of axes, sets the axis labels to X and Y, and scales both X- and Y-axes between 0.0 and 1.0 unless a prologue is read from the DATAPLOT (*.EXP) data file.

How to Plot an EXP file in POST

1. Go to the POLY-3 Module: At the SYS prompt type `Go Poly`.
2. Go to the POST module: At the POLY_3 prompt type `Post`.
3. At the POST prompt, type `Quick`.
4. Enter Prolog and Dataset numbers (if applicable). See QUICK_EXPERIMENTAL_PLOT.
5. AT the POST prompt, type `Plot`.

Using DATAPLOT Graphical Language

In this section:

DATAPLOT File Structure

A DATAPLOT file is a normal text file with the extension `EXP` that can be created with a text editor or by a program. The file must contain one or more `DATASETS` and possibly also one or more `PROLOGUES`. Each `PROLOGUE/DATASET` is an entity that can be individually selected for plotting.

A PROLOGUE/DATASET is identified by a unique positive number in the file. A PROLOGUE normally contains various DATASET commands for defining information about axis scaling, axis text, axis length, title and so on. A PROLOGUE is terminated by another PROLOGUE or by the first DATASET. This means that all PROLOGUES must be placed at the beginning of the file, before the first DATASET.

A DATASET normally contains DATASET commands that are associated to separate data points, as well as with one or more `BLOCKS` of data (calculated or experimental). A DATASET is terminated by another DATASET command or the end of file.

DATAPLOT Language Syntax

The DATAPLOT language consists of commands with or without parameters:

```
COMMAND {parameter(s)}
```

The basic graphical command consists of an X/Y coordinate pair and a Graphical Operation Code (GOC). With other commands, the interpretation of this basic command can be modified. There are separate commands to draw a polygon or a function and ways to get texts in different fonts.

To edit a DATAPLOT file, the graphical commands can be abbreviated.

A command (with parameters) must not exceed 80 characters. If it is too long (normally as writing necessary codes in a command's parameters for a complex expression), two or more lines can be edited.

Coordinate Systems

The DATAPLOT language accepts coordinates in three different coordinate systems, which are called *world*, *virtual* and *normalized*.

- The *world* coordinates are selected to represent any kind of data and be of “any” magnitude.
- The *virtual* coordinate system uses centimeters as units. However, the actual size of one unit is dependent on the implementation of the device driver in DIGLIB. It is not recommended to use this coordinate system if different output devices are used for preliminary and final plots.
- The *normalized* coordinate system goes from zero to one. When plotting, you interactively scale each axis by selecting the minimum and maximum word coordinates on the axis. In the normalized coordinate system, the minimum axis value is represented by zero and the maximum by one. DIGLIB draws a square between the four points (of the X and Y axes) that are determined by the coordinates zero and one in the normalized coordinates.

It is also possible to draw triangular plots as described below. However, in most places, it only references square diagrams. All data points within the minimum and maximum word coordinates are plotted inside this square. DIGLIB also writes tic marks and corresponding word values at such tic marks.

It may be convenient to use normalized coordinates to draw boxes and texts. You can give normalized coordinates outside zero and one if you want to write texts outside the area enclosed by the square. To ensure proper operation outside the normalized box, the clipping must be turned off.

Graphical Operation Codes

The Graphical Operation Code (`GOC`) determines how the coordinates are interpreted and what is done at the point determined by the coordinates. For an individual data point, its GOC codes must be given. For each data BLOCK, you define a default GOC that is used for the whole BLOCK, unless a GOC is explicitly defined for a specific point.

- If `S` is omitted, no symbol is plotted. A number selecting the symbol can optionally follow the character `S`. The DIGLIB software determines which symbol the number represents. See Plotting a Symbol.
- If any of the other characters are omitted, the default defined for the BLOCK is used. Absolute values imply the current coordinates; relative values mean that these are added to the current coordinates. The GOC must be written without any space between various characters, but the order for the characters is irrelevant.
- If no `GOC` is defined for a BLOCK, the system default is `MWA`, (Move Word Absolute), i.e., move to the given point that is interpreted as absolute word coordinates. `GOC=DNA` means draw a line from the current point to the new one interpreting the coordinates as normalized. After each draw or move operation, the so-called current point is the new point.
- The TEXT following the `'` command is interpreted and expanded by the DIGLIB software, if it includes any ^ operator or STRING names using the ~ descriptor. To get PostScript outputs, the TEXT must be edited by the LaTeX Text Formatting Program instead (see LaTeX Formatting Codes).

GOC Character Definitions

The GOC is a combination of the following characters:

Character	*Meaning*
`W`, `V` or `N`	To use world (`W`), virtual (`V`) or normalized (`N`) coordinates. `W` is the default.
`A` or `R`	XY are absolute (A) or relative (R) values. `A` is the default.
`M` or `D`	To perform a move (M) or draw (D) operation to XY. `M` is the default.
`B`	To apply “soft” splines on a line drawn between the coordinate pairs (used only on BLOCK data).
`S`	To plot default symbol at XY.

Character	***Meaning***
`S#`	To change default symbol to No # symbol and plot it at XY.
`` `TEXT ``	To plot `TEXT` at XY. It must be the last operation in a GOC code. The TEXT following the ’ command is interpreted and expanded by the DIGLIB software, if it includes any ^ operator or STRING names using the ~ descriptor.

Tables or Blocks

In many cases, you have (calculated or experimental) data in the form of tables, and want to plot one or several columns as X-axis and one or more columns as Y-axis. A single table can contain many sets of data records of the same kind of information for a specific data BLOCK. There can be many data BLOCKS in a DATASET.

By enclosing these tables in a data BLOCK, you can select which column(s) is the X-axis and which is the Y-axis. For example,

```
BLOCK X=C1; Y1=C3; Y2=C2; GOC=C4,DAW
```

Where the X-axis values are in column 1, the Y-axis values are in columns 2 and 3, and any GOC codes are in column 4. The default GOC for this BLOCK is Draw Absolute Word. The GOC code inside the table is only necessary if the default GOC is not applicable.

A more elaborate use of the table is shown in this example:

```
BLOCK X=C3; Y=1E3/(C3+273); GOC=C8,MAWS1
```

Where the X-axis values are in column 3, the Y-axis values are in column 1 with some additional calculations applied. Any GOC is in column 8, and the default GOC is Move Absolute Word and plot the symbol no. 1.

Columns in a table must be separated by one or more space characters and do not have to be justified.

It is possible to have tables with mixed text and numbers, but each word followed by a space is counted as one column. The columns used for plotting also must be numerical. An example of a legal line in a table is

```
298.15 This_is_the_second_column 11.5 This_is_the_fourth_column
```

A line in the table must not exceed 80 characters. A BLOCK must be terminated by a line with the BLOCKEND command.

See the Tips and Tricks: How to Plot Experimental Data blog post on our website for useful guidance about this topic.

Drawing a Polygon

Normally, each point is written on a separate line. But in order to draw a line in a more compact way, use the command DRAWLINE. DRAWLINE is followed by a couple of X/Y number pairs. The X/Y pairs must be separated by a space, and there must be a comma sign between the X and Y values. DRAWLINE makes a move operation to the first pair of X/Y coordinates, and then draws a line among all pairs up to the last one. All pairs must fit on one line of 80 characters, but there can be several consequent DRAWLINE commands.

Example 2 – Draw Polygons and Symbols

Drawing an Analytical Function

Use a BLOCK command to set an axis to a function. It is not necessary to use a value from any column in order to compute the function value to be plotted. Use the FUNCTION command to plot a function with an even increment of the independent variable.

Example 4 – Draw Curves Defined by Functions

Painting of an Enclosed Area

Use the PAINT command to paint or fill an area in a specified pattern in the plot. Available patterns are determined by the DIGLIB software. A related command to PAINT is PCFUNCTION.

Writing a Text

Use the TEXT command to write a text at the current point. You can write a text at any X/Y pair by appending a single quote followed by the text on the same line. For example:

```
1.1 1.0 NAM’This is a text
```

writes `This is a text` at the normalized coordinates (`1.1, 1.0`).

Use the command FONT to select the font used for the text, and CHARSIZE to select the size of the characters. Set this size of the symbols with SYMBOLSIZE.

If a text or a single character should be of a different font than all the other text, or to use subscripts or superscripts in a text, use the `^` operators or STRING command to create the text. The command STRING stores the text in a specified variable that includes all text-formatting information defined by the DIGLIB software.

Example 3 – Using Strings and Various Line Types and Example 5 – Use Included Files for Predefined Symbols.

However, if a graphical output is done on a PostScript device using the PostScript hardcopy fonts, special text formatting codes as LaTeX Formatting Codes should be used and the STRING formatting syntax is then not valid.

Plotting a Symbol

As described in Graphical Operation Codes, a GOC code in a data BLOCK may contain an `S` option to plot a symbol for an X/Y pair or the same symbols for the data BLOCK. A number selecting the symbol can optionally follow the character `S`. You can plot a symbol at any current X/Y position by appending a quote specified by the symbol number in the GOC code (e.g., `1.1 1.0 MANS5’This is a text`).

You can also insert DIGLIB symbols into LaTeX-edited documents.

Example 1 – Draw Lines and Symbols, Example 2 – Draw Polygons and Symbols and Example 8 - DIGLIB Symbols

Other Commands

General

- When plotting symbols representing various experimental data, it is important that the symbols are centered around the coordinate values.
- The dollar sign $ as the first character of a line stands for a comment character, which means the whole line is ignored when plotting.

ATTRIBUTE

Use the ATTRIBUTE command to change the coordinates where text is displayed. The default is the lower left corner of the first character in the text.

CLIP

Use the CLIP command to change the default where all data outside the normalized coordinates zero and one are not plotted.

COLOR

If you are using a color device, use the COLOR command to change color of the lines. On some black and white devices, colors are simulated with different width and dashing of the lines.

INCLUDE

Use the INCLUDE command to create libraries with texts and include these in similar plots.

LINETYPE

Use the LINETYPE command to define line types as solid, long dashed, short dashed or dotted.

Interactive Plotting

The DATAPLOT file is read into the POST module in the workspace with APPEND_ EXPERIMENTAL_DATA or QUICK_EXPERIMENTAL_PLOT. These commands ask for the name of the DATAPLOT file and also which PROLOGUE(S) and DATASET(S) are to be plotted.

Press F1 and search the Help for details.

By giving the PROLOGUE/DATASET number as `-1`, you get a list of the available PROLOGUES/DATASETS in the file. Note that if `DATASET 0` is in a DATAPLOT file, its data is always used even if other DATASETS are chosen.

Formatting DIGLIB Symbols in LaTeX Documents

When using the LaTeX editor, you can use the DIGLIB symbols in texts and in figures. This then refers to the corresponding LaTeX symbols (closest to those DIGLIB symbols which are plotted on a plot using the DATAPLOT Graphical Language) in the texts of LaTeX documents for publications/reports.

This topic shows how to generate some DIGLIB symbols in texts, through the attached LaTeX source file and its converted jpg file.

Example 8 - DIGLIB Symbols

DIGLIB_Sym.tex

```
\documentclass[dvips,12pt]{article}
\textwidth 165mm
\textheight 225mm
\oddsidemargin 1mm
\evensidemargin 1mm
\topmargin 1mm
%%\usepackage{amssymb}
%% next replace amssymb and to get udtimes
\usepackage[utopia]{mathdesign}
\usepackage{rotating}
\usepackage[latin1]{inputenc}
\usepackage{graphics}
\usepackage{graphicx,subfigure}% with figures
%\usepackage[draft]{graphicx}% without figures
\usepackage{subfigure}% with figures
\topmargin 1mm
\oddsidemargin 1mm
\evensidemargin 1mm
\begin{document}
{\Large \bf Diglib symbols and their corresponding LaTeX symbols}
\vspace{5mm}
```

The information below gives the closest corresponding LaTeX symbol. All symbols (except +) must be generated in math mode. Most of these require the package `amssymb`, i.e., you need a directive `usepackage{amssymb}` in the preamble. Two of the symbols require the more extensive `mathdesign` that can be included with `usepackage[utopia]{mathdesign}`.

```
\vspace{5mm}
{\Large
\begin{tabular}{llll}
Diglib & Latex & Latex name & Note\\
1& $\vartriangle$& $\backslash$vartriangle & amssymb \\
2& $\square$& $\backslash$square\\
3& {\Huge $\diamond$} & $\backslash$diamond & size $\backslash$Large \\
4& $\udtimes$& $\backslash$udtimes & mathdesign \\
5& $\triangledown$& $\backslash$triangledown & amssymb\\ 6 & +& normal + \\
7& $\ast$& $\backslash$ast & amssymb\\
8& $\times$& $\backslash$times \\
9& {\Huge $\circ$}& $\backslash$circ & size $\backslash$Large \\
10& {\Huge $\star$}& $\backslash$star & size $\backslash$Large, amssymb\\
11& $\curlyvee$& $\backslash$curlyvee & amssymb\\
12& $\Join$& $\backslash$Join\\
13&& - & nothing similar, overlapping $> <$\\
14&& - & nothing similar, 10-edged star \\
15& $\maltese$& $\backslash$maltese& mathdesign \\
16&& - & nothing similar, a pentagon \\
17& $\curlywedge$& $\backslash$curlywedge & amssymb\\
\end{tabular}}
\end{document}
```

LaTeX Formatting Codes

By default when using the LaTeX command, you are in math mode and Thermo-Calc automatically interprets the entered text as math. The above link uses the dollar sign ($) in all the examples but this is NOT required. For example, if you enter `$E=mc^2$` this is displayed including the $ instead of the equation.

As of Thermo-Calc 2015a the LTEXT text formatting is replaced by LaTeX. For existing users who may have plots and files that use the LTEXT format, and especially when using Console Mode, the following examples show the command changes from LTEXT and its LaTeX equivalent.

LTEXT vs LaTeX Commands for Labels

Symbol or text format	*LTEXT*	*LaTeX*
Subscripts in an axis text	S-A-TEXT Y N Mole-fraction Al^DO2O^DO3	S-A-TEXT Y N \latex \textsf{Mole-fraction } Al_2O_3
Label with subscript	add .13 .15 n c-ZrO^DO2$	add .13 .15 n \latex c-ZrO_2
Greek symbol	ADD .05 .50 N ^GRd$	ADD .05 .50 N \latex \delta

PROLOGUE Commands

In this section:

PROLOG

PROLOG is the beginning of a number of consequent lines of user-defined diagram layout commands. The lines are displayed with the `optional text` when using the `-1` option in the POST-processor as prompted for the PROLOG number with APPEND_EXPERIMENTAL_DATA or QUICK_EXPERIMENTAL_PLOT.

Examples of DATAPLOT Files and Outputs

See the Tips and Tricks: How to Plot Experimental Data blog post on our website for useful guidance about this topic.

Syntax	`PROLOGUE # optional text`
	`#` is an unsigned integer identifying the PROLOG.

DIAGRAM_TYPE

DIAGRAM_TYPE sets the diagram type to square (the default) or triangular.

Example 6 – Triangular Diagrams for Ternary Systems

Syntax	`DIAGRAM_TYPE type plot_3rd_axis clip_along_third-axis`
	`type` is a character string reading SQUARE (default) or TRIANGULAR. If `type` reads TRIANGULAR, then two additional parameters are given: `plot_3rd_axis` and `clip_along_third-axis` that are characters strings reading YES or NO.

TIC_TYPE

TIC_TYPE sets the relative length of the tic marks.

Syntax	`TIC_TYPE #`
	`#` is a real number. Default value is 1. Negative number gives tics on the inside of the diagram frame. 0 gives no tics.

TITLE

TITLE sets the title text string to be printed above the diagram.

Syntax	`TITLE text`
	`text` is an arbitrary text string that may contain text-formatting codes

XLENGTH

XLENGTH sets the X-axis length to approximately # centimeters.

Syntax	`XLENGTH #`
	`#` is a positive real number (the approximate X-axis length in centimeters).

XSCALE

XSCALE sets the scaling in word coordinates of the X-axis.

Syntax	`XSCALE min max`
	`min` and `max` are real numbers.

XTEXT

XTEXT sets the X-axis text.

Syntax	`XTEXT text`
	`text` is an arbitrary text string that may contain text-formatting codes.

XTYPE

XTYPE sets the X-axis type as linear (default), logarithmic or inverse.

Syntax	`XTYPE type`
	`type` is a character string reading LIN, LOG or INV.

YLENGTH

YLENGTH sets the Y-axis length to approximately # centimeters.

Syntax	`Y LENGTH #`
	`#` is a positive real number (the approximate Y-axis length in centimeters).

YSCALE

YSCALE sets the scaling in word coordinates of the Y-axis.

Syntax	`YSCALE min max`
	`min` and `max` are real numbers.

YTEXT

YTEXT sets the Y-axis text.

Syntax	`Y TEXT text`
	`text` is an arbitrary text string that may contain text-formatting codes.

YTYPE

YTYPE sets the Y-axis type as linear (default), logarithmic or inverse.

Syntax	`Y TYPE type`
	`type` is a character string reading LIN, LOG or INV.

DATASET Commands

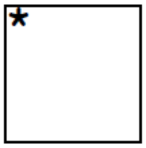
In this section:

ATTRIBUTE

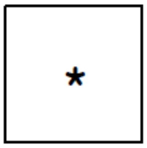
ATTRIBUTE specifies where the current XY position is in the character or symbol plotbox.

Example 2 – Draw Polygons and Symbols, Example 3 – Using Strings and Various Line Types, and Example 5 – Use Included Files for Predefined Symbols

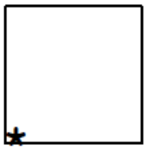
Syntax	ATTRIBUTE
Prompts	`attribute`
	`attribute` may be TOP, CENTER or BOTTOM. ATTRIBUTE CENTER is default for symbols; ATTRIBUTE BOTTOM is default for characters.



TOP



CENTER



BOTTOM

BLOCK

BLOCK defines how the following numeric data block shall be interpreted. The definitions of X and Y coordinates may also be expressed as a function of the column values, making it possible to perform transformations.

Syntax	`BLOCK X&=C#; ...; Y&=C#; ...; GOC=C#,@@@...`
	`&'` are optional unsigned integers that make it possible to plot several (maximum 9) X- or Y- axis columns. `#'` are unsigned integers identifying the column numbers. The column number # in “GOC=C#” is the location of any possible GOC codes in the current data BLOCK; @@@ stands for the default Graphical Operation Code (GOC) for the current BLOCK. The GOC code inside the current table is only necessary if the current default GOC is not applicable.

GOC Characters

The GOC is a combination of the following characters:

Character	*Meaning*
`W`, `V` or `N`	To use world (`W`), virtual (`V`) or normalized (`N`) coordinates. `W` is the default.
`A` or `R`	XY are absolute (A) or relative (R) values. `A` is the default.
`M` or `D`	To perform a move (M) or draw (D) operation to XY. `M` is the default.
`B`	To apply “soft” splines on a line drawn between the coordinate pairs (used only on BLOCK data).
`S`	To plot default symbol at XY.
`S#`	To change default symbol to No # symbol and plot it at XY.
`'TEXT`	To plot `TEXT` at XY. It must be the last operation in a GOC code. The TEXT following the ’ command is interpreted and expanded by the DIGLIB software, if it includes any ^ operator or STRING names using the ~ descriptor.

BLOCKEND

Use BLOCKEND to terminate the local definition of the graphical operation code defined by the earlier BLOCK command.

CHARSIZE

CHARSIZE redefines the default size of the characters in the plot. The character size has an initial default value, which may vary with the current font setting and the output device (the plot format).

Examples of DATAPLOT Files and Outputs

Syntax	`CHARSIZE $$`
	`$$` must be an unsigned real.

CLIP

CLIP turns clipping on or off. If it is OFF, it allows output outside the ordinary plot area defined by normalized coordinates zero and one.

Example 2 – Draw Polygons and Symbols and Example 9 - DIGLIB Fonts and Lines

Syntax	`CLIP CLP`
	`clp` is a character string reading ON or OFF.

COLOR

Use COLOR to redefine the current color setting. There are 22 legal color codes (from 0 to 21).

Example 7 – Color Codes

Syntax	`COLOR code`
	`code` is an unsigned integer number (from 0 to 21) identifying the color, or a character string specifying the color.

DIGLIB Color Codes

Code	***Color***	***Equivalent Character***
0	Background	Invisible
1	Black	Normal
2	Red	Very_Thick
3	Green	Thin
4	Blue	Thick
5	Yellow	Very_Thin
6	Magenta	Dashed
7	Cyan	Dotted
8	Purple	
9	Gold	
10	Turquoise	
11	Pink	
12	Gray	

Code	*Color*	*Equivalent Character*
13	Orange-red	
14	Maroon	
15	Plum	
16	Sea green	
17	Olive	
18	Sienna	
19	Orange	
20	Coral	
21	UserDef	
22 and higher	Any digit larger than 21 has the color effect as 1 (black).	

DATASET

DATASET indicates the beginning of a number of consequent lines comprising a set of user-defined data. The DATASET lines are displayed on the terminal along with the `optional text` when using the `-1` option in the POST-processor as prompted for the DATASET number in the APPEND_EXPERIMENTAL_DATA or QUICK_EXPERIMENTAL_PLOT command.

See the Tips and Tricks: How to Plot Experimental Data blog post on our website for useful guidance about this topic.

Syntax	`DATASET # optional text`
	`#` is an unsigned integer identifying this set of data.

DATAPOINT

DATAPOINT is not a DATASET command, but the basic DATAPLOT command (see synopsis below) performs an action at the current point determined by the specified X/Y-coordinates. A DATASET may contain various data points, in addition to one or more data BLOCKs. Such data points are separated and independent on each other.

Syntax	`X Y GOC`
	X and Y are unsigned real numbers identifying the X/Y-coordinates for the current data point. GOC stands for Graphical Operation Code (GOC) for the current point. Legal GOC characters. Example

```
0.7 0.95 N'Example 6

0.5 0.08 MNA'E^FS18^SQ(^SK^FS10A+5#8*C#^FS10 -!a^FS18)^FS11+B^DIa#b#$
```

DRAWLINE

DRAWLINE draws a line starting at (x1,y1) to (xn,yn) through (x2,y2) → (x(n-1), y(n-1)).

Example 1 – Draw Lines and Symbols and Example 2 – Draw Polygons and Symbols

Syntax	`DRAWLINE x1,y1 x2,y2 .... xn,yn`
	`x` and `y` may be reals or integers of any value. This is the same as connecting all points in a table:

```
x1   y1    M
x2   y2    D
...  ...   D
xn   yn    D
```

FONT

FONT redefines the default font setting in the POST-processor.

Example 9 - DIGLIB Fonts and Lines

Syntax	`FONT #`
	`#` is an unsigned integer.

Font Numbers

Number	*Font*
1	Bold
2	Normal
3	Italic
5	Bold and Italic
10	Monotype Normal
11	Monotype Italic
12	Monotype Bold
13	Monotype Bold and Italic
14	Narrow Normal
15	Narrow Italic

FUNCTION

FUNCTION defines and plots a user-defined function.

Example 4 – Draw Curves Defined by Functions

Syntax	`FUNCTION Y=f(X); start end number_of_XY_pairs; GOC;` `FUNCTION X=f(Y); start end number_of_XY_pairs; GOC;`
	`f(X)` or `f(Y)` are legal mathematical functions of X or Y, understandable by a FORTRAN program. `start` and `end` are unsigned real numbers, and `number_of_XY_pairs` an unsigned integer. `GOC` is a legal graphical operation code as defined with BLOCK.

GLOBALSIZE

GLOBALSIZE redefines the default global size of the plot. The global size has an initial default value.

Syntax	`GLOBALSIZE $$`
	`$$` must be an unsigned real.

INCLUDE

INCLUDE adds a file into the current input stream.

Example 5 – Use Included Files for Predefined Symbols.

Syntax	`INCLUDE filename`
	`filename` is a legal filename (with its correct path) for the operation system.

LINETYPE

LINETYPE redefines the current linetype in the plot.

Example 3 – Using Strings and Various Line Types, Example 8 - DIGLIB Symbols and Example 9 - DIGLIB Fonts and Lines

Syntax	`LINETYPE #`
	`#` must be an unsigned integer. Legal linetypes are (for both normal graphical outputs and for PostScript formats): • Solid (default) • Long dashed • Short dashed • Dotted

Line Types

Number	***Type***
1	Straight line
2	Dashed line
3	Dotted line
4	Dash-Dot line

PAINT

PAINT paints the area enclosed by the current path in the current pattern. The current path starts at the last MOVETO given and includes all subsequent DRAWs. This command only works for the PostScript format (as graphical files or on printed hardcopy).

PCFUNCTION

Syntax	`PAINT <code> <video> <mode>`
	<> denotes optional parameters. To set a new current pattern, supply any or all of the optional parameters. • `<code>` is a single letter 0-9, A-Z or a-t (if `<code>=t`, also supply a space and a number in the range 0.00-1.00). The default is `0`. • `<video>` is a string reading NORMAL (the default) or INVERSE. • `<mode>` is a string reading TRANSPARENT (the default) or OPAQUE.

PCFUNCTION

PCFUNCTION appends a user-defined function to the current path. It is used with PAINT.

Syntax	`PCFUNCTION Y=f(X); start end number_of_XY_pairs; GOC;` `PCFUNCTION X=f(Y); start end number_of_XY_pairs; GOC;`
	`f(X)` or `f(Y)` are legal mathematical functions of X or Y, understandable by a FORTRAN program. `start` and `end` are unsigned real numbers, and `number_of_XY_pairs` an unsigned integer. `GOC` is a legal graphical operation code as defined with BLOCK.

SYMBOLSIZE

SYMBOLSIZE redefines the current symbol size setting. The symbol size has an initial default value.

Example 3 – Using Strings and Various Line Types, Example 7 – Color Codes and Example 8 - DIGLIB Symbols

Syntax	`SYMBOLSIZE $$`
	`$$` must be an unsigned real.

STRING

STRING defines a string containing a text and operation codes (e.g., to change the default font settings).

Example 3 – Using Strings and Various Line Types and Example 5 – Use Included Files for Predefined Symbols

Syntax	`STRING name text_with_each_character_in_^S#^G^F#^U#^D#^R#^L#^N`
	`name` is a valid alphanumeric name (variable) to represent the text including all text formatting codes. It is highly recommended that all the characters in the name are in CAPITAL CASE (e.g. ACA2SO4); otherwise, the defined STRING can be incorrectly plotted. `text_with_each_character_in_^S#^G^F#^U#^D#^R#^L#^N` means the text is coded with each of its characters (and/or numeric numbers) that are formatted with various operators (`^S#`, `^G`, `^F#`, `^U#`, `^D#`, `^R#`, `^L#` and/or `^N`). `#’` are unsigned integers. `^` is the caret character and does not mean a control character. Between an `#` (in an operator) and a numeric number (as a part of the text), there must always be a comma sign (`,`) or the number is not plotted in the text, because the `#` with the number is interpreted as another incorrect #. In some of the commands, `#=0` resets the option to previous (or default) value.

String Operation Codes in the DIGLIB Software

For the PostScript hardcopy fonts, these operation codes are not valid; see LaTeX Formatting Codes:

Operator	*Operation*
`^S#`	Set character size to size #
`^G`	Set font to Greek
`^F#`	Set font to font number #
`^U#`	Move up # units
`^D#`	Move down # units
`^R#`	Move right # units
`^L#`	Move left # units

Operator	*Operation*
`^N`	Do not move, remain at current

Examples

```
STRING Alpha1 ^Ga^F0^D0^S8,1^S0^U0
```

is set to α_1

```
STRING M23C6 M^D0^S8,23^S0^U0C^D0^S8,6^S0^U0
```

is set to $M_{23}C_6$

```
STRING ACA2CO3 ^Ga^F0^D0^S8Ca^D0^S4,2^S0^U0^S8CO^D0^S4,3^S0^U0
```

is set to Ca_2CO_3

TEXT

TEXT outputs, at the current position, the text following the keyword TEXT or the text in the string `string_name` that is defined with STRING.

Syntax	`TEXT text` or `~string_name`
	It is possible to mix ^ operators and previously defined string names using the ~ operator.

Examples of DATAPLOT Files and Outputs

Once your Thermo-Calc software is installed you can open the Examples and PDF documentation (*Manuals*) from the main menu:

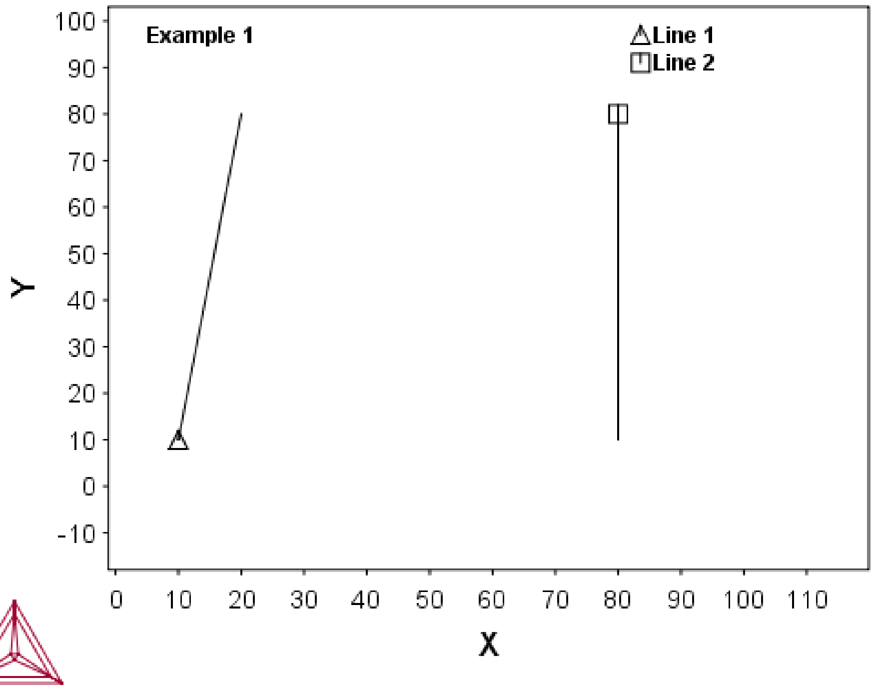
- To open the Manuals folder select **Help → Manuals Folder**. Note for Linux openSUSE users: This link is not functional. To access the folder, navigate to the default location based on your installation type
- To open the Examples based on whether you are in Console Mode or Graphical Mode, select **File → Examples Files** or **Help → Examples Files**.

In this section:

Example 1 – Draw Lines and Symbols

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 1 - Draw Lines and Symbols.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



Macro Text

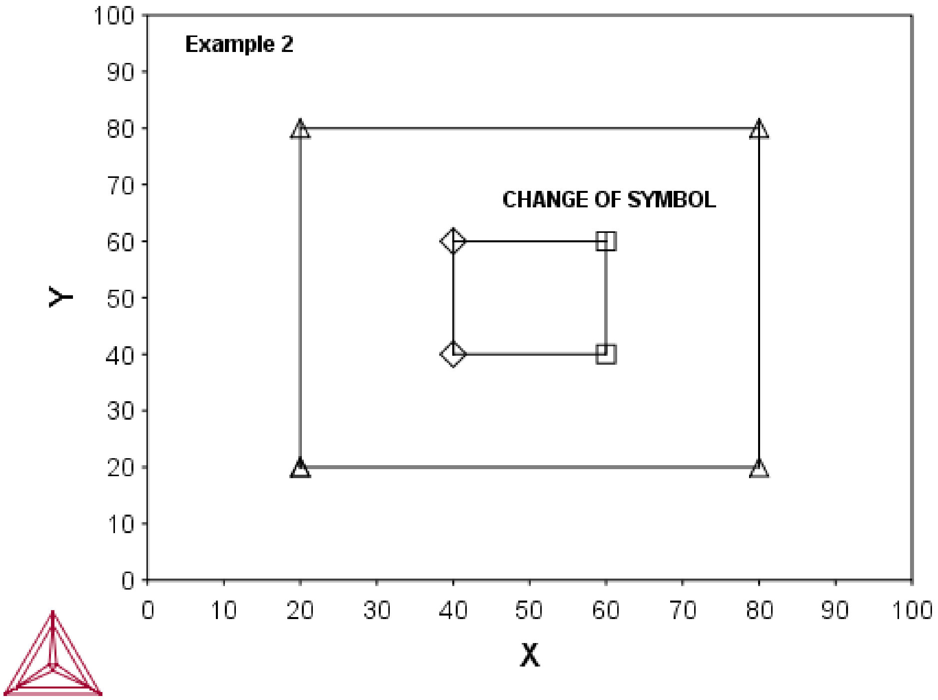
```
DATAPLOT Example 1
PROLOG 1 EXAMPLE 1 0<X<100, 0<Y<100
XSCALE 0.00000 100
YSCALE 0.00000 100
XTYPE LINEAR
YTYPE LINEAR
XLENGTH 11.5000
YLENGTH 11.5000
TITLE EXAMPLE 1
XTEXT X
```

```
YTEXT Y
DATASET 1 Two lines started with two symbols
ATTRIBUTE CENTER
0.05 0.95 N'Example 1
0.7 0.95 NS'Line 1
0.7 0.90 NS2'Line 2
10 10 S1
20 80 D
80 80 S2
80 10 D
50 60
```

Example 2 – Draw Polygons and Symbols

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 2 - Draw Polygons and Symbols.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



Macro Text

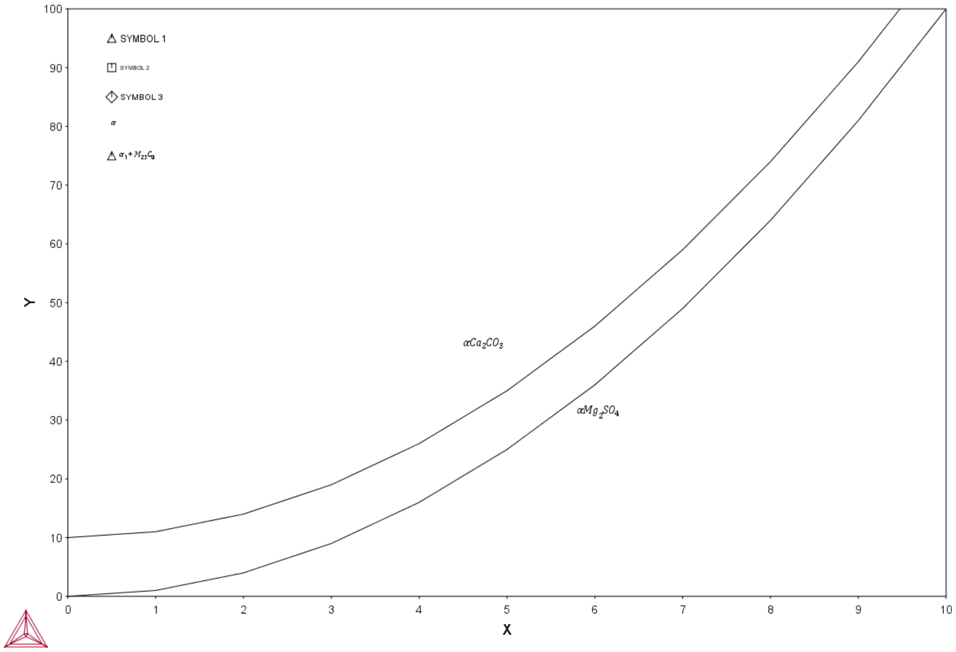
```
$DATAPLOT Example 2

PROLOG 2 EXAMPLE 2 0<X<100, 0<Y<100

XSCALE 0.00000 100

YSCALE 0.00000 100

XTYPE LINEAR

YTYPE LINEAR

XLENGTH 11.5000

YLENGTH 11.5000

TITLE EXAMPLE 2

XTEXT X
```

```
YTEXT Y
DATASET 2 Two ploygons with three types of symbols
ATTRIBUTE CENTER
CLIP OFF
0.05 0.95 N'Example 2
1.1 0.95 NS1'SYMBOL 1
1.1 0.90 NS2'SYMBOL 2
1.1 0.85 NS3'SYMBOL 3
BLOCK X=C1; Y=C2; GOC=C3,DSWA
40 40 M
40 60
60 60 S2'CHANGE OF SYMBOL
60 40
40 40 S0
BLOCKEND
BLOCK X=C1*100; Y=C2*100; GOC=C3,DSWA
0.2 0.2 MS1
0.2 0.8
0.8 0.8
0.8 0.2
0.2 0.2
BLOCKEND
$Draw an additional polygon:
DRAWLINE 20,10 30,15 40,30 50,80
DRAWLINE 50,80 60,60 90,30
```

Example 3 – Using Strings and Various Line Types

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 3 - Using String and Line Types.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



Macro Text

```
$DATAPLOT Example 3
PROLOG 3 EXAMPLE 3 0<X<10, 0<Y<100
XSCALE 0.00000 10
YSCALE 0.00000 100
XTYPE LINEAR
YTYPE LINEAR
XLENGTH 11.5000
YLENGTH 11.5000
TITLE EXAMPLE 3
XTEXT X
YTEXT Y
DATASET 3 Draw curves; plot formatted texts and symbols
```

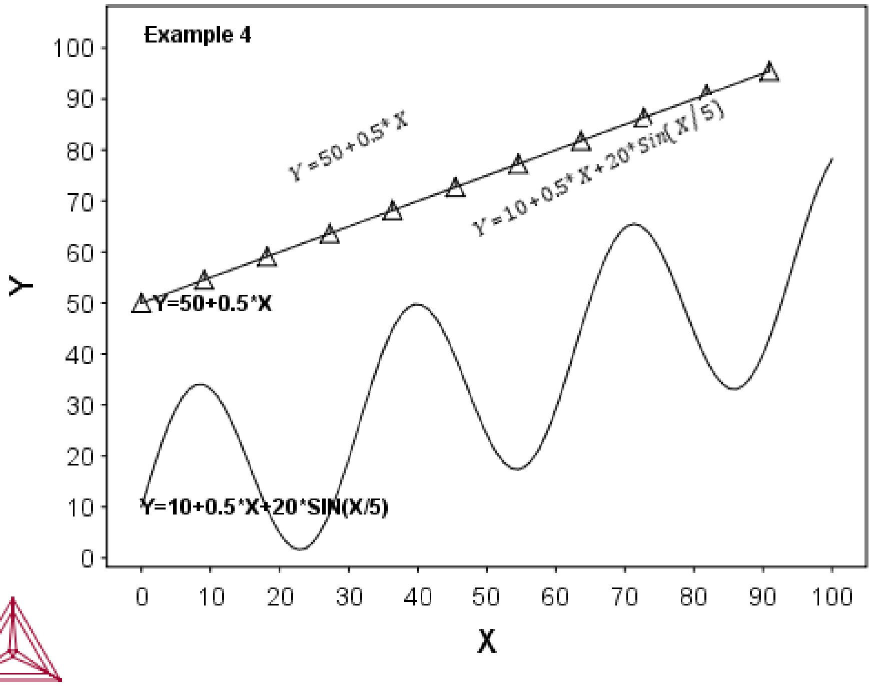
```
$Define some strings:
STRING BCC \latex \alpha
STRING BCC1 \latex \alpha_1 + M_23C_8
STRING M23C6 M_23C_6
STRING ACA2CO3 \latex \alpha Ca_2CO_3
STRING AMG2SO4 \latex \alpha Mg_2SO_4
ATTRIBUTE CENTER
CLIP OFF
FONT 2
0.05 0.95 NS1'SYMBOL 1
CHARSIZE 0.2
0.05 0.90 NS2' SYMBOL 2
CHARSIZE 0.3
0.05 0.85 NS3'SYMBOL 3
0.05 0.80 N' ~BCC
0.05 0.75 NS1'~BCC1
SYMBOLSIZE 0.4
CHARSIZE 0.4
0.45 0.42 N'~ACA2CO3
0.58 0.30 N'~AMG2SO4
CLIP ON
LINETYPE 1
BLOCK X=C1; Y=C1*C1; GOC=C2, DWA
0 M
1
2
3
4
5
6
7
8
9
10
BLOCKEND
```

```
LINETYPE 2
BLOCK X=C1; Y=C1*C1+10; GOC=C2, DWA
0 M
1
2
3
4
5
6
7
8
9
10
BLOCKEND
```

Example 4 – Draw Curves Defined by Functions

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 4 - Curves and Functions.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



Macro Text

```
$DATAPLOT Example 4
PROLOG 4 EXAMPLE 4 0<X<100, 0<Y<100
XSCALE 0.00000 100
YSCALE 0.00000 100
XTYPE LINEAR
YTYPE LINEAR
XLENGTH 11.5000
YLENGTH 11.5000
TITLE EXAMPLE 4
XTEXT X
```

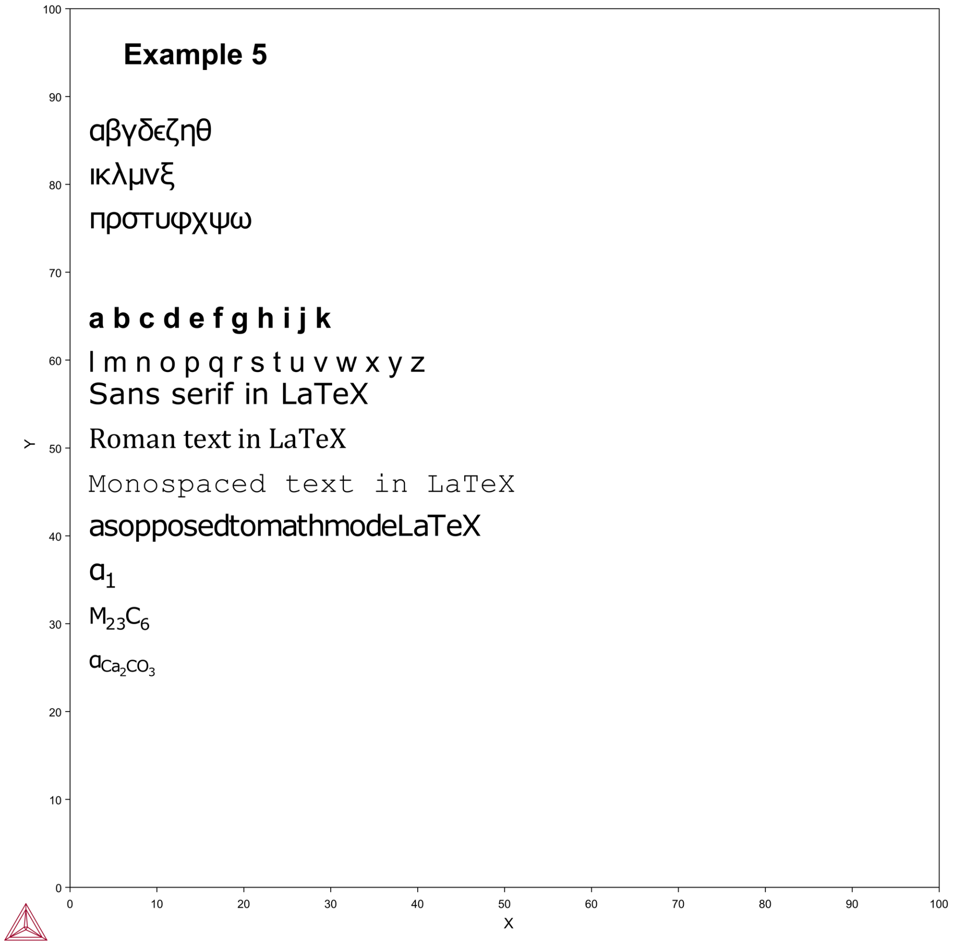
```
YTEXT Y
DATASET 4 Plot two functions as lines:
ATTRIBUTE CENTER
0.05 0.95 N'Example 4
$ Draw two lines defined by FUNCTIONS:
FUNCTION Y=10+0.5*X+20*Sin(X/5); 0 100 100; DWA;
FUNCTION Y=50+0.5*X; 0 100 10; DS1WA;
$ Write functions beside the lines:
$ Note the real rotation angle (27 degree) can be seen
$ only on the PostScript hardcopy
0.25 0.68 N'^RO27Y=50+0.5*X
0.25 0.45 N'^RO27Y=10+0.5*X+20*Sin(X/5)
```

Example 5 – Use Included Files for Predefined Symbols

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 5 - Predefined Symbols.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example

In the plot result, the hard-to-read LaTeX line is intended to highlight how to type readable text using LaTeX.



Macro Text

```
$DATAPLOT Example 5 Symbols
```

```
PROLOG 5 EXAMPLE 5 0<X<100, 0<Y<100

XSCALE 0.00000 100

YSCALE 0.00000 100

XTYPE LINEAR

YTYPE LINEAR

XLENGTH 11.5000

YLENGTH 11.5000

TITLE EXAMPLE 5

XTEXT X

YTEXT Y

DATASET 5 Write equations and strings with different properties

STRING TEST1A \latex \alpha \beta \gamma \delta \epsilon \zeta \eta \theta

STRING TEST1B \latex \iota \kappa \lambda \mu \nu \xi \omicron

STRING TEST1C \latex \pi \rho \sigma \tau \upsilon \phi \chi \psi \omega

STRING TEST2A a b c d e f g h i j k

STRING TEST2B l m n o p q r s t u v w x y z

STRING BCC1 \latex \alpha_1

STRING ACA2CO3 \latex \alpha_{Ca_2CO_3}

ATTRIBUTE CENTER

CHARSIZE 1

0.05 0.95 N'Example 5

CLIP OFF

0.01 0.85 N'~TEST1A

0.01 0.80 N'~TEST1B

0.01 0.75 N'~TEST1C

FONT 1

0.01 0.65 N'~TEST2A

FONT 2

0.01 0.60 N'~TEST2B

0.01 0.55 N'\latex \textsf{Sans serif in LaTeX}

0.01 0.50 N'\latex \textrm{Roman text in LaTeX}

0.01 0.45 N'\latex \texttt{Monospaced text in LaTeX}

0.01 0.40 N'\latex as opposed to math mode LaTeX

0.01 0.35 N'~BCC1

CHARSIZE 0.8
```

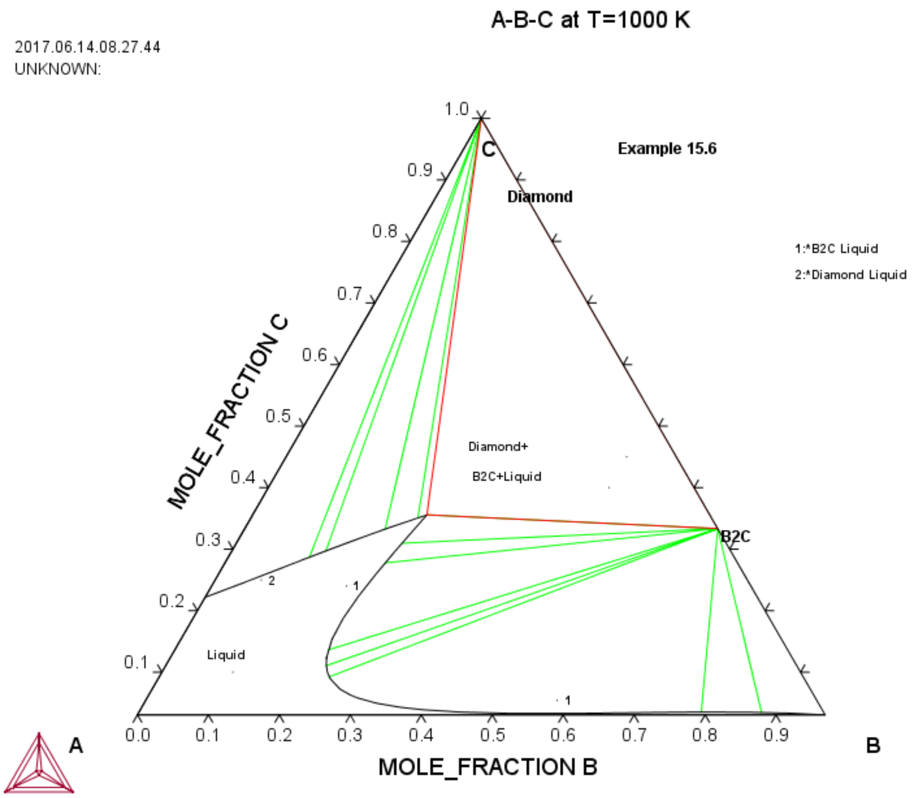
```
0.01 0.30 N'\latex M_{23}C_6
0.01 0.25 N'~ACA2CO3
```

Example 6 – Triangular Diagrams for Ternary Systems

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 6 - Ternary Plots.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example

In the DATAPLOT language, this type of diagram is only available for Console Mode.



Macro Text

```
$DATAPLOT Example 6 - Ternary Phase Diagram

PROLOG 6 EXAMPLE 6 0<X<0.969224, 0<Y<1.00000

XSCALE 0.00000 0.969224

YSCALE 0.307492E-01 1.00000
```

```
XTYPE LINEAR
YTYPE LINEAR
XLENGTH 11.5000
YLENGTH 11.5000
TITLE A-B-C at T=1000 K
XTEXT MOLE_FRACTION B
YTEXT MOLE_FRACTION C
DIAGRAM_TYPE TRIANGULAR YES YES
DATASET 6 Plot a ternary phase diagram
CLIP OFF
0.80 0.90 N'Example 6
0.86 0.31 N'B2C
0.52 0.97 N'Diamond
CHARSIZE 0.25
1.4E+01 1.10E+01 MVA'1:*B2C Liquid
1.4E+01 1.05E+01 MVA'2:*Diamond Liquid
0.10 0.10 N'Liquid
0.48 0.45 N'Diamond+
0.48 0.40 N' B2C+Liquid
5.80E-01 5.40E-02 MWA' 1
1.90E-01 2.40E-01 MWA' 1
0.65E-01 2.50E-01 MWA' 2
CHARSIZE 0.45
-0.10 -0.05 N'A
1.06 -0.05 N'B
0.48 1.05 N'C
CHARSIZE 0.35
```

```
$$ Calculated A-B-C Phase Equilibrium Data:
$ PHASE REGION FOR:
$F0 LIQUID
$E DIAMOND_A4
$F0 B2C
$ INVARIANT EQUILIBRIUM
COLOR 2
BLOCK X=C1; Y=C2; GOC=C3,WAD;
2.4555855989E-01 3.5568857193E-01 M
0.0000000000E+00 9.9999523163E-01
2.4555855989E-01 3.5568857193E-01 M
6.6666668653E-01 3.3333334327E-01
0.0000000000E+00 9.9999523163E-01 M
6.6666668653E-01 3.3333334327E-01
COLOR 1
BLOCKEND
$ PHASE REGION FOR:
$E LIQUID
$F0 B2C
BLOCK X=C1; Y=C2; GOC=C3,WAD;
$ PLOTTED COLUMNS ARE : X(LIQUID,B) and X(LIQUID,C)
2.2030337155E-01 1.2340000272E-01 M
2.2632879019E-01 1.1058768630E-01
2.3371633887E-01 9.9345825613E-02
2.4253317714E-01 8.9345827699E-02
2.6429468393E-01 7.2744041681E-02
2.8429466486E-01 6.2814079225E-02
```

```
2.9617273808E-01 5.8319382370E-02
3.2811737061E-01 4.9470417202E-02
3.6353862286E-01 4.3130427599E-02
3.9895987511E-01 3.8979098201E-02
4.5209178329E-01 3.5266116261E-02
5.2293431759E-01 3.3152002841E-02
6.1148744822E-01 3.3077053726E-02
6.4690870047E-01 3.3490389585E-02
6.8232995272E-01 3.4017231315E-02
7.3546189070E-01 3.4814555198E-02
7.5317251682E-01 3.5033416003E-02
8.0630439520E-01 3.5373892635E-02
8.5943627357E-01 3.4983776510E-02
9.1256815195E-01 3.3575300127E-02
9.6747112274E-01 3.0857827514E-02
9.6922445297E-01 3.0749246478E-02
2.2030337155E-01 1.2340000272E-01 M
2.1294665337E-01 1.5308913589E-01
2.1171525121E-01 1.8851040304E-01
2.1532440186E-01 2.2393165529E-01
2.2180187702E-01 2.5935292244E-01
2.2992117703E-01 2.9477417469E-01
2.3888295889E-01 3.3019542694E-01
2.4555855989E-01 3.5568857193E-01
$ PLOTTED COLUMNS ARE : X(B2C,B) and X(B2C,C)
6.6666668653E-01 3.3333334327E-01 M
6.6666668653E-01 3.3333334327E-01
```

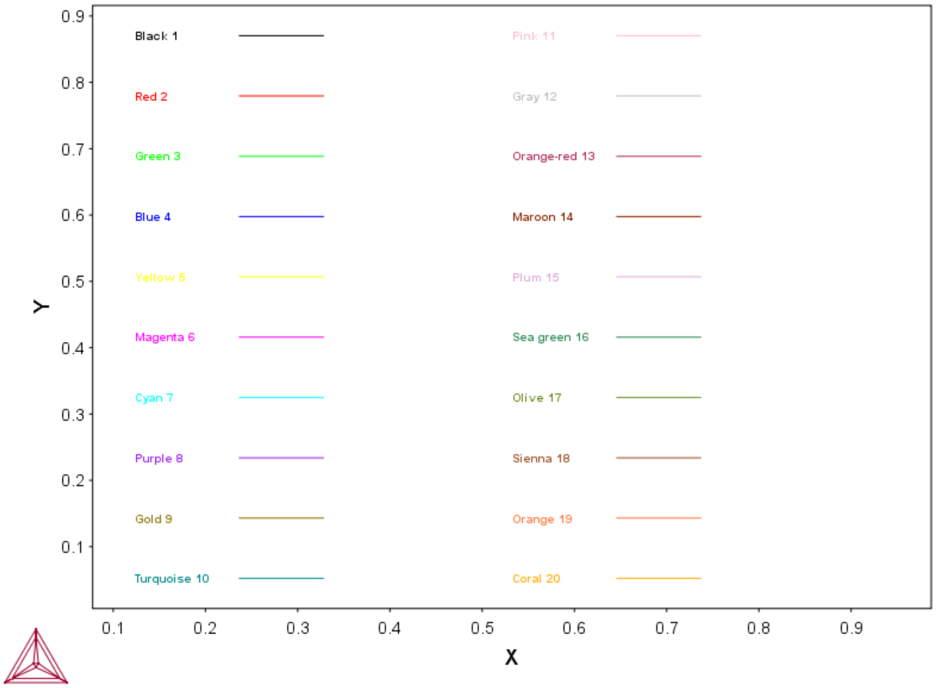
```
$ TIELINES
COLOR 3
6.6666668653E-01 3.3333334327E-01 M
8.7775242329E-01 3.4625384957E-02
6.6666668653E-01 3.3333334327E-01 M
7.9250496626E-01 3.5342670977E-02
6.6666668653E-01 3.3333334327E-01 M
2.4555824697E-01 3.5568737984E-01
6.6666668653E-01 3.3333334327E-01 M
2.3944084346E-01 9.2542596161E-02
6.6666668653E-01 3.3333334327E-01 M
2.3359020054E-01 3.0954307318E-01
6.6666668653E-01 3.3333334327E-01 M
2.2585247457E-01 2.7766343951E-01
6.6666668653E-01 3.3333334327E-01 M
2.1618695557E-01 1.3621240854E-01
2.2632879019E-01 1.1058768630E-01 M
6.6666668653E-01 3.3333334327E-01
COLOR 1
BLOCKEND
$ PHASE REGION FOR:
$F0 DIAMOND_A4
$E B2C
BLOCK X=C1; Y=C2; GOC=C3,WAD;
$ PLOTTED COLUMNS ARE : X(DIAMOND_A4,B) and X(DIAMOND_A4,C)
0.0000000000E+00 9.9999523163E-01 M
0.0000000000E+00 9.9999976158E-01
```

```
BLOCKEND
$ PHASE REGION FOR:
$E LIQUID
$F0 DIAMOND_A4
BLOCK X=C1; Y=C2; GOC=C3,WAD;
$ PLOTTED COLUMNS ARE : X(LIQUID,B) and X(LIQUID,C)
2.4555855989E-01 3.5568857193E-01 M
2.0263540745E-01 3.3483061194E-01
1.6243904829E-01 3.1375369430E-01
1.2243904918E-01 2.9153180122E-01
8.2439050078E-02 2.6854267716E-01
4.2439054698E-02 2.4548016489E-01
2.4390530307E-03 2.2313812375E-01
2.4999999937E-07 2.2181616724E-01
$ TIELINES
COLOR 3
0.0000000000E+00 9.9999511242E-01 M
2.3529186845E-01 3.5085919499E-01
0.0000000000E+00 9.9999469519E-01 M
1.9826586545E-01 3.3260950446E-01
0.0000000000E+00 9.9999409914E-01 M
1.3240024447E-01 2.9716023803E-01
0.0000000000E+00 9.9999397993E-01 M
1.1439975351E-01 2.8695335984E-01
BLOCKEND
```

Example 7 – Color Codes

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 7 - Color Codes.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



Macro Text

```
$DATAPLOT Example 7 - DIGLIB Colors

PROLOG 1 DIGLIB Colors

XSCALE 0.0 1.0

YSCALE 0.0 1.0

XTYPE LINEAR

YTYPE LINEAR

XLENGTH 15.5000

YLENGTH 11.5000

TITLE DIGLIB Colors

XTEXT X

YTEXT Y
```

```
DATASET 1 DIGLIB Colors:
$ DIGLIB Colors:
CHARSIZE 0.3
SYMBOLSIZE 0.5
COLOR 1
0.05 0.95 N' Black 1
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.95 M
0.275 0.95 D
BLOCKEND
COLOR 2
0.05 0.85 N' Red 2
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.85 M
0.275 0.85 D
BLOCKEND
COLOR 3
0.05 0.75 N' Green 3
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.75 M
0.275 0.75 D
BLOCKEND
COLOR 4
0.05 0.65 N' Blue 4
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.65 M
0.275 0.65 D
BLOCKEND
COLOR 5
0.05 0.55 N' Yellow 5
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.55 M
0.275 0.55 D
BLOCKEND
COLOR 6
```

```
0.05 0.45 N' Magenta 6
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.45 M
0.275 0.45 D
BLOCKEND
COLOR 7
0.05 0.35 N' Cyan 7
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.35 M
0.275 0.35 D
BLOCKEND
COLOR 8
0.05 0.25 N' Purple 8
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.25 M
0.275 0.25 D
BLOCKEND
COLOR 9
0.05 0.15 N' Gold 9
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.15 M
0.275 0.15 D
BLOCKEND
COLOR 10
0.05 0.05 N' Turquoise 10
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.05 M
0.275 0.05 D
BLOCKEND
COLOR 11
0.5 0.95 N' Pink 11
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.95 M
0.725 0.95 D
BLOCKEND
```

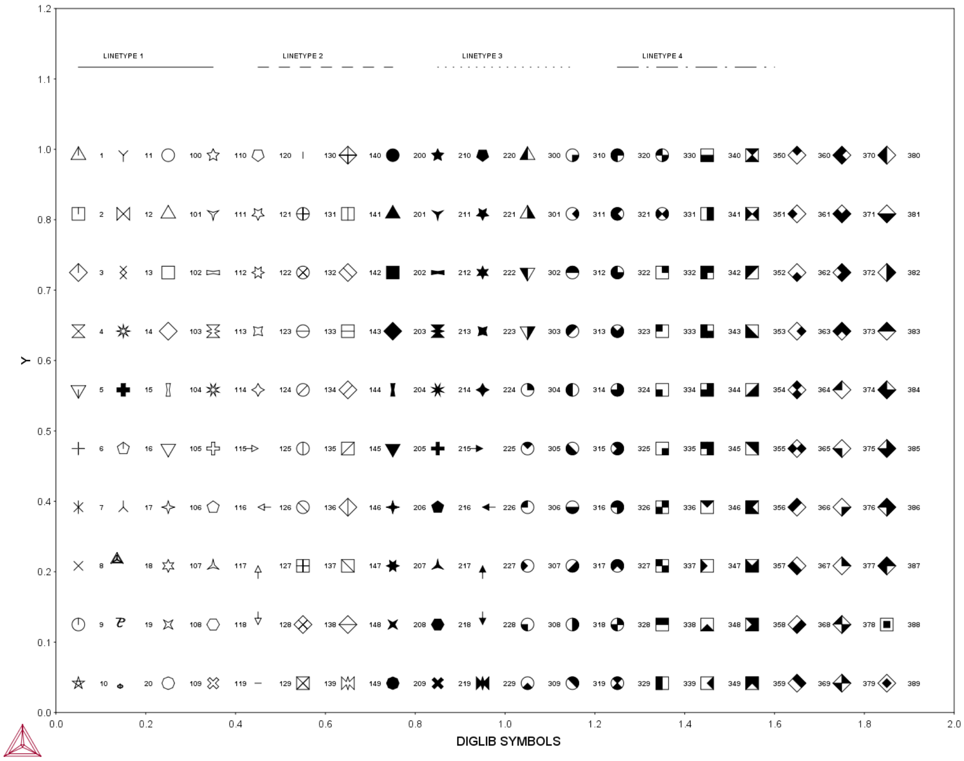
```
COLOR 12
0.5 0.85 N' Gray 12
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.85 M
0.725 0.85 D
BLOCKEND
COLOR 13
0.5 0.75 N' Orange-red 13
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.75 M
0.725 0.75 D
BLOCKEND
COLOR 14
0.5 0.65 N' Maroon 14
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.65 M
0.725 0.65 D
BLOCKEND
COLOR 15
0.5 0.55 N' Plum 15
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.55 M
0.725 0.55 D
BLOCKEND
COLOR 16
0.5 0.45 N' Sea green 16
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.45 M
0.725 0.45 D
BLOCKEND
COLOR 17
0.5 0.35 N' Olive 17
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.35 M
0.725 0.35 D
```

```
BLOCKEND
COLOR 18
0.5 0.25 N' Sienna 18
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.25 M
0.725 0.25 D
BLOCKEND
COLOR 19
0.5 0.15 N' Orange 19
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.15 M
0.725 0.15 D
BLOCKEND
COLOR 20
0.5 0.05 N' Coral 20
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.05 M
0.725 0.05 D
BLOCKEND
```

Example 8 - DIGLIB Symbols

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 8 - DIGLIB Symbols.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



A default symbol is the current symbol in the run of the software (it is usually the No 1 symbol if the POST-processor is switched on for the first time). S (i.e., # is not specified) means that the current symbol is plotted. S0 (i.e., #=0) means that no symbol is plotted.

Macro Text

```
$DATAPLOT DIGLIB Symbols 2

PROLOG 1 DIGLIB Symbols 2 0<X<2.0, 0<Y<1.2

XSCALE 0.0 2.0

YSCALE 0.0 1.2

XTYPE LINEAR

YTYPE LINEAR

XLENGTH 15.5000
```

```
YLENGTH 11.5000
TITLE DIGLIB Symbols
XTEXT DIGLIB SYMBOLS
DATASET 1 Various DIGLIB Symbols:
$ DIGLIB Symbols:
CHARSIZE 0.3
SYMBOLSIZE 0.5
0.05 0.95 WS1' 1
0.05 0.85 WS2' 2
0.05 0.75 WS3' 3
0.05 0.65 WS4' 4
0.05 0.55 WS5' 5
0.05 0.45 WS6' 6
0.05 0.35 WS7' 7
0.05 0.25 WS8' 8
0.05 0.15 WS9' 9
0.05 0.05 WS10' 10
0.15 0.95 WS11' 11
0.15 0.85 WS12' 12
0.15 0.75 WS13' 13
0.15 0.65 WS14' 14
0.15 0.55 WS15' 15
0.15 0.45 WS16' 16
0.15 0.35 WS17' 17
0.15 0.25 WS18' 18
0.15 0.15 WS19' 19
0.15 0.05 WS20' 20
0.25 0.95 WS100' 100
0.25 0.85 WS101' 101
0.25 0.75 WS102' 102
0.25 0.65 WS103' 103
0.25 0.55 WS104' 104
0.25 0.45 WS105' 105
0.25 0.35 WS106' 106
0.25 0.25 WS107' 107
```

```
0.25 0.15 WS108' 108
0.25 0.05 WS109' 109
0.35 0.95 WS110' 110
0.35 0.85 WS111' 111
0.35 0.75 WS112' 112
0.35 0.65 WS113' 113
0.35 0.55 WS114' 114
0.35 0.45 WS115' 115
0.35 0.35 WS116' 116
0.35 0.25 WS117' 117
0.35 0.15 WS118' 118
0.35 0.05 WS119' 119
0.45 0.95 WS120' 120
0.45 0.85 WS121' 121
0.45 0.75 WS122' 122
0.45 0.65 WS123' 123
0.45 0.55 WS124' 124
0.45 0.45 WS125' 125
0.45 0.35 WS126' 126
0.45 0.25 WS127' 127
0.45 0.15 WS128' 128
0.45 0.05 WS129' 129
0.55 0.95 WS130' 130
0.55 0.85 WS131' 131
0.55 0.75 WS132' 132
0.55 0.65 WS133' 133
0.55 0.55 WS134' 134
0.55 0.45 WS135' 135
0.55 0.35 WS136' 136
0.55 0.25 WS137' 137
0.55 0.15 WS138' 138
0.55 0.05 WS139' 139
0.65 0.95 WS140' 140
0.65 0.85 WS141' 141
0.65 0.75 WS142' 142
```

```
0.65 0.65 WS143' 143
0.65 0.55 WS144' 144
0.65 0.45 WS145' 145
0.65 0.35 WS146' 146
0.65 0.25 WS147' 147
0.65 0.15 WS148' 148
0.65 0.05 WS149' 149
0.75 0.95 WS200' 200
0.75 0.85 WS201' 201
0.75 0.75 WS202' 202
0.75 0.65 WS203' 203
0.75 0.55 WS204' 204
0.75 0.45 WS205' 205
0.75 0.35 WS206' 206
0.75 0.25 WS207' 207
0.75 0.15 WS208' 208
0.75 0.05 WS209' 209
0.85 0.95 WS210' 210
0.85 0.85 WS211' 211
0.85 0.75 WS212' 212
0.85 0.65 WS213' 213
0.85 0.55 WS214' 214
0.85 0.45 WS215' 215
0.85 0.35 WS216' 216
0.85 0.25 WS217' 217
0.85 0.15 WS218' 218
0.85 0.05 WS219' 219
0.95 0.95 WS220' 220
0.95 0.85 WS221' 221
0.95 0.75 WS222' 222
0.95 0.65 WS223' 223
0.95 0.55 WS224' 224
0.95 0.45 WS225' 225
0.95 0.35 WS226' 226
0.95 0.25 WS227' 227
```

```
0.95 0.15 WS228' 228
0.95 0.05 WS229' 229
1.05 0.95 WS300' 300
1.05 0.85 WS301' 301
1.05 0.75 WS302' 302
1.05 0.65 WS303' 303
1.05 0.55 WS304' 304
1.05 0.45 WS305' 305
1.05 0.35 WS306' 306
1.05 0.25 WS307' 307
1.05 0.15 WS308' 308
1.05 0.05 WS309' 309
1.15 0.95 WS310' 310
1.15 0.85 WS311' 311
1.15 0.75 WS312' 312
1.15 0.65 WS313' 313
1.15 0.55 WS314' 314
1.15 0.45 WS315' 315
1.15 0.35 WS316' 316
1.15 0.25 WS317' 317
1.15 0.15 WS318' 318
1.15 0.05 WS319' 319
1.25 0.95 WS320' 320
1.25 0.85 WS321' 321
1.25 0.75 WS322' 322
1.25 0.65 WS323' 323
1.25 0.55 WS324' 324
1.25 0.45 WS325' 325
1.25 0.35 WS326' 326
1.25 0.25 WS327' 327
1.25 0.15 WS328' 328
1.25 0.05 WS329' 329
1.35 0.95 WS330' 330
1.35 0.85 WS331' 331
1.35 0.75 WS332' 332
```

```
1.35 0.65 WS333' 333
1.35 0.55 WS334' 334
1.35 0.45 WS335' 335
1.35 0.35 WS336' 336
1.35 0.25 WS337' 337
1.35 0.15 WS338' 338
1.35 0.05 WS339' 339
1.45 0.95 WS340' 340
1.45 0.85 WS341' 341
1.45 0.75 WS342' 342
1.45 0.65 WS343' 343
1.45 0.55 WS344' 344
1.45 0.45 WS345' 345
1.45 0.35 WS346' 346
1.45 0.25 WS347' 347
1.45 0.15 WS348' 348
1.45 0.05 WS349' 349
1.55 0.95 WS350' 350
1.55 0.85 WS351' 351
1.55 0.75 WS352' 352
1.55 0.65 WS353' 353
1.55 0.55 WS354' 354
1.55 0.45 WS355' 355
1.55 0.35 WS356' 356
1.55 0.25 WS357' 357
1.55 0.15 WS358' 358
1.55 0.05 WS359' 359
1.65 0.95 WS360' 360
1.65 0.85 WS361' 361
1.65 0.75 WS362' 362
1.65 0.65 WS363' 363
1.65 0.55 WS364' 364
1.65 0.45 WS365' 365
1.65 0.35 WS366' 366
1.65 0.25 WS367' 367
```

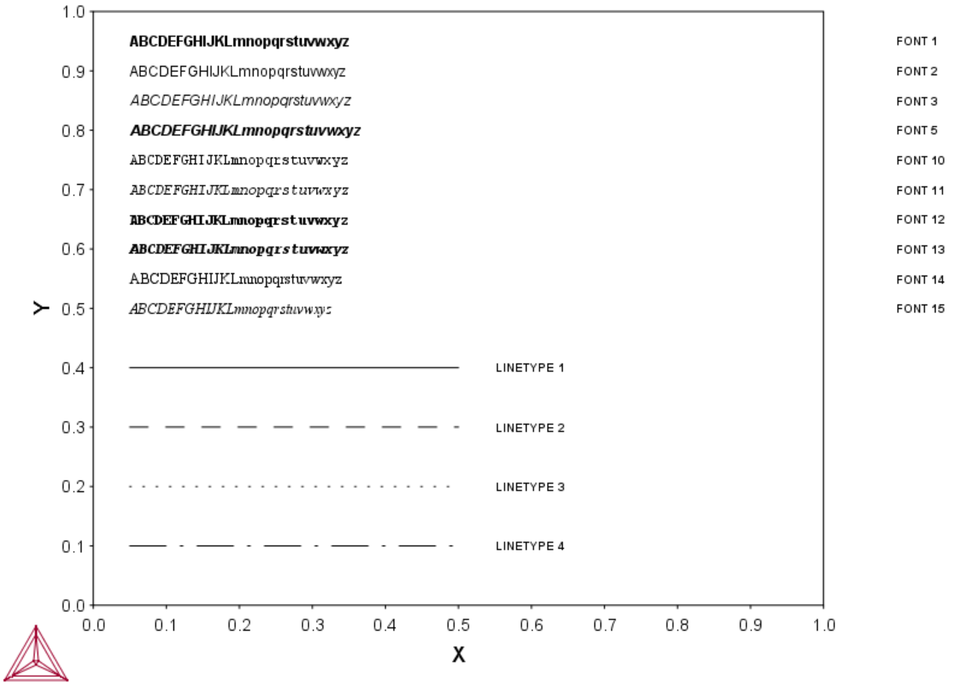
```
1.65 0.15 WS368' 368
1.65 0.05 WS369' 369
1.75 0.95 WS370' 370
1.75 0.85 WS371' 371
1.75 0.75 WS372' 372
1.75 0.65 WS373' 373
1.75 0.55 WS374' 374
1.75 0.45 WS375' 375
1.75 0.35 WS376' 376
1.75 0.25 WS377' 377
1.75 0.15 WS378' 378
1.75 0.05 WS379' 379
1.85 0.95 WS380' 380
1.85 0.85 WS381' 381
1.85 0.75 WS382' 382
1.85 0.65 WS383' 383
1.85 0.55 WS384' 384
1.85 0.45 WS385' 385
1.85 0.35 WS386' 386
1.85 0.25 WS387' 387
1.85 0.15 WS388' 388
1.85 0.05 WS389' 389
$ DIGLIB Line Types:
LINETYPE 1
BLOCK X=C1; Y=C2; GOC=C3,DWA
0.05 1.10 M
0.35 1.10
BLOCKEND
LINETYPE 2
BLOCK X=C1; Y=C2; GOC=C3,DWA
0.45 1.10 M
0.75 1.10
BLOCKEND
LINETYPE 3
BLOCK X=C1; Y=C2; GOC=C3,DWA
```

```
0.85 1.10 M
1.15 1.10
BLOCKEND
LINETYPE 4
BLOCK X=C1; Y=C2; GOC=C3,DWA
1.25 1.10 M
1.60 1.10
BLOCKEND
0.10 1.12 W' LINETYPE 1
0.50 1.12 W' LINETYPE 2
0.90 1.12 W' LINETYPE 3
1.30 1.12 W' LINETYPE 4
```

Example 9 - DIGLIB Fonts and Lines

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 9 - DIGLIB Fonts.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



Macro Text

```
$DATAPLOT Example 9 - DIGLIB Fonts
PROLOG 1 DIGLIB Fonts & Line Types 0<X<1, 0<Y<1
XSCALE 0.0 1.0
YSCALE 0.0 1.0
XTYPE LINEAR
YTYPE LINEAR
XLENGTH 11.5000
YLENGTH 11.5000
TITLE DIGLIB Fonts
XTEXT X
YTEXT Y
```

```
DATASET 1 Various DIGLIB Fonts and Line Types:
$ DIGLIB Fonts:
CHARSIZE .35
FONT 1
0.05 0.95 N'ABCDEFGHIJKLmnopqrstuvwxyz
FONT 2
0.05 0.90 N'ABCDEFGHIJKLmnopqrstuvwxyz
FONT 3
0.05 0.85 N'ABCDEFGHIJKLmnopqrstuvwxyz
FONT 5
0.05 0.80 N'ABCDEFGHIJKLmnopqrstuvwxyz
FONT 10
0.05 0.75 N'ABCDEFGHIJKLmnopqrstuvwxyz
FONT 11
0.05 0.70 N'ABCDEFGHIJKLmnopqrstuvwxyz
FONT 12
0.05 0.65 N'ABCDEFGHIJKLmnopqrstuvwxyz
FONT 13
0.05 0.60 N'ABCDEFGHIJKLmnopqrstuvwxyz
FONT 14
0.05 0.55 N'ABCDEFGHIJKLmnopqrstuvwxyz
FONT 15
0.05 0.50 N'ABCDEFGHIJKLmnopqrstuvwxyz
FONT 1
CLIP OFF
CHARSIZE .30
1.10 0.95 N'FONT 1
1.10 0.90 N'FONT 2
1.10 0.85 N'FONT 3
1.10 0.80 N'FONT 5
1.10 0.75 N'FONT 10
1.10 0.70 N'FONT 11
1.10 0.65 N'FONT 12
1.10 0.60 N'FONT 13
1.10 0.55 N'FONT 14
```

```
1.10 0.50 N'FONT 15
CLIP ON
$ DIGLIB Line Types:
LINETYPE 1
BLOCK X=C1; Y=C2; GOC=C3,DWA
0.05 0.40 M
0.50 0.40
BLOCKEND
$DRAWLINE 0.05,0.40 0.5,0.40
LINETYPE 2
BLOCK X=C1; Y=C2; GOC=C3,DWA
0.05 0.30 M
0.50 0.30
BLOCKEND
$DRAWLINE 0.05,0.30 0.5,0.30
LINETYPE 3
BLOCK X=C1; Y=C2; GOC=C3,DWA
0.05 0.20 M
0.50 0.20
BLOCKEND
$DRAWLINE 0.05,0.20 0.5,0.20
LINETYPE 4
BLOCK X=C1; Y=C2; GOC=C3,DWA
0.05 0.10 M
0.50 0.10
BLOCKEND
$DRAWLINE 0.05,0.10 0.5,0.10
0.55 0.40 N' LINETYPE 1
0.55 0.30 N' LINETYPE 2
0.55 0.20 N' LINETYPE 3
0.55 0.10 N' LINETYPE 4
```

Pourbaix Diagrams

Educational Material

Introduction to Pourbaix Diagrams

In this section:

About Pourbaix Diagrams in Thermo-Calc

This guide is for Thermo-Calc software users who know the basics of thermodynamics and want to know more about Pourbaix Diagrams.

You are introduced to the concept of a Pourbaix diagram and shown how to interpret such diagrams through a series of examples.

Materials corrosion occurs almost everywhere. It may lead to serious material damages, unexpected application failures, tremendous economic costs and environmental degradations. Consequently, scientists and engineers must often conduct expensive and time-consuming corrosion experiments as part of failure analyses, risk evaluations, quality improvements and application enhancements.

Under certain conditions, when a metal or alloy is exposed to an aqueous solution with a concentration of inorganic/organic mixture, corrosion phenomena occur at a corresponding degree. During corrosion, some metallic phases dissolve, the metal or alloy surface gets damaged and some secondary solid phases form at the solid-liquid interfaces (such as oxides, hydroxides, silicates, sulphides, sulphates, carbonates, nitrates, phosphates, borates, or halides). Such corrosive chemical or electrochemical reactions can be studied by means of the so-called Pourbaix diagrams if the reactions reach their equilibrium states [1973/1974Pou; 2003Cra; 2011Ver; 2011Tho].

GES5 and GES6 Calculation Engine Version

As of Thermo-Calc version 2019b, the default calculation engine is set to GES6. For POURBAIX module users, you need to use GES5. When you try to enter this module, you are instructed to switch to GES5 using the SET_GES_VERSION command.

About the Gibbs Energy System (GES) Module

To globally set the default from GES6 back to GES5, go to the **Options** window Global General Settings tab and click **Version 5** for the *Preferred Gibbs Energy System* setting. The SET_GES_VERSION Console Mode command is used to change GES versions for a single Thermo-Calc session.

Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.

GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features. However, not all GES5 functionality is implemented in GES6. In such cases (except for the POURBAIX module), GES6 falls back silently and uses functionality from GES5 in the background.

References

[1973Pou] M. Pourbaix, Lectures on Electrochemical Corrosion (Plenum Press, New York, 1973).

[1974Pou] M. Pourbaix, Atlas of Electrochemical Equilibria in Aqueous Solutions (National Association of Corrosion Engineers, Houston, TX, ed. 2, 1974).

[2003Cra] S. D. Cramer, B. S. Covino Jr., Eds., Corrosion: Fundamentals, Testing, and Protection: ASM Handbook, Volume 13A (ASM International, 2003).

[2011Ver] E. D. Verink Jr., "Simplified procedure for constructing Pourbaix diagrams", in Uhlig's Corrosion Handbook, R. W. Revie, Ed. (John Wiley & Sons, Inc., Hoboken, NJ, USA, ed. 3, 2011), pp. 93–101.

[2011Thom] W. Thompson, M. H. Kaye, C. W. Bale, A. Pelton, "Pourbaix diagrams for multielement systems" in Uhlig's Corrosion Handbook, Revi, Ed. (John Wiley & Sons, Hoboken, NJ, USA, 2011), pp. 103–109.

Pourbaix Diagrams

Marcel Pourbaix applied thermodynamics to predict materials corrosion resistance. He determined the phase stability relations in terms of varied pH and Eh values for an interaction system of metal and pure water or dilute aqueous solution. He presented the stability regions of metal and secondary phases (such as metal-oxides/hydroxides) on a pH-Eh diagram, which is now known as a Pourbaix diagram.

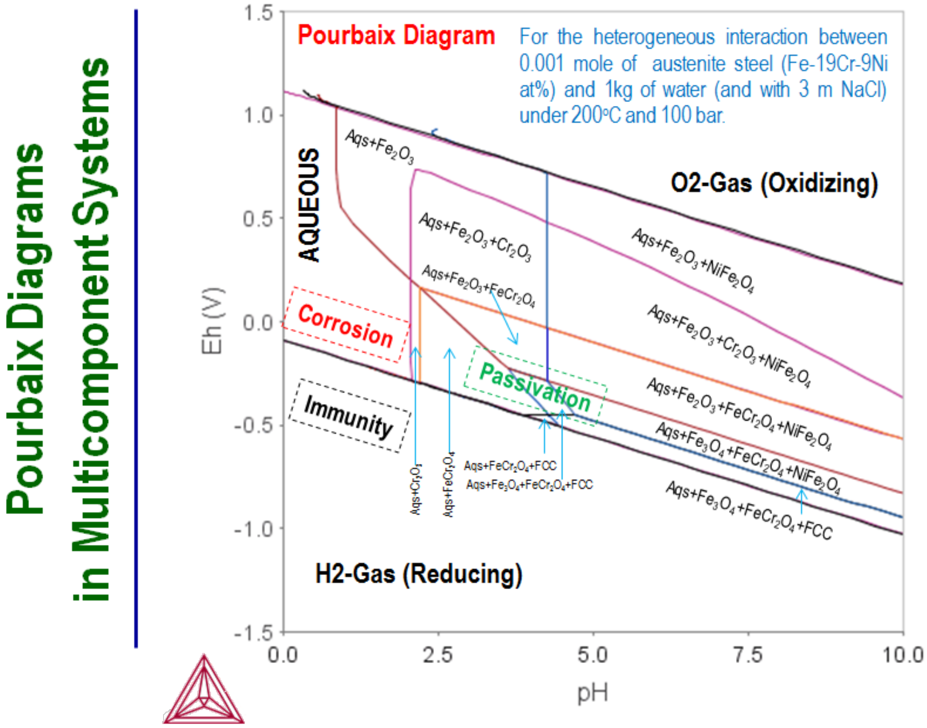
A Pourbaix diagram is a kind of phase diagram that shows the stability boundaries for a metal-aqueous interaction system. The phase boundaries are shown as a function of pH (acidity) and Eh (standard hydrogen electronic potential). An aqueous solution phase is always present in such a system. At a given pH and Eh, a metal may lose its stability to a soluble or corrosive aqueous solution, or be in equilibrium with either the aqueous solution (insoluble/immune) or with a secondary-phase file that has formed (consisting of oxides, hydroxides, sulphides or other solids). In the latter case, further dissolution of the passive or protective metal is prevented.

The speciation and partition in the aqueous solution and the interacting phases depend not only on pH and Eh, but also on other factors such as the bulk composition, temperature and pressure in the system. The interacting phases may be gas mixtures, stoichiometric solids or solid solutions.

A Pourbaix diagram is divided in regions of *immunity*, *corrosion* and *passivity*. These regions provides information about the stability of a particular metal or alloy in a specific aqueous electrochemical environment under certain pH, Eh, pressure and temperature conditions.

- The immunity region is the region in which there is no metal dissolution.
- The corrosion region is the region in which there is active metal dissolution.
- The passivation region is the region in which a protective metal-oxide film that prevents metal dissolution is formed.

The following shows these three regions in a Pourbaix diagram for the heterogeneous interaction between 0.001 mole of austenite steel (Fe-19Cr-9Ni [at%]) and 1 kg of water (with 3 m NaCl), at 200° C and 100 bar:



Depending on the system's bulk chemical composition, secondary phases may form during the transformation process. These can not only be oxides, but also be, for example, hydroxides, sulphides, sulphates, carbonates, nitrates, phosphates, borates, silicates, hydrous silicates and halides. Information about these secondary phases may help one understand the passivation behaviours in corrosion processes. For example, it may be important to understand whether any secondary phases are formed in different pH-Eh regions during hydrolysis, oxidation, reduction or other reaction processes.

In a Pourbaix diagram, the predominant ion boundaries are often represented by dashed and straight lines imposed on a traditional Pourbaix diagram for a simple interaction system (Pourbaix, 1973, 1974; Cramer and Covino, 2003; Verink, 2011; Thompson et al., 2011). Such a predominance boundary is normally an equal molality (or equal activity) line for a pair of two most-concentrated aqueous solute species (charged or neutral) involving a common metal. A line is then simply determined by a reaction constant of its corresponding electrochemical reaction in the homogeneous aqueous solution phase. However, this is not the case in Thermo-Calc.

You cannot get any information about predominant ion boundaries from a Pourbaix diagram in Thermo-Calc.

Working with Pourbaix Diagrams

With the Thermo-Calc software package, Pourbaix diagrams can be calculated over a wide range of pressure, temperature and composition conditions for complex heterogeneous interactions between multicomponent primary alloy solution or compound phases, concentrated aqueous solutions (with dissolved inorganic and organic substances), complicated secondary solids and oxidizing/reducing gaseous mixtures. In the Console Mode, diagrams can be calculated and plotted either using the response-driven POURBAIX module or directly using the DATA, GIBBS, POLY and POST modules.

This command or module is not available with GES6.

GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features. However, not all GES5 functionality is implemented in GES6. In such cases (except for the POURBAIX module), GES6 falls back silently and uses functionality from GES5 in the background.

It is possible in Thermo-Calc to set aqueous properties other than pH and Eh as axis variables. For example, the following properties can also be set as axis variables: `Ah` (electronic affinity), `pe` (electronic activity log10ACRe), `IS` (ionic strength), `TM` (total aqueous concentration, in molality), `OC` (Osmotic coefficient), activity or activity coefficient of solvent H2O, and activities or activity coefficients or concentrations in m (molality) of charged or neutral solute species.

Beside a concentrated aqueous solution phase handled by a proper thermodynamic model named SIT, HKF or PITZ, it is also possible to consider complex alloy solution phases or compound phases, as well as secondary solid phases and gaseous mixtures, which are treated by specific solution models.

Most frequently, a Pourbaix diagram is calculated for a specific alloyed phase with the initial alloying composition, such as the FCC solution phase in an austenite steel. However, it is possible to calculate a Pourbaix diagram for two co-existing phases, such as the FCC+BCC solution phases in a duplex steel for example, or even for more than two co-existing phases in a steel/alloy.

Each point on the line in a pH-Eh diagram in Thermo-Calc represents a certain minimum state of Gibbs energy. When a line is crossed, a phase transformation should occur. This means that a Pourbaix diagram in Thermo-Calc does not provide any information about any predominant ion boundary.

Key Concepts

The following are two key concepts important for understanding how aqueous solutions behave and how an aqueous-bearing heterogeneous interaction system is properly defined and calculated in Thermo-Calc.

Effective Interaction Ratio

A pH-Eh plot is always related to a certain amount of initial alloys or other condensed materials that has effectively reacted with an aqueous solution in the system. This is the amount of condensed material that is fully in equilibrium with the defined aqueous solution phase. The amount is specified relative to an aqueous solution that is normally comprised of 1 kg of water with certain specified solute concentrations at certain temperature and pressure conditions. (This is why a calculated Pourbaix diagram is typically presented for an initial amount of the interacting metal or alloy at a certain level, such as 10-6, 1E-3, 0.1 or 1 mole of metal or alloy.) It is called the *Effective Interaction Ratio* (between the initial alloy or alloyed phases and the initial aqueous solution) and it is expressed in terms of molality (mol/kg).

The Effective Interaction Ratio is important for two reasons. First, the ratio has implications for kinetic or dynamic effects such as chemical reaction mechanism and kinetics, fluid flow dynamics, surface area and interaction time. Secondly, the ratio, being expressed as 10-6 mole of metal (or alloy), is the solubility limit that can be detected for cathodic corrosion protection by immunity.

One should always be careful when setting initial amounts and compositions in the original condensed materials, as well as when setting the initial concentrations of dissolved solutes in the original aqueous solution phase. It is often useful to make a series of calculations for different levels of initial amount of the interacting metal/alloy while the conditions are fixed for other settings (such as initial aqueous concentration, pressure, temperature, pH, and Eh).

Solubility

When a heterogeneous equilibrium has a dissolving solution or mixture phase and a stoichiometric or solution phase, then the concept of solubility becomes important. A solubility of a phase (the solute) is its property of dissolving in the solvent phase. This concept concerns the constitution of a phase and is applied where one or several of the constituents are dominant (which is highly concentrated and dissolving) while there are only small amounts of the other remaining species (which are less concentrated and dissolved). The dissolving solution or mixture phase can be liquid, gas, aqueous or solid, as long as it has dissolving capacity. The stoichiometric or solution phase has some constituents which tend to be dissolved into the dissolving solution or mixture phase.

Key Points about Solubility

- Under certain temperature, pressure and composition conditions, a Fe- or Cr-dominant BCC phase can dissolve certain amounts of Ni and C from a carbide phase such as M23C6, M7C3 or M3C. The Ni and C elements in the carbides have the solubility defined relative to the BCC phase.
- An aqueous solution phase is always dominant in the solvent water, that is, H2O. Under specific temperature, pressure and aqueous composition conditions, any other element (such as Fe and C) or substance (such as a pure SO2 gas, stoichiometric phase Cu2S and solution phase (Fe,Ni)1(O,Va)1) have a certain solubility limit in the defined aqueous solution.
- Under certain temperature and pressure conditions, and under given certain concentrations of other dissolved species in the mixture, an O2-dominant gaseous mixture phase can dissolve certain amounts of Fe+2 or Fe+3 species from magnetite (Fe3O4). The magnetite solid has solubility defined relative to the gaseous mixture under the given conditions.
- Under certain temperature and pressure condition, under specific concentrations of other dissolved species in the liquid phase, a Fe-dominant liquid mixture phase can dissolve certain amounts of, for example, Cr and O. The Cr and O components have the solubility defined in the liquid mixture.

Basic Settings and Definitions

In a homogeneous aqueous solution or an aqueous-bearing heterogeneous interaction system, the most essential definition is for system-components there must be `H2O`, `H+1` and `ZE` (electron) plus those for elements dissolved in aqueous solution (such as `Na`, `Cl`, `S`) and associated in interacting metals/alloys (such as `Fe`, `Cr`, `Mn`, `Mg`, `Ni`, `Al`, `Si`, `Zn`). Three fundamental phases in a system are the `AQUEOUS` solution, the `GAS` mixture and the `REF_ELECTRODE`. The `REF_ELECTRODE` phase is used for setting the reference state for electrostatic potential in the system and for calculating the Eh condition (defined as `MUR(ZE)/RNF`). Other phases should be appropriately selected and retrieved from critically-assessed databases that cover not only the target phases (solution or stoichiometric) in interacting metals/alloys but also the secondary phases (solution or stoichiometric). The two public databases PAQ and PAQS are specially designed as single-database choices that cover all kinds of phases necessary for calculations. However, these databases are each limited to a framework of a very small number of elements. When it comes to simulations of complex multicomponent systems with a wide variety of elements and phases, the thermodynamic data must be selected and retrieved from several databases: `AQUEOUS` solution and `REF_ELCTRODE` phases must be retrieved from TCAQ or AQS; alloy phases (such as `FCC_A1`, `BCC_A2`, `HCP_A3`, `CEMENTITE`) from alloy solution databases (such as SSOL for general alloy phases, TCFE for steel/Fe-alloy phases, TCAL for Al-based alloy phases; TCMG for Mg-based alloy phases, and TCNI for Ni-based superalloy phases); gaseous mixture phase and secondary phases from specific substance or solution databases (such as SSUB for `GAS` phase and various solid compound phases or TCOX for oxide solution phases). Note that the `REF_ELECTRODE` phase should always be suspended in equilibrium calculations, while `GAS` phase could be set as `ENTERED`, `SUSPENDED` or `DORMANT`, depending on the purpose of the calculation.

When defining an interaction system, the initial condition for the `H2O` component is always set as 1 kg of water. The initial composition conditions for dissolving and interacting elements are normally defined in moles (such as `n(Fe)=0.009`, `n(Cr)=5E-4`, `n(Ni)=3E-4`, `n(Mn)=5E-5`, `n(S)=5E-5`, `n(Na)=3`, `n(Cl)=3`). This makes it straightforward and convenient to count various related aqueous solution properties based on molality. The initial conditions for the `H+1` and `ZE` components can be given as molar compositions (such as `n(H+1)=0`, `n(ZE)=0`) or their activities or potentials (such as `lnACR(H+1)=-9.21`, `MUR(ZE)=8400`).

The pH and Eh properties of the aqueous solution in the interacting system are always defined in the following way:

```
pH = -log10[ACR(H+1,AQUEOUS)*AH2O]]Eh = MUR(ZE)/RNF
```

The symbol `AH2O` is the molecular weight of solvent H2O (equals `55.508435`) and `RNF` is the Faraday constant (equals `96485.309`).

The activity of the solvent water (`ACRH2O`, `Aw`), the osmatic coefficient of aqueous solution (`OSMC`, `Os`), electronic affinity (`Ah`), electronic activity log10ACRe (`pe`), ionic strength (`IS`), total aqueous concentration, in molality (`TM`) and total alkaline concentrations under two definitions (`At1`/`AT2`) are calculated and listed for each equilibrium state.

POLY3 calculations for mass balances in Thermo-Calc are always based on site-fractions. Consequently, when functions for describing various properties of aqueous solutes are defined, such as molality (`MLi`), activity coefficient (`RCi`) and activity (`AIi`), they should be converted to molality-based quantities:

```
MLi = Y(AQUEOUS,i)*AH2O/YH2O

RCi = ACR(i,AQUEOUS)*YH2O/Y(AQUEOUS,i)

AIi = ACR(i,AQUEOUS)*AH2O
```

Here, `YH2O` is the site-fraction of solvent H2O and `AH2O` equals `55.508435`.

Many more variables, functions and tables can be entered for various purposes. For instance, an equilibrium constant for a homogeneous reaction or a solubility product for a solid dissolution reaction can be entered.

Thermodynamic Data Requirements

In this section:

Required Thermodynamic Data

To calculate a Pourbaix diagram, thermodynamic data for at least the following four types of phases must be available:

- The aqueous solution phase which applies a certain aqueous solution model. In Thermo-Calc, information about this phase could be retrieved from, for instance, the TCAQ or AQS database (these also include data for the `REF_ELECTRODE` phase that is used for setting the reference state of the standard hydrogen electrode).
- The alloy solution and/or compound phases for the primary matrix phases (and possibly also for the precipitated phases in the alloy. Examples of such phases include FCC_A1, BCC_A2, HCP_A3, SIGMA and CEMENTITE. In Thermo-Calc, information about such phases could be retrieved from, for example, the TCFE database for steels/Fe-alloys, the TCNI database for Ni-based superalloys, the TCAL database for Al-based alloys, the TCMG database for Mg-based alloys, the TCSLD for Sn-/Au-/Bi-/Zn-based solder alloys or the SSOL for general alloys.
- The secondary solid phases that would form as a result of the heterogeneous chemical or electrochemical reactions. These phases could be, for example, oxides, hydroxides, silicates, hydrous silicates, sulphides, sulphates, carbonates, nitrates, phosphates, borates or halides. In Thermo-Calc, information about such phases could be retrieved from, for example, the SSUB database for pure solid compounds or the TCOX database for complex oxide solids.
- The gaseous mixture phase. Information about this phase could be retrieved from, for example, the SSUB database. However, note that is also possible to perform Pourbaix diagram calculations that ignore the gaseous mixture phase.

All this thermodynamic data about the various phases must be critically assessed and internally consistent. Furthermore, when the data is retrieved from several databases, the data taken from each database must be consistent with the data taken from the other databases. When Pourbaix diagrams and other diagrams of steel corrosion processes are calculated, it is typically recommended that the TCAQ, TCFE, SSUB and TCOX databases or the AQS, TCFE, SSUB and TCOX are used in combination.

The public PAQ database contains thermodynamic data for all four phase types and can be used for calculating Pourbaix diagrams. They have been designed specifically for the purpose of demonstrating the POURBAIX module functionality in Thermo-Calc. However, these databases only allow you to perform test calculations for simple cases with major phases in which only a few elements can be considered.

Including or Excluding the Gas Phase

Under defined pressure and temperature conditions, the solvent water’s thermodynamic stability limits are determined by the following two electrochemical reactions:

```
H2O(water) + 2e- = H2(gas) + 2OH-1

2H2O(water) = O2(gas) + 4H+1 + 4e-
```

The first reaction describes the formation of H2-dominated gaseous mixture, under reducing conditions. The second reaction describes the formation of O2-dominated gaseous mixture, under oxidising conditions.

If the system reaches global equilibrium, then the water component is electrolyzed to H+ and O-2 at all pH conditions. The degree of electrolysis depends on the pH value in the aqueous solution phase. If Eh gets high enough, then the O-2 anion is oxidized to O2 (aqs). On the other hand, if Eh gets low enough, then the H+ cation is reduced to H2 (aqs). The major electrolysis and redox reactions are the following:

```
H2O (water) = H+ + OH- → Electrolysis of water at all pH.

H2O (water) = 2H+ + O-2 → Electrolysis of water at all pH.

O-2 - 2e- = 0.5O2 (aqs) → Oxidation or de-electronization of O-2 at high Eh.

2H+ + 2e- = H2 (aqs) → Reduction or electronization of H+ at low Eh.
```

At a critically high Eh value under a given pH condition, an aqueous solution phase with a high enough O2 activity becomes less stable than an O2-dominated gaseous mixture phase. At this point, the gas phase replaces the aqueous solution phase in the system. The replacement process can be characterised by the following phase-transformation on the aqueous-gas phase boundary and oxidation of remaining water:

```
O2 (aqs)  = O2 (gas)

H2O (water) - 2e- = 2H+(gas) + 0.5O2 (gas)
```

Similarly, at a critically low Eh value under a given pH condition, an aqueous solution phase with a high enough H2 activity becomes less stable than a H2-dominated gaseous mixture phase. At this point, the gas phase replaces the aqueous solution phase in the system, through the following phase-transformation on the aqueous-gas phase boundary and reduction of remaining water:

```
H2 (aqs)  = H2 (gas)

H2O (water) + 2e- = O-2 (gas) + H2 (gas)
```

The phase transformation from an aqueous solution phase to an O2- or H2-dominated gaseous mixture phase also depends on the total molar Gibbs energies of the phases (which are complex functions of the phase constituents, the temperature and the pressure). The Gibbs energy minimization technique used in Thermo-Calc ensures that the phase transformation is accurately simulated.

The following Pourbaix diagrams show the result of a calculation where the gaseous mixture phase was included. In the upper region (high Eh) and lower region (low Eh), the aqueous solution phase has been oxidized and reduced, respectively, to an O2- or H2-dominated gaseous mixture phase.

The two example diagrams show that the upper and lower boundaries between the aqueous phase (water) and the gas phase (dominated by either O2 or H2) can shift when solutes dissolve or when the temperature and pressure change.

Accordingly, if one does not take a gaseous mixture phase into account when performing a calculation of Pourbaix diagram (as above), then the aqueous solution phase may end up with an extremely high O2 (aqs) concentration at high Eh condition, or an extremely high H2 (aqs) concentration at low Eh condition. Under either of these two extreme circumstances, the concept of “aqueous solution phase” is no longer valid and consequently no proper aqueous solution model can actually be applied. Therefore, from a restrictive thermodynamic equilibrium point of view, one shall normally include a gaseous mixture phase in an aqueous-bearing heterogeneous interaction system. This is true for all types of equilibrium calculations for an aqueous-bearing heterogeneous interaction system, not only of Pourbaix diagram calculations.

Hence, to perform a completely accurate Pourbaix diagram calculation, the gaseous mixture phase must be taken into account. However, since these electrochemical reactions normally have much higher kinetic barriers and are slower than other electrochemical and chemical reactions in the interaction system, one can sometimes ignore the gaseous mixture phase in the calculation. Note that if the gaseous mixture phase is ignored in this way, then the Pourbaix diagram does not show the H2O-stability limiting lines.

Examples

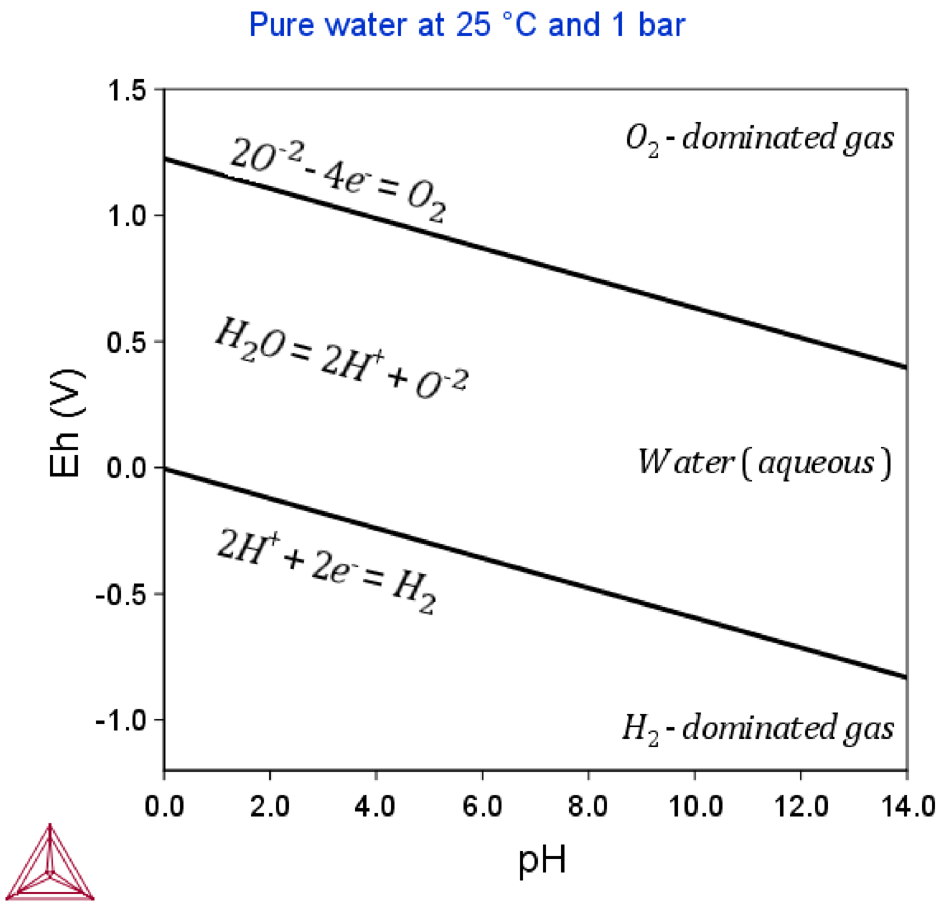


Figure 1: A pH-Eh diagram for pure water at 25° C and 1 bar.

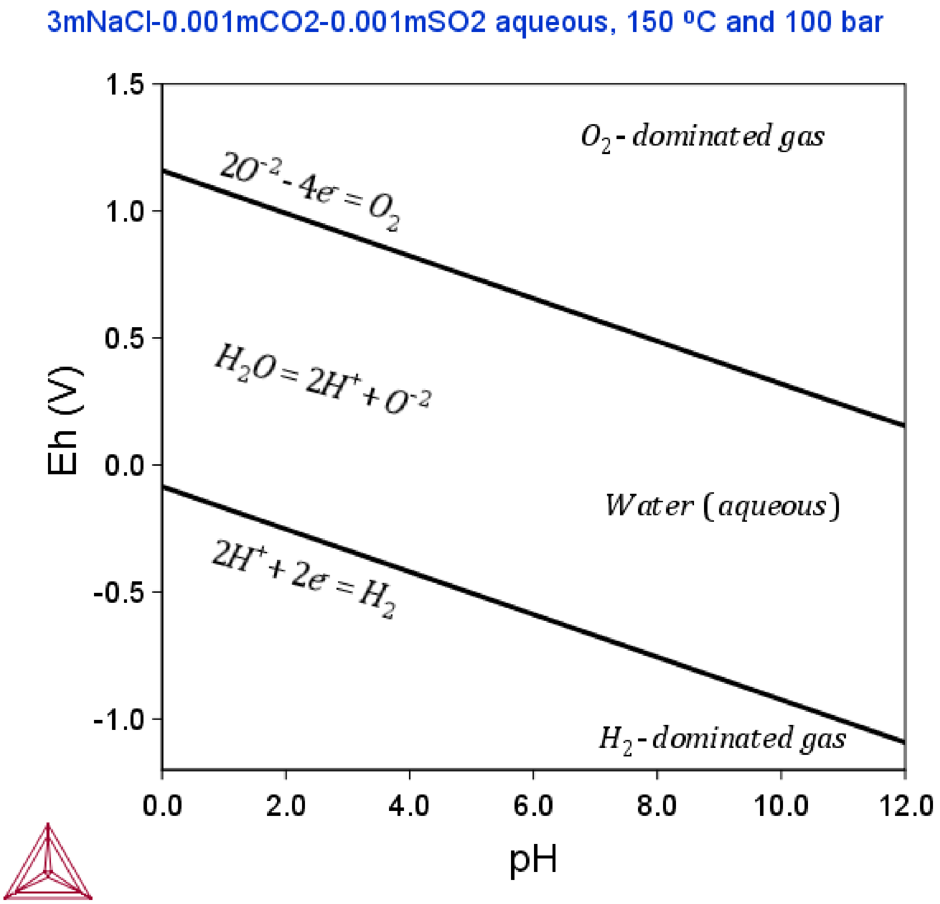


Figure 2: A pH-Eh diagram for 3mNaCl-0.001mCO2-0.001mSO2 aqueous solution at 150° C and 100 bar.

Examples of Pourbaix Diagrams for Fe

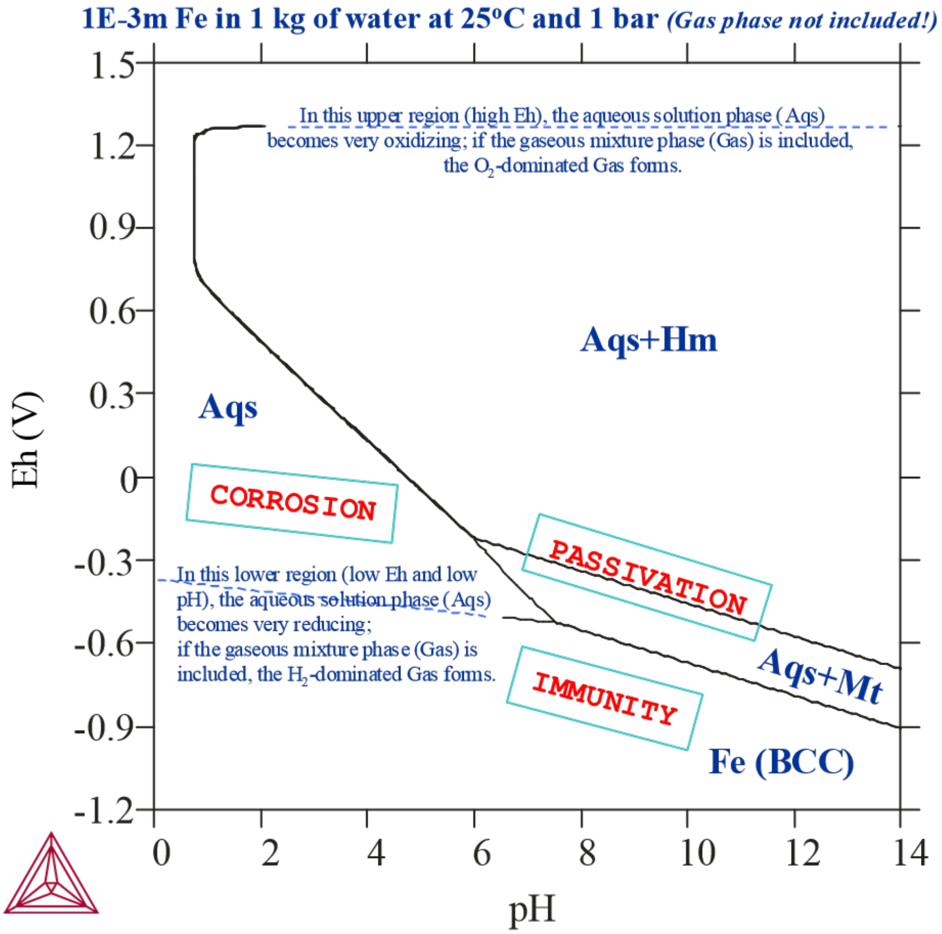
The following two topics are examples of Pourbaix diagrams for Fe. For the first example, the calculations on which the diagrams are based have not taken the gas phase into account. The diagrams in the second example are based on calculations that have taken the gas phase into account.

In this section:

Pourbaix Diagrams with Gas Phase Excluded

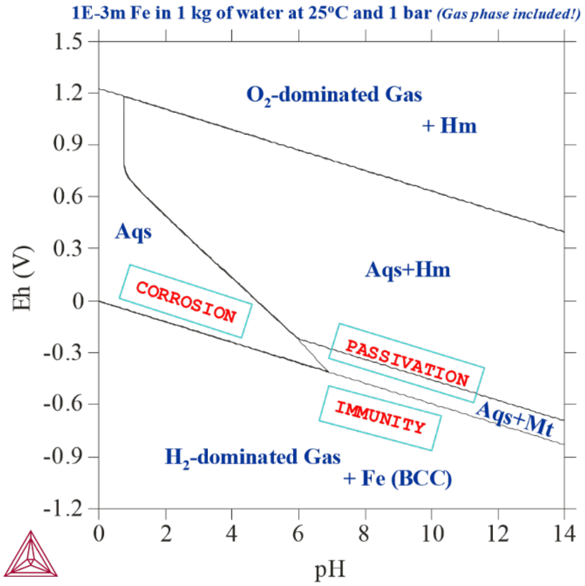
This is an example of a Pourbaix diagram of Fe, in which the gas phase has not been considered in the calculation. The system has 0.001 mole of Fe in 1 kg of pure water at a temperature of 25oC and a pressure of 1 bar. Magnetite (Mt, Fe3O4) and hematite (Hm, Fe2O3) co-exist with the Fe-containing dilute aqueous solution. The formation of magnetite and hematite represent the passivation of iron in the upper right pH-Eh field.

If pH is low and Eh is relatively high, then Fe eventually completely dissolves into the aqueous solution phase. Under conditions of low Eh, Fe remains in its stable solid state, the BCC phase, and neither dissolves into water nor into alternates to Fe (the immunity of Fe).



Pourbaix Diagrams with Gas Phase Included

With all the possible redox reactions involving the aqueous solution phase and gaseous mixture phase being considered in the equilibrium system, that is, the gaseous mixture phase is included in the calculation, the Pourbaix diagram of Fe in a system with 0.001 mole of Fe in 1 kg of pure water at 25oC and 1 bar.



Comparing this Pourbaix diagram with that from Basic Settings and Definitions, you can see that both diagrams are for the same interaction system under the same temperature-pressure condition, but the present diagram shows the results of calculations where the gaseous mixture phase has been included. It presents the complete Pourbaix diagram for the defined interaction system, in a full thermodynamic equilibrium. In the upper region (high Eh) and lower region (low Eh), the aqueous solution phase is oxidised and reduced to the O2- or H2-dominated gas phase. Hematite coexists with the O2-dominated gas, while Fe-BCC is stable with the H2-dominated gas. The stability field of magnetite may extend slightly into the H2-dominated gas region, where it coexists with the gaseous mixture instead of the aqueous solution. Its boundary with Fe (BCC) cannot be drawn due to the absence of aqueous solution phase.

It is not possible to calculate the pH value in both the O2- and H2-dominated gaseous mixture phase stability regions where the aqueous solution phase is absent. Hence, in a normal Pourbaix diagram, no line is drawn that indicates a phase boundary between the gas phase and the metallic phases or secondary phases (that is, metal-oxides).

Other Examples of Pourbaix Diagrams

In this section:

Variations of Pourbaix Diagrams

The shape of a Pourbaix diagram of an alloy or condensed material and the stability relations of various secondary phases depend upon the following system factors:

- Initial amount of the alloy or other condensed materials
- Initial composition of the alloy or other condensed materials
- Initial amount of the interacting aqueous solution phase
- Initial composition of the interacting aqueous solution phase
- Temperature and pressure conditions

In the interaction system that the diagrams in Pourbaix Diagrams with Gas Phase Excluded and Pourbaix Diagrams with Gas Phase Included are based on, the initial amount of pure Fe that was taken to have effectively reacted with 1 kg of pure water at 25° C and 1 bar was 0.001 m. The following diagrams are Pourbaix diagrams of Fe where other initial amounts of pure Fe have been used, or where the interacting aqueous solution compositions have been alternated, or the temperature and/or pressure have been changed. Gaseous mixture phases have been included in all the calculations that these diagrams are based on.

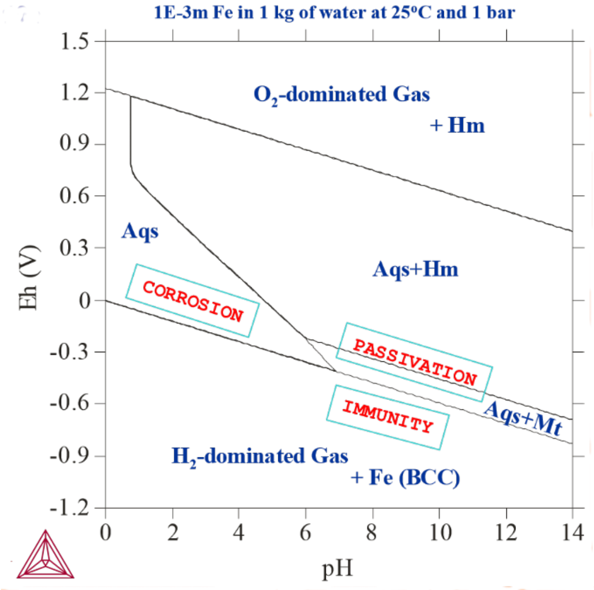


Figure 1: 1E-3 m Fe actively reacted with 1 kg of pure water at 25° C and 1 bar (as in the calculation in Pourbaix Diagrams with Gas Phase Included).

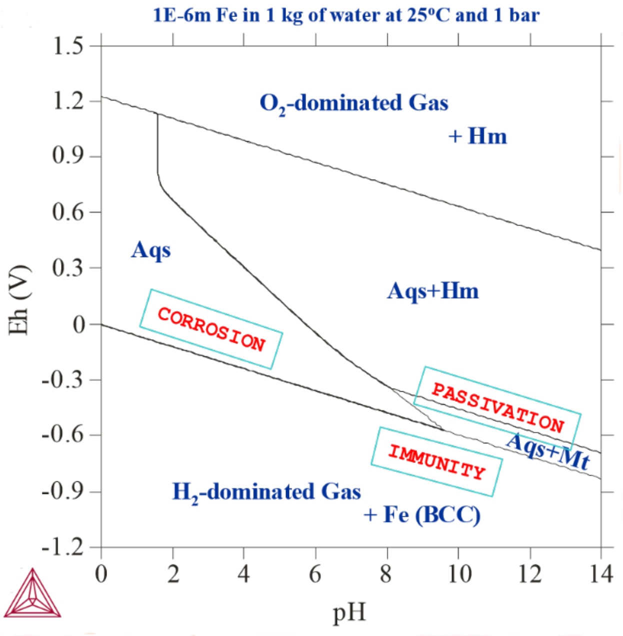


Figure 2: 1E-6 m Fe actively reacted with 1 kg of pure water at 25° C and 1 bar. Note that the active metal corrosion region gets enlarged as the initial Fe amount decreases from 1E-3m to 1E-6m.

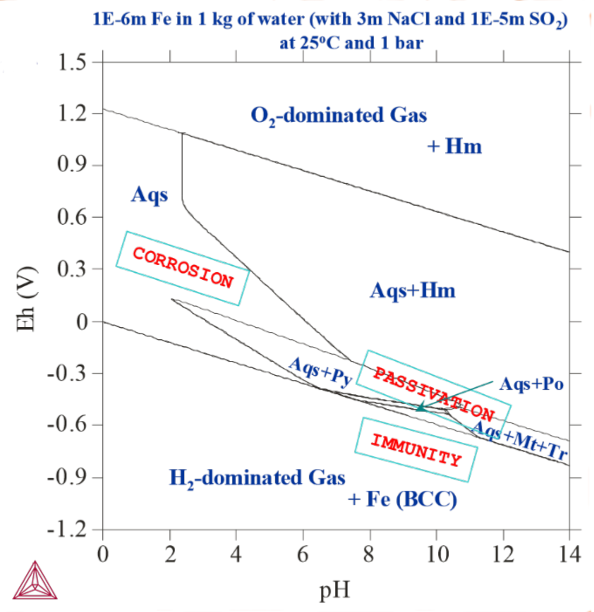


Figure 3: 1E-6 m Fe actively reacted with 1 kg of water, 3m NaCl and 1E-5 m SO2 at 25° C and 1 bar. Introducing SO2 into the system leads to the formation of various metal-sulphides (Py-pyrite, Popyrrhotite, Tr-troilite). In addition, the passivation region becomes larger.

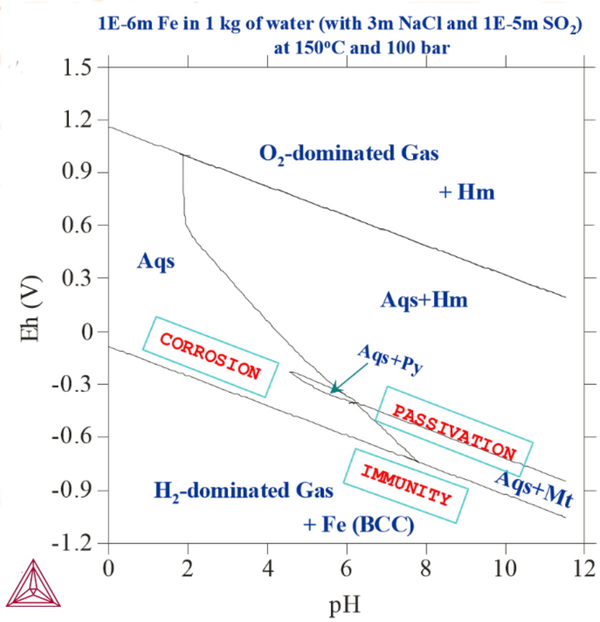


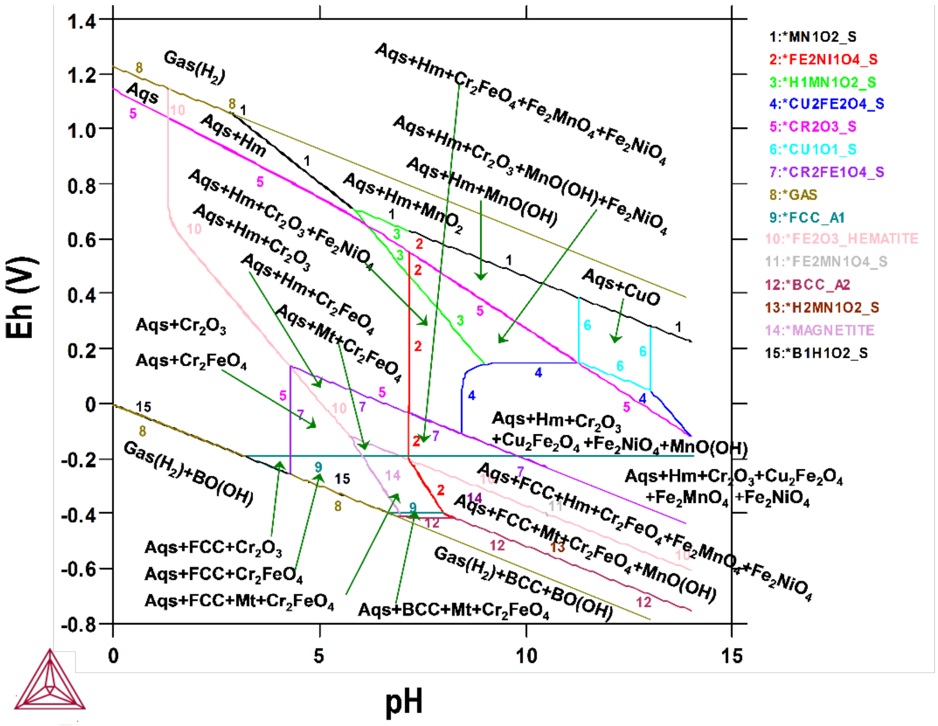
Figure 4: 1E-6 m Fe actively reacted with 1 kg of water, 3m NaCl and 1E-5 m SO2 at 150° C and 100 bar. Here, changing the temperature and pressure affects the stability fields of various Fe-oxides/sulphides.

As you can see from the figures, the aqueous-gas phase boundaries shift as the initial bulk compositions, pressure and temperature conditions in the interaction system change.

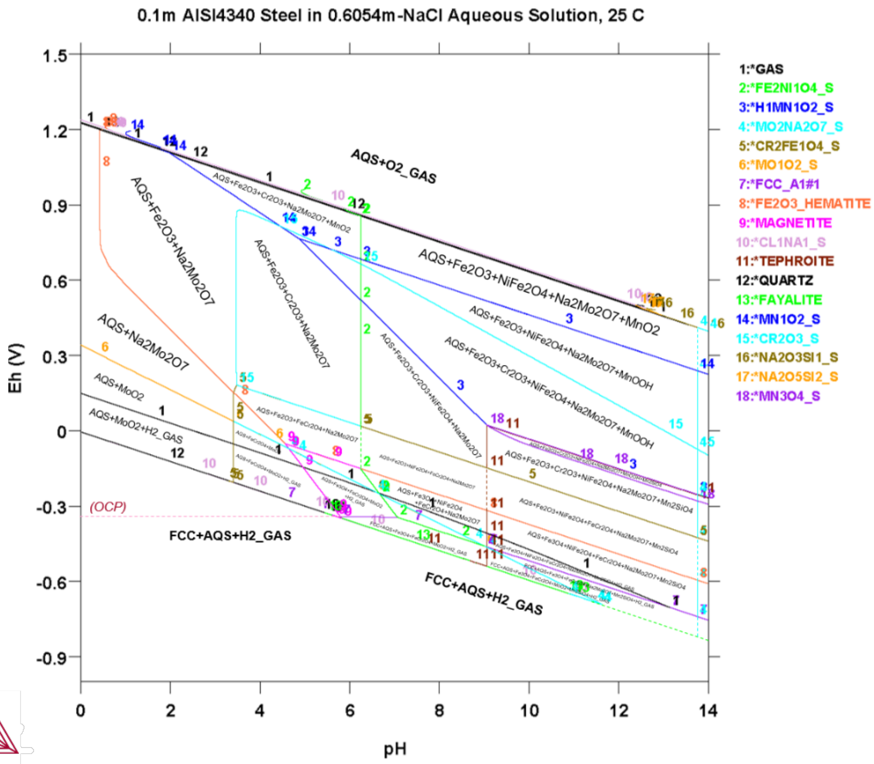
Pourbaix Diagrams for Complex Alloys

Thermo-Calc can not only be used to simulate how pure metals interact with pure water or simple aqueous solutions under normal pressure and temperature conditions. It can also be used to calculate how complex alloys and concentrated aqueous solutions interact over a very wide pressure, temperature and composition ranges. This is illustrated with the two examples.

The first example is a Pourbaix diagram calculated for the heterogeneous interaction between 0.001 mole of steel (Fe-7.676Cr-5.0Ni-2.1887Mn-1.0Cu [at%]) and 1 kg of water (and with 1.2 m H3BO3, 0.022 m Li and 0.001 m NH3), at 25° C and 1 bar. This application is particularly useful for safety assessments of nuclear reactors and nuclear waste repositories.



The next example is a Pourbaix diagram calculated for the heterogeneous interaction systems between 0.1 mole of AISI4340 stainless steel (Fe-0.80Cr-1.85Ni-0.70Mn-0.25Mo-0.25Si-0.40C [wt%]) and 1 kg of seawater (with the equivalent of 0.6054 m NaCl), at 25° C and 1 bar. This application is particularly useful for failure analysis of petroleum exploitation industry.



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Thermo-Calc: General Reference

Miscellaneous Information

Generally applicable to multiple applications within Thermo-Calc, i.e. in both Console Mode and Graphical Mode, or needed for a specific database calculation in Thermo-Calc (i.e. thermophysical properties), etc.

Parameters, Functions, and Variables

This section is applicable to both Console Mode and Graphical Mode with respect to understanding the format these are to be written in for Thermo-Calc to use the parameter, function, or variable. However, many of the sections are specific to Console Mode where the explicit use of these terms is more often used.

To learn about using variables and functions, in Graphical Mode, see T_07: User-Defined Functions and in Console Mode, see example 44.

In this section:

Specifying Parameters

This section or topic is specific to Console Mode.

Running a command typically requires that several parameter values are specified, which can be done directly in the command line after the command name. For example, to set an axis variable for a stepping or mapping operation, enter:

```
SET_AXIS_VARIABLE 1 X(FCC,FE) 0 0.89 0.025
```

You can also use SET_AXIS_VARIABLE and press <Enter>. At the command line prompt, you then specify the parameters one at a time.

On all command lines, you can enter a question mark (`?`) for help. For some parameters, enter two question marks (`??`) for more detailed information.

Default Parameters Values

When you are requested to specify a parameter, Thermo-Calc usually suggests an appropriate default value, which is displayed at the prompt between two slash signs (//). For example, this prompt means the default answer is `TERMINAL`:

```
OUTPUT FILE /TERMINAL/:
```

Press <Enter> to accept the default.

If you specify some parameters directly after the command name, then you can still choose to accept default values for some parameters.

To accept the default value for a parameter, type a comma (,) instead of a value for that parameter. For the comma to be interpreted correctly, type a blank space on each side of the comma. However, if you accept the default values for several parameters that follow each other, then the commas can be typed in without blank spaces separating them: (,,,) is interpreted in the same way as (, , ,).

For some commands and parameters, Thermo-Calc treats the values previously assigned as default values if the command is used again. For example, if the first stepping or mapping axis variable is specified as:

```
SET_AXIS_VARIABLE 1 X(FCC,FE) 0 0.89 0.025
```

Then if you want to change a parameter value for this axis variable, type:

```
SET_AXIS_VARIABLE 1 , 0.1 ,,,
```

This changes the minimum value from 0 to 0.1 at which a stepping or mapping operation halts. The other parameter values remain the same. Consequently, what is typed is equivalent to:

```
SET_AXIS_VARIABLE 1 X(FCC,FE) 0.1 0.89 0.025
```

About Operators and Functions

Sometimes you need to specify functions when setting up a system. For example, to make global conditions vary as a function of time.

The following operators can be used in writing functions. Use a semi-colon (`;`) to mark the end of a function.

Available Operators for Writing Functions

Operator	***Description***
+, -, *, /	Addition, subtraction, multiplication, division
**	Exponentiation, raising one quantity to the power of another, e.g. x^2.
ABS()	Absolute value
ERF(X)	Error function
EXP(X)	Exponential
LOG(X)	Natural logarithm
LOG10(X)	Base 10 logarithm
SIGN(X)	Sign function SIGN(X) is -1 when X<0, is 0 when X=0 and is 1 when X>0.
SIN(X), COS(X), TAN(X), ASIN(X), ACOS(X), ATAN(X)	• Trigonometric functions: sine, cosine, tangent • Inverse trigonometric functions: arcsine, arccosine, arctangent
SINH(X), COSH(X), TANH(X), ASINH(X), ACOSH(X), ATANH(X)	• Hyperbolic trigonometric functions • Inverse hyperbolic functions
SQRT(X)	Square root

Thermodynamic Variables

Thermophysical Properties Variables and Elastic Properties Variables

There are different thermodynamic variables in Thermo-Calc. Some are *state variables*, for example temperature, pressure and mole fraction. These characterize the equilibrium state of a system. You set them when you define your system in the POLY module before performing a calculation. They are also used in other modules such as DATA, GIBBS and PARROT. State variables that involve components can be used for the defined components, but not for any species. (To define new components in a defined system, use DEFINE_ COMPONENTS).

Other useful thermodynamic variables are derive from state variables with a mathematical function. Some derived variables are pre-defined by Thermo-Calc, such as normalized energetic and compositional extensive state variables for example. You use these by appending various normalizing suffixes to abbreviations that are associated with the state variables.

Thermodynamic variables can also be divided into extensive variables and intensive variables. An extensive variable is a variable whose value depends on the size of the system, whereas an intensive variable is a variable whose value is independent of system size.

More information about thermodynamic variables is available in the online help in Thermo-Calc Console Mode. Use the command INFORMATION, with a subject keyword such as one of the following as argument: STATE VARIABLES, INTENSIVE VARIABLES, EXTENSIVE VARIABLES, DERIVED VARIABLES, CONDITIONS (for condition settings), AXIS-VARIABLES (for stepping/mapping variable settings).

Common Thermodynamic Variables

The tables below list common thermodynamic variables. Most of these can be used to define equilibrium conditions in the POLY module unless otherwise indicated.

The variables are divided into the following tables:

- Intensive variables
- Energy-related extensive variables for whole system or for a phase
- Compositional extensive variables (overall amount of components in the whole system, or amount of a component in system or in a phase)
- Constitutional composition-related extensive variables (amount of a

constituent/species on a sublattice site in a phase)

- Special quantities

How to Read the Tables

- The *Abbrev*. column shows the abbreviation that you use in the POLY module for referring to the variable. If the variable must be given any arguments, then these are given in parenthesis directly after the abbreviation. For most variables, this is also the abbreviation that you use to refer to the variable in other modules. However, some variables are referred to with a different abbreviation in the POST module. If this is the case, then this is noted at the bottom of the table.
- Variables that are specific to a species, in which case the species is specified as an argument (*sp* in the table below). If there are two or more sublattices in a given phase, then this argument is given as `constituent#sublattice`. This indicates a constituent on a specific sublattice or site in the phase (referred to by the # sign and a digit). For example, `y(BCC,C#2)` stands for the site fraction of the C species on the second sublattice site of the BCC_A2 solution phase.
- The *Unit* column show which unit that you can use to express the variable in the POLY module. This unit is always the SI unit. In other modules, state variables may be expressed in other units.
- The *Suffix* column shows the suffixes you can append to the variables. The `R` suffix can be used with all compositional extensive state variables, but the suffix does not always change the value of the variable. This is indicated by putting the `R` in parenthesis.

These types of variables are listed in the following topics:

- Intensive Variables
- Extensive Variables
- Special Quantities
- The u-Fraction Variable
- Suffixes

Intensive Variables

V	Abbrev.	Unit	Descript.	Domain	Suffix
T	T[1]	K	Temperature	System	
P	P	Pa	Pressure	System	
µ	MU(comp)	J/mol	Chemical potential	Component	R
	MU(sp,ph)[2]			Species relative to a solution phase	R
a	AC(comp)	N/A	Activity	Component	R
	AC(sp,ph)[2]			Species relative to a solution phase	R
	LNAC (comp)[3]		ln(Activity)	Component	R
	LNAC (sp,ph) [2]			Species relative to a solution phase	R

[1] When plotting in POST, besides T (Kelvin), you can also use T_C or T_F to plot temperature in °C or °F.

[2] Only for single-substitutional-lattice solution phases such as AQUEOUS solution and GASeous mixture phases and for interacting species on the substitutional sublattice of two-sublattice solution phases (such as the phases BCC_A2 and M6C phases).

[3] In natural logarithm (lnAC=MU/RT)

Extensive Variables

Energy-Related Extensive Variables for Whole System or for a Phase

V	Abbrev.	Unit	Descript.	Domain	Suffix
V	V	m^3	Volume	System	M, W, V, R
	V(ph)[1]			Phase	M, W, F, R
	VP(ph) [2]			Phase	M, W, V, R
G	G	J	Gibbs energy	System	M, W, V, R
	G(ph) [1]			Phase	M, W, V, F, R
A	A	J	Helmholtz energy	System	M, W, V, R
	A(ph) [1]			Phase	M, W, V, F, R
U	U	J	Internal energy	System	M, W, V, R
	U(ph) [1]			Phase	M, W, V, F, R
H	H	J	Enthalpy[6]	System	M, W, V, R
	H(ph)			Phase	M, W, V, F
S	S	J/K	Entropy[6]	System	M, W, V, R
	S(ph) [1]			Phase	M, W, V, F, R
Cp	HM.T[3]	J/mol/K	Heat capacity at constant pressure	System	R
	HM(ph).T[3]			Phase	R
Cv	UM.T[4]	J/mol/K	Heat capacity at constant volume	System	R
	UM(ph).T[4]			Phase	R

V	Abbrev.	Unit	Descript.	Domain	Suffix
D	DG(ph) [5]	N/A	Driving force (thermodynamic factor)	Phase	Always use with M, W, V or F. R can also be used.

[1] For this variable, if the phase is unstable, then the variable gets a value of zero.

[2] Do not use VP(ph) as a condition in POLY. Instead, use CHANGE_STATUS PHASE <PHASE>=FIX <AMOUNT> where the fixed <AMOUNT> is roughly equal to VPF(ph), which cannot be directly evaluated or listed. If the phase is unstable, then VP(ph) and its normalized quantities get zero value.

[3] Use only if pressure has been set as a condition.

[4] Use only if volume has been set as a condition.

[5] Already divided by RT.

[6] When working in the POST module you can also enter the abbreviation for this variable into the Console, for example, `enth` or `enthalpy`, which corresponds to `HM`, and `entr` and `entropy`, which corresponds to `SM`.

Compositional Extensive Variables

These are for the overall amount of components in whole system, or amount of a component in system or in a phase.

Do not use NP(ph) or BP(ph) as conditions in the POLY module. Instead use CHANGE_STATUS PHASE <PHASE>=FIX <AMOUNT> where the fixed <AMOUNT> is roughly equal to NPF(ph) or BPF(ph), which cannot be directly evaluated or listed. If the phase is unstable, then NP(ph) or BP(ph) (and its normalized quantities) get zero value.

When plotting the following quantities in POST, refer to each as indicated:

- X(comp) -> `Mole-Fraction <comp>` (or `M_F`)
- W(comp) -> `Weight-Fraction <comp>` (or `W_F`)
- X%(comp) -> `Mole-Percent <comp>` (or `M_P`)
- W%(comp) -> `Weight-Percent <comp>` (or `W_P`).
- u-f(ph,comp) -> `U-F`

V	Abbrev.	Unit	Descript.	Domain	Suffix	Comment
n	N	mole	Moles	All	M, W, V,	

V	Abbrev.	Unit	Descript.	Domain	Suffix	Comment
				components	(R)	
	N(comp)			Component	M, W, V, (R)	
	N(ph,comp)			Component in a phase	M, W, V, (R)	
	NP(ph)[1]			Phase	M, W, V, (R)	See above
b	B	gram	Mass	All components	M, W, V, (R)	
	B(comp)			Component	M, W, V, (R)	
	B(ph,comp)			Component in a phase	M, W, V, (R)	
	BP(ph) [1]			Phase	M, W, V, (R)	See above
x	X(comp)	N/A	Mole fraction	Component	(R)	See above
	X(ph,comp)			Component in a phase	(R)	
w	W(comp)	N/A	Mass (weight) fraction	Component	(R)	See above
	W(ph,comp)			Component in a phase	(R)	
x%	X%(comp)[2]	N/A	Mole percent	Component	(R)	See above
w%	W%(comp)[2]	N/A	Mass (weight) percent	Component	(R)	See above
u	u-f (ph,comp)[1]	N/A	u-fraction	Component in a stable phase	(R)	See above
in	IN(sp)[2]	mole	Input mole number	Phase species in the system	(R)	See above

V	Abbrev.	Unit	Descript.	Domain	Suffix	Comment
im	IM(sp)[2]	gram	Input mass unit	Phase species in the system	(R)	See above

[1] Do not use as a condition in the POLY module.

[2] Only available in TQ-Interface.

Constitutional Composition-Related Extensive Variable

This is the amount of a constituent/species on a sublattice site in a phase.

V	Abbrev.	Unit	Descript.	Domain
y	Y(ph,cons#sub)	N/A	Site fraction	Constituent on a sublattice site (denoted by # and a digit) in a phase

Special Quantities

Variable	Abbrev.	Unit	Description or Example	Domain	Suffix
Q	QF(ph)[1]	n/a	Phase stability function	Phase	R Under a condition and system definition, QFR(ph) = QF(ph)
Tc	TC(ph) [2]	K	Curie temperature	Phase	R Under a condition and system definition, TCR(ph) = TC(ph)
Mb	BMAG(ph)[3]	n/a	Bohr magneton number	Phase	R Under a condition and system definition, BMAGR(ph) = BMAG(ph)
D1G	D1G(phase, site-fraction)	n/a	For example, D1G(FCC_A1#1, Cr#1) for first derivative of G for first composition set of FCC_A1 phase with respect to Cr site fraction on first sublattice. ? Search for TQGMDY in the *TQ-Interface Guide*	Phase	n/a
D2G	D2G(phase, site-fraction, site-fracton)	n/a	For example, D2G(FCC_A1#2, Cr#1, Cr#1) for second derivative of G for second composition set of	Phase	n/a

Variable	Abbrev.	Unit	Description or Example	Domain	Suffix
			FCC_A1 phase with respect to Cr site fraction on first sublattice. Search for TQDGYY in the *TQ-Interface Guide*		

[1] Negative when phase composition is inside a spinodal, otherwise positive. Can be used to find out if an equilibrium is within the miscibility gap for a solution phase. Cannot be used as a condition.

[2] Calculated for phases with magnetic contributions in an equilibrium state. Cannot be used as a condition, but can be plotted in POST or evaluated in POLY using SHOW_VALUE.

[3] Calculated for phases with magnetic contributions in an equilibrium state.

n/a = not applicable

The u-Fraction Variable

The u-fraction is an important quantity in some single-point or stepping paraequilibrium calculations in the POLY module and in the DICTRA module. You can apply the variable in a paraequilibrium calculation to the substitutional matrix component, the substitutional alloying components or the interstitial component. The u-fraction is denoted as ui for the i-th system component *n* of a whole system or of a specific phase in various equilibrium states (such as full-equilibria, partial-equilibria, para-equilibria, local-equilibria).

Generally, the u-fraction is defined as:

$$\frac{x_i}{\sum\limits_{j \in S} x_j}$$

The sum of x_{j} in the denominator is calculated for all substitutional alloying elements in the whole system or in a specific phase. The variable x_i in the numerator stands for the mole-fraction of the *i*-th component in the whole system or in the specific phase.

Suffixes

Suffixes may be appended to all extensive variables and to some intensive variables. Some suffixes can be used to enter the value of variables in normalized form. These are referred to as normalizing suffixes. If the variable that you create with a normalizing suffix is based on a state variable that can be set as a condition in POLY, then the normalized variable can also be set as a condition in POLY.

The normalizing suffixes are M (per mole), W (per mass in gram), V (per volume in m^3) and F (per mole formula unit). There is also a reference state suffix `R`, which you can use if you want the value of a thermodynamic variable to be calculated with respect to a reference state that have previously set.

Normalizing Suffixes

When variables that express system and phase quantities are normalized, the following general rules are used:

- System quantities are normalized by the total system size (in terms of N, B or V).
- Phase quantities are normalized by the phase amount [in terms of NP(ph), BP(ph) or VP(ph)].

The normalized quantities of G(ph), A(ph), U(ph), H(ph), S(ph) and V(ph) are calculated according to the thermodynamic model used for the phase (e.g. GM(ph), AM(ph), UM(ph), HM(ph), SM(ph) and VM(ph)). These quantities are calculated using the first derivatives of the Gibbs energy expressed for the phase with respect to the current composition of the system.

The tables describe the normalizing suffixes for the different state variables.

G, A, U, H, S and V of a Whole System

Suffix	Description	Example
M (per mole)	Total system size in terms of N.	GM is the Gibbs energy per mole of the system (J/mol). $\mathrm{GM} = \mathrm{G}/\mathrm{N}$
W (per mass in gram)	The total system size in terms of B.	GW is the Gibbs energy per mass of the system (J/g). $\mathrm{GW} = \mathrm{G}/\mathrm{B}$

Suffix	Description	Example
V (per volume in m^3)	The total system size in terms of V. VV does not have to be evaluated.	GV is the Gibbs energy per volume of the system (J/m^3). $\mathrm{GV} = \mathrm{G}/\mathrm{V}$

G(ph), A(ph), U(ph), H(ph), S(ph) and V(ph) of a Phase

Suffix	Example
M (per mole)	For example, GM(ph) is Gibbs energy of the phase per mole of the phase (J/mol). $\mathrm{GM(ph)} = \mathrm{G(ph)/NP(ph)}$
W (per mass in gram)	For example, GW(ph) is Gibbs energy of the phase per mass of the phase (J/mol). $\mathrm{GW(ph)} = \mathrm{G(ph)/BP(ph)}$
V (per volume in m^3)	For example, GV(ph) is Gibbs energy of the phase per volume of the phase (J/mol). $\mathrm{GV(ph)} = \mathrm{G(ph)/V(ph)}$
F (per mole formula unit)	For example, GF(ph) is the Gibbs energy of the phase per formula unit of the phase (J/mol). $\mathrm{GF(ph)} = \mathrm{G(ph)/NP(ph)^{*}NA}$

DG(ph) of a Phase

Suffix	Description	Example(s)
M (per mole)	Theoretically, the first derivative of the variable with regard to the phase amount in terms of NP(ph). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead. DGM(ph) cannot not be set as a condition since it is only calculated under a certain type of	DGM(ph) is driving force for precipitation of the phase per mole of components. $\mathrm{DGM(ph)} = \partial\mathrm{DG(ph)}/\partial\mathrm{NP(ph)}$

Suffix	Description	Example(s)
	equilibrium state.	
W (per mass in gram)	Theoretically, the first derivative of the variable with regard to the phase amount in terms of BP(ph). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead. DGW(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.	DGW(ph) is driving force for precipitation of the phase per mass of components. $\mathrm{DGW(ph)} = \partial \mathrm{DG(ph)} / \partial \mathrm{BP(ph)}$
V (per volume in m^3)	Theoretically, the first derivative of the variable with regard to the phase amount in terms of VP(ph). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead. DGV(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.	DGV(ph) is driving force for precipitation of the phase per volume of components. $\mathrm{DGV(ph)} = \partial \mathrm{DG(ph)} / \partial \mathrm{VP(ph)}$
F (per mole formula unit)	Theoretically, the first derivative of the variable with regard to the phase amount in terms of NP(ph) and NA (NA is the total atomic number in the phase formula). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead. DGF(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.	DGF(ph) is driving force for precipitation of the phase per formula unit of components. $\mathrm{DGF(ph)} = \partial \mathrm{DG(ph)} / \partial \mathrm{NP(ph)}^{*} \partial \mathrm{NA}$

N and B of a System

Suffix	Description	Example(s)
M (per mole)	The total system size in terms of N. NM does not have to be evaluated. BM cannot be set as a condition.	BM is mass (gram) of components per mole of the system (g/mol). $\mathrm{BM} = \mathrm{B}/\mathrm{N}$
W (per mass in gram)	The total system size in terms of B. BW does not have to be evaluated. NW cannot be set as a condition.	NW is mole number of components per mass of the system (mol/g). $\mathrm{NW} = \mathrm{N}/\mathrm{B}$
V (per volume in m^3)	The total system size in terms of V. BV is the density of the entire system.	NV is mole number of components per volume of the system (mol/m^3). $\mathrm{NV} = \mathrm{N}/\mathrm{V}$ BV is the density of the entire system (g/m^3). $\mathrm{BV} = \mathrm{B}/\mathrm{V}$

N (comp) and B(comp) of a Component in the System

Suffix	Description	Example(s)
M (per mole)	The total system size in terms of N. BM(comp) cannot be set as a condition.	NM(comp) is the mole of a component per mole of the system (i.e. mole fraction, which also is expressed as X(comp)). $\mathrm{NM(comp)} = \mathrm{N(comp)}/\mathrm{N}$
W (per mass in gram)	The total system size in terms of B. NW(comp) cannot be set as a condition.	BW(comp) is mass (gram) of a component per mass of the system (i.e. mass fraction, which also is expressed as W(comp)). $\mathrm{BW(comp)} = \mathrm{B(comp)}/\mathrm{B}$
V (per	The total system size	NV(comp) is mole number of a component per volume of the system

Suffix	Description	Example(s)
volume in m^3)	in terms of V.	(mol/m^3). $\mathrm{NV(comp) = N(comp)/V}$

NP(ph), BP(ph) and VP(ph) of a Phase in the System

Suffix	Description	Example(s)
M (per mole)	BPM(ph) and VPM(ph): The phase amount in terms of NP(ph). NPM(ph): The total system size in terms of N.	BPM(ph) is mass (gram) of a phase per moles of the system (g/mol). $\mathrm{BPM(ph) = BP(ph)/N}$ NPM(ph) is number of moles of a phase per moles of the system (mole fraction). $\mathrm{NPM(ph) = NP(ph)/N}$
W (per mass in gram)	NPW(ph) and VPW(ph): The phase amount in terms of BP(ph). BPW(ph):The total system size in terms of B.	VPW(ph) is volume (m^3) of a phase per mass of the system (m^3/g) $\mathrm{VPW(ph) = VP(ph)/B}$ BPW(ph) is mass (gram) of a phase per mass of the system (mass fraction) $\mathrm{BPW(ph) = BP(ph)/B}$
V (per volume in m^3)	NPV(ph) and BPV(ph): The phase amount in terms of VP(ph). VPV(ph): The total system size in terms of V.	NPV(ph) is number of moles of a phase per volume of the system (mol/m^3). $\mathrm{NPV(ph) = NP(ph)/V}$ VPV(ph) is volume (m^3) of a phase per volume of the system (volume fraction). $\mathrm{VPV(ph) = VP(ph)/V}$

N(ph,comp) and B(ph,comp) of a Component in a Phase

Suffix	Description	Example(s)
M (per	The phase amount in	NM(ph,comp) is number of moles of a component per mole of a

Suffix	Description	Example(s)
mole)	terms of NP(ph) of the phase.	phase (i.e. mole fraction of a component in a phase, which is equivalent to X(ph, comp)). $\mathrm{NM(ph,comp)} = \mathrm{N(ph,comp)/NP(ph)}$
W (per mass in gram)	The phase amount in terms of BP(ph) of the phase.	BW(ph,comp) is mass (gram) of a component per mass of a phase (i.e. mass fraction of a component in a phase, which is equivalent to W(ph,comp)). $\mathrm{BW(ph,comp)} = \mathrm{B(ph,comp)/BP(ph)}$
V (per volume in m^3)	The phase amount in terms of VP(ph) of the phase.	NV(ph,comp) is mole number of a component per volume of a phase (mol/m^3). $\mathrm{NV(ph,comp)} = \mathrm{N(ph,comp)/VP(ph)}$

The Reference State Suffix R

SET_REFERENCE_STATE

You can use the reference state suffix `R` for some thermodynamic variables to calculate their value with respect to a reference state that you have previously set for a system component with the SET_REFERENCE_STATE command in POLY (or in response-driven modules such as the POURBAIX module). The value of energy-related variables that are used with the `R` suffix depends on the reference states of all the components in the defined system.

It is possible to use an `R` suffix on all compositional extensive state variables as well, but the value of the state variable is always the same, with or without the suffix.

If the reference state for a system component is the default reference state (the stable reference state (SER) which is defined in a Thermo-Calc database), then MUR(comp)= MU (comp), ACR(comp)= AC(comp) and LNACR(comp)= LNAC(comp).

In the case of some thermodynamic variables, you can also use the `R` suffix to express chemical potentials and activities of species relative to some single-substitutional-lattice solution phases (such as aqueous solution, gaseous mixture, metallic liquid solution, slag mixture or MO solid solution). These state variables are MU(sp,ph), MUR(sp,ph), AC(sp,ph), ACR(sp,ph), LNAC(sp,ph) and LNACR(sp,ph).

The reference states and standard states of various solution species are pre-defined for some solution phases in some databases. For all solution species in any solution model in any database, it is always the case that MUR(sp,ph)= MU(sp,ph), ACR(sp,ph)= AC(sp,ph) and LNACR(sp,ph)= LNAC(sp,ph).

Derived Variables and Partial Derivatives

Many derived variables can be obtained easily by using partial derivatives of state variables, such as heat capacity, thermal expansivity, isothermal compressibility, among others.

Derivatives of state variables can be defined or evaluated by putting a dot (.) between two state variables. The variable after the dot must be a condition that you have set when you defined your system. For example, the heat capacity (at constant pressure or volume) of a system is the partial derivative of the state variable enthalpy with respect to temperature. To evaluate this derivative, use the designation HM.T, where temperature is a state variable that you have set already.

Any partial derivative of a state variable with respect to another can be defined or evaluated as a derived variable by using the dot (.) notation.

Derived Variables Dot Notation Examples

The following table shows some examples:

Derived Variable	Description
$\mathrm{HM.T} = \partial\mathrm{HM}/\partial\mathrm{T}$	Heat capacity for the system at either constant P if pressure is a condition or constant V if volume is a condition.
$\mathrm{HM(ph).T} = \partial\mathrm{HM(ph)}/\partial\mathrm{T}$	Heat capacity for a phase at either constant P if pressure is a condition or constant V if volume is a condition.
$\mathrm{H.T} = \partial\mathrm{H}/\partial\mathrm{T}$	Heat capacity for the system multiplied by total mole number of components, i.e., $\partial\mathrm{H}/\partial\mathrm{T} = \mathrm{C_p}{}^*\mathrm{N}$ if pressure is a condition in a closed system or $\partial\mathrm{H}/\partial\mathrm{T} = \mathrm{C_v}{}^*\mathrm{N}$ if volume is a condition in a closed system.
$\mathrm{H(ph).T} = \partial\mathrm{H(ph)}/\partial\mathrm{T}$	Heat capacity for a phase multiplied by the sum of $\mathrm{NP(ph)}$and $\mathrm{HM(ph)}^*\partial\mathrm{NP(ph)}/\partial\mathrm{T}$, i.e., $\mathrm{C_p\,(ph)^*NP(ph){+}HM(ph)^*\partial NP(ph)/\partial T}$ if pressure is a condition or $\mathrm{C_{v(ph)}{}^*NP(ph){+}HM(ph)^*\partial NP(ph)/\partial T}$ if volume is a condition.
$\mathrm{VM.T} = \partial\mathrm{VM}/\partial\mathrm{T}$	Thermal expansivity of the system (already multiplied by the total molar volume), i.e., $\partial\mathrm{VM}/\partial\mathrm{T} = \alpha^*\mathrm{VM}$.

Derived Variable	Description
$\mathrm{VM(ph).T} = \partial\mathrm{VM(ph)}/\partial\mathrm{T}$	Thermal expansivity of a phase (already multiplied by its molar volume), i.e., $\partial\mathrm{VM(ph)}/\partial\mathrm{T} = \alpha\mathrm{(ph)}^*\mathrm{VM(ph)}$.
$\mathrm{V.T} = \partial\mathrm{V}/\partial\mathrm{T}$	Thermal expansivity of the system (already multiplied by the total volume), i.e., $\partial\mathrm{V}/\partial\mathrm{T} = \alpha^*\mathrm{V}$.
$\mathrm{V(ph).T} = \partial\mathrm{V(ph)}/\partial\mathrm{T}$	Thermal expansivity of a phase (already multiplied by the phase volume) plus the $\mathrm{VM(ph)}^*\partial\mathrm{NP(ph)}/\partial\mathrm{T}$ term, i.e., $\partial\mathrm{V(ph)}/\partial\mathrm{T} = \alpha\mathrm{(ph)}^*\mathrm{V(ph)} = \alpha\mathrm{(ph)}^*\mathrm{VM(ph)}^*\mathrm{NP(ph)}+\mathrm{VM(ph)}^*\partial\mathrm{NP(ph)}/\partial\mathrm{T}$.
$\mathrm{VM.P} = -\partial\mathrm{VM}/\partial\mathrm{P}$	Isothermal compressibility of the system (already multiplied by the total molar volume), i.e.,$\partial\mathrm{VM}/\partial P - \kappa^*\mathrm{VM}$.
$\mathrm{VM(ph).P} = -\partial\mathrm{VM(ph)}/\partial\mathrm{P}$	Isothermal compressibility of a phase (already multiplied by its molar volume), i.e.,$\partial\mathrm{VM(ph)}/\partial\mathrm{P} = -\kappa\mathrm{(ph)}^*\mathrm{VM(ph)}$.
$\mathrm{V.P} = -\partial\mathrm{V}/\partial\mathrm{P}$	Isothermal compressibility of the system (already multiplied by the total volume), i.e.,$\partial\mathrm{V}/\partial\mathrm{P} = -\kappa^*\mathrm{V}$
$\mathrm{V(ph).P} = -\partial\mathrm{V(ph)}/\partial\mathrm{P}$	Isothermal compressibility of a phase (already multiplied by the phase volume) plus the $\mathrm{VM(ph)}^*\partial\mathrm{NP(ph)}/\partial\mathrm{P}$ term, i.e., $\partial\mathrm{V(ph)}/\partial\mathrm{P} = -\kappa\mathrm{(ph)}^*\mathrm{V(ph)} = -\kappa\mathrm{(ph)}^*\mathrm{VM(ph)}^*\mathrm{NP(ph)}+\mathrm{VM(ph)}^*\partial\mathrm{NP(ph)}/\partial\mathrm{P}$.
$\mathrm{T.X(comp)} = \partial\mathrm{T}/\partial\mathrm{X(comp)}$	Slope of a phase boundary on a T-X(comp) phase diagram with respect to mole fraction of the component in the system.
$\mathrm{T.W(comp)} = \partial\mathrm{T}/\partial\mathrm{W(comp)}$	Slope of a phase boundary on a T-W(comp) phase diagram with respect to mass of the component in the system.
$\mathrm{T.X(ph,comp)} = \partial\mathrm{T}/\partial\mathrm{X(ph,comp)}$	Slope of a phase boundary on a T-X(ph,comp) phase diagram with respect to mole fraction of the component in the phase.
$\mathrm{T.W(ph,comp)} = \partial\mathrm{T}/\partial\mathrm{W(ph,comp)}$	Slope of a phase boundary on a T-W(ph,comp) phase diagram with respect to mole fraction of the component in the phase.
$\mathrm{P.T} = \partial\mathrm{P}/\partial\mathrm{T}$	Slope of a phase boundary on a P-T phase diagram (Note that the equilibrium with phase assemblage must be calculated first).

Defining New Derived Variables and Functions

You can define additional derived variables or functions based on a state variable by using ENTER_SYMBOL. Any derived variable or function must have a unique name that starts with a letter and has a maximum number of eight characters. These characters can include both uppercase and lowercase letters, numerical digits and the underscore (_). No other characters are allowed.

The difference between new derived variables introduced with the ENTER_SYMBOL command and new functions introduced with the same command is as follows. Whenever Thermo-Calc calculates the value of a function (as part of an equilibrium calculation for example), all functions related to the defined system is evaluated. An entered derived variable, on the other hand, is only evaluated when it is defined and when it is re-evaluated with EVALUATE_FUNCTIONS.

Derived Variables for Aqueous Solutions

Standard state variables used for other phases can be directly applied to the aqueous solution phase. In addition, there are pre-defined derived variables for the aqueous solution phase in particular.

Examples of predefined derived variables for the aqueous solution phase are listed and briefly described in the following tables. Some derived variables for a gaseous mixture phase are also shown. This is because EOS (Equation of State) expressions, standard thermodynamic properties and transport properties of the pure solvent H2O are also expressions and properties of the pure gaseous species H2O.

For Aqueous Solution Phase

Name	Abbrev.	Units	Description	Comments
pH	PH	N/A	Acidity	of the aqueous solution phase pH = -log10(AC(H+)) = -log10 (ACR(H+,AQ))
Eh	EH	V, mV	Hypothetical electric potential	of the aqueous solution phase Eh = u(ZE)/96485.309
Pe	PE	N/A	Logarithm of the hypothetical electron activity	of the aqueous solution phase pe = u(ZE)/(2.3025851*RT)

Name	Abbrev.	Units	Description	Comments
Ah	AH	kJ, kcal	Thermodynamic affinity per electron	of a redox couple wrt the standard hydrogen electrode in the aqueous solution phase Ah = u(ZE)
yw	YH2O	N/A	Mole fraction	of the solvent H2O in the aqueous solution phase YH2O = Y(AQ,H2O)
Nw	AH2O	mole	Mole number	of 1.0 kg of solvent H2O AH2O = 55.508435
Nsp	NSH2O	mole	Mole number, NS(AQ,H2O)	of the solvent (H2O) in the aqueous solution phase NS(AQ,H2O) = YH2O*NP(AQ)
	NS#		Mole number, NS(AQ,sp)	of a solute species in the aqueous solution phase NS(AQ,sp) = Y(AQ,sp)*NP(AQ)
M	ML#	mol/kg_H2O	Molality, ML(AQ,sp)	of a solute species in the aqueous phase ML(AQ,sp) = Y (AQ,sp)*AH2O/YH2O
m*	TIM	equivalent molality	Total molality	of all solute species in the aqueous solution phase TIM = sum[ML(AQ,sp)]ions + sum[ML(AQ,sp)]complexes
mt	TIC#	equivalent molality	Total ionic concentration, TIC (AQ,sp)	of a cation I in the aqueous phase TIC(AQ,spI) = sum[ML (AQ,spJ)*V(spI-in-spJ)]
I	ISTR	N/A	Ionic strength	of the aqueous solution phase ISTR=1/2*sum[ML(AQ,sp)*Z (AQ,sp)**2]
γ	RCH2O	N/A	Activity coefficient,	of the solvent (H2O)

Name	Abbrev.	Units	Description	Comments
			RC(H2O,AQ)	RC(H2O,AQ) = ACR (H2O,AQ)/YH2O
	RC#		Activity coefficient, RC(sp,AQ)	of a solute species RC(sp,AQ) = ACR(sp,AQ)/Y (AQ,sp)*YH2O
αi	AIH2O	N/A	Activity, AI(H2O,AQ)	of the solvent (H2O), AI(H2O,AQ) = ACR(H2O,AQ)
	AI#		Activity, AI(sp,AQ)	of a solute species related to the aqueous solution phase, AI(sp,AQ) = ACR (sp,AQ)*AH2O
	LogAI#		Log10 Activity, LogAI(H2O,AQ), LogAI(sp,AQ)	of the solvent or a solute species related to the aqueous solution phase in common logarithm, LogAI(H2O,AQ) = log10[AI (H2O,AQ)] LogAI(sp,AQ) = log10[AI (sp,AQ)]
αw	AW	N/A	Activity	of H2O in the aqueous solution phase AW = ACR(H2O,AQ)
ϕ	OS	N/A	Osmotic coefficient	of aqueous solution phase OS = -55.508435*lnAW/TIM
At1	AT1	equil_mol/kg_ H2O	Titration alkalinity (definition 1)	of the aqueous solution phase Generally defined as the equivalent molality of carbonate and bicarbonate at the methyl orange endpoint (pH=4.5).
At2	AT2	equil_mol/kg_ H2O	Titration alkalinity (definition 2)	of the aqueous solution phase Generally defined as the equivalent molality of

Name	Abbrev.	Units	Description	Comments
				carbonate and bicarbonate, plus sulfide, at the methyl orange endpoint (pH=4.5).

For Gaseous Mixture Phase

Name	Abbrev.	Units	Description	Comments
γ	RA#	N/A	Activity coefficient, RA(sp,GAS)	of a gaseous species in the gaseous mixture RA(sp,GAS) = function(Y,T,P)
γ*	RF#	N/A	Fugacity coefficient, RF(sp,GAS)	of a pure gaseous species under TP RF(sp,GAS) = function(T,P/V)
F	FUG#	pa, bar, psi	Fugacity, FUG(sp,GAS)	of a gaseous species in the gaseous mixture FUG(sp,GAS) = RA(sp,GAS)*RF (sp,GAS)*Y(GAS,sp)*P
ft	TFUG	pa, bar, psi	Total gas fugacity	of the gaseous mixture phase TFUG = sum[FUG(sp,GAS)]

Defining New Derived Variables for Aqueous Solutions

You can define many different additional derived variables and functions. For instance, the partition coefficient of a component between two phases is defined as follows:

```
Pc<name> = X(phase1,component)/X(phase2,component)
```

Another example is the activity coefficient of a component in the system. It is defined as follows:

```
Rc<name> = ACR(component)/X(component)
```

The activity coefficient of a species in a solution phase depends on which model definitions on the reference states that are used and it depends on the standard states for the species. If the standard state of a species is defined to be the same as the pure species in a substitutional phase, then the activity coefficient of the species can be calculated as:

```
RC<name> = ACR(species,phase)/Y(phase,species)
```

In some cases, there are more than one sublattice in the phase and the reference states for the phase species cannot be presented by the pure species, as in the case of C in FCC [(Fe)1 (C,N,VA)1], where the model may end at fifty percent C and fifty percent Fe. In those cases, the chemical potential and activity of all phase constituents is not well defined and you cannot properly define the activity coefficients of the species in the phase.

For an aqueous solution phase, no matter what model is used, the reference state and standard state for both the solvent and solutes are defined in a special way in the Thermo-Calc software. The reference state for the solvent is set as pure water, the same as its standard state (according to Raoults's Law). The standard state for a solute species is set the hypothetical solute species, whilst its reference state is defined as the hypothetical state at unit molality (one mole dissolved into 1.0 kg of solvent) but in which the environment of each molecular is the same as at infinite dilution (according to Henry's Law). Under these definitions, the activity coefficients for solvent species can be calculated as follows:

```
RC<H2O> = ACR(H2O,aqueous)/ Y(aqueous,H2O)
```

The coefficients for the solute species can be calculated as follows:

```
RC<spec> = AI(species,aqueous)/ML(aqueous,species)
= ACR(species,aqueous)/ Y(aqueous,species)*Y(aqueous,H2O)
```

AI is here the activity of solute species calculated from the model, and ML is the molality of the species.

Thermodynamic Variables and Wildcard Characters

The ACR (species,phase) and the MUR (species,phase) quantities can only be appropriately and meaningfully applied to substitutional solution phases (such as GAS, AQUEOUS, LIQUID) and to solution phases without an interstitial sublattice set. This means that the wild card characters `*` and `$` normally don't work properly for the activity and/or chemical potential properties.

For example, do not use ACR(*,*) or MUR(*,*) for all the species relative to all phases, nor ACR(*,phase) or MUR(*,phase) for all the species relative to a specific phase, nor ACR (species,*) or MUR(species,*) for a specific species relative to all phases.

Instead, use specific names for species and (applicable) phase, as in the following examples:

```
SHOW_VALUE acr(fe+2,aqueous)Lists activity of the Fe+2 species referred to
AQUEOUS solution phase
```

```
SHOW_VALUE mur(c2,gas)Lists chemical potential of the C2 species referred to GAS
mixture phase
```

```
SET_AXIS_VAR y ac(o2,gas)Sets activity of the O2 species referred to GAS mixture
phase as Y-axis
```

Units of State Variables and Derived Variables

The units for the state variables in the Units column in the table in User-Specified Units are the SI units that are used in the POLY module. However, in the POST module, you can both use pre-defined symbols and define your own symbols which are based on state variables and derived variables. By doing this, you can express the value of the thermodynamic variables in non-default units. The following topic briefly describes how you can create your own symbols and suggests expressions that you can use to convert default units into other standard units which are not default units in Thermo-Calc.

The topic Examples of User-Defined Units describes some variables of specific species in a phase and the units in which they are expressed. These variables are not used in POLY or POST, but in the GIBBS, DATA, PARROT and ED_EXP modules.

User-Specified Units

You do not always need to use the default units for variables. Using ENTER_SYMBOL, you can convert the value of variable from the default unit to your preferred unit. (Some response-driven modules also allow you to set conditions in non-default units.) User-defined symbols in the form of functions can be used for plotting in the POST module, but they cannot be used as conditions in POLY. User defined symbols in the form of variables can be used as conditions.

For example, if you want pressure to be plotted in bar rather than Pa, then you define the following function `PB`:

```
Enter_symbol function PB = P/1E5 ;
```

If you wanted heat capacity of a system to be shown as in terms of J/mol/K, then you can define the following function Cp:

```
Enter_symbol function Cp = Hm.T ;
```

If the variable you want to convert is a function of one or more derivatives, then you must enter the symbol as a variable rather as a function. For instance, a symbol expressing heat capacity of a system in a unit of cal/mol/K can be defined as the following variable `Cp2`:

```
Enter_symbol variable Cp2 = Hm.T/4.1858 ;
```

Examples of User-Defined Units for information about entering conventional functions and the associated units.

Examples of User-Defined Units

The following tables give examples of expressions you can use to enter symbols. This enables you to show the values of thermodynamic variables in a variety of units.

Units of State Variables and Derived Variables and User-Specified Units

> You can also use thermodynamic variables with normalizing suffixes in the expression when you enter a symbol. However, the tables do not have examples of these expressions.

In the expressions these are defined as follows:

- `i` is for an auxiliary index or letter that corresponds to the component `c`
- `j` is for an auxiliary index or letter that corresponds to the phase `ph`, and
- `ij` stands for an auxiliary index or letter that corresponds to the component `c` in the phase `ph`.

Intensive and Extensive Variables of a Defined System

Quantity	Suggested Name and Expression	Unit
For Intensive Variables of a Defined System		
Temperature	TempC = T-273.15	Celsius (C)
	TempF = 1.8*T-459.67	Fahrenheit (F)
	TempF = 1.8*TempC+32	

Quantity	**Suggested Name and Expression**	**Unit**
Pressure	PB = P/1E5	bars (bar)
	PKb = P/1E8	kilobars (kbar)
	PAtm = P/101325	atmosphere (atm)
	PSI = P/6894.76	pounds/sq. inch (psi)
	PIHg = P/3342.11	inches of Hg
	PTor = P/133.322	Tors (millimeters of Hg)
For Extensive Variables of a Defined System		
Amount	BKg = 1E-3*B	kilograms (kg)
	BTon = 1E-6*B	tons
Volume	VDM = 1E-3*V	cubic decimeters (dm^3, l)
	VCM = 1E-6*V	cubic centimeters (cm^3)
	VMM = 1E-9*V	cubic millimeters (mm^3)
	VCI = 1.6387064E-5*V	cubic inches (in^3)
	VLi = 1E-3*V	liters (l)
Energy	GCal = G/4.1858	cal
	ACal = A/4.1858	cal
	UCal = U/4.1858	cal
	HCal = H/4.1858	cal
	SCal = S/4.1858	Cal/K

Quantity	Suggested Name and Expression	Unit
Heat Capacity	Cp2 = HM.T/4.1858	cal/mol/K
	Cp3 = HW.T/4.1858	cal/g/K
	Cp4 = HV.T/4.1858	cal/m^3/K
Thermal Expansion	A2 = VM.T*1E-6/VM	1/K
	A3 = VW.T*1E-6/VW	1/K
Isothermal Compressibility	B2 = -VM.P*1E-9/VM	1/Pa
	B3 = -VW.P*1E-9/VW	1/Pa

Intensive and Extensive Variables of a System Component

Quantity	Suggested Name and Expression	Unit
For Intensive Variables of a System Component		
Chemical Potential	MUi = MU(c)/4.1858	cal/mol
	MURi = MUR(c)/4.1858	cal/mol
Special quantity for aqueous solution	pH = -LOG10(ACR(H+1))	dimensionless
	Eh = MUR(ZE)/RNF where RNF=96485.309	volts (V)
For Extensive Variables of a System Component		

Quantity	Suggested Name and Expression	Unit
Amount	MFi = N(c)/N = X(c)	dimensionless
	MPi = N(c)/N*100	dimensionless
	WFi = B(c)/B = W(c)	dimensionless
	WPi = B(c)/B*100	dimensionless
	BKgi = 1E-3*B(c)	kilograms (kg)
	BToni = 1E-6*B(c)	tons

Extensive Variables of a Phase

Quantity	Suggested Name and Expression	Unit
Amount	MFj = NP(ph)/N	dimensionless
	MPj = NP(ph)/N*100	dimensionless
	WFj = BP(ph)/B	dimensionless
	WPj = BP(ph)/B*100	dimensionless
	BKgj = 1E-3*BP(ph)	kilograms (kg)
	BTonj = 1E-6*BP(ph)	tons
Volume	VCMj = 1E-3*V(ph)	cubic decimeters (dm^3, l)
	VCMj = 1E-6*V(ph)	cubic centimeters (cm^3)
	VMMj = 1E-9*V(ph)	cubic millimeters (mm^3)
Energy	GCalj = G(ph)/4.1858	cal
	ACalj = A(ph)/4.1858	cal

Quantity	Suggested Name and Expression	Unit
Isothermal Compressibility	B2j = -VM(ph).P/VM(ph)	1/Pa

Extensive Variables of a Component in a Phase

Quantity	Suggested Name and Expression	Unit
Amount	MFij = N(ph,c)/NP(ph) = X(ph,c)	dimensionless
	MPij = N(ph,c)/NP(ph)*100	dimensionless
	WFi = B(ph,c)/BP(ph) = W(ph,c)	dimensionless
	WPij = B(ph,c)/BP(ph)*100	dimensionless
	BKgij = 1E-3*B(ph,c)	kilograms (kg)
	BTonij = 1E-6*B(ph,c)	tons

Intensive and Extensive Variables of a Species in a Phase

Quantity	Suggested Name and Expression	Unit
For Intensive Variables of a Species in a Phase		
Chemical Potential	MUCalij = MU(sp,ph)/4.1858	cal/mol
	MUErgij = MU(sp,ph)*1E7	cal/mol
Fugacity	FAij = AC(sp,ph)*PATM	atmosphere (atm)
	FBij = AC(sp,ph)*PB	bars (bar)
	FCij = AC(sp,ph)*PKB	kilobars (kbar)
	FTij = AC(sp,ph)*PTOR	Tors (millimeters of Hg)

Quantity	Suggested Name and Expression	Unit
ln(Fugacity)	LnFAij = LNAC(sp,ph)+LN(PATM)	atmosphere (atm)
	LnFBij = LNAC(sp,ph)+LN(PB)	bars (bar)
	LnFCij = LNAC(sp,ph)+LN(PKB)	kilobars (kbar)
	LnFTij = LNAC(sp,ph)+LN(PTOR)	Tors (millimeters of Hg)
Special quantity for aqueous solution	AIij=ACR(FE+3,AQ)*AH2O	dimensionless
	RCij=ACR(FE+3,AQ)*YH2O/Y(AQ,FE+3) where AH2O=55.508435 and YH2O=Y(AQ,H2O)	dimensionless
	WRCalij = WR(AQ,sp)/4.1858 (WR(AQ,sp) is only valid for aqueous species in a system in which the AQUEOUS solution phase is considered)	cal/mol
For Extensive Variables of a Species in a Phase		
Special quantity for aqueous solution	MLij=Y(AQ,FE+3)*AH2O/YH2O	molality (m)
	ISTR=1*IS1+1*IS2+1*IS3 where AH2O=55.508435, YH2O=Y(AQ,H2O) and ISn=.5*MLi*Zi**2+.5*MLj*Zj**2+.5*MLk*Zk**2	molality (m)

Units for Variables of Specific Species in a Phase

In the GIBBS, DATA, PARROT and ED_EXP modules, there are quantities that describe various thermodynamic, physical, chemical and transport properties for a compound phase, and for a certain species or a given species combination in a specific solution phase. The following table describes the units for those variables.

These variables cannot be directly used in the POLY or POST modules.

Variables	Description and Unit
G(ph,sp) G(ph,sp;0) G(ph,sp1;sp2;...;0)	Gibbs energy (J/mol) of a pure substance or end-member.
G(ph,sp1,sp2,...) L(ph,sp1,sp2,...) G(ph,sp1,sp2,...;0) L(ph,sp1,sp2,...;0) G(ph,sp1,sp2,...;...;0) L(ph,sp1,sp2,...;...;0)	Zero-order interaction parameter (J/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
G(ph,sp1,sp2,...;i) L(ph,sp1,sp2,...;i) G(ph,sp1,sp2,...;...;i) L(ph,sp1,sp2,...;...;i)	The ith -order interaction parameter (J/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
TC(ph,sp) TC(ph,sp;0) TC(ph,sp1;sp2;...;0)	Curie temperature (K) of a pure substance or end-member.
TC(ph,sp1,sp2,...) TC(ph,sp1,sp2,...;0) TC(ph,sp1,sp2,...;...;0)	Zero-order Curie-temperature contribution (K) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
TC(ph,sp1,sp2,...;i) TC(ph,sp1,sp2,...;...;i)	The ith -order Curie-temperature contribution (K) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
BMAGN(ph,sp) BMAGN(ph,sp;0) BMAGN (ph,sp1;sp2;...;0)	Bohr magneton number (dimensionless) of a pure substance or end-member.
BMAGN(ph,sp1,sp2,...) BMAGN (ph,sp1,sp2,...;0)	Zero-order Bohr magneton number (dimensionless) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.

Variables	Description and Unit
BMAGN (ph,...;sp1,sp2,...;0)	
BMAGN (ph,sp1,sp2,...;i) BMAGN (ph,sp1,sp2,...;...;i)	The ith -order Bohr magneton number (dimensionless) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
V0(ph,sp) V0(ph,sp;0) V0(ph,sp1;sp2;...;0)	Molar volume (m^3) at 1 bar and reference T0 of a pure substance or end-member.
V0(ph,sp1,sp2,...) V0(ph,sp1,sp2,...;0) V0(ph,sp1,sp2,...;...;0)	Zero-order composition-dependent molar volume (m^3) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
V0(ph,sp1,sp2,...;i) V0(ph,sp1,sp2,...;...;i)	The ith-order composition-dependent molar volume (m^3) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VA(ph,sp) VA(ph,sp;0) VA(ph,sp1;sp2;...;0)	Integrated thermal expansivity (m^3/mol/K) of a pure substance or end-member.
VA(ph,sp1,sp2,...) VA(ph,sp1,sp2,...;0) VA(ph,sp1,sp2,...;...;0)	Zero-order composition-dependent thermal expansivity (m^3/mol/K) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VA(ph,sp1,sp2,...;i) VA(ph,sp1,sp2,...;...;i)	The ith -order composition-dependent thermal expansivity (m^3/mol/K) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VC(ph,sp)	High pressure fitting parameter (m^3/mol) of a pure substance or endmember.
VC(ph,sp1,sp2,...)	Zero-order composition-dependent high pressure fitting parameter (m^3/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VC(ph,sp1,sp2,...i)	The ith -order composition-dependent high pressure fitting parameter (m^3/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site

Variables	Description and Unit
	in a solution phase.
VK(ph,sp)	Isothermal compressibility (m^3/mol/Pa) of a pure substance or endmember.
VK(ph,sp1,sp2,...)	Zero-order composition-dependent isothermal compressibility (m^3/mol/Pa) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VK(ph,sp1,sp2,...i)	The ith -order composition-dependent isothermal compressibility (m^3/mol/Pa) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
WR(ph,sp) WR(ph,sp;0)	Standard Born function (J/mol) of a specific aqueous species in the AQUEOUS solution phase (always with a single sublattice) under the reference-state temperature and pressure.

State Variables for Scheil

Post processing is done the same way as POLY-3: specific variables for plotting in the Scheil module are listed.

POLY Module Commands

For a comparable list in Graphical Mode, see Scheil Calculator Available Plot Variables.

The variables can be plotted along the X- and Y-axes. In the table, *ph* is an abbreviation of *phase*, and *el* is an abbreviation of *element*. An asterisk (*) can be used as a wild character for *el* and *ph*. Use the abbreviations of the variables when you specify what the X- and Y-axes represent in a diagram.

Abbreviation	***State Variable***
T	Temperature in Celsius
NL/BL/VL	Mole/mass fraction of liquid
NS/BS/VS	Mole/mass fraction of all solid phases
NS(ph)/BS(ph)	Mole/mass fraction of a solid phase
VS(ph)	Volume fraction of a solid phase
W(ph,el)	Weight fraction of an element in a phase
X(ph,el)	Mole fraction of an element in a phase
Y(ph,el)	Site fraction of an element in a phase
NN(ph,el)	Distribution of an element in a phase
NH/BH	Total heat per mole/gram (top curve) and Latent heat per mole/gram (bottom curve)
CP/BCP	Apparent heat capacity per mole/gram
NV/NV(ph)	Molar volume of the system or a phase
DS/DS(ph)	Average density of the system or a phase
BT	Apparent volumetric CTE of the system

Abbreviation	***State Variable***
DVIS(ph)	Dynamic viscosity of a phase
KVIS(ph)	Kinematic viscosity of a phase
SURF(ph)	Surface tension of a liquid phase
ELRS/ELRS(ph)	Electrical resistivity of the system or a phase
ELCD/ELCD(ph)	Electrical conductivity of the system or a phase
THCD/THCD(ph)	Thermal conductivity of the system or a phase
THRS/THRS(ph)	Thermal resistivity of the system or a phase
THDF/THDF(ph)	Thermal diffusivity of the system or a phase
DGV	Driving force for evaporation
DHV	Evaporation enthalpy
MMG	Molar mass of gas
XAVG(el)	Mole fraction of an element in solid phases
WAVG(el)	Mass fraction of an element in solid phases

State Variables in Console Mode DICTRA

State variables in the DICTRA POST module are similar to those defined in Thermo-Calc POLY-3 module. Examples of state variables are temperature, mole fraction, enthalpy, etc. In POLY-3 a general notation method based on character mnemonics is designed for a predefined set of state variables.

The numerical values of some state variables, e.g. activity, chemical potential, and the energetic extensive properties, are given relative to some reference state which has been defined in the thermodynamic database file. Sometimes you may have specified a reference state using SET_REFERENCE_STATE. To get numerical values relative to the user-defined reference state, append an R to the mnemonic names as defined.

Intensive Properties

Mnemonic	Description
T	temperature
P	pressure
AC(component)	activity
MU(component)	chemical potential

Extensive Properties

NORMALIZATION of extensive properties: For all extensive properties a suffix can be added to the mnemonic name to indicate a normalized extensive property. The following tables describe each mnemonic .

Extensive Property `Z at Each Grid Point

Mnemonic	Description
Z	Extensive property `Z at each grid point.
ZM	Extensive property `Z per moles of atoms.
ZW	Extensive property `Z per mass (gram).

Mnemonic	Description
ZV	Extensive property `Z per volume (m^3).

Extensive Property `Z for a Phase at Each Grid Point

Mnemonic	Description
Z	Extensive property `Z for the current amount of the phase.
ZM	Extensive property `Z per mole of atoms of the phase.
ZW	Extensive property `Z per mass (gram) of the phase.
ZV	Extensive property `Z per volume (m^3) of the phase.
ZF	Extensive property `Z per mole formula unit of the phase.

Energetic Extensive Properties

Suffixes M, W, V and F can be applied.

Mnemonic	Description
S	entropy
S(phase)	entropy of a phase
V	volume
V(phase)	volume of a phase
G	Gibbs energy
G(phase)	Gibbs energy of a phase

Mnemonic	Description
H	enthalpy
H(phase)	enthalpy of a phase
A	Helmholtz energy
A(phase)	Helmholtz energy of a phase

Amount of Components

Suffixes M, W and V can be applied.

Mnemonic	Description
N(component)	Number of moles of a component.
N(phase,component)	Number of moles of a component in a phase.
B(component)	Mass of a component.
B(phase,component)	Mass of a component in a phase.

Total Amount

Suffixes M, W and V can be applied.

Mnemonic	Description
N	Number of moles
B	Mass

Mnemonic	Description
	The legal combination BW is not very interesting as it will always be unity. BV is the density

Amount of a Phase

Suffixes M, W and V can be applied.

The normalizing properties are calculated at each grid point.

Mnemonic	Description
NP(phase)	Number of moles of a phase.
BP(phase)	Mass of a phase.
VP(phase)	Volume of a phase.
Y(phase,species#sublattice)	site fraction This quantity is dependent upon the model chosen for the phase.

Constitution

This quantity is dependent upon the model chosen for the phase.

Mnemonic	Description
Y(phase,species#sublattice)	site fraction

Thermophysical Properties Data and Variables

In this section:

About Thermophysical Properties Data Parameters

Parameters, Functions, and Variables and Thermophysical Properties Variables

The so-called classic syntax is used in the examples below. It can be used in Console Mode or when using the APIs, e.g. TC-Python or TC-Toolbox for MATLAB®. Graphical Mode in Thermo-Calc has readable names for all of these.

You can find information on our website about the properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources are added on a regular basis so keep checking back or subscribe to our newsletter.

All Available Properties Data Parameters and Variables

Below is a summary of the available thermophysical parameters and variables for the databases when working in Thermo-Calc. There are differences when you are working in Console Mode versus Graphical Mode as well as if you use an SDK such as TC-Python or TC-Toolbox for MATLAB®.

Property (and Graphical Mode Variable Name)	***Model Parameters***	***Variables to Show or Plot in Console Mode or the SDKs (TC-Python, or TC-Toolbox for MATLAB®)******
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI
Electrical conductivity	ELQ**	ELCD for a system `ELCD(PHI)` for phase PHI
Electrical resistivity	ELRS, ESPD	ELRS for a system `ELRS(PHI)` for a phase PHI
Thermal conductivity	THCD	THCD for a system `THCD(PHI)` for phase PHI
Thermal resistivity		THRS for a system `THRS(PHI)` for phase PHI
Thermal diffusivity		THDF for a system `THDF(PHI)` for phase PHI

Property (and Graphical Mode Variable Name)	***Model Parameters***	***Variables to Show or Plot in Console Mode or the SDKs (TC-Python, or TC-Toolbox for MATLAB®)****
Surface tension	SIGM, XI*	`SURF(LIQUID)` `SURF(ION)` **
Dynamic viscosity	VISC	`DVIS(LIQUID)` `DVIS(ION)` **
Kinematic viscosity		`KVIS(LIQUID)` `KVIS(ION)` **

* XI is not used in the TCOX database (all versions). As of 2023b it is also not used starting with the following versions of these databases: TCFE13, TCNI12.1, TCTI5.1, TCNOBL3, TCPMAG2, and TCCU6. As of 2024a, TCMG7, TCAL9, and TCHEA7. As of 2024b, TCSLD5.

** `ION` is used in the TCS Metal Oxide Solutions Database (TCOX)

*** The examples listed for the SDKs are using Console Mode syntax. The quantities can also be accessed in both `ThermodynamicQuantity` and `ScheilQuantity` classes. See the various model descriptions or the SDK help for details.

Viscosity Model

? Viscosity of the Metallic Liquids Model

? Viscosity of the Ionic Liquids Model

To use this model, the database parameter VISC is needed. It can be used for liquids.

- Dynamic viscosity (DVIS)
- Kinematic viscosity (KVIS)

Examples in Console Mode:

- In POLY module: SHOW DVIS(LIQUID)
- Set as plot variable: SET-DIAGRAM-AXIS Y KVIS(LIQUID)

Thermal Conductivity Model

? Thermal Conductivity Model

To use the thermal conduction parameters, the database parameter THCD is needed. The other two related properties are derived from THCD. These properties can be obtained for a phase or for the whole system.

- Thermal conductivity (THCD)
- Thermal diffusivity (THDF)
- Thermal resistivity (THRS)

Examples in Console Mode:

- In POLY module: SHOW THCD
- Set as plot variable: SET-DIAGRAM-AXIS Y THDF(FCC_A1)

Electrical Conductivity and Electrical Resistivity Models

Electrical Resistivity Model

To use the electric properties parameters, the database parameter ELRS is needed. ELCD is derived from that. These properties can be obtained for a phase or for the whole system.

- Electrical conductivity (ELCD)
- Electrical resistivity (ELRS)

Examples in Console Mode:

- In POLY module: SHOW ELCD
- Set as plot variable: SET-DIAGRAM-AXIS Y ELRS(FCC_A1)

Electrical Conductivity of Molten Slag Model

Electrical Conductivity for Ionic Liquid Model

To use the electric properties parameters, the database parameter ELQ is needed. The model parameters are the activation Gibbs energy of end-members and excess activation Gibbs energy.

- Electrical conductivity of molten slags `ELCD(IONIC)`
- Electrical resistivity of molten slags `ELRS(IONIC)`

Surface Tension Model

- Surface Tension of Metallic Liquid Alloys Model
- Surface Tension Model for Oxide Slag

Surface tension for liquids can be calculated if the database contains the two database parameters SIGM and XI. From these, the surface energy is calculated:

- Surface energy (SURF)

> XI is not used in the TCS Metal Oxide Solutions Database (TCOX)

Examples in Console Mode:

- In POLY module: `SHOW SURF(LIQUID)`
- Set as plot variable: `SET-DIAGRAM-AXIS Y SURF(LIQUID)`

Thermophysical Properties Variables

The Thermo-Calc databases have a variety of properties data included such as molar volume, thermal conductivity, dynamic and kinematic viscosity, thermal resistivity, electrical resistivity, and surface tension. These properties data are being integrated into databases as each new version of a database is released.

Availability of properties data is dependent on both the database and its version. Some information is specific to use in Console Mode. There is more information also available for Graphical Mode, TC-Python, or TC-Toolbox for MATLAB® for each of the databases where the properties data is included. More advanced information is also contained in the *Database Manager User Guide* PARAMETER section included with this documentation set.

To determine if the database you are using has this properties data, search the help (press F1) to review the technical information. The availability of properties data is also included with the Database Overview document available on the Thermo-Calc website.

Variables	Abbrev.	Unit	Descript.	Domain
DVIS	DVIS(ph)	Pa·s	Dynamic viscosity	Liquid phase
KVIS	KVIS(ph)	m^2/s	Kinematic viscosity	Liquid phase
ELCD	ELCD	S/m	Electric conductivity	System
ELCD	ELCD(ph)	S/m	Electric conductivity	Phase
ELRS	ELRS	Ωm	Electric resistivity	System
ELRS	ELRS(ph)	Ωm	Electric resistivity	Phase
THCD	THCD	W/(mK)	Thermal conductivity	System

Variables	Abbrev.	Unit	Descript.	Domain
THCD	THCD(ph)	W/(mK)	Thermal conductivity	Phase
THRS	THRS	mK/W	Thermal resistivity	System
THRS	THRS(ph)	mK/W	Thermal resistivity	Phase
THDF	THDF	m^2/s	Thermal diffusivity	System
THDF	THDF(ph)	m^2/s	Thermal diffusivity	Phase
SURF	SURF(ph)	J/m^2	Surface tension	Liquid phase

Electrical Resistivity Model

The modeling starts with unaries in their stable and metastable structures. The temperature dependence of electrical resistivity is described with polynomials for each unary and each end-member of compounds. In order to guarantee the reliability of the extrapolation, experimental data were first fitted to a semi-empirical model, which was established based on relevant theories. The experimental data, together with the extrapolated values, are then used for deriving the polynomials that are saved in the database. The magnetic contribution to electrical resistivity can be separately treated with a model implemented in Thermo-Calc.

The composition dependence of electrical resistivity is described with the Redlich-Kister expression. All binary systems are modeled by using experimental data or theoretical estimations. Ternary and higher-order parameters can be used if necessary.

Electrical resistivity is modeled and its descriptions are stored in the databases. Electrical conductivity is derived from electrical resistivity and can be retrieved from calculated results as well.

Model Description

The semi-empirical model for electrical resistivity is built based on the Matthiessen's rule [1997DeB]. In general, the electrical resistivity of a metallic alloy consists of residual resistivity (ρ_0) and electron-phonon resistivity (ρ_{e-p}), as well as magnetic resistivity (ρ_m). The residual resistivity is due to the scatterings of impurities and defects that exist in well-annealed and high purity alloys, and the value of ρ_0 is generally considered independent of temperature.

[Eq. 1]

$$\rho = \rho_0 + \rho_{e-p} + \rho_m$$

ρ_{e-p} is described with the modified Bloch-Grüneisen equation [1928Blo; 1933Gru] and corrections can be made in cases where other types of scatterings play considerable roles.

[Eq. 2]

$$\rho_{e-p} = A \cdot \left(\frac{T}{\theta_R}\right)^5 \cdot J_5\left(\frac{\theta_R}{T}\right)$$

[Eq. 3]

$$A = \frac{\frac{3}{2} h q_D^6 (G')^2}{4e^2 (m^*)^2 n_c k_B \theta_D k_F^2 \nu_F^2}$$

[Eq. 4]

$$J_n\left(\frac{\theta_D}{T}\right) = \int_0^{\frac{\theta_D}{T}} \frac{x^n e^x}{(e^x - 1)^2} dx$$

The characteristic temperature θ_R plays a similar role and is also approximated as the Debye temperature (θ_D), which can be readily obtained from low-temperature heat capacity and elastic constants data as well as theoretical computations. The approximation of θ_R as θ_D indicates that transverse phonons play a role in electron scattering. k_F is the electron wave number at the Fermi surface. q_D is the phonon Debye wave number. h is the Planck constant. G' is a constant representing the strength of the e-p interaction and cannot be easily estimated. m^* is the electron effective mass. n_c is the number of unit cells per unit volume. v_F is the electron velocity at the Fermi surface.

To describe the drastic change of the magnetic resistivity (ρ_m) around the Curie (or Neel) temperature, T_C, of a magnetic alloy, an empirical model is proposed using the dimensionless temperature T/T_C and a parameter ρ_{spd} that stands for the resistivity due to spin disordering. According to this model, Eq. 5, ρ_m approaches ρ_{spd}, when the temperature is well above T_C, and is 0 when the temperature is far below T_C. ρ_{spd} depends only on composition and is described with the Redlich-Kister (R-K) expression. Apparently, ρ_{spd} has a positive value for magnetic elements, and compounds as well as endmembers, and is 0 for non-magnetic ones.

In a typical binary system made of a magnetic element A and a non-magnetic element B, ρ_{spd} decreases usually from ρ_{spd}^A to 0 at a certain composition (x_*). Such a behavior is also seen in magnetic moment and Curie temperature. ρ_{spd} is expected to be zero in the composition range from x_* to element B, and will be forced to zero when the R-K expansion leads inevitably to negative values over this composition range. T_C is available from the thermodynamic description in the database.

$$\rho_m = \rho_{spd} \cdot \left(1 - e^{\left(-\frac{3}{2}\left(\frac{T}{T_c}\right)^3\right)}\right)$$

[*Eq. 5*]

The semi-empirical model (as given in Eq. 1 to Eq. 5) is first fitted to experimental data. The description is then extrapolated to a wider temperature range if necessary, either to extreme temperatures where the structure is no longer stable or to where experimental data are missing. Polynomials are then derived with the experimental data, together with the extrapolated values, and stored in the database. The model as given in Eq. 5 is implemented in Thermo-Calc, so the magnetic contribution can be excluded from the polynomials and separately modeled, and it will be automatically included during the calculations.

Model Parameters

The extended TDB format accepts parameters describing electrical resistivity and thermal conductivity, together with spin disordering resistivity. Examples for unary and binary systems are given below:

```
ELRS(FCC_A1,AL:VA;0)
ELRS(FCC_A1,AL,CO:VA;0)
ESPD(FCC_A1,CO:VA;0)
ESPD(FCC_A1,AL,CO:VA;0)
```

Calculation and Plot Variables

- `ELRS` – Electrical resistivity
- `ELCD` – Electrical conductivity

All the above quantities can be calculated, retrieved, shown and plot in Thermo-Calc via the variables in the Console Mode or via the quantity names in the Graphical Mode (see sections below).

CONSOLE MODE

The quantities corresponding to the variables of `ELRS` and `ELCD` can be calculated in Console Mode for a phase, e.g. `ELRS(FCC_A1)`, or for a system, i.e. `ELRS`. The results can be shown in the POLY module with the command SHOW_VALUE or illustrated as a plot in the POST module with the command PLOT_DIAGRAM.

GRAPHICAL MODE

On the **Plot Renderer** in Graphical Mode, electrical resistivity, electrical conductivity, thermal conductivity, thermal resistivity, and thermal diffusivity can be selected from the axes lists, tabulated and plotted using the quantity names, with options for a specific phase, all phases or for a system.

TC-PYTHON AND TC-TOOLBOX FOR MATLAB®

With these Software Development Kits (SDKs), the quantities of `ELRS` and `ELCD` can be retrieved, for a phase, e.g. `ELRS(FCC_A1`), or for a system, i.e. `ELRS`, via `get_value_of()` or `get_values_of()`, from most phase equilibrium calculations in TC-Python, for instance,

- `with_single_equilibrium_calculation()`,
- `with_property_digram_calculation()` or
- `with_batch_equilibrium_calculation()`.

These can also be accessed in both `ThermodynamicQuantity` and `ScheilQuantity`classes. You can, for example, use `ThermodynamicQuantity.electrical_resistivity()` for electrical resistivity.

References

[1928Blo] F. Bloch, Über die Quantenmechanik der Elektronen in Kristallgittern (About the quantum mechanics of electrons in crystal lattices). Zeitschrift fur Phys. 52, 555–600 (1928).

[1933Gru] E. Grüneisen, The dependence of the electrical resistance of pure metals on the temperature. Ann. Phys. 16, 530–540 (1933).

[1997DeB] R. De-Bruyn-Ouboter, Heike Kamerlingh Onnes's discovery of superconductivity. Sci. Am., 98–103 (1997).

Electrical Conductivity for Ionic Liquid Model

The model for the electrical conductivity of molten slags is mainly based on the theory of the electrical conductivity of ionic solutions. The total conductivity is the sum of the contributions from all cations including those network-forming cations modeled as neutrals in the two sublattice ionic liquid model, such as liquid silicon oxide. For slags containing transition metal ions of different oxidation states, the electronic contribution due to the electron or hole exchange between these ions is also considered.

In short, the electrical conductivity of molten slags consists of the following:

1. Ionic conductions contributed by cations in the ionic liquid.
2. Electronic conductions from the cations having more than one oxidation states (Fe^{2+}-Fe^{3+}, Mn^{2+}- Mn^{3+} and so on).

The composition and temperature dependence of the total electrical conductivity of molten slags, σ, is represented by:

$$\sigma = \sum x_{C_i}\sigma_{C_i} - x_{MeO}y_{MeO_3}\sigma_{Me^{2+}} + x_{B_k^0}\sigma_{B_k^0}$$

$$= x_{\mathrm{Ca}^{2+}}\sigma_{\mathrm{Ca}^{2+}} + x_{\mathrm{Mg}^{2+}}\sigma_{\mathrm{Mg}^{2+}} + \ldots + x_{\mathrm{Fe}^{2+}}\sigma_{\mathrm{Fe}^{2+}} - x_{\mathrm{FeO}}y_{\mathrm{FeO}_3}\sigma_{\mathrm{Fe}}^{2+} + \ldots + x_{\mathrm{SiO}_2}\sigma_{\mathrm{SiO}_2}$$

where x_{Ci} is the mole fraction of cation C_i, and its electrical conductivity, σ_{Ci}, is written in the form of the Nernst-Einstein equation as:

$$\sigma_{C_i} = \frac{1}{RT}\exp\left[-\frac{Q_{C_i}}{RT}\right] = \frac{1}{RT}\exp\left[-\frac{\sum_j y_{C_i}y_{A_j}Q_{C_i:A_j} + \sum_j y_{C_i}y_{B_k^0}Q_{C_i:B_k^0} + Q_{C_i}^E}{RT}\right]$$

where Q_{Ci} is the activation Gibbs energy, of which the composition dependence has been expanded in a CALPHAD fashion.

Model Parameters

The model parameters are the activation Gibbs energy of end-members and excess activation Gibbs energy in the above equation. They can be entered in the GES module or TDB file by using the keyword `ELQ`, for example,

```
PARAM ELQ(IONIC_LIQ&Ca+2,CA+2:O-2;0)

PARAM ELQ(IONIC_LIQ&Ca+2,CA+2:SIO4-4;0)

PARAM ELQ(IONIC_LIQ&Ca+2,CA+2:SIO2;0)
```

Calculation and Plot Variables

All the quantities can be calculated, retrieved, shown and plot in Thermo-Calc via the variables in the Console Mode or via the quantity names in the Graphic Mode.

CONSOLE MODE

The electrical conductivity and resistivity of molten slags modeled as the ionic liquid phase can be calculated usually through a single point or step equilibrium calculation in Console Mode. The results can be shown or plotted by using the variables `ELCD(IONIC)` and `ELRS (IONIC)`, respectively.

GRAPHICAL MODE

On the **Plot Renderer** in Graphical Mode, the electrical conductivity and resistivity of molten slags modeled as the ionic liquid phase can be calculated by using the **Single** point or **One Axis** calculation type in Graphical Mode. The corresponding tabulation or plot variables are **Electrical Conductivity** and **Electrical Resistivity**, respectively.

TC-PYTHON AND TC-TOOLBOX FOR MATLAB®

With these Software Development Kits (SDKs), this property can be plotted using `property-diagram_calculation()` or `with_batch_ equilibrium_calculation()`. The plot variables are `ELCD(IONIC)` and `ELRS(IONIC)`.

These can also be accessed in both `ThermodynamicQuantity` and `ScheilQuantity`classes. You can, for example, use `ThermodynamicQuantity.electrical_conductivity("IONIC")` and `ThermodynamicQuantity.electrical_resitivity("IONIC")` for electrical conductivity and electrical resistivity, respectively.

You can also get the individual values e.g. from an equilibrium calculation and use in whatever way you want, e.g. feed into other models: `result.get_value_of("ELCD(IONIC_ LIQ)")`, where 'result' is the result of one equilibrium calculation. It matches SHOW_VALUE in Console Mode.

This can also be written `result.get_value_of(ThermodynamicQuantity.electrical_ conductivity("IONIC_LIQ"))` or `result.get_value_of (ThermodynamicQuantity.electrical_resitivity("IONIC_LIQ"))`.

Thermal Conductivity Model

The modeling starts with unaries in their stable and metastable structures. The temperature dependence of thermal conductivity is described with polynomials for each unary and each end-member of compounds. Thermal resistivity and thermal diffusivity can be derived from thermal conductivity and retrieved from calculated results. The composition dependence is described with the Redlich-Kister expression in the CALPHAD spirit, but the relation is applied to thermal resistivity (or the inverse of thermal conductivity).

Model Description

Experimental data of thermal conductivity are used to derive descriptions in polynomials, which are stored in the database, despite that it consists of two components, electronic thermal conductivity (κ_e) and lattice thermal conductivity κ_g. In other words, they are not separately treated.

In cases where experimental data are absent or sparse, however, κ_e and κ_g can be separately predicted and summed up to give the total thermal conductivity. κ_e can be predicted from ρ or vice versa, by employing the Wiedemann-Franz Law [1853Fra; 1985Jon], respectively, to the residual resistivity, magnetic resistivity and intrinsic resistivity.

[Eq. 1]

$$\frac{1}{\kappa_e} = W_e = \frac{\rho_0 + \rho_m + \rho_i}{L_0 T}$$

L_0 is known as the Sommerfeld value of the Lorenz number: $2.4453 \times 10^{-8} W\Omega/K^2$.

[Eq. 2]

$$\rho_i = \frac{A}{L_0 T} \cdot \left(\frac{T}{\theta_R}\right)^5 \cdot J_5\left(\frac{\theta_R}{T}\right) \cdot f$$

[Eq. 3]

$$f = 1 + \frac{3}{\pi^2} \cdot \left(\frac{k_F}{q_D}\right)^2 \cdot \left(\frac{\theta_R}{T}\right)^2 - \frac{1}{2\pi^2} \cdot \frac{J_7\left(\frac{\theta_R}{T}\right)}{J_5\left(\frac{\theta_R}{T}\right)}$$

The intrinsic resistivity (ρ_i) is based on Eq. 4

[Eq. 4]

$$\rho_{e-p} = A \cdot \left(\frac{T}{\theta_R}\right)^5 \cdot J_5\left(\frac{\theta_R}{T}\right)$$

for the e-p processes, but corrections are provided, as given in Eq. 3: the first term corresponds to large-angle scattering that satisfies the original Wiedemann-Franz Law; the second one is due to inelastic small-angle (vertical processes) and has no counterpart in the electrical resistivity; the third term is a correction that accounts for situations where large-angle scattering can reverse the electron direction without actually assisting to restore the distribution back to equilibrium.

κ_g can be predicted with the Slack model in a temperature range where only anharmonic Umklapp phonon-phonon interactions are important. In other words, normal processes are neglected as a first approximation [1979Sla; 2002Mor]. The most reasonable version among several ones is given below [1965Jul].

[*Eq. 5*]

$$\kappa_p^U = A' \cdot \frac{M_a \cdot \theta_D^3 \cdot \delta}{\gamma^2 \cdot n_c^{\frac{2}{3}}} \cdot \frac{1}{T}$$

[*Eq. 6*]

$$A' = \frac{2.43 \cdot 10^{-5}}{1 - \frac{0.514}{\gamma} + \frac{0.228}{\gamma^2}}$$

The Debye temperature, θ_D can be obtained from low-temperature heat capacity or elastic constant data. M_a is the average atomic mass, δ^3 the volume per atom, n_c the number of atoms in a unit cell, and γ the Grüneisen coefficient. A typical value for A' is evaluated to be 3×10^{-5} using $\gamma = 2$ as the Grüneisen coefficient, and can be used in the absence of experimental information. It can also be obtained from e.g. DFT calculations of elastic properties.

Model Parameters

The extended TDB format accepts parameters describing electrical resistivity and thermal conductivity, together with spin disordering resistivity. Examples for unary and binary systems are given below:

```
THCD(FCC_A1,AL:VA;0)
THCD(FCC_A1,AL,CO:VA;0)
```

Calculation and Plot Variables

- `THCD` – Thermal conductivity
- `THRS` – Thermal resistivity
- `THDF` – Thermal diffusivity

All the above quantities can be calculated, retrieved, shown and plot in Thermo-Calc via the variables in the Console Mode or via the quantity names in the Graphic Mode (see sections below).

CONSOLE MODE

The quantities corresponding to the variables of `THCD`, `THRS`, and `THDF` can be calculated in Console Mode for a phase, e.g. `THCD(FCC_A1)`, or for a system, i.e. `THCD`. The results can be shown in the POLY module with the command SHOW_VALUE or illustrated as a plot in the POST module with the command PLOT_DIAGRAM.

GRAPHICAL MODE

On the **Plot Renderer** in Graphical Mode, electrical resistivity, electrical conductivity, thermal conductivity, thermal resistivity, and thermal diffusivity can be selected from the axes lists, tabulated and plotted using the quantity names, with options for a specific phase, all phases or for a system.

TC-PYTHON AND TC-TOOLBOX FOR MATLAB®

The quantities of `THCD`, `THRS`, and `THDF` can be retrieved, for a phase, e.g. `THCD(FCC_A1)`, or for a system, i.e. `THCD`, via `get_value_of()` or `get_values_of()`, from most phase equilibrium calculations in these Software Development Kits (SDKs), for instance,

- `with_single_equilibrium_calculation()`,
- `with_property_diagram_calculation()` or
- `with_batch_equilibrium_calculation()`.

These can also be accessed in both `ThermodynamicQuantity` and `ScheilQuantity` classes. You can, for example, use `ThermodynamicQuantity.thermal_resistivity()` for thermal resistivity.

References

[1852Fra] R. Franz, G. Wiedemann, Ueber die Wärme-Leitungsfähigkeit der Metalle. Ann. der Phys. und Chemie. 165, 497–531 (1853).

[1965Jul] C. L. Julian, Theory of Heat Conduction in Rare-Gas Crystals. Phys. Rev. 137, A128–A137 (1965).

1979[Sla] G. A. Slack, The Thermal Conductivity of Nonmetallic Crystals, in Solid State Physics Volume 34, 1–71 (1979).

[1985Jon] W. Jones, N. H. March, Theoretical Solid State Physics (Courier Dover Publications, 1985).

[2002Mor] D. T. Morelli, J. P. Heremans, G. A. Slack, Estimation of the isotope effect on the lattice thermal conductivity of group IV and group III-V semiconductors. Phys. Rev. B. 66, 195304 (2002).

Surface Tension of Metallic Liquid Alloys Model

In general, for liquid metal alloys, the surface tension is assessed for all the elements and binary systems where experimental data are available. When experimental data are not available, the Butler model [1932But] is used to estimate the composition dependence of the surface tension. The experimental or estimated data are modeled with either the modified Guggenheim model [2019Ver] or the Redlich-Kister-Muggianu sub-regular solution model [1948Red; 1975Mug].

Search the help (press F1) to review the technical information for the database you are using.

Modified Guggenheim Model Description

The surface tension of metallic liquid alloys by the modified Guggenheim model [2019Ver] and is expressed as:

$$\sigma(x_i^B,T) = -\frac{RT}{S(x_i^B,T)}\ln\left[x_1^B\exp\left(-(1+\Xi_1\cdot x_2^S(x_i^B,T))\frac{\sigma_1(T)S_1(T)}{RT}\right)\right.$$
$$\left.+x_2^B\exp\left(-(1+\Xi_2\cdot x_1^S(x_i^B,T))\frac{\sigma_2(T)S_2(T)}{RT}\right)\right]$$

where

- x_i^B is the bulk composition
- σ_i is the surface tension
- S and S_i are the total and the partial molar surface of species i defined as

$$S_{(i)} = 1.901\cdot N_A^{1/3}\cdot V_{m,(i)}^{2/3}$$

- N_A being the Avogadro number and $V_{m,(i)}$ the molar volume of the system or the species i.
- x_i^S is the composition of i in surface, which is a function of bulk composition and T and defined as follows:

$$x_i^{S,id}(x_i^B,T) = \frac{x_i^B}{x_i^B+x_j^B\exp\left(\frac{S(x_i^B,T)[\sigma_i(T)-\sigma_j(T)]}{RT}\right)}$$

- Ξ_1 and Ξ_2 are called damping factors and these parameters are fitted for species 1 and 2 of binary systems.

The extrapolation to higher-order systems is straightforward. The ideal surface composition for a multicomponent system is:

$$x_i^{S,id}(T, x_i^B, x_j^B, \dots) = \frac{x_i^B}{x_i^B + \sum_{j \neq i} x_j^B \exp\left(\frac{S_{ij}(x_i^B, T) \cdot [\sigma_i(T) - \sigma_j(T)]}{RT}\right)}$$

and the surface tension of a multicomponent alloy is obtained from:

$$\sigma(T, x_i^B, x_j^B, \dots) = -\frac{RT}{S(T, x_i^B, x_j^B, \dots)} \cdot$$

$$\ln\left[\sum_{i=1}^{n} \sum_{j \neq i} x_i^B \exp\left(-(1 + x_j^S(T, x_i^{B,ij}) \cdot \Xi_i^{ij}) \frac{\sigma_i(T) S_i(T)}{RT}\right)\right]$$

Corresponding Variable - Modified Guggenheim

The corresponding variable for surface energy of pure elements is `SIGM`. For instance, the surface tension of pure A is written as `SIGM(LIQUID,A;0)`. The corresponding X_1 and X_2 parameters for A-B binary system are respectively written as following:

```
PARAMETER XI(LIQUID,A,B:0)
PARAMETER XI(LIQUID,A,B:1)
```

Redlich-Kister-Muggianu Model Description

In the case of using the Redlich-Kister-Muggianu (R-K-M) [1948Red; 1975Mug] sub-regular solution model for modeling the surface tension, the surface tension is given by:

$$\sigma = \sum y_i \sigma_i + \sigma^E$$

where y_i and σ_i are the site fraction and surface tension for pure component i, and the excess term is expressed using (R-K) for binary and (R-K-M) for ternary interactions.

Corresponding Variable Redlich-Kister-Muggianu

The corresponding variable for surface energy of pure elements is `SIGM`. For instance, the surface tension of pure A is written as `SIGM(LIQUID,A;0)`. The corresponding L parameters for the A-B binary system are written as follows:

```
PARAMETER SIGM (IONIC_LIQ, A, B; 0)
```

```
PARAMETER SIGM (IONIC_LIQ, A, B; 1)
PARAMETER SIGM (IONIC_LIQ, A, B; 2)
```

Plot Variables (Both Models)

Console Mode

The surface energy can be calculated through various calculations in Console Mode, e.g. a step. The plot variable is `SURF(LIQUID)`.

Graphical Mode

On the **Plot Renderer** in Graphical Mode, the plot variable **Surface tension** can be selected from the axes lists, tabulated and plotted using the quantity names, with options for a specific liquid phase based on the database.

TC-Python and TC-Toolbox for MATLAB®

The quantity `SURF(LIQUID)` can be retrieved, for a liquid phase, e.g. `SURF(LIQUID)`), via `get_value_of()` or `get_values_of()`, from most phase equilibrium calculations in these Software Development Kits (SDKs), for instance,

- `with_single_equilibrium_calculation()`,
- `with_property_diagram_calculation()` or
- `with_batch_equilibrium_calculation()`.

These can also be accessed in both `ThermodynamicQuantity` and `ScheilQuantity` classes. You can, for example, use `ThermodynamicQuantity.surface_tension("LIQUID")`.

Graphical Mode and Console Mode Examples

There are two basic examples included with your software installation and that use demonstration (DEMO) databases.

Search the help (press F1 when in Thermo-Calc) for brief descriptions of these examples, or browse to the examples located in your installation. From the main menu, **Help→ Examples Files**:

- Graphical Mode **T_11_Surface_tension_in_Cu-Zr.tcu**
- Console Mode `tcex56`

References

[1932But] J. A. V. Butler, The thermodynamics of the surfaces of solutions. Proc. R. Soc. London. Ser. A, Contain. Pap. a Math. Phys. Character. 135, 348–375 (1932).

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[1975Mug] Y. M. Muggianu, M. Gambino, J. P. Bros, Enthalpy of formation of liquid Bi-Sn-Ga alloys at 723 K, choice of an analytical expression of integral and partial excess quantities of mixing. J. Chim. Phys. 72, 83–88 (1975).

[2019Ver] M. Vermot des Roches, A. E. Gheribi, P. Chartrand, A versatile multicomponent database for the surface tension of liquid metals, Calphad. 65, 326–339 (2019).

Surface Tension Model for Oxide Slag

The model for TCS Metal Oxide Solutions Database (TCOX) surface tension of oxide slag:

$$\sigma = \sum y_i \sigma_i + \sigma^E$$

$$\sigma^E = \sum_i y_A \cdot y_B (y_A - y_B)^i \cdot SIGM^i$$

where y_i and σ_i indicate the site fraction and surface tension for pure component i. For pure component, the surface tension is described with $a + b * T$. The excess term is expressed using Redlich-Kister polynomial, as one can find the example of a binary A-B.

SIGM is the parameter used for optimization, for example,

```
PARAMETER SIGM (IONIC_LIQ, A;0)
PARAMETER SIGM (IONIC_LIQ, B;0)
PARAMETER SIGM (IONIC_LIQ, A:B,0)
```

The user can calculate the surface tension of liquid oxide by calling the variable `SURF (IONIC)`.

Viscosity of the Metallic Liquids Model

This section provides details about calculating the dynamic and kinematic viscosities.

Model Description

The viscosity of metallic liquid alloys is modeled as follows:

$$RT\ln\eta = RT\ln\eta_0 + E$$

where

- η is the dynamic (or shear) viscosity of the liquid,
- η_0 is the viscosity at finite temperatures,
- E is the activation energy in J/mole,
- R is the gas constant, and
- T is the absolute temperature.

The SI unit of viscosity is pascal.second (Pa.s). The viscosity parameters are expanded via Redlich-Kister polynomials.

For example, viscosity of a liquid A-B alloy is:

$$\begin{aligned} RT\ln\eta_{alloy} &= x_A(E_A + RT\ln\eta_0^A) \\ &+x_B(E_B + RT\ln\eta_0^B) \\ &+x_Ax_B(L_0 + (x_A - x_B)\cdot L_1) \end{aligned}$$

The two first terms are the contributions for the end-members, A and B elements and the last term accounts for the excess viscosity. Basically, the activation energies are optimized. L_0 and L_1 etc. are the parameters that are optimized to fit the viscosity data.

The kinematic viscosity, ν, is the ratio of the dynamic viscosity, η, to the density, ρ, of the alloy:

$$\nu = \eta/\rho$$

The SI unit of kinematic viscosity is square meter per second (m^2/s).

Calculation and Plot Variables

Both the dynamic viscosity and kinematic viscosity can be calculated, retrieved, shown, and plotted in Thermo-Calc via the variables in Console Mode, using the quantity names in Graphical Mode, and also via the quantities in the SDKs.

CONSOLE MODE

The values for dynamic viscosity and kinematic viscosity in Console Mode are obtained with the variables `DVIS` (dynamic viscosity) and `KVIS` (kinematic viscosity). For example, once the equilibrium is calculated in Console Mode, you can get the viscosity value by `show DVIS (LIQUID)` or `show KVIS(LIQUID)`.

GRAPHICAL MODE

On the **Plot Renderer** in Graphical Mode, the dynamic viscosity and kinematic viscosity each can be directly plotted when the variables are available to select.

TC-PYTHON AND TC-TOOLBOX FOR MATLAB®

The quantities of `DVIS` (dynamic viscosity) and `KVIS` (kinematic viscosity) can be retrieved, for a phase, e.g. `DVIS(FCC_A1)`, or for a system, i.e. `DVIS`, via `get_value_of()` or `get_values_of()`, from most phase equilibrium calculations in these Software Development Kits (SDKs), for instance,

- `with_single_equilibrium_calculation()`,
- `with_property_diagram_calculation()` or
- `with_batch_equilibrium_calculation()`.

These can also be accessed in both `ThermodynamicQuantity.kinematic_viscosity ("LIQUID")` or `ThermodynamicQuantity.dynamic_viscosity("LIQUID")`.

Graphical Mode and Console Mode Examples

There are two basic examples included with your software installation and that use demonstration (DEMO) databases.

Search the help (press F1 when in Thermo-Calc) for brief descriptions of these examples, or browse to the examples located in your installation. From the main menu, **Help→ Examples Files**:

- Graphical Mode **T_12_Viscosity_in_Cr-Ni.tcu**
- Console Mode `tcex55`

Viscosity of the Ionic Liquids Model

The model for TCS Metal Oxide Solutions Database (TCOX) viscosity of slag:

$$RTln\eta = RTln\eta_0 + E$$

where η is viscosity, $\eta_0 = \frac{hN_A}{V_m}$ and E is activation energy.

The excess parameters are expanded via R-K. An example of viscosity of A-B liquid oxide:

$$RTln\eta_{A-B} = y_A(RTln\eta_0^A + E_A) + y_B(RTln\eta_0^B + E_B) + \sum_i y_A \cdot y_B(y_A - y_B)^i \cdot VISC^i$$

The parameter of *VISC* stands for *R· T· ln(viscosity)*. In Thermo-Calc software, VISC is implemented as *VISC(ionic)*. In order to quickly acquire the actual viscosity, the parameter of *DVIS(ionic)* should be used. By coupling to the database, it makes use of the site fractions of each species, which reflects the structural change in the oxide melt.

Units for the viscosity of oxide slag:

- Pa·s (pascal-second) is the SI unit, mostly used for oxide slag
- CGS unit is poise (P), 1 poise=0.1 Pa·s
- Centipoise is also common (cP) because it is equivalent to mPa·s.

Molar Volume Model

Molar volume can be used to establish a connection with some significant physical properties, for example, viscosity, electrical conductivity and surface tension. It is the reciprocal of density multiplied by molar mass.

Model Description

The model used to describe the molar volume at ambient pressures is:

$$V_m(T) = V_0 exp(\int_{T_0}^{T} 3\alpha dT)$$

A simple polynomial is used to model non-magnetic volumetric expansivity above 298 K:

$$3\alpha = a + bT + cT^2 + dT^3 + eT^{-2}$$

The model described above is implemented in Thermo-Calc software with two parameters, V0 and VA, and α is the linear thermal expansivity at 1 bar and 3α is the volumetric thermal expansivity.

Molar Volume Descriptions

Parameter	***Unit***	***Description***
V0 (phase, constituent array)	m^3/mol	Volume at 1 bar and reference temperature T0
VA (phase, constituent array)	None	$\int_{T_0}^{T} 3\alpha dT$

Elastic Properties Variables

In this section:

Elastic Properties Variables

As of Thermo-Calc version 2025b, elastic properties are available with Thermo-Calc and the TCS Ti/TiAl-based Alloys Database (TCTI) (TCTI6 and newer), TCS Steel and Fe-alloys Database (TCFE) (TCFE14 and newer), TCS High Entropy Alloys Database (TCHEA) (TCHEA8 and newer), and TCS Ni-based Superalloys Database (TCNI) (TCNI13 and newer). These elastic properties will be added to additional databases over time. Subscribe to our newsletter to be kept up-to-date on the latest product releases, webinars, user group meetings, applications examples, and more.

You can find information on our website about the properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources are added on a regular basis so keep checking back or subscribe to our newsletter.

About the Elastic Properties.

For information about thermophysical properties such as surface tension, viscosity, etc, see About Thermophysical Properties Data Parameters.

Elastic Constants and Moduli Variables

The so-called classic syntax is used in the examples below. It can be used in Console Mode or when using the APIs, e.g. TC-Python or TC-Toolbox for MATLAB®. Graphical Mode in Thermo-Calc has readable names for all of these.

The quantities corresponding to individual elastic constants and elastic moduli (derived from the elastic constants) can be calculated in Console Mode for individual phases or for all phases. The results can be shown in the POLY module with the command SHOW_VALUE or shown as a plot in the POST module with the command PLOT_DIAGRAM using:

- `Cij(<phase name>)` or `Cij(*)`
- Bulk modulus: `BULKMOD(<phase name>)` or `BULKMOD(*)`
- Shear modulus: `SHEARMOD(<phase name>)` or `SHEARMOD(*)`
- Young's modulus: `YOUNGMOD(<phase name>)` or `YOUNGMOD(*)`

Variables	Unit	Description
`BULKMOD`	Pascal	Bulk modulus
`SHEARMOD`	Pascal	Shear modulus
`YOUNGMOD`	Pascal	Young's modulus
`Cij`	Pascal	Elastic constants i.e. C11, C12, C13, C33, or C44

About the Elastic Properties

As of Thermo-Calc version 2025b, elastic properties are available with Thermo-Calc and the TCS Ti/TiAl-based Alloys Database (TCTI) (TCTI6 and newer), TCS Steel and Fe-alloys Database (TCFE) (TCFE14 and newer), TCS High Entropy Alloys Database (TCHEA) (TCHEA8 and newer), and TCS Ni-based Superalloys Database (TCNI) (TCNI13 and newer). These elastic properties will be added to additional databases over time. Subscribe to our newsletter to be kept up-to-date on the latest product releases, webinars, user group meetings, applications examples, and more.

To use the elastic properties parameters, the database parameter `ECij` is needed. The elastic stiffness tensor is described by its independent tensor elements (elastic constants) given by the indices ij in Voigt notation. Both indices i and j run from 1 to 6 and the number of independent tensor elements depends on the symmetry of the crystal lattice (i.e., three independent constants for cubic crystals and five for hexagonal crystals). The elastic moduli are derived from the elastic constants.

Elastic properties are only available for cubic (FCC and BCC) or hexagonal (HCP) phases.

Elastic Properties Model

The modeling process begins with determining the independent elastic constants for each phase.

- For cubic (FCC, BCC) phases, the independent elastic constants are: C_{11}, C_{12}, C_{44}.
- For hexagonal (HCP) phases, the independent elastic constants are: $C_{11}, C_{12}, C_{13}, C_{33}, C_{44}$.

The temperature dependence of the elastic constants is represented by exponential and polynomial functions for each phase's end-member. To ensure reliable interpolation and extrapolation, both experimental and theoretical data are fitted to a robust model based on relevant theories, following the CALPHAD methodology. For magnetic materials, the magnetic contribution to the elastic constants is treated separately and incorporated into the model implemented in Thermo-Calc [2021Joh].

The elastic constants assessed for single crystalline phases are related to the polycrystalline elastic moduli (bulk, shear, and Young's moduli) using the Voigt-Reuss-Hill averaging method. These moduli are expressed in terms of the Voigt (upper bound) and Reuss (lower bound) limits of the elastic moduli as follows:

Bulk modulus

$$B = \frac{1}{2}(B_V + B_R)$$

Shear modulus

$$G = \frac{1}{2}(G_V + G_R)$$

Young's modulus

$$E = \frac{9BG}{3B+G}$$

Cubic Symmetry

The Voigt and Reuss bounds depend on crystal symmetry. For cubic (FCC, BCC) phases with 3 independent elastic constants (C_{11}, C_{12}, C_{44}), the Voigt and Reuss bounds are given as:

$$B_V = B_R = \frac{1}{3}(C_{11} + 2C_{12})$$

$$G_V = \frac{1}{5}(C_{11} - C_{12} + 3C_{44})$$

$$G_R = \frac{5\left(C_{11} - C_{12}\right)C_{44}}{3(C_{11} - C_{12}\big) + 4C_{44}}$$

Hexagonal Symmetry

For hexagonal (HCP) phase with 5 independent elastic constants ($C_{11}, C_{12}, C_{13}, C_{33}, C_{44}$), the Voigt and Reuss bounds are calculated as:

$$B_V = \frac{1}{9}[2(C_{11} + C_{12}) + 4C_{13} + C_{33}]$$

$$G_V = \frac{1}{30}(7C_{11} - 5C_{12} - 4C_{13} + 2C_{33} + 12C_{44})$$

$$B_R = \frac{(C_{11}+C_{12})C_{33} - 2C_{13}^2}{C_{11}+C_{12}-4C_{13}+2C_{33}}$$

$$G_R = \frac{\frac{5}{2}hC_{44}C_{66}}{3B_V C_{44}C_{66} + h(C_{44}+C_{66})}$$

Where the symmetry relation $C_{66} = (C_{11} - C_{12})/2$ and help function $h = (C_{11} + C_{12})C_{33} - 2C_{13}^2$ are used to further condense G_R.

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases. Also visit the video tutorials on our website or our YouTube playlist.

Model Parameters

The extended TDB format accepts parameters describing elastic constants and magnetic ordering effects. Examples for unary and binary systems are given below for C11:

```
EC11(HCP_A3,TI:VA;0)

EC11(HCP_A3,TI,MO:VA;0)

EC11(BCC_A2,FE:VA;0)

EC11MAG(BCC_A2,FE:VA;0)

EC11(BCC_A2,FE,CR:VA;0)
```

Where `EC11MAG` is the scaling factor for the magnetic contribution.

PARAMETER in the *Database Manager User Guide*.

Calculation and Plot Variables

- Elastic constants (Cij)
- Bulk modulus
- Shear modulus
- Young’s modulus

All of the above quantities can be calculated, retrieved, shown, and plotted in Thermo-Calc via the variables in Console Mode or via the axes quantity names in Graphical Mode.

Elastic Properties Variables

Graphical Mode

In the **Plot Renderer** in Graphical Mode, elastic constants and moduli can be selected from the drop-down list of axis variables.

The independent elastic constants are selected on the **Plot Renderer** as an axis variable **Elastic constant** and then choose an option (**C11**, **C12**, **C13**, **C33**, or **C44**) from the drop-down list.

The elastic moduli, **Bulk modulus**, **Shear modulus**, and **Young's modulus**, are directly available from the **Axis variable** list.

All can be tabulated and plotted using the quantity names, with options for a specific phase or all phases.

Console Mode

The quantities corresponding to the individual elastic constants and elastic moduli (derived from the elastic constants) can be can be calculated in Console Mode for individual phases or all phases. The results can be shown in the POLY module with the command SHOW_VALUE or shown as a plot in the POST module with the command PLOT_DIAGRAM using:

- `Cij(<phase name>)` or `Cij(*)`
- Bulk modulus: `BULKMOD(<phase name>)` or `BULKMOD(*)`
- Shear modulus: `SHEARMOD(<phase name>)` or `SHEARMOD(*)`
- Young's modulus: `YOUNGMOD(<phase name>)` or `YOUNGMOD(*)`

TC-Python and TC-Toolbox for MATLAB®

For the Software Development Kits (SDKs), i.e. TC-Python and TC-Toolbox, the quantities of elastic constants, bulk modulus, shear modulus, and Young’s modulus can be retrieved for individual phases or all phases via `get_value_of()` or `get_values_of()` from any equilibrium calculation types using:

- `Cij(<phase name>)` or `Cij(ALL_PHASES/*`)
- `ThermodynamicQuantity.bulk_modulus(<phase name>)` or `ThermodynamicQuantity.bulk_modulus(ALL_PHASES/*)`
- `ThermodynamicQuantity.shear_modulus (<phase name>)` or `ThermodynamicQuantity.shear_modulus(ALL_PHASES/*)`
- `ThermodynamicQuantity.youngs_modulus(<phase name>)` or `ThermodynamicQuantity.youngs_modulus(ALL_PHASES/*)`

See the relevant SDK documentation for details.

Units

When plotting or tabulating the elastic moduli in Graphical Mode you can choose between several units of pressure. The default unit for elastic moduli in the Plot Renderer and Table Renderer is GPa.

The elastic moduli and elastic constants are given in SI units, i.e. the values calculated in TC-Python, TC-Toolbox, and Console Mode are in Pascal.

Specific Database Use Case Examples

Each of the following databases have examples available to show how the elastic properties are applied within Thermo-Calc.

Titanium and Titanium Aluminide-based Alloys (TCTI)

The *TCS Ti/TiAl-based Alloys Database (TCTI) Validation and Calculation Examples Collection* has examples using elastic properties. You can find a description of these either in the Thermo-Calc help or via the Examples Collection PDF, which is available on our website.

An example of the effect of oxygen concentration on Young's modulus in HCP_A3 titanium is included with the Thermo-Calc installation. The installed *T_19_Elastic_Properties_ YoungsModulus_Ti-O.tcu* example is available from the **Thermo-Calc** Examples folder.

Steel and Fe-Alloys (TCFE)

The *TCS Steel and Fe-alloys Database (TCFE) Validation and Calculation Examples Collection* has an example using elastic properties. You can find it either in the Thermo-Calc help or via the Examples Collection PDF, which is available on our website.

High Entropy Alloys (TCHEA)

The TCS High Entropy Alloys Database (TCHEA) Validation and Calculation Examples Collection has an example using elastic properties. You can find it either in the Thermo-Calc help or via the Examples Collection PDF, which is available on our website.

Nickel-Based Alloys (TCNI)

The TCS Ni-based Superalloys Database (TCNI) Validation and Calculation Examples Collection has an example using elastic properties. You can find it either in the Thermo-Calc help or via the Examples Collection PDF, which is available on our website.

Reference

[2021Joh] E. Johansson, PhD thesis, Theoretical studies of the coupling between electronic, vibrational, configurational and structural effects in metal borides, Linköping University (2021).

Database Files

In this section:

About the Database Files

Database Manager User Guide

Encrypted vs Unencrypted Database Files

Any licensed databases purchased from Thermo-Calc Software are encrypted in files with the extension `.TDC`; these files cannot be edited. These are referred to as *encrypted databases*.

Unencrypted databases have the file extension `.TDB` and can be edited. For example, PURE5 or PG35 (the free databases), or a user-defined database file.

Editing the Database Initialization File or Unencrypted Database File

If you develop your own databases on a regular basis, also see About the TDB Editor.

Database Initialization File

The *database initialization file* is called `tc_initd.tdb`. Individual licenses are still required to use each database.

The file is used differently by the program depending on whether you are working with databases in Console Mode or Graphical Mode. For this reason, editing the file can be problematic if you do not understand the differences.

About Cached Database Files and Editing the Database Initialization File or Unencrypted Database File

User Database Files

A user-defined database is considered to be an unencrypted database because you can make changes to it.

In Graphical Mode you can add user databases via the **Options** window. Once you have added the user database it is available from the database list in the System Definer Configuration window.

Global Settings: System Definer to add a user database.

In Console Mode, users can decide to add their own user-defined database to the database initiation file, which then makes it available in the Console window.

Editing the Database Initialization File or Unencrypted Database File

Custom Databases: GES5 and GES6 Calculation Engine Version

As of Thermo-Calc version 2019b, the default calculation engine is set to GES6. For custom database users, you may sometimes see messages in the log indicating that additional preparation is being done by Thermo-Calc prior to a calculation. The preparation is carried out automatically; it is usually fast and only needed the first time a custom database is used after a modification. While databases with warnings are tolerated, databases that contain errors can only be loaded by GES6 after the errors are corrected.

The Database Checker tool uses the same parser as GES6 and can be used to verify the consistency and correctness of databases during development, before the databases are actually used.

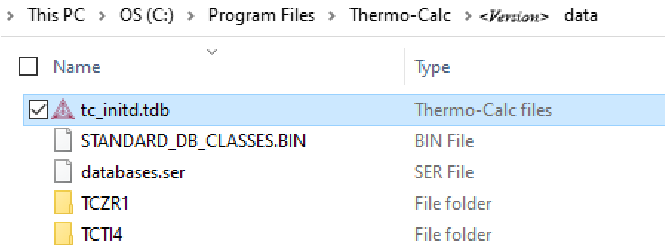
Database Checker

To globally set the default from GES6 back to GES5, go to the **Options**window Global General Settings tab and click **Version 5** for the *Preferred Gibbs Energy System* setting. The SET_GES_VERSION Console Mode command is used to change GES versions for a single Thermo-Calc session.

Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.

Database Installation Folder

The standard Thermo-Calc databases and the database initialization file `tc_initd.tdb` are located in a subfolder to the Thermo-Calc installation. For example, in a Windows Standalone installation, you can find these in a folder called **data** where the file path is *C:\Program Files\Thermo-Calc\<version>\data*.



› This PC › OS (C:) › Program Files › Thermo-Calc › <Version> data

☐ Name	Type
☑ tc_initd.tdb	Thermo-Calc files
STANDARD_DB_CLASSES.BIN	BIN File
databases.ser	SER File
TCZR1	File folder
TCTI4	File folder

About Cached Database Files

This is applicable to Graphical Mode.

Also see Global Settings Global General Settings where you can set the default database directory path. There is also an option to clear the database cache, which may be helpful if you are having issues.

The first time you open a database in Graphical Mode it can take a little while for it to load, especially if it is one of the large databases such as TCFE or TCNI. However, the next time the database opens quickly because the databases are now cached, or stored, in Graphical Mode.

Think of a cache as an intermediate storage area. Once a database cache is established the file is made easily accessible, even if you close the software program. It is the same concept as when you load a web page for the first time. The next time the page opens faster. This is also how it works for the databases in Thermo-Calc Graphical Mode.

Thermo-Calc caches the database files, both encrypted and unencrypted types, at two points—when you first open a database, sometimes called an *in-memory cache*, and then as a *disk-based cache*. The disk-based cache is what speeds up database loading and it is at this point that Thermo-Calc refers to the database initialization file for information. The disk-based cache uses a lookup key to find the abbreviated database name (e.g. TCFE or TCNI) contained in this initialization file.

It is important to understand the way databases are cached in Graphical Mode to ensure best practices for those who also use Console Mode, especially if the database initialization file is edited. If you plan to edit this file, see Editing the Database Initialization File or Unencrypted Database File.

Editing the Database Initialization File or Unencrypted Database File

Some advanced users may decide to edit the database initialization file, for example to reorder the list of encrypted databases displaying in the Console window or to add a user-defined database for use in Console Mode. It is important to understand that changes to this file impact the database caching process used in Graphical Mode.

? About the Database Files

? About Cached Database Files

The following recommendations are also applicable if you edit an unencrypted database file, which includes user databases and free databases such as PURE5 or PG35.

Best Practice Recommendations

? Database Installation Folder

If you edit the database initialization file (`tc.initd.tdb` in Windows or `initd.tdb` in Mac and Linux), then:

- If a user database is added to the file, it is subject to the same caching as the encrypted databases. This means that further changes (to the user database) are not detected when you are working with databases in the System Definer in Graphical Mode.

If you have a user database, which is subject to regular updates, then:

- If you make changes to a user database, you then need to clear the cache.
- It is recommended that you create a separate directory to store unencrypted database files.

If you edit an unencrypted database file included with the installation (such as the PURE5 and PG35 files):

- Do not edit the file in the installation folder. Instead make a local copy and load it into the application as a user database.

Database Checker

The Thermo-Calc software package includes a program to check that the syntax of unencrypted database files is correct. The program applies the syntax rules set out in the *Database Manager User Guide* and reports errors and issues warnings. This program is intended for advanced users who develop and manage databases.

Thermo-Calc accepts some deviations from these syntax rules. Although warnings can be ignored, errors must be corrected. Reported errors must be corrected in the TDB file before the database can be loaded by the application. Sometimes the warnings can also reveal the need for additional corrections as shown in the example below.

For example, a warning is generated if a phase name is detected that is also an abbreviation of another phase name in the database. Although allowed, it is not recommended as this can (in some cases) lead to unexpected results because abbreviations are also used when entering commands in the Console and included in macro files. The following shows why in this case an abbreviation is not recommended.

Imagine that a macro file uses the abbreviation `ABC` to refer to a phase in a database that is named `ABCDE`. As long as there is no other phase in the database with the same exact name or initial abbreviation, it works. But if a new phase is added to the database and is actually named `ABC` then the macro can in error refer to the wrong phase. The macro still runs but now refers to the phase `ABC` instead of `ABCDE` because `ABC` is an exact match, *which takes precedence over abbreviations*. The Database Checker displays a warning because this situation can only occur when one phase name is an abbreviation of another.

With respect to using this tool, the executable `DatabaseChecker` file is found in the Thermo-Calc home directory.

The program can also be launched by selecting **Tools →** **Database Checker**from the main menu in Thermo-Calc.

Database Manager User Guide

Global Settings

In the **Options** window you can globally set general settings for Graphical Mode as well as default settings for any new activities for both Graphical Mode and Console Mode.

To open the **Options** window:

- Windows: Select **Tools** → **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

In this section:

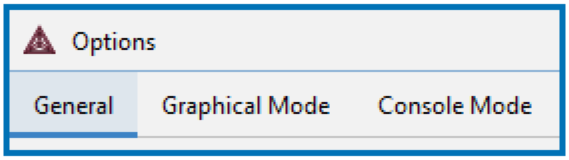
Global General Settings

Make global changes to the various defaults used for the settings for both Graphical Mode and Console Mode.

To open the **Options** window:

- Windows: Select **Tools** → **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

then click the **General** tab.



TOOLTIPS ENABLED

Select whether to turn on tooltips information. By default the **Tooltips enabled** checkbox is selected. Hover the cursor above some buttons or other settings to display text with more information about the settings.

LOCALIZATION

To change the GUI language from the **Localization** list choose **English** (the default), **Swedish**, **Spanish**, **German**, **Russian**, **Chinese**, **Japanese**, or **French**.

LOOK AND FEEL

To change the **Look and feel** of the GUI layout, choose **Light** (the default) or **Dark**.

For macOS, there are also the options **macOS Light** and **macOS Dark**.

The primary difference for the macOS themes is that the buttons and panels are a closer match to the Mac operating system. In addition, macOS Dark is darker than the standard Dark (more black than gray), although the macOS Light version is only slightly darker. It is recommended that users experiment with the options to determine which is best for your needs.

Also see Global Plot Settings: Design the Look and Feel for details about the **Color switching options** available and related to the **Light** and **Dark** modes. The use of these modes is also related to being able to right-click and access the **Plot Properties** options for local plots. See Changing the Plot Properties.

LOG LEVEL

Select the level and type of information to display in the **Event Log** window using the **Log level** slide bar. Choose from a **Debug**, **Info** (the default), **Warning**, or **Error** level of detail.

DATABASE DIRECTORY

In the **Database directory** field, the default path is to the **data** directory where all the database files and data are located. Click **Modify**to open the default folder to change this default but first review the important information below.

MODIFYING THE DATABASE DIRECTORY PATH (GRAPHICAL MODE ONLY)

Important Note: Database Directory Path (Graphical Mode only)

When you open a database for the first time, it is stored in a cache (an intermediate storage area), that is maintained even if you close the program. This improves the speed of loading the next time you open that database. The cache is used for all databases that are listed in the database initialization file, typically all the standard databases that are included with Thermo-Calc.

If you modify your own user-defined database, or if you choose to edit an unencrypted database, it is recommended that you create a separate directory to store these database files. This way the most recent version of the user-defined or edited databases are loaded into the program when the System Definer is performed.

About the Database Files

MODEL DIRECTORY

In the **Model directory** field, this is the default file location where the predefined and custom Property Models (used with the Property Model Calculator or TC-Python) are saved and stored. Click **Modify** to open the default folder or to create a custom folder for your own models.

All Property Models (whether these are predefined or custom models) must be located in a subdirectory of the Property Model directory. For that reason it is recommended that you do not change the directory location.

See Property Model Calculator for information about using the predefined models. Also see the TC-Python help on the website for details about creating custom models.

TEMPORARY DIRECTORY

In the **Temporary directory** field this is the default file path to the temporary folder, where files are stored during calculation, such as Console Mode state files (e.g. `State_4064824901731140183.POLY3`), log files, and so forth.

Click **Modify** to open the default folder, which is set during installation and based on your operating system.

PROPERTY MODEL PYTHON INTERPRETER

This is the path to the executable Python file that is needed to work with custom property models.

See the **Property Model Framework → Best Practices** section in the TC-Python help on the website.

CHECK UPDATE INTERVAL

From the **Check update interval** list, choose **Do not check** (the default) or **On startup**.

You can also manually check for updates – choose **Help** → **Check for Updates**.

PREFERRED GIBBS ENERGY SYSTEM

Use this setting to globally set the default GES version to be either GES6 (**Version 6** the default) or GES5 (**Version 5**).

About the Gibbs Energy System (GES) Module

This setting is useful if you are using the POURBAIX module (aqueous solutions) or if you have a custom database that is not compatible with GES6. The SET_GES_VERSION Console Mode command can also be used to change GES versions for a single Thermo-Calc session.

Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.

PARALLEL CALCULATION FOR PROPERTY MODEL CALCULATOR

By default, the **Parallel calculation** (Property Model Calculator Configuration window) and **Parallel calculation for Property Model Calculator** (Options window for a Global setting) checkbox is selected.

The number of parallel branches (the **No. of worker processes**) can only be changed globally via the Options window. The default number of worker processes is based on the number of physical cores available on the computer. You can adjust the number of worker processes as needed, however it is still dependent on the available cores on the computer.

This checkbox is used for all the calculation types available with the Property Model Calculator in Graphical Mode. When you click **Perform**, the grid points calculated are distributed among these worker processes, which enables parallel calculations and speeds up the calculation. Click to deselect the checkbox as needed to not use these worker processes.

RESET ALL SETTINGS AND THE DATABASE CACHE TO DEFAULTS

Click **Factory reset** to reset all the settings to the original defaults, including clearing the database cache. The changes are applied when Thermo-Calc is restarted.

This may be useful when there are several versions of Thermo-Calc installed and there are conflicts between settings or loading databases becomes problematic. See About Cached Database Files.

RESET TO ORIGINAL SETTINGS

Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button. For local plot settings, there is a **Reset** button available instead.

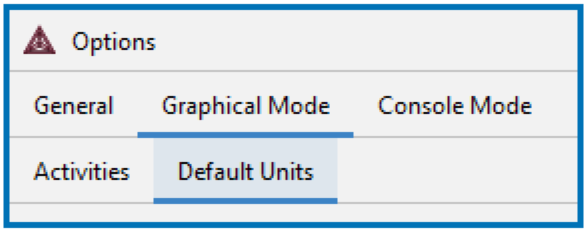
Graphical Mode: Default Units

Make global changes to the default units used for the settings.

To open the **Options** window:

- Windows: Select **Tools** → **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

then click the **Graphical Mode** → **Default Units** tabs.



RESET TO ORIGINAL SETTINGS

Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button. For local plot settings, there is a **Reset** button available instead.

Setting	***Options***
Temperature	**Kelvin** (the default), **Celsius**, or **Fahrenheit**
Pressure	**Pascal** (the default), **Atmospheres**, or **Bar**
Amount	**Mole** (the default), **Gram**, **Kilogram**, **Tonne**, or **Pound**
Mass	**Tonne** (the default), **Kilogram**, **Gram**, or **Pound**
Composition	**Mass percent** (the default), **Mole percent**, **Mass fraction**, or **Mole fraction**
Mass composition	**Mass percent** (the default) or **Mass fraction**

Setting	***Options***
Energy	**Joule** (the default), **Calorie**, **Electron volt**, **Gigajoule**, **Watt hour**, or **Kilowatt hour**
Power	**Watt** (the default), **Kilowatt**, or **Megawatt**
Volume	**Cubic meter** (the default), **Cubic decimeter**, **Cubic centimeter**, or **Normal cubic meter**
Density	**Kilogram per cubic meter**, **Gram per cubic meter**, **Gram per cubic centimeter**(the default), or **Pound per cubic inch**.
Heat capacity	**Joule per mole Kelvin** (the default), **Calorie per mole Kelvin**, **Joule per kilogram Kelvin**, or **BTU per pound Fahrenheit**
Entropy	**Joule per Kelvin** (the default), **Calorie per Kelvin**, or **Electron volt per Kelvin**
Dynamic viscosity	**Pascal-second** (the default), **milliPascal-second**, **Poise**, or **centiPoise**
Kinematic viscosity	**Square meter per second** (the default), **Stokes**, or **Centistokes**
Length	**Meter** (the default), **Millimeter**, **Micrometer**, **Nanometer**, or **Ångström**
Time	**Seconds** (the default), **Minutes**, **Hours**, or **Days**
Velocity	**m/s** (the default), **mm/s**, **µm/s**, or **nm/s**
Strength	**Mega Pascal** (the default) or **Kilogram-force per square millimeter**
Vickers hardness	**Mega Pascal** (the default) or **Kilogram-force per square millimeter**
Surface tension	**Joule per m^2** (the default) or **Millijoule per m^2**
Surface energy	**Joule per m^2** (the default) or **Millijoule per m^2**

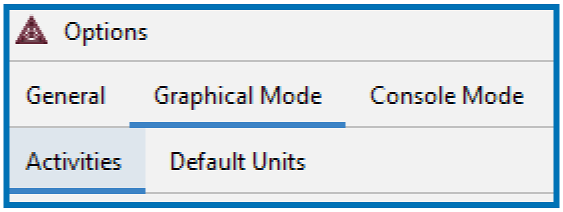
Graphical Mode: Activities

Make global changes to the various defaults used for the settings.

To open the **Options** window:

- Windows: Select **Tools** → ☰ **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

then click the **Graphical Mode** → **Activities** tabs.



Under **Default Configurations**, there are **System definition**, **Calculation**, **Precipitation**, **Diffusion**, **Scheil**, **Process Metallurgy**, **Plotting**, and **Tabulation** setting nodes. These are described individually.

- Global Settings: System Definer
- Global Settings: Equilibrium Calculator
- Global Settings: Precipitation Calculator
- Global Settings: Diffusion Calculator
- Global Settings: Scheil Calculator
- Global Settings: Process Metallurgy
- Global Settings: Graphical and Console Mode Plotting
- Global Settings: Tables

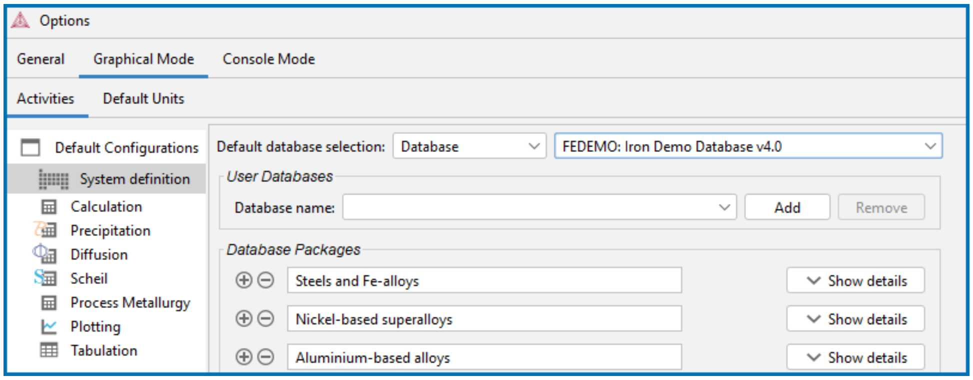
Global Settings: System Definer

When you create a new System Definer, the default databases are taken from these defaults. The database selections for each System Definer can then be configured individually. Once created, the specific (local) settings for a System Definer are not affected if you later make changes to the global defaults.

To open the **Options** window:

- Windows: Select **Tools** → ☰ **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

then click the **Activities** tab and the **System definition** node in the tree.



Default database selection: Database | FEDEMO: Iron Demo Database v4.0

Database name:

Steels and Fe-alloys

Nickel-based superalloys

Aluminium-based alloys

System Definer

Creating a Database Package and Clearing a Database Package Message

Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button. For local plot settings, there is a **Reset** button available instead.

DEFAULT DATABASE SELECTION

The **Default database selection** can be either for a **Database** or a **Database Package**.

- If you choose **Database**, then select the default installed database to use globally for all System Definer nodes. For example, choose the latest version of the TCS Steel and Fe-alloys Database (TCFE) from the list if you have a license.
- If you choose **Database Package**, select an option from the list. These Database Packages are defined in the *Database Packages* section described below.

USER DATABASES

Under *User Databases*, define the **Database name** after adding a custom database.

Click **Add** to navigate to a custom database on your computer. After you have added the user database it is available from the list to choose as the default.

Once a user database is added to the **Database name** list, you can also click the **Remove** button to delete it from your project.

DATABASE PACKAGES

Based on the installed databases, there are also default *Database Packages* available. Use this section to organize your own sets of databases that you use together often.

Create and remove *Database Packages* by clicking the **Add a database package** ⊕ button or **Remove this database package** ⊖ button.

> ❗ The addition or removal of a database package does not take effect until a new System Definer node is defined.

Click **Show Details** to display the list of databases included with the package. Click **Hide Details** to only display the name of the package.

? Creating a Database Package

Global Settings: Equilibrium Calculator

When you create a new Equilibrium Calculator, its initial settings are taken from these defaults. The settings of each Equilibrium Calculator can then be configured individually. Once created, the specific (local) settings for an Equilibrium Calculator are not affected if you later make changes to the global defaults.

To open the **Options** window:

- Windows: Select **Tools** → **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

then click the **Activities** tab and the **Calculation** node in the tree.

The available default settings are described in the topic Options Tab Settings.

Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button. For local plot settings, there is a **Reset** button available instead.

Global Settings: Diffusion Calculator

When you create a new Diffusion Calculator, its initial settings are taken from these defaults. The settings for each Diffusion Calculator can then be configured individually. Once created, the specific (local) settings are not affected if you later make changes to the global defaults.

To open the **Options** window:

- Windows: Select **Tools** → **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

then click the **Activities** tab and the **Diffusion** node in the tree.

The available default settings are described in the topic Options Tab Settings.

Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button. For local plot settings, there is a **Reset** button available instead.

Global Settings: Precipitation Calculator

When you create a new Precipitation Calculator, some of its initial settings are taken from these defaults. The settings for each Precipitation Calculator can then be configured individually. Once created, the specific (local) settings for a Precipitation Calculator are not affected if you later make changes to the global defaults.

To open the **Options** window:

- Windows: Select **Tools** → **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

then click the **Activities** tab and the **Precipitation** node in the tree.

The available default settings are described in the topics Matrix Phase Settings and Precipitate Phase Settings

Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button. For local plot settings, there is a **Reset** button available instead.

Global Settings: Scheil Calculator

When you create a new Scheil Calculator, its initial settings are taken from these defaults. The settings of each Scheil Calculator can then be configured individually. Once created, the specific (local) settings for a Scheil Calculator are not affected if you later make changes to the global defaults.

To open the **Options** window:

- Windows: Select **Tools** → **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

then click the **Activities** tab and the **Scheil** node in the tree.

The available default settings are described in the topic Advanced Options.

Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button. For local plot settings, there is a **Reset** button available instead.

Global Settings: Process Metallurgy

When you create a new Process Metallurgy Calculator, its initial settings are taken from these defaults. The settings for each Process Metallurgy Calculator can then be configured individually. Once created, the specific (local) settings are not affected if you later make changes to the global defaults.

To open the **Options** window:

- Windows: Select **Tools** → **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

then click the **Graphical Mode**and **Activities** tabs, followed by the **Process Metallurgy** node in the tree.

The available default settings are described in the topic Options Tab.

Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button. For local plot settings, there is a **Reset** button available instead.

Global Settings: Tables

When you create a new Table Renderer, its initial settings are taken from these default settings. The settings of each Table Renderer can then be configured individually. Once created, the settings of a Table Renderer are not affected by changes in the default settings.

To open the **Options** window:

- Windows: Select **Tools** → **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

then click the **Activities** tab and the **Tabulation** node in the tree.

Configuration Settings

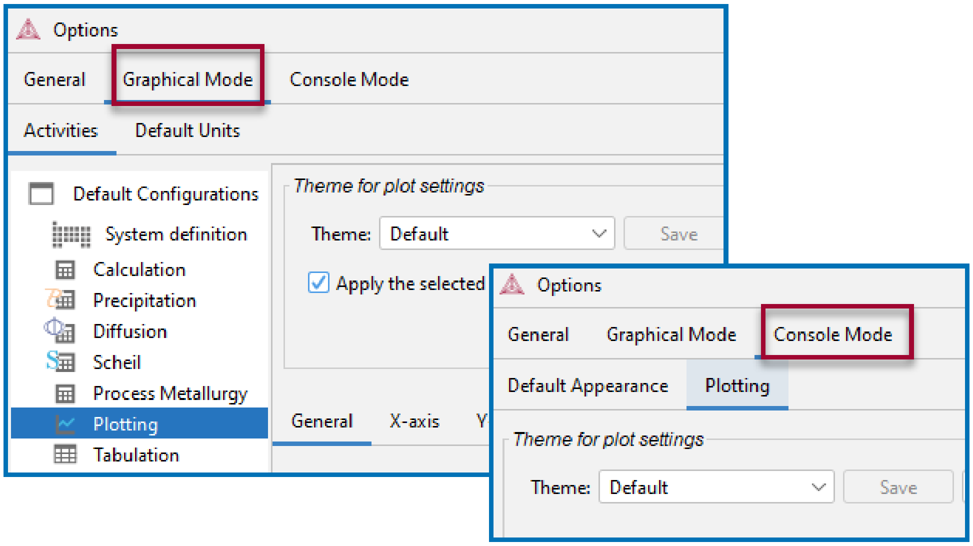
Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button. For local plot settings, there is a **Reset** button available instead.

Global Settings: Graphical and Console Mode Plotting

Globally configure several default plot settings or work with a **Theme**.

To open the **Options** window:

- Windows: Select **Tools** → **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.



On the **Options** window you can access the same settings either from the **Graphical Mode** or **Console Mode** tabs.

- Click the **Graphical Mode** → **Activities** tabs and then click the **Plotting** node in the tree, or
- Click the **Console Mode** → **Plotting** tabs.

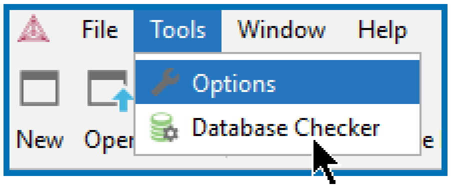
> The Console Mode and Graphical Mode plot settings are independent of each other once you start making changes to any predefined or custom Themes, or when applying changes to individual plots in either Mode.

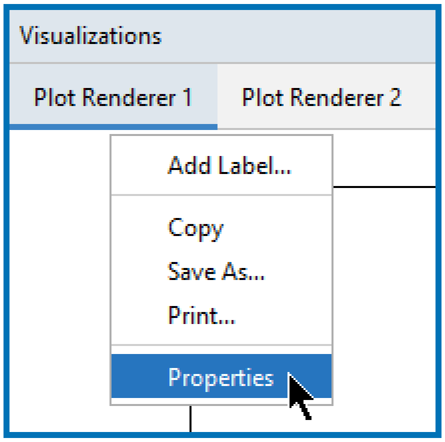
There are many options available and these are generally divided into these topics:

- Global Plot Settings: Design the Look and Feel to set a variety of options for titles, legends, labels, fonts, colors, lines, grids, data points, anchors, data points, numbers, and to adjust image quality.
- Global Plot Settings: Themes to create, edit, import, export, rename, or delete plot themes.
- Global Plot Settings: Plot Area Size to set the Plot Area Size.

Global vs Local Plot Settings

For both Graphical Mode and Console Mode, you can work with plots and themes from both the global or local settings windows. Global settings are accessed on the **Options** window and local plot settings from the **Visualizations** window when you right-click an individual plot and choose **Properties**.





Local Plot Property Settings

Plot Renderer (Graphical Mode)

> When you create a new Plot Renderer in Graphical Mode, its initial settings are taken from the default settings and theme. The settings can then be configured individually. Once created, the settings of a Plot Renderer are not affected by changes to the default global settings unless you are working with themes and then save or create a custom theme. See Global Plot Settings: Themes.

Visualizations Window Individual Plots (Graphical or Console Mode)

To make local changes to the appearance of a specific plot for either Graphical Mode or Console Mode, in the **Visualizations** window right-click a plot and select **Properties**. In the **Plot Properties** window a variety of settings can be made. These are mostly the same settings as in the **Options** window.

You can also edit some properties for individual plot lines (the color, the line width and type, and whether data points are included). In the **Visualizations** window, hover the mouse over a plot line. The crosshair cursor turns into a cursor resembling a pointing hand when it is over a line that can be clicked. Alternatively, hold down the <Ctrl> key while you move the cursor around the plot to only display it as a crosshair and prevent unintended edits.

When changes are made that differ from the plot theme applied (i.e. a predefined or custom theme) then blue text next to the theme section alerts you to the change. See Global Plot Settings: Themes for details.

Reset to Original Settings

Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button. For local plot settings, there is a **Reset** button available instead.

Global Plot Settings: Themes

Make global changes to the various defaults used for the settings.

To open the **Options** window:

- Windows: Select **Tools** → **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

On the **Options** window you can access the same settings either from the **Graphical Mode** or **Console Mode** tabs.

- Click the **Graphical Mode** → **Activities** tabs and then click the **Plotting** node in the tree, or
- Click the **Console Mode** → **Plotting** tabs.

> ❗ The Console Mode and Graphical Mode plot settings are independent of each other once you start making changes to any predefined or custom Themes, or when applying changes to individual plots in either Mode.

About Plot Themes

Location of Local and Global Theme Settings

Plot **Theme** settings are accessed in the *Theme for plot settings* section:

- Locally on the **Plot Properties** window (right-click any plot in the **Visualizations** window).
- Globally on the **Options** window for both Graphical Mode and Console Mode.

Predefined Plot Themes

There are these predefined plot themes available: **Default**, **Large**, **Small**, or **Publication**. For these themes, you can use them as a template to create your own custom theme or export the json file for use elsewhere.

The predefined plot themes have many of the same settings where key differences include font sizes, plot area size and type, scaling, data point marker radius, tick mark length, and line width. For all predefined themes, the default font is SansSerif with the style Plain (normal).

See Predefined Theme Settings for details and differences.

Custom Themes

You can create, edit, delete, rename, import, and export custom themes.

Plotting Input is Changed: Ignore, Create, Update, or Discard the Changes

When any change is made to a predefined or custom theme, either locally or globally, a blue text message under the *Theme for plot settings* section reminds you that *at least one plotting input has changed*.

When you see this blue text you can:

- Ignore it and apply the local changes to a specific plot. In this case when you click **Perform** or **Perform Tree** to update the plot in the **Visualizations** window the change only applies to this one plot. The blue text continues to be visible.
- Create a new custom theme (click **Save as**). If this is done locally on the **Plot Properties** window, the new theme is added to the global list but only applied locally to the plot. The blue text is gone.
- Update an existing custom theme (click **Save**). If this is done on the **Plot Properties** window, the changes are applied globally and applied locally to the plot. The blue text is gone.
- Discard the changes and click **Reset to original settings** (for global **Options** windows you may need to scroll, it is in the bottom right of the window) or **Reset** (for local settings on the **Plot Properties** window). The blue text is gone.

Working with Plot Themes

Whether working with a predefined or custom theme, there are common tasks you can do such as using a theme as a template to create a new custom theme, or you can import and export .json files.

Once created, there is more flexibility with the custom themes.

Applying Predefined or Custom Themes to a Plot Globally or Locally

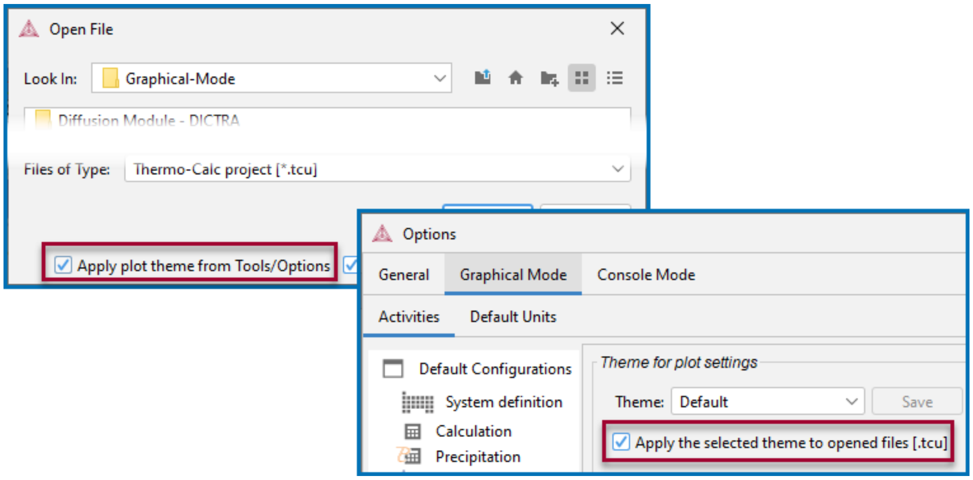
1. In the *Theme for plot settings* section, choose an option from the **Theme** list.
2. Click **OK** to apply the theme. Click close (X) or **Cancel** to exit without saving, or **Reset** to revert any changes to the original saved settings.

- On the **Options** window this is applied globally.
- On the **Plot Properties** window this is applied locally to the specific plot in the **Visualizations** window.

Applying Plot Themes to Project Files (Graphical Mode Only)

When opening project files, a predefined or custom plot theme can be automatically applied to all plots. There are two checkboxes that control this, one is a global setting and one is a local setting applied to a specific file as it is opened.

If you double-click or drag and drop to open a project file it automatically uses the global settings in Thermo-Calc (which may or may not be to apply a theme). This means you may inadvertently apply a theme to your plots without realizing it.



Look In: Graphical-Mode

Files of Type: Thermo-Calc project [*.tcu]

☑ Apply plot theme from Tools/Options

Theme: Default

☑ Apply the selected theme to opened files [.tcu]

There is some interaction between these checkboxes as detailed in the table below.

Checkbox	***Location***	***Actions***	***Comments***
Apply the selected theme to opened file [.tcu]	**Options** window.	Select the checkbox to apply a theme globally to all project files being opened. Click to clear the checkbox to allow each file to keep existing plot settings.	When this checkbox is selected or deselected, it also changes the **Apply plot theme from Tools/Options** checkbox to match, i.e. these are connected in one direction.
Apply plot theme from Tools/Options	**Open File** window. See Opening Project Files	Select the checkbox to apply a theme locally to the specific project file being opened. Click to clear the checkbox to allow the specific file to keep existing plot settings.	If this checkbox is selected or deselected it only applies to the specific project file being opened, i.e. the **Apply the selected theme to opened file [.tcu]** checkbox does not change.

If you have a project file with calculated results and local settings applied to plots i.e. applied from the **Visualizations** window to a specific plot via the **Plot Properties** settings window, then click to clear the local setting as you open the file using **Apply plot theme from Tools/Options** checkbox. Otherwise the default global settings are applied to all plots and you would need to individually change these settings back to your original design. Alternatively, experiment with applying a predefined theme, e.g. **Publication**, as this could be sufficient for your final output.

Creating a Custom Plot Theme in Thermo-Calc

To create a custom theme, you start by making changes to the selected theme type and then save it with a new name using the **Save as** option.

> You can work with themes from both the global or local settings windows. Global settings are accessed on the **Options** window (Windows: **Tools** → **Options**; Mac: **Thermo-Calc** *<version>* → **Preferences**) and local plot settings accessed from the **Visualizations** window when you right-click an individual plot and choose **Properties**.

For example, the **Background color** is changed to RGB **#FF4EE2** for the **Default** theme. Next to the *Theme for plot settings* section, a message in blue alerts you that *at least one plotting input has changed*.

To save the new settings including the change to the background color (you cannot replace the predefined themes), you also must make sure to click **OK** at the end.

HOW TO CREATE A CUSTOM PLOT THEME

1. In the *Theme for plot settings* section, click **Save as**. The **New theme plot setting** window opens.
2. In the **Theme name** field enter the new custom theme name. The new theme is now available from the list.
3. On the **Plot Properties** or **Options** window, click **OK** to finish. Click close (X) or **Cancel** to exit without saving, or **Reset** to revert any changes to the original saved settings.

Importing a Custom Theme

Use the **Import** option to add your own theme with the file type of *.json. Once the file is imported, you can make further changes and save the new theme settings as needed. If you import a theme that uses the same name one already in the list (e.g. **Publication**), the imported theme name is changed automatically by adding a number at the end of its name (e.g. **Publication_1**). You can then **Rename** the theme to give it a unique name.

HOW TO IMPORT A CUSTOM PLOT THEME

1. In the *Theme for plot settings* section, click **Import**.
2. Navigate to where you saved the .json file, select it, then click **Open**.
3. During the import, and if there are incorrect input values, you are prompted with an error message describing the issue with the file.

   This could be for various reasons, such as entering a value that is not available (i.e. it is out of bounds), or the file contains information about an unavailable setting. In particular these settings must be correctly entered in the import file: font sizes, tie line, number of decimals, border width, data points marker radius, x and y axis tick marks length, and jpeg compression level.

4. If it is a successful import, click **Rename** to give the theme a unique name.
5. On the **Plot Properties** or **Options** window, click **OK** to finish. Click close (X) or **Cancel** to exit without saving, or **Reset** to revert any changes to the original saved settings.

Exporting a Theme

Use the **Export** option to export an existing theme or after creating a custom theme.

> You can also export an existing theme, edit it in a text editor (making sure to save the file with file extension .json), and then **Import** this new .json file. However, it is better to use the Graphical User Interface to prepare your custom theme in order to minimize errors during import.

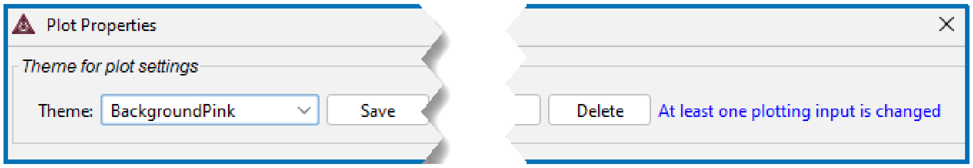
HOW TO EXPORT A PLOT THEME

1. In the *Theme for plot settings* section, select the **Theme** to export.
2. Click **Export**.
3. Navigate to where you want to save the .json file. Enter a **File name** as required then click **Save**.

Deleting a Custom Theme

After you have created a custom theme, it can be deleted from the list. Predefined themes cannot be deleted.

If the selected theme is deleted from the global Options section, and you open a project or plot that uses the now deleted theme, the default theme is selected but it includes the message in blue next to the section to remind you that *at least one plotting input has changed*. In the example the custom theme, **BackgroundPink**, was deleted at the global level but at the local level for the specific plot open in the **Visualizations** window the settings are retained and the message displays.



At least one plotting input is changed

How to Delete a Custom Plot Theme

1. In the *Theme for plot settings* section, select the **Theme** to delete.
2. Click **Delete**.
3. Click **OK** on the window that opens.
4. On the **Plot Properties** or **Options** window, click **OK** to finish. Click close (X) or **Cancel** to exit without saving, or **Reset** to revert any changes to the original saved settings.

Renaming a Custom Theme

After you have created or imported a custom theme, it can be renamed. Predefined themes cannot be renamed.

How to Rename a Custom Plot Theme

1. In the *Theme for plot settings* section, select the custom **Theme** to rename.
2. Click **Rename**.
3. Enter the new name in the field. Click **OK**.
4. On the **Plot Properties** or **Options** window, click **OK** to finish. Click close (X) or **Cancel** to exit without saving, or **Reset** to revert any changes to the original saved settings.

Predefined Theme Settings

The following lists the applied attributes for each of the predefined themes: **Default**, **Large**, **Small**, or **Publication**.

? Global Plot Settings: Themes

Image Quality

Plot Setting	*Default*	*Large*	*Small*	*Publication*
Default file format and DPI	.png and Use default resolution (300 DPI)	.png and Use default resolution (400 DPI)	.png and Use default resolution (300 DPI)	.png and 600 DPI

Fonts, Style, Size, and Format

Plot Setting	*Default*	*Large*	*Small*	*Publication*
Title font (SansSerif) and Style (Plain/normal). The size is different for each.	18	26	16	24
Legend font (SansSerif) and Style (Plain/normal). The size is different for each	11	22	9	20
Label font (SansSerif) and Style (Plain/normal). The size is different for each.	16	24	14	22
Header font (SansSerif) and Style (Plain/normal). The size is different for each.	12	18	10	16
X and Y Axis Label font (SansSerif) and Style (Plain/normal). The size is different for each.	18	28	16	26
X and Y Axis Tick Label font (SansSerif) and Style (Plain/normal). The size is different for each.	14	24	12	22
Title format, Label format, Axis label format (X- and Y-axis)	Plain text			

Colors

Plot Setting	*Default*	*Large*	*Small*	*Publication*
Title color, Legend color, Label color, Header color, Border color, Axis label color (X- and Y-axis), Axis tick label color (X- and Y-axis)	rgb ff000000			
Legend background color, Background color, and Canvas color	rgb ffffffff			
Color option	Vivid (in json file it is PlotColorOption 6)			

Checkbox Selections

Selected = Yes

Plot Setting	*Default*	*Large*	*Small*	*Publication*
Show grid	No			
Show legend	Yes			
Show anchor	Yes			
Retain labels	Yes			
Show header	No			
Show tick labels (X- and Y-axis)	Yes			
Tick marks outside (X- and Y-axis)	Yes			

Plot Area Size

Plot Setting	*Default*	*Large*	*Small*	*Publication*
Fit the plot area size to the enclosing window (selected), with the plot area height and width preset as indicated	400 x 400	700 x 700	400 x 400	Not selected. By default it is 600 x 600

Plot Setting	Default	Large	Small	Publication
Fit the plot area size to a square with a width/height of the enclosing window	Not selected (in json file it is plotAreaSizeType: Window_Fit)			Selected (in json file it is Square_ Fit)
Define the plot area size	Not selected			
Scale plot attributes using the system scaling factor	yes			

Other Settings

Plot Setting	Default	Large	Small	Publication
Show every Nth tieline (only relevant for phase diagrams)	1			
Border width	1	1	1	3
Data points marker	None (in json file this is called Symbol and set to 0)			
Legend phase caption style	None (in json file it is set to 0)			
Data points marker size (if you choose a data points marker symbol, then this is the default size applied)	3	5	3	5
Tick mark length (X- and Y-axis)	6	8	4	6
Number of decimals	2			
Numeric format	Auto (in json file it is 2)			
Line width	0	2	0	3

Global Plot Settings: Plot Area Size

Make global changes to the various defaults used for the settings.

To open the **Options** window:

- Windows: Select **Tools** → **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

On the **Options** window you can access the same settings either from the **Graphical Mode** or **Console Mode** tabs.

- Click the **Graphical Mode** → **Activities** tabs and then click the **Plotting** node in the tree, or
- Click the **Console Mode** → **Plotting** tabs.

> The Console Mode and Graphical Mode plot settings are independent of each other once you start making changes to any predefined or custom Themes, or when applying changes to individual plots in either Mode.

For local or global application, the default settings applied in the *Plot Area Size* section are initially based on the selected predefined theme. Once a custom theme is available from the list, these default settings can also be related to how the custom theme is set up.

See Predefined Theme Settings for details and differences between the predefined themes initially available in the list.

In the *Plot Area Size* section, choose an option.

Click **Fit the plot area size to the enclosing window** and as the **Visualizations** window is resized, the plot moves and adjusts at the same time. This setting is the default for the **Default**, **Large**, and **Small** themes.

Click **Fit the plot area size to a square with a width/height of the enclosing window**. With this option, the minimum value of the width and height of the **Visualizations** window is used as the dimension of the fixed plot area and in a square.

Click **Define the plot area size** to enter a **Plot area height** and **Plot area width (not applicable to triangular plots**. The units are pixels and the size is kept as the size on the screen (96 dpi). This is the default for the **Publication** theme.

For the predefined themes this is already set for each as indicated below. As needed, you can change these defaults for one plot or create a new theme.

- **Default** and **Small** are set to 400 x 400
- **Large** is set to 700 x 700
- **Publication** is set to 600 x 600

Click to deselect the **Scale plot attributes using the system scaling factor** checkbox to scale all plot attributes (i.e. labels, font size, axes, tick marks, etc.) independently of the screen size and resolution. This maintains consistent attribute sizing between different plots.

The minimum value of the width and height of the **Visualizations** window, or the fixed plot is used for resizing, in the following parts of the plot:

- X- and Y-axis label
- Legend font
- Tick label font
- Tick mark length
- Title
- Header
- Line width
- Data point width
- Experiment data size
- Logo

Global Plot Settings: Design the Look and Feel

Make global changes to the various defaults used for the settings.

To open the **Options** window:

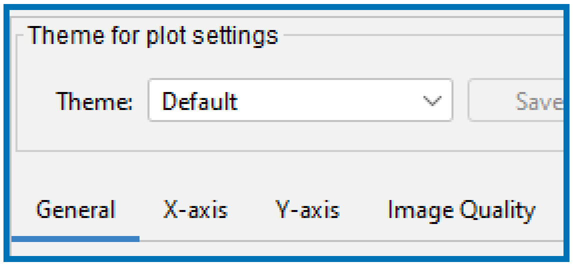
- Windows: Select **Tools** → **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

On the **Options** window you can access the same settings either from the **Graphical Mode** or **Console Mode** tabs.

- Click the **Graphical Mode** → **Activities** tabs and then click the **Plotting** node in the tree, or
- Click the **Console Mode** → **Plotting** tabs.

> The Console Mode and Graphical Mode plot settings are independent of each other once you start making changes to any predefined or custom Themes, or when applying changes to individual plots in either Mode.

The following global design settings are available for both Graphical Mode and Console Mode from the **General** tab or as indicated for the **X-axis**, **Y-axis**, and **Image Quality** tabs.



Theme: Default

The plot settings listed below are grouped into these general categories

- Titles, Legends, Headers, and Labels
- Fonts and Colors
- Lines and Grids
- Data Points, Anchors, and Numbers
- Image Quality

Titles, Legends, Headers, and Labels

TITLE FORMAT, LABEL FORMAT, AND AXIS LABEL FORMAT

On the **General** tab (**Title format** and **Label format**) and the **X-axis** and **Y-axis** tabs (**Axis label format**) select **Plain text** (the default) or **LaTeX formatted text**.

> For **LaTeX formatted text** you can use the LaTeX math text to enter text. See ADD_LABEL_TEXT and Plot Labels for more details.

SHOW LEGEND

Select the **Show legend** checkbox to include a legend on the plot. By default no legend is displayed.

TICK MARK LENGTH, LOCATION, AND SHOW TICK LABELS

On the **X-axis** and **Y-axis** tabs, choose or enter a **Tick mark length** (**6** is the default).

The defaults are to have the **Tick marks outside the chart** and to **Show tick labels**. Click to clear the checkboxes as required.

LEGEND PHASE CAPTION STYLE

For the **Legend phase caption style**, choose **None**, **All**, **Constitution description**, or **Ordering description**.

About Legend Styles

RETAIN LABELS

By default the **Retain labels** checkbox is selected. Plot labels are kept (retained) when plots are updated. It can be applied globally or locally to individual plots.

SHOW HEADER

Click to select the **Show header** checkbox to display the basic details about the plot along the top. This includes the date and time the plot is generated, the database used, and the properties.

Fonts and Colors

COLOR SWITCHING

This is related to the **Light** and **Dark** look and feel modes set under **Tools → Options** then on the **General** tab. See Global General Settings.

This section is about Global changes to the default output for all plots for any future project files. Global settings take effect for *new* project files and/or *new* plots *added* to existing projects. That is, the default setting only affects how the plots start out initially. Once a plot is created the settings are locked to the mode and can only be changed locally.

You can locally change an existing plot in a project. See Changing the Plot Properties for details.

Select a **Color switching** option: **Switch automatically between Light mode and Dark mode** (the default), **Always use Light mode colors**, or **Always use Dark mode colors**.

Tie lines and invariant lines are the same color for both Light and Dark modes, i.e. these colors do not change.

Use the **Color switching** option to override the look and feel settings that may not be optimal. For example, when preparing a plot for publication, the **Dark** mode plot or line colors may not work well or do not follow a journal's guidelines. In other words, you can view and export the plot with **Light** mode color settings even though the interface is using Dark mode, and vice versa.

FONTS: TITLE, LEGEND, LABEL, HEADER, AXIS LABEL, AND TICK LABEL

On the **General** tab (**Title**, **Legend**, **Label**, **Header**, and on the **X-axis** and **Y-axis** tabs (**Axis Label**, **Tick Label**, click **Modify** to edit the **Font Name**, **Style**, **Size**, and **Color**.

LEGEND BACKGROUND COLOR, BACKGROUND COLOR, CANVAS COLOR, BORDER COLOR

To change various background color attributes, click **Modify** to choose a color or enter a specific color.

Lines and Grids

SHOW GRID

Click to select the **Show grid** checkbox to include a grid on the plot. By default no grid is displayed.

SHOW EVERY NTH TIELINE

Tielines are only applicable to phase diagrams.

Choose an integer value ranging from 0 to 99.

COLOR OPTION (PLOT LINES)

For the for plot line colors, choose a **Color option** from the list: **Legacy**, **Printer friendly**, **JFree chart**, **Pastel**, **Medium dark**, **Bright dark**, **Vivid**, or **Earth**.

This option is also available for specific plot lines. To change the color of an individual plot line double-click it in the **Visualizations** window and use the color palette to define it or enter a specific color.

BORDER WIDTH

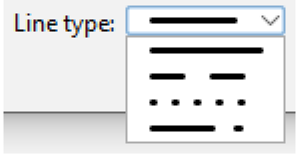
Choose a plot **Border width** between **1** (thin, the default) and **10** (thick).

LINE WIDTH

For the plot line width, choose a **Line width** from the list. These options are also available for specific plot lines. To change an individual plot line width double-click it in the **Visualizations** window.

LINE TYPE

This option is only available for individual plot lines. To change an individual plot line type double-click it in the **Visualizations** window and choose a **Line type** from the list.



Data Points, Anchors, and Numbers

SHOW ANCHOR

Click to select the **Show anchor** checkbox. By default, an anchor between the label and the plot point is displayed.

DATA POINTS MARKER

From the **Data points marker** list, scroll to select a symbol to use to display the data points on plot lines. This option is also available for specific plot lines. To show data points on an individual plot line double-click it in the **Visualizations** window and select a symbol from the **Marker** list.

DATA POINTS MARKER SIZE

Choose the **Data points marker size** between **1** (small) and **10** (large). The default is 3.

NUMBER OF DECIMALS

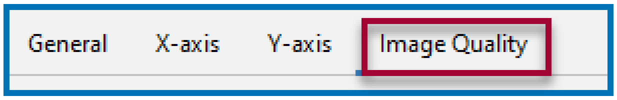
Choose the **Number of decimals** to display in the plot. The default is 2.

NUMERIC FORMAT

Choose the **Numeric format** to display in the plot **Auto**, **Decimal**, or **Scientific**.

Image Quality

Click the **Image Quality** tab to access the settings below.



Choose a **Default file format**: **Portable Network Graphics .png** (the default), **Graphical Interchange Format .gif**, **Enhanced Windows Metafile .emf**, **Portable Document Format .pdf**, **PostScript .ps**, **Scalable Vector Graphics .svg**, or **Joint Photographic Experts Group .jpg**.

The following settings are only available for .png and .jpg file formats.

To change the resolution of a *.png or *.jpg image, click to clear the **Use default resolution** checkbox. Then enter a numerical value in the **Dots per inch (DPI)** field. For .*jpg files, you can also use the slider to choose a number between 0 and 1 for the **JPG quality**. The default is 0.9. The lower the number, the smaller the file.

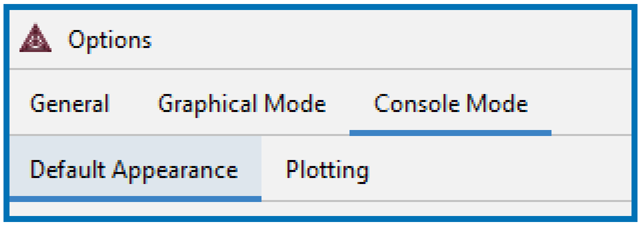
Global Settings: Console Mode Default Appearance

Make global changes to the various defaults used for the settings.

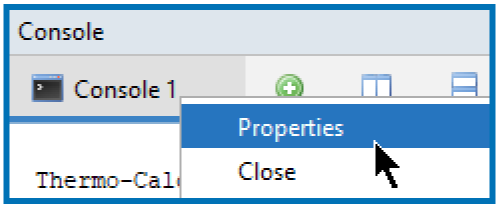
To open the **Options** window:

- Windows: Select **Tools** → ☷ **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

then click the **Console Mode** → **Default Appearance** tabs.



To change these defaults for an individual Console tab, in Console Mode, right-click the tab and select **Properties**.



Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to scroll or expand the window to see the button. For local plot settings, there is a **Reset** button available instead.

CONSOLE NAME

The default **Console name** prefix is `Console` or enter another name to display as the tab label.

BUFFER SIZE

The default **Buffer size** is 40,000.

In Console Mode, sometimes the output overflows the window text buffer. This is how to increase the buffer size.

1. In the Console window right-click the tab to edit. For example, if this is the first tab, it is labeled **Console 1**.
2. Select **Properties** and either enter a number in the field or use the arrows to increase or decrease the **Buffer size**.

FONTS: SYSTEM OUTPUT, COMMAND PROMPT, OR USER INPUT

Click **Modify** to open the **Select Font** window and makes changes to the **Font Name**, **Style**, **Size**, or choose from a variety of color options for the font as required. The **Show only fonts that support Greek characters** checkbox is selected by default.

BACKGROUND COLOR

Click **Modify** to open the **Select Color** window to choose a background color for the Console Mode window where you enter commands.

DEFAULT DIRECTORY

Click **Modify** to change the default directory file path to where the various file types are saved.