Precipitation Module (TC-PRISMA) User Guide

Thermo-Calc Version 2024a

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Contents

Introduction to the Precipitation Module (TC-PRISMA)

In this section:

About the 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

> The configuration of the Yield Strength Property Model is completed on the Property Model Calculator and then accessed as a variable with the Plot Renderer or Table Renderer.

In order to perform a simulation in the Precipitation 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.

Precipitation, formation of particles of a second phase, or second phases from a supersaturated solid solution matrix phase, is a solid state phase transformation process that has been exploited to improve the strength and toughness of various structural alloys for many years. This process is thermochemically driven and fully governed by system (bulk and interface) thermodynamics and kinetics.

Typically, a precipitation process has three distinctive stages: nucleation, growth, and coarsening. However, under certain conditions, these can also happen at the same time. With the Precipitation Module, the kinetics of concurrent nucleation, growth, and coarsening can be simulated by calculating the evolution of the probability distribution of the particle number densities, usually called particle size distribution (PSD). The simulation results can be used to understand and guide how to obtain desirable precipitates with certain PSD or to avoid undesirable precipitations during heat treatments of alloys such as aging and tempering.

A summary for the input and output of the Precipitation Module is shown.

Input and Output of the Precipitation Module

Input

- Alloy composition
- Temperature
- Simulation time
- Thermodynamic data
- Kinetic data
- Property data
- Nucleation sites
- Grain size
- Dislocation density
- Initial microstructure

Precipitation Module (TC-PRISMA)

Output

- Particle size distribution
- Grain size distribution
- Number density
- Average particle size
- Volume fraction
- Matrix composition
- Precipitate composition
- Nucleation rate
- Critical radius
- Driving force
- TTT/CCT diagrams
- Yield stress

The Precipitation Module relies on CALPHAD-based software tools and databases to provide the necessary bulk thermodynamic and kinetic data for phases in multicomponent systems. The CALPHAD approach has been developed for more than 50 years and is routinely applied to design new alloys and optimize existing materials within various metal industries, such as steels and alloys of nickel, titanium, aluminum and magnesium.

The power of this approach is due to the adopted methodology where free energy and atomic mobility of each phase in a multicomponent system can be modeled hierarchically from lower order systems, and model parameters are evaluated in a consistent way by considering both experimental data and ab-initio calculation results. The Precipitation Module is directly integrated into Thermo-Calc, a CALPHAD-based computer program for calculating phase equilibrium. Another Add-on Module, the Diffusion Module (DICTRA) is available for diffusion controlled phase transformation in multicomponent systems.

With Thermo-Calc and the accompanying thermodynamic and mobility databases, almost all fundamental phase equilibrium and phase transformation information can be calculated without unnecessary and inaccurate approximations. For example you can calculate:

- Driving forces for nucleation and growth

- Operating tie-lines under local equilibrium conditions

- Deviations from local equilibrium at interfaces due to interface friction

- Atomic mobilities or diffusivities in the matrix phase

In addition to bulk thermodynamic and kinetic data, a few other physical properties, such as interfacial energy and volume, are needed in precipitation models. These additional physical parameters can be obtained by experiments or other estimation models or first principles calculations. Volume data are available in most of our thermodynamic databases . The Precipitation Module has an estimation model available for interfacial energy.

📄 This guide is a supplement to the full Thermo-Calc documentation set. It is recommended that you use the Online Help, which you can access in Thermo-Calc by pressing F1 or from the main menu choose **Help → Online help**.

❓ See "Help Resources" on page 13 to learn how to access this information if you have not already done so.

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.
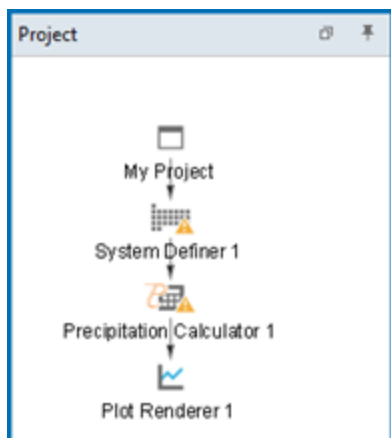
Precipitation Calculator

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.
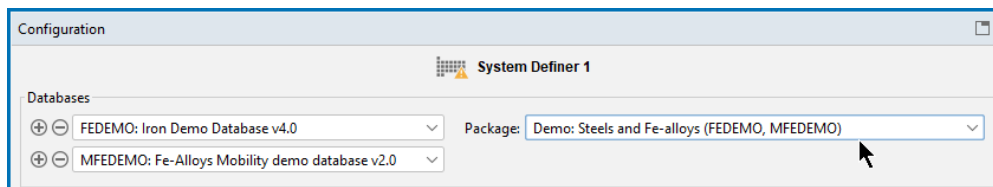
Demonstration (Demo) Mode

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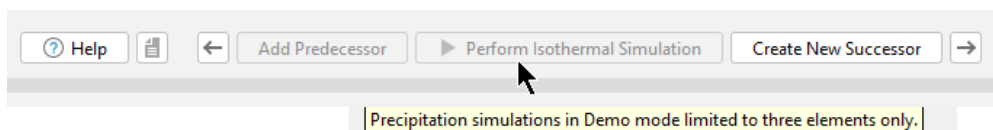
Even if you have more than three elements, the Plot Renderer or Table Renderer **Perform** button is still available. However, if you click the button and try to run the simulation the Event Log displays an error message.

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.

Network License Restrictions

The Precipitation Module (TC-PRISMA) 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 Precipitation 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 Precipitation Calculator is available with three elements.

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

Help Resources

'Online' 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:

- 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**.

> 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.

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.

Convention	Definition
Read More	Read more at the link, which may be to our website or another source of general information.
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.

Convention	Definition
Property Models	This indicates that the information relates to the Property Models. This includes the Steel Model Library and Nickel Model Library as well as the general Models included with all installations.
Additive Manufacturing (AM) Module	This indicates that the information relates to the Add-on Additive Manufacturing (AM) Module.

Using the Precipitation Calculator

In this section:

Precipitation Calculator

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.

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" on page 21

    (?)   "Precipitate Phase Settings" on page 28

    (?)   "Calculation Type Settings" on page 38

Options

Modify *Numerical Parameters* that determine how the conditions are calculated.

    (?)   "Numerical Parameters on the Options Tab" on page 46

Plot Renderer

There are also unique settings available for this calculator once you add a "Precipitation Calculator Plot Renderer" on page 48.

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" on page 40

    *   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" on page 48.

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.
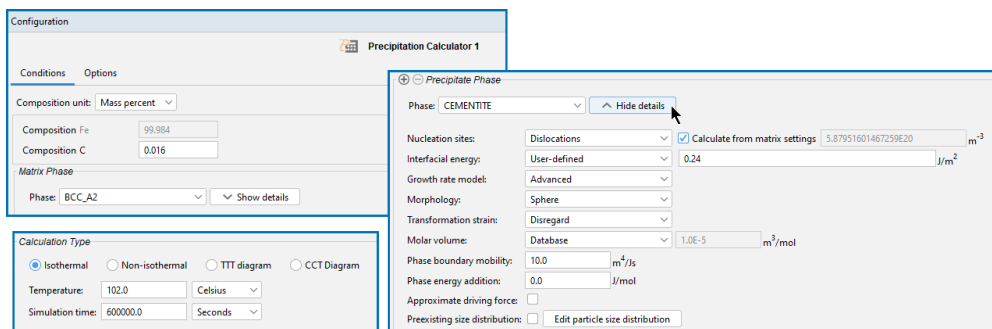
This is the three distinct settings areas for the Configuration window for example P_04_ Precipitation_Fe-C_Cemetite.tcu. In this case, Show Details is expanded to show the Precipitate Phase settings.

> 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 " on page 27

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

(?) See "Homogeneous Nucleation" on page 62 for theory.

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 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.

> **(?)** See "Precipitation Morphology" on page 96 and "The Number of Available Heterogeneous Nucleation Sites" on page 73 for theory.

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.

> **(?)** See "Precipitation Morphology" on page 96 and "The Number of Available Heterogeneous Nucleation Sites" on page 73 for theory.

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}.

> See "Precipitation Morphology" on page 96 and "The Number of Available Heterogeneous Nucleation Sites" on page 73 for theory.

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.

❓ See "Normal Grain Growth" on page 99 and "Zener Pinning" on page 101 for theory.

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)" on page 35.

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.

See "Normal Grain Growth" on page 99 for theory.

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.

See Grain Boundary Mobility Values for theory and recommended values.

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.

See "Zener Pinning" on page 101 for theory.

"P_14: Grain Growth and the Zener Pinning Effect" on page 206

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

See "Homogeneous Nucleation" on page 62 and "Heterogeneous Nucleation" on page 69 for theory.

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

See "Estimation of Coherent Interfacial Energy" on page 95 and "Interfacial Energy Anisotropy" on page 84 for theory.

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*.

(?) See "Growth" on page 77.

Morphology

(?) See "Precipitation Morphology" on page 96 for theory.

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.

(?) If **Sphere** is selected, there is an option to use a **3D → 2D** conversion on the Plot or Table Renderer for certain variables. See "Stereology" on page 104 for theory details.

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.

(?) See "Particle Shape Determination" on page 83 for theory.
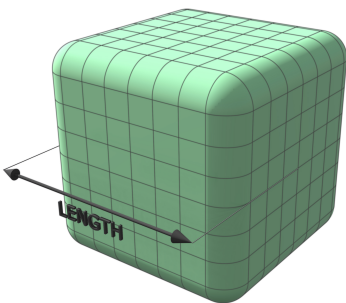
Figure 1: The cuboid shape is described by a supersphere. Cuboids have six faces, which form a convex polyhedron.
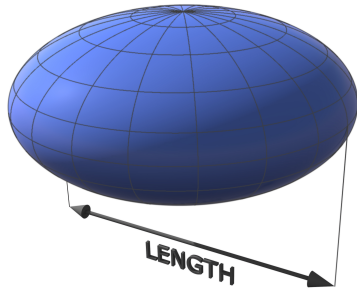
Figure 2: The plate is described as oblate spheroid. Oblate spheroids have rotational symmetry around an axis from pole to pole.
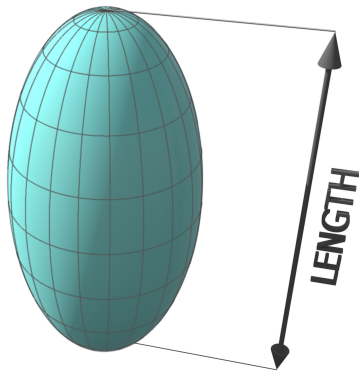
Figure 3: The needle shape is described as prolate spheroid. A prolate spheroid is a surface of revolution obtained by rotating an ellipse about its major axis.

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**.

❓   See "Particle Shape Determination" on page 83 for theory.

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 : 7×10^{-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.

See "Zener Pinning" on page 101 for theory.

"P_14: Grain Growth and the Zener Pinning Effect" on page 206

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.

See "Simplified Growth Rate Model" on page 78 for theory.

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.

See "Simplified Growth Rate Model" on page 78 for theory.

Approximate Driving Force

Select the checkbox to include this if simulations with several compositions sets of the same phase create problems.

See "Nucleation Theory" on page 61.

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.

Particle Size Distribution (PSD)

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 entered as a pre-defined distribution, by importing a file, or by manually entering information into a table.

Accessing the 'Pre-existing Size Distribution' Settings

1. To the right of the *Precipitate Phase* settings fields, click **Show Details**.

2. At the bottom of the *Precipitate Phase* section, click to select the **Preexisting size distribution** checkbox. Then click **Edit particle size distribution**.

3. The **Preexisting Particle Size Distribution** window opens as shown for example P_10.
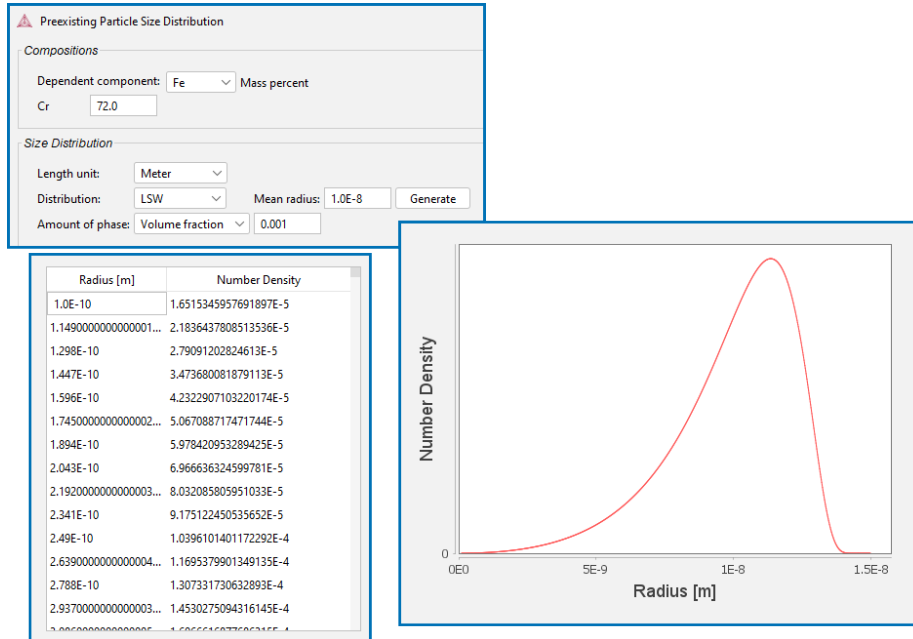
Defining the Preexisting Size Distribution

1. Under *Compositions*, choose a **Dependent component** from the list and enter the composition for the other component.

2. Under *Size Distribution* define the following:

   a. Choose a **Length unit**: **Meter**, **Micrometer**, **Nanometer**, or **Ångström**.

   b. Choose a **Distribution**: **LSW** (Lifshitz-Slyozov-Wagner), **Normal**, **Log normal**, **Weibull**, or **From file**. You can also click in the table to manually enter numbers into the cells instead of importing a file.

   c. Then based on the **Distribution** selected, enter additional settings:

   - **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.

d. 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.

e. For all options, choose an **Amount of phase**: **Volume percent** or **Volume fraction** and then enter a number in the field.

f. Once the **Distribution** is defined, click **Generate**.

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" on page 40.

Non-isothermal

> (?) "Nucleation During a Non-isothermal Process" on page 75

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" on page 40 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" on page 135

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'" on page 156.

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 a **Simulation time** and choose a unit: **Seconds**, **Minutes**, **Hours**, or **Days**.

   The profile is displayed on the **Precipitation Calculator** tab in the **Visualizations** window showing the constant temperature entered.
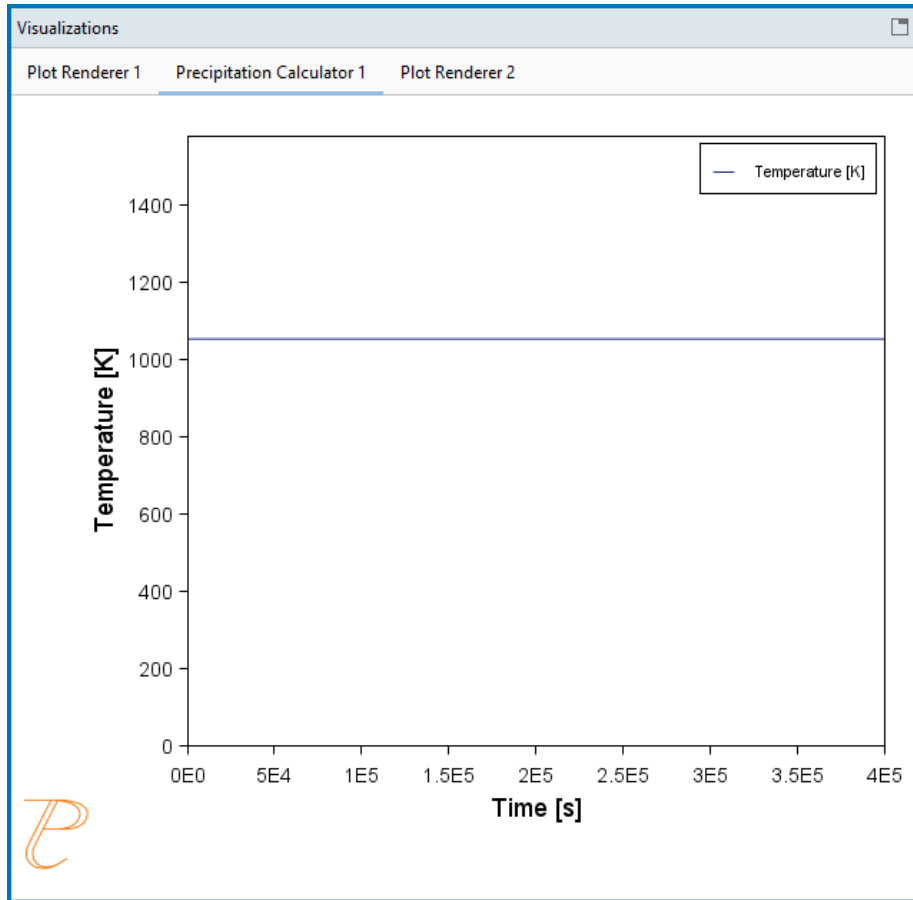
5. For this calculation type this completes the settings you need to enter for the Thermal Profile.

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 a total **Simulation time** and choose a unit: **Seconds**, **Minutes**, **Hours**, or **Days**.

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" on page 44.

    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.
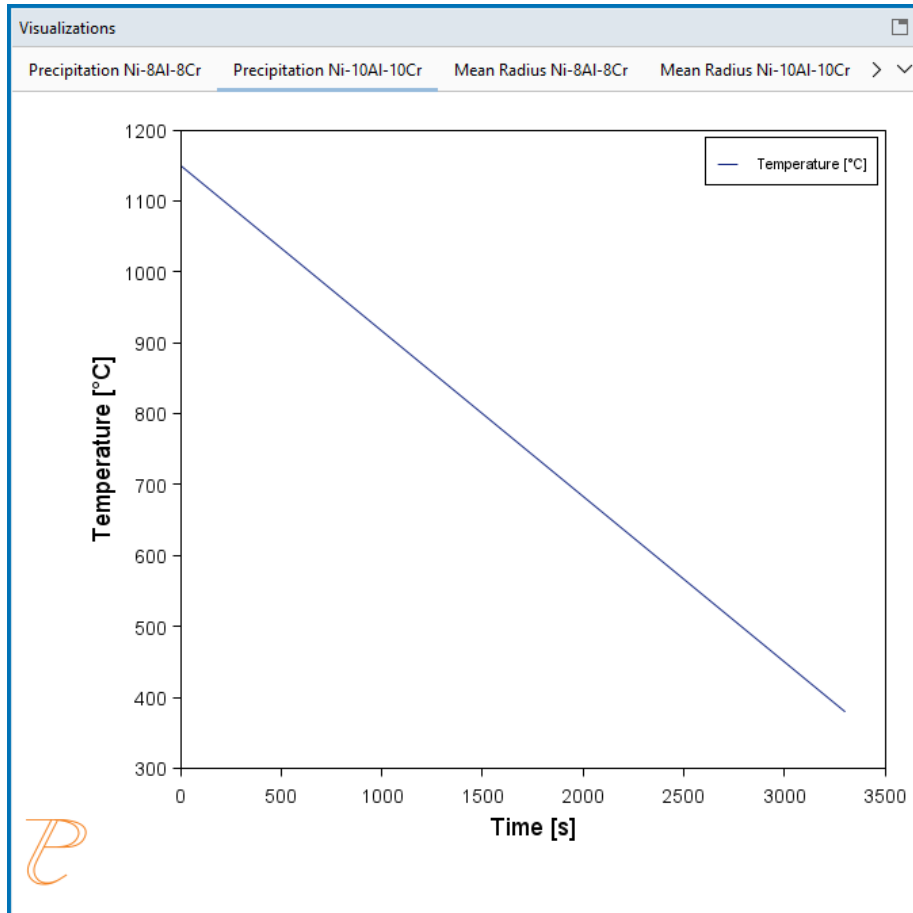
This is from the non-isothermal calculation example, *P_06_Precipitation_Ni-Al-Cr_Non-isothermal_Gamma-Gamma_prime*.

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.

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 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.
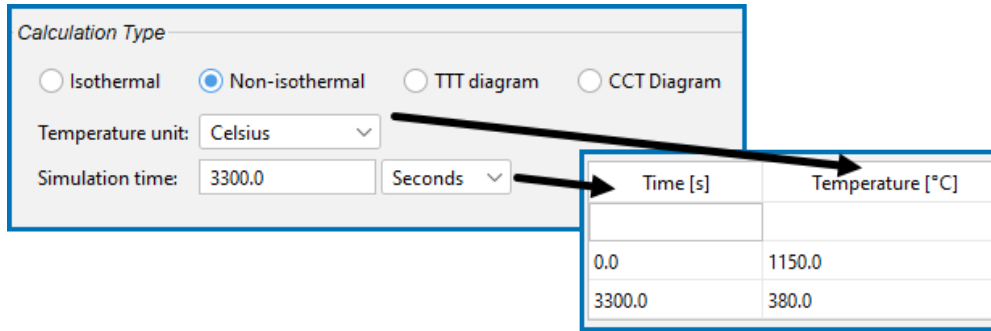
Figure 5: The units shown on the Configuration window for the Time and Temperature correspond to settings that can ONLY be selected on the Configuration window. The data file does not contain any information about the units.

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 Celsius, which is the unit chosen in the example shown in Figure 5

Numerical Parameters on the Options Tab

The Precipitation Calculator *Numerical Parameters* settings are located on the **Configuration** window → **Options** tab.

> For equations and details about these settings, see "Numerical Method" on page 90.

> You can change these settings locally for a specific Precipitation Calculator or globally for some defaults in the **Options** window settings.

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.

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**.

There are also specific settings related to that are detailed in this topic.

Plot Settings

Legend Option

Select whether the diagram's legend displays **On** or **Off**.

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.

Below are additional details related to the *Axis variable* chosen.

Separate Multimodal PSD

If you select **Mean radius**, **Number density**, **Size distribution**, **Number density distribution**, or **Normalized number density distribution** then select the **Separate multimodal PSD** checkbox to enter settings for **Points**, **Excess kurtosis**, **Valley depth ratio** and **Minimum peak**.

> There are additional settings described for .

3D → 2D

For a spherical morphology, and if you select **Mean radius**, **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 for settings.

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. 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.
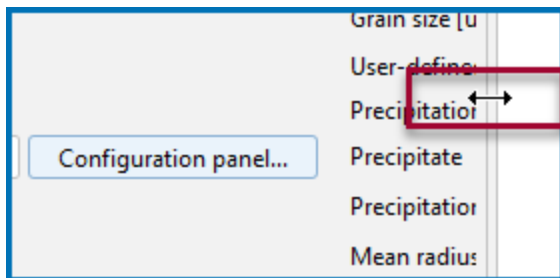
- Total yield strength
- Intrinsic strength
- Solid solution strengthening
- Solid solution strengthening FCC
- Solid solution strengthening BCC
- Solid solution strengthening HCP
- Grain boundary strengthening
- Total precipitation strengthening
- Precipitation strengthening per phase
- Constant strength addition

> 📈 The **P_01: Isothermal Precipitation of Al3Sc** example demonstrates the use of this Yield Strength Model.

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 micrograph.

> 📖   The stereological conversion is described in the theory for spherical particles. See "Stereology" on page 104.

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.

- **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.

Axis Variables

- **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.

- **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.

Non-Isothermal Simulations

When doing non-isothermal simulations it is common that particles grow in different generations. This results in multimodal size distributions. To correctly estimate the properties of these different generations of particles you need to separate the peaks of multimodal distributions.

Separate Multimodal PSD

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 checked for multimodal peaks. These are separated and used to calculate the specified property.

"P_06: Precipitation of γ' in Ni Superalloys - Non-isothermal" on page 148

It can be applied on the following plot properties:

- Mean radius

- Size distribution

- Number density

- Volume fraction

Points

This field is available when **Mean radius**, **Number density**, or **Volume fraction** is selected as the **Axis 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.

Time

This field is available when **Size distribution** or **Number density distribution** is selected as the **Axis 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" on page 173

For example, if you enter `100.0 1000.0 1.0E7` in the field:

When you click **Perform** the times are plotted:
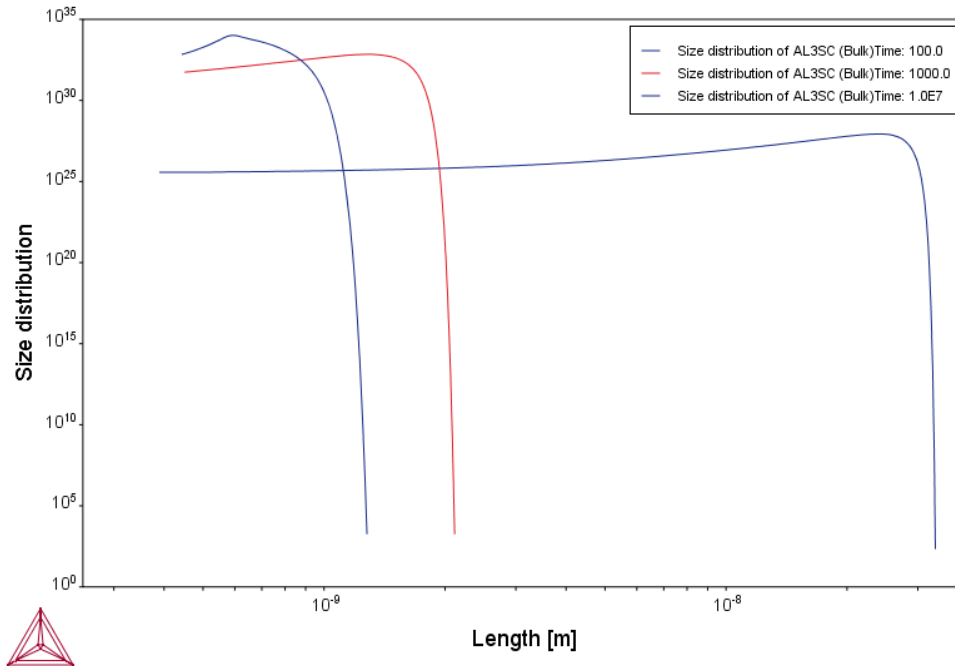
Excess Kurtosis

The **Excess kurtosis** number specifies the sensitivity when the program evaluates whether a curve is bimodal or not. The evaluation process calculates the excess kurtosis of the given size distribution and compares it with the input value. If the value is lower than the given value, the distribution is split. The excess kurtosis is a statistical measure that measures how *peaked* and *how heavy tail* a distribution has. For the definition used see [Wikipedia article](). The default is 25.0.

Minimum Separation Limit (Valley Depth Ratio)

The **Minimum separation limit** is a rough method to prevent that noise or wiggles are interpreted as different distributions. If a local minima is encountered above this value the following peak is not interpreted as a new distribution. The valley depth ratio is the ratio of the minimum separation limit to the peak value. The default is 0.01.

Minimum Peak

Any separated peak below the entered **Minimum peak** value is removed. The default is 100000.0.

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.

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.
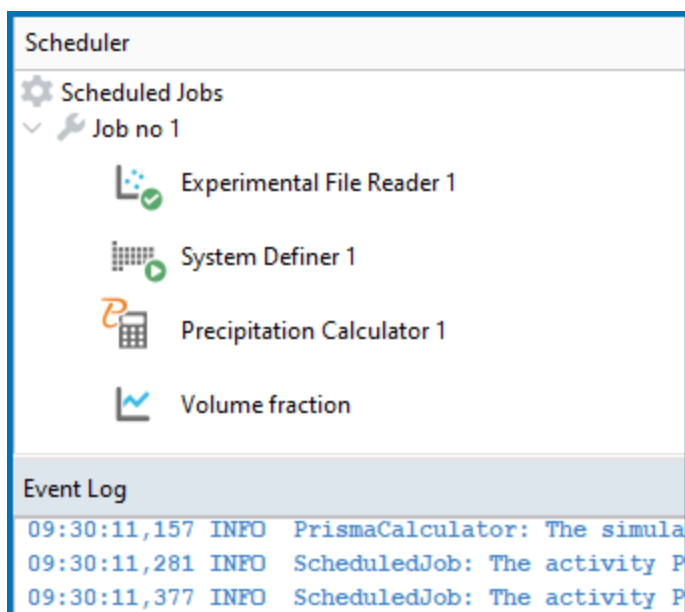
2. In the **Project** window, click the **Precipitation Calculator** node.

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**.
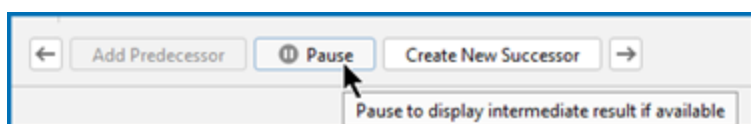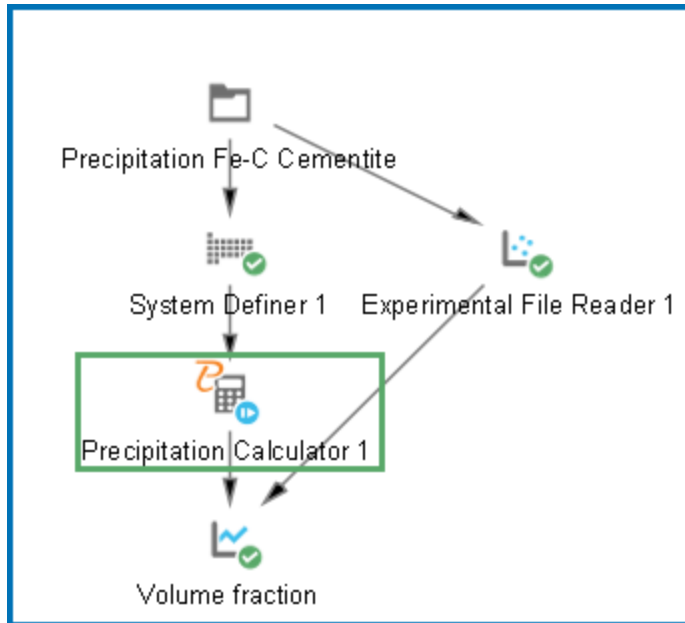
4. When pausing the calculation, you can make changes to a variety of settings under the *Matrix Phase* or *Precipitate Phase* sections (click **Show Details**), plus the **Interfacial energy**, **Temperature** (for non-isothermal calculations), and **Simulation time**. The rest of the **Configuration** 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).
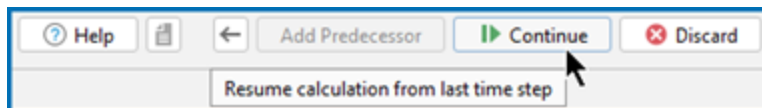
To Cancel a Job

- In the **Scheduler** window, right-click the job you want to cancel and select **Cancel Job**.
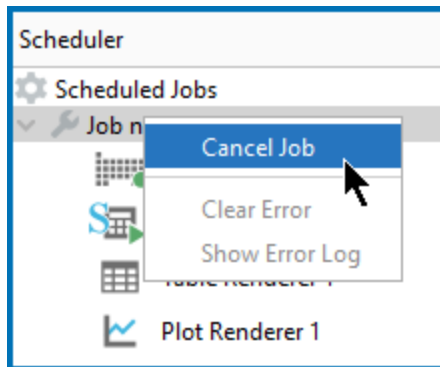
Theoretical Models and Numerical Methods

In this section:

Introduction to the Theory

Based on the theory from Langer-Schwartz [1980Lan] the Precipitation Module (TC-PRISMA) adopts Kampmann-Wagner numerical (KWN) [2013Wag] method to simulate the concomitant nucleation, growth, and coarsening of precipitates in multicomponent and multiphase alloy systems. The KWN method is an extension of the original Langer-Schwartz (LS) approach and its modified (MLS) form, where the temporal evolution of the mean radius and particle density over the whole course of precipitation are predicted by solving a set of rate equations derived with certain assumptions for the rates of nucleation and growth, as well as the function of particle size distribution (PSD). The MLS approach differs from the LS with respect to the Gibbs-Thomson equations used for calculating equilibrium solubilities of small particles. The former applies the exact exponential form, whereas the latter takes the convenient linearized version. Instead of assuming a PSD function *a priori* and working with rate equations for determining only mean radius and particle density, the KWN method extends the LS and MLS approaches by discretizing the PSD and solving the continuity equation of the PSD directly. Therefore, the time evolution of the PSD and its nth moment (*0*: number density; *1*st: mean radius; *3*rd: volume fraction) can be obtained altogether during the simulation. The key elements of the KWN method are the models for nucleation and growth under the mean field mass balance condition and the numerical algorithm for solving the continuity equation of the PSD. Coarsening comes out naturally without any *ad hoc* treatment.

The key elements of the KWN method and their relationship as implemented in the Precipitation Module (TC-PRISMA).
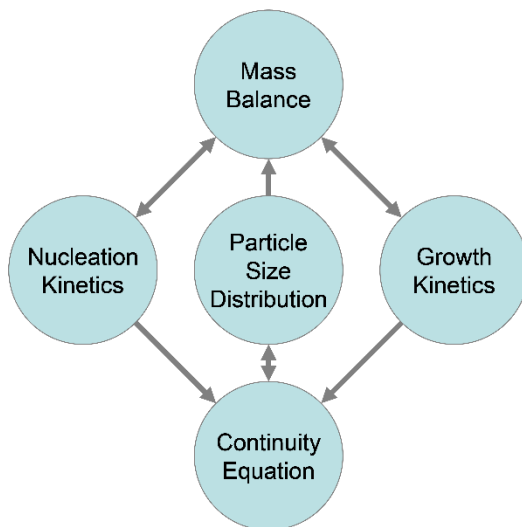
Integration of the Precipitation Module into Thermo-Calc

Precipitation Module (TC-PRISMA) is integrated with Thermo-Calc in order to directly get all necessary thermodynamic and kinetic information required in the KWN method. For industry relevant multicomponent alloys, thermodynamic and kinetic databases and calculation tools have to be used in order to obtain various quantities in the multicomponent models for nucleation and growth, such as the driving forces for the formation of embryos and their compositions, the atomic mobilities or diffusivities in the matrix, the operating interface compositions under local equilibrium conditions, the Gibbs-Thomson effect, and the deviation from local equilibrium due to interface friction etc. With Thermo-Calc and the Diffusion Module (DICTRA) as well as the accompanying databases, all these properties and effects can be calculated without unnecessary and inaccurate approximations.

In the following topics, various models and numerical methods implemented in Precipitation Module (TC-PRISMA) are introduced. Unless specified, spherical particles are assumed in the discussion.

References

[1980Lan] J. S. Langer, A. J. Schwartz, Kinetics of nucleation in near-critical fluids. Phys. Rev. A. 21, 948–958 (1980).

[2013Wag] R. Wagner, R. Kampmann, P. W. Voorhees, 'Homogeneous second phase precipitation', in Materials Science and Technology, R. W. Cahn, P. Haasen, E. J. Kramer, Eds. (Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany, 2013), pp. 213–304.

Nucleation Theory

Precipitation starts from the nucleation of clusters that can be considered as embryos of new phases with distinctive structures or compositions. In a perfect single crystal, nucleation happens homogeneously. In an imperfect crystal or polycrystalline materials, nucleation tends to occur heterogeneously due to the presence of dislocations, grain boundaries, grain edges, and grain corners. These imperfections or defects reduce the nucleation barrier and facilitate nucleation. However, if supersaturation or driving force is very large homogeneous nucleation is also possible since all sites including those inside a grain can be activated.

The following sections further elaborate on this theory.

- "Homogeneous Nucleation" on the next page
- "Heterogeneous Nucleation" on page 69
- "Nucleation During a Non-isothermal Process" on page 75

Homogeneous Nucleation

The classic nucleation theory (CNT) [2000, Kashchiev; 1980, Russell] has been extended for the purpose of modeling nucleation in multicomponent alloy systems. The time-dependent nucleation rate $J(t)$ is given by

$$J(t) = J_s exp\left(\frac{-\tau}{t}\right)$$

[Eq. 1]

where

- J_s is the steady state nucleation rate,

- τ is the incubation time for establishing steady state nucleation conditions, and

- t is the time.

The steady state nucleation rate J_s is expressed by

$$J_s = Z\beta^* N exp\left(\frac{-\Delta G^*}{kT}\right)$$

[Eq. 2]

where

- Z is the Zeldovich factor,

- β^* is the rate at which atoms or molecules are attached to the critical nucleus,

- N is the number of available nucleation sites (of a particular type) per unit volume. In the case of homogeneous nucleation, initially, each atom in the whole volume of the mother phase is a potential nucleation site. As precipitation proceeds, the number of available nucleation sites decreases due to the occupancy of part of the matrix volume by formed secondary phase particles. In the case of heterogeneous nucleation, the initial number can also be estimated, given the grain size or dislocation density in the matrix phase. It decreases also with time but at different rates.

- ΔG^* is the Gibbs energy of formation of a critical nucleus,

- k is Boltzmann's constant,

- T is absolute temperature.

The Gibbs energy of formation of a critical nucleus is expressed as

$$\Delta G^* = \frac{16\pi\sigma^3}{3\left(\Delta G_m^{\alpha\to\beta}/V_m^\beta\right)^2}$$

[Eq. 3]

where

- σ is the interfacial energy,

- $\Delta G_m^{\alpha\to\beta}$ is the molar Gibbs energy change for the formation of the β precipitate of the critical composition X_i^β from the α matrix, i.e. the maximum driving force for the $\alpha\to\beta$ phase transformation

- V_m^β is the molar volume of the β precipitate phase.

If elastic strain energy is excluded, $\Delta G_m^{\alpha\to\beta}$ is the chemical driving force for nucleation. There are two ways to calculate the nucleation driving force $\Delta G_m^{\alpha\to\beta}$ and the critical composition X_i^β, as shown in Figure 6 for a prototype binary system. The standard calculation in Figure 6 is to obtain the maximum driving force by finding the parallel tangent lines or surfaces passing through the alloy composition of the matrix, which is a routine calculation in the Thermo-Calc software. The approximate calculation in Figure 6 is performed by using the Gibbs energy difference corresponding to the equilibrium composition in the precipitate phase. It can be used when the standard calculation fails, mostly within a miscibility gap. Additionally, the standard calculation is also used for driving force under paraequilibrium conditions, while the approximate calculation is used for driving force under NPLE (Non-Partitioning Local Equilibrium) conditions.

(?) "Growth" on page 77
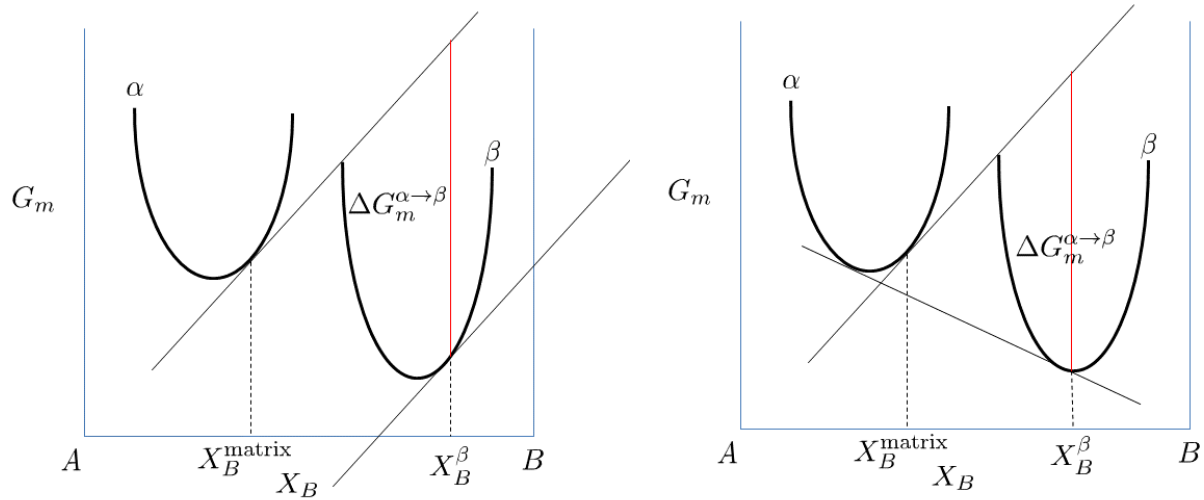
Figure 6: Methods to calculate the nucleation driving force $\Delta G_m^{\alpha \to \beta}$ and the critical composition X_i^{β}. The standard calculation (left) and an approximate calculation (right).

Nucleation is a stochastic process and can be considered formally as a diffusion process or Brownian movement in the particle size space. Supercritical nuclei with radius slightly larger than the critical radius have a probability of passing back across the free energy barrier and dissolve in the matrix. The Zeldovich factor (Z) is a measure of such probability and is related solely to the thermodynamics of the nucleation process in

[Eq. 4]
$$Z = \frac{V_m^{\beta}}{2\pi N_A r^{*2}} \sqrt{\frac{\sigma}{kt}}$$

where N_A is the Avogadro number and r^*, the critical radius, is given by

[Eq. 5]
$$r^* = -\frac{2\sigma V_m^{\beta}}{\Delta G_m^{\alpha \to \beta}}$$

The atomic or molecular attachment rate β^* reflects the kinetics of mass transport in the nucleation process and is given by Svoboda et al. [2004Svo].

[Eq. 6]
$$\beta^* = \frac{4\pi r^{*2}}{a^4} \left[\sum_{i=1}^{k} \frac{(X_i^{\beta/\alpha} - X_i^{\alpha/\beta})^2}{X_i^{\alpha/\beta} D_i} \right]^{-1}$$

where

- a is the lattice parameter,

- $X_i^{\beta/\alpha}$ and $X_i^{\alpha/\beta}$ are the mole fractions of element *i* at the interface in the precipitate and matrix, respectively.

- D_i is the corresponding diffusion coefficient in the matrix.

The incubation time τ for an isothermal reaction is

$$\tau = \frac{1}{\theta Z^2 \beta*}$$

[Eq. 7]

where θ differs from one derivation to another. The value 2 from Feder et al. [1966Fed] is adopted.

Elastic Strain Energy

Elastic strain energy, E_{el}, reduces the nucleation driving force, $\Delta G_m^{\alpha \to \beta}$ in Eq. 3, hence affecting nucleation rate and nuclei size. It also changes the shape of the particle by competing with interfacial energy.

Cuboid Particle

"Precipitation Morphology" on page 96

The numerical simulations by Onaka et al. [2003Ona] indicate that the elastic strain energy is reduced almost linearly with increasing cubic factor η. Since the numerical simulations are computationally expensive, we assume that the elastic strain energy follows the linear relationship with η, and the elastic strain energy for spherical ($\eta = 1$) and cubic ($\eta = \sqrt{2}$) are calculated based on Khachaturyan's approximation [1983/2008Kha].

$$E_{el} = \tfrac{1}{2}(c_{11} + 2c_{12})\epsilon_0^2 V[A_1 + A_2]$$

[Eq. 8]

where

- ϵ_0 is the lattice misfit strain,

- c_{11}, c_{12}, c_{44} are elastic constants in a cubic system,

- V is particle volume,

- A_1 and A_2 are expressed as

$$A_1 = 2\frac{c_{11}-c_{12}}{c_{11}} - 12\frac{c_{11}+2c_{12}}{c_{11}}\frac{c_{11}-c_{12}-2c_{44}}{c_{11}+c_{12}+2c_{44}}I_1$$

$$A_2 = -54 \frac{c_{11}+2c_{12}}{c_{11}} \frac{(c_{11}-c_{12}-2c_{44})^2}{(c_{11}+c_{12}+2c_{44})(c_{11}+2c_{12}+4c_{44})} I_2$$

with

Sphere

$$I_1 = \frac{1}{15} \qquad I_2 = \frac{1}{105}$$

Cubic

$$I_1 = 0.006931 \qquad I_2 = 0.000959$$

Ellipsoidal Particle (Plate and Needle)

(?)   "Precipitation Morphology" on page 96

Since they are ellipsoidal shape, it is convenient to use Eshelby's theory [1957/1959Esh] with a reasonable computational cost. The Eshelby's tensor can be calculated by simply performing a surface integral over a unit sphere

$$D_{ijkl} = -\frac{abc}{4\pi} \int_0^\pi \int_0^{2\pi} \Omega_{ij} n_k n_l \frac{\sin\theta}{\beta^3} d\phi d\theta$$

[Eq. 9]

where

- a, b, c are ellipsoid axes,

- $n_i (i = 1, 2, 3)$ are unit directional vector normal to the spherical surface and

$$\beta = \sqrt{(a^2 \cos^2 \phi + b^2 \sin^2 \phi) \sin^2 \theta + c^2 \cos^2 \theta}$$

For matrix phase with cubic crystal symmetry, we have for $\Omega_{ij}(i, j = 1, 2, 3)$. See [1983Kha].

$$\Omega_{ii}(\vec{n}) = \frac{c_{44}+(c_{11}-c_{44})(n_j^2+n_k^2)+\xi(c_{11}+c_{12})n_j^2 n_k^2}{c_{44}D(\vec{n})}$$

$$\Omega_{ij}(\vec{n}) = -\frac{(c_{12}+c_{44})(1+\xi n_k^2)}{c_{44}D(\vec{n})} n_i n_j$$

where

$$\xi = \frac{c_{11}-c_{12}-2c_{44}}{c_{44}}$$

$$D(\vec{n}) = c_{11} + \xi(c_{11}+c_{12})(n_1^2 n_2^2 + n_1^2 n_3^2 + n_2^2 n_3^2) + \xi^2(c_{11}+2c_{12}+c_{44})n_1^2 n_2^2 n_3^2$$

The Eshelby S tensor can then be calculated as

[Eq. 10] $$S_{ijmn} = -\tfrac{1}{2}C_{lkmn}\left(D_{iklj} + D_{jkli}\right)$$

The total strain ϵ_{ij} at each location inside the particle is related to its transformation strain (eigenstrain) ϵ_{ij}^* as

[Eq. 11] $$\epsilon_{ij} = S_{ijkl}\epsilon_{kl}^*$$

Combined with elastic stress calculated as

$$\sigma_{ij} = C_{ijkl}\left(\epsilon_{kl} - \epsilon_{kl}^*\right)$$

The elastic strain energy can be then obtained

[Eq. 12] $$E^{el} = -\tfrac{1}{2}\sigma_{ij}\epsilon_{ij}^* V$$

with V the particle volume.

Spherical Approximation for Nuclei

In the Precipitation Module, the user-input or calculated interfacial energy is assumed to be the coherent interfacial energy that applies to the habit plane, $\sigma_{\text{coh}}^{\text{sph}}$, consistent with the approximation made by the embedded interfacial energy model. When calculating the critical nuclei, the interfacial energy in Eq. 3 is assumed to be that of a spherical particle with constant specific interfacial energy $\sigma_{\text{coh}}^{\text{sph}}$. This is consistent with the fact that the nuclei tend to be spherical due to dominant interfacial energy. Interfacial energy penalty assuming a nucleus with pre-defined, and most likely large, aspect ratio is thus over-estimated, and has been found to shut down nucleation event abnormally.

Under spherical approximation, the elastic strain energy is calculated using spherical expression in Eq. 8 for spherical and cuboidal particles, or by setting $a = b = c$ in Eq. 9 for ellipsoidal particles.

References

[1957Esh] J. D. Eshelby, The Determination of the Elastic Field of an Ellipsoidal Inclusion, and Related Problems. Proc. R. Soc. A Math. Phys. Eng. Sci. 241, 376–396 (1957).

[1959Esh] J. D. Eshelby, The Elastic Field Outside an Ellipsoidal Inclusion. Proc. R. Soc. A Math. Phys. Eng. Sci. 252, 561–569 (1959).

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[1980Rus] K. C. Russell, Nucleation in solids: The induction and steady state effects. Adv. Colloid Interface Sci. 13, 205–318 (1980).

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[2003Ona] S. Onaka, N. Kobayashi, T. Fujii, M. Kato, Energy analysis with a superspherical shape approximation on the spherical to cubical shape transitions of coherent precipitates in cubic materials. Mater. Sci. Eng. A. 347, 42–49 (2003).

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Heterogeneous Nucleation

All equations remain the same for the calculation of heterogeneous nucleation rate within the framework of classic nucleation theory (CNT), but the nucleation energy and available nucleation site are different.

To a first approximation, the nucleation energy may be calculated by assuming an effective interfacial energy for each heterogeneous nucleation site.

For a rigorous treatment of heterogeneous nucleation the effect of wetting angles need to be considered.

Non-Spherical Particles and the Effect of Wetting Angle

? "Precipitation Module (TC-PRISMA) References" on page 111

Non-spherical particles have been considered for grain boundary (GB) precipitation. Three morphologies are implemented for grain boundary, grain edge and grain corner precipitation, respectively, as shown in Figure 7. The parameter that defines the deviation from spherical shape is wetting angle (or dihedral angle), θ, as described in Figure 8 and taken from Clemm and Fisher [1955Cle].

(a)   (b)   (c)
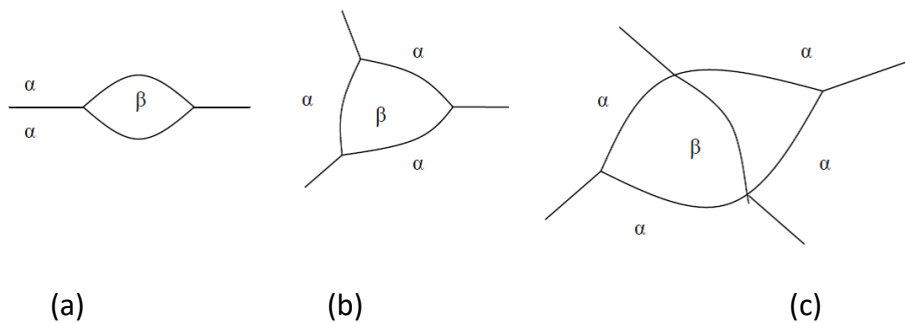
Figure 7: Non-spherical particles (β) that precipitate at grain boundaries of matrix phase(α) (a) grain boundary (two-grain junction) (b) grain edge (three-grain junction) (c) grain corners (four-grain junction). Images from [2004Zan].
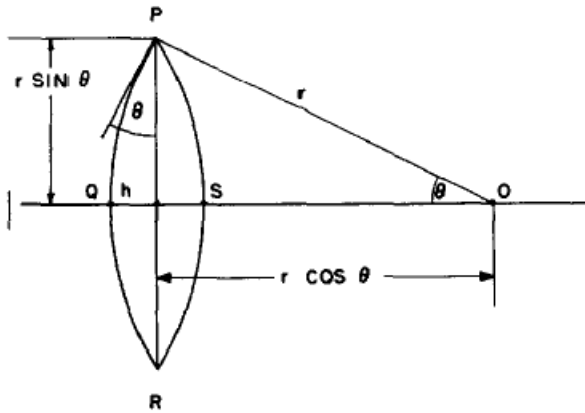
Figure 8: The nucleus at the grain boundary. Image from [1955Clem].

Some physical parameters, mainly in nucleation models, have to be modified for the effect of the wetting angle. The following discussions contribute to this effect.

Shape Factors

Following Clemm and Fisher, the eliminated grain boundary area between $\alpha - \alpha$ grains due to the formation of nucleus of a new phase β is:

[Eq. 1] $\quad A_{\alpha\alpha} = ar^2$

Where r is the radius of curvature of the nucleus. The surface area of the nucleus is:

[Eq. 2] $\quad A_{\alpha\beta} = br^2$

and the volume of the nucleus is

[Eq. 3] $\quad V = cr^3$

The expression of a, b, c in Eq. 1 and Eq. 3 for grain boundary (two-grain junction), grain edge (three-grain junction) and grain corner (four-grain junction) can be found in the paper by Clemm and Fisher [1955Cle].

Critical Radius and Activation Energy

The energy change due to the formation of the new particle is thus

[Eq. 4] $\quad \Delta F = \dfrac{\Delta G_m^{\alpha \to \beta}}{V_m} \cdot cr^3 + br^2 \sigma_{\alpha\beta} - ar^2 \sigma_{\alpha\alpha}$

where $\sigma_{\alpha\beta}$ and $\sigma_{\alpha\alpha}$ are the interfacial energy and grain boundary energy, respectively.

Then the critical radius should be

$$r^* = -\frac{2\left(b\sigma_{\alpha\beta} - a\sigma_{\alpha\alpha}\right)V_m}{3c\Delta G_m^{\alpha\to\beta}}$$

[Eq. 5]

And the activation energy barrier for nucleation is

$$W = \frac{4}{27}\frac{\left(b\sigma_{\alpha\beta} - a\sigma_{\alpha\alpha}\right)^3 V_m^2}{c^2\left(\Delta G_m^{\alpha\to\beta}\right)^2}$$

[Eq. 6]

The interfacial energy, grain boundary energy and wetting angle can be related as

$$k = \cos\theta = \frac{\sigma_{\alpha\alpha}}{2\sigma_{\alpha\beta}}$$

[Eq. 7]

i.e.

[Eq. 8] $$\sigma_{\alpha\alpha} = 2k\sigma_{\alpha\beta}$$

which can be replaced into Eq. 5 and Eq. 6.

$$r^* = -\frac{2\left(b - 2ak\right)\sigma_{\alpha\beta}V_m}{3c\Delta G_m^{\alpha\to\beta}}$$

[Eq. 9]

$$W = \frac{4}{27}\frac{\sigma_{\alpha\beta}^3 V_m^2}{\left(\Delta G_m^{\alpha\to\beta}\right)^2}\frac{\left(b - 2ak\right)^3}{c^2}$$

[Eq. 10]

The bulk, spherical precipitation equation is recovered by:

[Eq. 11] $$a = 0, \quad b = 4\pi, \quad c = \frac{4\pi}{3}$$

so that

$$r^* = -\frac{2\sigma_{\alpha\beta}V_m}{\Delta G_m^{\alpha\to\beta}}$$

[Eq. 12]

$$W = \frac{16\pi}{3}\frac{\sigma_{\alpha\beta}^3 V_m^2}{\left(\Delta G_m^{\alpha\to\beta}\right)^2}$$

[Eq. 13]

And also the grain boundary precipitation with spherical shape (with weighting angle $90°$) follows Eq. 12 and Eq. 13 by $k = \cos\theta = 0$.

Zeldovich Factor

The Zeldovich factor is modified as

[Eq. 14] $$Z = Z_b \sqrt{f}$$

with Z_b the original value, and f the volume factor that is the ratio of the c in Eq. 3 to the spherical shape factor $4\pi/3$.

[Eq. 15] $$f = \frac{3c}{4\pi}$$

Impingement Rate

The surface area factor in impingement rate calculation is changed from $4\pi(r^*)^2$ to $b(r^*)^2$.

Nucleation Site Density

In each time step, the occupied grain boundary area

[Eq. 16] $$A_{\text{red}} = a \cdot nr^2$$

is deducted when calculating available nucleation site density.

Growth Rate

The radius r defined in previous equations is the curvature of the precipitate surface (the Big radius) as shown in Figure 8. It is exactly the definition in the growth rate whose coarsening consideration relates to the curvature effect. Therefore, the growth rate equation can be directly used with r being defined here. Again, for bulk, spherical precipitation it automatically corresponds to the particle radius.

Output

The volume of the precipitate should be calculated appropriately as cr^3 with r being the curvature of the particle surface as defined above. For output of the particle size (mean radius, critical radius and particle size distribution) in the user interface, it seems better to use the radius of the eliminated grain boundary area, i.e.

$$r' = \sqrt{\frac{a}{\pi}} \cdot r$$

[Eq. 17]

With a defined in Eq. 1.

For example, the size of the precipitate at grain boundary (two-grain junction) is the radius of the lens shown in Figure 8.

$$r' = r\sin\theta = r\sqrt{1-k^2}$$

The Number of Available Heterogeneous Nucleation Sites
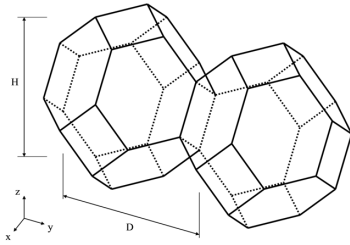
Figure 9: An example of tetrakaidecahedron approximation of grains.

The number of different nucleation sites is dependent on the shape and size of grains in the matrix. Assuming all grains are equally large tetrakaidecahedra with the distance between one pair of square faces as H, and that between the other two pairs as D we obtain the densities ρ_2, ρ_1, and ρ_0 for the grain boundary area, edge length, and grain corner number, respectively in

$$\rho_2 = \frac{6\sqrt{1+2A^2}+1+2A}{4A}D^{-1}$$

[Eq. 18]

$$\rho_1 = 2\frac{\sqrt{2}+2\sqrt{1+A^2}}{A}D^{-2}$$

[Eq. 19]

$$\rho_0 = \frac{12}{A}D^{-3}$$

[Eq. 20]

where $A = H/D$ is the aspect ratio, defining the degree of elongation of the grains.

By default, the aspect ratio is set to 1 and the densities are then the same as obtained by Cahn [1956Cah]. Once the densities are known, if taking boundary thickness as one atomic layer, the available nucleation sites can be calculated by

$$N_i = \rho_i \left(\frac{N_A}{V_m^\alpha} \right)^{i/3} \quad i = 2, 1, 0$$

[Eq. 21]

where V_m^α is the molar volume of the matrix phase and N_A is the Avogadro number.

For a crystalline material, given a dislocation density ρ_d, the number of nucleation sites at the dislocations N_d can be calculated with the same form as in

$$N_d = \rho_d \left(\frac{N_A}{V_m^\alpha} \right)^{1/3}$$

[Eq. 22]

References

[1955Cle] P. J. Clemm, J. C. Fisher, The influence of grain boundaries on the nucleation of secondary phases. Acta Metall. 3, 70–73 (1955).

[1956Cah] J. W. Cahn, Transformation kinetics during continuous cooling. Acta Metall. 4, 572–575 (1956).

[2004Zan] L. Zang, Lecture 13: Heterogeneous Nucleation: Effects of Grain Boundaries and Surface Defects, The University of Utah, (2004), (available at http://www.eng.utah.edu/%7B$~$%7Dlzang/images/lecture-13.pdf).

Nucleation During a Non-isothermal Process

Under non-isothermal conditions, temperature dependency of key parameters such as nucleation driving force, solute diffusivities and solute concentrations, etc., have been taken into account, and are updated automatically during a simulation.

Another important parameter that depends on thermal history is the incubation time, defined by

$$\tau = \frac{1}{\theta Z^2 \beta^*}$$

[Eq. 1]

for an isothermal condition. In a non-isothermal process, the exact calculation of the incubation time requires a solution to the Fokker-Planck equation. In the Precipitation Module, an approximation approach has been employed to deal with the transient nucleation, which gives the incubation time as an integral form of past thermal history [2004Jou] as in

$$\int_o^{\tau} \beta^*(t')dt' = \frac{1}{\theta Z^2(\tau)}$$

[Eq. 2]

where

τ is the incubation time, β^* is the impingement rate for solute atoms to the critical cluster as defined in

$$\beta^* = \frac{4\pi r^{*2}}{a^4}\left[\sum_{i=1}^{k}\frac{\left(X_i^{\beta/\alpha} - X_i^{\alpha/\beta}\right)^2}{X_i^{\alpha/\beta}D_i}\right]^{-1}$$

[Eq. 3]

and Z is the Zeldovich factor, previously defined in

$$Z = \frac{V_m^{\beta}}{2\pi N_A r^{*2}}\sqrt{\frac{\sigma}{kT}}$$

[Eq. 4]

but now as a function of τ derived from temperature change.

The starting point of the integral $t' = 0$ is either the starting time if there is an initial nucleation driving force, or the latest time when the nucleation driving force is vanished.

Reference

[2004Jou] H.-J. Jou, P. Voorhees, G. B. Olson, Computer simulations for the prediction of microstructure/property variation in aeroturbine disks. Superalloys, 877–886 (2004).

Growth

Spherical Particles

The growth rate models implemented in the Precipitation Module are called **Advanced**, **Simplified**, **General**, **Para-eq**, **NPLE**, and **PE Automatic**. All models treat a spherical particle (precipitate) of stoichiometric composition or with negligible atomic diffusivity.

> 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*.

Advanced Growth Rate Model

The *Advanced* model is proposed by Chen, Jeppsson, and Ågren (CJA) [2008Che]. In this 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.

According to the CJA model, the interface velocity v can be obtained together with interface concentrations by numerically solving $2n - 1$ equations, comprising of the flux balance equations for $n - 1$ independent components and the local equilibrium conditions for all n components as in

[Eq. 1]
$$v(c_i^{\beta/\alpha} - c_i^{\alpha/\beta}) = c_i^{\alpha/\beta} M_i \frac{\mu_i^\alpha - \mu_i^{\alpha/\beta}}{\xi_i r}$$

[Eq. 2]
$$\mu_i^{\alpha/\beta} = \mu_i^{\beta/\alpha} + \frac{2\sigma V_m^\beta}{r}$$

where

- $c_i^{\beta/\alpha}$ and $c_i^{\alpha/\beta}$ are the volume concentrations of component i at the interface in the precipitate and matrix, respectively,

- M_i is the corresponding atomic mobility in the matrix,

- μ_i^{α} and $\mu_i^{\alpha/\beta}$ are the chemical potentials in the matrix of the mean-field concentration and at the interface, respectively.

- $\mu_i^{\beta/\alpha}$ is the chemical potential at the interface in the precipitate.

In the above local equilibrium condition, the multicomponent Gibbs-Thomson effect has been taken into account by adding a curvature induced pressure term to the Gibbs energy of the precipitate phase.

The introduced effective diffusion distance factor, ξ_i, for each independent component is given by

$$\xi_i = \frac{\Omega_i}{2\lambda_i^2}$$

[Eq. 3]

where

$$\Omega_i = \frac{c_i^{\alpha} - c_i^{\alpha/\beta}}{c_i^{\beta/\alpha} - c_i^{\alpha/\beta}}$$

is the so-called dimensionless supersaturation for an individual component, and λ_i is obtained via

[Eq. 4] $$2\lambda_i^2 - 2\lambda_i^3\sqrt{\pi}\exp\left(\lambda_i^2\right)\mathrm{erfc}(\lambda_i) = \Omega_i$$

Simplified Growth Rate Model

In some cases, the **Advanced** model fails to find the solution to flux-balance equations. Even when it does, the calculation can be time consuming. Therefore, a simple and efficient, albeit less rigorous, model is preferred in many applications. The **Simplified** model [2022Ågr], in a pseudo-steady state approximation, is developed by solving Laplace equation along radial direction, and is expressed as

[Eq. 5] $$v = \frac{K}{r}\left[\Delta G_m - \frac{2\sigma V_m^{\beta}}{r}\right] = \frac{2\sigma V_m^{\beta}K}{r}\left[\frac{1}{r^*} - \frac{1}{r}\right]$$

where ΔG_m is the nucleation driving force and r^* is the radius of critical nuclei. K is the kinetic parameter that is related to solute composition and mobility. Neglecting cross diffusion, it is expressed as

$$K = K_{\text{sphere}}^{\text{simplified}} = \left[\sum_i \frac{\left(X_i^{\beta/\alpha}(r) - X_i^{\alpha/\beta}(r) \right)^2 \xi_i}{X_i^{\alpha/\beta}(r) M_i} \right]^{-1}$$

[Eq. 6]

The interface compositions (mole fractions) $X_i^{\beta/\alpha}(r)$ and $X_i^{\alpha/\beta}(r)$ for precipitate and matrix phase, respectively, are tie-line compositions across the matrix composition. To avoid time-consuming equilibrium calculations and also realizing that precipitate composition $X_i^{\beta/\alpha}(r)$ only appears in the difference term

$$\left(X_i^{\beta/\alpha}(r) - X_i^{\alpha/\beta}(r) \right)$$

Equation 6 is further simplified by replacing $X_i^{\beta/\alpha}(r)$ with nuclei composition from nucleation driving force calculation, and $X_i^{\alpha/\beta}(r)$ with matrix composition.

> The K constant defined here relates growth rate to driving force in $v = \frac{K}{r} \left[\Delta G_m - \frac{2\sigma V_m^\beta}{r} \right]$, which is not to be confused with coarsening rate constant relating mean particle radius cubed to time.

For the *Precipitation Calculator → Precipitate Phase* settings, **Phase energy addition** G_m^a and **Phase boundary mobility** M^B shifts the Gibbs energy of the precipitate β phase by $G_m^a + vV_m^\beta/M^B$. As a result, the driving force ΔG_m is reduced by $G_m^a + vV_m^\beta/M^B$, and the equilibrium compositions $c_i^{\beta e}$ and $c_i^{\alpha e}$ are shifted.
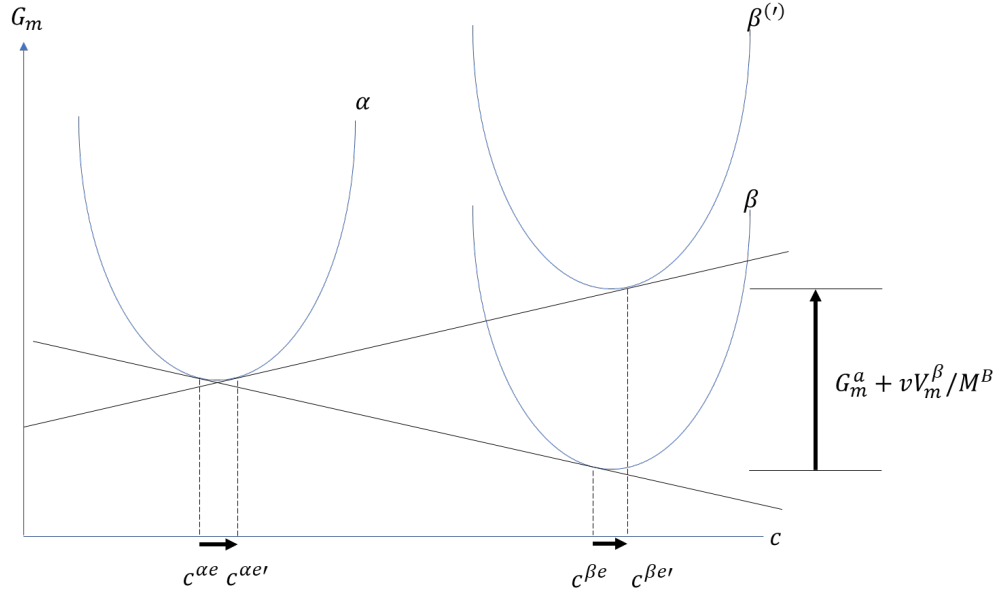
Figure 10: Effects of "Phase energy addition" G_m^a and "Phase boundary mobility" M^B .

General Growth Rate Model

The **General** model is based on the existing coarsening models [1993Uma; 1994Mor; 1995Mor], which follows the same quasi-steady state approximation as the **Simplified** model, but improves by taking into account the cross diffusion. The growth rate equation has thus the same format as that in the Simplified model, i.e., Eq. 5, with the kinetic parameter K defined as

[Eq. 7]
$$K = K_{\text{sphere}}^{\text{general}} = \frac{1}{(\Delta X^{\alpha\beta}][\ddot{G}][D]^{-1}[\Delta X^{\alpha\beta})}$$

where $(\Delta X^{\alpha\beta}]$ and $[\Delta X^{\alpha\beta})$ are $n-1$ row and column vector, respectively, whose ith element is the composition difference $\left(X_i^{\beta/\alpha}(r) - X_i^{\alpha/\beta}(r)\right)$ as described in Eq. 6. $[\ddot{G}]$, a $(n-1) \times (n-1)$ matrix, is based on thermodynamic factor matrix $[G^\alpha]$ with a correction factor

[Eq. 8] $$[\ddot{G}] = f[G^\alpha]$$

where thermodynamic factor matrix is defined as the secondary derivative of free energy with respect to composition in the matrix phase

$$[G^\alpha]_{ij} = \frac{\partial^2 G_m^\alpha}{\partial X_i^\alpha \partial X_j^\alpha}$$

$[G^\alpha]$ is evaluated at the far-field matrix composition to consider the multicomponent Gibbs-Thomson effect [1995Mor]. For a particle with critical nuclei size r^*, the Gibbs-Thomson equation is

[Eq. 9] $(\Delta X^{\alpha\beta}][G^\alpha][\Delta X^\alpha) \approx \frac{2\sigma V_m}{r^*} = \Delta G_m$

where $[\Delta X^\alpha)$ is a $n-1$ column vector representing the difference between the far-field matrix composition $[X^\alpha)$ and the equilibrium (tie-line) composition of the matrix phase $[X^{\alpha/\beta})$. It has been found that Eq. 9 is not numerically accurate and sometimes the deviation can be quite significant. Therefore, a correction factor is introduced as

$f = \frac{\Delta G_m}{(\Delta X^{\alpha\beta}][G^\alpha][\Delta X^\alpha)}$

which then appears in Eq. 8.

$[D]^{-1}$ in Eq. 7 is the inverse of the chemical diffusivity matrix $[D]$. In some alloy systems, diffusivity is strongly composition dependent, so that an effective diffusivity is necessary. A series of numerical simulations in comparison with DICTRA calculations indicates that a good approximation can be achieved if $[D]$ is the arithmetic mean of the diffusivity with far-field matrix composition and diffusivity with equilibrium (tie-line) composition

$[D] = \frac{1}{2}\left\{[D]_{(X^\alpha)} + [D]_{(X^{\alpha/\beta})}\right\}$

Paraequilibrium Growth Rate Model

> The paraequilbrium (**Para-eq**) growth rate model is only available for alloy systems where Fe is the major element and C is the only interstitial element, which also partitions into the precipitate phase.

The intersitial elements, e.g. C, N, etc., usually have remarkably faster diffusion rate than the substitutional elements. Meanwhile, they are assumed to have negligible volume contribution, and as a result the composition variables in Eq. 6 to Eq. 9 are replaced by *u*-fractions when interstitial elements are included in the system. The paraequilbrium growth rate model is designed specifically to address the fast diffusion of C in Fe alloys. Based on the *Simplified growth rate model*, it holds a paraequilbrium condition [1953Hil] at the migrating interface, in that, instead of assuming that all alloying elements are in equilibrium at the interface as the regular ortho-equilibrium condition states, only C assumes equilibrium state, while the substitutional elements are immobile and thus have the same compositions (*u*-fractions) across the interface. Therefore, only composition of C and its mobility appear in Eq. 6.

PE Automatic Growth Rate Model

The tempering of martensite in steels induces the precipitation of cementite particles. The growth kinetics initially follows the paraequilbrium (abbreviated here as PE) condition due to the fast diffusion of interstitial C, and gradually transforms to regular Local Equilibrium (LE), i.e. Ortho-equilibrium (OE), condition so that substitutional elements can reach equilibrium partitioning at the migrating interface. The **PE Automatic** model enables the smooth transition from *Paraequilibrium growth rate model* to *Simplified growth rate model*. The rate of transition process is dependent on the relative differences in diffusion between C and substitutional elements, as well as the differences in driving force between PE and OE.

NPLE Growth Rate Model

> The Non-Partitioning Local Equilibrium (NPLE) growth rate model is only available for alloy systems where Fe is the major element and at least one interstitial element partitions into the precipitate phase.

The **NPLE** growth model is designed specially to deal with the fast diffusion of interstitial element (C, N, etc.) in Fe alloys. Based on the *Simplified* growth model, it still holds a local equilibrium condition at the migrating interface, but chooses a tie-line under NPLE condition [1958Kir] that the *u*-fractions of all substitutional elements and minor interstitial elements in the precipitate phase are the same as those in the far-field matrix phase (i.e. the overall instantaneous matrix composition).

Model Selections

The most efficient model is the **Simplified** model, which is the default and applicable to most alloy systems under conditions that either the supersaturation is small, or the alloying elements have comparable diffusivity. If all alloying elements are substitutional but they have remarkable diffusivity difference, e.g. in Al-Zr system, or the diffusivity is strongly composition dependent, the **General** model is preferred. If the supersaturation is high, and meanwhile there are fast-diffusing interstitial elements such as C, the **Advanced** model is more appropriate to capture the NPLE mechanism.

> In some cases with the **General** model, you may need to switch to another model if the matrix composition passes through a spinodal composition space where the thermodynamic factor becomes negative, thus leading to an abnormal growth rate. When this happens, Thermo-Calc alerts you that the *Matrix Composition in Spinodal Zone*. It is then recommended to switch to other models.

Non-Zero Volume Correction

The non-zero volume correction to the velocity according to Chen and Voorhees [1993Che] is taken into account and it follows as

[Eq. 10]
$$v' = v\left(1 + r\sqrt{4\pi N_V \langle r \rangle}\right)$$

where

- v' is the corrected velocity
- $\langle r \rangle$ is the mean radius
- N_V is the number density

Non-Spherical Particles

> A reference for this section can be found in [2018Wu].

Particle Shape Determination

The shape of the cuboid particles, the cubic factor, is determined by the minimization of combined interfacial energy and elastic strain energy. If you choose **Calculated from molar volume** for the **Transformation strain** as the *Precipitation Calculator → Precipitate Phase* settings, the lattice misfit is then calculated from difference in molar volume between matrix and precipitate phase, and the elastic strain energy is calculated accordingly. If you disregard the transformation strain, the elastic strain energy is neglected and hence the particles remain spherical in shape.

If you select the **Calculated aspect ratio from elastic energy** checkbox for either a plate or needle **Morphology** on the *Precipitation Calculator → Precipitate Phase* settings, the particle

shape is determined by the minimization of combined interfacial energy and elastic strain energy. Otherwise, if you enter a value for aspect ratio, the particle shape is fixed except for nucleation calculation in which a spherical particle is always assumed.

Interfacial Energy Anisotropy

Isotropic interfacial energy is always assumed for spherical and cuboidal particles. For plate and needle, when the aspect ratio becomes larger than 1, the interfacial energy anisotropy occurs, so that the interfacial energy at the edge is larger than that at the broad face (habit plane). This increases the overall interfacial energy which is given as follows for each morphology.

Plate

$$E_{\text{int}} = 4\pi\sqrt[3]{\alpha^2}\sigma_0^{\text{sph}}r^2$$

Needle

$$E_{\text{int}} = 4\pi\sqrt[3]{\alpha}\sigma_0^{\text{sph}}r^2$$

Where

- α is the aspect ratio
- σ_0^{sph} is the interfacial energy of the habit plane, i.e., the plane normal to the shorter axis
- r is the radius of a sphere with equivalent volume

Growth Rate Adjustment

For non-spherical particles, the growth rate equations for spherical particles are still applicable, but adjustment parameters are introduced to take into account the shape effect. The cuboid particles arise from "symmetry preserving" transformation, e.g., FCC_A1 to L1$_2$, and are thus highly isotropic and assumed growth rate equal to that of spherical particles. The plate and needle particles, on the other hand, arise from "symmetry breaking" transformations, e.g., cubic to tetragonal transformation, and are thus anisotropic leading to a significant increase of growth rate.

We define r as the radius of a sphere with equivalent volume of the non-spherical particle, so that the format of Eq. 5 keeps unchanged. In our current model, two effects are considered contributing to the growth rate for plate and needle particles, from interfacial energy anisotropy and particle shape effect. The kinetic parameter K defined in Eq. 5 is thus given as

[Eq. 11] $\qquad K = K_\sigma \cdot K_{\text{shp}} \cdot K_{\text{sphere}}$

with K_{sphere} defined in Eq. 6 and Eq. 7. The interfacial energy σ in Eq. 5 is that of habit plane, i.e., the plane that is normal to the shorter axis of the particle. K_σ is the parameter that takes into account the Gibbs-Thomson effect due to interfacial energy anisotropy, based on Johnson [1965Joh].

Plate

$$K_\sigma = \sqrt[3]{\alpha^2}$$

Needle

$$K_\sigma = \sqrt[3]{\alpha}$$

where α is the aspect ratio of the ellipsoidal particle. K_{shp} is the parameter that takes into account the non-spherical concentration field around the particle. Assuming a shape-conserving concentration field and thus following the derivation by Ham [1958 and 1959], it is given as

Plate

$$K_{\text{shp}} = \frac{e\sqrt[3]{\alpha}}{\arccos(0) - \arccos(e)}$$

Needle

$$K_{\text{shp}} = \frac{2\sqrt[3]{\alpha^2}e}{\ln(1+e) - \ln(1-e)}$$

where e is the eccentricity of the ellipsoidal particle.

$$e = \sqrt{1 - \frac{1}{\alpha^2}}$$

References

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Coarsening

Physically speaking, coarsening or Ostwald ripening where big particles grow and small particles shrink is a process driven by lowering the total surface energy of the system. From a thermodynamic point of view, the Gibbs-Thomson effect leads to inhomogeneous chemical potentials in the system if the particle sizes are not uniform. Solutes at the interface in the matrix near a particle of a radius smaller than critical radius have a higher chemical potential than that corresponding to the mean concentration of the matrix. As a result, the solutes diffuse from the precipitate/matrix interface to the inside of the matrix and cause dissolution of the particle. Conversely, particles with a radius larger than the critical size have lower interface potentials, and the solutes diffuse to the interface and cause growth of the particles.

Since it is not possible to find a closed form analytic solution for the problem of diffusion-controlled spherical particle dissolution [1970Aar], we simply apply the Growth equations 1 to 5 with the absolute value of Ω_i to calculate the interface velocity for particles of all sizes.

As can be easily seen, if $r < r^*$, then the Gibbs-Thomson Equation 1 gives $\mu_i^{\alpha/\beta} > \mu_i^\alpha$, and a negative velocity results from Equation 2 for particles having $r < r^*$, which means that they shrink.

Results for particles having $r > r^*$ are obtained vice versa. In all situations, when the absolute values of Ω_i are very small, the steady-state solution for either growth or dissolution are recovered. In conclusion, the dissolution is treated as the reverse of growth (1970Aar, Ibid.), and the coarsening comes out naturally either together with nucleation and growth or as a dominant process finally in the course of the evolution of the PSD.

Reference

[1970Aar] H. B. Aaron, Diffusion-Limited Phase Transformations: A Comparison and Critical Evaluation of the Mathematical Approximations. J. Appl. Phys. 41, 4404 (1970).

Continuity Equation

Let $f(r)$ be the PSD of a precipitate phase, N the number of particles per unit volume, $\langle r \rangle$ the mean radius and ϕ the particle volume fraction, is expressed as

[Eq. 1] $N = \int_0^\infty f(x)dr$

[Eq. 2] $\langle r \rangle = \int_0^\infty rf(r)dr$

[Eq. 3] $\phi = \int_0^\infty \left(\frac{4\pi}{3}\right)r^3 f(r)dr$

The time evolution of $f(r)$ follows the continuity as in Langer and Schwartz [1980Lan].

[Eq. 4] $\frac{\partial f}{\partial t} = -\frac{\partial}{\partial r}[v(r)f(r)] + j(r)$

Where $v(r)$ is the growth rate of a particle of size r, and $j(r)$ is the distributed nucleation rate, which is defined by

[Eq. 5] $J = \int_{r*}^\infty j(r)dr$

where J is the nucleation rate.

Reference

[1980Lan] J. S. Langer, A. J. Schwartz, Kinetics of nucleation in near-critical fluids. Phys. Rev. A. 21, 948–958 (1980).

Mass Conservation

The matrix concentration is updated at each time step according to the law of mass conservation. If the alloy concentration, i.e. initial mole fraction of component i in the matrix phase is X_i^0, the new concentration X_i can be obtained from the following mass balance shown in

$$X_i^0 = \left(1 - \sum_p \int_0^\infty \frac{4\pi r_p^3 f(r_p)}{3V_m^p} dr_p\right) X_i + \sum_p \int_0^\infty \int_0^{t_j} \frac{4\pi r_p^2 f(r_p,t)v(r_p,t)}{V_m^p} X_i^p(r_p,t) dt dr_p$$

where

- $X_i^p(r_p,t)$ is the mole fraction of element i at the interface in the precipitate phase p of particle size r_p at time t. $f(r_p,t)$, $v(r_p,t)$ and V_m^p are the PSD function, growth rate, and molar volume of the precipitate phase p, respectively.

- t_j is the time at time step j.

Apparently, the new matrix concentration, and thus the updated supersaturation, nucleation rate, and interface velocity are all functions of the PSD function. This inevitably leads to the complex non-linear behavior of and great difficulty in solving the continuity equation.

Numerical Method

Since it is impossible to have a general close form solution, the complex non-linear continuity equation (see "Continuity Equation" on page 88) of the particle size distribution (PSD) function has to be solved numerically. Different numerical methods can be found in the literature to solve this equation, such as finite difference and method of characteristics. In all approaches, the continuous PSD is discretized into a sufficiently large number of size classes, and then integrated discretely in the time space. The Precipitation Module utilizes the method of characteristics, where the number of particles in each size class is kept constant unless particles of the same size have been nucleated.

An adaptive geometric grid allocation method has been used for particle size discretization since from nucleation to coarsening the particle size can span several orders of magnitude. In this approach, the new size grids are allocated evenly in a logarithmic scale and the number of grid points over one order of magnitude is kept almost constant during the whole process by class merging and splitting. The time step is controlled by several adjustable numerical parameters based on mechanistic quantities.

Summarized below are all numerical parameters used in this approach to control either the size grid distribution or time steps.

Maximum Time Step Fraction

$$P_{dt}^{max}$$

Maximum time step allowed for time integration as fraction of the simulation time.

Number of Grid Points Over One Order of Magnitude in r

$$P_{Nr}$$

Default number of grid points for every order of magnitude in size space. The number determines a default ratio between two adjacent grid points. When there is a need to create new grid points, such as nucleating at a new radius not covered by the current range of PSD, this default ratio is used to add these new radius grid points. A larger value of this parameter enforces a finer grid to allow better numerical accuracy. However, this also comes with performance penalty, since finer grid in the size space often requires smaller time step to resolve the calculations.

Maximum Number of Grid Points Over One Order of Magnitude in r

$$P_{Nr}^{max}$$

The maximum allowed number of grid points in size space. This parameter determines a lower bound limitation for the ratio of every two next nearest grid points in order to maintain adequate computational efficiency. When a ratio of two next nearest grid points is less than this limit, the middle grid point is removed and the corresponding size class merged with the two neighboring ones.

Minimum Number of Grid Points Over One Order of Magnitude in r

$$P_{Nr}^{min}$$

The minimum allowed number of grid points in size space. This parameter determines an upper bound limitation for the ratio of every two adjacent grid points in order to maintain proper numerical accuracy. When a ratio of two adjacent grid points exceeds this limit, a new grid point is then inserted between the two adjacent grids to keep the required resolution.

Maximum Relative Radius Change

$$P_r$$

The maximum value allowed for relative radius change in one time step. This parameter limits the time step according to the following relation, which is controlled by the particle growth:

$$\Delta t \leq P_r \times r/(|dr/dt|) \text{ for } r > r_{dt}$$

where r_{dt} is a cut-off subcritical size defined by the next parameter. The growth rates of supercritical particles (with $r > r_c$) are always bounded, and there is a size class and the corresponding growth rate that controls the time step. The subcritical particles (with $r < r_c$), however, has a mathematical singularity (negative infinity) in growth rate as r approaches 0. This means that the time step can become extremely small if applying the above criterion to very small subcritical particles. In open literature, several researchers have tried mathematical transformation to avoid this singularity. Unfortunately, the transformation also complicates the formulation of the models. The Precipitation Module implementation uses a simple approach to deal with this issue by defining a cut-off size r_{dt}. All the particles with $r < r_{dt}$ may disappear within one time step. is determined by the next input parameter.

Maximum Relative Volume Fraction of Subcritical Particles Allowed to Dissolve in One Time Step

$$P_{rdt}$$

This parameter represents the portion of the volume fraction that can be ignored when determining the time step. It is used to calculate the cut-off subcritical size, r_{dt}, for the above time step control that allows a maximum relative radius changes for all particles:

$$(\int_0^{r_{dt}} fr^3 dr)/(\int_0^\infty fr^3 dr) = P_{rdt}$$

Relative Radius Change for Avoiding Class Collision

$$P_{cc}$$

For the supercritical particles, the growth rate is non-linear – usually, it first increases with r and then decreases after a certain size. In the region(s) with growth rate decreasing with r, it is possible that the smaller size grid point can catch up with the larger size grid, if the time step is not controlled. To prevent this from happening, an additional parameter, P_{cc}, can be used to set a limit on time step according to the following relation:

$$\Delta t \le P_{cc} \times (r_{i+1} - r_i)/(dr_i/dt - dr_{i+1}/dt)$$

for

$$r_{i+1} > r_{i+1}$$

and

$$dr_{i+1}/dt < dr_i/dt$$

Maximum Overall Volume Change

$$P_\nu$$

This parameter defines the maximum absolute (not ratio) change of the volume fraction allowed during one time step. This parameter is also used in controlling allowable variation in volume fraction due to the newly created particles within one time step. That is

$$\Delta t \le P_V/10/(4\pi r_{eff}^3 J/3)$$

where r_{eff} and J are effective radius and nucleation rate, respectively.

Maximum Relative Change of Nucleation Rate in Logarithmic Scale

P_{logJ}

This parameter ensures accuracy for the evolution of effective nucleation rate. It sets a limit on time step so that the relative change of nucleation rate does not exceed the specified value, based on the information of previous step. That is

$$\Delta t \le P_{logJ} \times \Delta t_{previous}/(|log(J_1/J_2)|)$$

where nucleation rate J_1 and J_2 occurs at the beginning and end of $\Delta t_{previous}$.

Maximum Relative Change of Critical Radius

P_{rc}

During the nucleation under high supersaturation, the critical radius can vary dramatically. Hence, this parameter can be used to place a constraint on how fast the critical radium can vary, and thus put a limit on time step:

$$\Delta t \le P_{rc} \times \Delta t_{previous}/(|r_{c1} - r_{c2}/r_{rc1}|)$$

Minimum Radius for a Nucleus to be Considered as a Particle

P_{rmin}

The cut-off lower limit of precipitate radius. Particles with radius smaller than the value specified for this parameter are discarded. In reality, the particle cannot be smaller than an atom; hence, there is no reason to keep track of particles of unphysical sizes.

Maximum Time Step During Heating Stages

P_{htmax}

The upper limit of the time step that has been enforced in the heating stages. The current algorithm may over-estimate the subsequent time increment when temperature is increased. It is thus required to reduce this value when the calculation terminates unexpectedly during or after a heating stage.

Numerical Control Parameters Default Values

Default value for numerical parameters that controls the size grid distribution and time step.

Parameter	Default value
P_{dt}^{max}	0.1
P_{Nr}	200
P_{Nr}^{max}	300
P_{Nr}^{min}	100
P_r	0.01
P_{rdt}	0.01
P_{cc}	0.5
P_ν	0.001
P_{logJ}	0.5
P_{rc}	0.1
P_{rmin}	5e-10m
P_{htmax}	1.0s

Estimation of Coherent Interfacial Energy

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).

Precipitation Morphology

As the spherical particle is the default morphology, for precipitations within the grain, three non-spherical shapes are considered: *cuboid*, *plate* and *needle*.

(?)   "Growth" on page 77

(?)   "Homogeneous Nucleation" on page 62

(?)   "Precipitate Phase Settings" on page 28

Cuboid
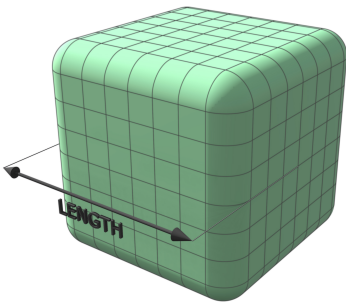
Figure 11: Cuboids have six faces, which form a convex polyhedron.

The cuboid shape is described by a supersphere

$$x_1^p + x_2^p + x_3^p = R^p \qquad (p \geq 2)$$

with p=2 being spherical shape. The larger the *p*, the more cubic the shape. Sometimes it is useful to define the cubical character as

$$\eta = \sqrt{2} \cdot 2^{-1/p}$$

Which gives a spherical shape when $\eta = 1$, and a cubic shape when $\eta = \sqrt{2}$.

Plate
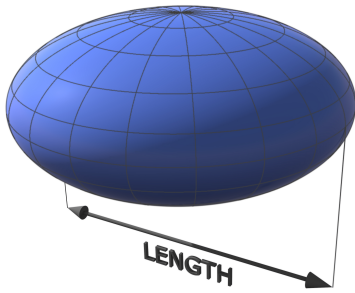
Figure 12: Oblate spheroids have rotational symmetry around an axis from pole to pole.

The plate is described as oblate spheroid

$$\frac{x_1^2}{l^2} + \frac{x_2^2}{l^2} + \frac{x_3^2}{r^2} \leq 1 \qquad l > r$$

with aspect ratio

$$\alpha = \frac{l}{r} > 1$$

Needle
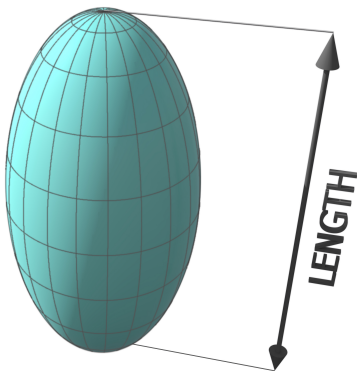
Figure 13: A prolate spheroid is a surface of revolution obtained by rotating an ellipse about its major axis.

The needle shape is described as prolate spheroid

$$\frac{x_1^2}{r^2} + \frac{x_2^2}{r^2} + \frac{x_3^2}{l^2} \leq 1 \qquad l > r$$

with aspect ratio

$$\alpha = \frac{l}{r} > 1$$

Precipitations at a Grain Boundary, Edge or Corner

For precipitations at a grain boundary, grain edge, or grain corner, non-spherical particles are considered based on wetting angle.

⊙   "Heterogeneous Nucleation" on page 69

⊙   "Matrix Phase Settings" on page 21

Normal Grain Growth

The normal grain growth model in the Precipitation Module (TC-PRISMA) uses a similar approach to its precipitation counterpart (see "Introduction to the Theory" on page 59) in that it calculates 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.

The boundary motion of a grain with radius R_i without considering pinning forces from precipitate particles, is driven by curvature and can be modeled as [1957Fel; 1965Hil]

[Eq. 1] $$\frac{dR_i}{dt} = \alpha M \gamma \left(\frac{1}{R_{cr}} - \frac{1}{R_i} \right)$$

where

- M is grain boundary mobility (m^4/Js)

- γ is the grain boundary energy (J/m^2)

- α is a dimensionless constant

If it should be satisfied that $k = M\gamma$, which is the parabolic growth rate of average grain size at steady-state

[Eq. 2] $$\bar{R}^2 - \bar{R_0}^2 = kt$$

It was found that $\alpha \approx 2$ [1965Hil].

R_{cr} in Eq. 1 is the critical grain size, which, not necessarily the average grain size, is determined by volume conservation [2008Jep]

[Eq. 3] $$\frac{dV}{dt} = 4\pi \sum_i \frac{R_i^2 dR_i}{dt} = 0$$

where the index i covers all the grains at each time step. Substituting Eq. 1 into Eq. 3, R_{cr} is obtained at each time step.

Grain Boundary Mobility Values

The grain boundary mobility M can be calculated as:

[Eq. 4] $$M = M_0 exp(-\frac{Q}{RT})$$

where

- M_0 is the prefactor (m^4/Js)
- Q is the activation energy (J/mol)

The recommended values of M_0 and Q in high purity metals such as ferritic iron, austenitic iron, nickel, and aluminum are shown in the table below.

> **❗** Since grain growth is significantly affected by grain boundary segregation, precipitation, and grain boundary complexion, the accuracy of the mobility data used for the recommended values is not guaranteed.

> **📄** If the grain size is in nanoscale, these parameters may not be applicable since the effects of grain boundary junction and complexion cannot be ignored in nanocrystals. For some alloys, such as Al, the parameters can also be sensitive to temperature. The temperature range in the table is the suggested best fit.

Recommended grain growth parameters for mobility prefactor M_0 and activation energy Q.

	Matrix Phase	Temperature Range (K)	Prefactor M_0 (m^4/Js)	Activation Energy Q (J/mol)	Reference
High purity iron	BCC_A2	625 ~ 875	4E-3	242000	[1997Mal]
Low alloying steel (Cr-Mo)	FCC_A1	1173 ~ 1473	3.6E-3	228302	[2008Lee]
Pure Ni	DIS_FCC_ A1/FCC_L12	1098 ~ 1323	4.12E-8	123050	[2008Ran]
High purity aluminum	FCC_A1	300 ~ 548	1.02E-14	27430	[2004Yu]
		573 ~ 773	1.25E-8	73080	

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Zener Pinning

Zener [1948Smi] proposed a pinning force due to second-phase particles, so that the normal grain growth would be completely inhibited when the grain size reached a critical maximum grain size R_z. In general form, it can be expressed as [1998Man]

[Eq. 1]
$$R_z = K \frac{r}{f^m}$$

Where

- r is the radius of the pinning particles

- f the volume fraction of the particles

- K is a dimensionless constant

- m an exponential index for f

The original Zener pinning theory gives

$$K = 4/3, m = 1$$

which has been found to be inconsistent with the experimental information and thus needs refinement.

For simplicity, the average particle radius $\bar{r}_j$ of a precipitate phase j has been used to calculate the pinning force arising from all the particles of this phase. The pinning force, z_j, can be evaluated as the inverse of $R_{z,j}$

$$z_j = \frac{1}{R_{z,j}} = \frac{1}{K_j} \frac{f_j^{m_j}}{\bar{r}_j}$$

When there are multiple precipitate phases, the overall pinning effect is the sum of that from all precipitate particles,

$$z_j = \sum_j z_j = \sum_j \frac{1}{K_j} \frac{f_j^{m_j}}{\bar{r}_j}$$

The retarding force due to Zener pinning, RF_z, is therefore [1965Hil]

$$RF_z = \sigma \cdot z = \frac{\sigma}{R_z}$$

where σ is the grain boundary energy.

Realizing that the drag force resists the grain boundary motion, no matter in the growing (positive velocity) or shrinking (negative velocity) direction, the overall growth rate is expressed as [1965Hil]

$$\frac{dR_i}{dt} = \alpha M \sigma \left[\left(\frac{1}{R_{cr}} - \frac{1}{R_i} \right) \pm \frac{1}{R_z} \right]$$

The negative sign holds when

$$\left(\frac{1}{R_{cr}} - \frac{1}{R_i} \right) - \frac{1}{R_z} > 0$$

while positive sign holds when

$$\left(\frac{1}{R_{cr}} - \frac{1}{R_i} \right) + \frac{1}{R_z} < 0$$

And $\frac{dR_i}{dt} = 0$ when R_i lies between these two limits.

In the Precipitation Module (TC-PRISMA), you can input parameters K_j and m_j for each precipitate phase. An additional parameter, *cutoff radius* (unit= m), can be used so that precipitates with a smaller size than this value are excluded from the calculation of pinning force. This adjustment avoids an unreasonably large pinning force calculated from very small precipitates (e.g. nuclei).

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Stereology

Stereology is the science of assessing the three-dimensional (3D) geometry and morphology of objects utilizing data descriptive of a cross-section of the material. It is common to characterize a precipitate dispersion utilizing quantitative image analysis of micrographs obtained from light or scanning electron microscopy. In these cases, the data describes the precipitates found in a cross-section taken through the sample.
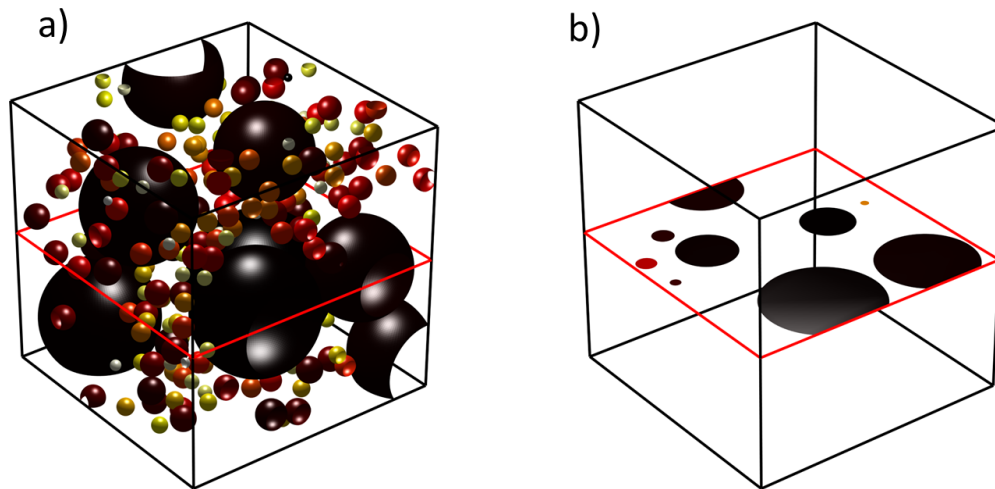
Figure 14: a) A 3D dispersion of non-penetrating polydisperse particles. b) A cross-section taken through the dispersion.

Stereological considerations are important when seeking greater quantitative accuracy comparing model calculations and experimental data. The two-dimensional (2D) size distribution is of interest for the calculation of mechanical properties as it represents the size distribution of obstacles encountered by a dislocation on a slip system.

The size of the precipitates can be expressed as the equivalent radius of a circle with the same cross-sectional area as measured from the micrograph. Figure 15, Figure 16, and Figure 17 compare the 3D and 2D size distributions of a spherical dispersion considering a left skewed, a normal, and a right-skewed distribution. Observe the changes in shape of the distribution in addition to the smaller 2D mean radius compared to the true 3D size.

> The 3D to 2D conversion implementation considers spherical particles. Although the precipitates may be approximated as spherical for the approximation of the 2D size distribution, there may be a large error for geometries that differ largely from spheres.

The **3D → 2D** checkbox that is available to use this feature requires (1) that the *Precipitate Phase* **Morphology** is set to **Sphere** on the Precipitation Calculator, and then (2) one of these axis variables is selected on either the Plot or Table Renderer: **Mean radius**, **Size distribution**, **Number density distribution**, or **Normalized number density distribution**.
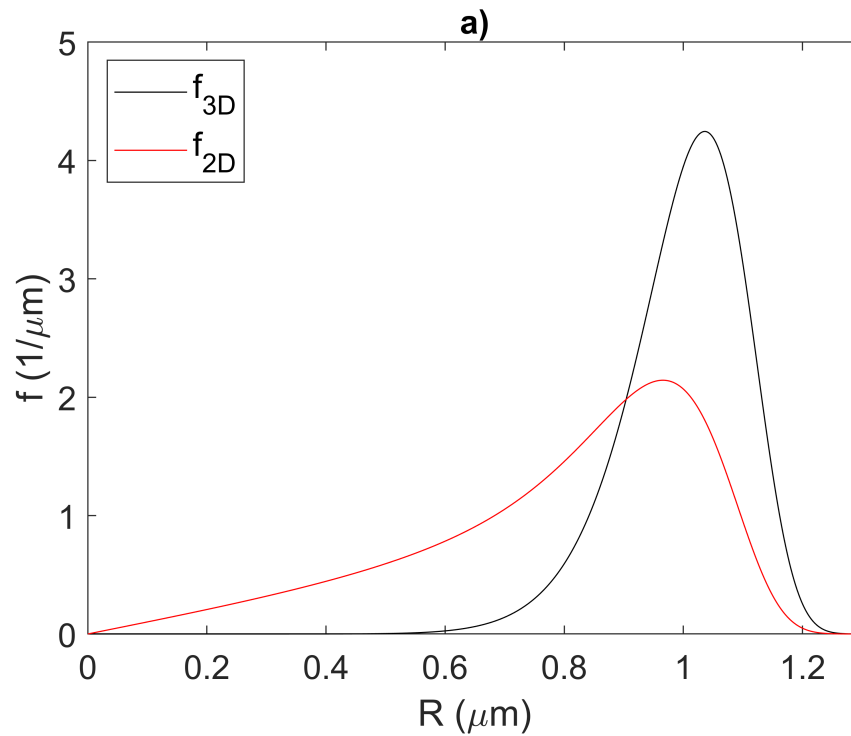

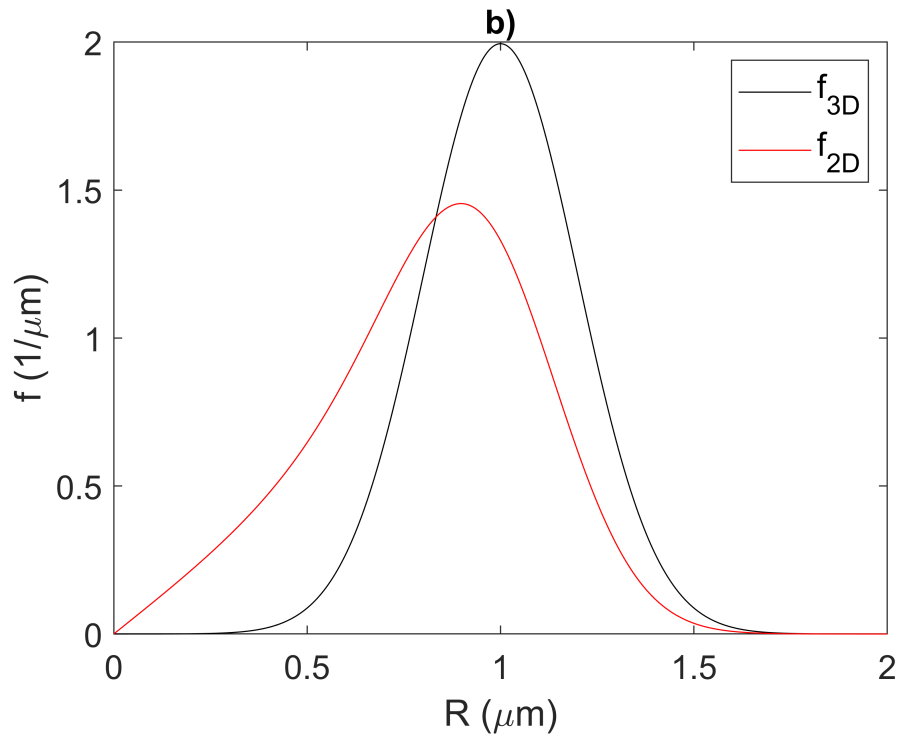*Figure 15: A comparison of the 3D and 2D particle size distributions considering a left-hand skewed Weibull distribution.*

Figure 16: A comparison of the 3D and 2D particle size distributions considering a normal distribution
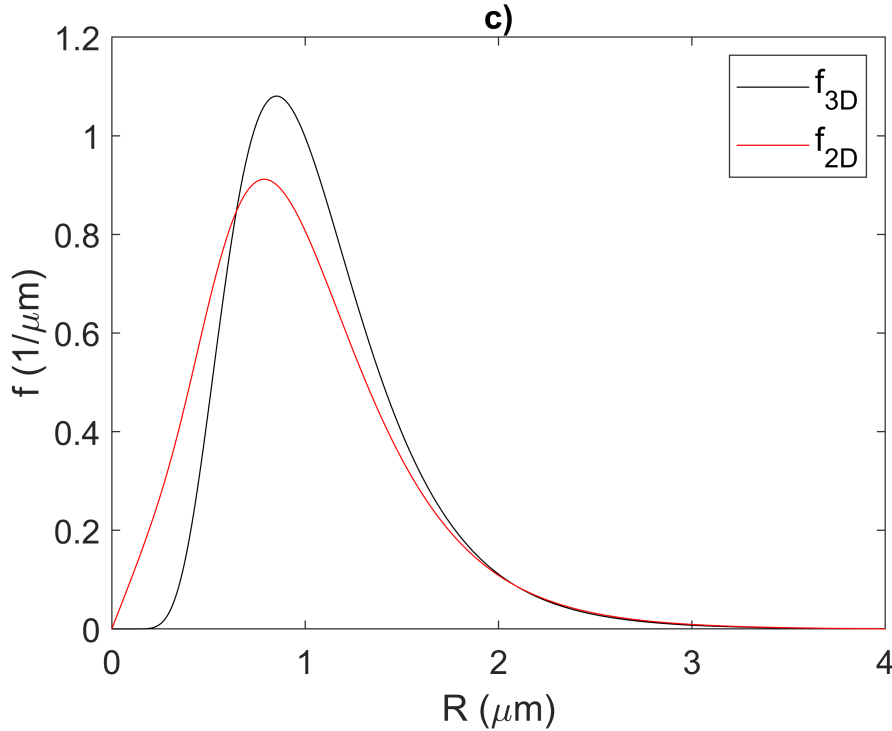
Figure 17: A comparison of the 3D and 2D particle size distributions considering a right-hand skewed log-normal distribution.

Analytical solutions exist for the determination of the 2D size distribution of impenetrable polydisperse spheres [1958Sal; 1925Wic]. Thermo-Calc has implemented the Jeppsson-Mannesson-Borgenstam-Agren (JMBA) [2011Jep] Saltykov conversion method to calculate the 2D size distribution.

Let $F_{3D}(r)dr$ describe the number of particles with radius varying between r and $r + dr$ within a unit volume. The corresponding 2D size distribution is given by $F_{2D}(r)dr$, describing the number of particle cross-sections with a radius varying between r and $r + dr$ within a unit area. Following the Saltykov method, the 2D size distribution is obtained from the following matrix calculation:

$$\underline{F_{2D}} = \underline{\underline{\alpha}}\,\underline{F_{3D}}$$

where $\underline{\underline{\alpha}}$ is a matrix of probabilities for the conversion and $\alpha_{i,j}$ describe the likelihood of obtaining a 2D cross-section of radius r_i from 3D grains of radius r_j . The JMBA model derived these probabilities as:

$$\alpha_{i,j} = \begin{cases} 2r_i \dfrac{\Delta \mathrm{rb_i}}{\Delta rb_j} \dfrac{\sqrt{r_i^2 - b_{j-1}^2} - \sqrt{r_j^2 - b_j^2}}{r_i} & i < j \\[2em] \dfrac{\Delta b_j 4\pi r_j^3 / 3 - \sum_{i=1}^{j-1}\left(\pi r_j^2 b_i \Delta b_{i-1} \alpha_{i,j}\right)}{\Delta b_j \pi r_j^2} & i = j \\[2em] 0 & i > j \end{cases}$$

Where b_i and b_{i+1} describe the lower and upper boundaries to the particle radii class r_i. Δr_i and Δb_i are the spacing between radii midpoints and class boundaries, respectively. For a linear discretization, $\Delta b_i = \Delta r_i$.

It is assumed that the 2D cross-section is a perfect cut through the material however there may be some error in this approximation. Figure 18 presents the idealized case with a 3D and 2D size distribution with a mean radius of 1.5 µm. In Figure 19, it is assumed that the minimum size of particles that can be quantified in the micrograph is 0.25 µm. This crops off the left-hand tail of the 2D distribution. Etching away the matrix reveals sub-surface particles. Figure 20 shows the impact of etching a depth of 30 nm, further exposing particles that have a center below the cross-section of the cut.
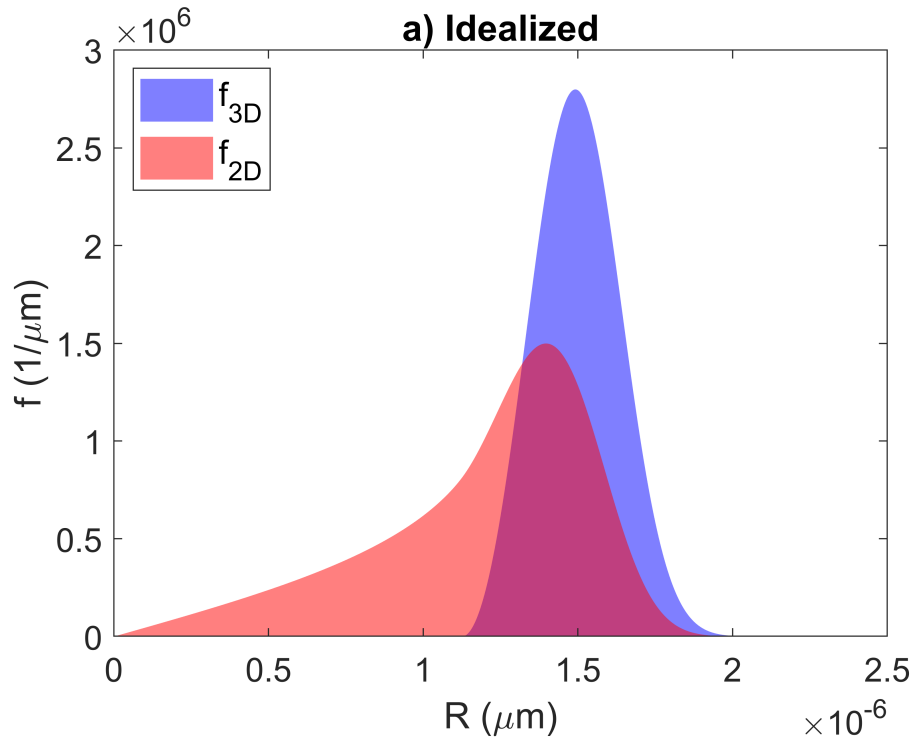
Figure 18: Potential causes of error in micrographs showing the idealized 2D size distribution.
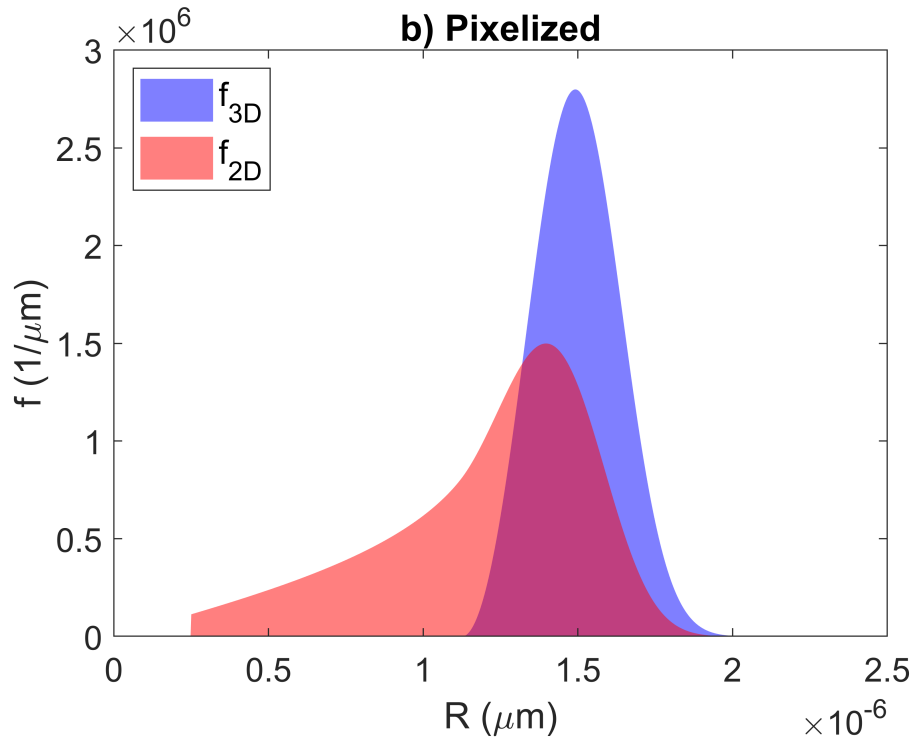
Figure 19: Potential causes of error in micrographs showing the cropped left-hand tail caused by a limiting size that can be measured from the micrograph.
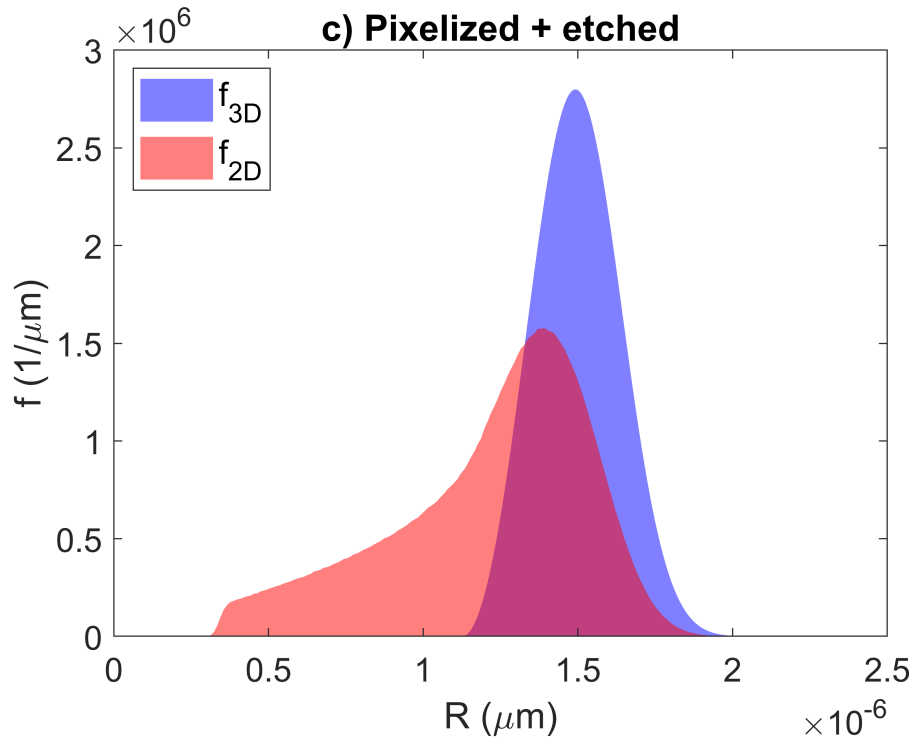
Figure 20: Potential causes of error in micrographs showing how the left-hand tail can be blurred due to etching.

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Precipitation Module Examples

🔑 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 Al₃Sc

This example simulates the kinetics of precipitation of Al$_3$Sc 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.

Open the example project file and click **Perform Tree** to generate the plots associated with it.

Project File, Step-By Step Instructions, and Video Tutorial Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: *P_01_Precipitation_Al-Sc_AL3SC.tcu*

This example is included as a Precipitation Module (TC-PRISMA) tutorial on our website and as part of the playlist on our YouTube channel.

You can also use the step-by-step instructions included in a PDF to follow the video or compare to the project file in Thermo-Calc.

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

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.
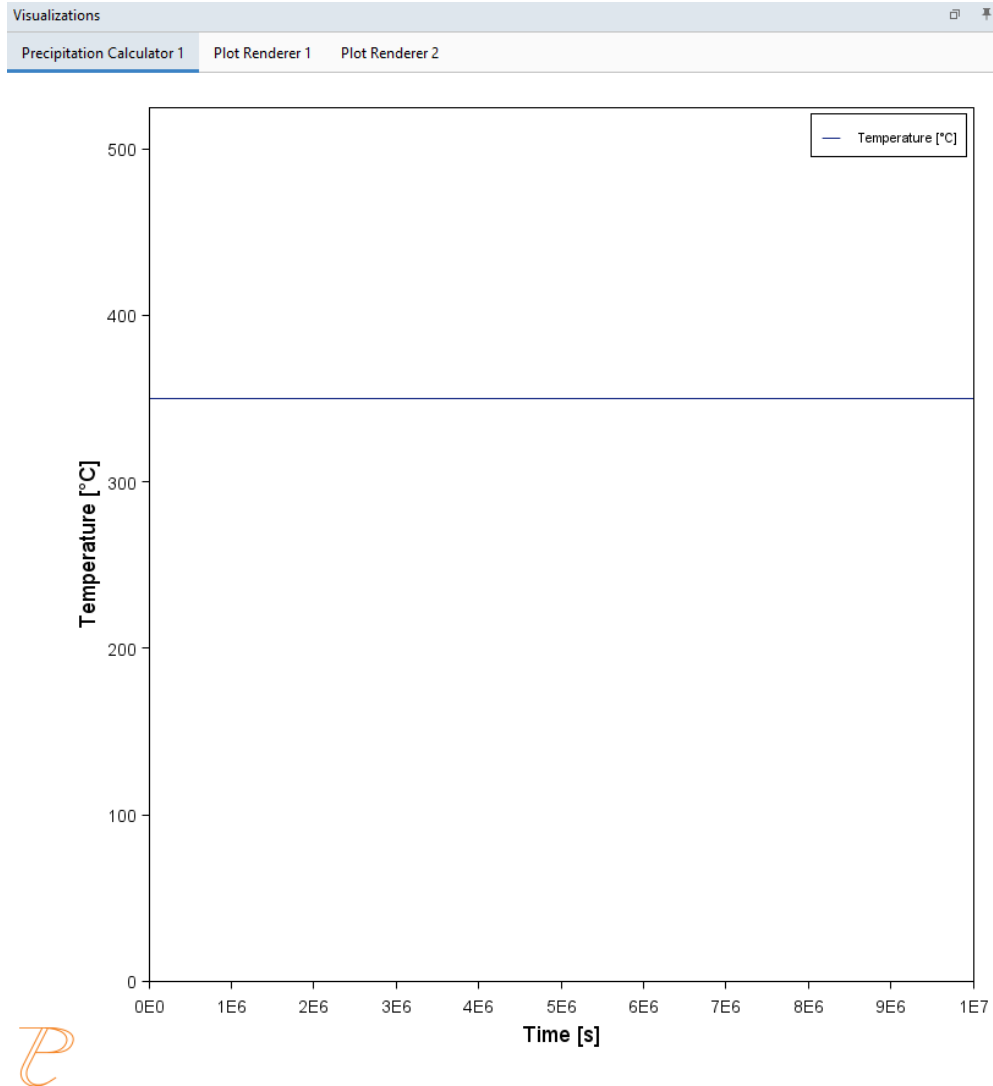
Figure 21: During set up of the calculation, you can preview the Thermal Profile. Click the tab in the Visualizations window to preview it and adjust settings on the Precipitation Calculator Configuration window. For an Isothermal Thermal Profile this shows the constant temperature as entered.
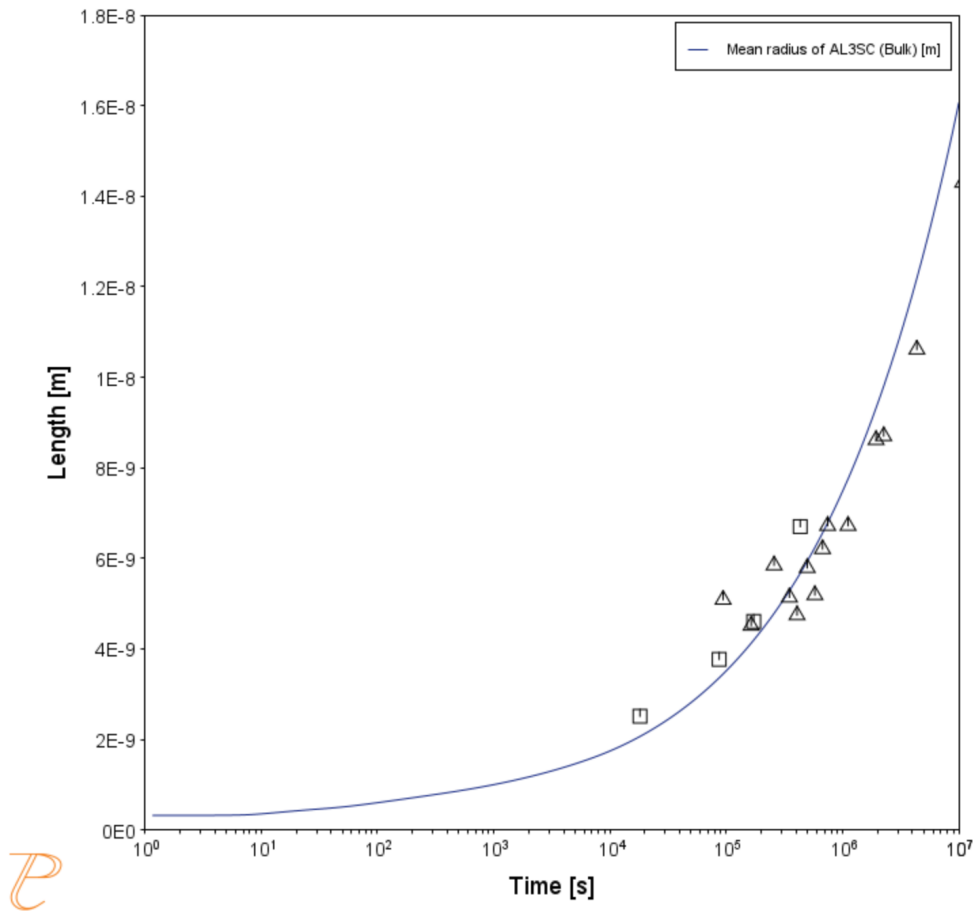
Figure 22: After performing the calculation, you can view the final Plot Renderer result on the applicable tab. This plot shows the mean radius of the AL3SC precipitate as a function of time.
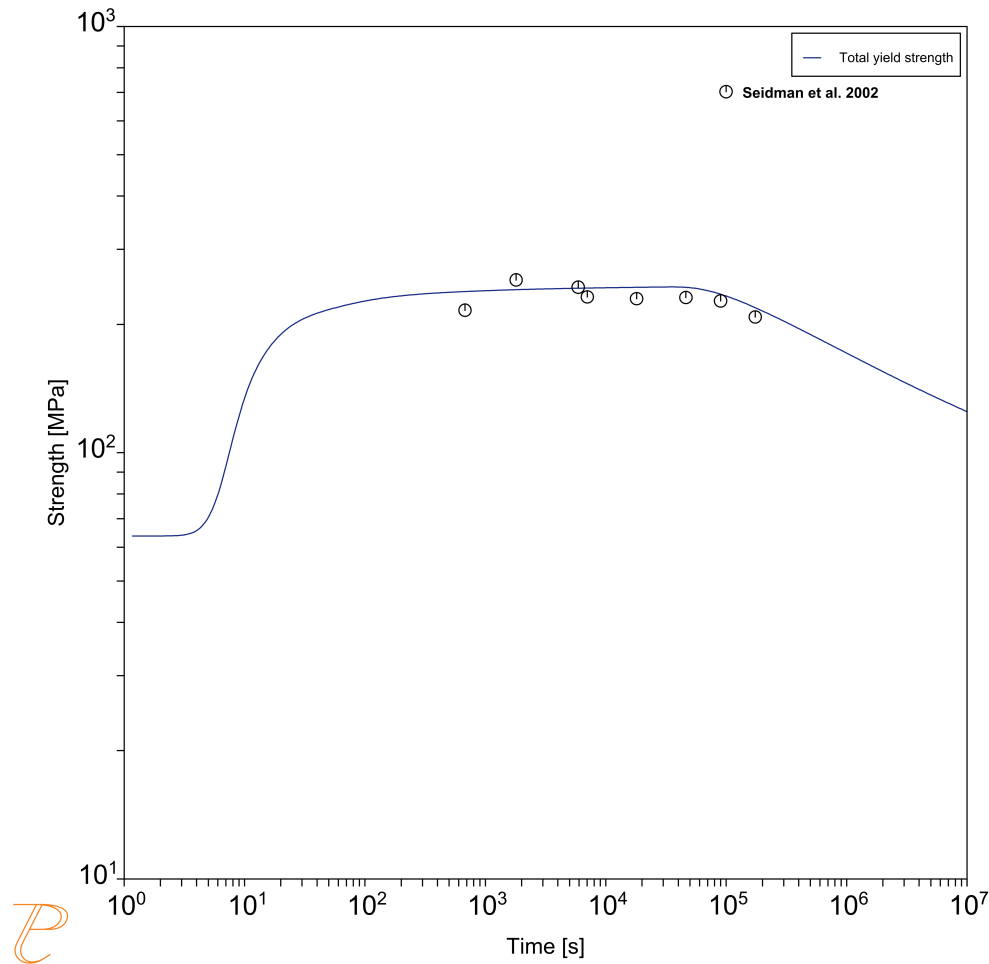
Figure 23: After performing the calculation, you can view the final Plot Renderer result on the applicable tab. This plot shows the total yield strength of the AL3SC precipitate as a function of time compared to experimental data from Siedmen et al. [2002Sei]. The model captures the over-tempering behavior from excessive coarsening of the strengthening precipitates.

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Isothermal Precipitation Calculation: Example P_01 – Precipitation Al-Sc AL3SC

This example shows you how to set up an isothermal precipitation calculation for the formation of AL$_3$SC in an aluminium-scandium alloy at 350° using the Precipitation Module (TC-PRISMA).

The end of the example also shows how to use the results of the calculation to model Yield Strength.

This is one of the most basic calculations using the Precipitation Module (TC-PRISMA), so it is a good place to start if you are new to this simulation type.

HELPFUL INFORMATION

- **All users can run this calculation,** even those who do not have a license for the Precipitation Module (TC-PRISMA).
- **A companion video** is available for this example , which can be watched here: https://www.youtube.com/playlist?list=PLfv6McToaTGSpqvuLoY3b_UV-8xpgLUkJ

This calculation is based on Precipitation Module example *P_01 – Precipitation Al-Sc AL3SC*, which is included in your installation.

1. To run the example file, open Thermo-Calc and select **Help > Examples Files** or click **Example Files** on the **My Project Configuration** window.
2. Open the *Precipitation Module (TC-PRISMA)* folder. Double-click the example file to open it.
3. In Thermo-Calc at the bottom center of the **Configuration** window click **Perform Tree**.
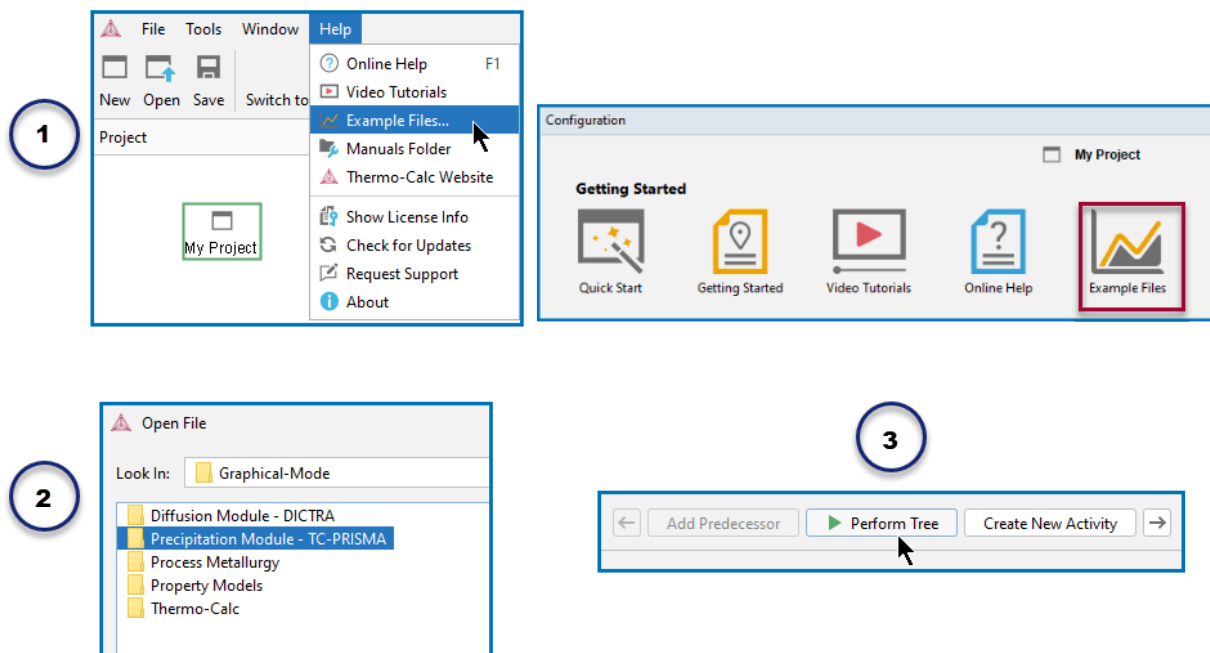
ABOUT THE EXAMPLE

This example simulates the kinetics of precipitation of Al_3Sc from an FCC_A1 solution phase. The results of the simulation are also used to model yield strength.

SETTING UP THE SYSTEM

1. Open Thermo-Calc in Graphical Mode.
2. On the **My Project Configuration** window under **Non-Equilibrium**, click **Precipitation**.
3. All the nodes for a precipitation calculation are added to the **Project** window:
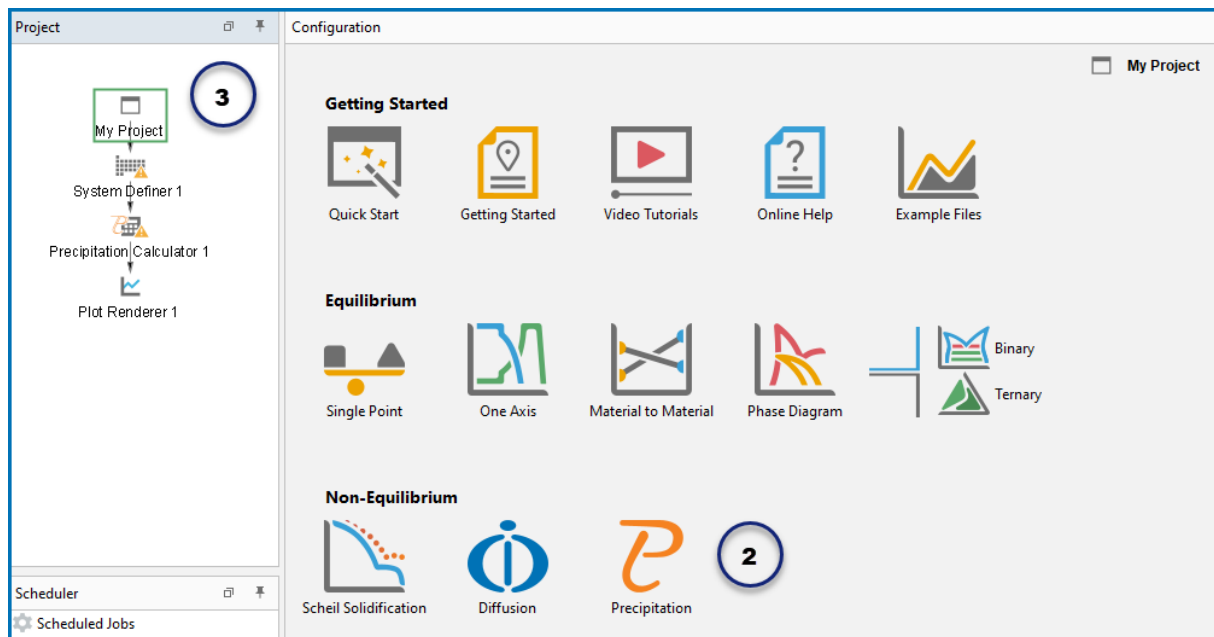
4. In the **Project** window, click the **System Definer 1** node.
5. On the **Configuration** window from the *Package* list, select **Demo: Aluminium-based alloys (ALDEMO, MALDEMO).** This loads both thermodynamic and kinetic demonstration aluminium databases.
6. In the **Periodic Table**, select the elements in the following order.
   Select Al first so that it is the dependant element:
   a. **Al** (aluminium)
   b. **Sc** (scandium).
7. From the *Amount* list (to the right of the Periodic Table), select **Mole percent**.
8. Enter 0.18 for **Sc**. This automatically sets **Al** to 99.82.
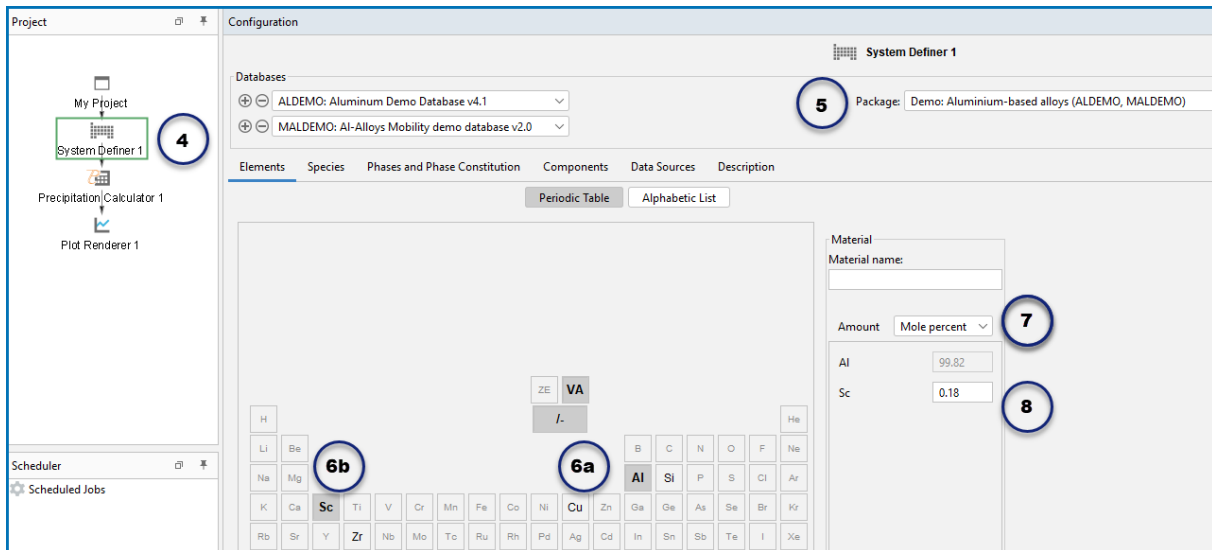
The system is now defined. However, before starting the precipitation calculation, it is recommended to run a one axis calculation to find the phases present around 350° C.
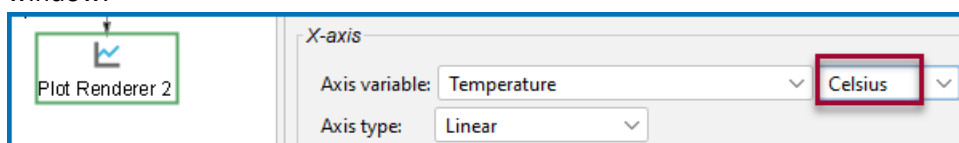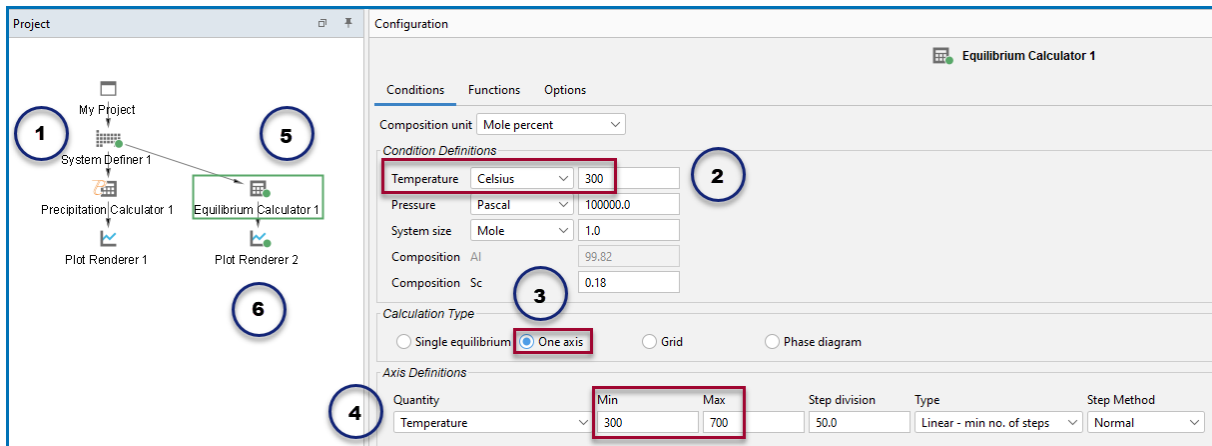
ONE AXIS CALCULATION

Why We Do This

In order to set up an isothermal precipitation calculation, you need to know which phases are present at 350 °C. A *one axis* calculation provides this information. Note that this step is not included with the P_01 example. This is an additional exercise.

Setting up a One Axis Calculation

1. In the **Project** window, right-click the **System Definer 1** node, and select **Create New Successor** > **Equilibrium Calculator**.
2. In the **Configuration** window, set *Temperature* to **Celsius** and enter 300.
3. Under *Calculation Type*, click **One axis**.
   You now want to find the phases present around 350 °C.
4. Under *Axis Definitions,* enter the **Temperature** range from **Min** 300 to **Max** 700.
   Keep the default values for everything else. The system is now defined.
5. Right-click the **Equilibrium Calculator** node and select **Create New Successor > Plot Renderer**.
6. In the **Project** window, click the **Plot Renderer 2** node you just created. In the **Configuration** window, set the *X-axis variable* for **Temperature** to **Celsius**. Then right-click the **Plot Renderer 2** node select **Perform Now**. Or click **Perform** at the bottom of the **Configuration** window.

Interpreting the Results of the One Axis Calculation

Once the calculation is complete, a plot is displayed in the **Results** window. This plot shows you which phases are present at each temperature between 300° and 700° and the amount of that phase at each temperature.

If you hover your cursor over any of the lines on the plot, a label gives you the name of the phase, the temperature and the amount of the phase at that temperature.

We can see that there are two phases present at 350°. **FCC_A1** is at the very top of the plot and makes up more than 99% of the system. The remainder of the system is made up of **Al₃SC**, which is near the very bottom of the plot and is the precipitate phase in the alloy we are considering.

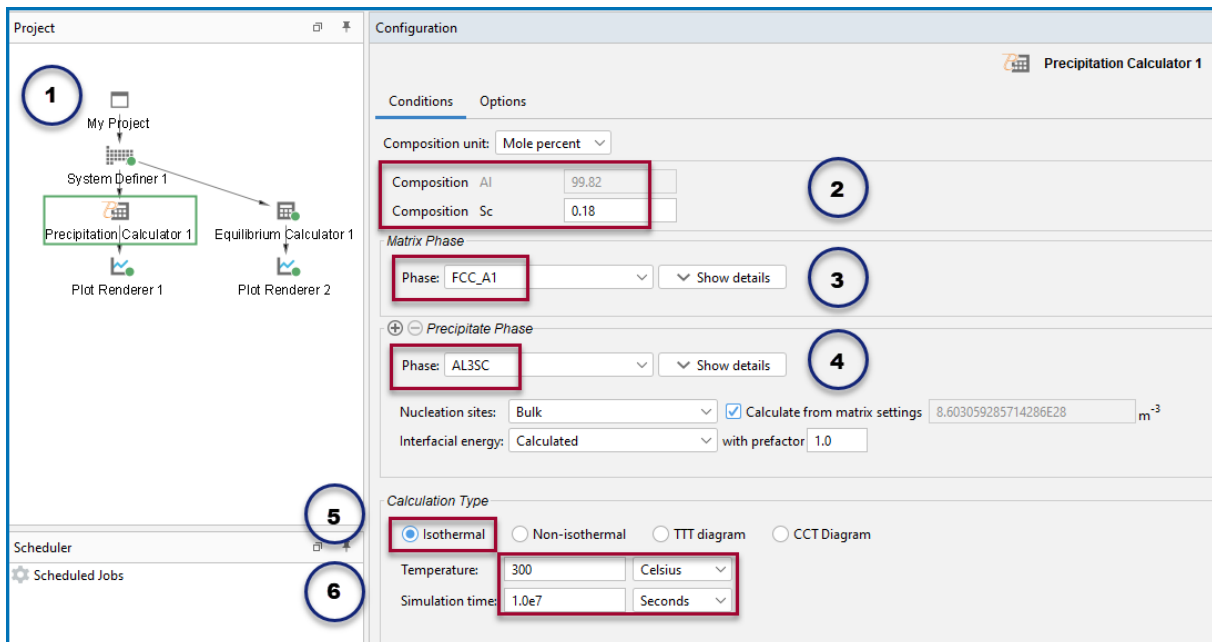Remember these two phases because these are used in the precipitation calculation.
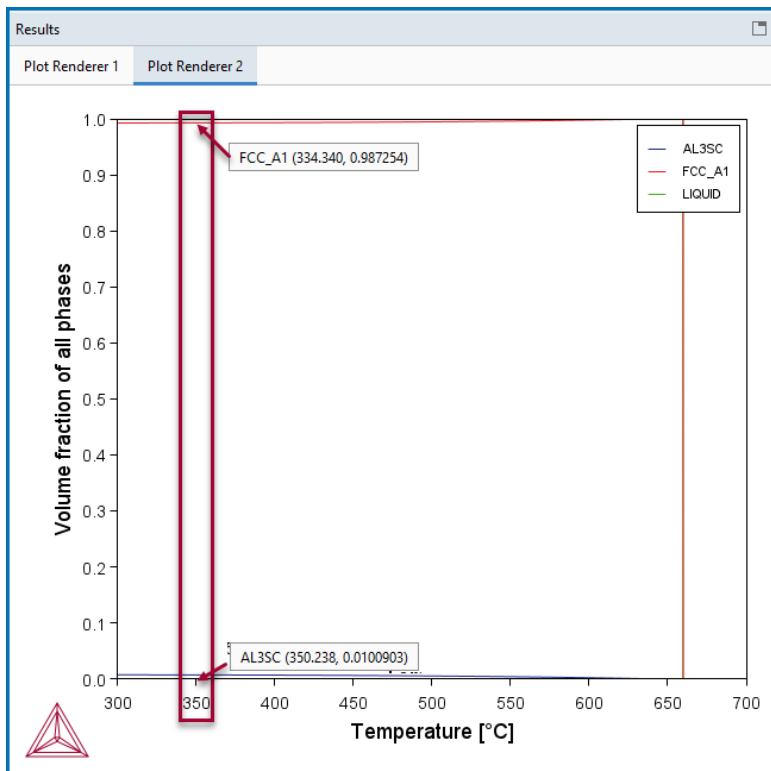
PRECIPITATION CALCULATION

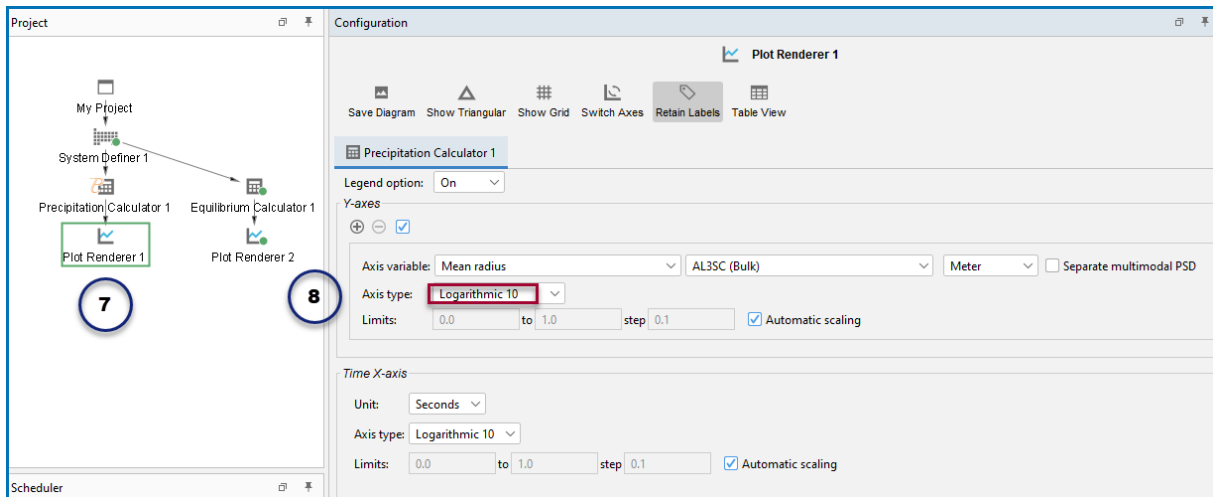### *Setting up the Precipitation Calculation*

1. In the **Project** window, click the **Precipitation Calculator 1** node.
2. Notice that the *Composition* set in the *System Definer* auto-populated here.
3. Under *Matrix Phase*, the *Phase* defaults to **FCC_A1**, which is the primary phase present in the one axis calculation.

NOTE: If you do not see any phases listed here it is probably because you do not have a kinetic database selected. If so, go back to the *System Definer* and add a kinetic (mobility) database. In this example it should be the **MALDEMO** database.

4. Under *Precipitate Phase,* select **AL3SC** from the *Phase* list because that is the other phase present around 350 °C, as shown in the one axis calculation.
5. Accept the rest of the default settings in the *Precipitate Phase* section. You could choose to define your own interfacial energy settings if you have them.
6. Under *Calculation Type*, make sure **Isothermal** is selected.
7. Enter:
   a. `350` as the *Temperature* and select **Celsius**.
   b. `1.0E7` as the *Simulation time* and select **Seconds**, which is ten million seconds.
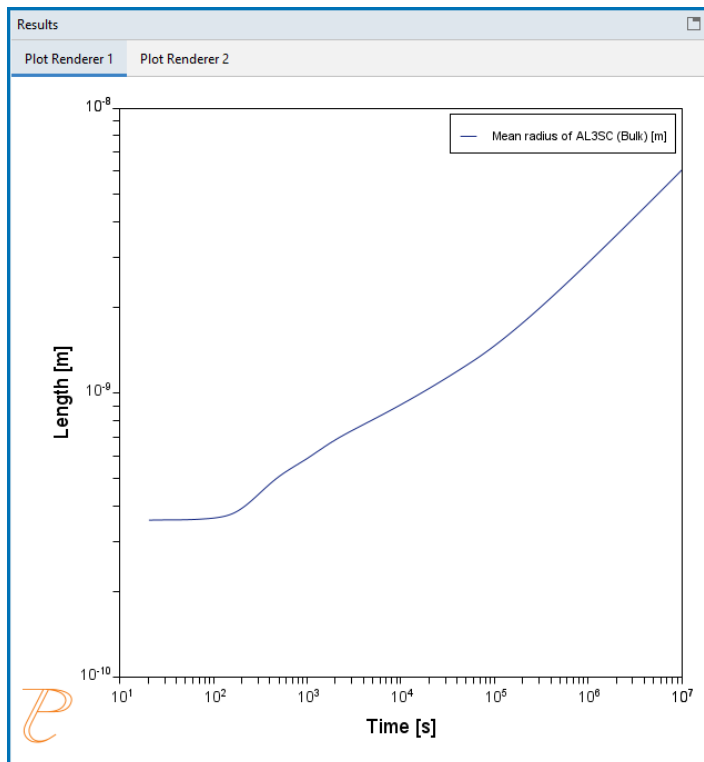

8. In the **Project** window, click the **Plot Renderer 1** node.
9. Under *Y-axes*, from the *Axis type* menu select **Logarithmic 10** for a better view of the plot.
10. Click **Perform** at the bottom, center of the **Configuration** window.

Interpreting the Results of the Precipitation Calculation

Once the calculation is complete, your plot is shown in the **Results** window.

*This plot shows the Mean radius of the AL3SC precipitate as a function of time.*

At the beginning, which is the left-most side of the plot, the mean radius is quite small and then grows rapidly over time, which is represented by moving rightward on the plot.

Setting Other Variables in the Precipitation Module (TC-PRISMA)

The Precipitation Module (TC-PRISMA) offers many variables that you can plot for the same calculation.

1. Click the **Plot Renderer 1** node.
2. Under *Y-axes*, click the *Axis variable* menu to see the other available options in the list.

3. Once you have made your selection, click **Perform** at the bottom, center of the **Configuration** window to create a new plot.
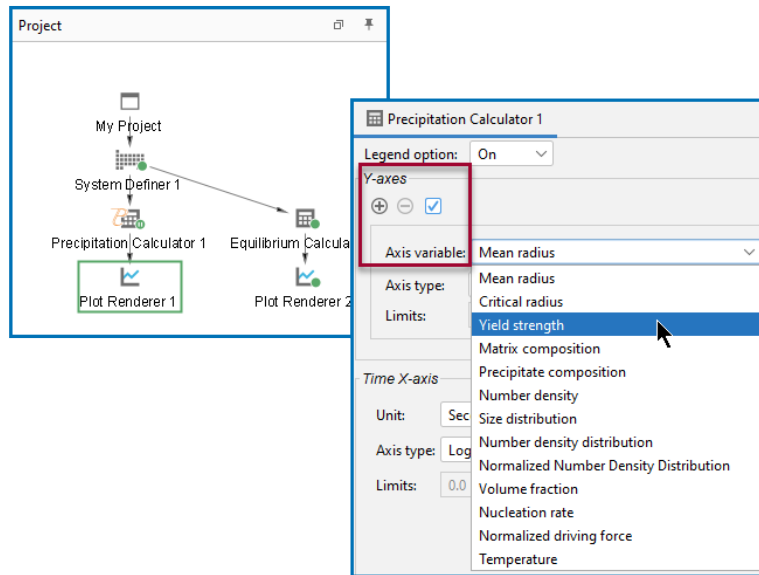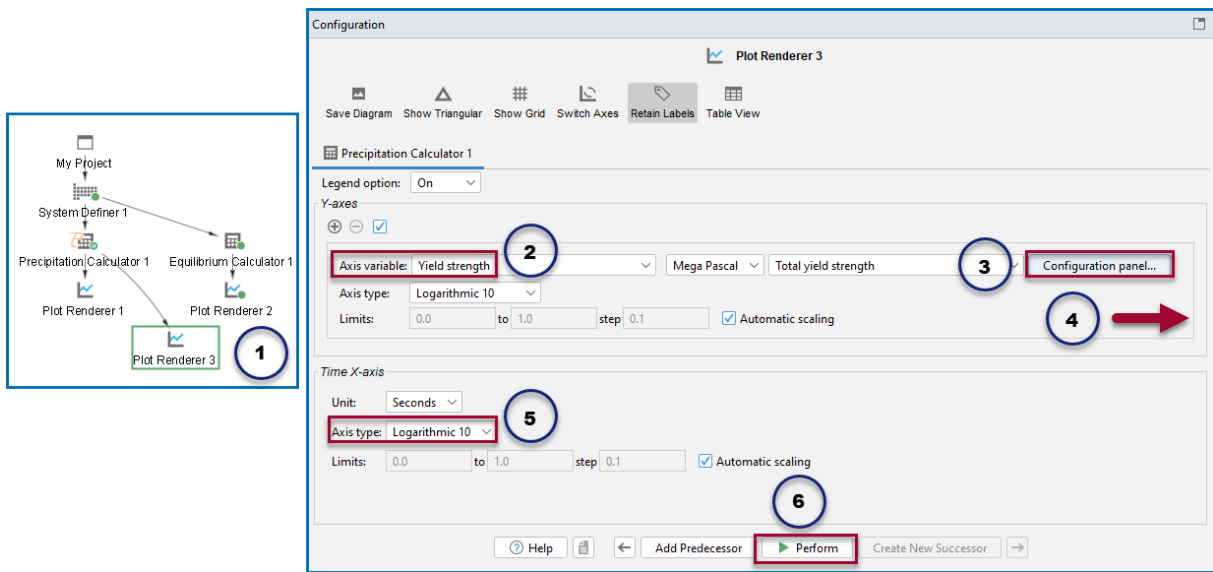

Model Yield Strength

Beginning with Thermo-Calc 2020b, results of a precipitation simulation can be used as input to model yield strength using the Yield Strength Property Model. The following simulation requires a license for Thermo-Calc 2020b or newer.

1. Right click the **Precipitation Calculator 1** node and select **Create New Successor > Plot Renderer**.
2. Under *Y-axes*, from the *Axis variable* menu, select **Yield strength** (as in the figure above but for **Plot Renderer 3)**.
3. Click the *Configuration panel* button.
4. If required, expand the **Plot Renderer Configuration** window. Then from the *Precipitation strengthening model* menu select **Seidman model (Al-base)**.
5. Under *Y-axes*, from the *Axis type* menu, select **Logarithmic 10**.
6. Click **Perform** at the bottom, center of the program.

The program uses the results from the precipitation simulation as the input for the Yield Strength model.

Interpreting the Results of the Yield Strength Model

Once the calculation is complete, your plot is shown in the **Results** window.
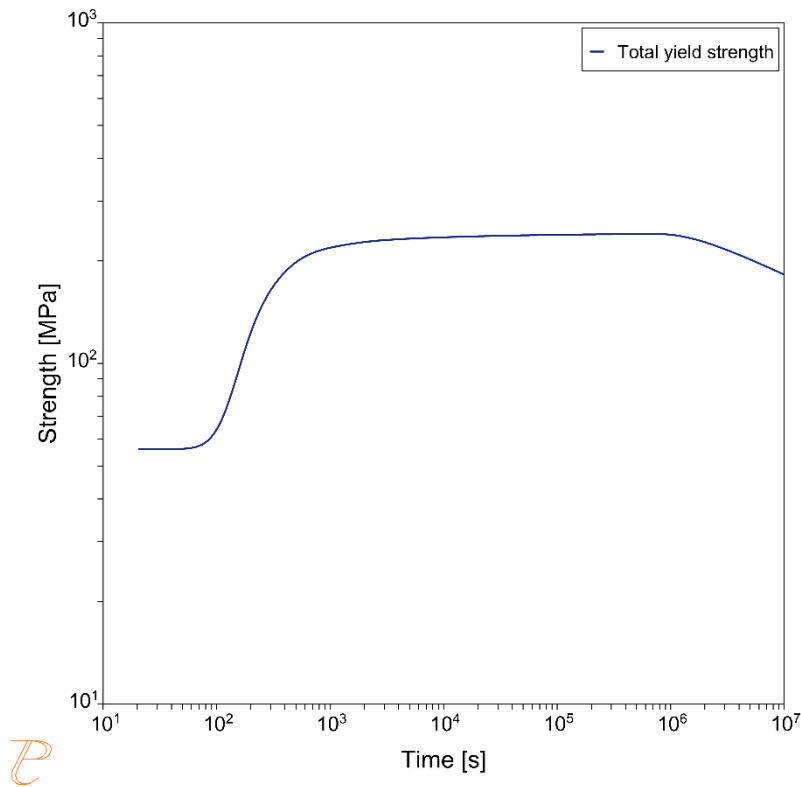
This plot shows the yield strength of the AL3SC precipitate as a function of time.

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.

Open the example project file and click **Perform Tree** to generate the plots associated with it.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: *P_02_Precipitation_Fe-C-Cr_Cementite-M7C3-M23C6.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.

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	1.0E-4 m

setting)	
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

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.
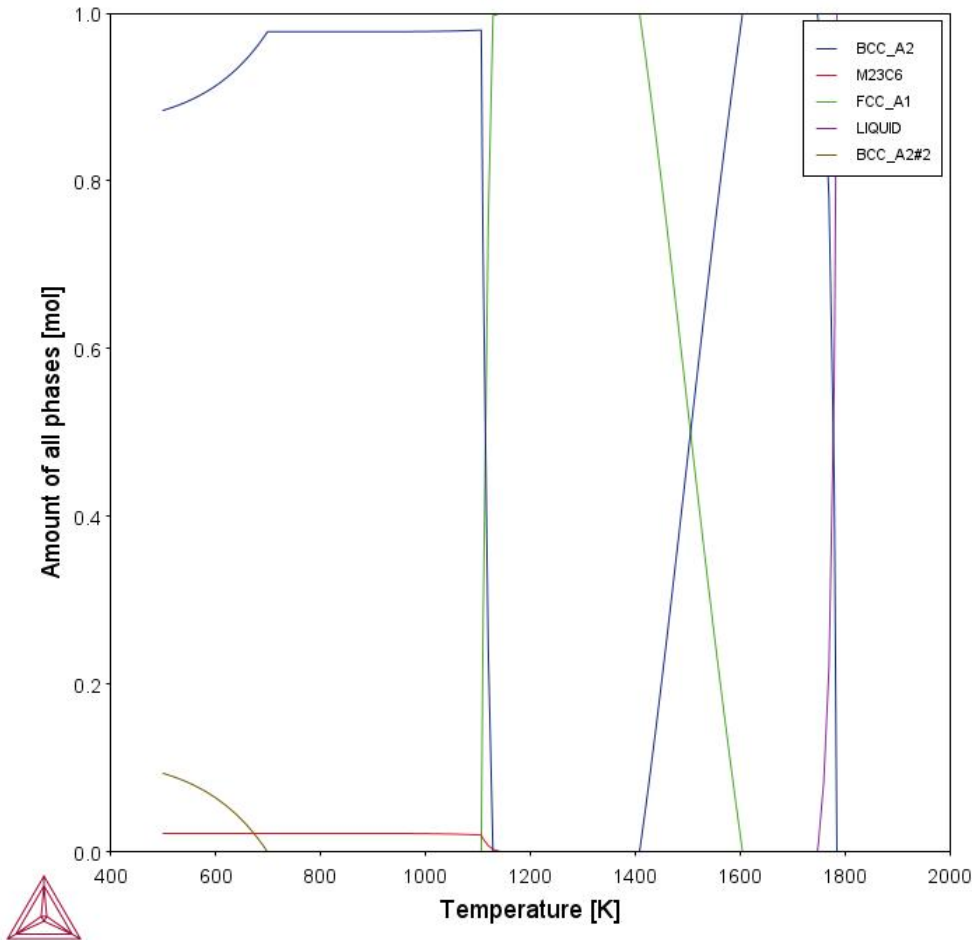

Figure 24: After performing the calculation, you can view the final Plot Renderer result on the applicable tab. This shows the equilibrium property diagram for the Fe-C-Cr alloy, highlighting what phases are predicted to be at equilibrium for a range of temperatures. The calculation shows that at 1053 K, M23C6 is the stable carbide.
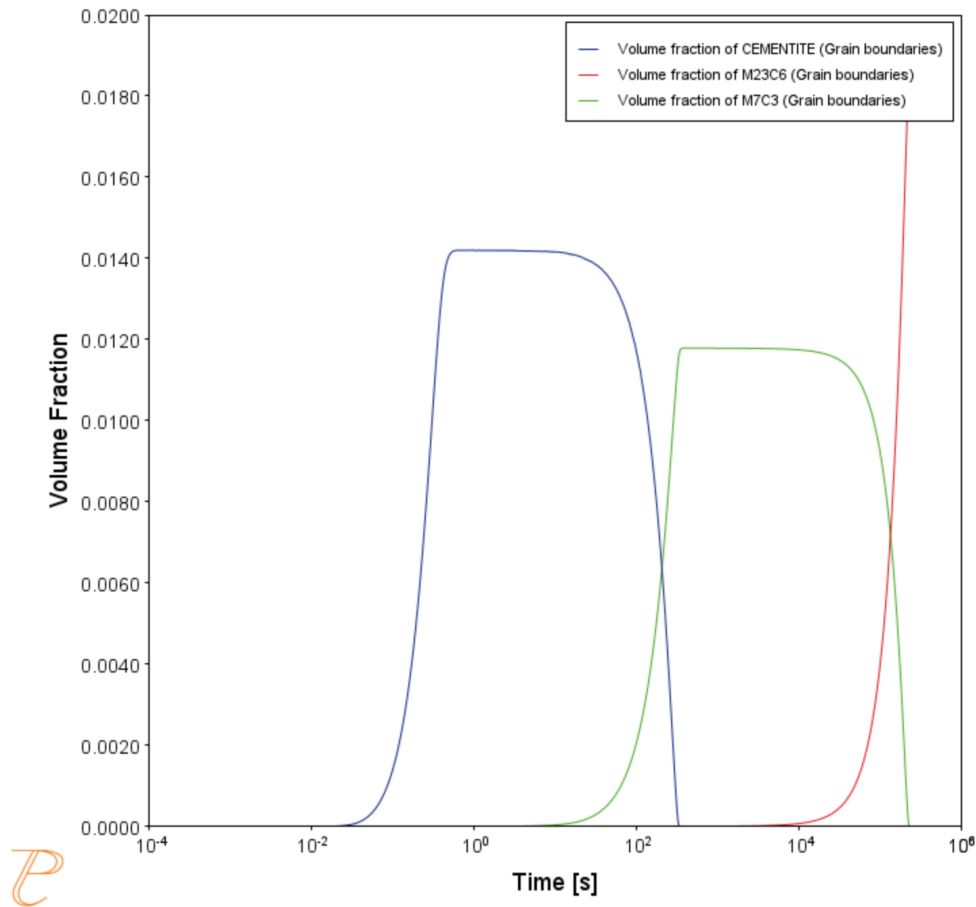
Figure 25: After performing the calculation, you can view the final Plot Renderer result on the applicable tab. This shows the evolution of the volume fraction of cementite, M7C3, and M23C6 during an isothermal heat treatment of an Fe-C-Cr alloy at 1073 K. The cementite and M7C3 are metastable at this 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 **Tempeature**, as well as **Max annealing time**. In **Stop criterion**, choose **Volume fraction of phase** and enter the value.

Open the example project file and click **Perform Tree** to generate the plots associated with it.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**

- File name: *P_03_Precipitation_Fe-C-Cr_TTT_Cementite-M7C3-M23C6.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](#).

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

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.
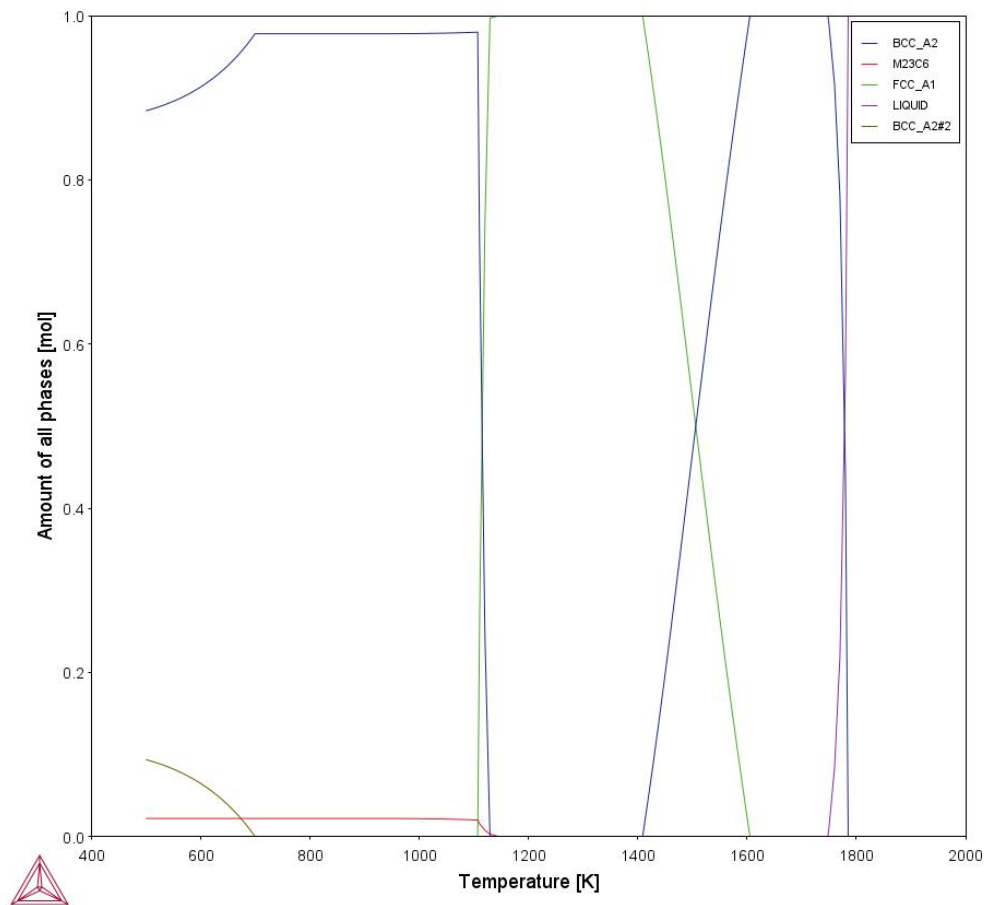

Figure 26: After performing the calculation, you can view the final Plot Renderer result on the applicable tab. Here the results from the equilibrium calculator are shown, which assesses the stability of phases across the temperature range of interest.
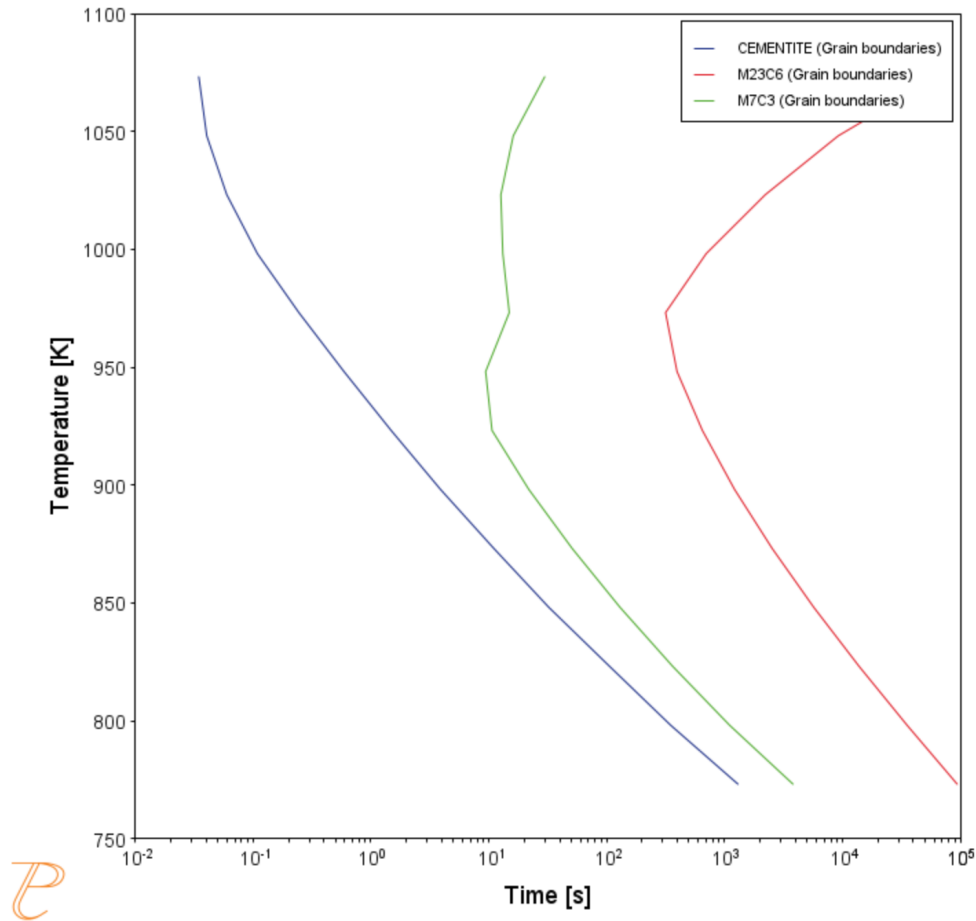
Figure 27: After performing the calculation, you can view the final Plot Renderer result on the applicable tab.This shows results from a TTT (Temperature-Transformation) simulation using the Precipitation Calculator to examine the sequence of phase transitions considering the formation of cementite, 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.

Open the example project file and click **Perform Tree** to generate the plots associated with it.

> ⧗ When you run (Perform) this example, it takes a few minutes for the calculations to complete.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: *P_04_Precipitation_Fe-C_Cemetite.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.

▌ 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

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.
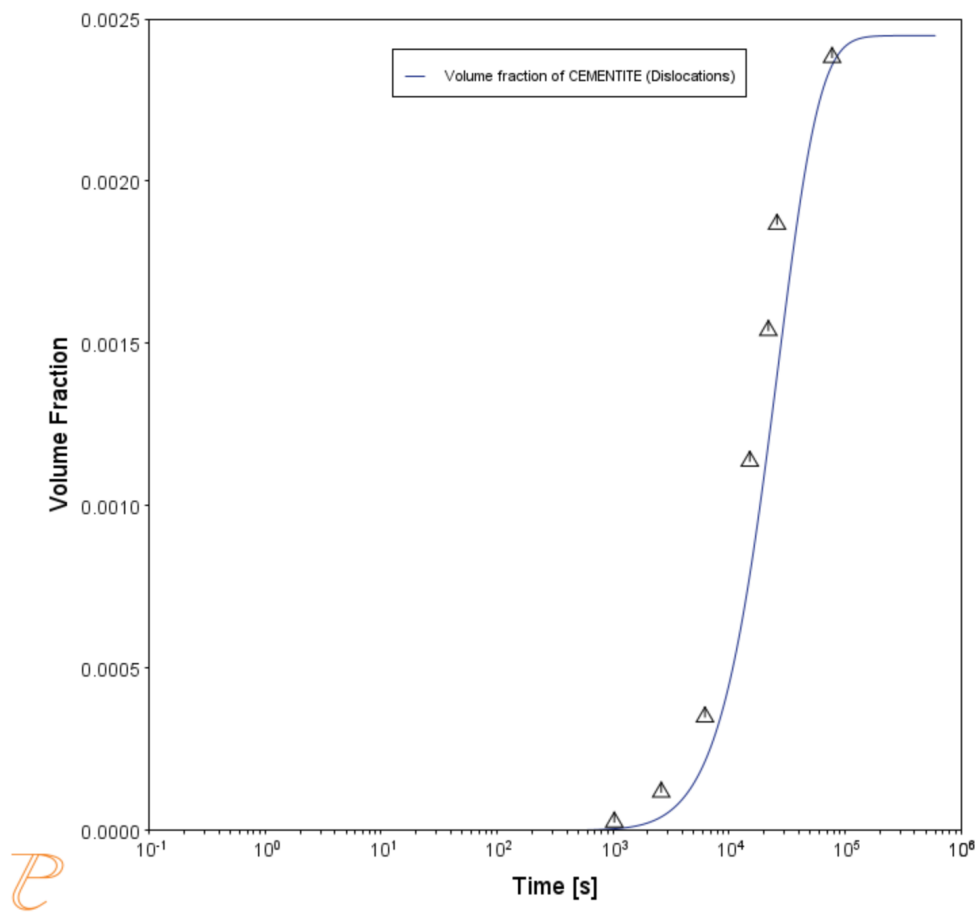

Figure 28: After performing the calculation, you can view the final Plot Renderer result on the applicable tab. The result compares the predicted evolution of the volume fraction of cementite with the measurements of [1949Wer].

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 " on page 27 for details.

Open the example project file and click **Perform Tree** to generate the plots associated with it.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**

- File name: *P_05_Precipitation_Ni-Al-Cr_Isothermal_Gamma-Gamma_prime.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.

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 " on page 27

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

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.
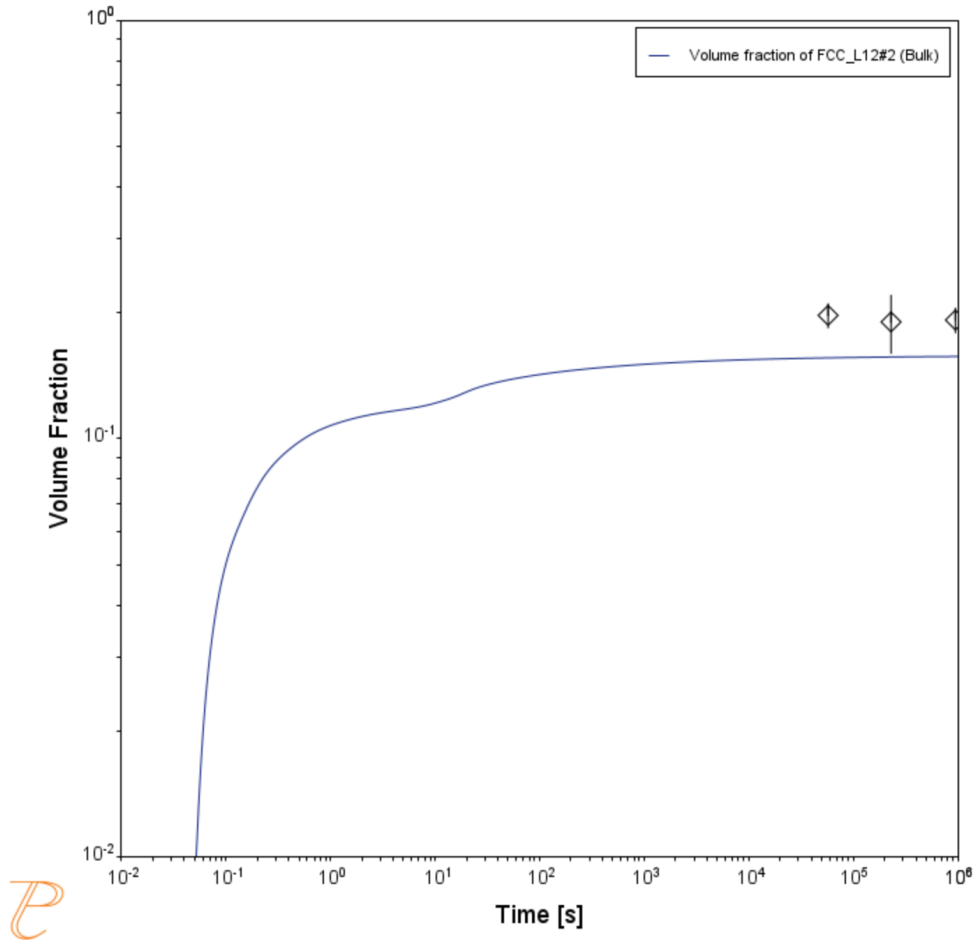
Figure 29: After performing the calculation, you can view the final Plot Renderer result on the applicable tab. This plot compares the predicted evolution of the volume fraction of gamma prime with the measurements of [2008Sud].
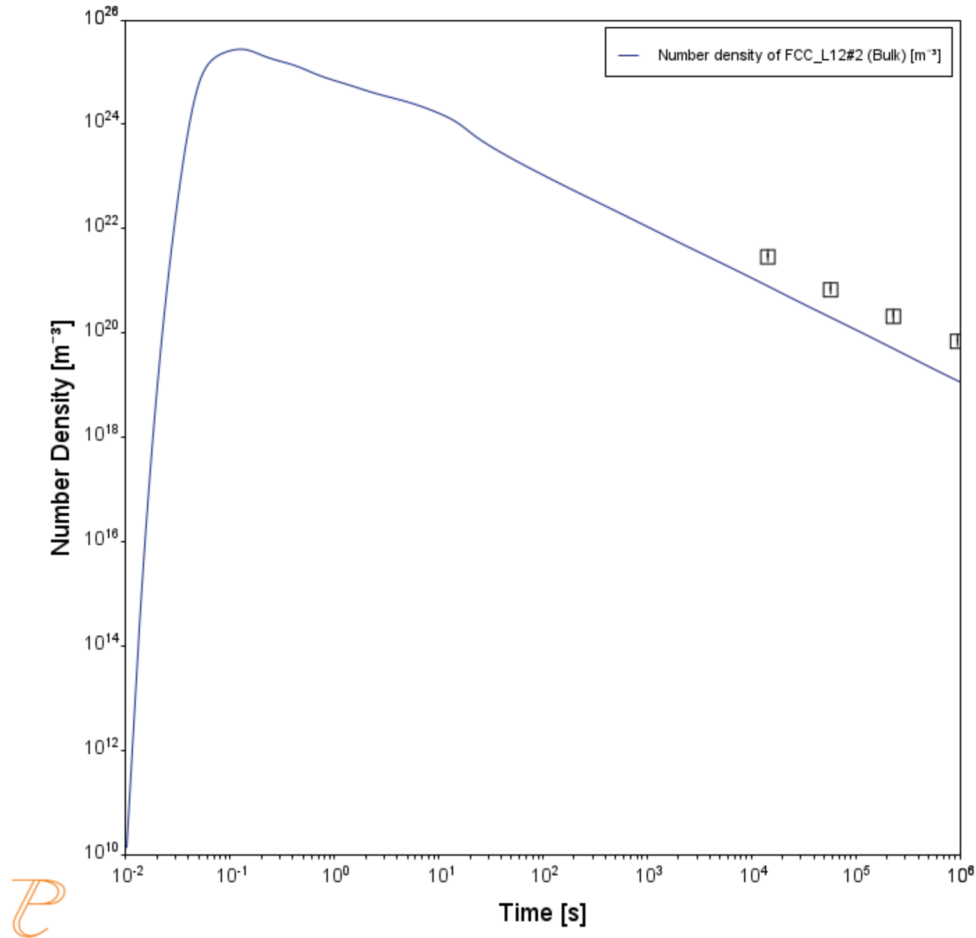
Figure 30: After performing the calculation, you can view the final Plot Renderer result on the applicable tab. This plot compares the predicted evolution of the number density of gamma prime with the measurements of [2008Sud].
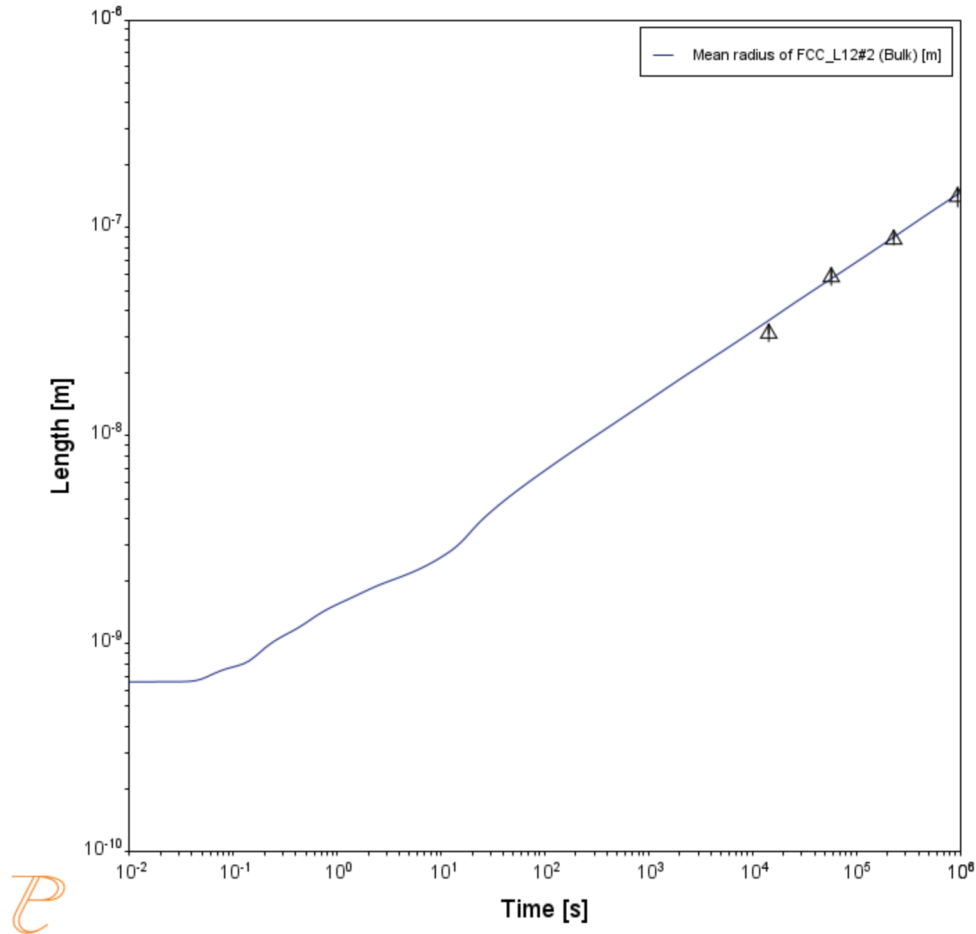
Figure 31: After performing the calculation, you can view the final Plot Renderer result on the applicable tab. This plot compares the predicted evolution of the mean particle radius of gamma prime with the measurements of [2008Sud].

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. The simulation results can be compared with experimental results from Rojhirunsakool et al. [2013Roj].

📄 DIS_FCC_A1 needs to be selected on the System Definer. See "Selecting the Disordered Phase as a Matrix Phase " on page 27 for details.

Open the example project file and click **Perform Tree** to generate the plots associated with it.

⧖ When you run (Perform) this example, it takes a few minutes for the calculations to complete.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**

- File name: *P_06_Precipitation_Ni-Al-Cr_Non-isothermal_Gamma-Gamma_prime.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.

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 " on page 27
Precipitate phase	FCC_L12#2

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 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 for 8Al-8Cr	The **Valley depth ratio** is set to 0.05 for both plots (mean radius and PSD) for this alloy. The number of **Points** is increased to 200 for an

	average radius plot.
Separate multimodal PSD for 10Al-10Cr	The **Valley depth ratio** is set to 0.18 for both plots (mean radius and PSD) for this alloy.

Visualizations

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.
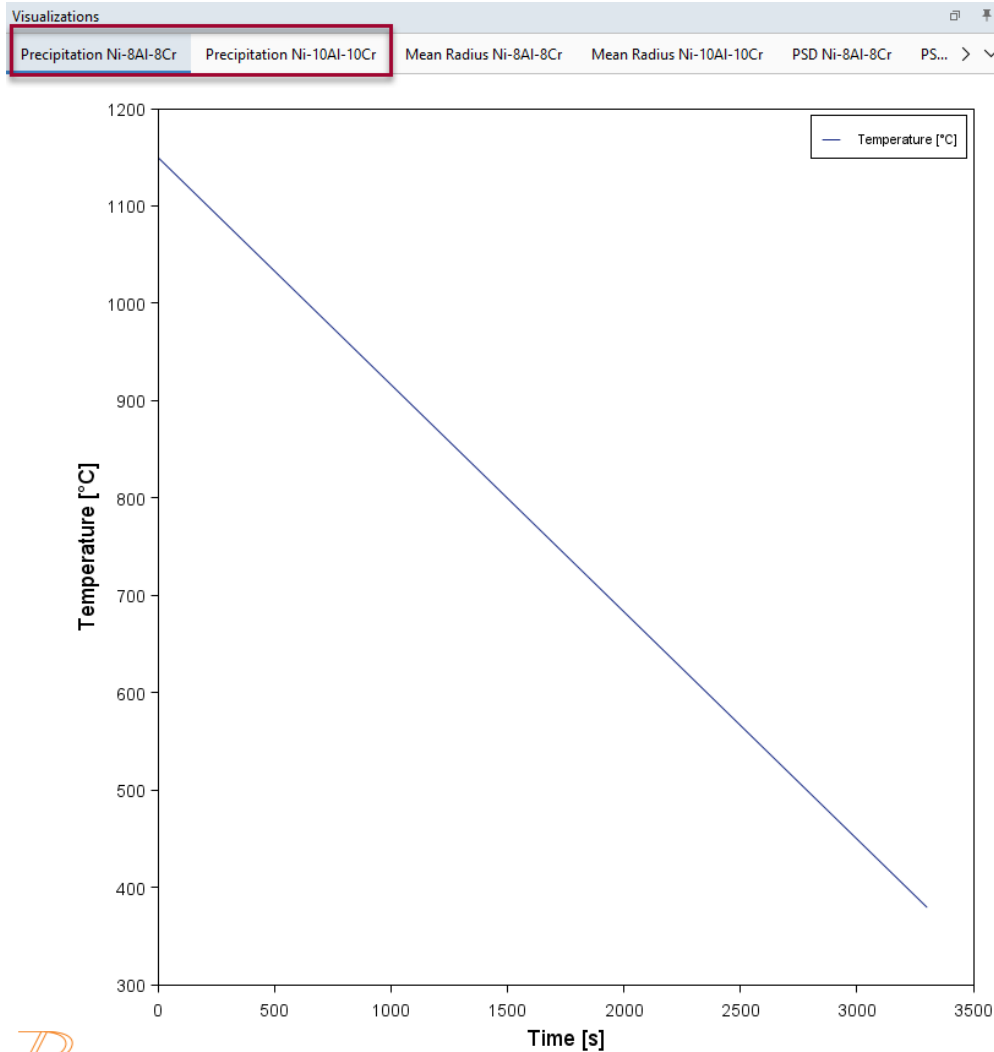
> For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **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 32: 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.
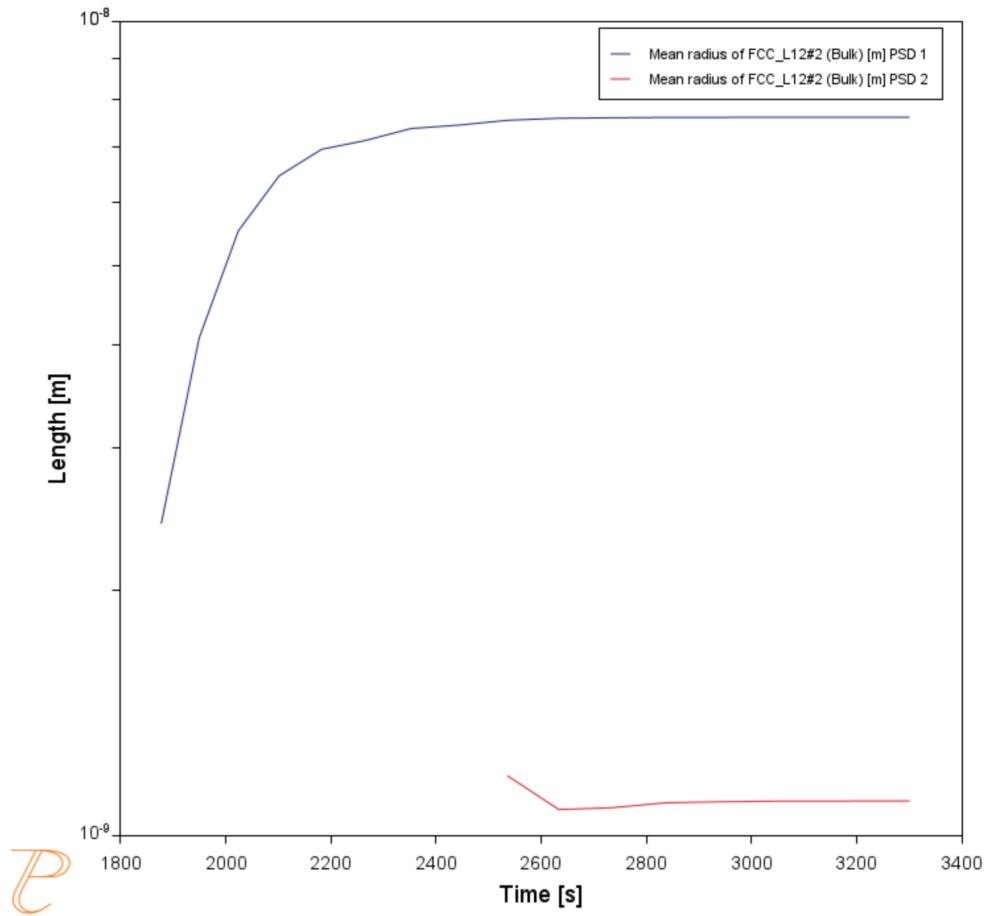
Figure 33: These results show the predicted evolution of the mean radius of gamma prime populations nucleating during the quench for the Ni-8Al-8Cr alloy. Note that the tertiary particles (second particle population) are very small, and this dispersion would appear monomodal without TEM characterization.
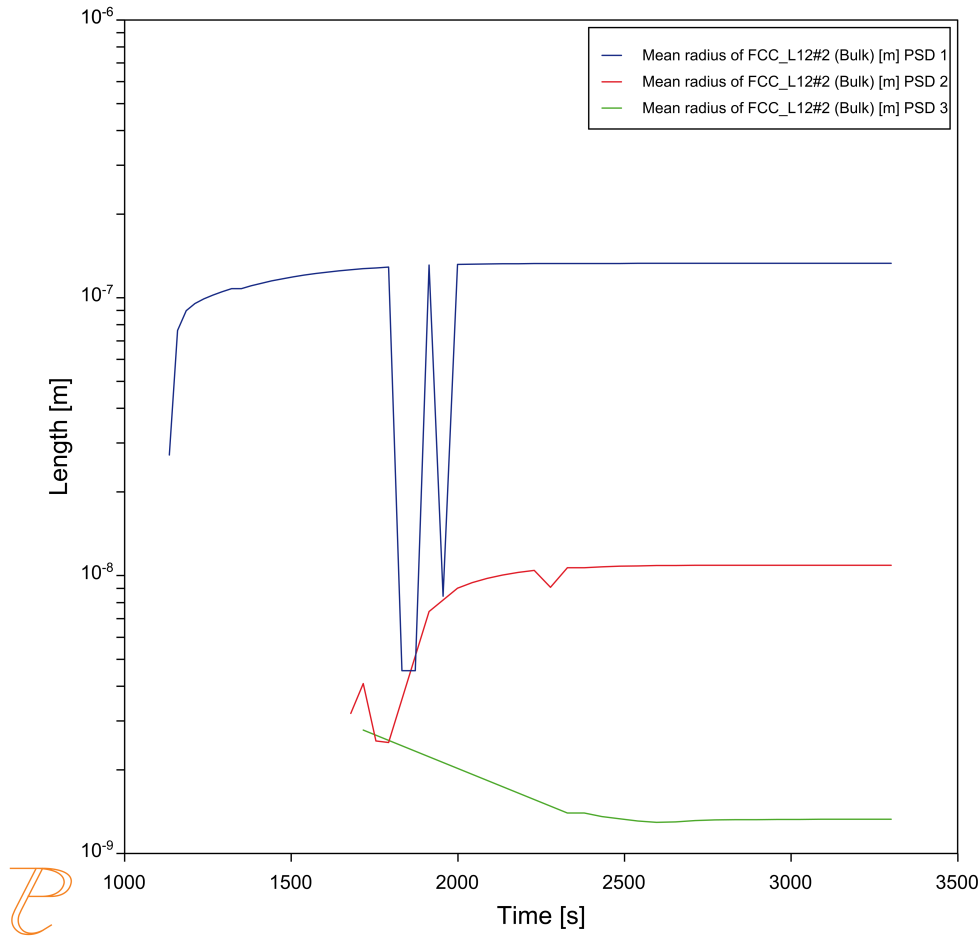
Figure 34: These results show the predicted evolution of the mean radius of gamma prime populations nucleating during the quench for the Ni-10Al-10Cr alloy. In this case three distinct particle populations are simulated to form, agreeing with [2013Roj].
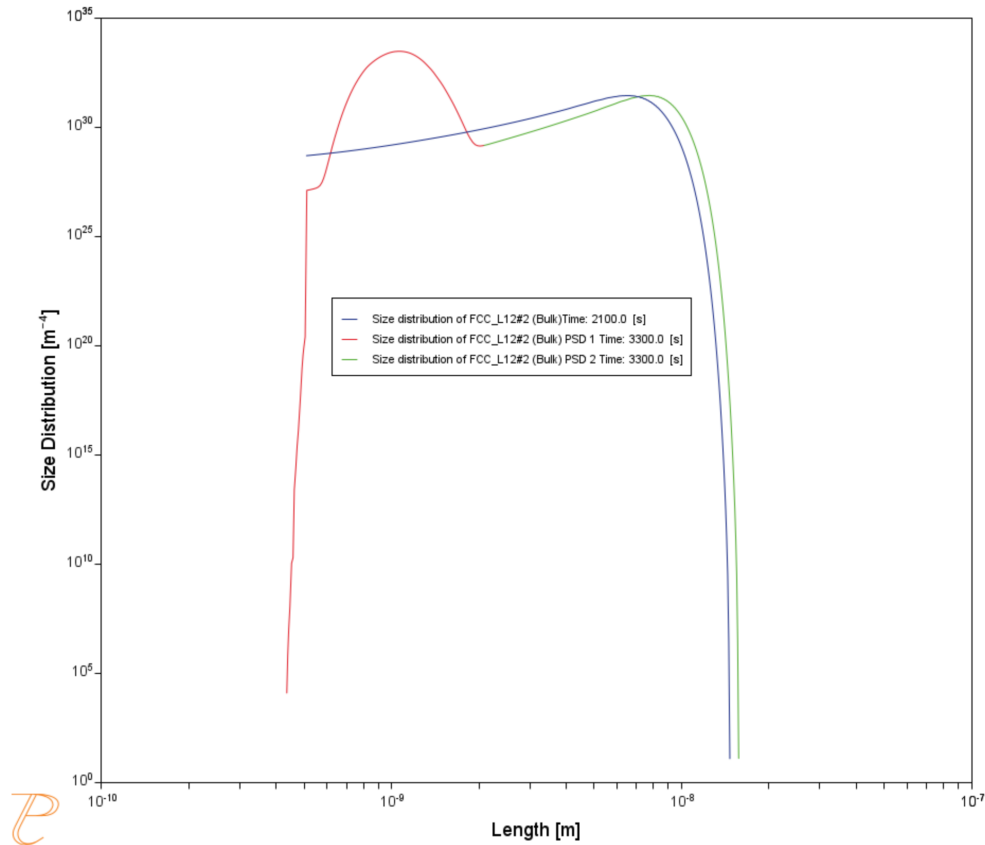
Figure 35: These results show the predicted size distributions of precipitates at different times during the quench of the for the Ni-8Al-8Cr alloy. The individual particle populations are distinguished using the "Separate multimodal PSD" option showing a bimodal distribution with very small nano-meter sized tertiary particles.
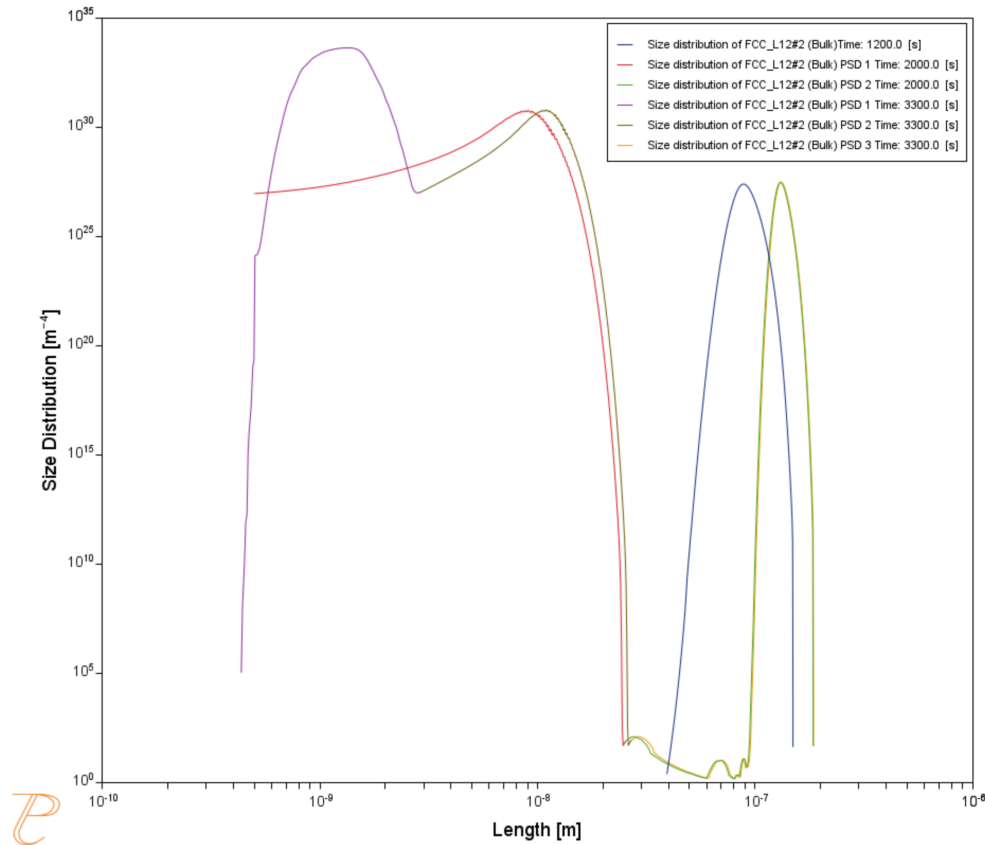
Figure 36: These results show the predicted size distributions of precipitates at different times during the quench of the for the Ni-10Al-10Cr alloy. The individual particle populations are distinguished using the "Separate multimodal PSD" option showing three large notable particle populations.

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.

Open the example project file and click **Perform Tree** to generate the plots associated with it.

> ⧗   When you run (Perform) this example, it takes a few minutes for the calculations to complete.

Project File, Step-By Step Instructions, and Video Tutorial Information

- Folder: **Precipitation Module - TC-PRISMA**

- File name: *P_07_Precipitation_Ni-Al-Cr_CCT_Gamma-Gamma_prime.tcu*

▶   This example is included as a Precipitation Module (TC-PRISMA) tutorial on our [website](#) and as part of the playlist on our [YouTube channel](#).

𝒫   You can also use [the step-by-step instructions](#) included in a PDF to follow the video or compare to the project file in Thermo-Calc.

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

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.
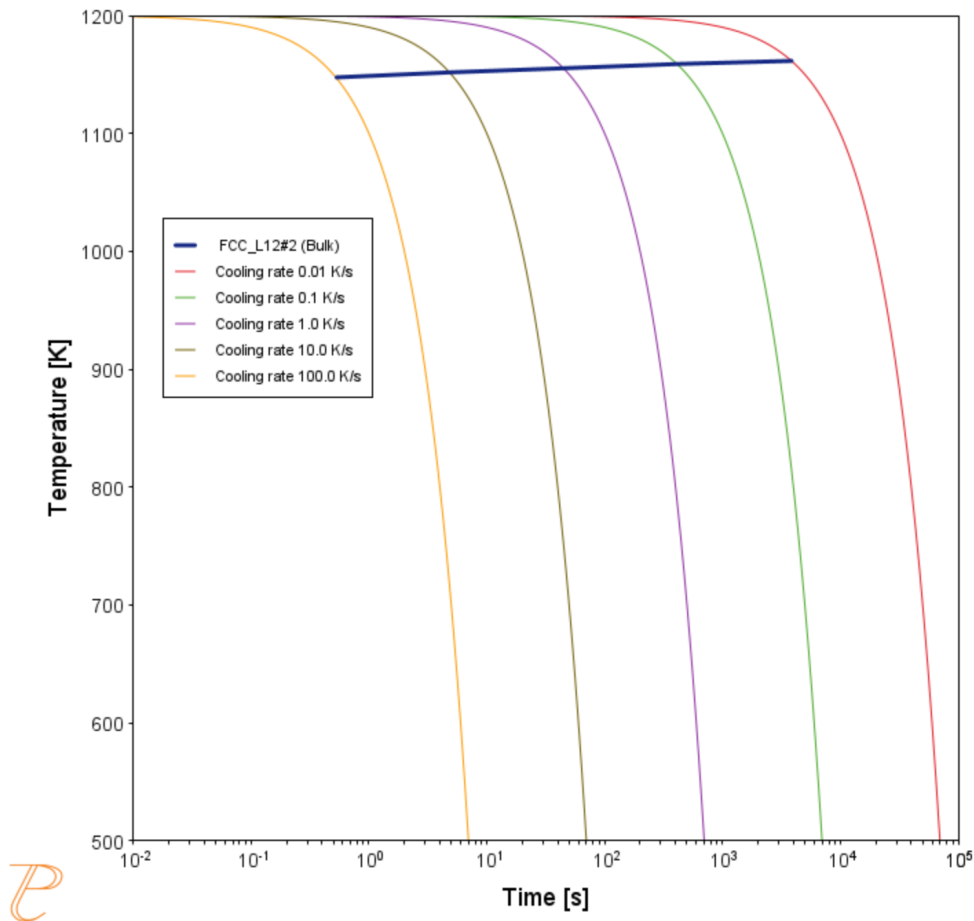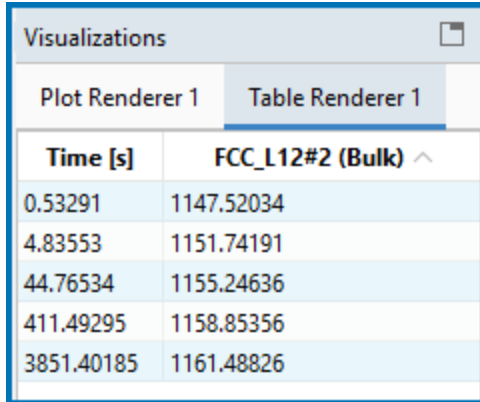
Figure 37: In this plot, the blue horizontal line shows the time it takes for γ' to transform at each of the cooling rates according to the stop criteria, which is set as 1e-4 volume fraction. The cooling rates are represented by the multicoloured curved lines.

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 38: 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.

Continuous Cooling Transformation (CCT) Diagram of Ni-Al-Cr γ-γ': Precipitation Example P_07

HELPFUL INFORMATION

- **All users can run this calculation,** even those who do not have a license for the Precipitation Module (TC-PRISMA).
- **A companion video** is available for this example , which can be watched here: https://www.youtube.com/playlist?list=PLfv6McToaTGSpqvuLoY3b_UV-8xpgLUkJ
- This calculation is based on Precipitation Module example *P_07 – Precipitation NI-Al-Cr_CCT_Gamma-Gamma_prime*, which is included in your installation.
1. To run the example file, open Thermo-Calc and select **Help > Examples Files** or click **Example Files** on the **My Project Configuration** window.
2. Open the *Precipitation Module (TC-PRISMA)* folder. Double-click the example file to open it.
3. In Thermo-Calc at the bottom center of the **Configuration** window click **Perform Tree**.
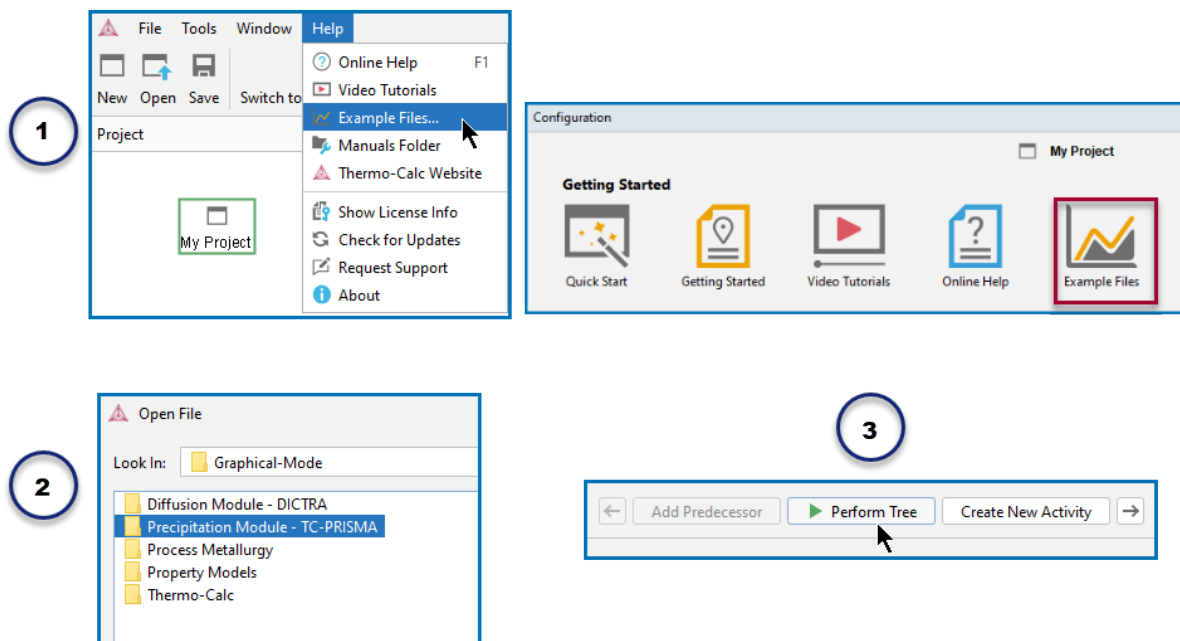

ABOUT THE EXAMPLE

This example shows you how to simulate a CCT diagram for gamma prime (γ') precipitation in a Ni-Cr-Al alloy using the Precipitation Module known as TC-PRISMA.

CCT stands for Continuous Cooling Transformation and is a calculation that maintains the same cooling rate the entire time.
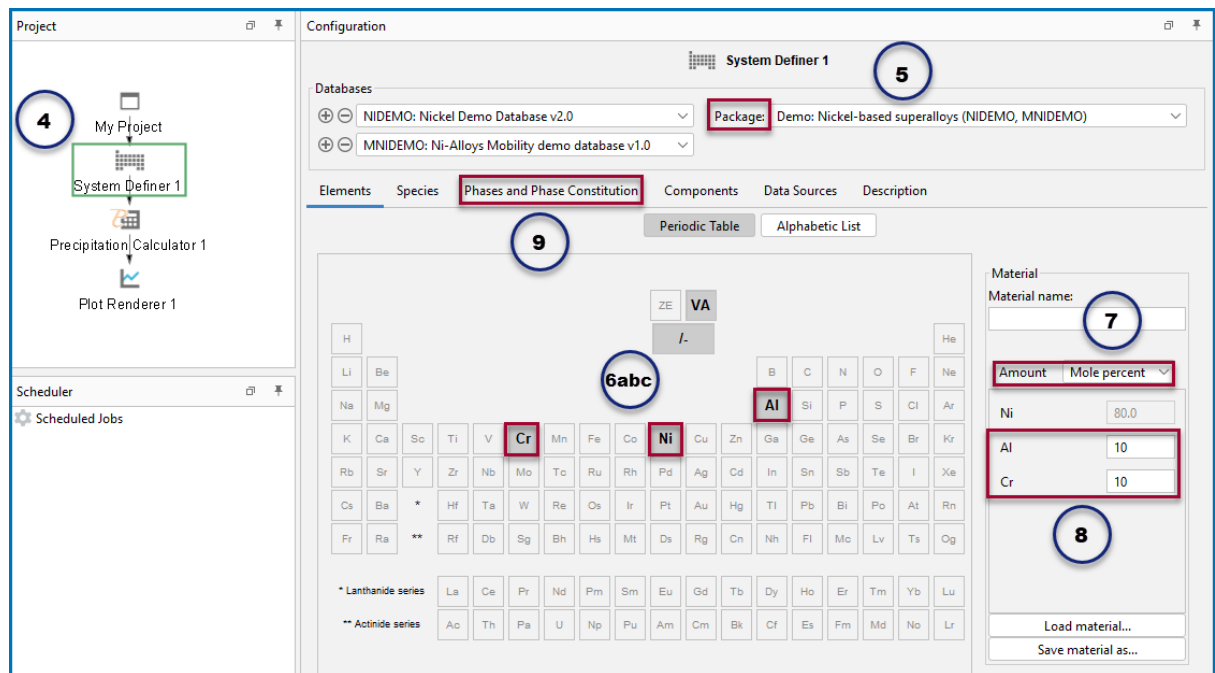
The system is a Ni-10Al-10Cr γ - γ' alloy and it is calculated and plotted with superimposition of the cooling rate values using the Precipitation Module (TC-PRISMA).
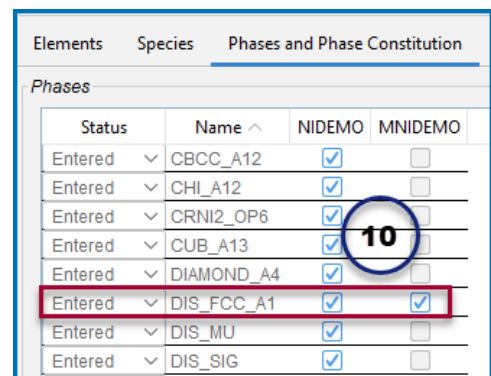
SETTING UP THE SYSTEM

1. Open Thermo-Calc in Graphical Mode.
2. On the **My Project Configuration** window under **Non-Equilibrium**, click **Precipitation**.
3. All the nodes for a precipitation calculation are added to the **Project** window:
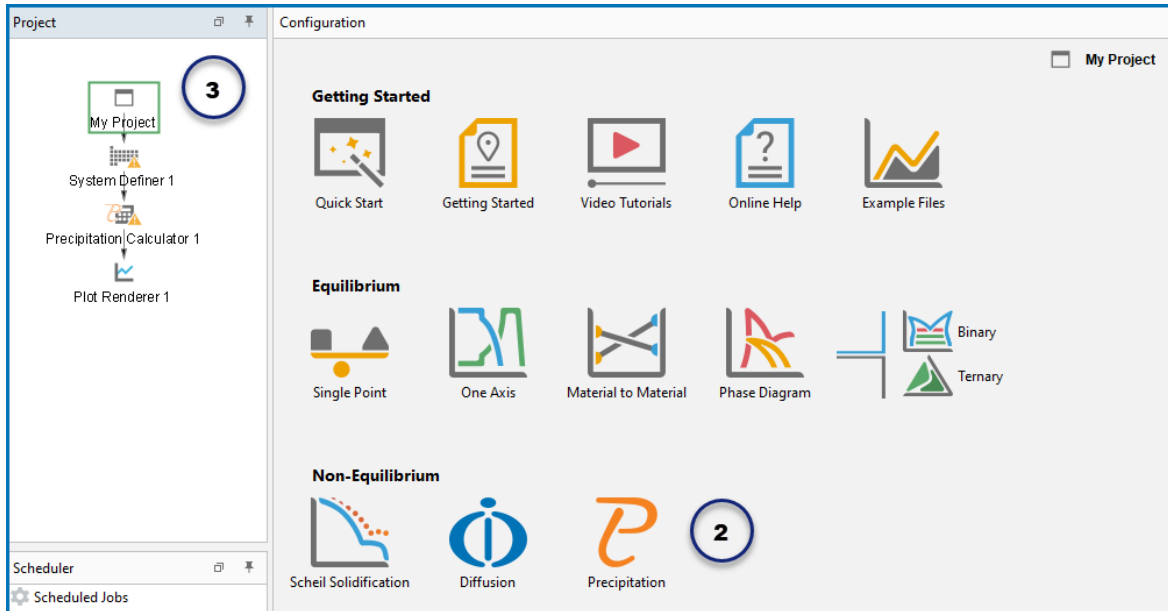
4. In the **Project** window, click the **System Definer 1** node.
5. On the **Configuration** window from the *Package* list, select **Demo: Nickel-based alloys (NIDEMO, MNIDEMO).** This loads both thermodynamic and kinetic demonstration nickel databases.
6. From the **Periodic Table**, select the elements in the following order.
   Select Ni first so that it is the dependant element.
   a. **Ni** (nickel)
   b. **Al** (aluminium) then
   c. **Cr** (chromium).
7. From the *Amount* list (to the right of the Periodic Table), select **Mole percent**.
8. Enter 10 for **Al** and 10 for **Cr**, which automatically sets **Ni** to 80 mole percent.

9. Click the **Phases and Phase Constitution** tab.
10. Under *Phases* click to select both check boxes next to the disordered FCC phase, **DIS_FCC_A1**.
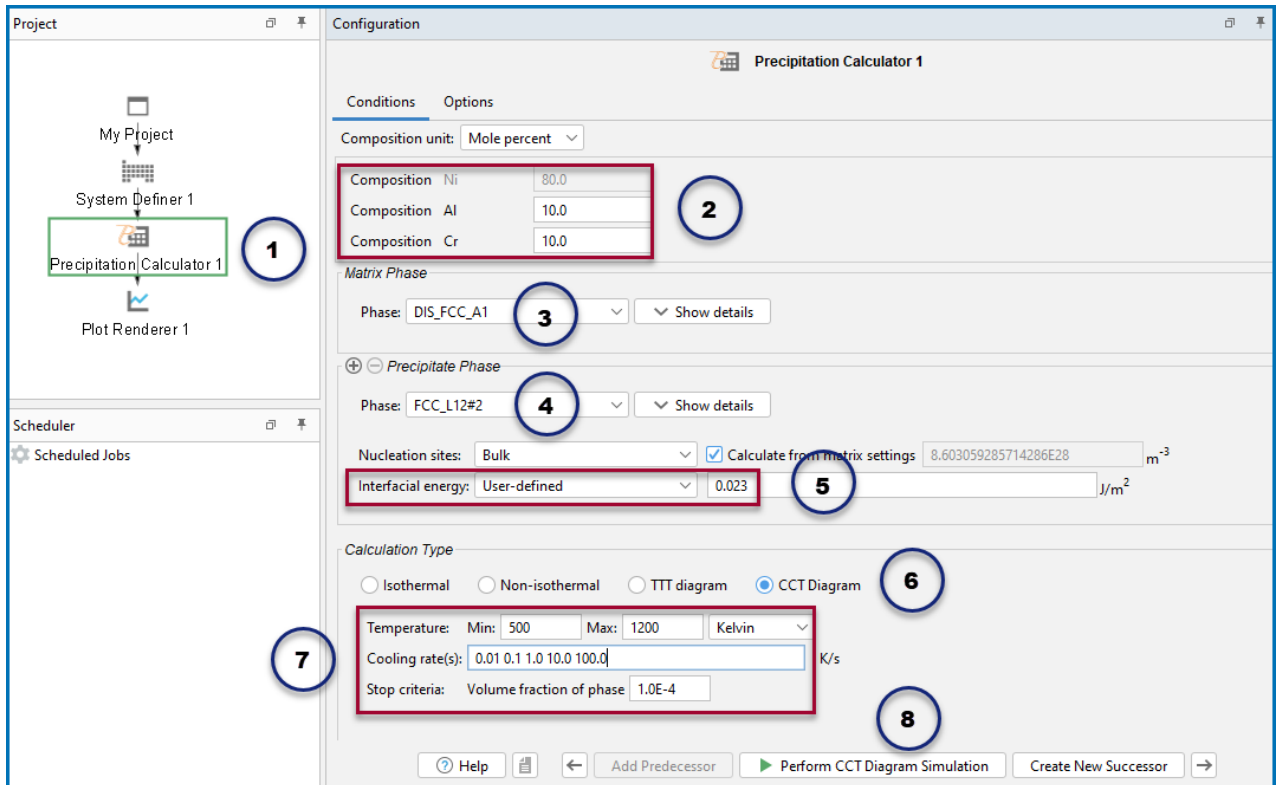

The system is now defined. The next step is to set up the precipitation calculations.

SETTING UP THE PRECIPITATION CALCULATION

1. In the **Project** window, click the **Precipitation Calculator 1** node.
2. Notice that the composition set in the *System Definer* auto-populated here.
3. Under *Matrix Phase*, from the *Phase* list select **Dis_FCC_A1**, which is the disordered FCC phase.
4. Under *Precipitate Phase* from the *Phase* list scroll to select **FCC_L12#2**.
5. Change the *Interfacial energy* to **User-defined** then enter 0.023 in the field.
6. Under *Calculation Type*, click **CCT Diagram**, which stands for Continuous-Cooling-Transformation and means that the same cooling rate is maintained throughout the calculation.
7. In the fields set:
    a. *Min* (minimum) *Temperature* to 500.
    b. *Max* (maximum) *Temperature* to 1200.
    c. Keep the default **Kelvin** as the temperature unit.
    d. Enter several cooling rates for the calculation. The rates are separated by a space. Enter these values as shown: .01 .1 1 10 100.

      e.   Keep the default **Stop criteria** of `1E-4` volume fraction of the γ' phase.

8. The calculation is now set. At the bottom, center of the **Configuration** window click **Perform CCT Diagram Simulation**.

INTERPRETING THE RESULTS OF THE PRECIPITATION CALCULATION
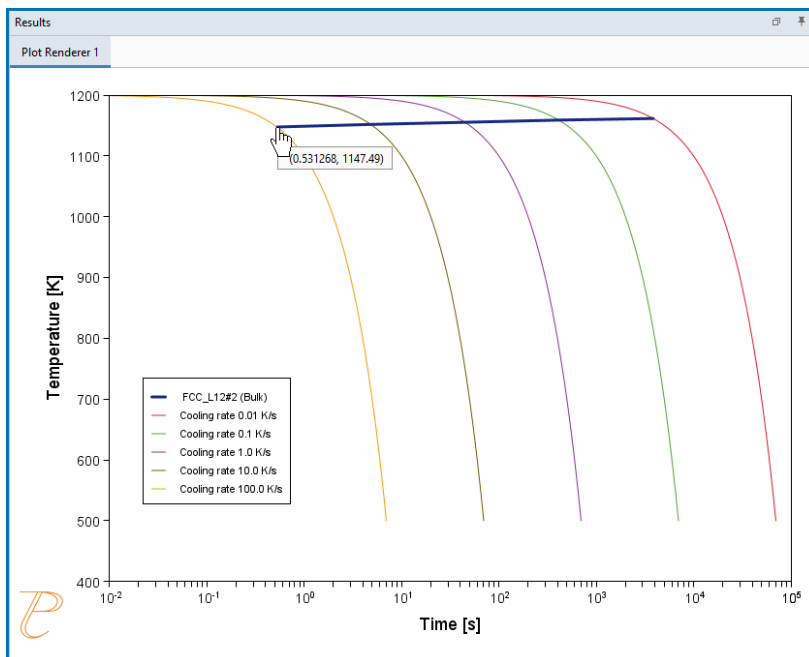
In this plot, the blue, horizontal line shows the time it takes for gamma prime (γ') to transform at each of the cooling rates according to the stop criteria, which we set as 1e-4 volume fraction.

In this plot, the blue 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 multi-coloured 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. In the image above, you can see a time of 0.531268 seconds and a temperature of 1147.49 Kelvin for the cooling rate of 100.0 K/s, which is represented by the yellow line.

SHOWING THE RESULTS AS A TABLE

You can also view these results in the form of a table, which gives you more precise results.
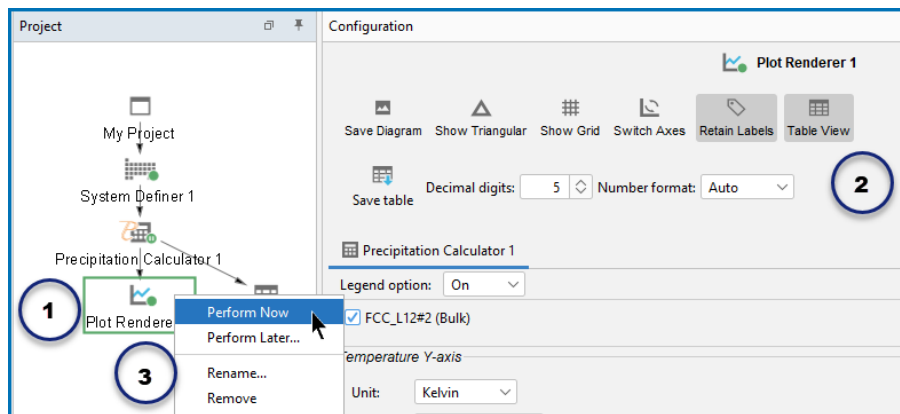
1. In the **Project** window, right-click the **Precipitation Calculator 1** node and select **Create New Successor>Table Renderer**.
2. Right-click the **Table Renderer 1** node and select **Perform Now**.

The table is shown in the **Results** window and 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.

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

Tip! You can also convert the plot data into a table format that includes all the points.

1. On the **Project** window, click **Plot Renderer 1.**
2. On the **Configuration** window, click the **Table View** button
3. After clicking the button, click **Perform** at the bottom of the window or right-click the **Plot Renderer 1** node and select **Perform Now**.
4. View the converted data on the **Results** window.

Time [s]	FCC_L12#2 (Bulk)	Time [s] [1]	Cooling rate 0.01 K/s	Time [s] [2]	Cooling rate 0.1 K/s
0.53291	1147.52034	0.01000	1199.99990	0.01000	1199.99900
4.83553	1151.74191	0.01082	1199.99989	0.01070	1199.99893
44.76534	1155.24636	0.01172	1199.99988	0.01145	1199.99886
411.49295	1158.85356	0.01268	1199.99987	0.01225	1199.99878
3851.40185	1161.48826	0.01373	1199.99986	0.01311	1199.99869

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" on page 96.

Open the example project file and click **Perform Tree** to generate the plots associated with it.

> ⧗ When you run (Perform) this example, it takes a few minutes for the calculations to complete.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**

- File name: *P_08_Precipitation_Cu-Ti_CU4TI1_Sphere_Needle.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.

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**.

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

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 39: The predicted evolution of the morphology of needle shaped precipitates, showing how the mean aspect ratio changes during the isothermal heat treatment.
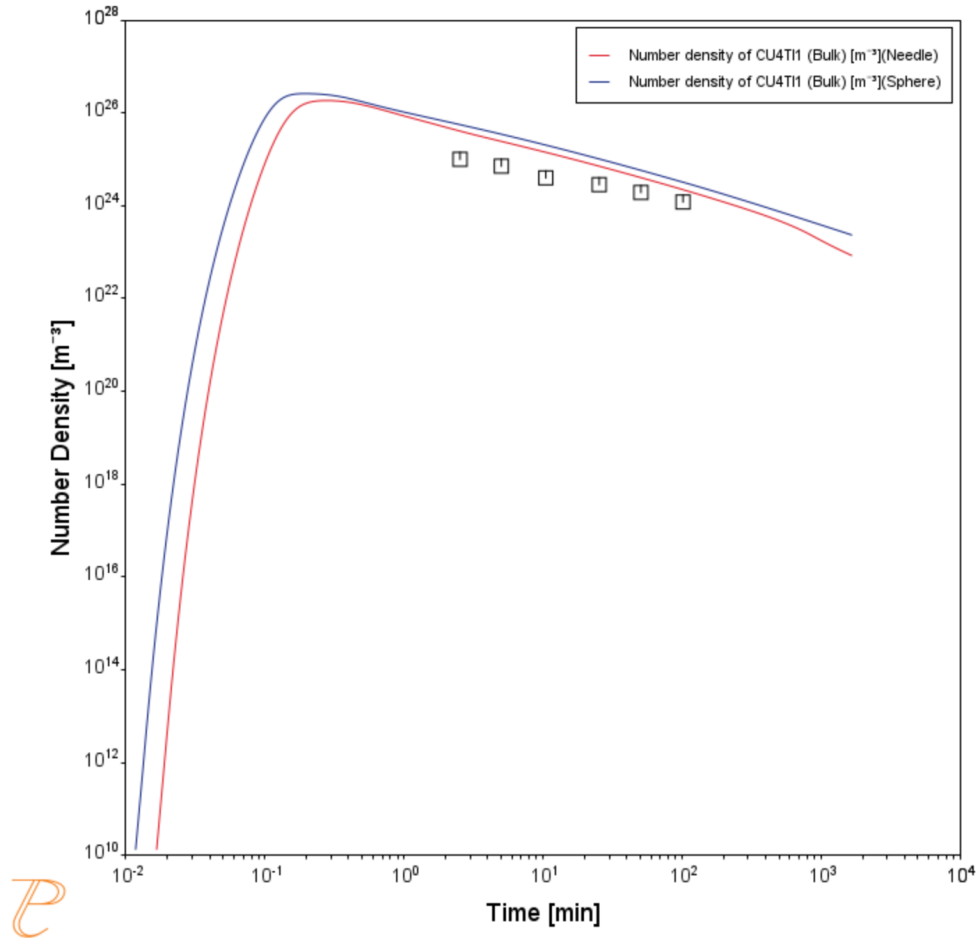
Figure 40: The results compare the predicted evolution of the mean size of precipitates with the experimental data from [1987Kam], comparing the spherical and needle shaped approximations of the precipitate morphology. Note how the needle shape approximation is closer to the experimental data.
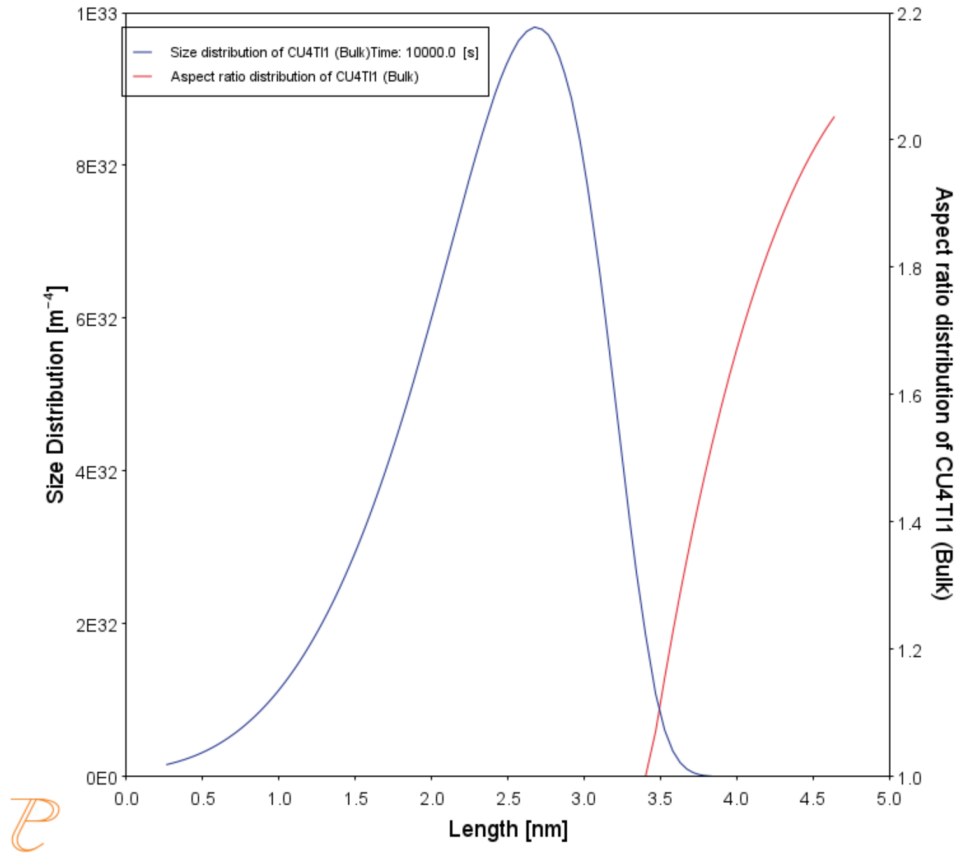
Figure 41: These results show both the predicted final particle size distribution from the needle shape simulation and the predicted relationship between the length of the precipitate and the needle aspect ratio.
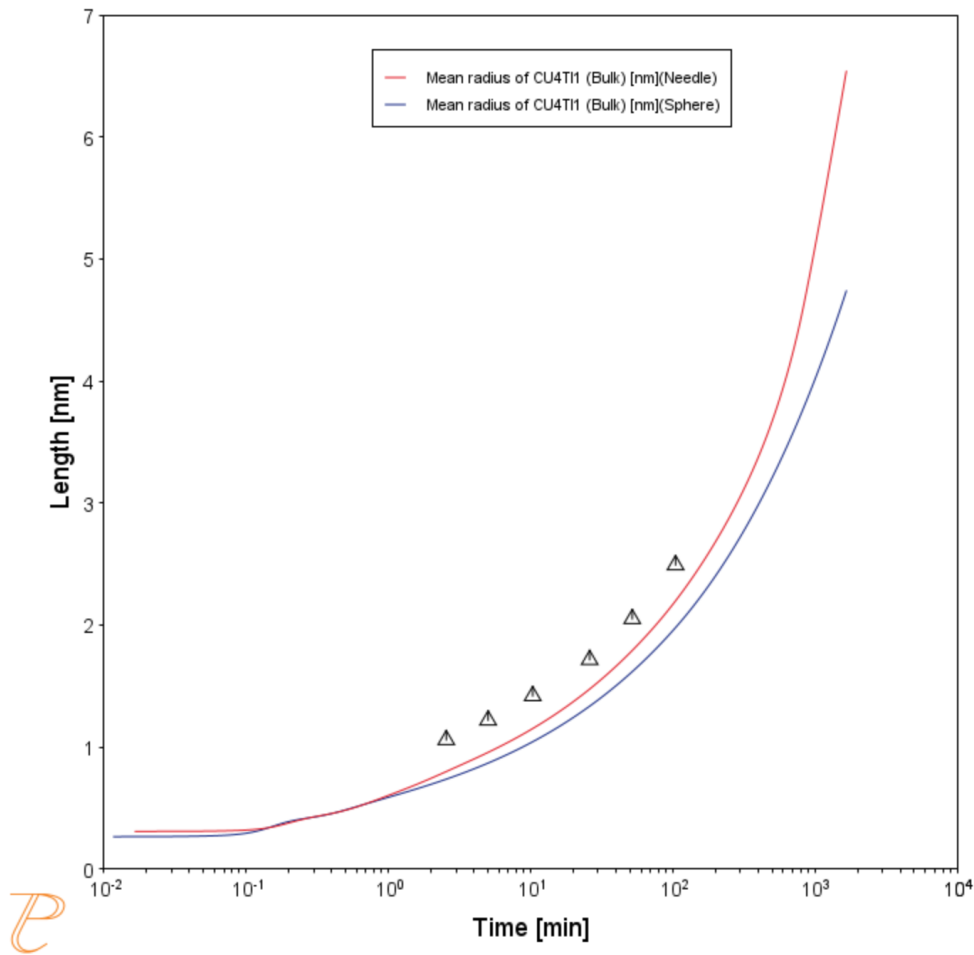
Figure 42: This shows the approximates the size of the needle shaped precipitates as a sphere of equivalent volume, and compares the experimental results of [1987Kam] with those obtained from a spherical and needle shaped approximation.

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" on page 96.

Open the example project file and click **Perform Tree** to generate the plots associated with it.

Project File, Step-By Step Instructions, and Video tutorial Information

- Folder: **Precipitation Module - TC-PRISMA**

- File name: *P_09_Precipitation_Al-Sc_AL3SC_Sphere_Cuboid.tcu*

▶️   This example is included as a Precipitation Module (TC-PRISMA) tutorial on our website and as part of the playlist on our YouTube channel.

𝒫   You can also use the step-by-step instructions included in a PDF to follow the video or compare to the project file in Thermo-Calc.

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

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 43: 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.
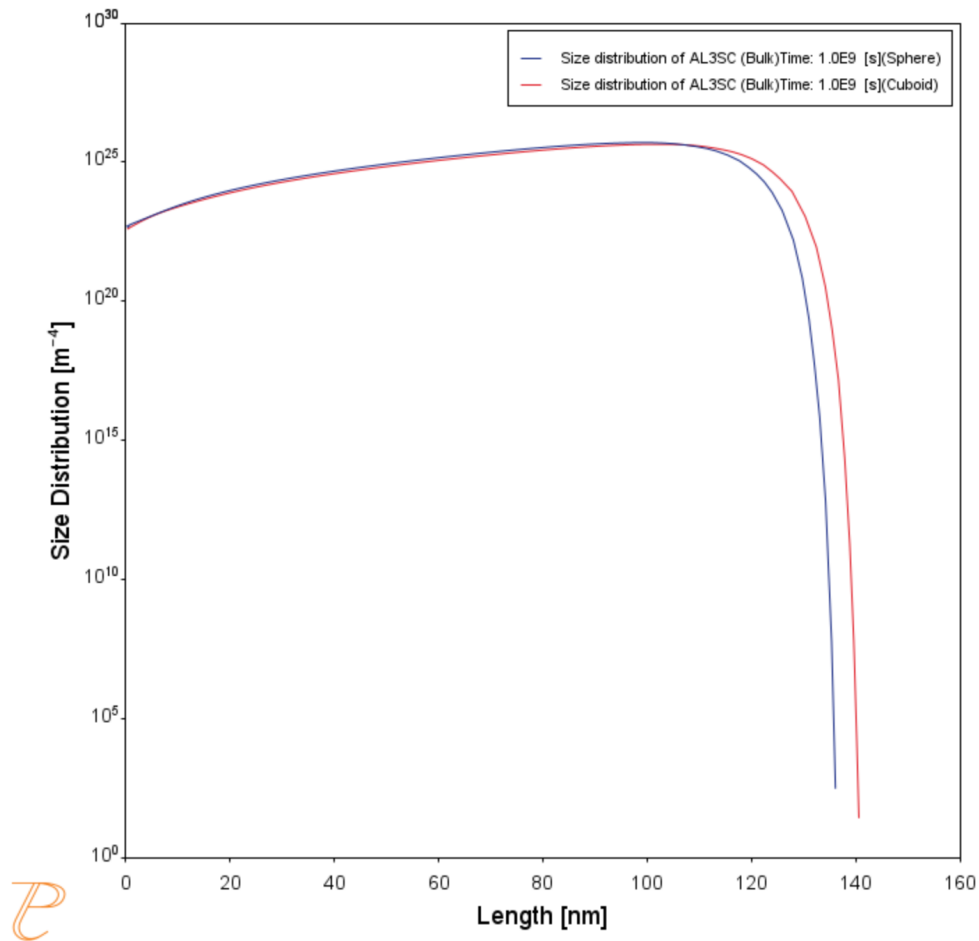
Figure 44: These results compare the predicted size distributions after heat treatment considering the spherical and cuboidal approximations of the precipitate morphology.
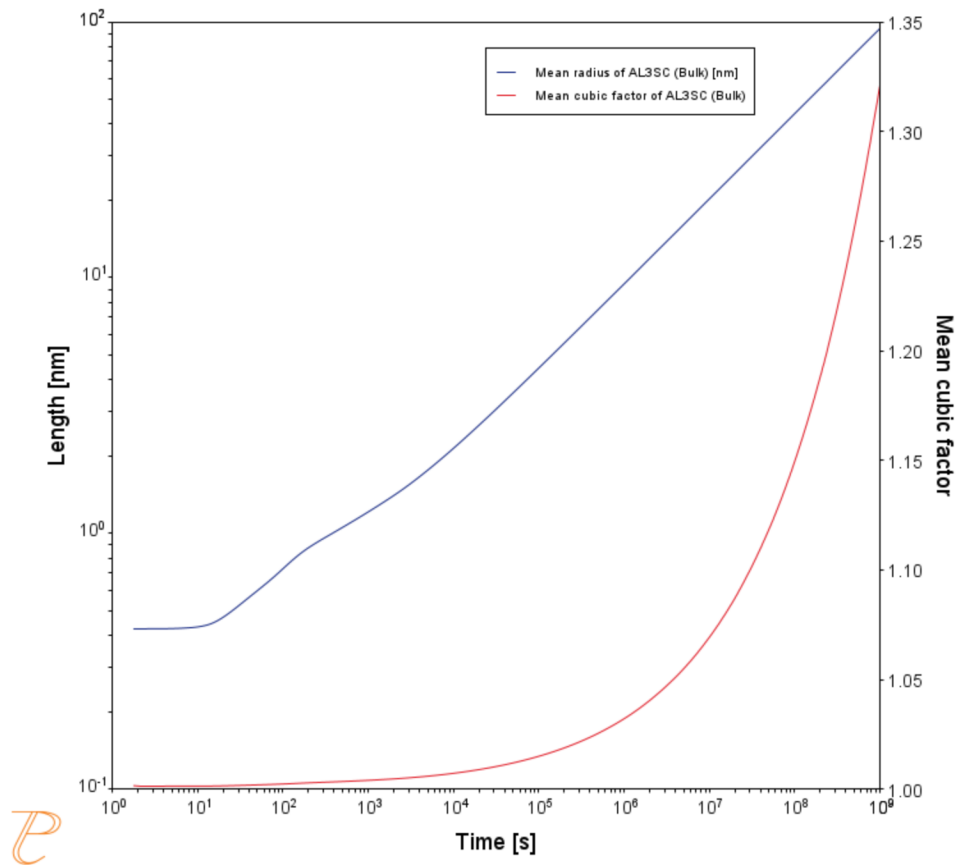
Figure 45: These results compare the predicted evolution of the mean particle radius and mean aspect ratio from using the cuboidal approximation of the precipitate morphology. In this case, the radius of a sphere of equivalent volume to the cuboidal precipitate is shown.
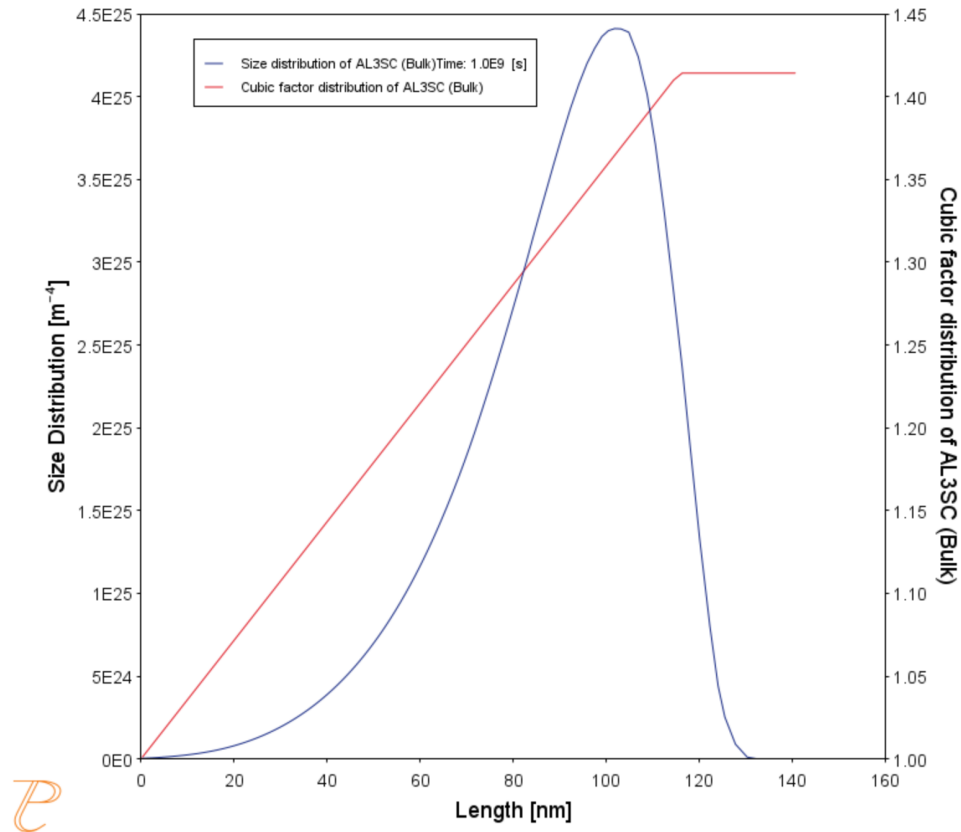
Figure 46: These results show the predicted size distribution of the precipitates obtained from the cuboidal approximation of the precipitate morphology. Also shown is the calculated size dependent cubic factor of the cuboids associated with this dispersion.

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).

Precipitation of Al-Sc AL3SC with Assumption
of Sphere and Cuboid Morphologies
Precipitation Example P_09

Precipitation of Al-Sc AL3SC with Assumption of Sphere and Cuboid Morphologies: Precipitation Example P_09

HELPFUL INFORMATION

- **All users can run this calculation**, even those who do not have a license for the Precipitation Module (TC-PRISMA).
- **A companion video** is available for this example , which can be watched here: https://www.youtube.com/playlist?list=PLfv6McToaTGSpqvuLoY3b_UV-8xpgLUkJ
- This calculation is based on Precipitation Module example *P_09 – Precipitation_Al-Sc_AL3SC_Sphere_Cuboid*, which is included in your installation.
1. To run the example file, open Thermo-Calc and select **Help > Examples Files** or click **Example Files** on the **My Project Configuration** window.
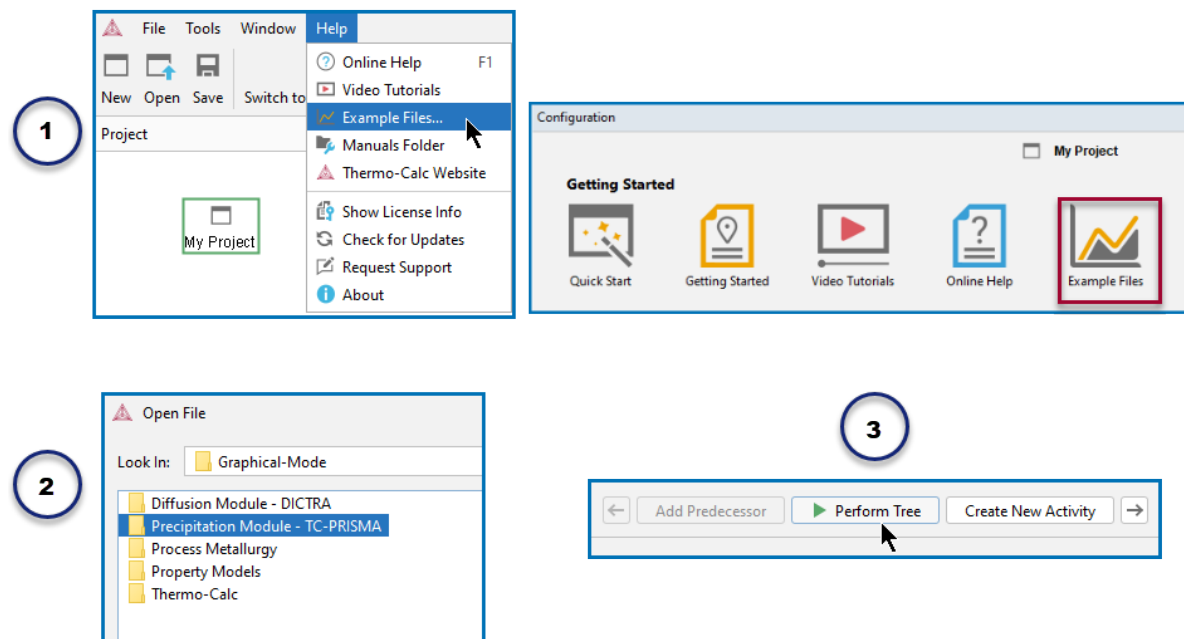2. Open the *Precipitation Module (TC-PRISMA)* folder. Double-click the example file to open it.
3. In Thermo-Calc at the bottom center of the **Configuration** window click **Perform Tree**.

ABOUT THE EXAMPLE

This example shows you how to calculate the precipitation of Al_3Sc phase from FCC_A1 matrix phase in an Al-Sc binary alloy using the Precipitation Module (TC-PRISMA).

Two separate calculations are performed so you can make a comparison of the results, 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.

In addition, mean cubic factor and cubic factor distribution are plotted for cuboid shape to illustrate the spherical-cuboidal transition during precipitation.

Precipitation of Al-Sc AL3SC with Assumption
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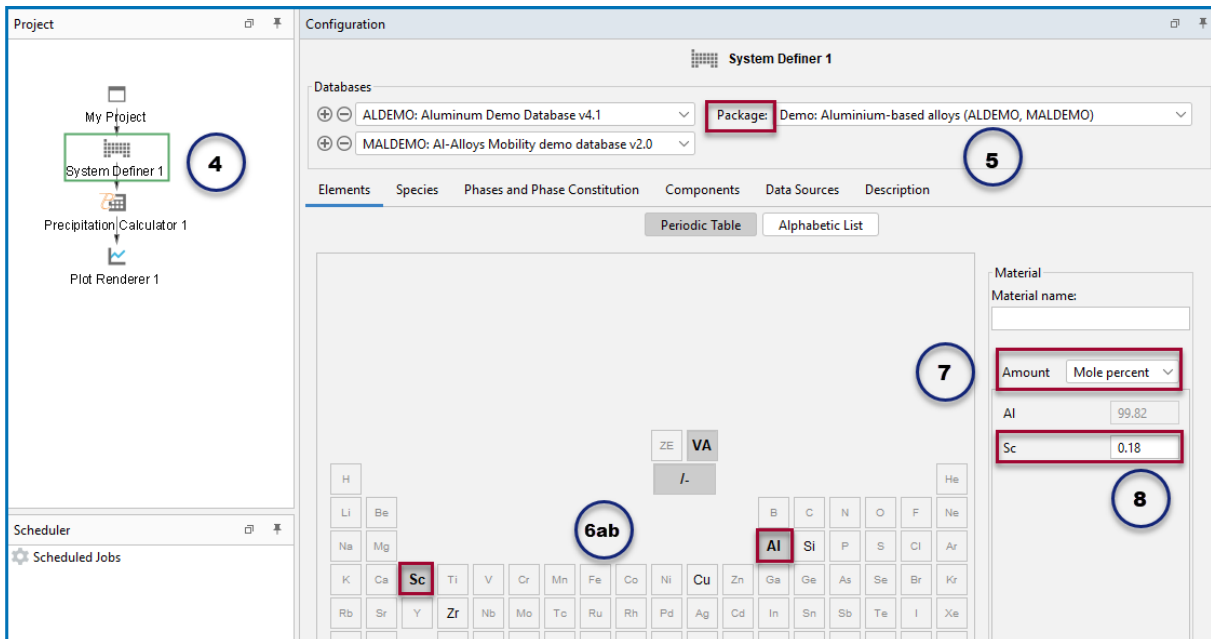
If you run the example file included in your software, the simulation results are compared with experimental data collected from Marquis and Seidman (2001) and Novotny and Ardell (2001).

SETTING UP THE SYSTEM

1. Open Thermo-Calc in Graphical Mode.
2. On the **My Project Configuration** window under **Non-Equilibrium**, click **Precipitation**.
3. All the nodes for a precipitation calculation are added to the **Project** window:
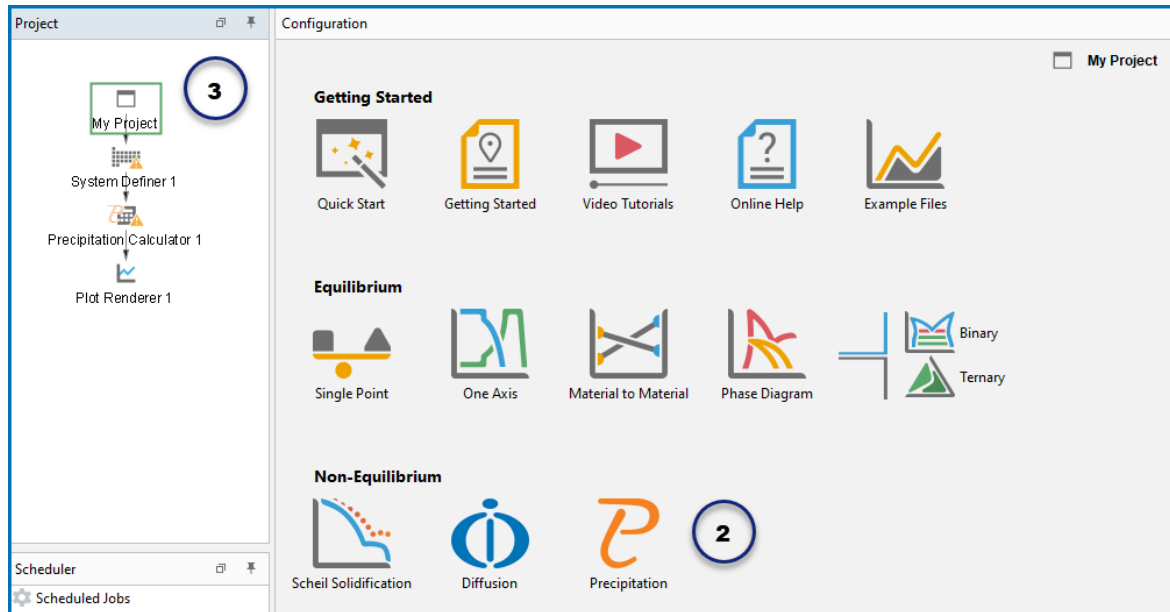
4. In the **Project** window, click the **System Definer 1** node.
5. Set the database *Package* to **Demo: Aluminium-based alloys (ALDEMO, MALDEMO)**, which loads both thermodynamic and kinetic demonstration aluminium databases.
6. From the **Periodic Table**, select the elements in the following order.
   Select Al first so that it is the dependant element:
   a. **Al** (aluminium)
   b. **Sc** (scandium).
7. From the *Amount* list (to the right of the Periodic Table), select **Mole percent**.
8. Enter 0.18 for **Sc**. This automatically sets **Al** to 99.82.

Precipitation of Al-Sc AL3SC with Assumption
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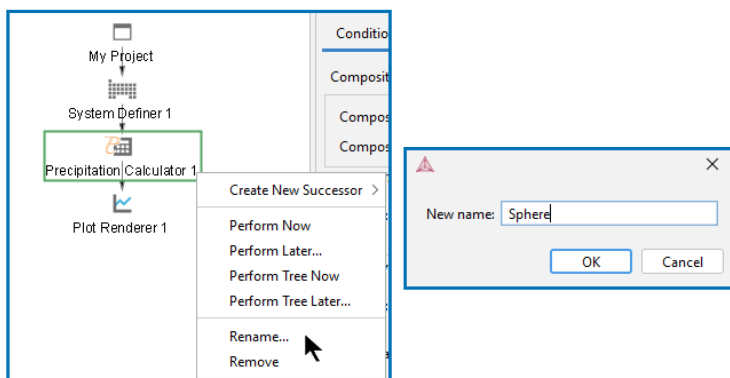
Our system is now defined. Now set up the precipitation calculations.

SETTING UP THE PRECIPITATION CALCULATIONS

There are two precipitation calculations in this example, 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 results are then compared for both calculations.

Setting up the Precipitation Calculation with Spherical Morphology

1. In the **Project** window, right-click the **Precipitation Calculator 1** node and select **Rename.** Enter `Sphere`, then press enter or click **OK**.

2. Notice that the composition set in the *System Definer* auto-populated on the Precipitation Calculator.
3. Under *Matrix Phase* from the *Phase* list it defaults to **FCC_A1**.
4. Under *Precipitate Phase* from the *Phase* list select **AL3SC**.
5. Under *Calculation Type*, make sure **Isothermal** is selected, which means that the same temperature is maintained throughout the calculation.
6. Enter
    a. `350` as the *Temperature* and select **Celsius**.

Precipitation of Al-Sc AL3SC with Assumption
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Precipitation Example P_09
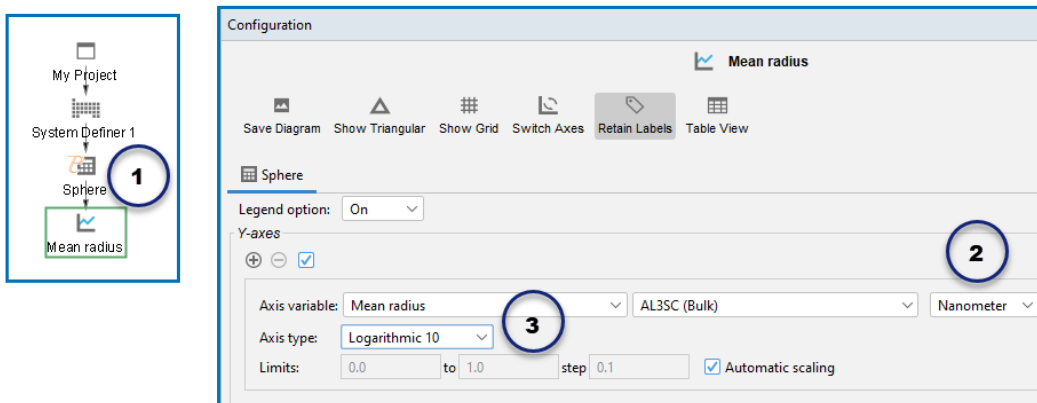
b. `1.0E9` as the *Simulation time* and select **Seconds**.

Our first calculation is set, so next configure the plot.

Configuring the Plot

1. In the **Project** window, right-click **Plot Renderer 1** and select **Rename**. Name the plot `Mean radius` then press enter or click **OK**.
2. Under *Y-axes* change the units to **Nanometer** (nm).
3. From the *Axis type* list select **Logarithmic 10***.*

The plot is now set, but before running the simulation you set up another calculation and link it to the same Plot Renderer.

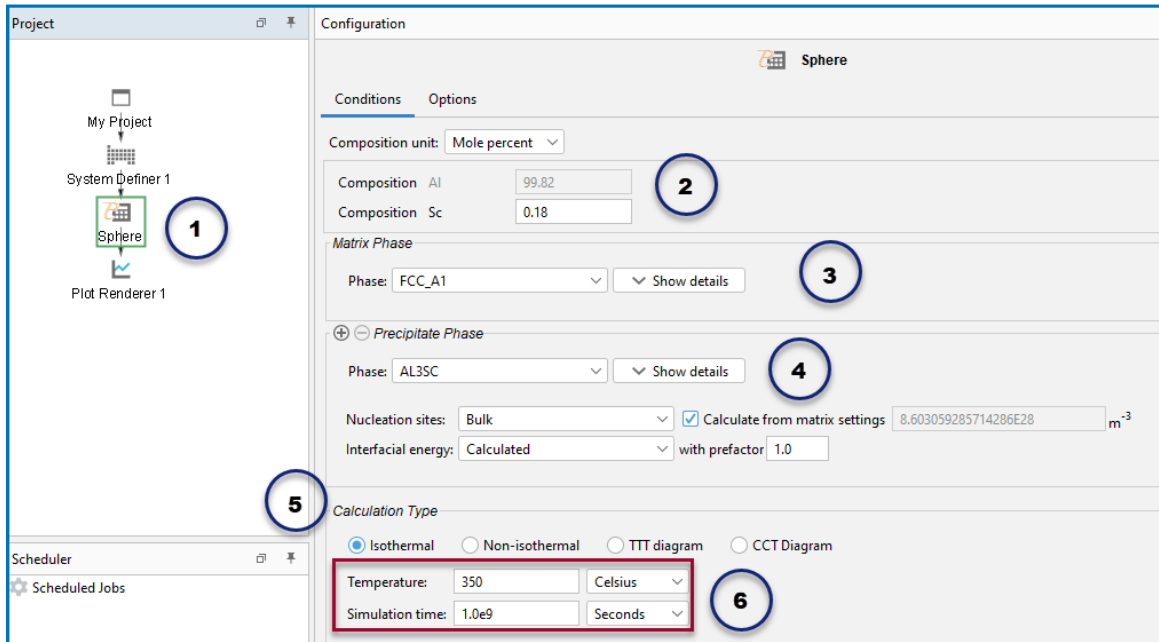### Setting up the Precipitation Calculation with Cuboid Morphology

1. In the **Project** window, right-click the **Sphere** node and select **Clone**.
    a. Right-click the **Sphere 1** node and select **Rename**.
    b. Name the node `Cuboid` and press enter or click **OK**.
2. On the **Configuration** window to the right of *Matrix Phase* click **Show Details***.*

Precipitation of Al-Sc AL3SC with Assumption
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3. From the *Elastic Properties* list select **Cubic**. Keep the suggested default values. Click **Hide details**.
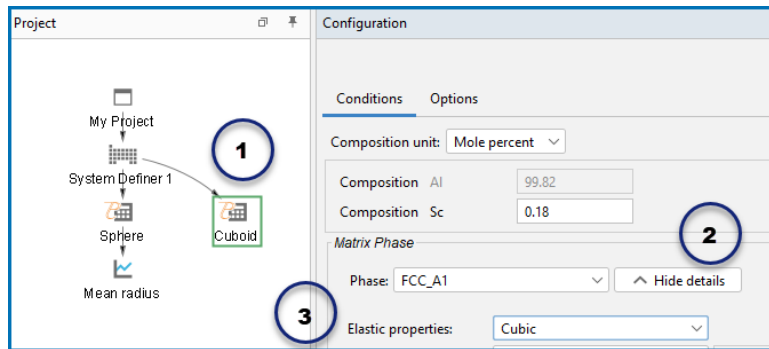
4. To the right of *Precipitate Phase*, click **Show details**.
5. From the *Morphology* list select **Cuboid**.
6. From the *Transformation strain* list select **Calculate from molar volume**.
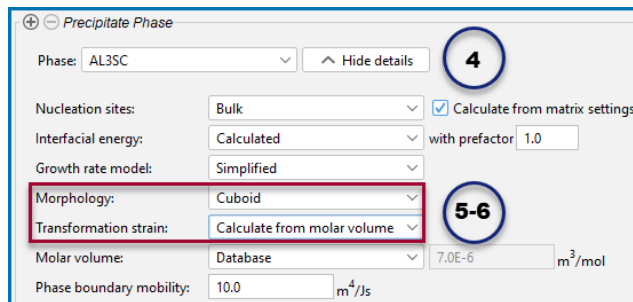
The second calculation is now set up, so now link it to the Plot Renderer node.

Linking the Plot to the Calculation with Cuboid Morphology

1. In the **Project** window, right-click the **Mean radius** node and select **Add Predecessor >Cuboid**.
2. Notice that in the **Configuration** window there are two tabs associated with this plot, one for **Sphere** and one for **Cuboid**. The Sphere settings are already configured, so you just need to set up the Cuboid tab.
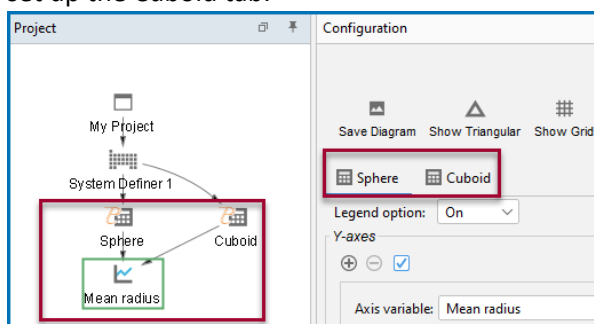
3. Click the **Cuboid** tab.
4. Under *Y-axes* change the units to **Nanometer** (nm).
5. From the *Axis type* list select **Logarithmic 10**.
6. The calculation is now ready to run. Right-click the **Mean radius** node and select **Perform Now** or click **Perform** on the **Configuration** window.

Precipitation of Al-Sc AL3SC with Assumption
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INTERPRETING THE RESULTS OF THE PRECIPITATION CALCULATIONS
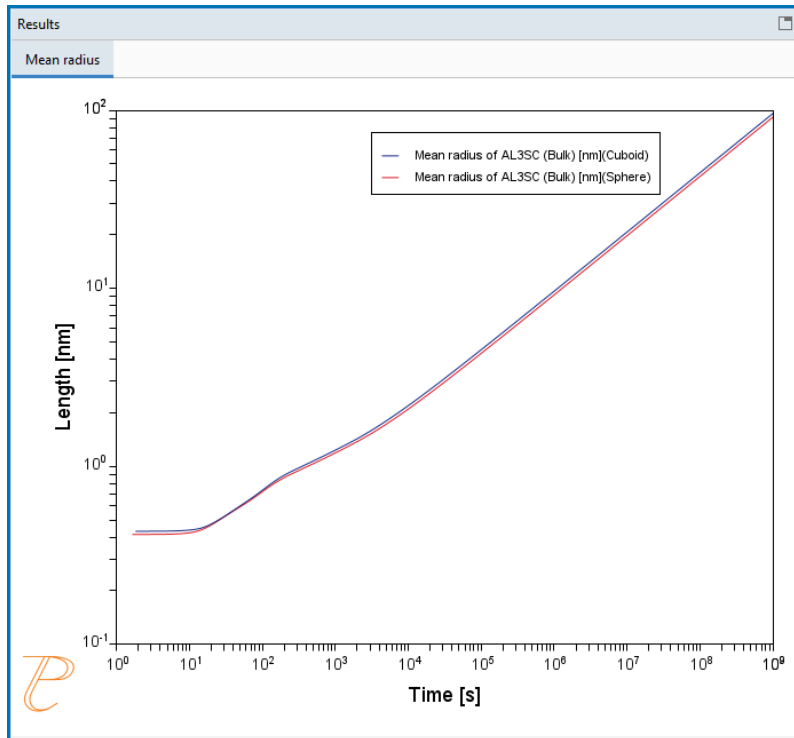
In this plot, the blue line represents the sphere calculation and the red line represents the cuboid calculation. You can see that, in this instance, they are almost identical.

In this plot, the blue line represents the sphere calculation and the red line represents the cuboid calculation. You can see that, in this instance, these are almost identical.

By 'radius for non-spherical particles' it means the radius of equivalent spheres with the same volume.

If you run the example file that is included in your software, the plot also contains an experimental file, which you can see closely matches the calculations.

PLOTTING ADDITIONAL VARIABLES

Now you use the same calculation to set up additional plots using the many available variables. The examples below include two Y-axes each.

Plotting Mean Radius and Cuboid Factor

This plot has two Y-axes: *Mean radius* and *Cuboid factor*.

1. Right-click the **Cuboid** node and add a **Plot Renderer**.
2. Right-click the new node and rename it `Mean radius and Cuboid factor`.
3. Under *Y-axes* click the plus sign to add another axis.
4. Keep *Mean radius* as the first axis variable but change the units to **Nanometer** (nm) and set the axis type to **Logarithmic 10**.
5. Set the second *Axis variable* to **Mean cubic factor**.
6. Click to clear the *Automatic scaling* check box. In the fields, enter the *Limits* from `1` to `1.41` and the *step* to `0.1`.
7. The plot is now set. Click **Perform**.

Precipitation of Al-Sc AL3SC with Assumption
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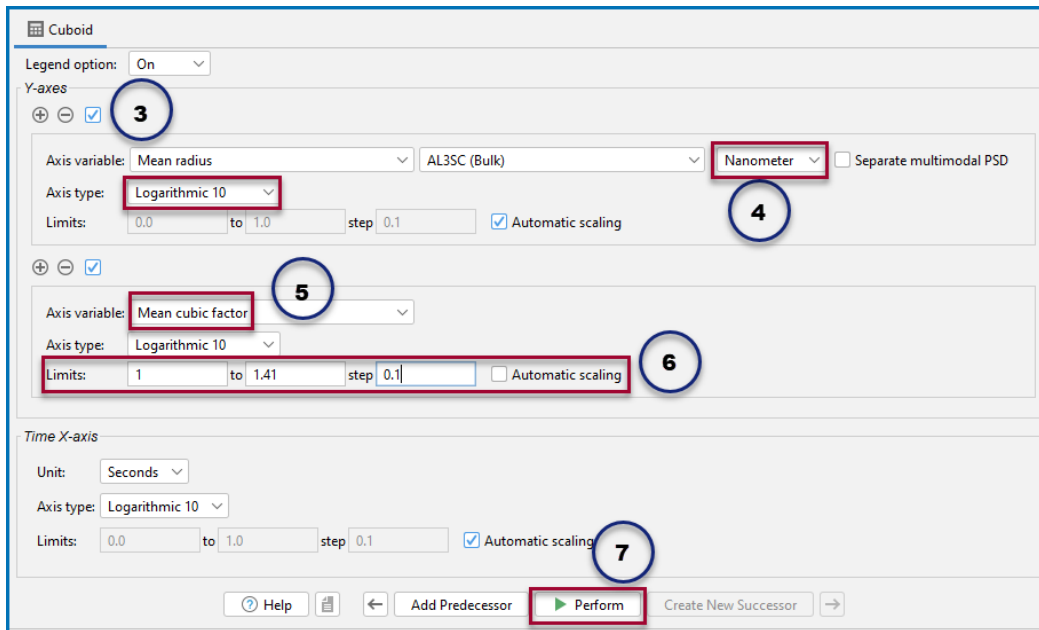
Interpreting the Results of Mean Radius and Cuboid Factor
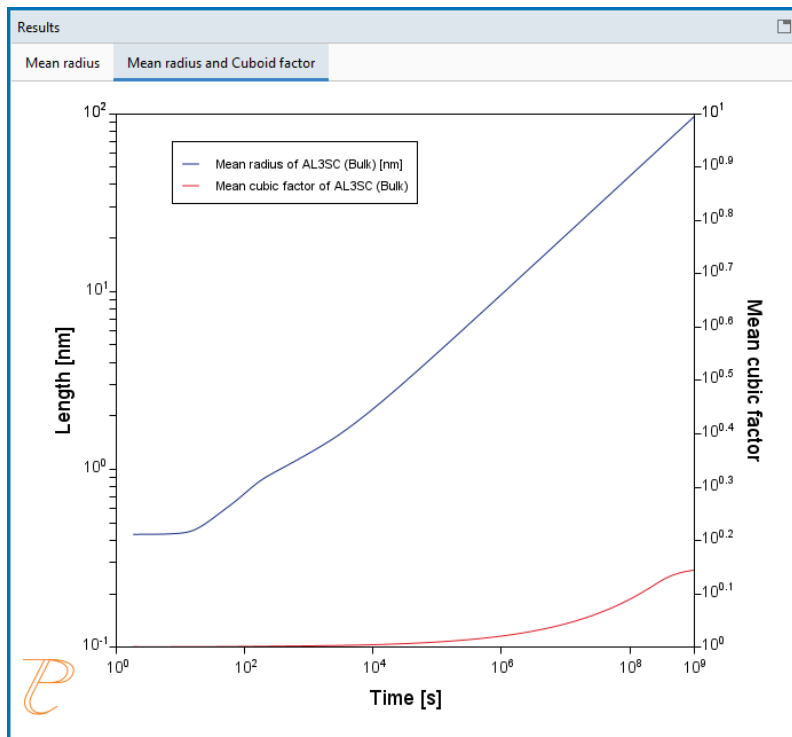
In this plot, the blue line represents the evolution of the average radius of the cubic particles as a function of time. The red line shows the average cubic factor as a function of time.

The blue line represents the evolution of the average radius of the cubic particles as a function of time. Again, for non-spherical precipitates this means the radius of equivalent spheres with the same volume.

The red line shows the average cubic factor as a function of time. A value of one represents a spherical shape. A square root of two represents a cubic shape.

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The evolution of the shape when the particles grows is determined by competition between interfacial energy and elastic strain energy. In general, the shape is close to spherical at small particle sizes because the interfacial energy term dominates.
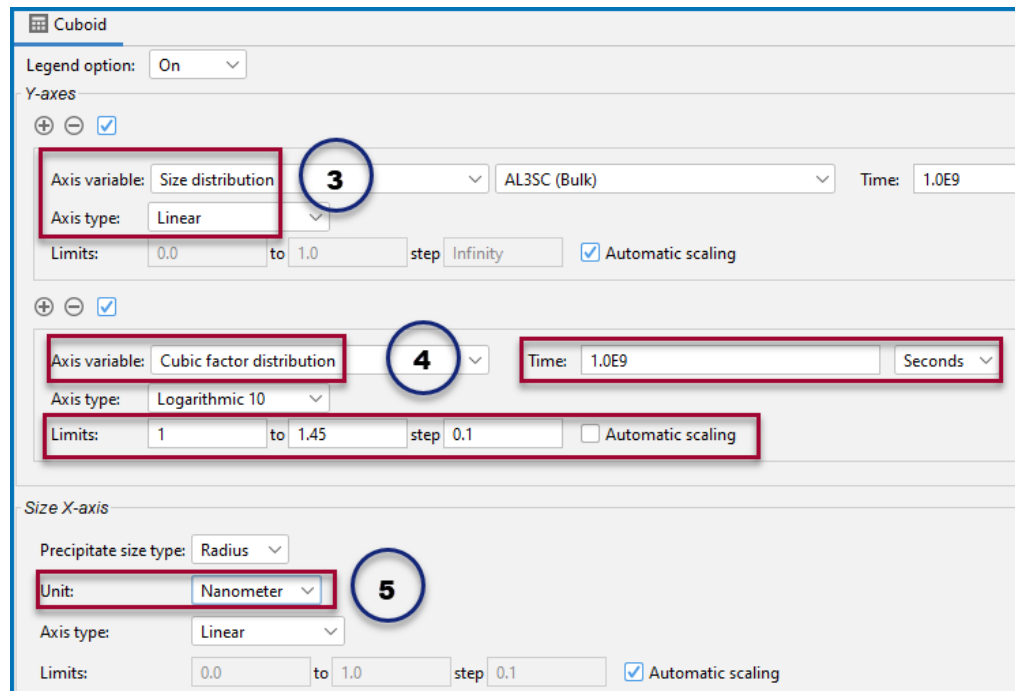
At large sizes the elastic energy dominates and it is therefore more favourable with a non-spherical shape. You can see that the particles get a more cubic form at later times when they grow to larger sizes.

Plotting Particle Size and Cubic Factor Distribution

This final plot shows the particle size distribution (PSD) and cubic factor distribution at the end of the simulation.

This plot also has two Y-axes, so you can clone the previous plot.
1. Right-click the **Mean radius and Cuboid factor** node and select **Clone**.
2. Right-click the new node and rename it `PSD and Cuboid factor`.
3. Under the *Y-axes*
    a. Select **Size distribution** as the first *Axis variable*.
    b. Change the *Axis type* to **Linear**.
4. Set the second Y-axis to **Cubic factor distribution** and enter a *Time* of `1e9` **Seconds**.
5. Keep the *Automatic Scaling* check box cleared. Enter the *Limits* from `1` to `1.45` and the *step* to `0.1`.
6. Under *Size X-axis*, change the unit to **Nanometer** (nm).
7. Click **Perform** at the bottom center of the **Configuration** window.

Precipitation of Al-Sc AL3SC with Assumption
of Sphere and Cuboid Morphologies
Precipitation Example P_09

Interpreting the Results of Particle Size Distribution and Cuboid Factor
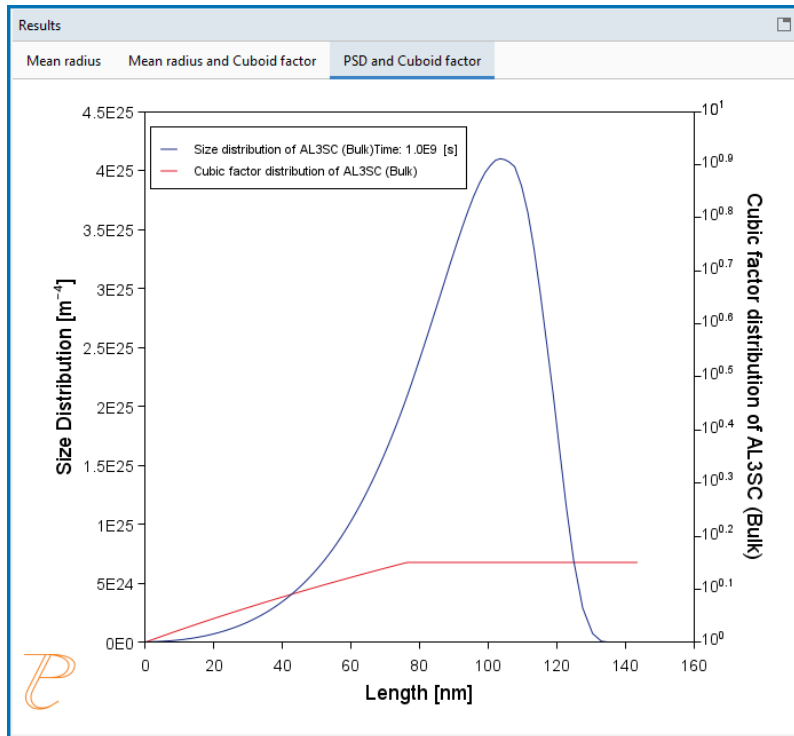
In this plot, the blue curve shows the particle size distribution and the red line shows the cubic factor distribution.

The blue curve, which shows the particle size distribution, is close to the regular LSW size distribution that is expected for spherical particles.

The cubic factor distribution shows that the smallest particles are closer to spherical and that the larger ones get more and more cubic.

References

1. Marquis, E.A, and D.N Seidman. 2001. "Nanoscale Structural Evolution of Al3Sc Precipitates in Al(Sc) Alloys." *Acta Materialia* 49 (11): 1909–19.
2. Novotny, Gabriel M., and Alan J. Ardell. 2001. "Precipitation of Al3Sc in Binary Al–Sc Alloys." *Materials Science & Engineering, A*: Structural Materials: Properties, Microstructure and Processing 318 (1–2): 144–54.

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, M23C6, and M7C3, are included in the calculations for competitive precipitations, and the precipitation kinetics are compared with or without initial particle size distribution.

Open the example project file and click **Perform Tree** to generate the plots associated with it.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**

- File name: *P_10_Precipitation_Initial_PSD_FeCrC.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.

Example Settings

The example illustrates the use of the PSD setting. You can import data from a spreadsheet or text file (.xls, .xlsx, .csv or .txt formats are acceptable). The **Preexisting Particle Size Distribution** window shown below, provides a graphical representation of the radius versus corresponding frequencies.

"Particle Size Distribution (PSD)" on page 35
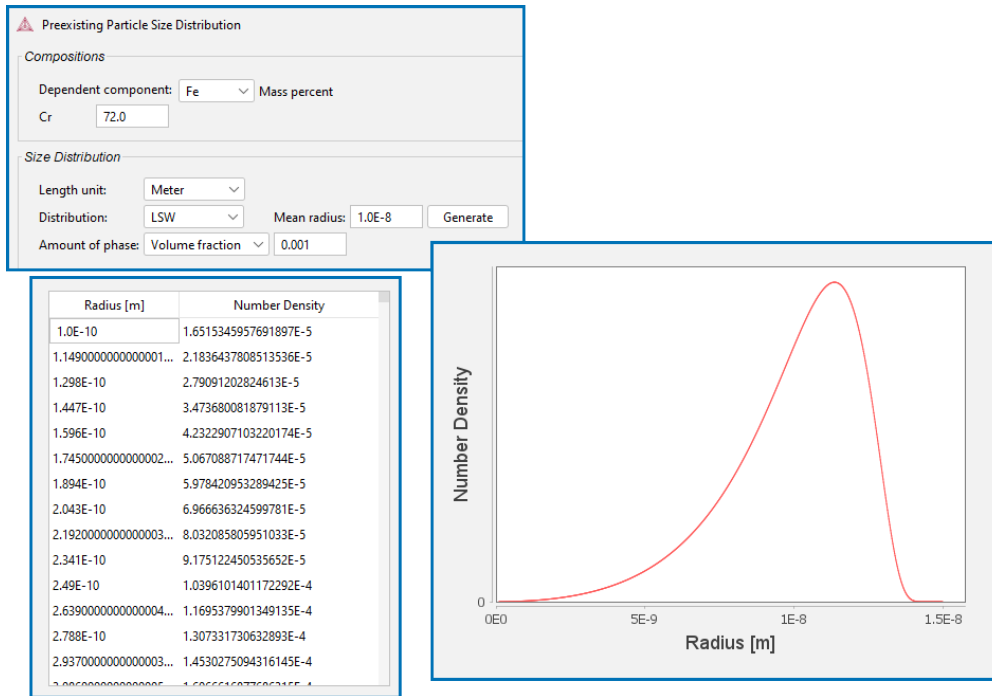
Figure 47: The Preexisting Particle Size Distribution (PSD) settings window for example P_10.

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, 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.
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	1053 K
Simulation time	400 000 seconds

Visualizations

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 48: 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.

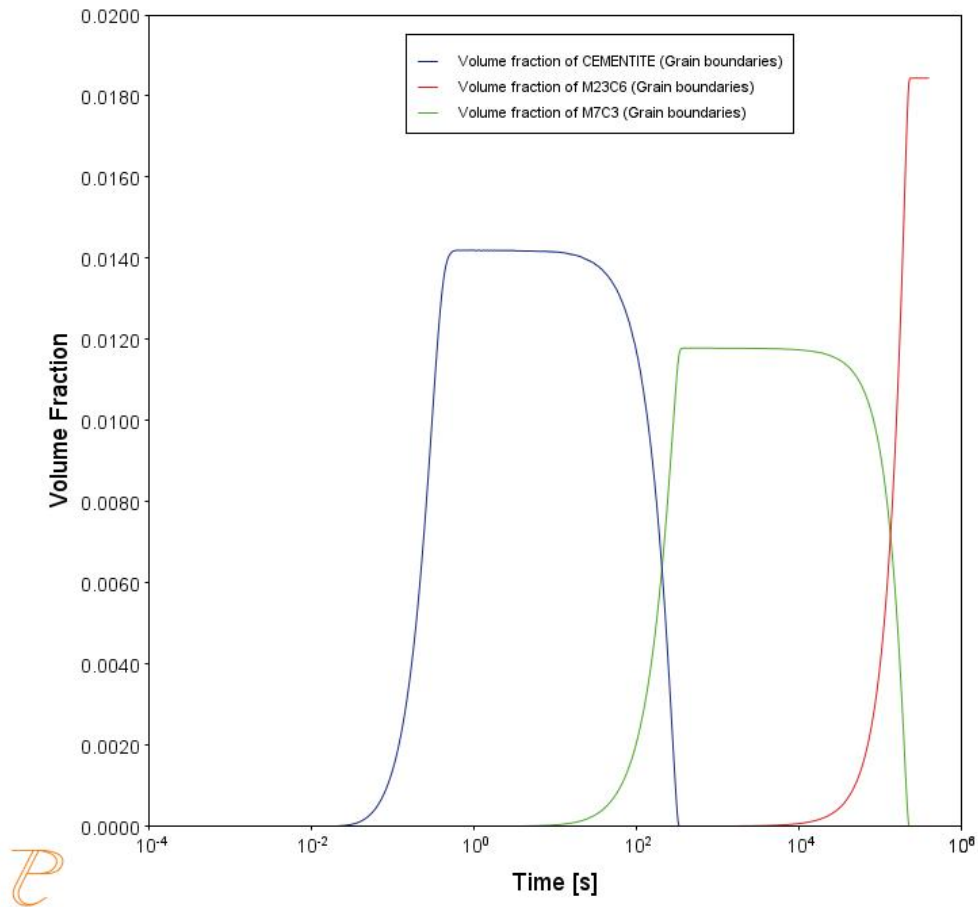*Figure 49: The predicted volume fraction of cementite, M23C6, and M7C3 during an isothermal aging with no precipitates in solution in the initial condition.*

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" on page 84

Open the example project file and click **Perform Tree** to generate the plots associated with it.

> ⏳   When you run (Perform) this example, it takes a few minutes for the calculations to complete.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**

- File name: *P_11_Interfacial_energy_function.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.

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

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.
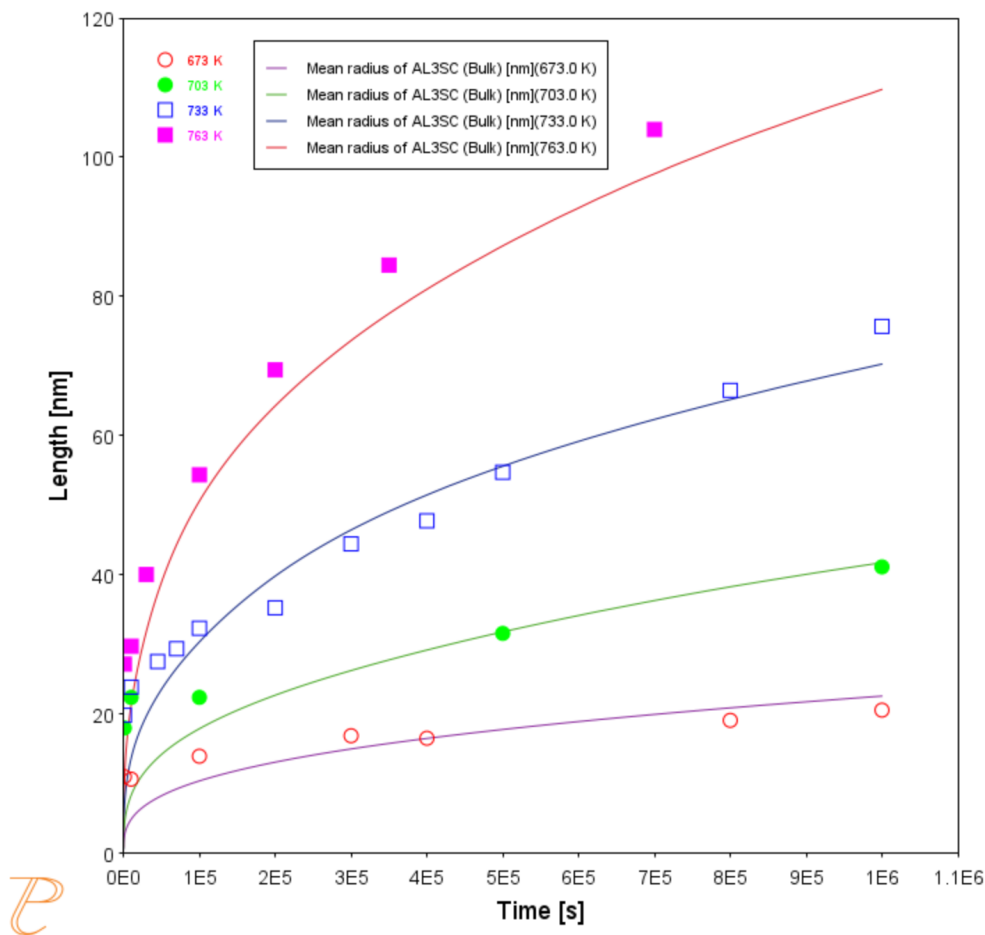

Figure 50: The results of an isothermal calculation to examine the mean radius of an Al-0.12Sc system with experimental data from [2004Iwa].

Reference

[2004Iwa] Iwamura, S, and Y Miura. 2004. "Loss in Coherency and Coarsening Behavior of Al3Sc Precipitates." *Acta Materialia* 52 (3): 591–600.

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" on page 77.

Open the example project file and click **Perform Tree** to generate the plots associated with it.

> ⧗   When you run (Perform) this example, it takes a few minutes for the calculations to complete.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**

- File name: *P_12_Precipitation_Al-Zr_GrowthRateModel_comparison.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.

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

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 51: 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" on page 77.

Open the example project file and click **Perform Tree** to generate the plots associated with it.

> ⏳ When you run (Perform) this example, it can take over two hours to complete the calculations.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**

- File name: *P_13_Precipitation_Fe-C-Cr_Paraequilibrium_Precipitation_of_Cementite.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.

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 Click **Show Details** to select the **Growth rate model** (**Simplified** and **Para-eq**). 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

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.
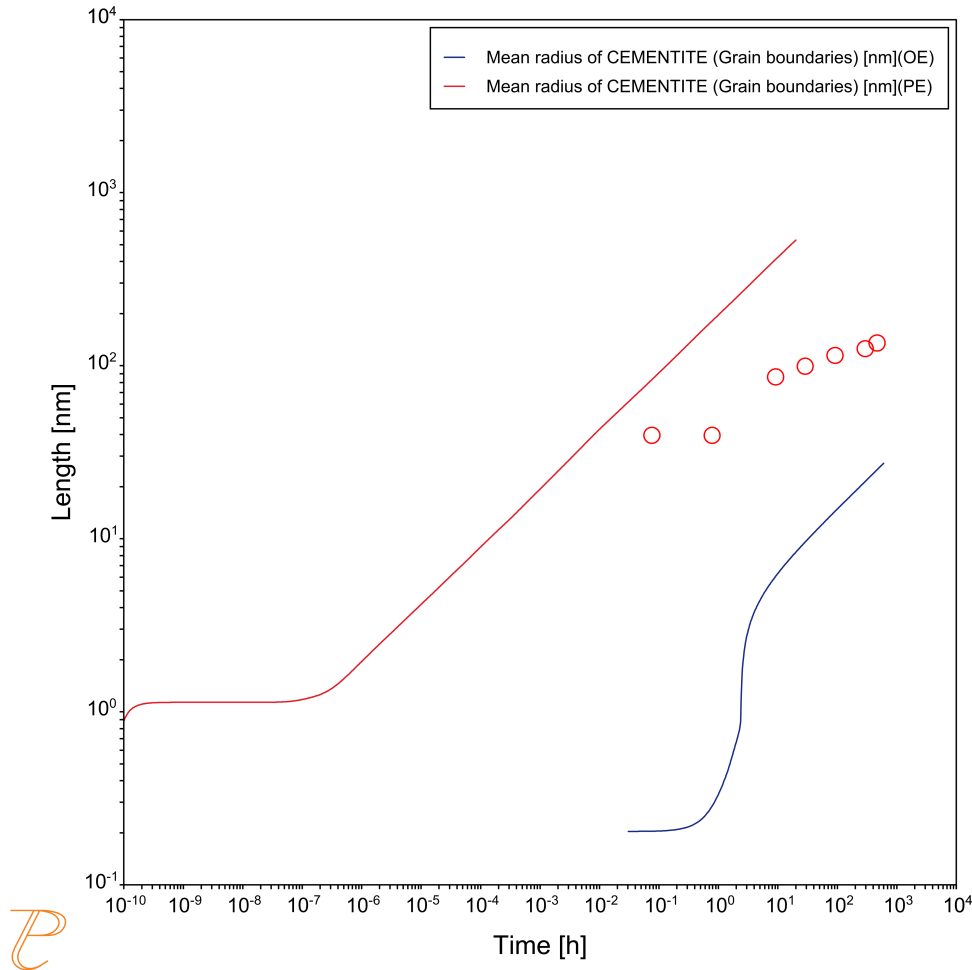
Figure 52: These results compare the predicted and measured evolution of the mean radius of cementite with the experimental data from [1980Sak] to simulation predictions obtained from the ortho-equilibrium (OE), and para-equilibrium (PE) approximations of the precipitate composition. The precipitate 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.

> 📖 For more details, see the theory described in "Normal Grain Growth" on page 99 and "Zener Pinning" on page 101.

> 💡 Open and run this example in Thermo-Calc to follow along with the description and to experiment with the available settings.

> ⏳ When you run (Perform) this example, it takes a few minutes for the calculations to complete.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: *P_14_Precipitation_Fe-C-Ferrite-Grain_Growth_with_Zener_Pinning.tcu*

> ▶️ This example is included as a Precipitation Module (TC-PRISMA) tutorial on our website and as part of the playlist on our YouTube channel.

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 x 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

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.

Results Discussion

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 53)
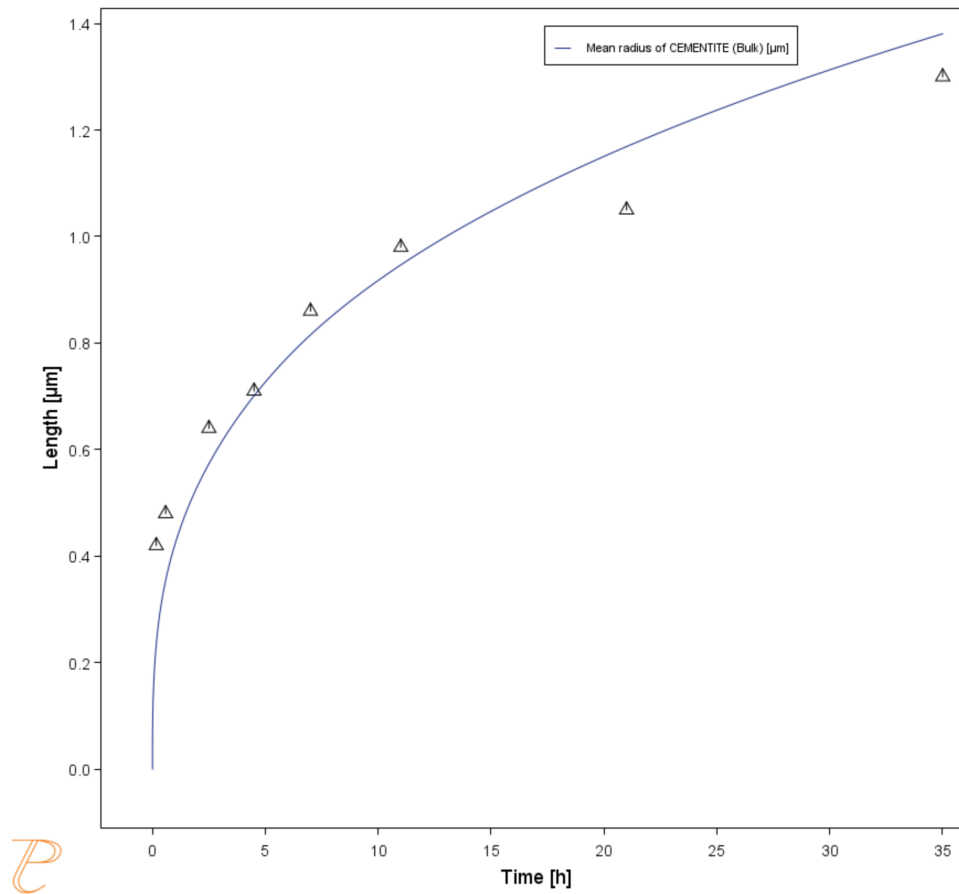
Figure 53: The evolution of the mean radius of cementite comparing the experimental data from [1975Hel] with the Precipitation Calculator results.

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.
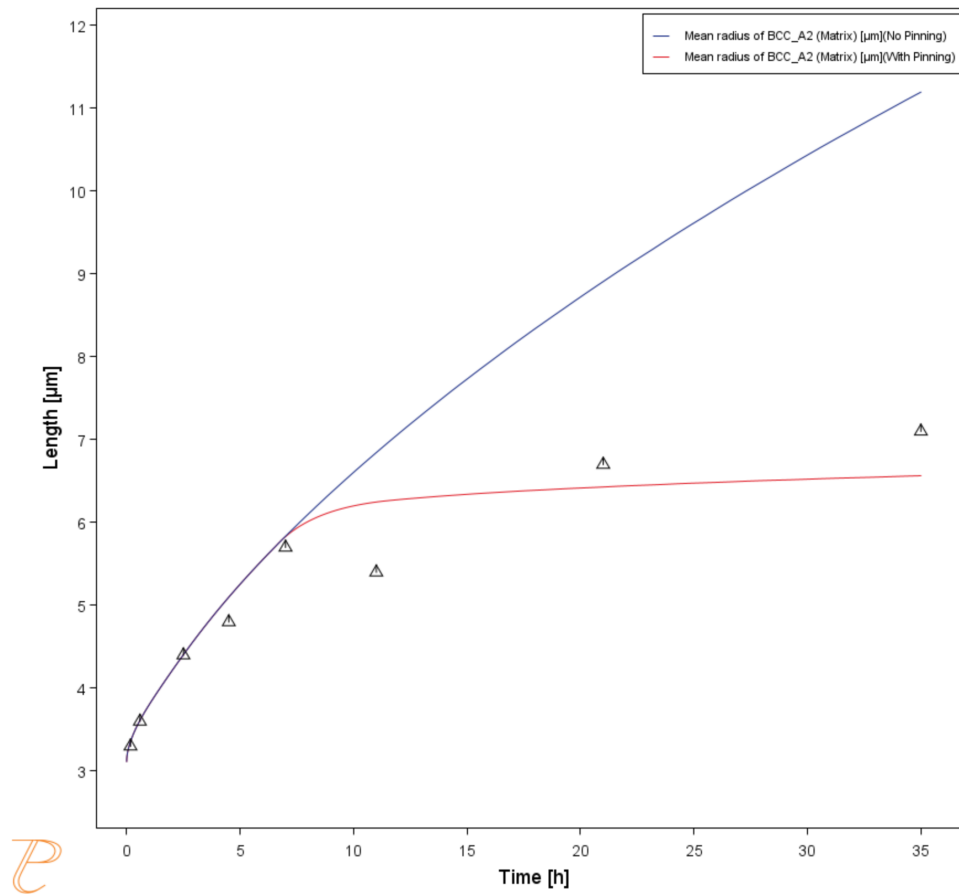
Figure 54: The evolution of the mean grain radius of ferrite comparing the experimental data from [1975Hel] with predictions made with and without Zener pinning from an evolving dispersion of cementite precipitates.

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.

> 📖 For more details, see PE Automatic Growth Rate Model described in the "Growth" on page 77 theory section.

> 💡 Open and run this example in Thermo-Calc to follow along with the description and to experiment with the available settings.

> ⧗   When you run (Perform) this example, it takes a few minutes for the calculations to complete.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**

- File name: *P_15_Precipitation_Fe-C-Mn_PE-OE_Precipitation_of_Cementite.tcu*

▶   This example is included as a Precipitation Module (TC-PRISMA) tutorial on our [website](#) and as part of the playlist on our [YouTube channel](#).

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 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

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.
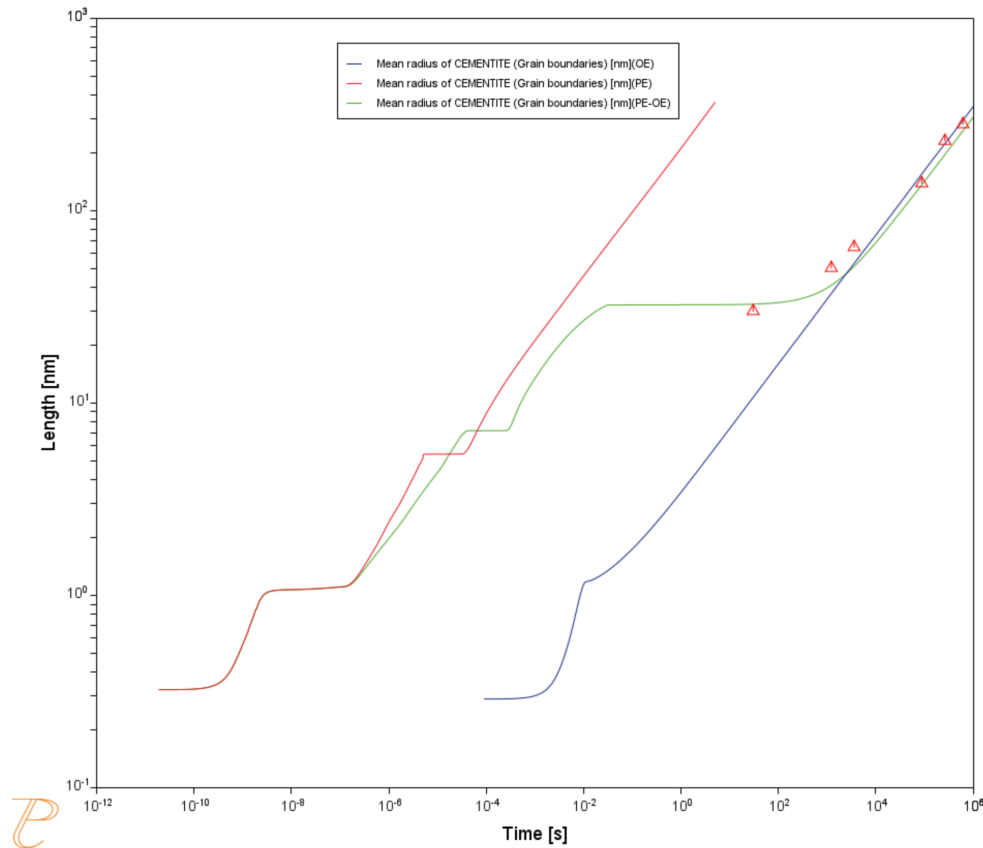

Figure 55: A comparison between the measurements of mean cementite radius from [2007Miy] with the simplified (OE), para-eq (PE), and PE Automatic (PE-OE) growth models. The PE-OE model is needed to capture the nucleation, growth, and coarsening behavior of cementite.
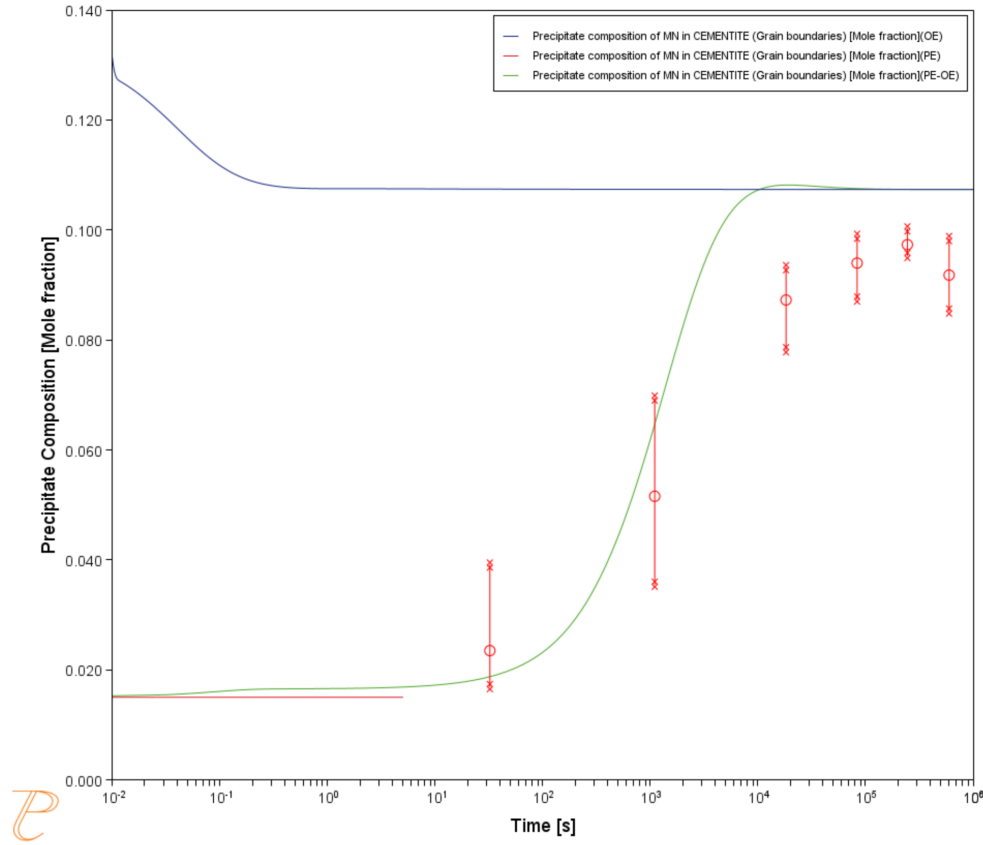
Figure 56: A comparison of the evolution of the cementite Mn composition during isothermal aging at 923.15 K between the experimental data from [2007Miy] with model predictions obtained from the simplified (OE) growth model, the para-eq (PE) growth model, and the PE Automatic (PE-OE) growth model. The 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" on page 104.

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.

> 🔆 Open and run this example in Thermo-Calc to follow along with the description and to experiment with the available settings.

> ⧗ When you run (Perform) this example, it takes a few minutes for the calculations to complete.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: *P_16_Precipitation_Ni-Al-Cr_Stereology.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.

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

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.
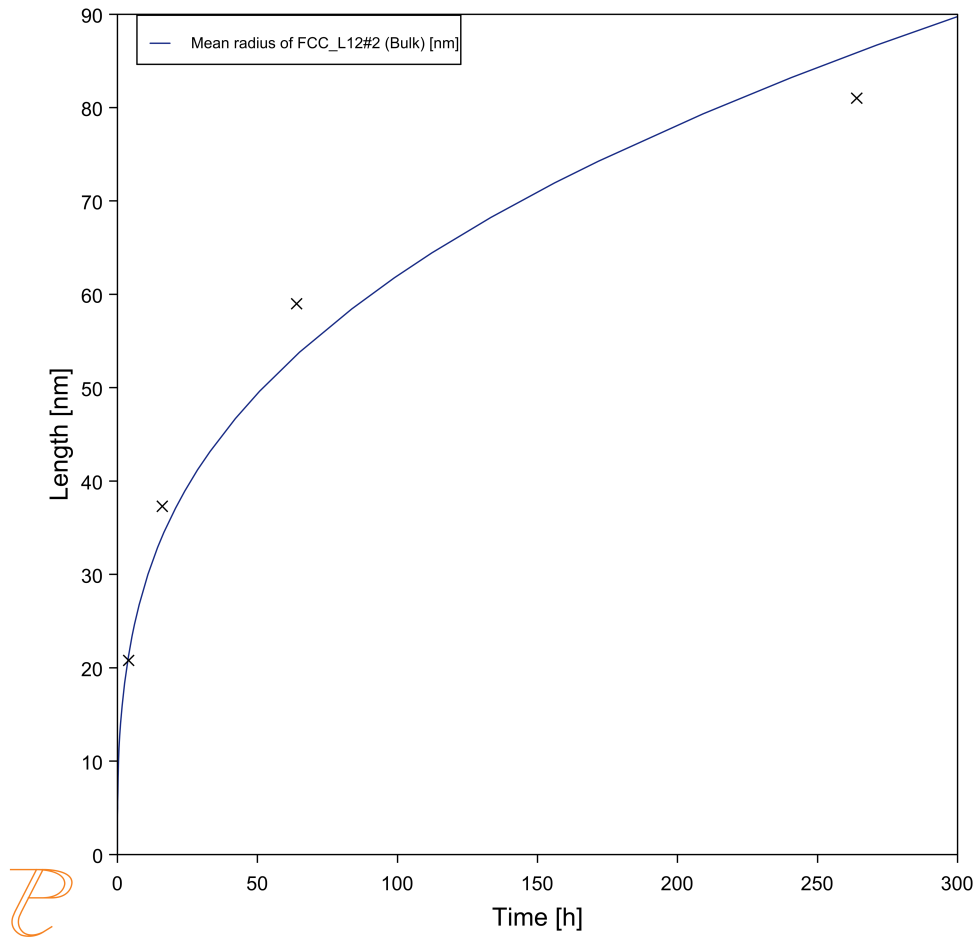
Figure 57: A comparison of the evolution of the mean 2D precipitate radius measurements of [2008Sud] with model predictions.
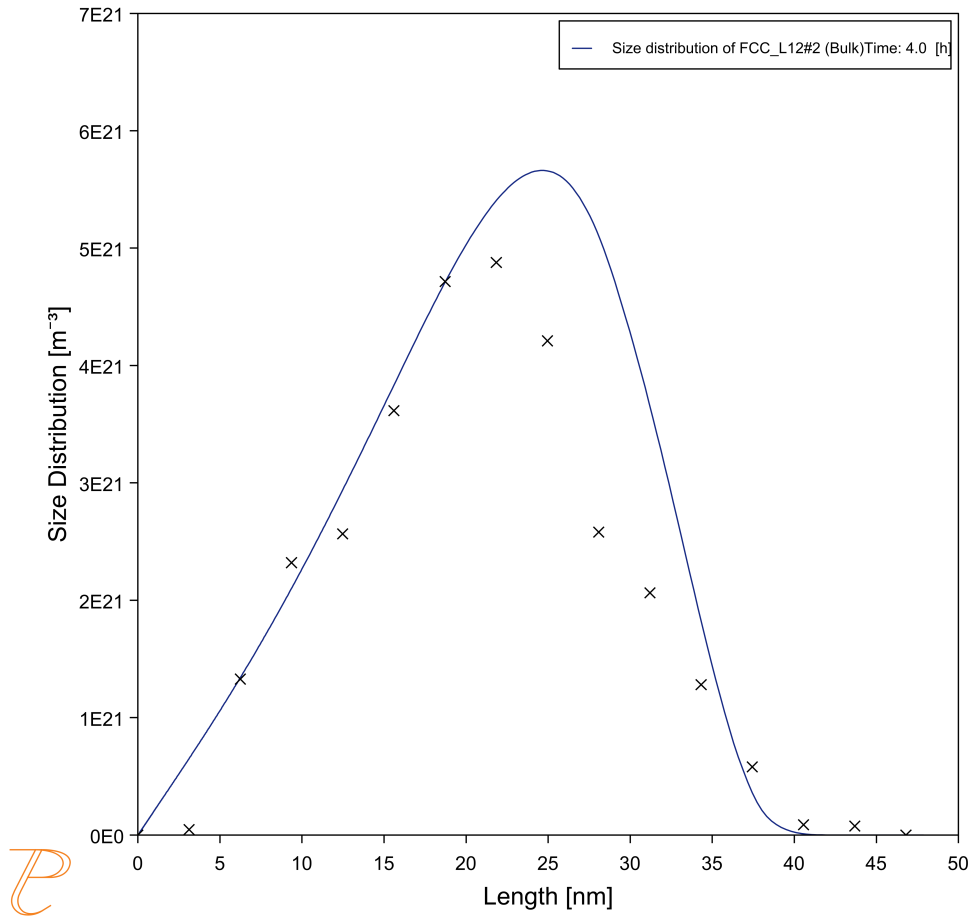
Figure 58: A comparison of the predicted and measured 2D size distribution after 4 h of aging.
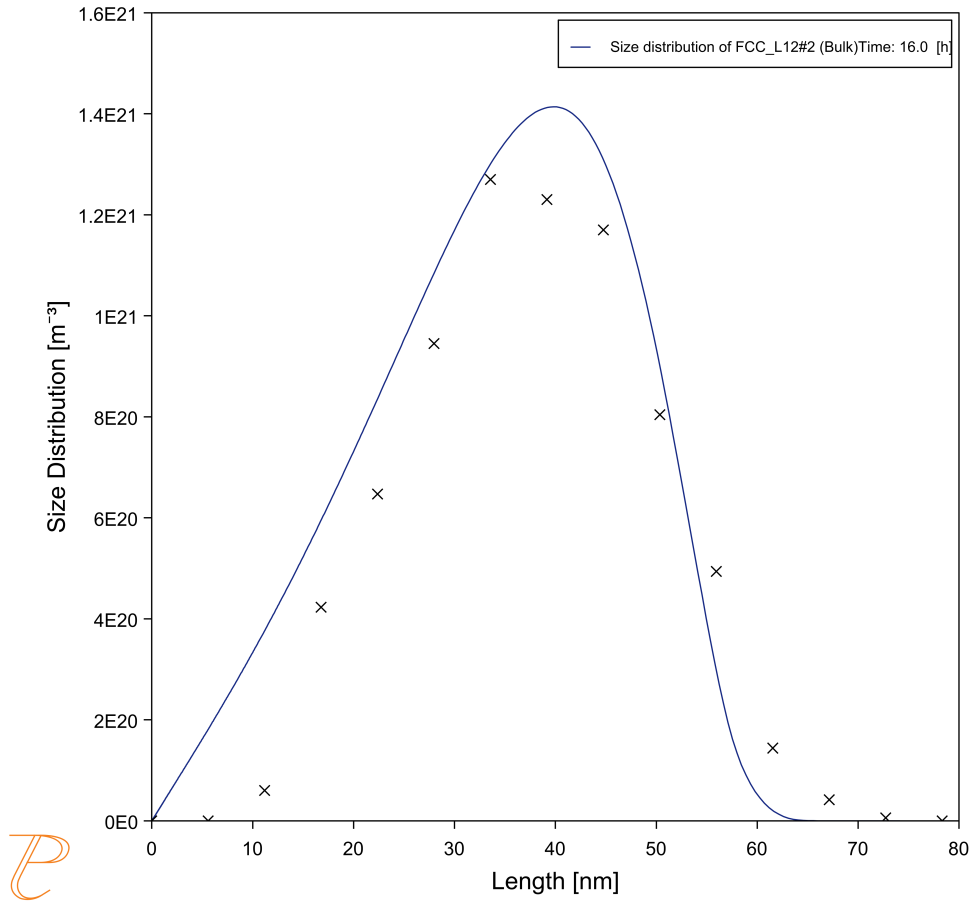
Figure 59: A comparison of the predicted and measured 2D size distribution after 16 h of aging.
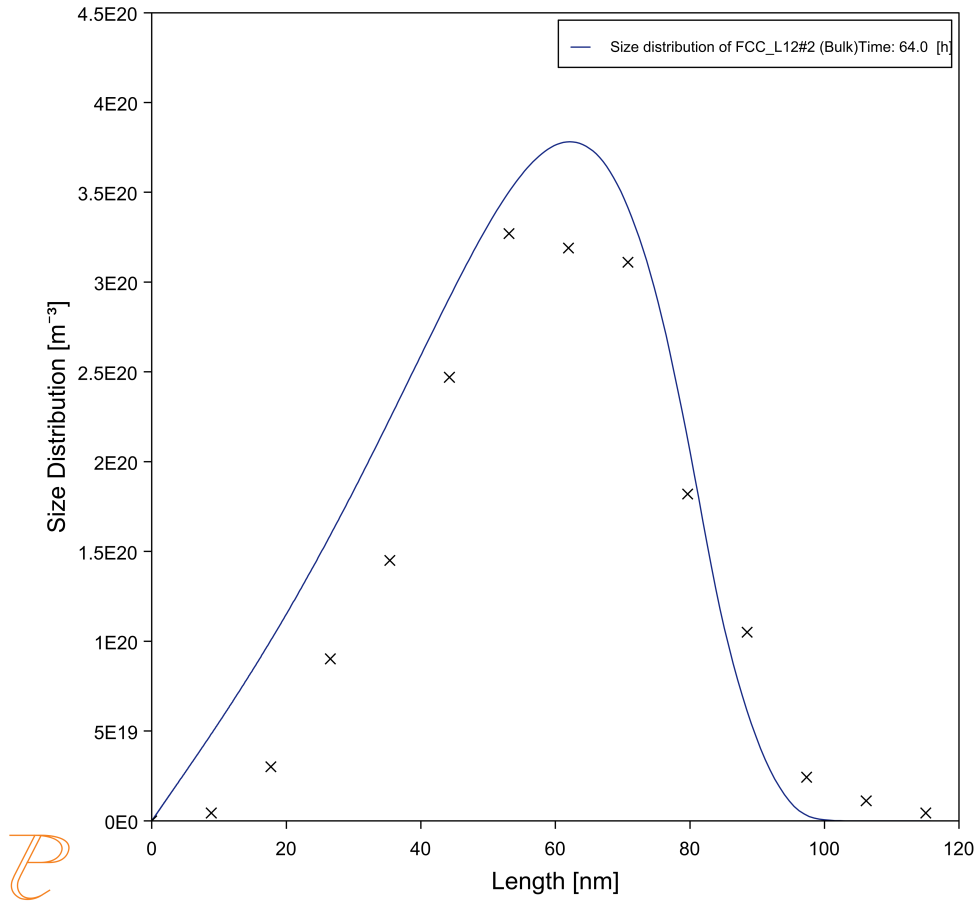
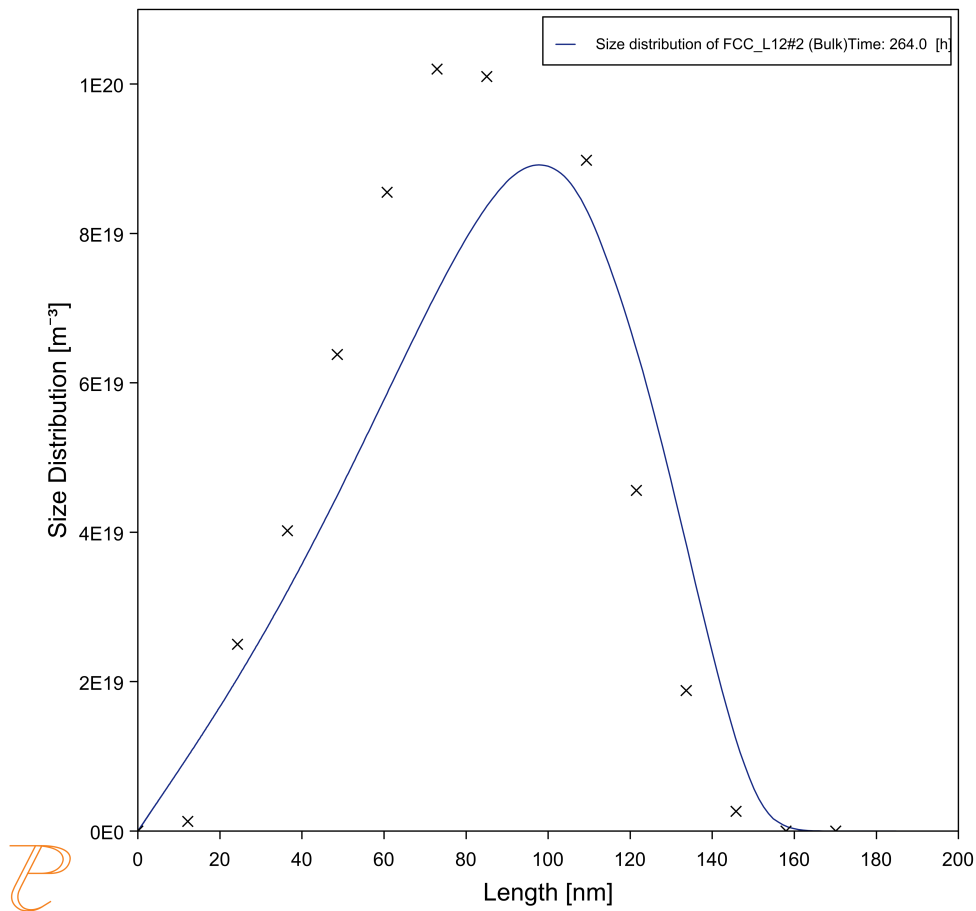*Figure 60: A comparison of the predicted and measured 2D size distribution after 64 h of aging.*

Figure 61: 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).