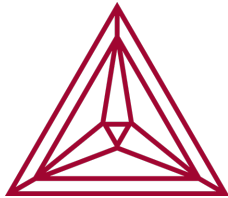


# **Thermo-Calc Console Mode Examples Guide**

**Thermo-Calc Version 2019a**



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## About the Thermo-Calc Console Mode Examples

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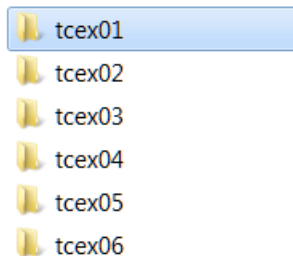
There are many examples to examine and to help you learn Thermo-Calc in Console Mode.

### OPENING THE MACRO FILE

To open an example macro file for Thermo-Calc:

1. Open Thermo-Calc.
2. Confirm you are in Console Mode. If not, click the **Switch to Console Mode** button.
3. From the main menu, select **File** → or **Help** → **Examples Files**. The Console Mode folder opens.
4. Open the **Thermo-Calc** folder to see the available examples contained in separate folders.

Name



For the Diffusion Module (DICTRA) examples (\*.DCM macro files), open the **Diffusion Module - DICTRA** folder.

5. In the folder, double-click the \*.TCM file or click **Open**.
6. Follow the prompts in the Console window i.e. keep pressing <Enter> to run the macro and produce a plot in the **Console Results** window.

Each topic has a brief description of the example and includes some or all of the commands used in the macros. As you progress through the examples, sometimes only new commands are highlighted.

Topic	TCEX Examples included
<a href="#">"Examples of Binary Systems" on page 3</a>	1, 4, 10, 11, 13, 16, 18, 26, 34, 51
<a href="#">"Examples Using Functions and Variables" on</a>	2, 44

Topic	TCEX Examples included
<a href="#">page 10</a>	
<a href="#">"Examples of the Gibbs Energy System (GES) Module" on page 11</a>	31, 38, 39, 49, 52
<a href="#">"Examples of Multicomponent Systems" on page 9</a>	6, 7, 47
<a href="#">"Example using the PARROT and EDIT EXPERIMENT Modules" on page 15</a>	36a
<a href="#">"Pourbaix Module Examples" on page 20</a>	40, 53
<a href="#">"Pourbaix Module Examples TCEX40A to 40E" on page 21</a>	40A to 40E (additional examples related to TCEX40)
<a href="#">"Examples of Property and Potential Diagrams" on page 8</a>	8, 35
<a href="#">"Examples of Scheil-Gulliver Calculations" on page 14</a>	15, 30a, 30b, 48
<a href="#">"Examples with Specialized Databases" on page 18</a>	20, 22, 25, 27, 29, 50,
<a href="#">"General Examples Using the Steel Database" on page 7</a>	9, 23, 28, 32, 37, 41
<a href="#">"Example of the Tabulate Reaction (TAB) Module" on page 16</a>	12
<a href="#">"Example of the Reactor Module" on page 17</a>	24
<a href="#">"Examples of Ternary Systems" on page 5</a>	3, 5, 14, 17, 19a, 19b, 21, 33, 42, 43, 45, 46,

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# Examples of Binary Systems

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## TCEX01 - CALCULATING THE BINARY FE-C PHASE DIAGRAM

This example calculates the binary Fe-C phase diagram using the Binary module. The TCBIN database is used and included with your installation.

## TCEX04 - CALCULATING THE FE-CR MISCIBILITY GAP

This example calculates the miscibility gap in the Fe-Cr system. The FEDEMO database is used and included with your installation.

## TCEX10 - PREVENTING Cr<sub>2</sub>O<sub>3</sub> CLOGGING IN A CONTINUOUS CASTING PROCESS

The example calculates an equilibrium with suspended or dormant phases and shows how to avoid Cr<sub>2</sub>O<sub>3</sub> clogging in a continuous casting process.



This uses the SLAG database. A license is required to run the example.

The origin of this example is that a manufacturer wanted to increase the Cr content of a material from 18 to 25 weight percent but the continuous casting of this material was problematic because solid Cr<sub>2</sub>O<sub>3</sub> was formed. Using Thermo-Calc to calculate the equilibria in the steel/slag system, a simple correction was found: modify the Mn or Si content to decrease the oxygen potential.

In Thermo-Calc, you can FIX a phase with zero amount to simulate how to avoid forming this phase. You then release one of the conditions, usually one of the compositions, and this composition is determined by the equilibrium calculation.

## TCEX11 - OXIDATION OF Cu<sub>2</sub>S WITH AN H<sub>2</sub>O/O<sub>2</sub> GAS MIXTURE

This example demonstrates the oxidation of Cu<sub>2</sub>S with an H<sub>2</sub>O/O<sub>2</sub> gas mixture. Thermo-Calc is used to find the optimum O/H ratio (i.e. oxygen potential) as certain oxygen potential values can desulphurize Cu<sub>2</sub>S without forming copper oxides.

In Thermo-Calc, the problem reduces to perform equilibria calculations in a Cu-S-H-O system. The amounts of the components should be kept to correct ratio corresponding to Cu<sub>2</sub>S and H<sub>2</sub>O using a command SET\_INPUT\_AMOUNTS in POLY3. Initially, O/H = 0.5 is given. Optimum O/H ratio is calculated with the desired calculation conditions. For example, to simulate one phase disappearing, you can FIX the phase with zero amount.

The *tcex11.TDB* file is used to access data and this is included with your installation.

## TCEX13 - THE BINARY AL-TI PHASE DIAGRAM AND ITS G CURVE

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This example calculates an Al-Ti binary phase diagram and G curve using the BINARY module. The TCBIN database is used and included with your installation.

### **TCEX16 - SECOND ORDER TRANSITION OF THE AL-FE SYSTEM**

This example calculates the second order transition line in the Bcc field of the Al-Fe system.



This uses the SSOL database. A license is required to run the example.

### **TCEX18 - A3 TEMPERATURE OF A STEEL**

This example calculates the A3 temperature of a steel and examines the influence of each alloying element on this temperature.

A3 temperature is the temperature where ferrite starts to form from austenite. You can easily read A3 from an Fe-C phase diagram. However, for complex multicomponent steels no simple diagram can be used. Using POLY, it is easy to find out the influence of each alloying element on the A3 temperature. This information is useful if you want to modify the compositions of a steel but keep A3 unchanged.



This uses the TCFE database. A license is required to run the example.

### **TCEX26 - THE AS-GA PHASE DIAGRAM: PLOTTING THE PARTIAL PRESSURES OF A GAS SPECIES**

This is an example of plotting the partial pressures of a gas species along the solubility lines in the As-Ga phase diagram. The calculation makes it possible to monitor the input gases to a process of depositing solid As-Ga.

### **TCEX34 - THE AL-ZN PHASE DIAGRAM AND ITS G CURVE**

This example uses the BINARY module to calculate the phase diagram and G curves in the Al-Zn system. It uses the TCBIN database included with your installation.

### **TCEX51 - CALCULATION OF MOLAR VOLUME, THERMAL EXPANSIVITY AND DENSITY**

This example uses the POLY3 module to calculate the molar volume, thermal expansivity and density of the FCC\_A1, BCC\_A2 LIQUID and liquid phases of C-Fe.



This uses the TCFE database. A license is required to run the example.

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# Examples of Ternary Systems

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## **TCEX03 - CALCULATING AN ISOTHERMAL SECTION WITH THE TERNARY MODULE**

This example calculates an isothermal section using the Ternary module. The FEDEMO database is used and included with your installation.

## **TCEX05 - CALCULATING A VERTICAL SECTION IN THE AL-CU-SI SYSTEM**

This example calculates a vertical section in the Al-Cu-Si system and of a vertical section from Al to 10% Cu<sub>2</sub>Si. The ALDEMO database is used and included with your installation.

In addition to various commands used in the previous examples, the LIST\_AXIS\_VARIABLE command is used.

## **TCEX14 - VARIATIONS IN SOLIDIFICATION OF AN AL-MG-SI ALLOY**

This example calculates the heat and heat capacity variations during solidification of an Al-Mg-Si alloy. The ALDEMO database is used and included with your installation.

## **TCEX17 - THE PSEUDO-BINARY SYSTEM - CaO-SiO<sub>2</sub>**

This example calculates the pseudo-binary system CaO-SiO<sub>2</sub> using the OXDEMO database, which is included with your installation.

The oxide demo (Oxdemo) database can be used both for pseudo-binary systems like the one in this case, CaO-SiO<sub>2</sub>, or for full ternary systems like Ca-Fe-O.

## **TCEX19A AND TCEX19B - MAPPING OF UNIVARIANT EQUILIBRIA WITH THE LIQUID IN AL-CU-SI**

- Part A. Step-by-step calculation using the POLY-3 module.
- Part B. Using the TERNARY module, you can get the information on invariant reactions, such as temperature and compositions.

## **TCEX21 - CALCULATING A TERNARY ISOTHERM IN Fe-Cr-Ni**

This example calculates a ternary isotherm in Fe-Cr-Ni with a user-defined database included with the example in the file named *tcex21.TDB*.

## **TCEX33 - AN Fe-Cr-C ISOPLETH**

This example is a benchmark calculation of an isopleth in the Fe-Cr-C system. The

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FEDEMO database is used and included with your installation.

#### **TCEX42 - PARAEQUILIBRIUM CALCULATION - FORMATION OF PARA-PEARLITE - ISOPLETH**

(This is the Drop-down text)

This example uses an Fe-Mn-C system at 2.5%Mn Mass u-fraction to show a paraequilibrium calculation where there is formation of para-pearlite. It is an isopleth calculation and shows the STEP\_WITH\_OPTIONS command using the Paraequilibrium option.



This uses the TCFE database. A license is required to run the example.

#### **TCEX43 - PARAEQUILIBRIUM CALCULATION - FORMATION OF PARA-PEARLITE - ISOTHERMAL**

This example uses an Fe-Mn-C system at 700 C to show a paraequilibrium calculation where there is formation of para-pearlite. It is an isothermal calculation and shows the STEP\_WITH\_OPTIONS command using the Paraequilibrium option.



This uses the TCFE database. A license is required to run the example.

#### **TCEX45 - 3D DIAGRAM WITH THE GAMMA VOLUME IN THE FE-CR-C SYSTEM**

This example calculates the gamma volume in the Fe-Cr-C system and plots it in 3D. The FEDEMO database is used and included with your installation.



To view the generated file, *tcex45.wrl*, install a WRML (Wirtual Reality Modelling Language) viewer to the web browser.

#### **TCEX46 - 3D DIAGRAM WITH THE LIQUIDUS SURFACE OF THE FE-CR-C SYSTEM**

This example calculates the liquidus surface of the Fe-Cr-C system and plots it in 3D.



To view the generated files, *tcex46\_tri.wrl* and *tcex46\_sqrt*, install a WRML (Wirtual Reality Modelling Language) viewer to the web browser.



This uses the TCFE database. A license is required to run the example.

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# General Examples Using the Steel Database

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## **TCEX09 - CALCULATING A DEW POINT WITH THE POLY3 MODULE**

This is an example calculating the dew point in the POLY3 module. The SUBDEMO database is used and included with your installation.

## **TCEX23 - CALCULATING A PARAEQUILIBRIUM AND THE T0 TEMPERATURE IN A LOW ALLOYED STEEL**

This example calculates a paraequilibrium and the T0 temperature in a low alloyed steel.



This uses the TCFE database. A license is required to run the example.

## **TCEX28 - PITTING RESISTANCE EQUIVALENCE (PRE) FOR A DUPLEX STAINLESS STEEL**

This example calculates the Pitting Resistance Equivalence (PRE) for a duplex stainless steel.



This uses the TCFE database. A license is required to run the example.

## **TCEX32 - CALCULATING OXIDE LAYERS ON STEEL**

This example calculates oxide layers on a steel and shows how to append databases.



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

## **TCEX37 - CALCULATING AN ISOTHERMAL SECTION IN CONSOLE MODE**

This example shows how to use command lines to enter and calculate an isothermal section using the POLY3 module. The FEDEMO database is used and included with your installation.

## **TCEX41 - CALCULATING A SOLUBILITY PRODUCT**

Calculation of a solubility product. Shows the STEP\_WITH\_OPTIONS command using the T-zero option.



This uses the TCFE database. A license is required to run the example.



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# Examples of Property and Potential Diagrams

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## Property Diagrams

### TCEX08 - PROPERTY DIAGRAMS FOR A HIGH SPEED STEEL

This example shows how to calculate property diagrams for a high speed steel i.e. phase fraction plots, activity vs temperature, and so forth.



This uses the TCFE database. A license is required to run the example.

## Potential Diagram

### TCEX35 - CALCULATING A POTENTIAL DIAGRAM

This example uses the POTENTIAL module to calculate a potential diagram. Note that there are no commands for this module, you just follow the prompts. The SUBDEMO database is used and included with your installation.

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## Examples of Multicomponent Systems

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### TCEX06 - AN ISOPLETH IN LOW ALLOYED FE-MN-SI-CR-NI-C STEEL

This example calculates a multicomponent phase diagram using the `DEFINE_MATERIAL` command in `POLY` and the TCFE steel database. The material contains 1.5 %Cr + 0.4 %Mn + 3.5 %Ni + 0.3 %Si and 1 %C (by weight). These conditions and the temperature are set by the `DEFINE_MATERIAL` command.

After the first equilibrium results, a phase diagram is calculated with one axis variable as temperature and the other as the carbon content.



This uses the TCFE database. A license is required to run the example.

### TCEX07 - SINGLE EQUILIBRIA IN LOW ALLOYED FE-MN-SI-CR-NI-C STEEL

This example shows how to calculate a single equilibria in a low alloyed Fe-Mn-Si-Cr-Ni-C steel. There are two common ways to perform a single equilibrium calculation:

- Get data from a database, then in `POLY` use `SET_CONDITION` and `COMPUTE_EQUILIBRIUM`.
- Go directly to `POLY` and use `DEFINE_MATERIAL`.

The `COMPUTE_TRANSITION` command is also used to determine the temperature or composition where one phase forms or disappears. It is the same as the `CHANGE_STATUS` → `SET_CONDITION` → `COMPUTE_EQUILIBRIUM` sequence of commands.

A `STEP_WITH_OPTIONS` command using the option *normal* is also used in addition to the other commands that should be becoming more familiar as you work through the examples.



This uses the TCFE database. A license is required to run the example.

### TCEX47 - 3D-QUATERNARY DIAGRAM WITH THE GAMMA VOLUME IN THE FE-CR-NI-C SYSTEM AT 1373K

The example calculates the gamma volume in the Fe-Cr-Ni-C system at 1373K and plots a 3D-quaternary diagram. The FEDEMO database is used and included with your installation.



To view the generated file, *tcex47.wrl*, install a WRML (Wirtual Reality Modelling Language) viewer to the web browser.

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# Examples Using Functions and Variables

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## TCEX02 - PLOTTING THERMODYNAMIC FUNCTIONS

This example shows how to plot thermodynamic functions in unary, binary and ternary systems. It also involves working with partial derivatives and partial quantities.



This uses the SSOL database. A license is required to run the example.

## TCEX44 - EXPLORING VARIABLES AND FUNCTIONS

This example uses variables and functions to predict properties e.g. proof strength for an austenitic stainless steel at elevated temperatures (20-550° C). The example was created using an expression from Eliasson and Sandström (2000)<sup>1</sup>.



This uses the TCFE database. A license is required to run the example.

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1. "Proof strength values for austenitic stainless steels at elevated temperatures", *Steel Res.*, 71(6–7), 249–254.

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# Examples of the Gibbs Energy System (GES) Module

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## TCEX31 - USING THE GES MODULE TO CALCULATE CVM

Using the Gibbs energy system (GES) module, this example calculates the CVM and compares it with the sublattices of a fictitious A B system. You also learn how to overlay diagrams from two calculations.

## TCEX38 - CALCULATING THE MORRAL "ROSE"

This example uses the Gibbs energy system (GES) module to calculate the Morral rose, which are miscibility gaps.

## TCEX39 - CALCULATING REVERSIBLE CARNOT CYCLES OF A HEAT ENGINE

This example shows how to calculate the reversible Carnot cycle of a heat engine using one mole of an ideal gas with two fictitious species A and A2. The GES, POLY3 and POST modules are used, as well as the SUBDEMO database, which is included with your installation.

One application of the Second Law is to the efficiencies of heat engines, pumps and refrigerators. Whenever there is a difference of temperature, work can be produced - the principle of heat engines. The Gibbs energy also enables the prediction of the maximum work that a process may achieve. The goal of this example is to help relate the results to different thermodynamic quantities.

## TCEX49 - QUASICHEMICAL MODEL USING THE GIBBS ENERGY SYSTEM (GES) MODULE

This example shows how to enter parameters for a FACT quasichemical liquid model and how to calculate the sulfur activity using the GIBBS\_ENERGY\_SYSTEM (GES) module commands.

## TCEX52 - CHANGING THE EXCESS MODELS FOR INTERACTION PARAMETERS IN A SOLUTION PHASE

This example shows how to change the excess models for binary and ternary interactions in a solution phase, either

- through direct interactive amendments of phase descriptions within the GIBBS\_ENERGY\_SYSTEM (GES) module, or
- enforced by specific type-definitions given in a database file retrieved by the DATABASE\_RETRIEVAL module (also called the TDB module).

---

For binary excess models, the example changes it from the default *R-K model* to a *Mixed-Excess-Model*. The phase has to be a substitutional phase in this case.

For ternary extrapolation models, the example changes it from the default *R-K-M model* to a *Toop\_Kohler model*.

### ***Notes related to the example***

The following is included in the macro file as part of the instructions but may be of use to new users:

#### ***Amending the binary excess model***

The default binary excess model is the Redlich-Kister Model for all the three associated binary interaction pairs (A-B, A-C and B-C) in the substitutional LIQUID solution phase (without sublattice) that consists of three elements (A, B and C).

Before changing this default binary excess model for the ternary LIQUID solution phase, one must have already entered the G parameters (for standard Gibbs energies of all pure end-members) and L parameters (for binary R-K excess interaction energies), as shown in the example.

In this particular example, we want to change from the default R-K binary excess model to the Mixed-Excess-Model (with three different binary excess models, namely Legendre, Polynom and Redlich-Kister models, applied to the A-B, A-C and B-C binaries, respectively), as demonstrated below:

For the A-B interaction, the Legendre binary excess model should be used (rather than the default Redlich-Kister Model), with the first species (i.e. A) as the independent constituent and the second species (i.e. B) as the dependent constituent, while the L parameters for the A-B interaction shall remain the same as those handled by the R-K model.

For the A-C interaction, the Polynom binary excess model should be used (rather than the default Redlich-Kister Model), with the second species (i.e. C) as the independent constituent and the first species (i.e. A) as the dependent constituent, while the L parameters for the A-C interaction shall remain the same as those handled by the R-K model.

#### ***Amending the ternary extrapolation model***

The default ternary excess model is the Redlich-Kister\_Muggianu Model (i.e., the MUGGIANU\_RESTOR method for ternary extrapolation based on binary parameters) for the associated ternary interaction terms; when no ternary L parameter is entered for that, such a default Redlich-Kister\_Muggianu Model is thus to be used for extrapolation from binary excess energies to ternary interactions in the substitutional LIQUID solution phase (without sublattice) that consists of three elements (A, B and C).

---

However, in this particular example as illustrated in the following, we shall change from this default R-K-M ternary excess model to the TOOP-KOHLER method for the ternary extrapolation method, with the species C as the Toop constituent, while the species A and B as the Kohler constituents (entering A and B, or B and A, as the basis constituent and first interacting constituent). This will implicitly enforce that, during the ternary extrapolation, only the A-B binary interaction parameters are utilized in accordance with the Kohler ternary extrapolation formula for A-B-C ternary interaction, while any other binary interaction parameters used in line with the Toop-Kohler ternary extrapolation formula (for the A-C-B and B-C-A ternary interactions). This makes the extrapolated ternary excess interaction terms different from those handled either by the default MUGGIANU\_RESTOR method or by the alternative KOHLER-ALL method.

Note that only when all the relevant binary excess energies in a ternary system are treated by the default Redlich-Kister Model (i.e., the Mixed-Excess-Model should have not been used), the MUGGIANU\_RESTOR method for ternary extrapolations is equivalent to the Redlich-Kister\_Muggianu Model, or the KOHLER-ALL method to the Redlich-Kister\_Kohler Model.

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## Examples of Scheil-Gulliver Calculations

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### TCEX15 - SIMULATING THE SOLIDIFICATION OF A CR-NI ALLOY WITH THE SCHEIL MODULE

This is an example of a solidification simulation of a Cr-Ni alloy. There is no back diffusion in the solid, i.e. Scheil-Gulliver model is used.



This uses the TCFE database. A license is required to run the example.

### TCEX30A AND 30B - SCHEIL CALCULATION FOR AN AL-4MG-2SI-2CU ALLOY

These examples show two ways to do a Scheil calculation for an Al-4Mg-2Si-2Cu alloy. In part A, you use the POLY3 module and the STEP\_WITH\_OPTIONS command with an EVALUATE option. Then in part B you use the SCHEIL module commands to do the same thing. Data from the COST2 database is used and included with the example in the file named *tcex30\_cost2.TDB*.

### TCEX48 - SCHEIL SOLIDIFICATION WITH C BACK DIFFUSION

This is an example of Scheil solidification with C back diffusion in solid phases. The results are compared between a simple Scheil and equilibrium calculation. The FEDemo database is used and included with your installation.

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## Example using the PARROT and EDIT\_EXPERIMENT Modules

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### TCEX36A - USING THE PARROT AND EDIT EXPERIMENTS MODULES



The example is divided into parts corresponding to the files in the **tcex36a** folder. It is recommended you read *tcex.36.readme* before continuing with this advanced exercise.

▶ Also see the *Data Optimization User Guide*.

Each problem has "selected" experimental data. The example uses a fictitious binary A-B system where element A is BCC until it melts. Element B is BCC up to 1100 K and FCC above. There is a compound A<sub>2</sub>B stable in a limited temperature range.

- The creation of the "setup" file is described (*tcex36a.TCM*) where you enter the elements and phases into the Gibbs Energy System (GES) module
- The creation of the experimental data file is described (*tcex 36b.TCM*). When you run the TCEX36a macro, the contents of this macro file is automatically launched and the experimental data file created.
- The actual run in the PARROT module in order to obtain the result (*tcex 36cpd.TCM*)



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## Example of the Tabulate Reaction (TAB) Module

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### TCEX12 - TABULATION OF THERMODYNAMIC DATA FOR REACTIONS

This example shows a number of independent cases using the TABULATE\_REACTION (TAB) module to tabulate thermodynamic data for reactions.



This uses the SSUB database. A license is required to run the example.

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## Example of the Reactor Module

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### TCEX24 - SIMULATION OF THE SILICON ARC FURNACE USING THE REACTOR MODULE

This is a simple reactor model with output of gases at the top and output of condensed phases at the bottom. The gas phase from one segment flows to higher segments, 80% reacts in the first above, 15% in the second above and 5% in the third above.

The condensed phases flow downwards and all of it goes to the next lowest segment. Heat can be added at any module. The only way to specify the initial state of the reactants added to the reactor is to specify the heat content.



This uses the SSUB database. A license is required to run the example.

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## Examples with Specialized Databases

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### TCEX20 - ADIABATIC DECOMPRESSION IN A GEOLOGICAL SYSTEM

This example calculates the adiabatic decompression in a geological system using the geochemical database. The database is included with the file named PGEO.TDB, which is in the same folder as this example.

### TCEX22 - CALCULATING AN ADIABATIC FLAME TEMPERATURE

This example examines a heat balance when  $C_3H_8$  is burned in oxygen by calculating the adiabatic flame temperature.



This uses the SSUB database. A license is required to run the example.

### TCEX25 - SIMULATING THE REFINEMENT OF STEEL

This example is based on a typical steel refining process. Raw iron used to produce steel usually has high carbon and silicon content, which is why oxygen is blown into the furnace to burn off carbon. Lime (CaO) is added to form a slag with silica, and the slag can be removed. Alloying elements, such as Mn, Ni, Cr and V are added to produce the desired steel. Since the reaction between O and C increases the temperature, scrap iron is added to keep the temperature constant (it is assumed the furnace is isolated and no heat is lost to the environment).

This example simulates blowing oxygen into a liquid steel of one metric ton (1e6 grams) with 4 w/o C, 2 w/o Si and 1 w/o Mn. 100 moles of CaO (equivalent to 5.6 kg) is added. Keeping the enthalpy constant is the way to simulate the isolation of the furnace. The oxygen reacts with carbon and increases the temperature. After blowing a certain amount of oxygen, scrap iron is added to keep the temperature constant.



This uses the SLAG database. A license is required to run the example.

### TCEX27 - CALCULATING CHEMICAL VAPOR DEPOSITIONS (CVD)

This example calculates the chemical vapor deposition (CVD).



This uses the SSUB database. A license is required to run the example.

### TCEX29 - CALCULATING THE SPECIATION OF A GAS

---

This example shows how to calculate the speciation of a gas.



This uses the SSUB database. A license is required to run the example.

### **TCEX50 - QUASICHEMICAL MODEL USING THE DATABASE RETRIEVAL (TDB) MODULE**

This example shows the quasichemical model using the DATABASE\_RETRIEVAL module (also called the TDB module).

The example replicates figures 3 and 4 from Kongoli, Pelton and Dessureault (1998)<sup>1</sup>.

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1. "Thermodynamic modeling of liquid Fe-Ni-Cu-Co-S mattes", *Metall. Mat. Trans. B*, 29(3), 591–601.

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# Pourbaix Module Examples

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## TCEX40 - USING THE POURBAIX MODULE

This is the first in a series of examples to demonstrate the advanced POURBAIX module calculations and plotting. This example automatically calculates and plots a Pourbaix diagram for 0.001 m Fe in a 0.1 m NaCl aqueous solution at 25° C and 1 bar. Other diagrams, along various phase boundaries for the same interactions resulted from the same Pourbaix module calculation, are also plotted.



It is recommended you read the text file *TCEX40-README.txt*, which is located in the **Extended** subfolder.

A so-called Pourbaix diagram is actually a phase diagram with independently-varied acidity (pH) and electropotential (Eh), for a heterogeneous interaction system at a certain bulk composition (that is by default always set as 1 kg of water dissolving a specified amount of metals and other solutes), under a defined temperature and pressure condition.

### The PAQ2 Database

The example uses the PAQ2 (TCS Public Aqueous Solution Database using the SIT aqueous solution model) included with your installation. The database contains an AQUEOUS solution phase and REF\_ELECTRODE phase (as a reference for electron in aqueous electrolyte systems), as well as some data for various solid phases (solution or stoichiometric) and gaseous mixture phase. The PAQ2 is specially designed for these example calculations of the so-called Pourbaix diagrams (i.e., pH-Eh plots) and other types of phase diagrams or property diagrams in some aqueous-bearing multicomponent heterogeneous interaction systems within the limited chemical framework of Fe-Co-Cr-Ni-C-N-S-H<sub>2</sub>O-NaCl, via the Single-Database Option in the advanced POURBAIX module or through the normal TDB-GES-PLOY-POST routine.

### Additional Examples in this Series

Additional examples (TCEX40A, TCEX40B, TCEX40C, TCEX40D and TCEX40E) are provided to demonstrate options and features in the Pourbaix module and to show more advanced applications of the TCAQ and AQS aqueous solution databases [in the Multiple-Database Option, i.e., with appended data from the SSOL and SSUB databases]. See ["Pourbaix Module Examples TCEX40A to 40E" on the next page](#).

## TCEX53 - POURBAIX DIAGRAM CALCULATIONS FOR A HETEROGENEOUS INTERACTION SYSTEM

This example uses the PAQ2 database to calculate some Pourbaix diagrams. The DATABASE\_

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RETRIEVAL (TDB), GIBBS\_ENERGY\_SYSTEM (GES), POLY3, and POST modules are used for the Fe-X-H<sub>2</sub>O-NaCl heterogeneous interaction system, where X = Cr-Ni-Co.



The initial bulk composition of Fe-based alloy in this calculation is just preliminarily assigned, in which the BCC\_A2 and/or FCC\_A1 solution phase(s) are considered as of primary interest. For practical calculations, one shall have more precise inputs for the initial bulk compositions of alloys.

#### *Step 1: Single-Point Calculations for H<sub>2</sub>O-NaCl system*

To demonstrate how to define the molality of NaCl in an aqueous-bearing heterogeneous interaction system.

#### *Step 2: Single-Point Calculations for Fe-X (X = Cr-Ni-Co) system*

To demonstrate how to define the initial amount of alloy in an aqueous-bearing heterogeneous interaction system. In this example, we are interested in only the BCC\_A2 and FCC\_A1 phases in the Fe-based alloy.

#### *Step 3: Single-Point Calculations for Fe-Cr-Ni-Co + H<sub>2</sub>O-NaCl system*

#### *Step 4: Pourbaix Diagram Mapping for Fe-Cr-Ni-Co + H<sub>2</sub>O-NaCl system - define the variables*

From the same mapping calculations you arrive at by the end of the example, you can plot more diagrams using a variety of X-Y axis variables.



For a list of pre-defined symbols, go to the end of the tcex53.TCM macro file (open it in a text editor).

## **Pourbaix Module Examples TCEX40A to 40E**

These are the extended examples that are described in ["Pourbaix Module Examples" on the previous page](#).

### **TCEX 40A**

This example shows you how to use Option 1 where you **start a completely new calculation**. It uses a single database. The Pourbaix diagram for 0.001 m Fe in a 0.1 m NaCl solution at 25C and 1 bar is automatically calculated and plotted.



A more advanced version of 40A can be found in TCEX40E, which also uses Option 1 but with multiple databases. However, licenses are required for three types of commercial Thermo-Calc databases.

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A so-called Pourbaix diagram is actually a phase diagram with independently-varied electropotential (Eh) and acidity (pH), for an heterogeneous interaction system at a certain bulk composition (that is by default always set as 1 kg of water solving a specified amount of metals and other solutes), under defined temperature and pressure conditions. Some property diagrams, along various phase boundaries for the same interactions resulting from the same Pourbaix module calculation, are also plotted, without leaving Option 1.



At the end of this example, a new POLY3 file called *POURBAIX.POLY3* is automatically saved. For Windows users this is saved to the Documents folder. The following examples (TCEX40B, TCEX40C and TCEX40D) use this same POLY3 file for the calculations. Therefore it is important to make four copies of this file and rename these to TCEX40A.POLY3, TCEX40B.POLY3, TCEX40C.POLY3 and TCEX40D.POLY3. This must be done outside of the Thermo-Calc software and after the TCEX40A calculation and plotting is complete. This is so that the required POLY3 file structure is not lost.



The reason you do not save from within Thermo-Calc is because of how the file is saved. When the command sequence (GO POLY3>SAVE TCEX40A.POLY3>Y) is used, the POLY3 workspace of the POURBAIX calculation results in the POLY3 module monitor and all the initial equilibrium points and the mapping/stepping calculation results are lost as well as parts of the POLY3 file structure (e.g., some definitions of the previously defined POURBAIX-type calculation system).

## TCEX 40B

This example shows you how to use Option 2 where you **Open an old (existing) file and plot other property diagrams**.

Example 40A calculated and plotted the Pourbaix diagram for 0.001 m Fe in a 0.1 m NaCl solution at 25° C and 1 bar. Example 40B reads the original POURBAIX.POLY3 file, and uses the calculated results to plot property diagrams for the same heterogeneous interaction system.



For example 40B, the POLY3 file is not modified. However, it is still recommended that a copy of the original POLY3 file is used so you do not lose the file structure and calculated results.



If you have a POLY3 file generated after choosing Option 4, that file can also be used for Option 2, and vice versa.

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## TCEX 40C

This example shows you how to use Option 3 where you **Open an old file and make another Pourbaix calculation**. The previously calculated (and copied) POURBAIX.POLY3 file from TCEX40A is edited to make another Pourbaix calculation and plot.

The same chemical system is used (Fe-H<sub>2</sub>O-NaCl) but with different P-T-X (pressure-temperature-composition) conditions and without the Gaseous mixture phase. The new conditions are 0.01 m Fe in a 1 m NaCl solution at 200° C and 1 kbar.



In this example, the Gaseous mixture phase for the Pourbaix diagram is not considered.



The POLY3 file is modified and rewritten with the new conditions. As previously recommended, make a copy of the original POLY3 file and rename it (e.g. TCEX40C.POLY3) so you do not lose the file structure and new calculated results.

After the default Pourbaix diagram is generated and refined, you can also use Option 3 to plot property diagrams along different phase boundaries for the same system. These settings are possible from within Option 3 and you do not need to go back to Option 2.

## TCEX 40D

This example shows you how to use Option 4 where you **Open an old file and make another stepping calculation**. The previously calculated (and copied) POURBAIX.POLY3 file from TCEX40A is edited to make a stepping calculation and plot.

The same chemical system is used (Fe-H<sub>2</sub>O-NaCl) but with different P-T-X (pressure-temperature-composition) conditions and using a POLY3 stepping calculation. The new conditions are 0.01 m Fe in a 0.1 m NaCl solution at 1 kbar and under varied temperature (from 0 to 400° C). The equilibrium conditions are modified and two stepping calculations are done. The same stepping calculation is used to plot property diagrams for the heterogeneous interaction system.

The example also explores settings such as editing the definitions for some system components and their initial bulk composition conditions. This is done through the direct and internal POURBAIX-POLY3 intersection, for a Stepping (or Mapping) calculation inside the Pourbaix module.



The POLY3 file is modified and rewritten with the new conditions. As previously recommended, make a copy of the original POLY3 file (from example TCEX40A) and rename it (e.g. to TCEX40D.POLY3) so you do not lose the file structure and new calculated results.





If you have a POLY3 file generated after choosing Option 2, that file can also be used for Option 4 and vice versa.

## TCEX 40E

This example shows you how to use Option 1 where you **start a completely new calculation**. It uses multiple databases (TCAQ, SSUB and SSOL). The Pourbaix diagram for 0.001 m Fe<sub>90</sub>Co<sub>5</sub>Ni<sub>5</sub> alloy (9E-3 m Fe + 5E-4 m Co + 5E-4 m Ni) in an aqueous solution with 2E-2 m H<sub>2</sub>S and 3 m NaCl at 25° C and 1 bar is automatically calculated and plotted.

You need licenses for three Thermo-Calc databases, i.e.

- A: AQS (TGG Aqueous Solution Database; HKF model) or TCAQ (TCS Aqueous Solution Database; SIT model);
- B: SSUB (SGTE Pure Substances Database)
- C: SSOL (SGTE Alloy Solutions Database) or TCFE (TCS Steels/Fe-Alloys Database) or similar.

The TCAQ database contains only an AQUEOUS solution phase (using the SIT model) and REF\_ELECTRODE phase (as a reference state for electron in aqueous electrolyte systems). The SSUB database is appended for the GASEOUS mixture phase and some pure solid phases (so-called secondary phases formed during aqueous-involving interaction processes), and the SSOL database is appended for various solid solution phases.

The Pourbaix module inside the software also accepts the AQS2 aqueous solution database (using the complete Revised HKF model) in the Multiple Database Option, in addition to the TCAQ2 aqueous solution database (using the SIT model).