Thermo-Calc Software

Graphical Mode Examples Guide

Thermo-Calc Version 2022a

Graphical Mode Examples

This guide includes descriptions of the following examples.

Category	*Example number*
Thermo-Calc Graphical Mode Examples Collection includes binary and ternary system examples, Scheil, the Equilibrium Calculator, Material to Material Calculator, plus more	T_01 to T_14
Thermo-Calc General Property Model Examples Collection: General Models Library	General Models: PM_G_01 to PM_G_12
Steel Model Library Examples Collection	Steel Models: PM_Fe_01 to PM_Fe_08
Nickel Model Library Examples Collection	Nickel Models: PM_NI_01 to PM_Ni_02
Process Metallurgy Module Examples Collection	PMET_01 to PMET_08
Diffusion Module (DICTRA) Graphical Mode Examples	D_01, D_02, D_03 (the Quick Start Guide Examples) D_04 to D_08
Precipitation Module (TC-PRISMA) Graphical Mode Examples	P_01 to P_14

Thermo-Calc Graphical Mode Examples Collection

In this section:

T_01: Calculating a Single-Point Equilibrium

This example shows the result from a single-point equilibrium calculation in the Fe-C system. It demonstrates the use of the Equilibrium Calculator and generates a Table Renderer in the **Results** window. The number of equilibrium conditions is C+2 where C is the number of components, meaning that four conditions are needed in this example:

- **Temperature** is 1000 K
- **Pressure** is 100000 Pa
- **System size** is 1 mole
- **Mass percent carbon** is 0.1%

This example is included as a tutorial on our website and as part of the Graphical Mode Examples playlist on our YouTube channel.

Project File Information

- Folder: Thermo-Calc
- File name: *T_01_Single-point_equilibrium.tcu*

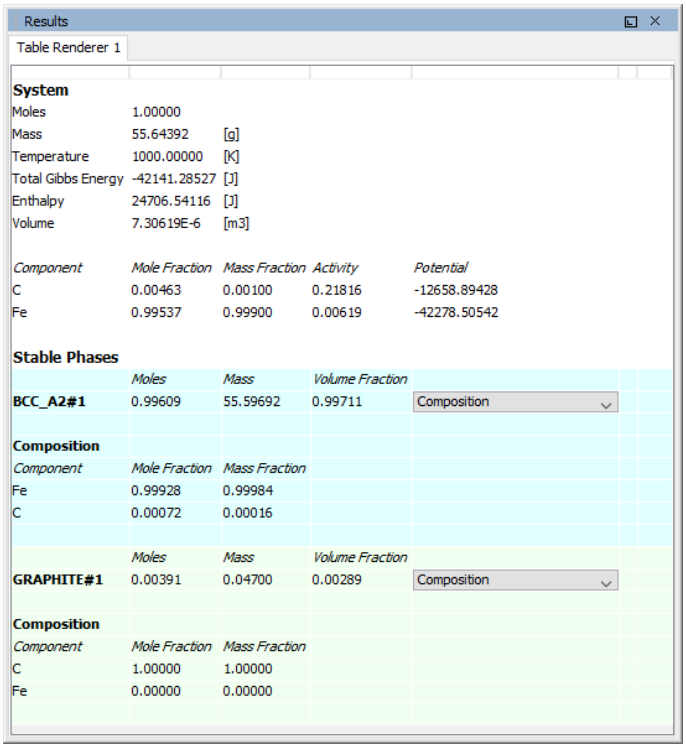


Figure 1: The displayed results of the calculation show that the BCC_A2 (ferrite) and GRAPHITE phases are stable for this set of equilibrium conditions.

T_02: Stepping in Temperature in the Fe-C System

This example shows how the fractions of stable phases vary for an Fe-0.1 mass-% C alloy when the temperature is varied between 500 and 2000 K. It demonstrates the use of the Equilibrium Calculator. To allow temperature to vary, the corresponding **Axis Definition** check box is selected.

This example is included as a tutorial on our website and as part of the Graphical Mode Examples playlist on our YouTube channel.

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

Project File Information

- Folder: Thermo-Calc
- File name: *T_02_Step_in_temperature_in_Fe-C.tcu*

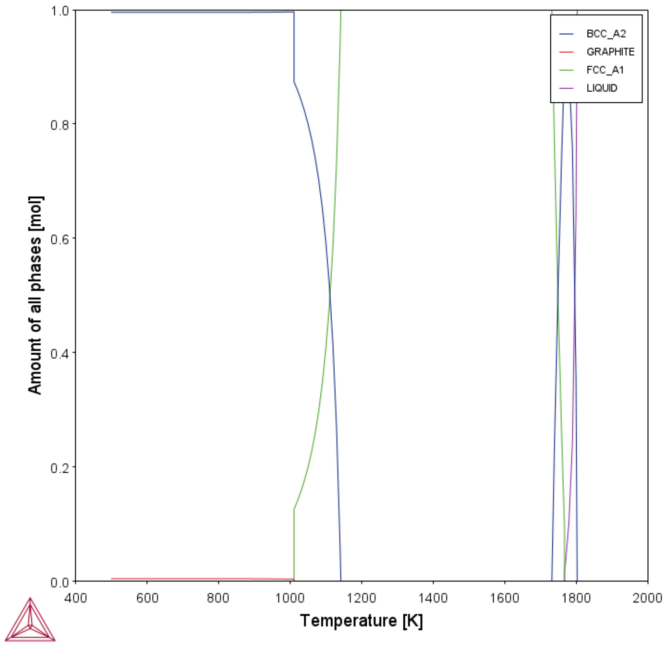


Figure 2: In this example, results are displayed graphically using a Plot Renderer activity.

If you want, you can use a Table Renderer to generate text results instead, as shown in this example after adding a Table Renderer to the Equilibrium Calculator and clicking **Perform**.

Results

Plot Renderer 1 | Table Renderer 1

Temperature [K]	Amount of BCC_A2 [mol]	Amount of FCC_A1 [mol]	Amount of GRAPHITE [mol]	Amount of LIQUID [mol]
1000.00000	0.99609		0.00391	
1010.00000	0.99618		0.00382	
1011.17630	0.99620		0.00380	
1011.17630	0.99620	0.00000	0.00380	
1011.17630	0.87367	0.12633	0.00000	
1011.17630	0.87367	0.12633		
1020.00000	0.86050	0.13950		
1030.00000	0.84335	0.15665		
1040.00000	0.82359	0.17641		
1050.00000	0.80085	0.19915		
1060.00000	0.77399	0.22601		
1070.00000	0.74184	0.25816		
1080.00000	0.70282	0.29718		
1090.00000	0.65470	0.34530		
1100.00000	0.59418	0.40582		
1110.00000	0.51618	0.48382		
1120.00000	0.41250	0.58750		
1130.00000	0.26894	0.73106		
1140.00000	0.05863	0.94137		
1142.15538	0.00000	1.00000		
1142.15538		1.00000		
1150.00000		1.00000		
1160.00000		1.00000		
1170.00000		1.00000		
1180.00000		1.00000		
1190.00000		1.00000		
1200.00000		1.00000		
1210.00000		1.00000		
1220.00000		1.00000		

T_03: Fe-C Phase Diagrams

This example shows the stable Fe-C phase diagram (stable meaning that the graphite phase is entered in the calculation). The same diagram is calculated using the Binary Calculator activity and then using a System Definer and Equilibrium Calculator.

In both cases, a Plot Renderer is used to display results. The purpose of the Binary Calculator is to simplify common calculations for binary systems. In the Equilibrium Calculator two axes are defined: *Mass percent C* and *Temperature*. An axis variable must also be an equilibrium condition.

This example is included as a tutorial on our website and as part of the Graphical Mode Examples playlist on our YouTube channel.

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

Project File Information

- Folder: Thermo-Calc
- File name: *T_03_Fe-C_phase_diagram.tcu*

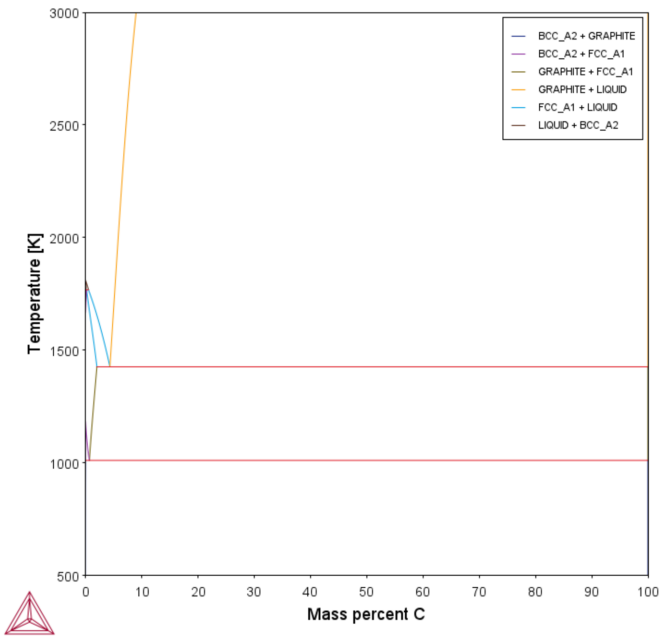


Figure 3: The plot result of the System Definer and Equilibrium Calculator.

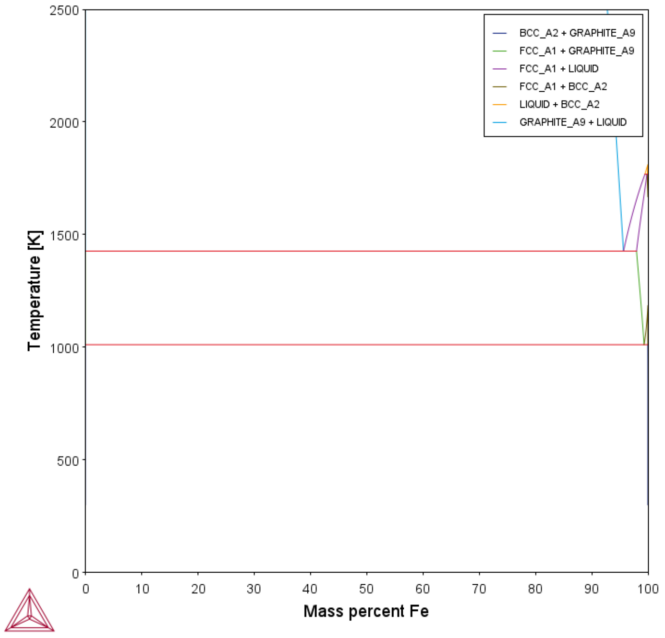


Figure 4: The plot result of the Binary Calculator simulation.

T_04: Fe-Cr-C Ternary Phase Diagram at 1000 K

This example shows a ternary phase diagram in the Fe-Cr-C system at 1000 K. Similar to example T_03: Fe-C Phase Diagrams, the same diagram is calculated using a Ternary Calculator and then using a System Definer and Equilibrium Calculator. Two Plot Renderer activities are added to create two plots.

This example is included as a tutorial on our website and as part of the Graphical Mode Examples playlist on our YouTube channel.

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

Project File Information

- Folder: Thermo-Calc
- File name: *T_04_Fe-Cr-C_ternary_phase_diagram.tcu*

Try practicing with two features on the Plot Renderer Configuration window. To toggle between a triangular and a rectangular diagram, click the **Show Triangular** button then click **Perform** to see what happens. To toggle the X and Y axis variables, click the **Switch Axes** button and then click **Perform**.

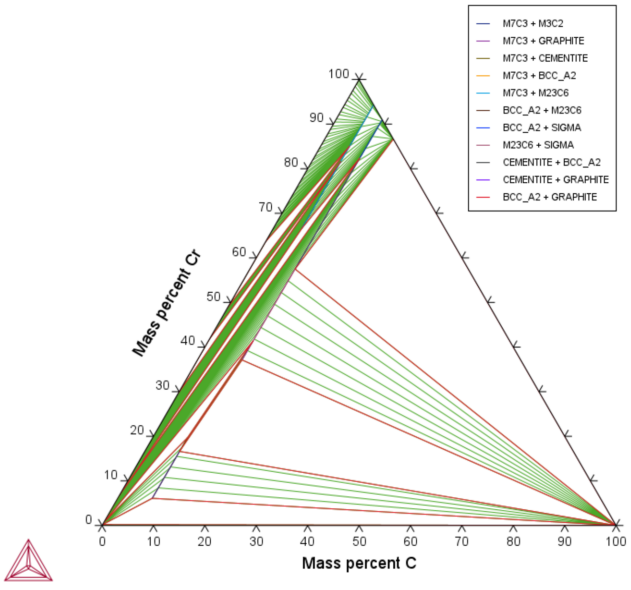


Figure 5: Ternary Calculator

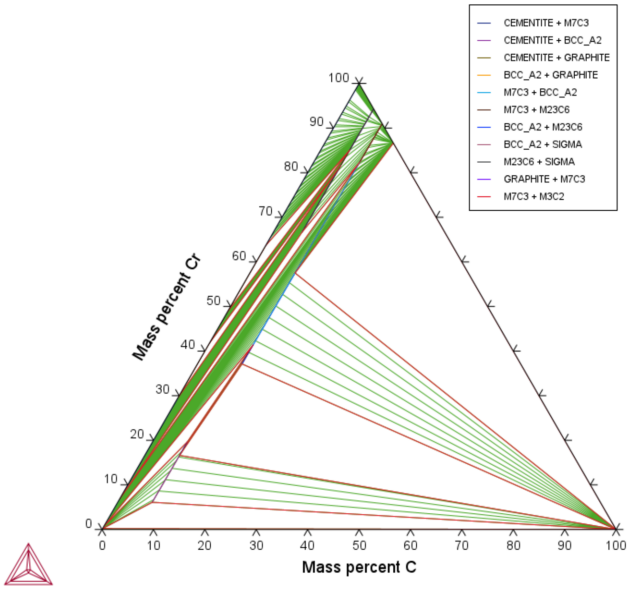


Figure 6: Equilibrium Calculator

T_05: Stable and the Metastable Fe-C Phase Diagrams

This example shows how to overlay results from two calculations in the same plot using the Equilibrium Calculator.

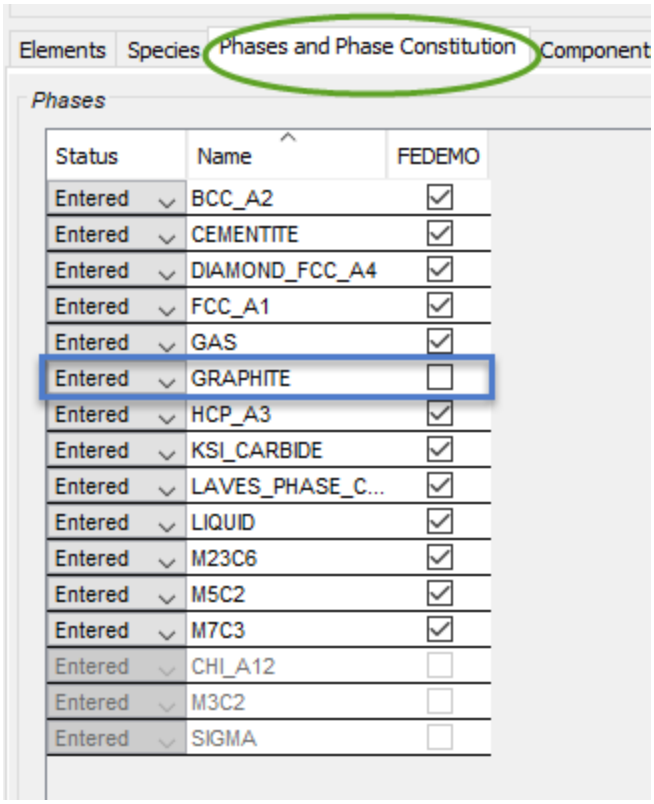
This example is included as a tutorial on our website and as part of the Graphical Mode Examples playlist on our YouTube channel.

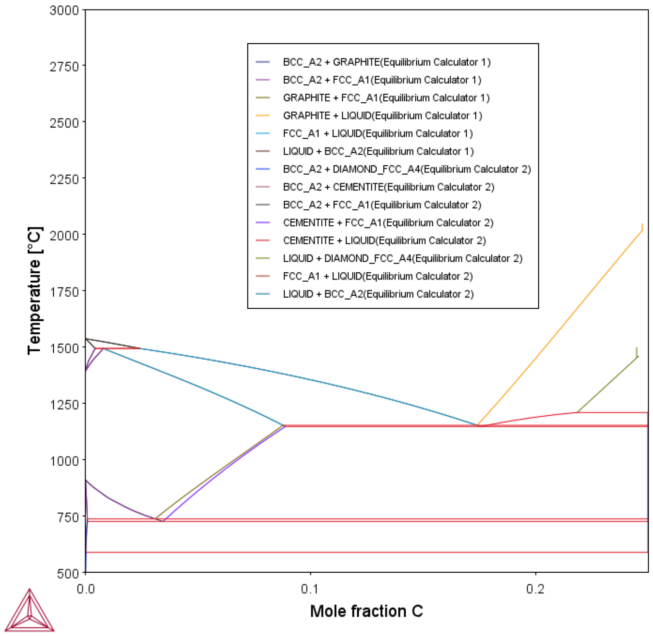
Open the example project file and click **Perform Tree** to generate the plots associated with it.

Project File Information

- Folder: Thermo-Calc
- File name: *T_05_Fe-C_stable_and_metastable_phase_diagram.tcu*

1. The Plot Renderer activity is first created as a successor to Equilibrium Calculator 1.
2. Then right-click the Plot Renderer node and select **Add predecessor** and the results from both equilibrium calculators are in the same plot. In **Equilibrium Calculator 1** the stable phase diagram is calculated and in **Equilibrium Calculator 2** the metastable phase.
3. The metastable diagram is obtained by deselecting the graphite phase on System Definer2 → **Phases and phase constitution** tab.




BCC_A2 + GRAPHITE(Equilibrium Calculator 1)
BCC_A2 + FCC_A1(Equilibrium Calculator 1)
GRAPHITE + FCC_A1(Equilibrium Calculator 1)
GRAPHITE + LIQUID(Equilibrium Calculator 1)
FCC_A1 + LIQUID(Equilibrium Calculator 1)
LIQUID + BCC_A2(Equilibrium Calculator 1)
BCC_A2 + DIAMOND_FCC_A4(Equilibrium Calculator 2)
BCC_A2 + CEMENTITE(Equilibrium Calculator 2)
BCC_A2 + FCC_A1(Equilibrium Calculator 2)
CEMENTITE + FCC_A1(Equilibrium Calculator 2)
CEMENTITE + LIQUID(Equilibrium Calculator 2)
LIQUID + DIAMOND_FCC_A4(Equilibrium Calculator 2)
FCC_A1 + LIQUID(Equilibrium Calculator 2)
LIQUID + BCC_A2(Equilibrium Calculator 2)
Temperature [°C]
3000
2750
2500
2250
2000
1750
1500
1250
1000
750
500
0.0
0.1
0.2
Mole fraction C

T_06: Serially Coupled Equilibrium Calculators

Sometimes there are multiple solutions for a given set of equilibrium conditions. In other cases the equilibrium calculation does not converge. You can then aid the final calculation by, in effect, telling the software where it should start the search for the equilibrium.

This example shows how to serially couple two Equilibrium Calculator nodes together for more complex equilibrium conditions. For each calculation, the output is to a Table Renderer.

This example is included as a tutorial on our website and as part of the Graphical Mode Examples playlist on our YouTube channel.

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

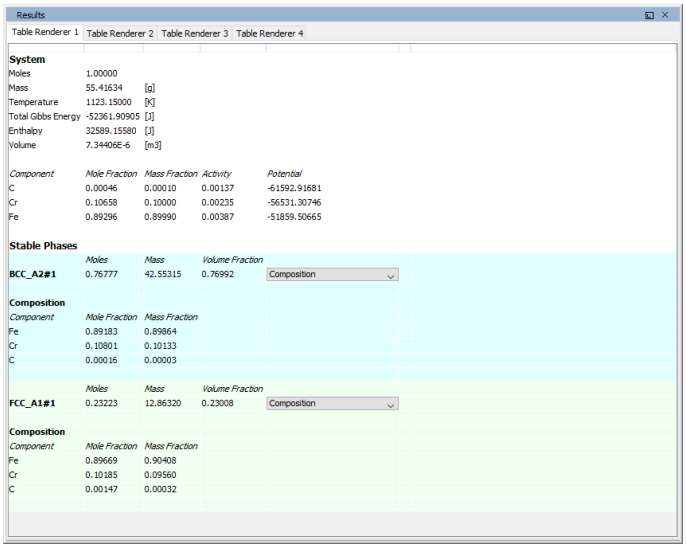
Project File Information

- Folder: Thermo-Calc
- File name: *T_06_Serial_equilibrium_calculators.tcu*

Table Renderer Results

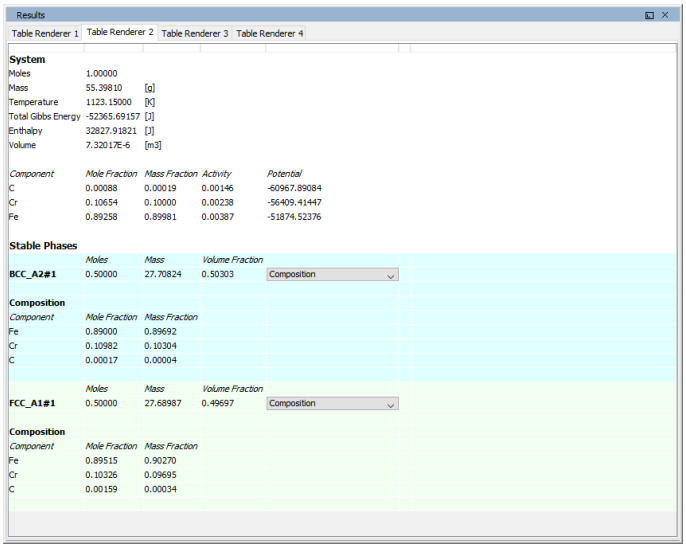
Equilibrium Calculator 1

In the first example, the objective is to calculate the equilibrium at 850° C where the mole fractions of the FCC A1 and BCC A2 phases are 0.5 each for an Fe-Cr-C steel with 10% chromium. In Equilibrium Calculator 1 a simple set of equilibrium conditions (temperature, pressure, system size and composition) are used to find a carbon content where only the FCC A1 and BCC A2 phases are stable. The results from this preliminary calculation are displayed in Table Renderer 1.



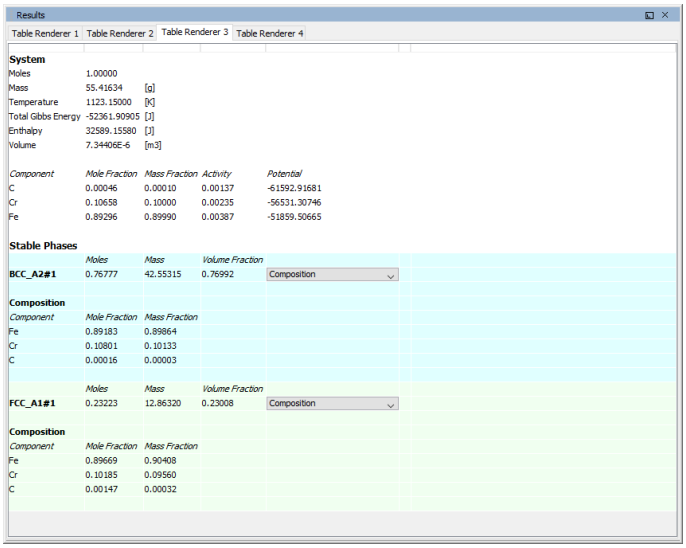
Equilibrium Calculator 2

In Equilibrium Calculator 2 the carbon content equilibrium condition is replaced by the condition that the numbers of moles of the BCC A2 phase should be 0.5. The final result is displayed in Table Renderer 2. In this case, the final objective is to calculate the solidus temperature of an Fe-Cr-C steel with 10% Cr and 0.01% C.



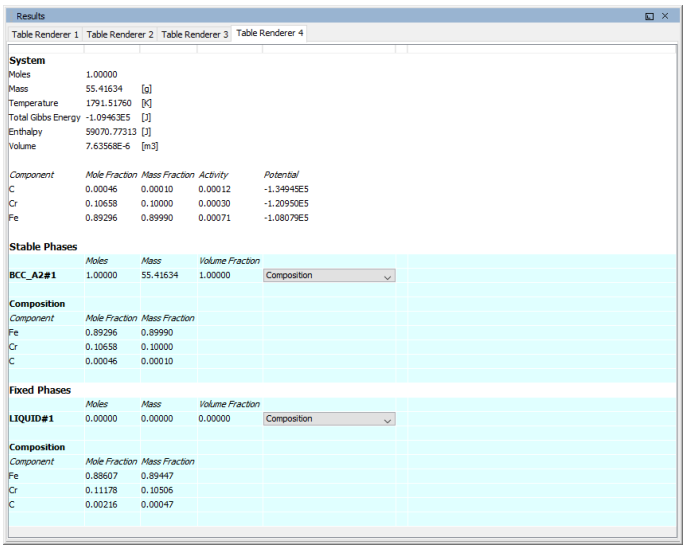
Equilibrium Calculator 3

In Equilibrium Calculator 3 the state at 2000 K is calculated and the result is displayed in Table Renderer 3.



Equilibrium Calculator 4

In Equilibrium Calculator 4 the temperature equilibrium condition is replaced by the condition *Fix phase / liquid / 0.0*, meaning that liquid should be stable in an amount of zero moles, i.e. the solidus temperature. The final result is displayed in Table Renderer 4.



T_07: User-Defined Functions

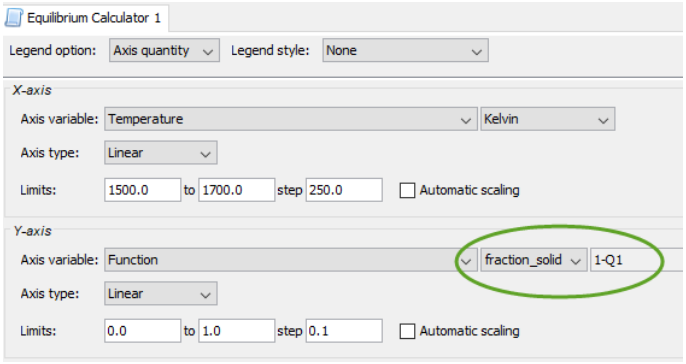
This example shows how to implement user-defined functions. A series of equilibria for an Fe-Cr-C alloy are calculated by varying temperature between 500 and 3000 K. In the configuration window of the Equilibrium Calculator under the **Functions** tab, two identically meaning functions are defined, *fraction solid* and *f solid*, the values of which are plotted against temperature in two Plot Renderer activities. Functions can be entered in terms of *QuantitiesQ1*, *Q2*, *Q3* and so forth, or by using the Thermo-Calc syntax.

This example is included as a tutorial on our website and as part of the Graphical Mode Examples playlist on our YouTube channel.

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

Project File Information

- Folder: Thermo-Calc
- File name: *T_07_User_defined_functions.tcu*



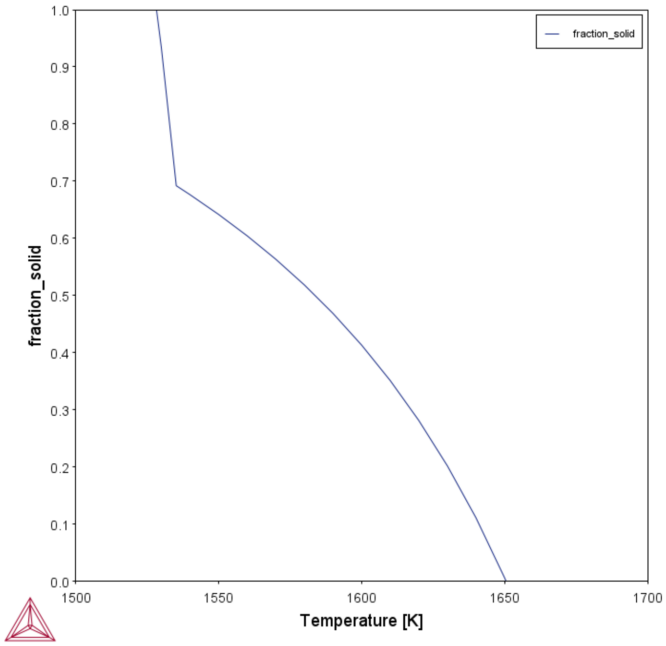


Figure 7: The result of the fraction_solid function.

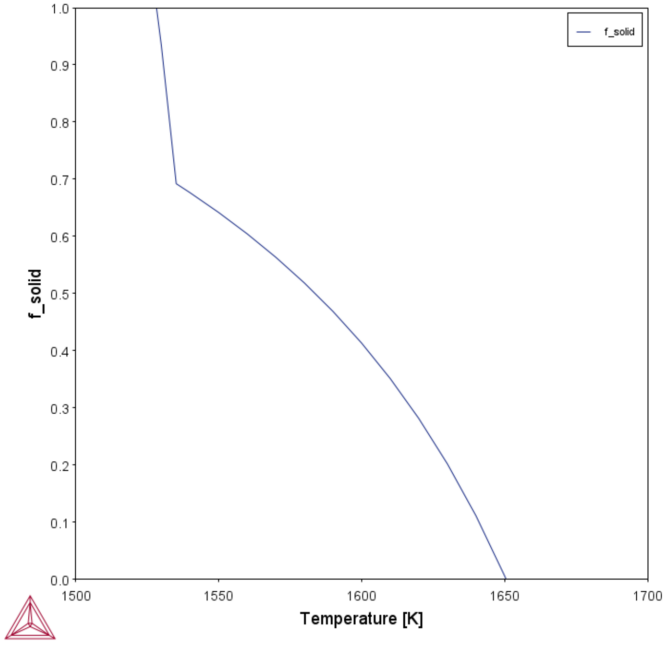


Figure 8: The result of the f_solid function.

T_08: Scheil and Equilibrium Solidification

This example shows a comparison for an Al-Si alloy solidified under full local equilibrium and under the Scheil assumptions, i.e. zero diffusion in the solidified material and infinitely fast diffusion in the liquid. The example uses the Scheil Calculator and adds a Plot and Table Renderer.

This example is included as a tutorial on our website and as part of the Scheil Solidification Simulations playlist on our YouTube channel.

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

Project File Information

- Folder: Thermo-Calc
- File name: *T_08_Scheil_and_equilibrium_solidification.tcu*

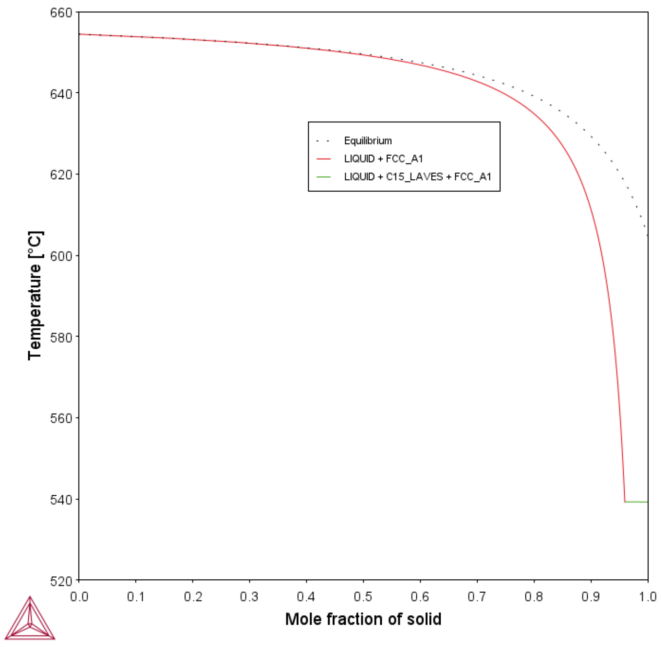
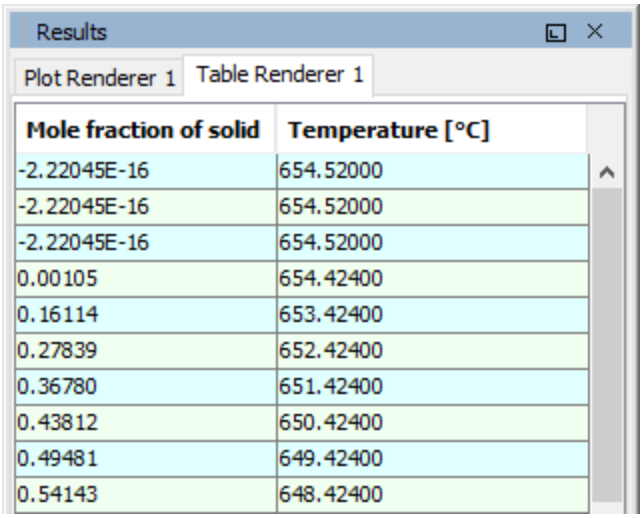


Figure 9: The plot compares the mole fraction of a solid vs temperature.



Mole fraction of solid	Temperature [°C]
-2.22045E-16	654.52000
-2.22045E-16	654.52000
-2.22045E-16	654.52000
0.00105	654.42400
0.16114	653.42400
0.27839	652.42400
0.36780	651.42400
0.43812	650.42400
0.49481	649.42400
0.54143	648.42400

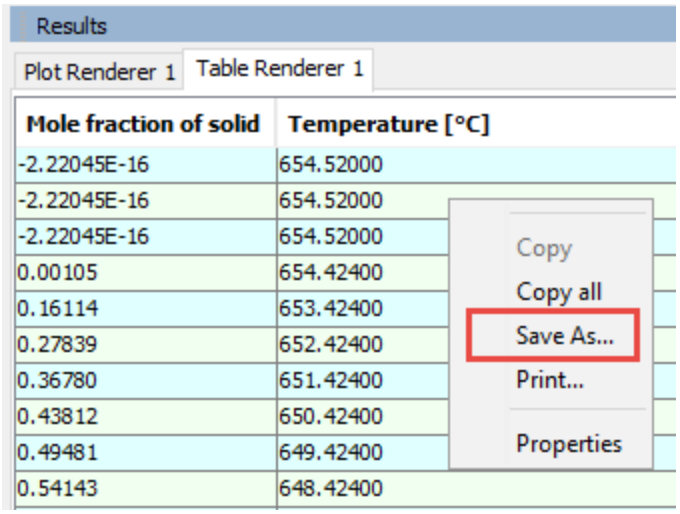
Figure 10: The table provides the data, which you can also export.

To Save the Table (via Table Renderer)

There are two ways to save the table from the Table Renderer **Results** or **Configuration** windows.

Method 1

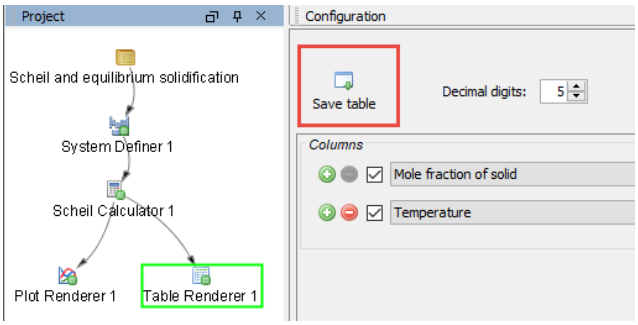
In the **Results** window, right click the table and select **Save As...**



Mole fraction of solid	Temperature [°C]
-2.22045E-16	654.52000
-2.22045E-16	654.52000
-2.22045E-16	654.52000
0.00105	654.42400
0.16114	653.42400
0.27839	652.42400
0.36780	651.42400
0.43812	650.42400
0.49481	649.42400
0.54143	648.42400

Method 2

1. In the **Project** window, click the **Table Renderer**.
2. In the **Configuration** window, click **Save table**.



T_09: Carbide Driving Force Heat Map

This is an example of using *Grid* calculations to plot the driving force for a carbide as a function of two composition variables. With the *Grid* calculation type, a 2D grid is generated from the two calculation axes. After the calculation is done, an equilibrium is calculated in each grid point. A Plot Renderer connected to a grid calculation plots the *z*-axis property for each equilibrium as a function of the two calculation axes.

This example is included as a tutorial on our website and as part of the Graphical Mode Examples playlist on our YouTube channel.

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

Project File Information

- Folder: Thermo-Calc
- File name: *T_09_Heat_map_of_carbide_driving_force.tcu*

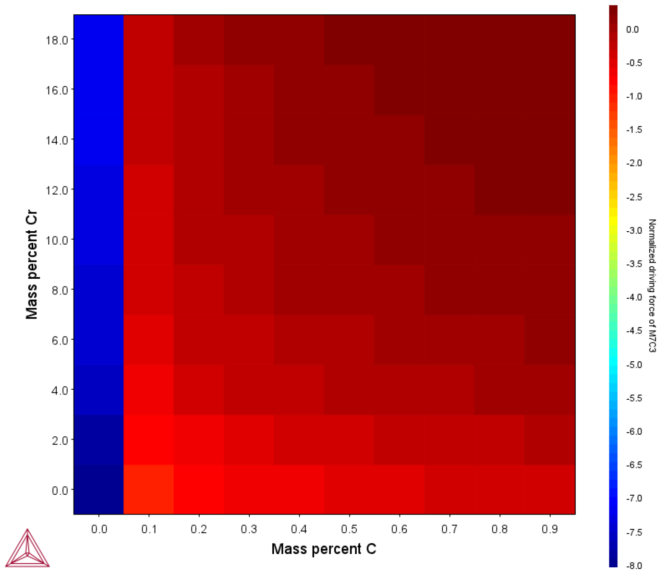


Figure 11: The results are plotted as a heat map. Alternatively, a contour plot type can be selected on the Plot Renderer.

T_10: Scheil Solidification with Back Diffusion

This is an example of a Scheil solidification simulation of a Al-2.1Cu-1Si alloy including back diffusion in the primary phase.

The example uses two of the Scheil Calculator activity nodes with different cooling rates, 10 K/s and 0.005 K/s. The lower cooling rate produces a solidification curve that is closer to the equilibrium curve as shown in the plot result. Both a thermodynamic ALDEMO (aluminum demo) and mobility MALDEMO (Al-alloys mobility) database are used for this calculation.

The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. this model requires the use of a mobility database.

This example is included as a tutorial on our website and as part of the Scheil Solidification Simulations playlist on our YouTube channel.

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

Project File Information

- Folder: Thermo-Calc
- File name: *T_10_Scheil_with_back_diffusion.tcu*.

Running the example itself does not require an additional license.

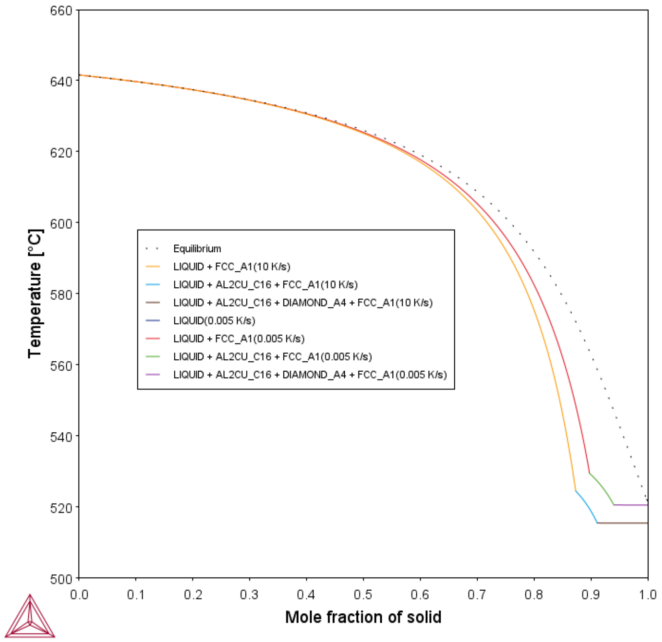


Figure 12: Scheil solidification. The lower cooling rate produces a solidification curve that is closer to the equilibrium curve .

T_11: Surface Tension in Cu-Zr

This is an example of including surface tension in the calculations. This property, and others, are progressively being added to the Thermo-Calc databases starting with Thermo-Calc software version 2020a.

Using the ALDEMO database, which is the free demonstration version of the TCS Al-based Alloy Database (TCAL), the surface tension of liquid metallic is plotted at 1373 K for Cu-Zr and compared to experimental data from [2005Kra].

Reference

[2005Kra] V. P. Krasovskyy, Y. V. Naidich, N. A. Krasovskaya, "Surface tension and density of copper–Zirconium alloys in contact with fluoride refractories," J. Mater. Sci. 40, 2367–2369 (2005).

You can learn more about the surface tension model by searching the help (press F1 when in Thermo-Calc).

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

Project File Information

- Folder: Thermo-Calc
- File name: *T_11_Surface_tension_in_Cu-Zr.tcu*

The same example is also provided in Console Mode as `tcex56`.

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 you can go to the website or our YouTube channel.

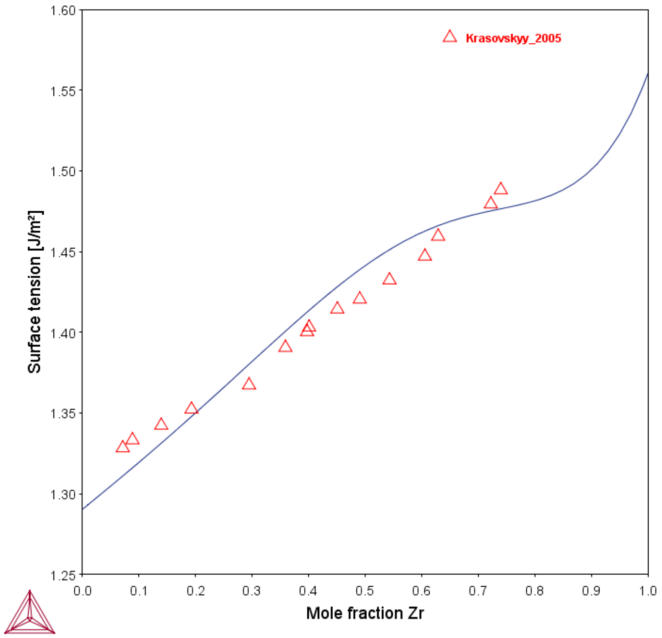


Figure 13: Surface tension of liquid metallic at 1373 K for Cu-Zr and compared to experimental data from [2005Kra].

T_12: Viscosity in Cr-Ni

This is an example of including viscosity in the calculations. This property, and others, are progressively being added to the Thermo-Calc databases starting with Thermo-Calc software version 2020a.

Using the FEDEMO database, which is the free demonstration version of the TCS Steel and Fe-alloys Database (TCFE), the viscosity of metallic liquids is plotted at 1873 K for Cu-Ni and compared to experimental data from [2005Sat].

Reference

[2005Sat] Y. Sato, K. Sugisawa, D. Aoki, T. Yamamura, "Viscosities of Fe–Ni, Fe–Co and Ni–Co binary melts," Meas. Sci. Technol. 16, 363–371 (2005).

You can learn more about the viscosity model by searching the help (press F1 when in Thermo-Calc).

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

Project File Information

- Folder: Thermo-Calc
- File name: *T_12_Viscosity_in_Cr-Ni.tcu*

The same example is also provided in Console Mode as `tcex55`.

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 you can go to the website or our YouTube channel.

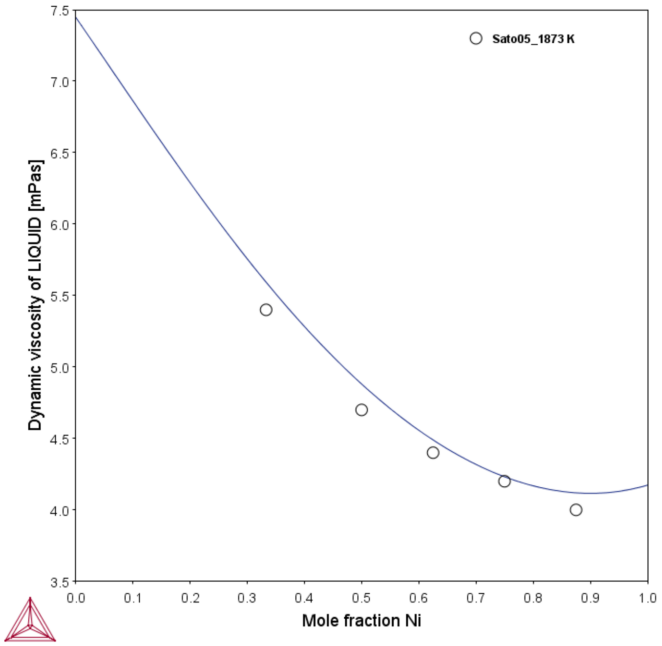


Figure 14: The viscosity of metallic liquids at 1873 K for Cu-Ni and compared to experimental data from [2005Sat].

T_13: Scheil Solidification with Solute Trapping

In Graphical Mode, you use the **Scheil Calculator** to set up the various Scheil solidification simulations.

This example shows the use of the *Scheil with solute trapping* option with an Al-7.5Si-0.2Cu alloy as compared to a Classic Scheil calculation. The thermodynamic ALDEMO (Aluminum demo) database, available to all users, is selected for this calculation to simulate the effect of solute trapping in the primary phase. This type of simulation is useful for additive manufacturing applications.

This example shows how the alloy starts to solidify at a lower temperature compared to a classic Scheil simulation, an effect which increases with increasing solidification speed. The solidification speed is calculated from user supplied scanning speed and angle between the solid/liquid interface and the scanning direction.

This example is included as a tutorial on our website and as part of the Scheil Solidification Simulations playlist on our YouTube channel.

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

Project File Information

- Folder: Thermo-Calc
- File name: *T_13_Scheil_with_Solute_Trapping.tcu*

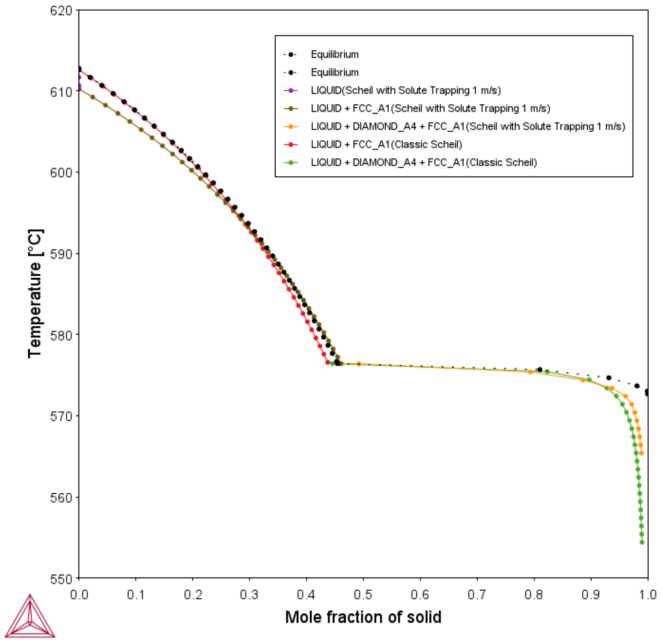


Figure 15: The effect of Scheil solidification with solute trapping of a Al-7.5Si-0.2Cu alloy compared to equilibrium and a Classic Scheil calculation.

T_14: Fe-Cr-Ni Transition Comparison Using the Material to Material Calculator

In Graphical Mode, you use the **Material to Material Calculator** to perform calculations and examine how two materials transition from one into the other. The calculations in this example search for potential deleterious phases during heat treatment of alloys joined together. In this example, the calculation steps between a model martensitic stainless steel (Fe-17Cr-2Ni) and a model Alloy 800 composition (Fe-35Ni-19Cr). Neither alloy is predicted to form the deleterious sigma phase at 600 °C. However sigma is predicted to form at a wide range of mixtures of these two materials, which could have an impact on mechanical properties if it forms.

The example, as defined when you open it, uses a **One axis**calculation (also known as a property diagram), a temperature of 650 °C, to compare the volume fraction of all phases to the mass fraction of Alloy 800. The **Fraction of the second material** (Alloy 800) is set to 50% (0.5), which for a **One axis** calculation is used as the start value.

As with all the examples, you can adjust the settings to plot a variety of combinations of output to see how the Material to Material Calculator works before defining your own project.

The plot for this calculation compares the volume fraction of all phases of Material 1 (martensitic stainless steel) to the mass fraction of Material 2 (Alloy 800). In the plots you can see where each phase (FCC_A1, SIGMA_D8B, and BCC_A2) evolves. As you step from Material 1 to Material 2, the FCC_A1 phase starts forming at about 5% (0.05), SIGMA-D8B phase starts to evolve at about 19% (0.19), and the BCC_A2 transitions from Material 1 to Material 2 where it stops forming at approximately 24% (0.24). The purpose of the calculation is to determine at what fraction of Alloy 800 the deleterious sigma phase forms and this is shown for these compositions.

This example is included as a tutorial on our website and as part of the Graphical Mode Examples playlist on our YouTube channel.

Project File Information

- Folder: Thermo-Calc
- File name: *T_14_Fe-Cr-Ni_Material_to_Material.tcu*

The default plot shows the volume fraction of all phases as a function of the mass fraction of the second material, which in this case, is Alloy 800. You can see that the martensitic stainless composition is BCC at this temperature, and the highly alloyed stainless is FCC. Neither material is expected to form any deleterious phase on its own at 650 °C.

However, mixtures of these two materials, which could arise from a graded transition joint, weld, or potentially a diffusion couple, show some stability for the deleterious sigma phase at this temperature. You can try to make small adjustments to the initial chemistry to reduce the potential for sigma phase to form.

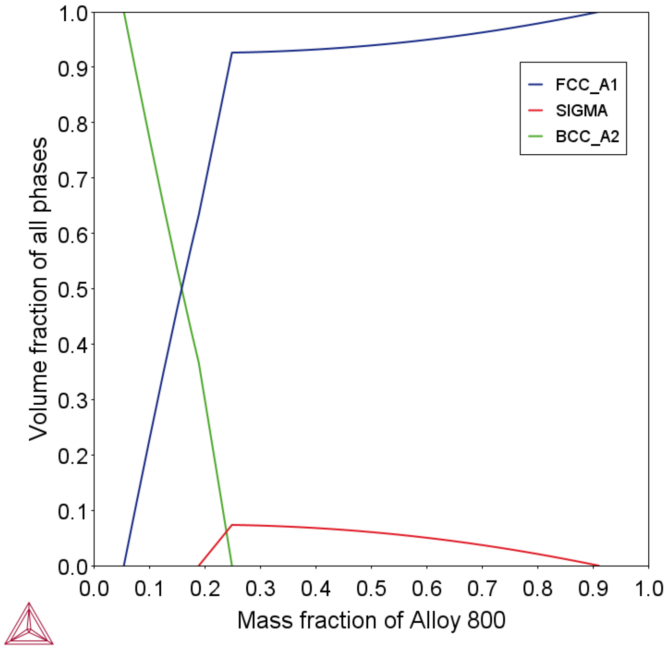


Figure 16: This plot shows the volume fraction of phases when changing composition from the Martensitic Steel (First material) to the Alloy 800 (Second material). This calculation uses the Material to Material Calculator to examine the transition of phases for two compositions of Fe-Cr-Ni. The purpose is to determine at what fraction of Alloy 800 does the deleterious sigma phase start to form. See the text for details.

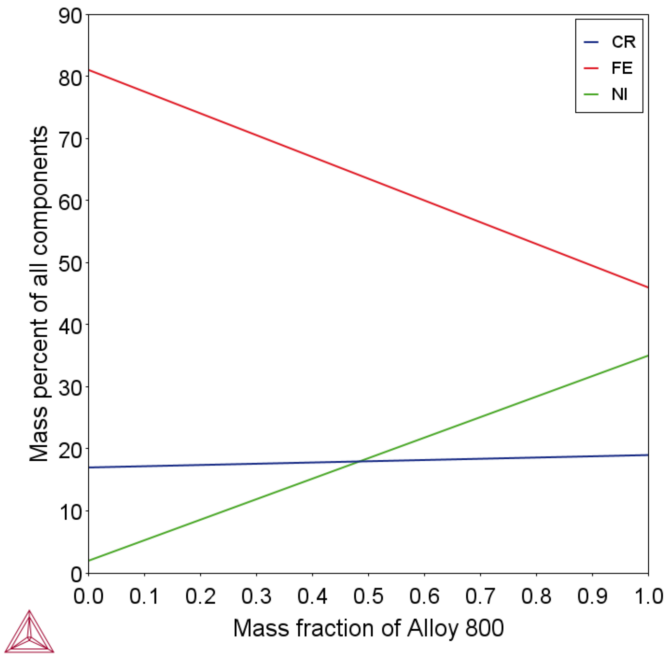


Figure 17: The composition varies linearly when the composition is changed from the Martensitic steel to the Alloy 800 using the Material to Material Calculator. See the text for details.

Thermo-Calc General Property Model Examples Collection

The **General Models** are available to all users.

To run calculations with the **Steel Models** (as part of the Steel Model Library) requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. To run calculations with the **Nickel Models** (as part of the Nickel Model Library) requires a valid maintenance license plus licenses for both the TCNI (version 11 and newer) and MOBNI (version 5 and newer) databases.

These examples use the **Property Model Calculator**, an activity available with Thermo-Calc.

In this section:

PM_G_01: Phase Transition

The example uses the Property Model Calculator to predict the transition temperature to the unwanted brittle sigma phase. The example shows how the temperature is influenced by changes to a steel alloy's composition using the *uncertainty* calculation type and how to create either a *histogram* (frequency diagram) or *probability* plot.

This example is included as a Property Model tutorial on our website and as part of the Property Model Calculator playlist on our YouTube channel.

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

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_01_Phase_Transition.tcu*

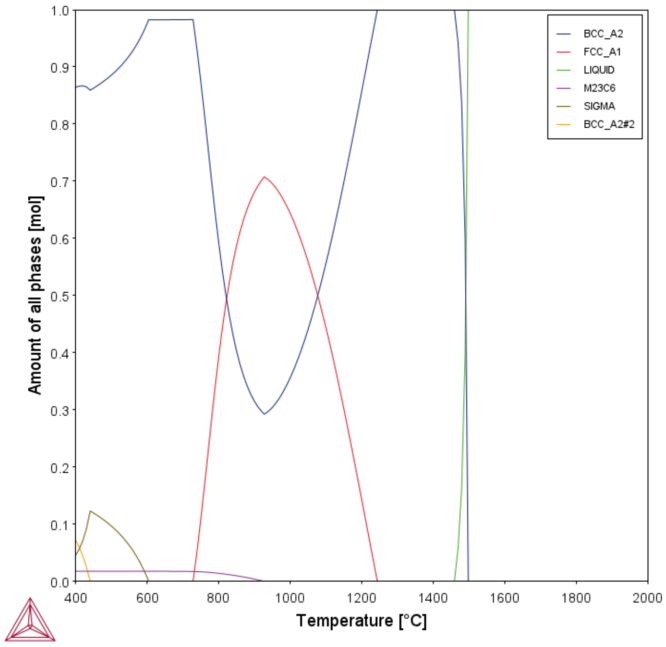


Figure 18: A property diagram as a result of using the Equilibrium Calculator with a One-axis calculation to determine a good starting temperature of the SIGMA phase.

Once you set up the Property Model Calculator, but before running a Grid calculation, it is recommended you run a Single calculation to make sure the calculation is valid. If `the subprocess completed normally` displays in the **Event Log**, it means it worked correctly. You will also see in the Log,

the result "Relaxed Condition", which refers to the variable, in this case, temperature. If the calculation did not work, you will see NAN (not a number) display instead. Check your configurations and run it again before moving on to the more complicated calculation.

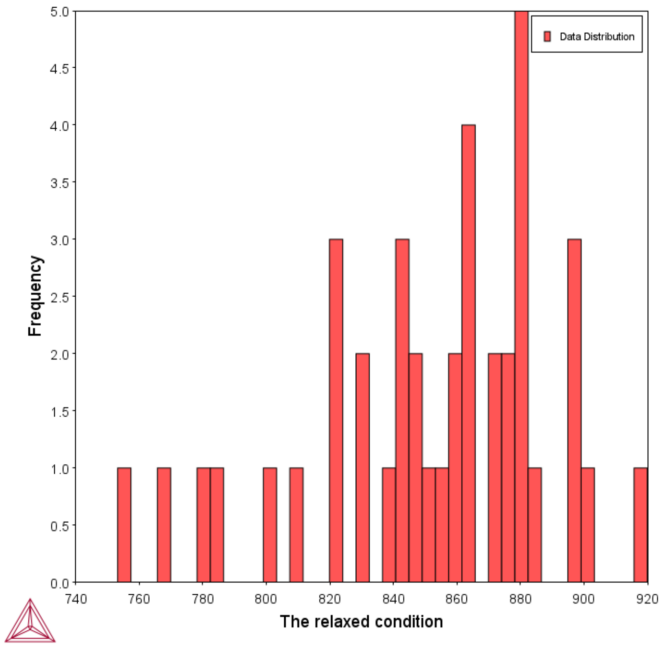


Figure 19: Using the Property Model Calculator with the Phase Transition Model to plot a histogram showing how the transition temperature of sigma varies when you vary the composition. The plot changes each time you run the calculation because it is taking a random sampling from the composition range set.

Note that the X-axis is labeled the **Relaxed Condition**, which you can see on the Configuration window it is **Temperature** for the **Condition to Vary** setting. The Y-axis shows the Frequency, which is the number of samples out of 40 where the composition transitions at each temperature. You can see that the transitions occur more frequently near the 600 degree starting point and less frequently at the edges.

PM_G_02: Coarsening and Interfacial Energy

The example uses the Property Model Calculator and both thermodynamic (FEDEMO) and kinetic (MFEDEMO) demonstration steel databases. Using a *Grid* calculation type it produces these plots: a *heat map*, a *contour plot* and a *cross plot with contour* (where both the interfacial energy and coarsening rate is shown). It also creates a diagram to show the phase fractions vs time and a 3D plot comparing the coarsening rate coefficient.

This example is included as a Property Model tutorial on our website and as part of the Property Model Calculator playlist on our YouTube channel.

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

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_02_Coarsening_and_Interfacial_energy.tcu*

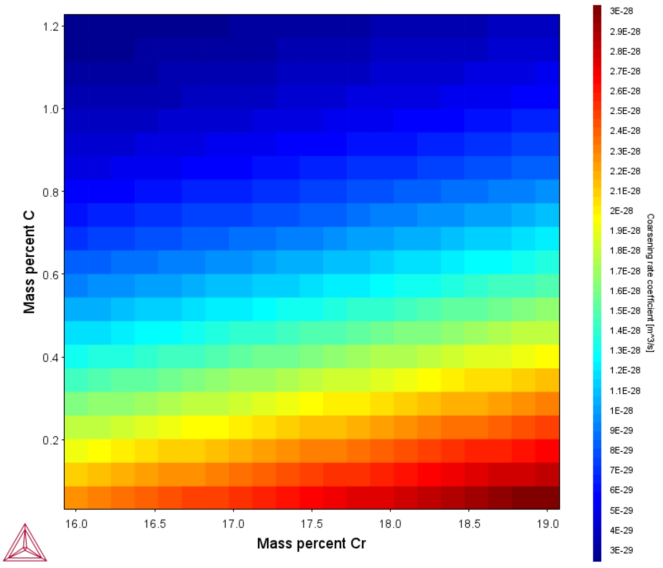


Figure 20: Coarsening rate coefficient (heat map plot).

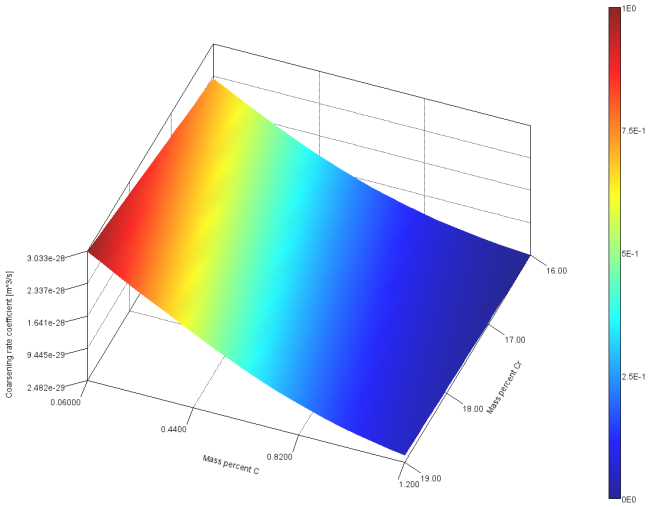


Figure 21: Coarsening rate coefficient (3D plot).

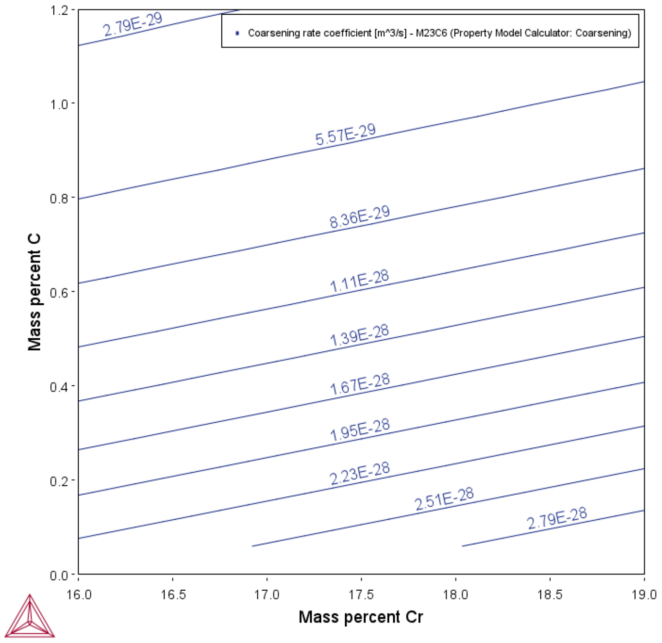


Figure 22: Coarsening rate coefficient (contour plot).

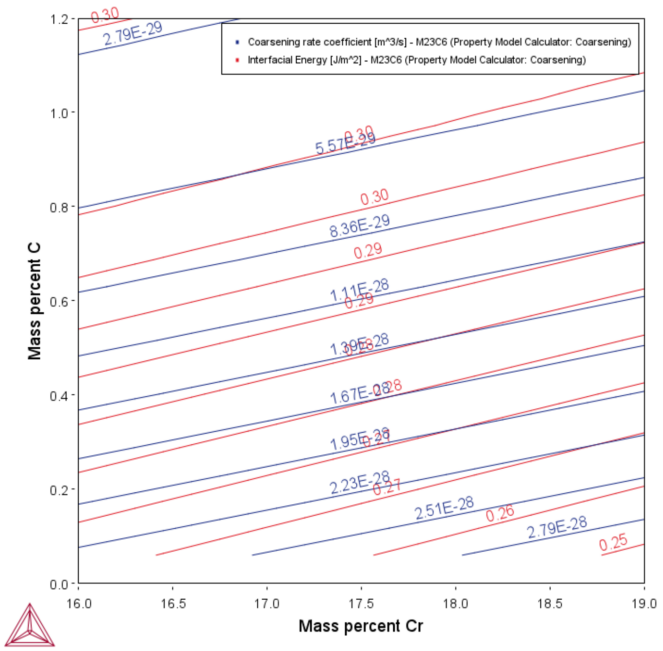


Figure 23: The coarsening rate coefficient and interfacial energy in overlaid plots.

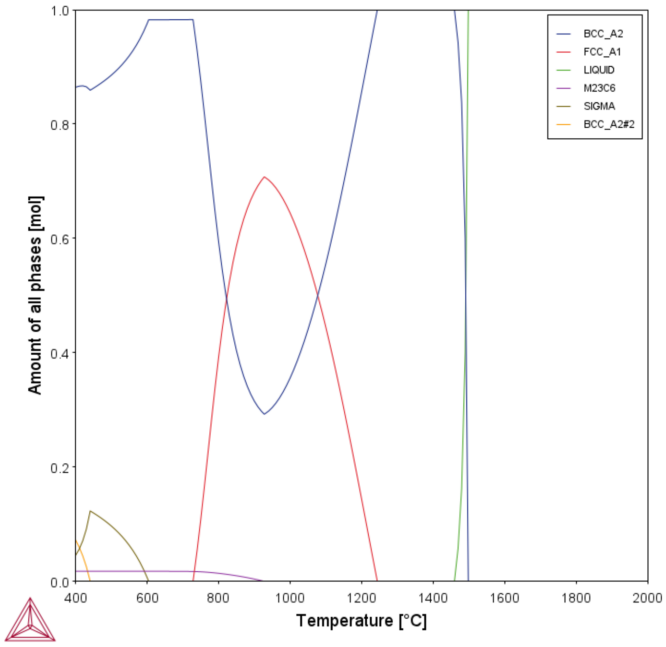


Figure 24: Phase fractions vs T (one axis).

PM_G_03: Driving Force and Interfacial Energy

The example uses the Property Model Calculator and a thermodynamic demonstration steel database (FEDEMO). Using a *grid* calculation type it produces a *contour* plot comparing the driving force and interfacial energy.

This example is included as a Property Model tutorial on our website and as part of the Property Model Calculator playlist on our YouTube channel.

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

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_03_Driving_force_and_Interfacial_energy.tcu*

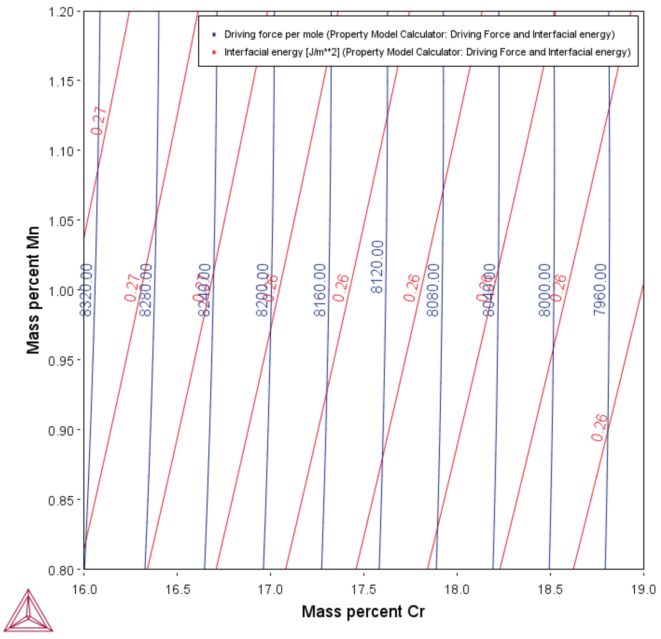


Figure 25: A contour plot.

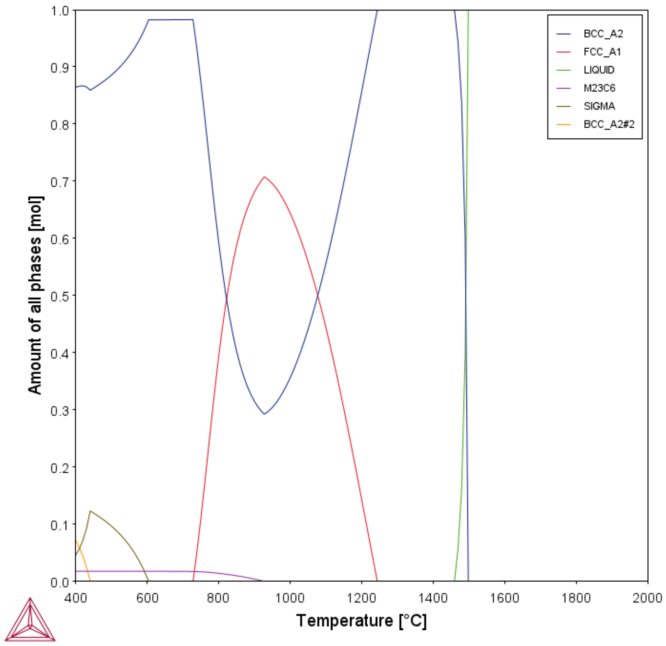


Figure 26: Phase fraction.

PM_G_04: Yield Strength

The example uses the **Property Model Calculator** and the **Yield strength** Property Model with a thermodynamic demonstration aluminum database (ALDEMO).

This example compares the **Simplified** and **Seidman** models yield strength versus precipitate radius to experimental data for an Al-0.3wt%Sc alloy homogenized at 648 °C for 24 hours and subsequently aged at 350 °C. Although the experimental set up is designed to eliminate grain boundary and solid solution strengthening, these are also included by optimizing the model parameters.

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

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_04_Yield_Strength.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 you can go to the website or our YouTube channel.

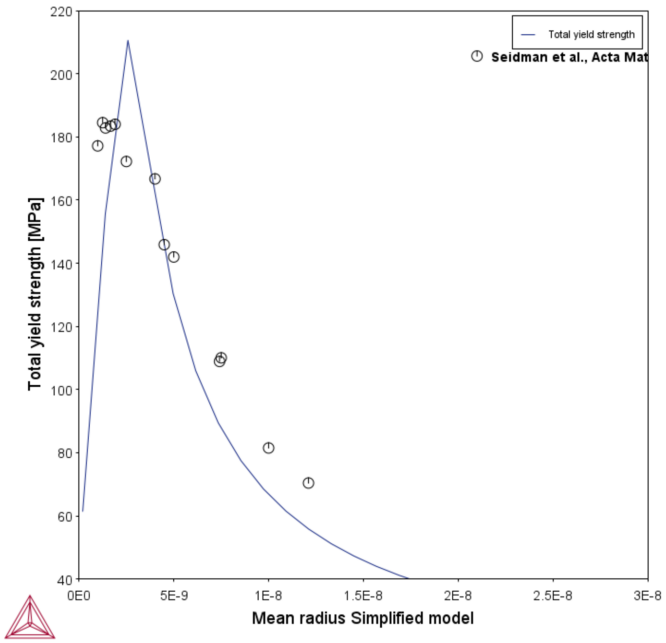


Figure 27: Strength vs Radius - Simplified compared to experimental data from [2002Sei].

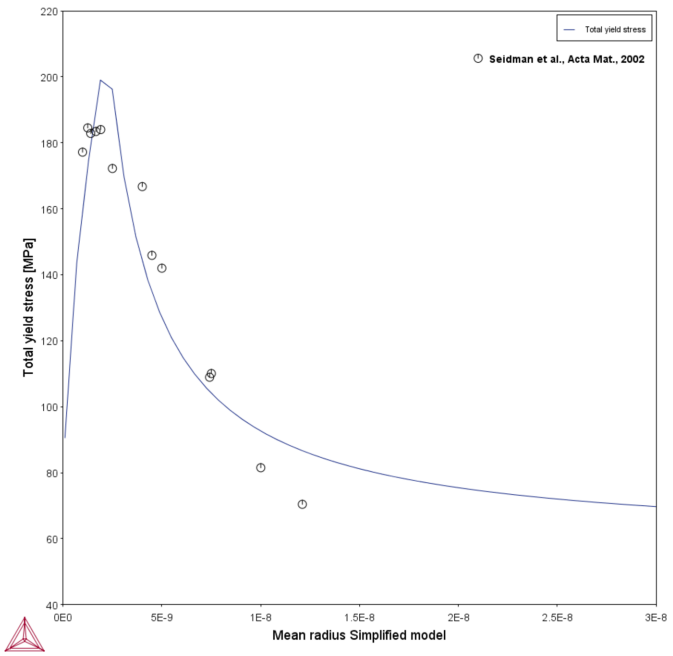


Figure 28: Strength vs Radius - Seidman compared to experimental data from [2002Sei].

Reference

[2002Sei] Seidman, D. N., Marquis, E. A. & Dunand, D. C. "Precipitation strengthening at ambient and elevated temperatures of heat-treatable Al(Sc) alloys," Acta Mater. 50, 4021–4035 (2002).

PM_G_05: Yield Strength NiAlCr

The example uses the **Property Model Calculator** and the **Yield strength** Property Model with a thermodynamic demonstration nickel database (NIDEMO).

The Reppich model is developed for calculation of precipitation strengthening in Ni-based super alloys consisting mainly of gammaprime precipitates in a gamma matrix. The example shows a calculation of the precipitation strengthening vs precipitate radius in a Ni-10at%Al-10at%Cr alloy.

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

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_05_Yield_Strength_NiAlCr.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 you can go to the website or our YouTube channel.

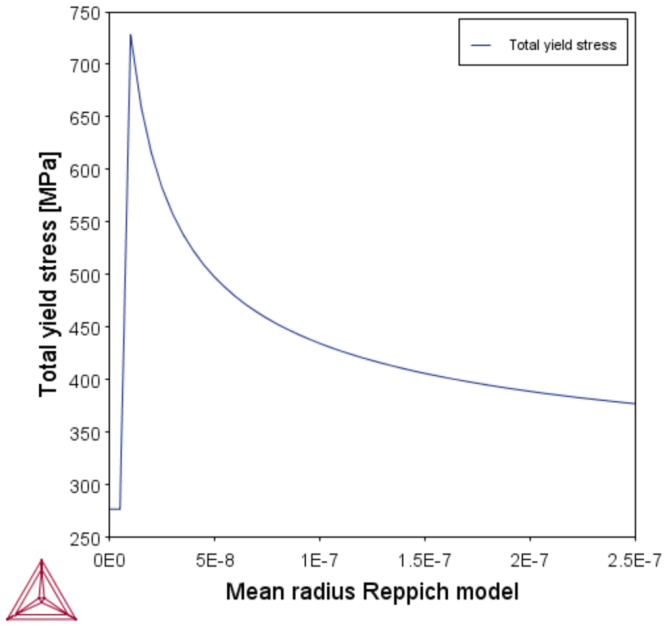


Figure 29: Reppich model plotted with results and experimental data for PE16, all data is normalized with the square root of the volume fraction of precipitate.

PM_G_06: Yield Strength HEA

The example uses the **Property Model Calculator** and the **Yield strength** Property Model with the thermodynamic TCS High Entropy Alloys Database (TCHEA). It is an example of solid solution strengthening, which is the contribution to total strength due to the elastic strains in the crystal lattice caused by alloying elements of a lattice parameter differing from the main constituent. The example shows the solid solution strengthening over the full solubility range for the Mo-Ta system as compared to experimental data [2017Wal].

This example requires the use of the TCS High Entropy Alloys Database (TCHEA). A license is required to run the example.

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

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_06_Yield_Strength_HEA.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 you can go to the website or our YouTube channel.

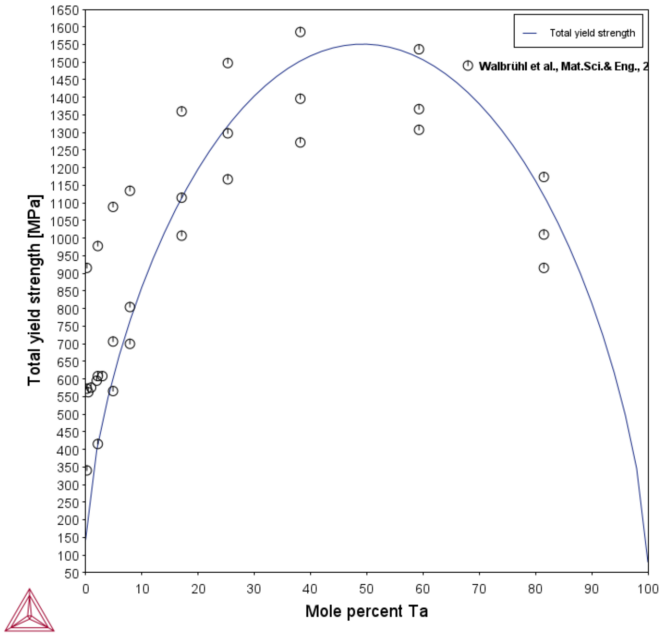


Figure 30: The solid solution strengthening over the full solubility range for the Mo-Ta system as compared to experimental data [2017Wal].

Reference

[2017Wal] Walbruhl, M., Linder, D., Ågren, J. & Borgenstam, A. "Modelling of solid solution strengthening in multicomponent alloys," Mater. Sci. Eng. A 700, 301–311 (2017).

PM_G_07: Hot Crack Susceptibility

The example uses the **Property Model Calculator** and the **Crack Susceptibility Coefficient** Property Model to calculate the hot tearing tendency during solidification for an Al-Si alloy. The **ALDEMO: Aluminum Demo Database** is used and this example is available to all users.

Hot tearing is one of the most common and serious defects encountered during the casting of, for example, aluminum alloys. In general, it is defined by the formation of a macroscopic fissure in a casting as a result of stress and the associated strain, generated during cooling, at a temperature above the non-equilibrium solidus.

The Model is based on the publication by Yan and Lin [2006Yan] and uses experimental data [1955Pum; 1976Feu; 2004Bar] from this paper.

The experimental hot cracking susceptibility of an alloy is defined as the ratio between the cracking length for that alloy and the maximum cracking length in the alloy system studied. Considering the uncertainties and difficulties in hot tearing measurements, the calculated hot tearing tendencies are in excellent agreement with the experimental data. The typical L-shaped curve is well reproduced in the current prediction. It rapidly increases at a low solute content and has a maximum at a composition of around 0.5 wt pct Si.

This example is included as a Property Model tutorial on our website and as part of the Property Model Calculator playlist on our YouTube channel.

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

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_07_Hot_Crack_Susceptibility.tcu*

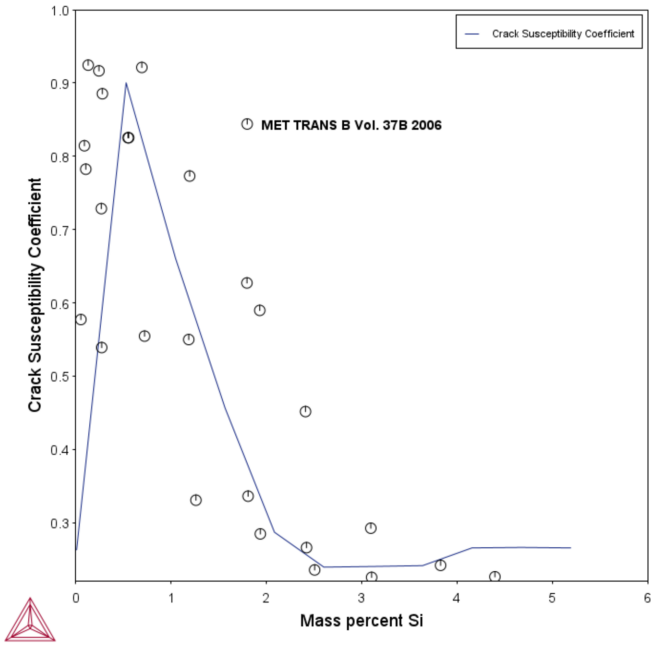


Figure 31: The plot compares the predicted cracking susceptibility/composition curve for the Al-Si system with the experimental hot tearing tendencies [1955Pum; 1976Feu; 2004Bar].

References

[1955Pum] W.I. Pumphrey: ‘‘The Aluminum Development Association Report No. 27,’’ Aluminum Development Association, London, 1955.

[1976Feu] V. Feurer: Giessereiforschung, 1976, vol. 28, pp. 75-80.

[2004Bar] S. R. Barnett, J. A. Taylor, and D. H. St. John: Solidification of Aluminum Alloys, M.G. Chu, D.A. Granger, and Q. Han, eds., TMS, Warrendale, PA, 2004, pp. 201-09.

[2006Yan] X. Yan and J. C. Lin, “Prediction of hot tearing tendency for multicomponent aluminum alloys,” Metall. Mater. Trans. B, vol. 37, no. 6, pp. 913–918, Dec. 2006.

PM_G_08: Spinodal

The example uses the **Property Model Calculator** and the **Spinodal** Property Model to calculate the so-called spinodal curve for the BCC_A2 miscibility gap in the system Fe-Cr. The **FEDEMO: Iron Demo Database** is used and this example is available to all users.

Two Property Model Calculators are used in this example. The spinodal curve (a **One axis** calculation), is overlaid on top of a the Fe-Cr **Phase diagram** calculation. As can be seen in the plot, the spinodal curve for BCC goes through the one-phase region for Sigma. This is because the spinodal curve for a phase is calculated when all other phases are suspended.

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

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_08_Spinodal.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 you can go to the website or our YouTube channel.

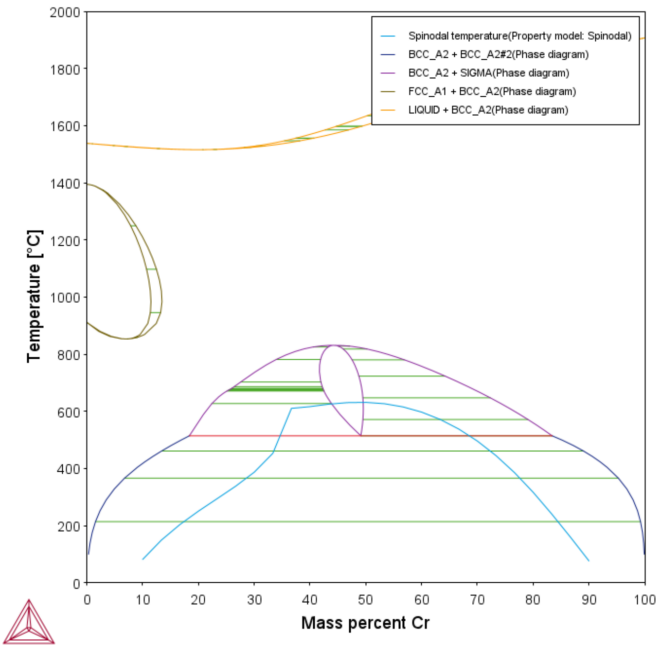


Figure 32: An Fe-Cr spinodal curve for BCC goes through the one-phase region for Sigma.

PM_G_09: T-Zero Temperature

The example uses the **Property Model Calculator** and the **T-Zero Temperature** Property Model to calculate the so-called T_0 line for the two-phase field FCC_A1 and BCC_A2 in the Fe-Ni system. The line is plotted together with the phase diagram for the same Fe-Ni system. The **FEDEMO: Iron Demo Database** is used and this example is available to all users.

The T_0 temperature is defined as the temperature where two phases of identical chemical composition have the same molar Gibbs free energy. This temperature is an important quantity in the field of diffusionless phase transformations, e.g. martensitic transformation, since it is the upper limit where diffusionless phase transformations can occur.

Two Property Model Calculators are used in this example. The T_0 line (a **One axis** calculation) for the two-phase field FCC_A1 and BCC_A2 is overlaid on top of a the Fe-Ni **Phase diagram** calculation.

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

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_09_T-Zero_temperature.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 you can go to the website or our YouTube channel.

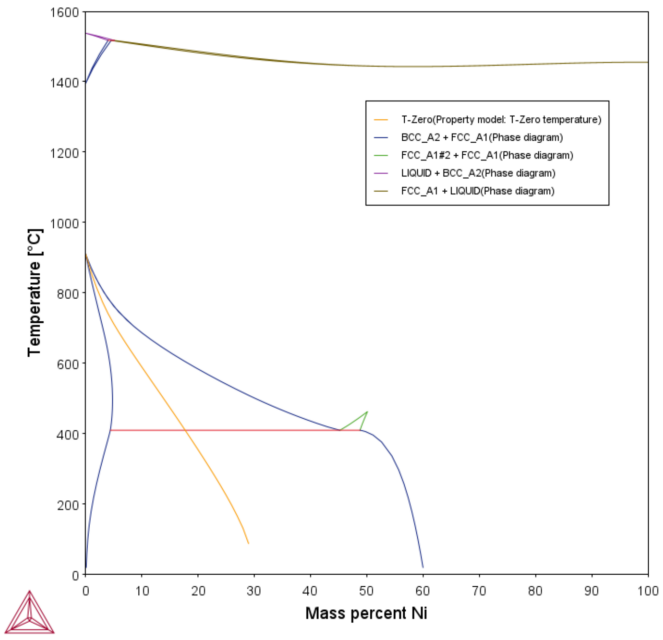


Figure 33: In this plot for the Fe-Ni system, the T_0 line for the FCC_A1 and BCC_A2 phases is located in the middle of the two-phase region. No solution for the T_0 temperature exists above about 30 mass% Ni.

PM_G_10: Freeze-in Thermal Conductivity

The example uses the **Property Model Calculator** and the **Equilibrium with Freeze-in Temperature** Property Model to compare the use of the model with thermal conductivity with and without grain boundary (GB) phase scattering being included in the calculation.

The TCS Al-based Alloy Database (TCAL) is used to evaluate a 7075_T6 alloy (Al-1.6Cu-2.5Mg-5.6Zn-0.25Fe-0.15Mn-0.23Cr-0.2Ti-0.2Si) mass%. The "T6" in the alloy name means that the alloy has been artificially peak-aged, i.e. the matrix is almost depleted. The heating is assumed to be at a typical artificial aging temperature of 150 °C. The temperature has then been increased for measuring of the reported values thermal conductivity at 400, 500, and 532 °C.

The thermal conductivity due to grain boundary phase scattering is approximated as a scattering constant times the total volume fraction of the grain boundary phases. The contribution to thermal conductivity is assumed to be related to that to electrical resistivity, following the Wiedemann-Franz law.

The calculation set up assumes that the alloy reaches equilibrium at the peak-age temperature, i.e. that the amounts of phases and their composition freeze-in at 150 °C and that these do not change for the evaluation of thermal conductivity at the temperatures 400, 500, and 532 °C. Calculations are compared between accounting and ignoring contributions from grain boundary (GB) phase scattering.

As can be seen in Figure 34, the calculation including the approximate effect of grain boundary phase scattering is close to the experimentally measured values. Excluding the effect of grain boundary phase scattering slightly overestimates the thermal conductivity. Experimental data is from [2008ASM].

The TCS Al-based Alloy Database (TCAL) is used in this example. A valid license for version 7 (TCAL7) or newer is required to run the example.

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

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_10_Freeze_In_Thermal_Conductivity.tcu*

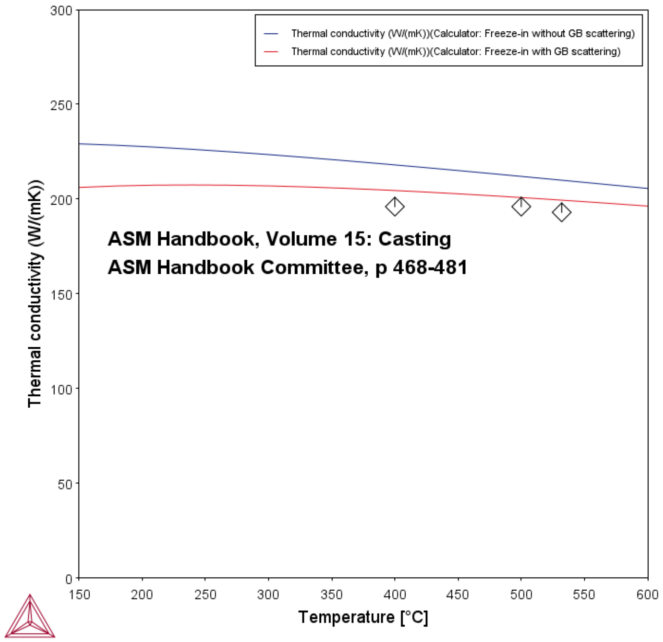


Figure 34: Comparing the freeze-in temperature for the 7075_T6 alloy with and without grain boundary (GB) scattering included in the calculations.

Reference

[2008ASM] ASM Handbook Committee, ASM Handbook Volume 15: Casting. ASM International, p. 468-481, 2008, ISBN 978-0-87170-711-6.

PM_G_11: Freeze-in Electrical Resistivity

The example uses the **Property Model Calculator** and the **Equilibrium with Freeze-in Temperature** Property Model to compare the use of the model for electrical resistivity with and without grain boundary (GB) scattering being included in the calculation.

The TCS Al-based Alloy Database (TCAL) is used to evaluate a 4032-O alloy (Al-0.9Cu-1.0Mg-0.9Ni-12.2Si) mass%. The "O" in the alloy name means that the Al alloy has been heat-treated at a typical temperature of 350 °C. The measurement of electric resistivity is usually performed at room temperature.

The electrical resistivity due to grain boundary phase scattering is approximated as a scattering constant times the total volume fraction of the grain boundary phases.

The calculation set up assumes that the alloy reaches equilibrium at the "O" heat-treated temperature, i.e. that the amounts of phases and their composition freeze-in at 350 °C and that these do not change for the evaluation of electrical resistivity at the room temperature. Calculations are compared between accounting and ignoring contributions from grain boundary (GB) scattering.

As can be seen from Figure 35, the calculated electrical resistivity at room temperature, including grain boundary phase scattering, is very close to the experimentally measured value (4.3E-8) for the alloy. Excluding the grain boundary phase scattering somewhat underestimates the electrical resistivity for the alloy. Experimental data is from [1993Dav].

The TCS Al-based Alloy Database (TCAL) is used in this example. A valid license for version 7 (TCAL7) or newer is required to run the example.

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

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_11_Freeze_In_Electric_Conductivity.tcu*

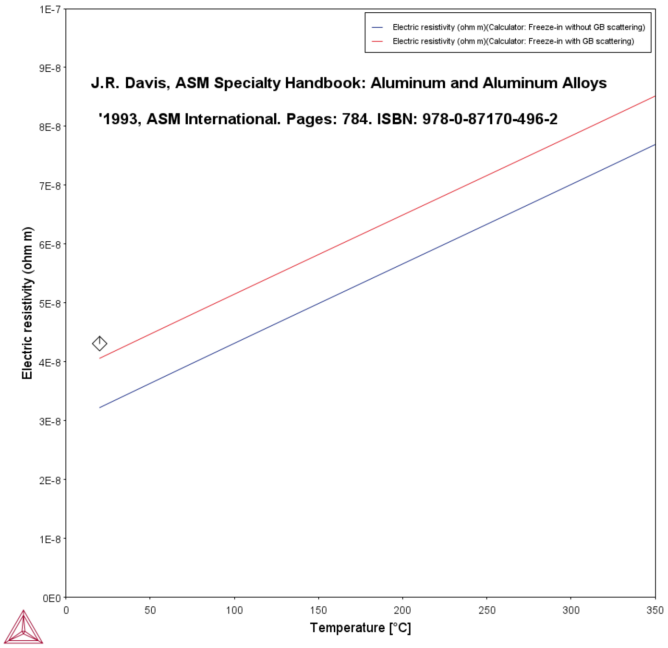


Figure 35: Comparing the freeze-in temperature for the 4032-O alloy with and without grain boundary (GB) scattering included in the calculations.

Reference

[1993Dav] J.R. Davis, ASM Specialty Handbook: Aluminum and Aluminum Alloys, 1993, ASM International. Pages: 784. ISBN: 978-0-87170-496-2.

PM_G_12: Solidus and Liquidus Batch Calculation

The example uses the **Property Model Calculator** and the **Liquidus and Solidus Temperature** Property Model to demonstrate the use of the **Batch** calculation type.

The thermodynamic demonstration steel database (FEDEMO) is used along with a randomized set of experimental data points that are shown on the **Configuration** window in a table. The data showing in this example is imported from a data file prepared with specific data entry requirements.

A variety of compositions for an Fe-Cr-Mn-Ni-C alloy is used for the calculations; these compositions are also taken from the same data file. When the heading includes `Exp`, then these columns are considered experimental data by Thermo-Calc, where in this example it is the columns titled `Exp Liq temp C` and `Exp Sol temp C`. This experimental data can then be plotted as a function of the calculated solidus/liquidus temperature and compared on the plot using a **Cross plot mode**, which is selected on the Plot Renderer. The limits are shown using the setting RMS (root mean square).

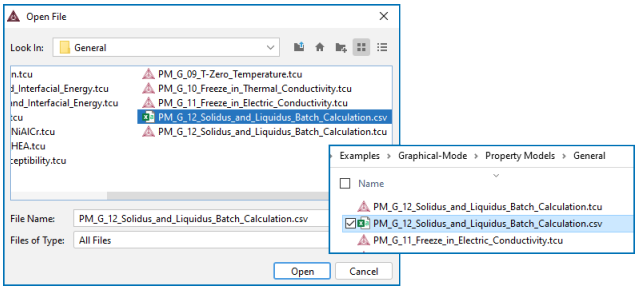
The experimental data entered into the batch data file is unitless even though the actual experimental data unit is Celsius (as written in the header text). In order for the plot and calculations to match, Celsius is chosen as the temperature unit when defining the **Solidus/Liquidus** Property Model and all the axes manually scaled to the same limits (1360 → 1520).

This example is included as a Property Model tutorial on our website and as part of the Property Model Calculator playlist on our YouTube channel.

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

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_12_Solidus_and_Liquidus_Batch_Calculation.tcu*
- There is also a `.csv` file with the same name available in this folder that is used with this example. You can navigate to use it as a template for other data files or just to see its format.



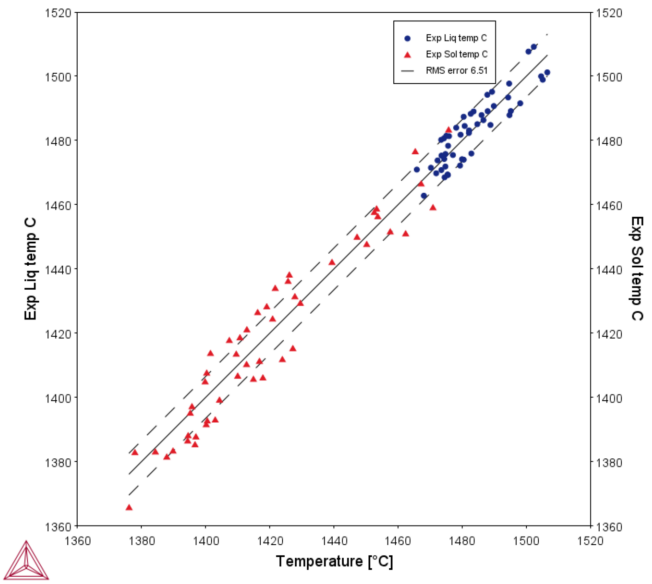


Figure 36: A comparison of experimental liquidus and solidus data using the Cross plot mode with a Batch calculation. A root mean square (RMS) setting shows the distribution of the data points.

Steel Model Library Examples Collection

The **General Models** are available to all users. To run calculations with the **Steel Models** (as part of the Steel Model Library) requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases.

These examples use the **Property Model Calculator**, an activity available with Thermo-Calc plus Property Models in the Steel Model Library.

In this section:

PM_Fe_01: Fe-Cr-C Martensite with Intercritical Annealing

The example uses the **Property Model Calculator** with the **Martensite Fractions** and **Martensite Temperatures** Models to calculate martensite fractions and martensite temperatures [martensite start (Ms) and 90% transformation temperature (M90)].

The alloy is first intercritically annealed and then quenched. Austenite composition is determined by an equilibrium calculation at the annealing temperature. Martensite fraction is calculated as a function of temperature which the alloy is quenched to. The example also shows how Cr content in the alloy influences Ms and M90 after intercritical annealing.

This example is included as a Property Model tutorial on our website and as part of the Property Model Calculator playlist on our YouTube channel.

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

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Project File Information

- Folder: **Property Models>Steel**
- File name: *PM_Fe_01_Fe-Cr-C_martensite_intercritical_annealing.tcu*

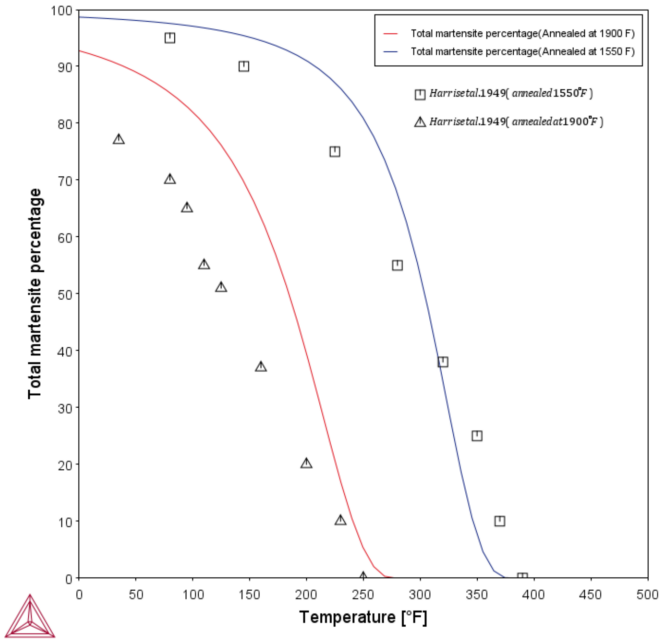


Figure 37: The transformation curves plot showing Fe-Cr-C martensite with intercritical annealing.

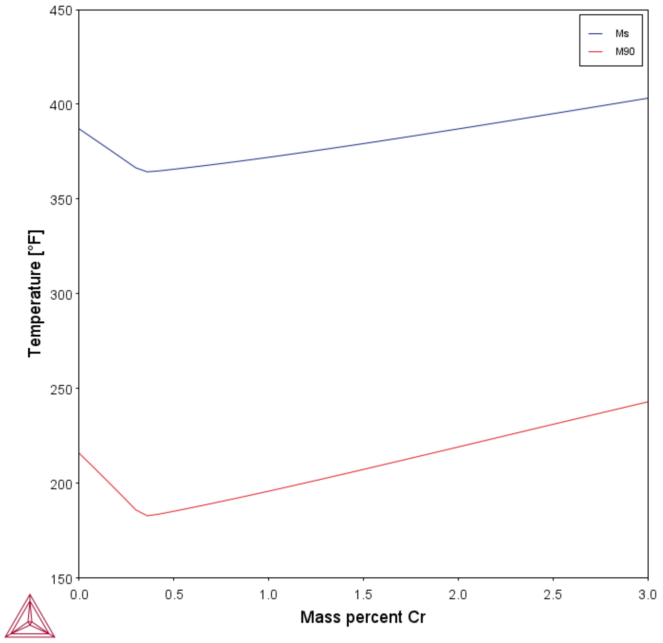


Figure 38: Comparing Martensite start (Ms) to Martensite finish (Mf).

Reference

[1949Har] Harris, William J, and Morris Cohen. 1949. “Stabilization Of The Austenite-Martensite Transformation.” Trans. AIME 180: 447–70.

PM_Fe_02: Fe-Mn Martensite Morphologies

The example uses the **Property Model Calculator** with the **Martensite Temperatures** Property Model to calculate the Ms temperatures of different types of martensites: lath, plate, and ε (HCP), compared with experimental ε Ms values taken from several sources.

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

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Project File Information

- Folder: **Property Models>Steel**
- File name: *PM_Fe_02_Fe-Mn_martensite_morphologies.tcu*

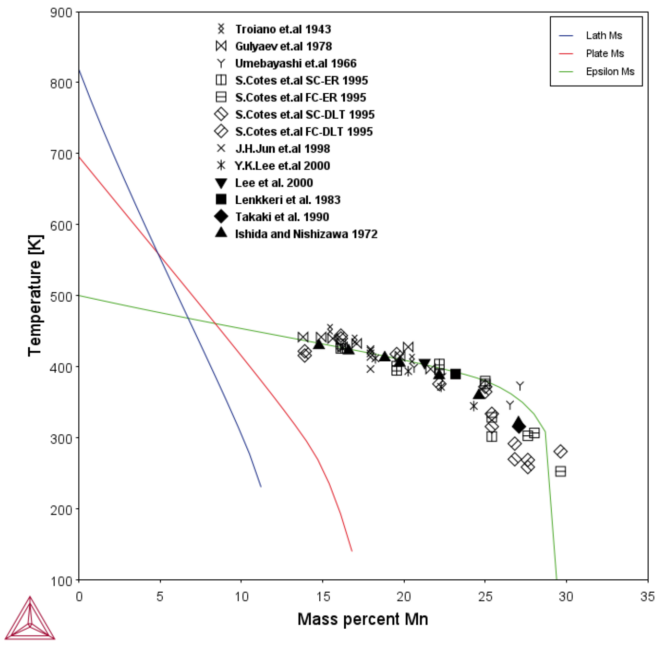


Figure 39: A diagram showing all the Ms temperatures of different types of martensite morphologies (lath, plate and epsilon (HCP) compared with experimental epsilon Ms values.

PM_Fe_03: Fe-C-Mn Pearlite

The example uses the **Property Model Calculator** and with the **Pearlite** Property Model and shows how to calculate pearlite growth rate, lamellar spacing, and times of start (2% transformation) and finish (98% transformation) as functions of isothermal heat treating temperature in an Fe-0.69C-1.80Mn alloy (mass %). With *maximize growth rate* set as the *criterion*, the model gives maximal growth rate and minimal lamellar spacing. With *optimal pearlite* as the *pearlite mode*, the model optimizes partitioning of substitutional alloying element(s) (Mn in this example) according to the criterion, which realizes a smooth transition between ortho-pearlite at high temperature and para-pearlite at low temperature.

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

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

Project File Information

- Folder: **Property Models>Steel**
- File name: *PM_Fe_03_Fe-C-Mn_Pearlite.tcu*

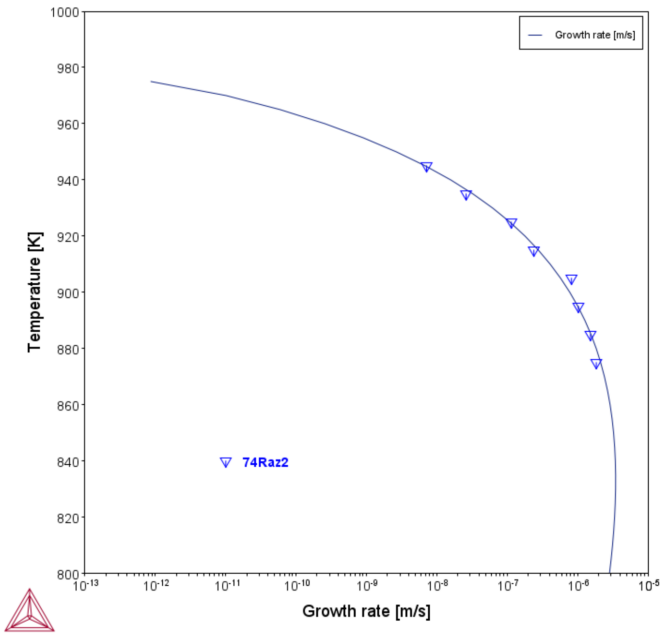


Figure 40: Growth rate as a function of temperature.

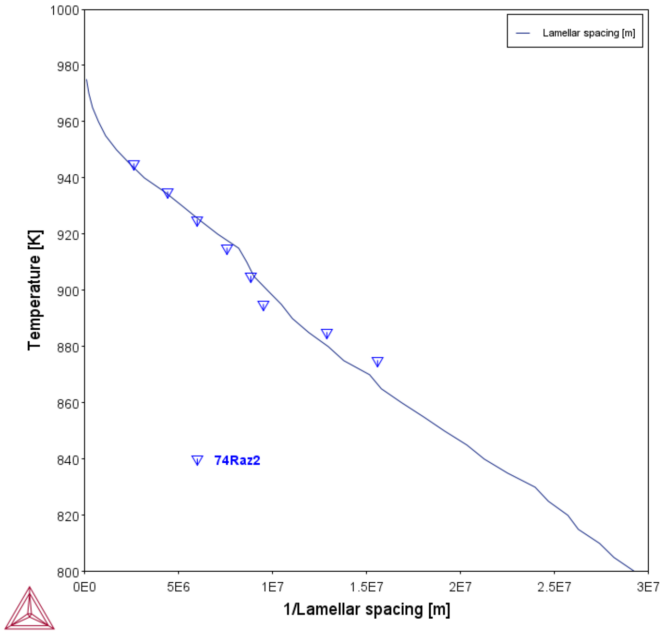


Figure 41: Lamellar spacing as a function of temperature.

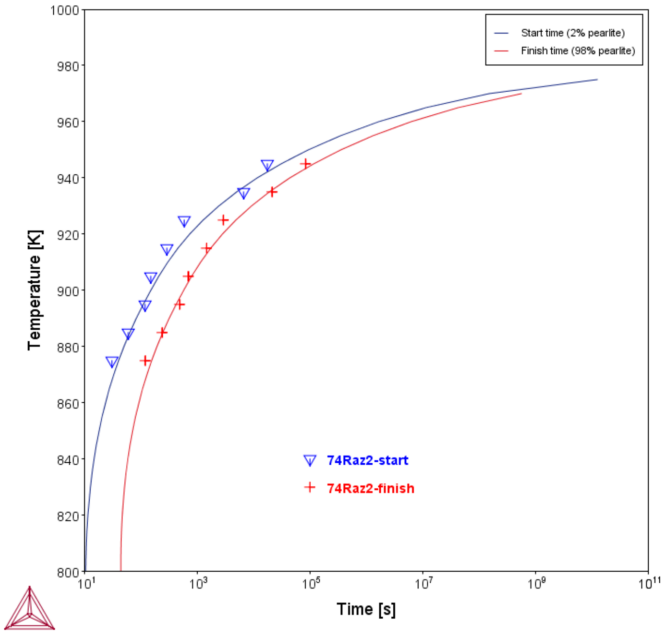


Figure 42: The TTT (time-temperature-transformation) diagram showing times of start (2% transformation) and finish (98% transformation) as functions of isothermal heat treating temperature in an Fe-0.69C-1.80Mn alloy (mass %).

Reference

[1974Raz] Razik, N.A, G.W. Lorimer, and N Ridley. 1974. “An Investigation of Manganese Partitioning during the Austenite-Pearlite Transformation Using Analytical Electron Microscopy.” Acta Metallurgica 22 (10): 1249–58.

PM_Fe_04: Critical Temperatures

The example uses the **Property Model Calculator** and the **Critical Transformation Temperatures** Model to calculate the distribution of the typical phase transition temperatures for a low alloy steel (Fe-0.3Cr-1.0Mn-0.3Mn-0.18C) when the composition is varied within the specification for the alloy.

In the set up of the example, the **Critical Transformation Temperatures** model is used with a Property Model Calculator **Uncertainty** calculation to plot a histogram showing the distribution of A1- and A3-temperatures (Figure 43). As a comparison, an Equilibrium Calculator, **One axis** calculation results in a property diagram showing the phase transitions for the nominal composition (Figure 44).

The phase transition temperatures are defined as:

- Liquidus: First austenite or ferrite transformation from the liquid
- Solidus: Liquid fully transformed to solid
- A0: Magnetic transition temperature (Curie temperature) of cementite. The cementite is paramagnetic above A0 and ferromagnetic below
- A1: Austenite (FCC_A1) transforms to ferrite (BCC_A2) + carbide (cementite or graphite or M23C6)
- A2: Magnetic transition temperature (Curie temperature) of ferrite (BCC_A2). Paramagnetic above A2 and ferromagnetic below
- A3: Austenite (FCC_A1) transforms to ferrite (BCC_A2)

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

The **FEDEMO: Iron Demo Database** is used and this example is available to all users. However, in general a license is required to run the Steel Models.

Project File Information

- Folder: **Property Models>Steel**
- File name: *PM_Fe_04_Critical_Temperatures.tcu*

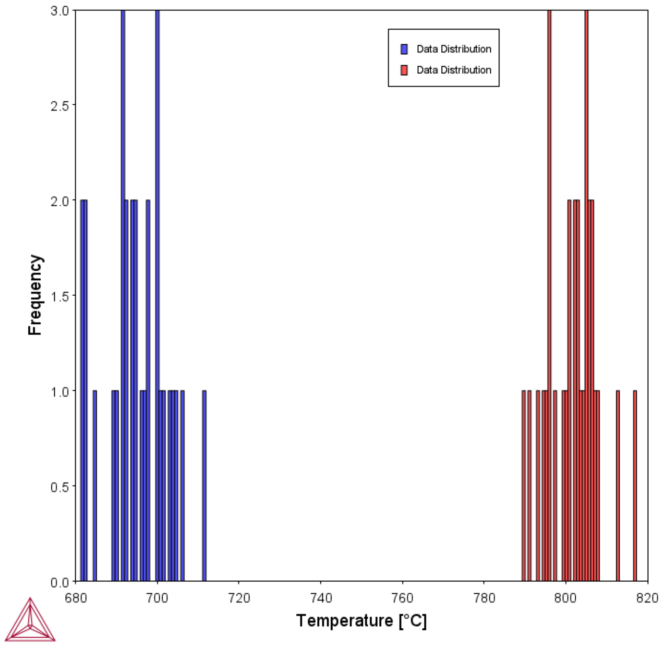


Figure 43: The distribution of the A1 and A3 phase transition temperatures for a low alloyed steel (Fe-0.3Cr-1.0Mn-0.3Mn-0.18C) when the composition is varied within the specification. This plot uses the Critical Transformation Temperatures model with the Property Model Calculator.

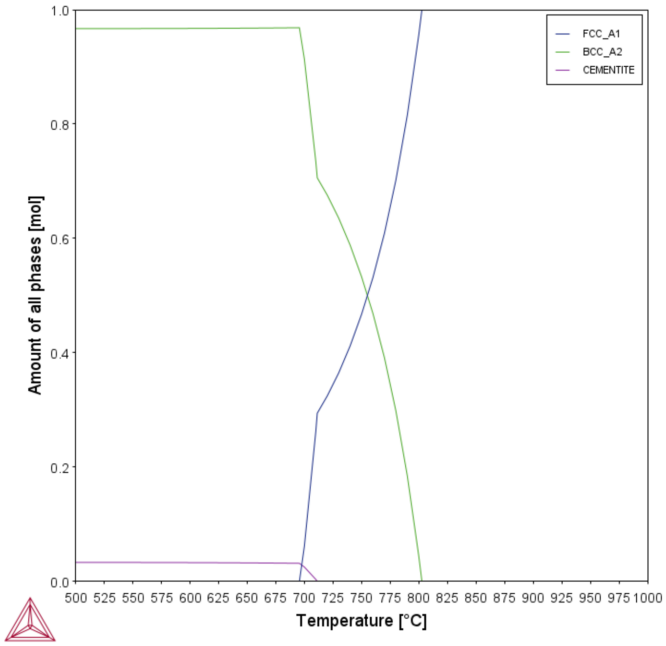


Figure 44: This plot uses an Equilibrium Calculator to show an alternate visualization of the phase transitions in a property diagram for the nominal composition.

PM_Fe_05: Fe-C-Mn-Si-Ni-Cr-Mo Bainite

The example uses the **Property Model Calculator** and the **Bainite** Steel Model to calculate a Time-Temperature-Transformation (TTT) diagram for an Fe-0.97C-0.72Mn-0.32Si-1.54Ni-0.8Cr-0.26Mo alloy. The result is compared to experimental results from [1948Jaf]. Other elements with low amount in the experimental alloy are omitted for the calculation.

Considered elements: Fe, C, Mn, Si, Cr, Ni, and Mo. Other elements in the system are neglected for bainite by mass percent.

A Property Model Calculator is used with a *One axis* calculation and the *TTT mode* selected on the Plot Renderer to plot the TTT diagram.

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

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

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

Project File Information

- Folder: **Property Models>Steel**
- File name: *PM_Fe_05_Fe-C-Mn-Si-Ni-Cr-Mo_Bainite.tcu*

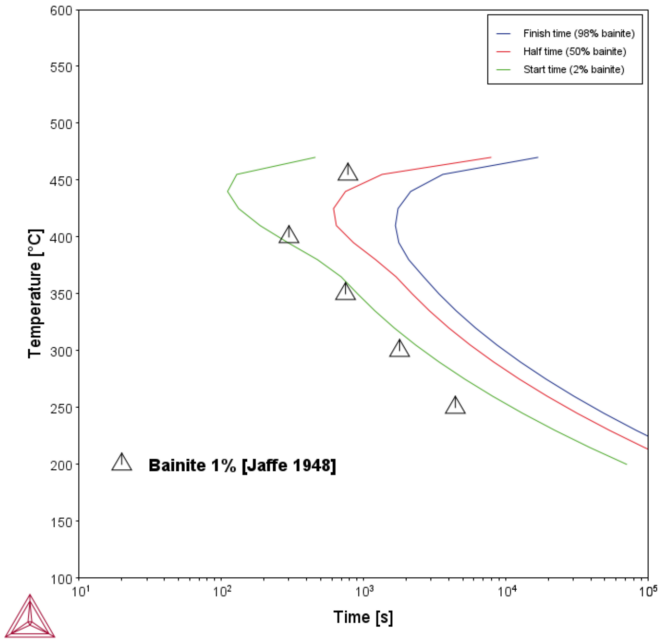


Figure 45: The bainite TTT diagram for an Fe-0.97C-0.72Mn-0.32Si-1.54Ni-0.8Cr-0.26Mo alloy.

Reference

[1948Jaf] L. D. Jaffe, Anisothermal formation of bainite and proeutectoid constituents in steels, Trans. AIME, vol. 176, pp. 343–383 (1948).

PM_Fe_06: TTT Diagram Property Model

The example uses the **Property Model Calculator** and the **TTT Diagram** Property Model to calculate a Time-Temperature-Transformation (TTT) diagram for an Fe-C-Mn-Si-Cr-V alloy (Steel 42CrV6). The calculation is compared to an experimental TTT diagram for the same steel (with some other impurities) from data in [1958Wev].

A *One axis* calculation is selected on the Property Model Calculator and then the *TTT mode* selected on the Plot Renderer in order to plot the final TTT diagram shown in the figure below.

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

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

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

Project File Information

- Folder: **Property Models>Steel**
- File name: *PM_Fe_06_Fe-C-Mn-Si-Cr-V_TTT.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 you can go to the website or our YouTube channel.

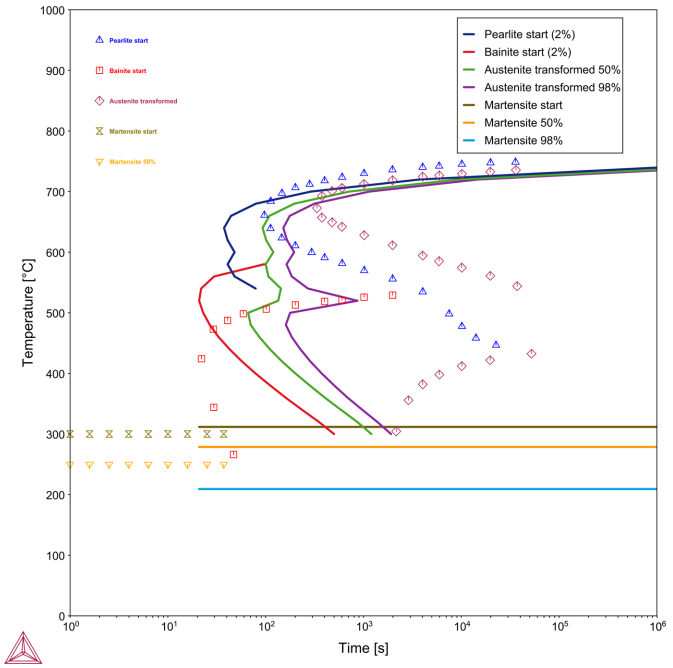


Figure 46: The TTT diagram for an Fe-C-Mn-Si-Cr-V alloy comparing the calculation with experimental data from [1958Wev].

Reference

[1958Wev] F. Wever, A. Rose, Atlas zur Wärmebehandlung der Stähle: 1954/56/58 (Verlag Stahleisen, Düsseldorf, 1958), p. II-112.

PM_Fe_07: Hardenability Design of Steel

This application example, which is showcased on our website, shows how the Steel Model Library in Thermo-Calc can be used to find the optimal compositions for an Fe-Mn-C steel to achieve high hardenability for the purpose of strength.

This example focuses on the hardenability design of steel using the Steel Model Library in Thermo-Calc. It shows how to find the optimal compositions for Fe-Mn-C steel to achieve high hardenability for the purpose of strength. Hardenability refers to the ability of steel to form martensite on quenching. It is a measure of the capacity of a steel to be hardened in depth when quenched from its austenitizing temperature. Among various factors, composition is one of the most important factors which has great influence on the hardenability of the steel. In this example, we use the Steel Model Library to investigate the possible composition ranges of Fe-C-Mn alloys to reach a fully martensitic microstructure.

To fulfil the requirement, room temperature martensite fraction should be large and the amount of retained austenite should be small. Meanwhile, other products of austenite decomposition should be avoided during continuous cooling. Such transformation products can be suppressed by fast quenching, yet the cooling rate is usually limited by the capacity of facilities or other problems such as cracking. Therefore, for hardenability purposes, it is desirable to achieve a fully martensitic structure with a relatively low cooling rate. This is done by promoting martensite formation while retarding other transformations through adjusting the steel composition.

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

Although this example uses the FEDEMO and MFEDEMO databases, running the calculation requires a license for Thermo-Calc 2021b or newer and for the Steel Model Library.

Project File Information

- Folder: **Property Models>Steel**
- File name: *PM_Fe_07_Hardenability_Design_of_Steel.tcu*

The resulting plots and details related to setting up this example are available either via the dedicated web page, or you can read the more in depth step-by-step documentation as a PDF, also available via our website.

PM_Fe_08: CCT Diagram Property Model

The example uses the **Property Model Calculator** and the **CCT Diagram** Property Model to calculate a Continuous-Cooling-Transformation (CCT) diagram for an Fe-C-Mn-Si-Cr-V alloy (Steel 42CrV6). The calculation is compared to an experimental CCT diagram for the same steel (with some other impurities) from data in [1958Wev].

A *One axis* calculation is selected on the Property Model Calculator and then the *CCT mode* selected on the Plot Renderer in order to plot the final CCT diagram shown in the figure below.

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

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and newer) and MOBFE (version 4 and newer) databases. Also see our website to learn more about the Steel Model Library and other related examples.

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

Project File Information

- Folder: **Property Models>Steel**
- File name: *PM_Fe_08_Fe-C-Mn-Si-Cr-V_CCT.tcu*

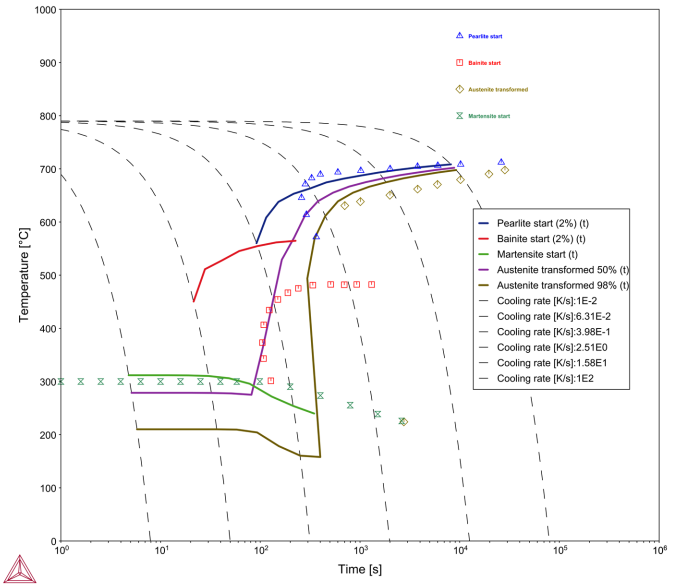


Figure 47: The CCT diagram for an Fe-C-Mn-Si-Cr-V alloy comparing the calculation with experimental data from [1958Wev].

Reference

[1958Wev] F. Wever, A. Rose, Atlas zur Wärmebehandlung der Stähle: 1954/56/58 (Verlag Stahleisen, Düsseldorf, 1958), p. II-112.

Nickel Model Library Examples Collection

The **General Models** are available to all users. To run calculations with the **Nickel Models** (as part of the Nickel Model Library) requires a valid maintenance license plus licenses for both the TCNI (version 11 and newer) and MOBNI (version 5 and newer) databases.

These examples use the **Property Model Calculator**, an activity available with Thermo-Calc plus the available Property Models in the Nickel Model Library.

In this section:

PM_Ni_01: Lattice Parameter of γ/γ'

The example uses the **Property Model Calculator** with the **Equilibrium with Freeze-in Temperature - Ni** Model.

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

To run calculations with the **Nickel Models** requires a valid maintenance license plus licenses for both the TCNI (version 11 and newer) and MOBNI (version 5 and newer) databases. Also see our website to learn more about the Nickel Model Library.

Project File Information

- Folder: **Property Models>Nickel**
- File name: *PM_Ni_01_Lattice_Parameter_of_Gamma_Gamma_Prime.tcu*

The lattice parameters are measured experimentally for γ/γ' in a Ni0.6Mo0.92Ta12.5Al1.83Ti10.5Cr3.3W alloy.

The thermodynamically stable equilibrium will not be reached for this alloy during the experimental heat treatment; only the phases γ and γ' are noticed in the experiment. The γ/γ' microstructure is in this calculation example assumed to freeze-in at 1000 °C where the phase compositions do not change during cooling to room temperature.

Some of the key settings to note in this example:

- The **Subset of phases** is selected as **Gamma and gamma-prime only** to match the experimental observations.
- The **Freeze-in temperature** is set to 1000 °C.
- A **One axis** calculation is used where the evaluation temperatures are within a range of 20 °C to 1000 °C.

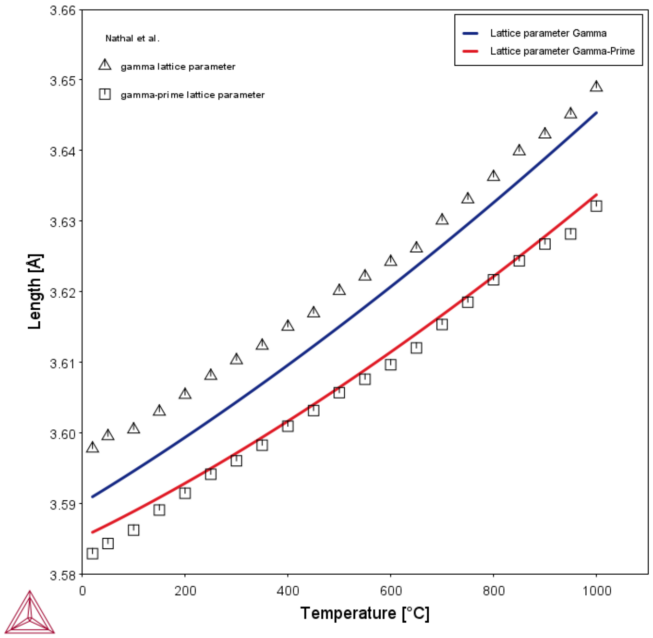


Figure 48: The lattice parameters for γ and γ' are plotted against experimental data from [1985Nat].

Reference

[1985Nat] M. V. Nathal, R. A. Mackay, R. G. Garlick, Temperature dependence of γ-γ’ lattice mismatch in Nickel-base superalloys. Mater. Sci. Eng. 75, 195–205 (1985).

PM_Ni_02: Antiphase Boundary Energy of γ'

The example uses the **Property Model Calculator** with the **Antiphase Boundary Energy - Ni** Model.

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

To run calculations with the **Nickel Models** requires a valid maintenance license plus licenses for both the TCNI (version 11 and newer) and MOBNI (version 5 and newer) databases. Also see our website to learn more about the Nickel Model Library.

Project File Information

- Folder: **Property Models>Nickel**
- File name: *PM_Ni_02_Antiphase_Boundary_Energy_of_Gamma_Prime.tcu*

This example shows a calculation of the antiphase boundary energy for an Al75Ni alloy at room temperature with increasing amounts of Ti. The plot shows the (111) APB energy in $Ni_3Al_{1-x}Ti_x$ over the whole compositional range together with first-principle calculations from Chandran and Sondhi [2011Cha] and Vamsi and Karthikeyani [2012Vam] evaluated at 0 K. The trend with increasing 111 APBE with an increasing amount of Ti is predicted by all calculations but the absolute values between the first principle calculations are quite different.

Some of the key settings to note in this example:

- γ' is the only stable phase for these compositions. FCC_L12 is therefore selected as the only phase in the System Definer.
- The **Freeze-in temperature** and evaluation temperature are both set at 20 °C with the **Subset of phases** for **All phases**.
- A **One axis** calculation is used with **Mole percent Ti** between 0 and 25 in 20 steps.
- The plotting quantity **APBE for 111 plane (1/2)** is then compared with the first principle calculations.

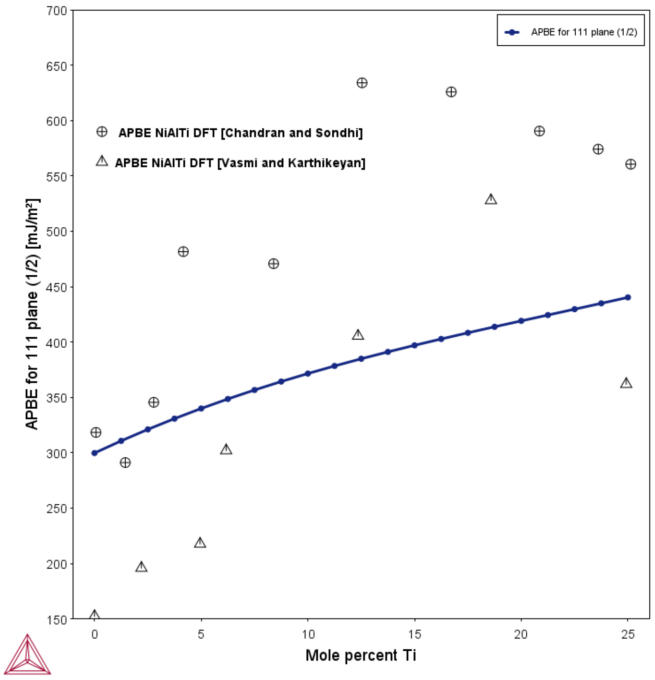


Figure 49: Composition of Ti (mole %) compared to antiphase boundary surface energy for 111 plane and experimental data from [2011Cha; 2012Vam].

References

[2011Cha] M. Chandran, S. K. Sondhi, First-principle calculation of APB energy in Ni-based binary and ternary alloys. Model. Simul. Mater. Sci. Eng. 19, 025008 (2011).

[2012Vam] K. V. Vamsi, S. Karthikeyan, Effect of Off-Stoichiometry and Ternary Additions on Planar Fault Energies in Ni3Al, in Superalloys 2012 (John Wiley & Sons, Inc., Hoboken, NJ, USA, 2012; pp. 521–530.

Process Metallurgy Module Examples Collection

The Process Metallurgy Module requires both a valid Maintenance and Support Subscription (M&SS) and a license for the TCS Metal Oxide Solutions Database (TCOX8 or newer).

All users can test the Process Metallurgy Module with the included OXDEMO database, which is limited to these elements: Al, C, Ca, Fe, O, S, and Si. For more information about this and other products visit our website.

In this section:

PMET_01: Basic Oxygen Furnace (BOF)

The example uses the **Process Metallurgy Calculator** to demonstrate a simplified steelmaking process in a Basic Oxygen Furnace (BOF).

This application example in its various forms is showcased on our website. There are two application examples (one equilibrium, one kinetic) showing how the Process Metallurgy Module can be used to calculate the BOF process.

This basic example uses equilibrium calculations to gain a general understanding of your BOF process and help you determine optimal operation conditions and predict and optimize costs of raw materials and recycling. The other set of examples gives detailed instructions on how to simulate the kinetics of the BOF process using the kinetic process simulation (see PMET_04: Basic Oxygen Furnace (BOF) Kinetics).

Project File Information

Open the example project file(s) from Thermo-Calc **Help** → **Example Files** → **Process Metallurgy** → **PMET_01_Basic_Oxygen_Furnace.tcu**.

Choose a, b, or c versions of the example based on your license.

- **PMET_01a_Basic_Oxygen_Furnace** is included in a regular Thermo-Calc installation as well as the free Educational version of Thermo-Calc. This is a highly simplified example and uses the OXDEMO database, and only considers the elements Fe, C, and O.
- **PMET_01b_Basic_Oxygen_Furnace** is also a simplified calculation but uses the OXDEMO database. It requires a full license of Thermo-Calc 2021b and newer.
- **PMET_01c_Basic_Oxygen_Furnace** requires the TCOX11 database and newer and a full license of Thermo-Calc 2021b and newer.

The resulting plots and details related to setting up this example are available either via the dedicated web page, or you can read the more in depth step-by-step documentation as a PDF, also available via our website.

PMET_02: Desulphurization in a Ladle Furnace (LF)

The example, which is also showcased on our website, uses the **Process Metallurgy Calculator** to demonstrate the use of a Ladle Furnace (LF) with the Process Metallurgy Module.

The ladle furnace fulfils many purposes in the steelmaking process. Desulphurization, which we will focus on in this example, is merely one of them.

Desulphurization is usually performed by transferring S that is dissolved in the liquid metal to a CaO-rich slag phase. For this process to be successful, two conditions need to be fulfilled:

1. The slag must be fully liquid (liquid fraction > 0.9). This is required for kinetic reasons. The slag phase must be fluid so that it can emulsify with the liquid steel and form a large surface area where the reaction between steel and slag can take place.
2. The slag must take up a large amount of S from the liquid steel (have a “high sulphur capacity”) so that a significant amount of sulphur will move from the liquid steel to the slag phase.

It is difficult to decrease the S content in the liquid steel during steelmaking in a basic oxygen converter (BOF) or an electric arc furnace (EAF) because conditions are predominantly very oxidizing. Desulphurization is therefore usually performed in a subsequent step, during steel refining in a ladle furnace or a vacuum degasser after the steel has been fully killed by a suitable deoxidizing agent and the oxygen activity is low.

The following example explores these two conditions for an equilibrium between liquid steel and slag in a ladle furnace, trying to find good slag compositions.

Project Files

Open the example project files from Thermo-Calc **Help** → **Example Files** → **Process Metallurgy** → **PMET_02a_Ladle_Furnace.tcu** or **PMET_02b_Desulphurization_in_Ladle_Furnace.tcu**.

Choose a or b versions of the example based on your license

- **PMET_02a_Ladle_Furnace.tcu** can be run with OXDEMO database but requires the full license for Thermo-Calc 2021b and newer.
- **PMET_02b_Desulphurization_in_Ladle_Furnace.tcu** requires the TCOX11 database and a full license for Thermo-Calc 2021b and newer.

The resulting plots and details related to setting up this example are available either via the dedicated web page, or you can read the more in depth step-by-step documentation as a PDF, also available via our website.

PMET_03: Argon Oxygen Decarburization (AOD)

The Argon Oxygen Decarburization (AOD) process is a converter process applied in stainless steel making. In this process the oxidation of chromium in the steel melt needs to be prevented while carbon is oxidized. This is achieved by reducing the oxygen partial pressure by having a high Ar-content in the blowing gas. It is a highly exothermic process that requires adiabatic modeling. In this example the conversion of carbon-rich steel scrap is modeled together with additions of Ferronickel and Ferrochrome to a stainless steel. The example uses the **Process Metallurgy Calculator**.

Visit the website Application Examples→Process Metallurgy page for more background information as well as more in depth analyses of this and other examples. Also visit the Process Metallurgy Module page to access resources such as training videos, presentations, publications, webinars, and much more.

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.

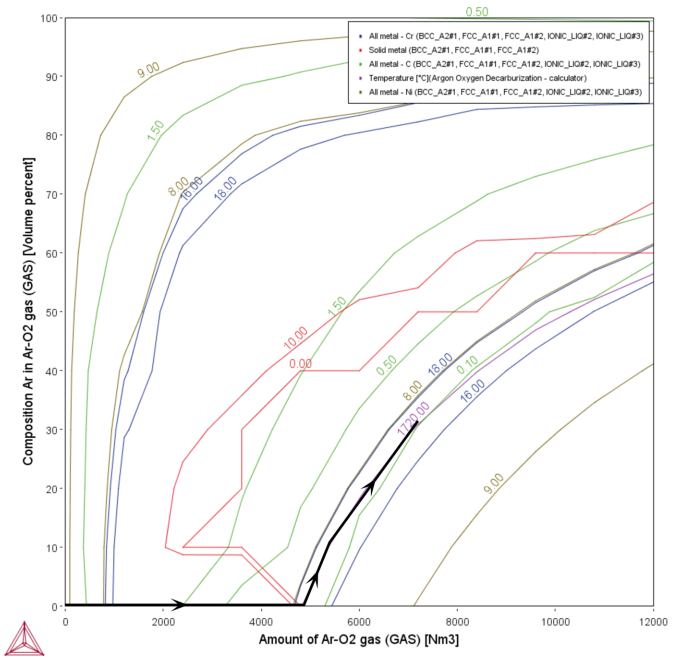
Project File Information

Open the example project file from Thermo-Calc **Help** → **Example Files** → **Process Metallurgy** → **PMET_03_Argon_Oxygen_Decarburization.tcu**.

This example does NOT require a license to run the simulation. It works with both the TCS Metal Oxide Solutions Database (TCOX versions 8 and newer) as well as the free OXDEMO database.

Background Description

The AOD-process is characterized by an initially high O_2-content of the blowing gas, which is gradually replaced by Ar. The maximum temperature of the process is typically around 1720 °C. A grid plot of an adiabatic calculation is well suited to model the required simultaneous change of amount of gas and its composition during this process. The black line in the plot above indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.



In principle, this plot could be used to control the blowing gas flow in a plant process. However, note that the simulation only considers a global gas phase, i.e. additional gas is added but never removed. This means that the given gas phase composition is an average one and not identical to the composition of the gas flowing in at each point in time. Additionally there is a certain impact on the resulting equilibria from the fact that all gas remains in the system and is not removed.

Slag Basicity

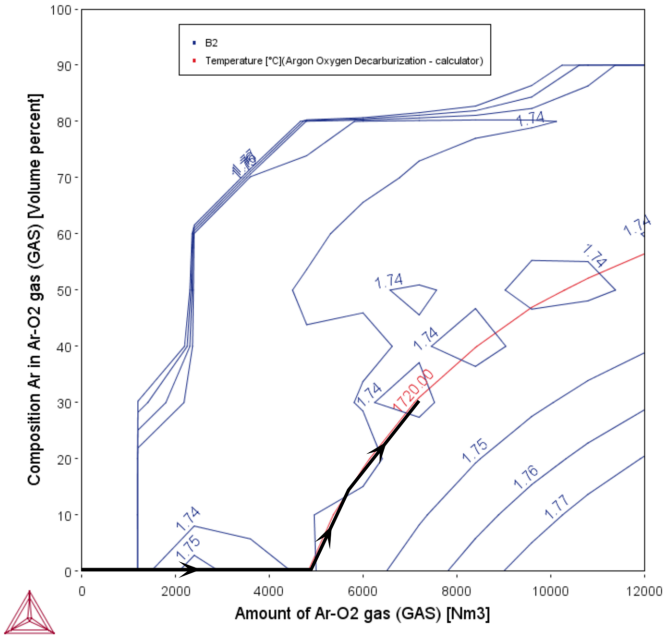


Figure 50: The Slag Basicity plot shows the basicity of the slag (which is a measure for the sulphur capacity of the slag). The process achieves a final basicity of 1.74 which is typical for an AOD-process. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

S Content in Steel

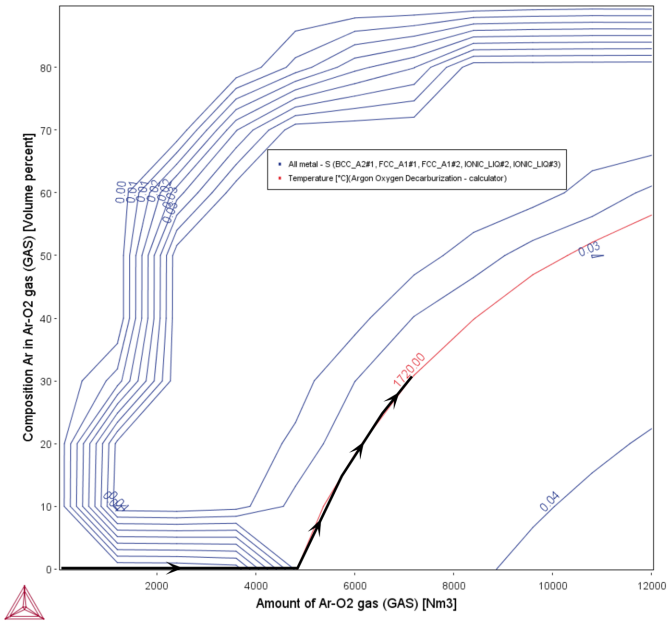


Figure 51: In the S Content in Steel plot, the sulphur content in the steel melt is slightly reduced during the process from 0.056% in the initial steel scrap to finally ca. 0.035%. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

Cr Content in Slag

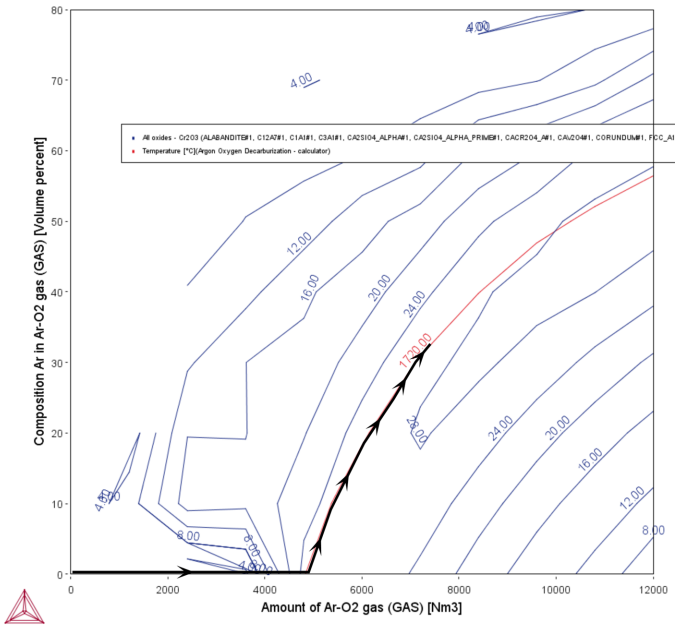


Figure 52: In the Cr Content in Slag plot, the Cr2O3-content in the slag reaches at the end of the process ca. 26 wt-%. This is typical for the AOD-process and requires an additional Cr-recovery step after the conversion to reduce the loss of chromium. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

Amount of Slag

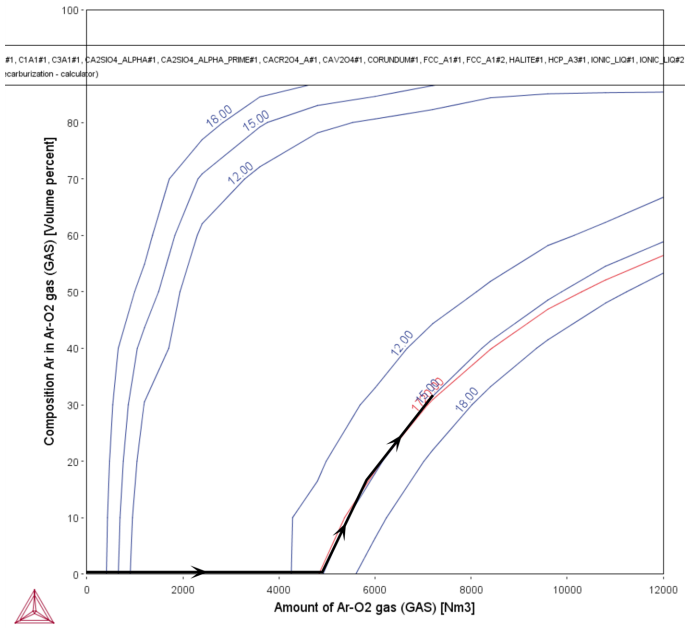


Figure 53: In the Amount of Slag plot, you can see that the process generates about 15 tons of slag in the total. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

Liquid Slag Fraction

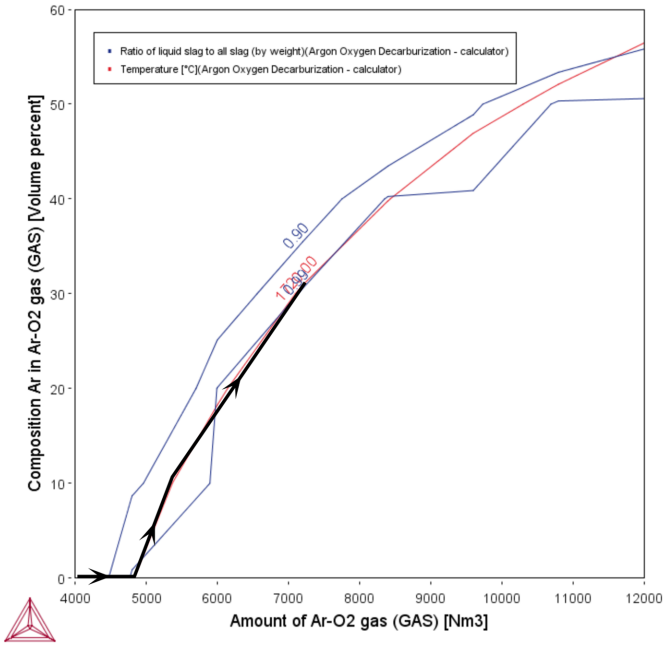


Figure 54: In the Liquid Slag Fraction plot, you can see that towards the end of the process the slag is calculated to be mostly liquid. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

PMET_04: Basic Oxygen Furnace (BOF) Kinetics

The example uses the **Process Metallurgy Calculator** to demonstrate the steelmaking process in a Basic Oxygen Furnace (BOF).

This application example in its various forms is showcased on our website. There are two application examples (one equilibrium, one kinetic) showing how the Process Metallurgy Module can be used to calculate the BOF process.

This example simulates the kinetics of the BOF process, whereas the other only considers equilibrium. For information about the equilibrium examples, see PMET_01: Basic Oxygen Furnace (BOF).

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

Project File Information

Open the example project file(s) from Thermo-Calc **Help** → **Example Files** → **Process Metallurgy** →.

Choose a, b, or c versions of the example based on your license.

- **PMET_04a_Basic_Oxygen_Furnace_Kinetics** is included in a regular Thermo-Calc installation as well as the free Educational version of Thermo-Calc. This only considers the elements Fe, C, and O.
- **PMET_04b_Basic_Oxygen_Furnace_Kinetics** needs a full license of Thermo-Calc 2021b or newer, but uses the free OXDEMO database. It considers the elements Fe, C, O, Ca, Al, Si, and S.
- **PMET_04c_Basic_Oxygen_Furnace_Kinetics** requires both a full license of Thermo-Calc 2021b or newer and a license for the TCOX11 database and newer. This simulation corresponds pretty much to a real BOF process with the elements Fe, Mn, C, O, Ca, Al, Mg, Si, S, and P considered.

The resulting plots and details related to setting up this example are available either via the dedicated web page, or you can read the more in depth step-by-step documentation as a PDF, also available via our website.

PMET_05: Lab Scale Ladle Furnace (LF) Kinetics

Using the **Process Metallurgy Calculator** and the **Process simulation** branch, this example is based on the publication by Piva et al [2017Piv] where a lab scale sample of pure iron is first deoxidized with Si-Mn and then a synthetic top slag is added to the steel. Generally, by using the project file and the information below, you can get an idea about how to set up a ladle furnace simulation using the Process Metallurgy Module.

Visit the website Application Examples→Process Metallurgy page for more background information as well as more in depth analyses of this and other examples. Also visit the Process Metallurgy Module page to access resources such as training videos, presentations, publications, webinars, and much more.

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

To open this project file, from the Thermo-Calc menu, go to **Help** → **Example Files** → **Process Metallurgy** → **PMET_05_Lab_Scale_Ladle_Furnace_Kinetics.tcu**.

This example requires a license to run the simulation. It works with TCS Metal Oxide Solutions Database (TCOX) versions 8 and newer.

About the Plot Results

Many different aspects of the reactions taking place in the LF can be plotted and analyzed. After you run the project file and obtain the plots, you can experiment by adjusting the settings on each Plot Renderer to see what happens in each case. There is more analysis about this and other examples available at the links to our website.

For an example of a more realistic industry scale, see PMET_06: Ladle Furnace (LF) Kinetics.

Setting Up the LF Process Simulation

In the paper by Piva et al. [2017], it is experimentally investigated how the steel and inclusion composition changes in function of time as the Si-Mn killed steel reacts with the slag. This experiment can serve as a model for the production of SiMn killed steel with subsequent top-slag deoxidation.

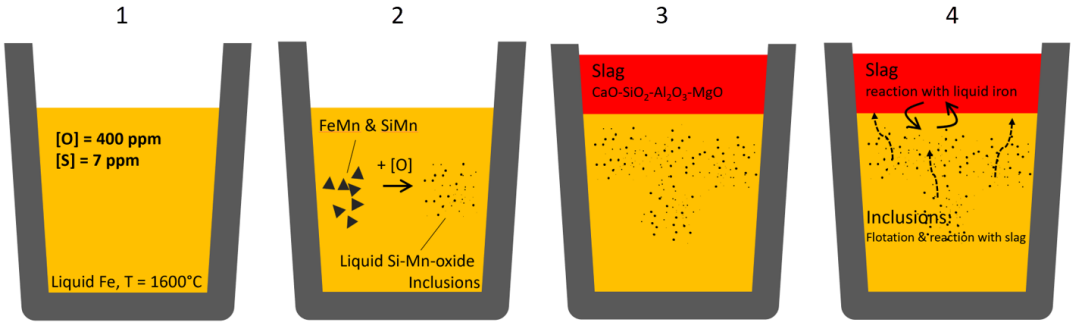


Figure 55: Diagram of the experiment performed by Piva et al. [2017]. The sequence as described in the text is: (1) liquid Fe with dissolved oxygen; (2) FeMn and SiMn added to deoxidize Fe; (3) top slag added after 360s; and (4) gradual reaction between steel, slag and inclusions.

According to the publication the following reaction sequence is expected as shown in the diagram:

1. The deoxidizing agents dissolve and react with the oxygen in the steel forming oxide inclusions, thereby reducing the amount of dissolved oxygen ("killing" the steel). The kinetics are fast, and it can be assumed that the reaction proceeds to thermodynamic equilibrium.
2. The inclusions formed in (1) slowly start to float upwards and are removed out of the liquid steel.
3. After adding the slag (360 s after killing the steel in (1) the liquid steel starts reacting with the slag.
4. The inclusions continue to float up out of the liquid steel and combine with the slag.

   According to the authors the most important reaction that takes place is the dissolution of Al out of the slag and its transferal into the liquid steel, where it reacts with the inclusions and changes the chemistry.

In this example only the last reaction is simulated after adding the slag. The kinetic parameters, compositions of all materials and process schedule are all taken from the publication.

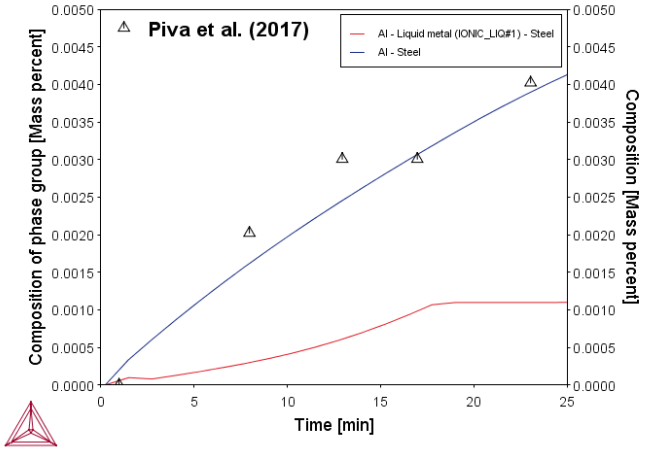
Results and Experimental Analysis

The plots below compare the Al content in the liquid steel with the experimentally determined amount. The bottom plot shows how the Al_2O_3 from the slag phase is gradually reduced to metallic Al that dissolves in the liquid steel.

In this example, only part of the Al in the liquid steel is dissolved as metallic Al. With the Process Metallurgy Module, it is possible to plot both dissolved Al and also total Al.

In the steel industry this fraction of Al in the liquid steel is often termed *dissolved Al*. The rest of the Al reacts with the oxygen in the liquid steel and forms oxide inclusions. The amount of dissolved Al plus the Al bound up in oxide inclusions is often termed *total Al*. The difference between total Al minus dissolved Al is an important measure for the steel cleanness.

Total Al is what was measured by Piva et al. [2017] and their experimental data are compared to the calculated values below.



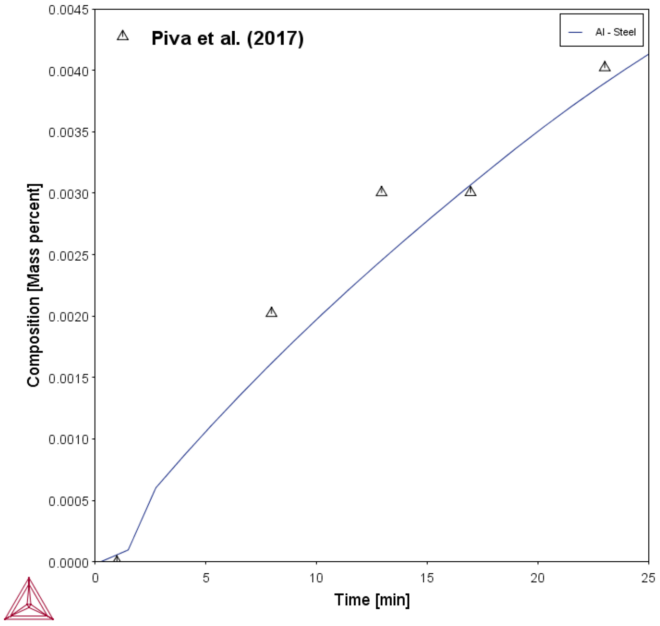


Figure 56: Total Al in the steel compared with experimental data (blue/top curve). If only the fraction of dissolved Al is to be plotted (red/bottom curve), this is done by selecting "Composition of phase group" and "Liquid metal". The bottom figure is available with the example.

Immediately after killing the steel with SiMn and FeMn, the liquid steel contains liquid Si-Mn-oxide inclusions only. As the liquid steel picks up Al from the slag phase in function of time, the inclusions get richer and richer in Al. This experimentally verified change in inclusion chemistry is well reproduced by this simulation.

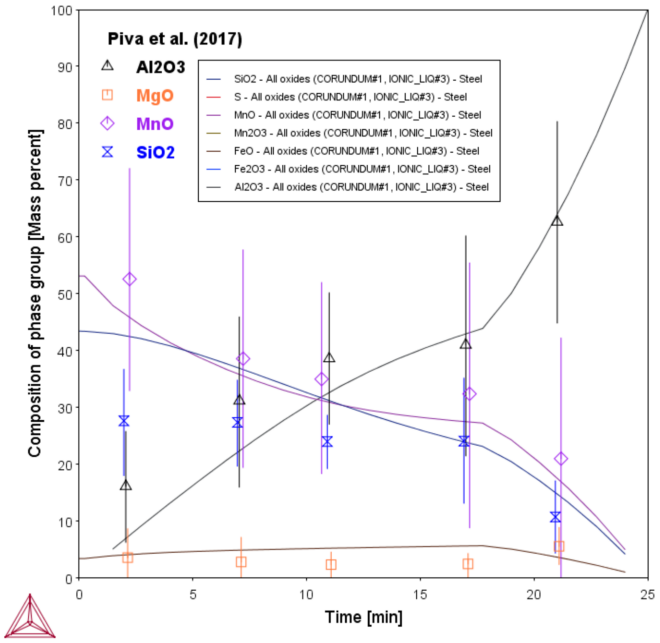


Figure 57: Calculated composition of non-metallic inclusions in function of processing time compared to experimental data [2017Piv].

It is also possible to calculate the amount and type of inclusions present in the liquid steel. At the beginning of the process all the inclusions are liquid oxides. After about 20 minutes processing time, the first solid corundum (Al_2O_3) inclusions start appearing. After 25 minutes almost no liquid inclusions remain. The total amount of inclusions decreases in function of time as they float up out of the liquid steel and combine with the slag floating on top of the steel.

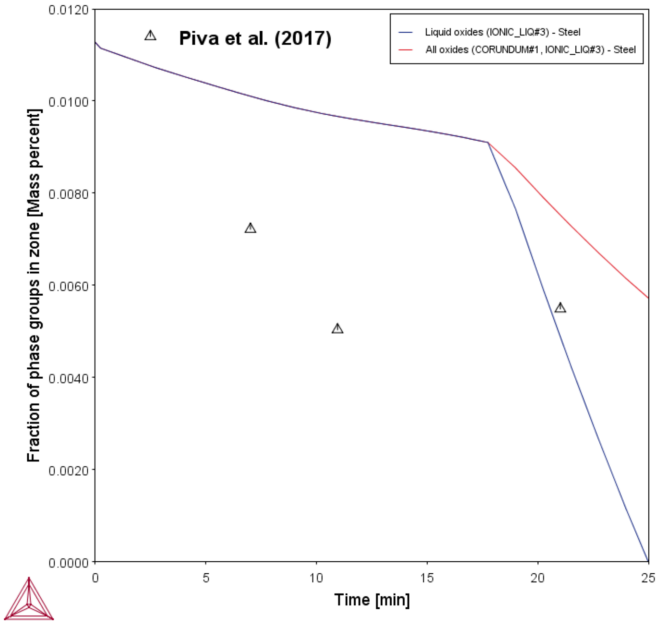


Figure 58: Amount of inclusions in the liquid steel in function of processing time. The total amount of inclusions (red line) and liquid oxide inclusions (blue line) are plotted. Up to about 20 min all inclusions are liquid oxide type, then they are replaced by solid corundum (Al_2O_3) inclusions. Experimental data from [2017Piv].

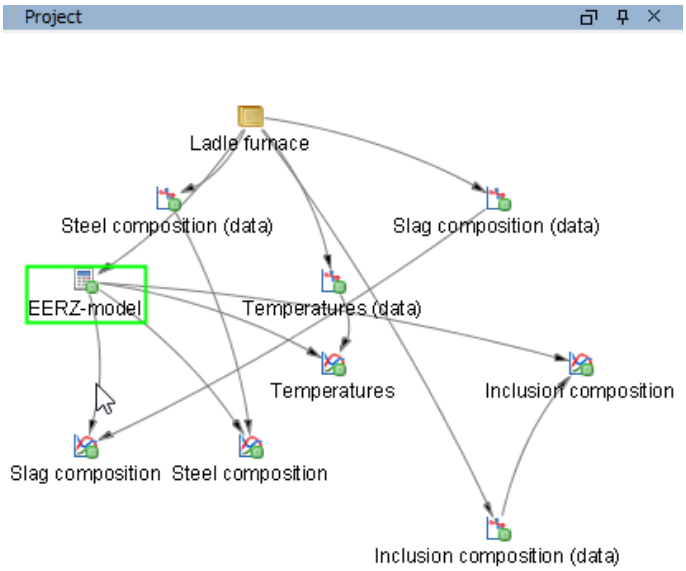
Reference

[2017Piv] Piva, S. P. T., Kumar, D. & Pistorius, P. C. "Modeling Manganese Silicate Inclusion Composition Changes during Ladle Treatment Using FactSage Macros," Metall. Mater. Trans. B 48, 37–45 (2017).

PMET_06: Ladle Furnace (LF) Kinetics

This in-depth example, which is also showcased on our website, uses the **Process Metallurgy Calculator** to show how to set up a full kinetic simulation of steel refining in a ladle furnace using the Process Metallurgy Module in Thermo-Calc. The Process Metallurgy Module uses the Effective Equilibrium Reaction Zone model (EERZ) to simulate the kinetics of the process. In this example, a full kinetic simulation of the LF refining process is set up using the Process Metallurgy Module.

For a simpler process that describes a lab-scale ladle furnace process, see PMET_05: Lab Scale Ladle Furnace (LF) Kinetics.



The nodes in the Project window for this example. The Process Metallurgy Calculator is renamed to EERZ model. If you click this node the Configuration window opens, which is where all the settings for the process simulation are located. This advanced example also uses three Experimental Data Reader nodes to read the experimental data that is included in the simulation results. After setting up the system and accessing the experimental data, you then add Plot Renderers to the calculator to generate the output in the Results window.

Project File Information

To open this project file, from the Thermo-Calc menu, go to **Help** → **Example Files** → **Process Metallurgy** → **PMET_06_Ladle_Furnace_Kinetics.tcu**.

This example requires the database TCOX10 or newer, a full license of Thermo-Calc 2020b or newer, plus a license for the Process Metallurgy Module.

The resulting plots and details related to setting up this example are available either via the dedicated web page, or you can read the more in depth step-by-step documentation as a PDF, also available via our website.

Background Overview

After steelmaking, which is mostly performed in a basic oxygen furnace (BOF) or electric arc furnace (EAF), the steel is usually tapped into a ladle where certain additions are made (deoxidation agents, slag formers, certain alloying elements) and then transferred to the ladle furnace (LF). The LF fulfils many purposes in the steel refining process, the most important being:

- Temperature control / heating by an electrical arc.
- Mixing by Ar or N2 bubbling through porous plugs in the bottom of the ladle to achieve homogeneous temperature and composition throughout the ladle.
- Removal of unwanted non-metallic phases / inclusions such as corundum (Al2O3), liquid oxide inclusions, spinel, on so on, by flotation, aided by Ar or N2 bubbling.
- Modification / engineering of non-metallic inclusions so that they are not detrimental for the downstream processing and/or the final product.
- Removal of unwanted volatile elements such as Pb, Zn, Sn, and so on. Due to their high vapor pressure, these elements are enriched in the rising Ar or N2 bubbles. After the gas escapes out of the ladle and cools, they condense, forming copious amounts of dust.
- Removal of unwanted elements such as sulphur by liquid steel / slag reactions.
- Lowering of the dissolved gas content. In the LF this is mainly achieved through chemical reactions. For direct removal of dissolved gas, vacuum degassing (VD) is usually required.
- Alloying and trimming of the steel to achieve the exact alloy composition required by the specification of the steel that is to be produced.

The reactions taking place in a LF are a complex interplay between equilibrium thermodynamics that define the direction of chemical reactions, and kinetics that define how fast the equilibrium state is approached.

PMET_07: Vacuum Oxygen Decarburization Kinetics

This application example, which is showcased on our website and uses the **Process Metallurgy Calculator**, shows how the Process Metallurgy Module in Thermo-Calc can be used to simulate the Vacuum Oxygen Decarburization (VOD) process for a stainless steel.

This example, based on data of a real VOD process published by Ding et al. [2000Din], shows how to set up the VOD process in Thermo-Calc's Process Metallurgy Module. Use of the following features in the Process Metallurgy Module are highlighted in this example:

- Change of pressure as a function of time during the process
- Change of reaction kinetics as a function of time during the process
- Selection of zone where degassing is allowed

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

Project File Information

Open this project file, from the Thermo-Calc menu, go to **Help** → **Example Files** → **Process Metallurgy** → **PMET_07_Vacuum_Oxygen_Decarburization_Kinetics.tcu**.

This example requires a license for Thermo-Calc 2021a or newer, the database TCOX10 or newer, and a license for the Process Metallurgy Module.

The resulting plots and details related to setting up this example are available either via the dedicated web page, or you can read the more in depth step-by-step documentation as a PDF, also available via our website.

Reference

[2000Din] R. Ding, B. Blanpain, P. T. Jones, P. Wollants, Modeling of the vacuum oxygen decarburization refining process. Metall. Mater. Trans. B. 31, 197–206 (2000).

PMET_08: Steel Deoxidation on Tapping

This application example, which is showcased on our website and uses the **Process Metallurgy Calculator**, shows a few of the ways the Process Metallurgy Module in Thermo-Calc can be used to investigate steel deoxidation (killing) on tapping.

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

Project File Information

Open the project files, from the Thermo-Calc menu, go to **Help** → **Example Files** → **Process Metallurgy** → **PMET_08_Steel_Deoxidation_on_Tapping.tcu**.

Choose a or b versions of the example based on your license.

- **PMET_08a_Steel_Deoxidation_on_Tapping.tcu** is included in a regular Thermo-Calc installation as well as the free Educational version of Thermo-Calc. It is a simplified version that uses the OXDEMO database.
- **PMET_08b_Steel_Deoxidation_on_Tapping.tcu** requires a full license of Thermo-Calc version 2021b or newer and database TCOX11 or newer.

The resulting plots and details related to setting up this example are available either via the dedicated web page, or you can read the more in depth step-by-step documentation as a PDF, also available via our website.

About Deoxidation or "Killing" of Steel

Deoxidation of steel, also known as killing of steel, occurs toward the end of the steelmaking process, but before desulphurization. After primary steelmaking, for example in a basic oxygen furnace (BOF) or electric arc furnace (EAF), the liquid steel contains a large amount of dissolved oxygen [O] (400 to over 1000 ppm, see PMET_04: Basic Oxygen Furnace (BOF) Kinetics). This oxygen must be removed from the liquid steel for several reasons, including:

- Desulphurization is not effective with high oxygen content in the steel (see example on desulphurization)
- Continuous casting of un-killed steel is not possible and will result in "boiling" of the steel in the mould and massive porosity, as shown in the figure.

The two most widely applied methods of deoxidizing or killing the steel are adding Al (Al-killed steel) to the steel and adding Si (Si-killed steel) to the steel. These elements readily react with oxygen to form oxides that precipitate within the liquid steel. This does not reduce the total amount of oxygen in the liquid steel; it simply transforms the dissolved oxygen into an oxide precipitate. This oxide precipitate then needs to be removed from the steel by flotation during secondary metallurgy in the ladle furnace (LF).

In this example we look at how the Process Metallurgy Module can be used to investigate these two widely applied methods of deoxidizing or killing the steel: adding Al (Al-killed steel) or adding Si (Si-killed steel). This, however, can result in the formation of damaging inclusions that cause problems during further processing, so we go on to look at two simple and very common processes that are used to transform the solid SiO_2 and Al_2O_3 inclusions into liquid oxides so that they are less damaging.

Diffusion Module (DICTRA) Graphical Mode Examples

Examples using up to three elements are available to all users. The other examples require a Diffusion Module (DICTRA) license to calculate and plot results.

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

These examples use the **Diffusion Calculator**. All examples use demonstration database packages included with your installation no matter what licenses you have.

In this section:

D_01: Homogenization of a Binary Fe-Ni Alloy

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

This example is included as a Diffusion Module (DICTRA) tutorial on our website and as part of the playlist on our YouTube channel.

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

Project File Information

- Folder: Diffusion Module - DICTRA
- File name: *D_01_Diffusion_Single_Phase.tcu*

This example is part of the *Diffusion Module (DICTRA) Quick Start Guide* available to all users. A version of the example is also available for Console Mode.

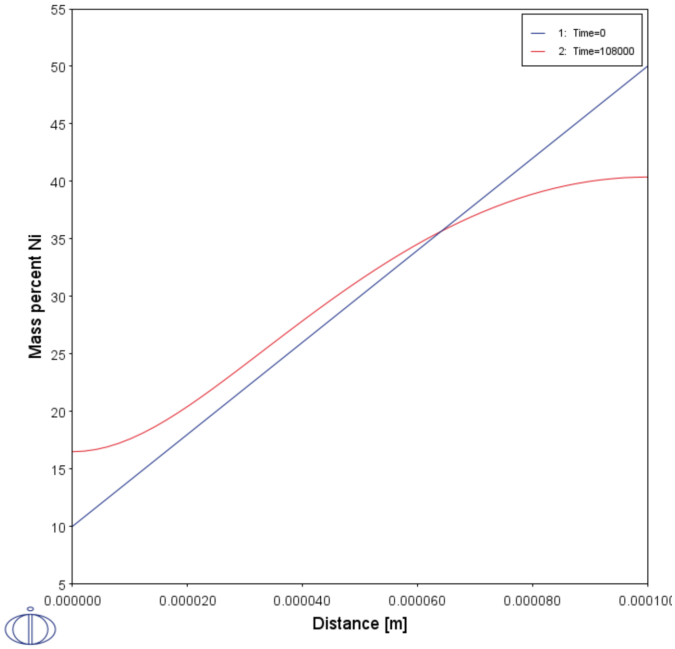


Figure 59: Composition of Ni vs Distance.

D_02: Ferrite(bcc)/Austenite(fcc) Transformation in a Binary Fe-C Alloy

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

This example is included as a Diffusion Module (DICTRA) tutorial on our website and as part of the playlist on our YouTube channel.

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

Project File Information

- Folder: Diffusion Module - DICTRA
- File name: *D_02_Diffusion_Moving_Boundary.tcu*

This example is part of the *Diffusion Module (DICTRA) Quick Start Guide* available to all users. A version of the example is also available for Console Mode.

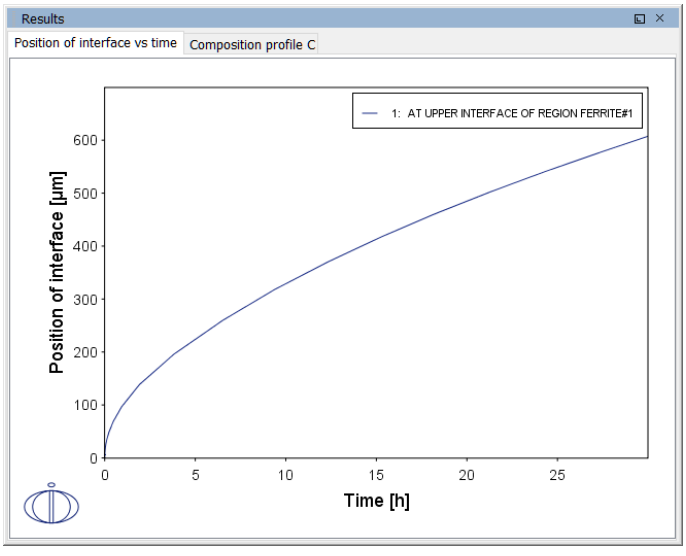


Figure 60: Position of interface vs time.

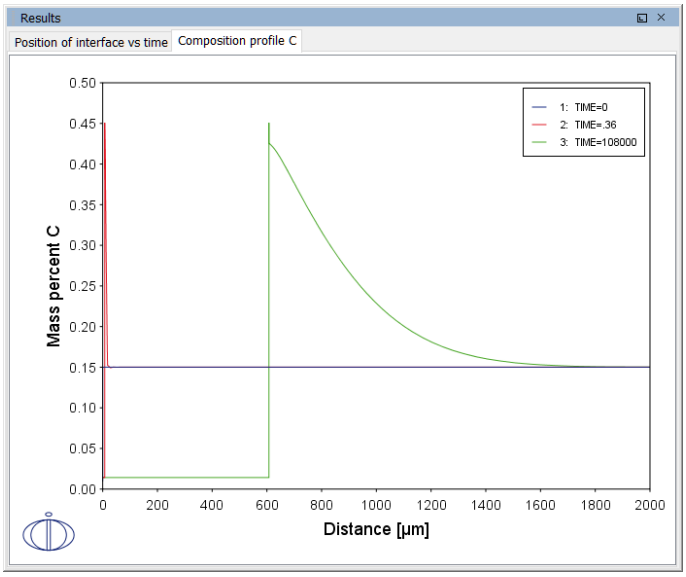


Figure 61: Composition profile C.

D_03: Evolution of an Fe-Cr-Ni Diffusion Couple

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

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

More details about the homogenization model for multiphase simulations can be found in Larsson and Engström [2006Lar] and Larsson and Höglund [2009Lar]. Experimental data is from Engström [1995Eng].

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

Project File Information

- Folder: Diffusion Module - DICTRA
- File name: *D_03_Diffusion_Multiphase.tcu*

This example is part of the *Diffusion Module (DICTRA) Quick Start Guide* available to all users. A version of the example is also available for Console Mode.

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 you can go to the website or our YouTube channel.

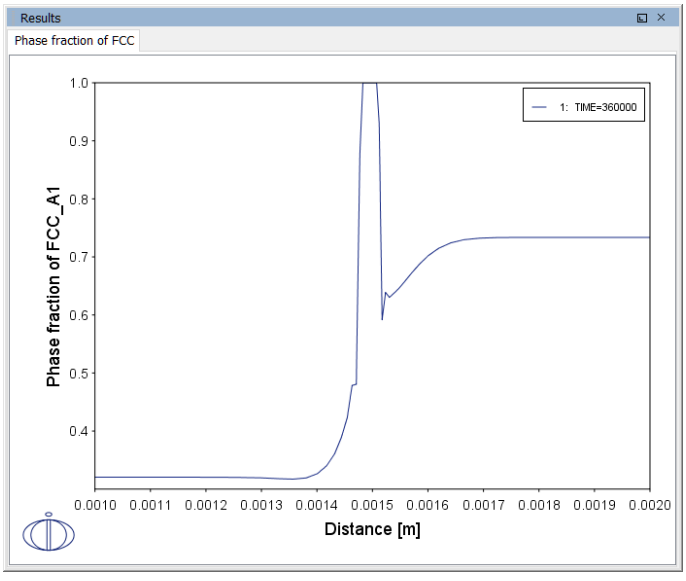


Figure 62: Phase fraction of FCC.

References

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

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

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

D_04: Fe-C Moving Boundary: Austenite to Ferrite

This example simulates the austenite to ferrite transformation in a Fe-0.01 mass% C steel during continuous cooling. The simulation starts at a temperature where only austenite is stable, ferrite nucleates and grows into the austenite during cooling in the two phase region. Plots of thermal and carbon composition profiles are generated.

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

Project File Information

- Folder: Diffusion Module - DICTRA
- File name: *D_04_Diffusion_Fe-C_Moving_Boundary_Austenite_to_Ferrite.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 you can go to the website or our YouTube channel.

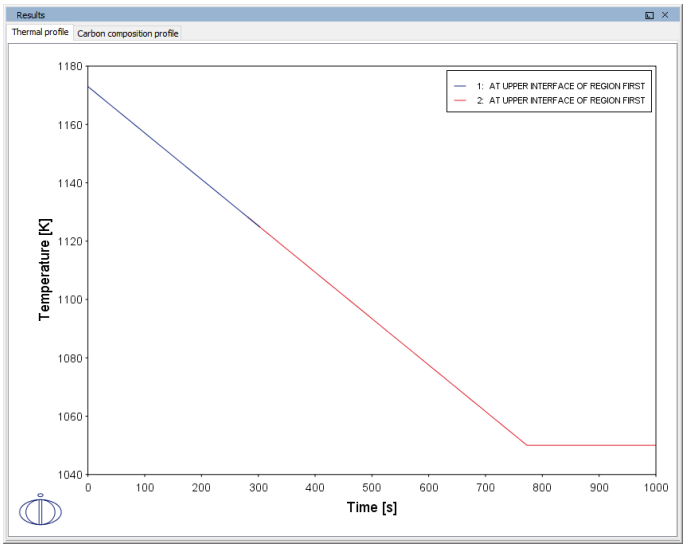


Figure 63: Thermal profile.

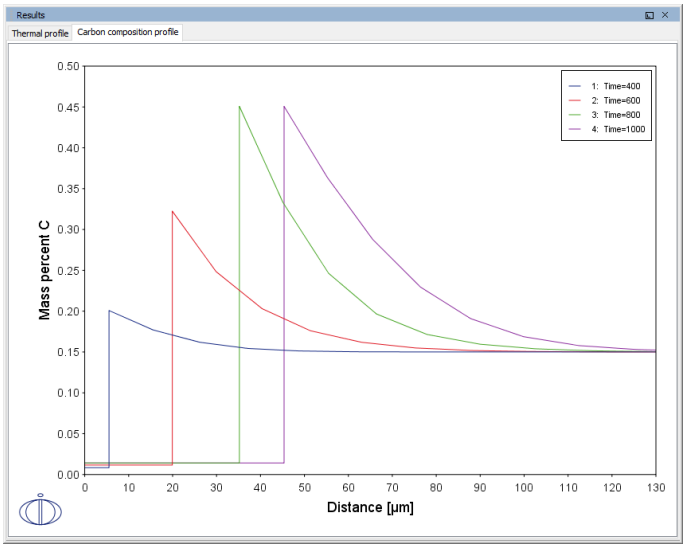
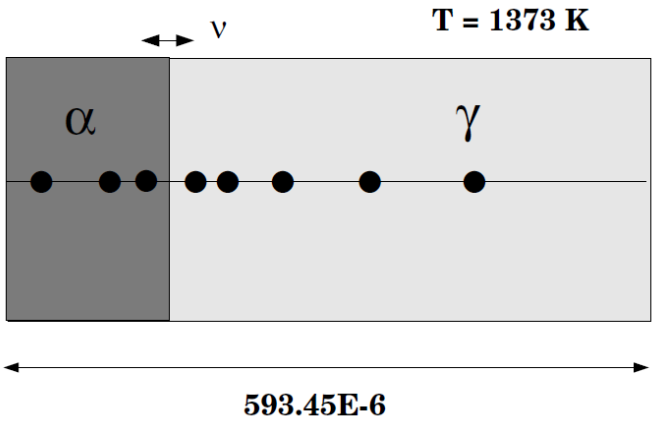


Figure 64: Carbon composition profile.

D_05: γ/α/γ Diffusion Couple of Fe-Ni-Cr alloys

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

This set up corresponds to diffusion couple in Kajihara et al. [1993aKaj] and Kajihara and Kikuchi [1993bKaj].



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: Diffusion Module - DICTRA
- File name: *D_05_Diffusion_Fe_Ni_Cr_Moving_Boundary_Diffusion_Couple.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 you can go to the website or our YouTube channel.

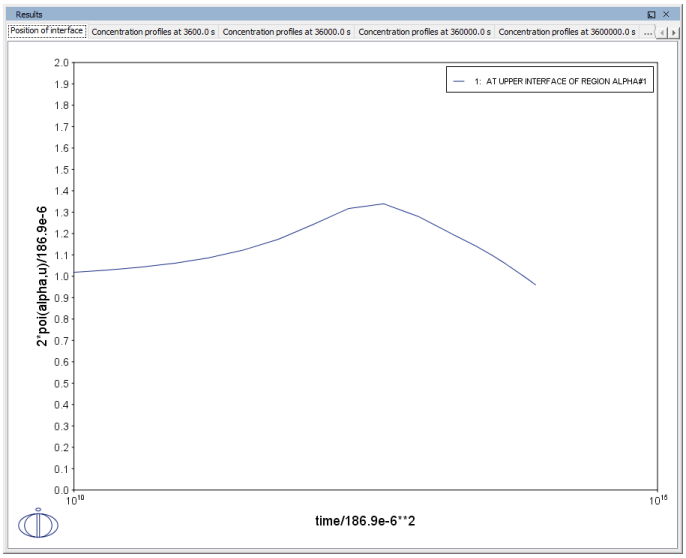


Figure 65: Interface position.

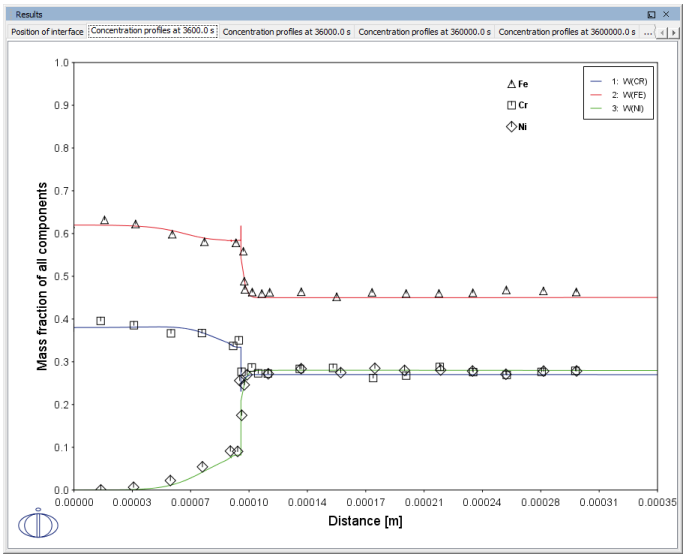


Figure 66: Concentration profiles at 3600 s.

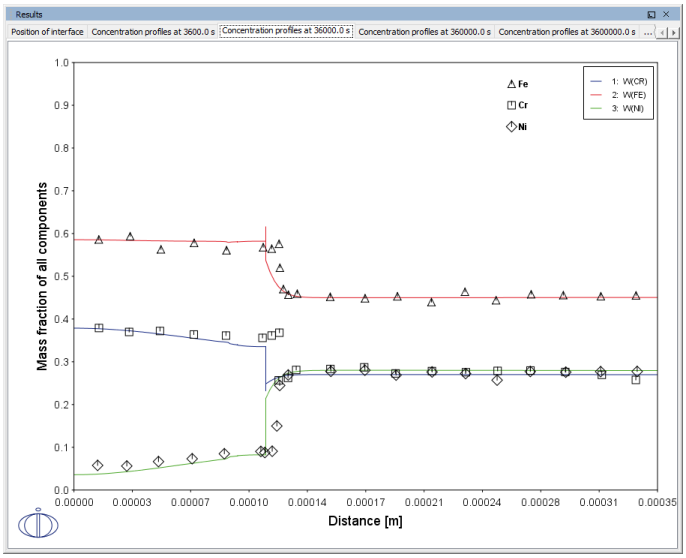


Figure 67: Concentration profiles at 36 000 s.

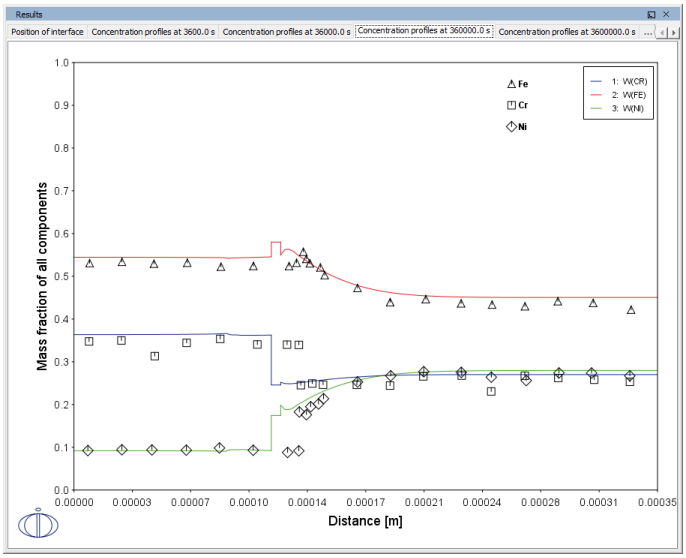


Figure 68: Concentration profiles at 360 000 s.

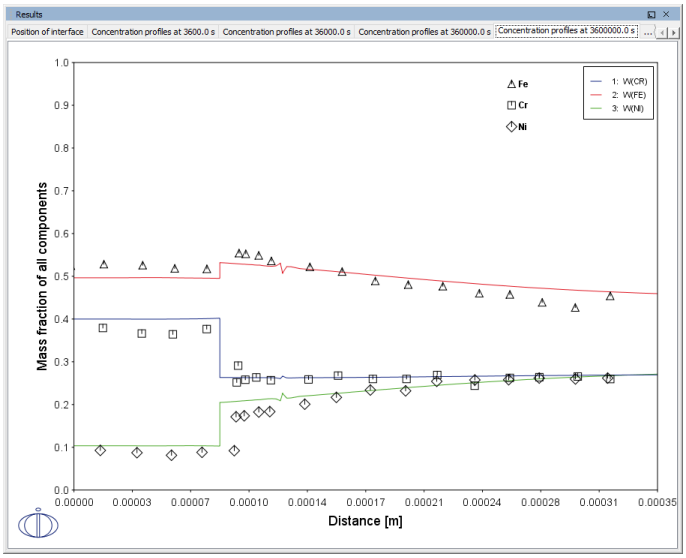


Figure 69: Concentration profiles at 3 600 000 s.

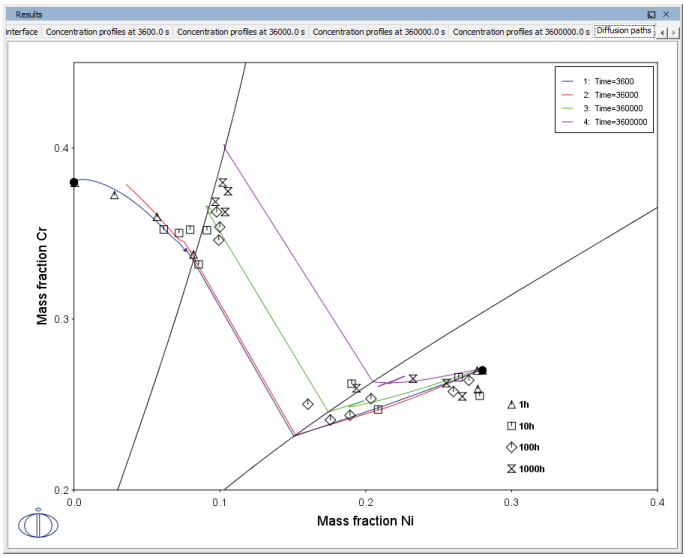


Figure 70: Diffusion paths.

References

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

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

D_06: Diffusion Through a Tube Wall

This is a simple example of diffusion through a tube wall. The tube material is an Fe-0.06Mn-0.05C alloy. Two plots comparing distance to the U-fraction of manganese and composition of carbon are generated to visualize the austenite region. A *cylindrical* geometry is used with *mixed zero flux and activity* boundary conditions.

On the inside wall a carbon activity of 0.9 is maintained whereas on the outside the carbon activity is very low. This example demonstrates the use of boundary conditions, advanced plotting and tables.

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

Project File Information

- Folder: Diffusion Module - DICTRA
- File name: *D_06_Diffusion_Carburization_Tube.tcu*

This example is based on Console Mode exab6. When in Console Mode, you can open the example from Thermo-Calc (**File → Examples Files → Diffusion Module**).

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 you can go to the website or our YouTube channel.

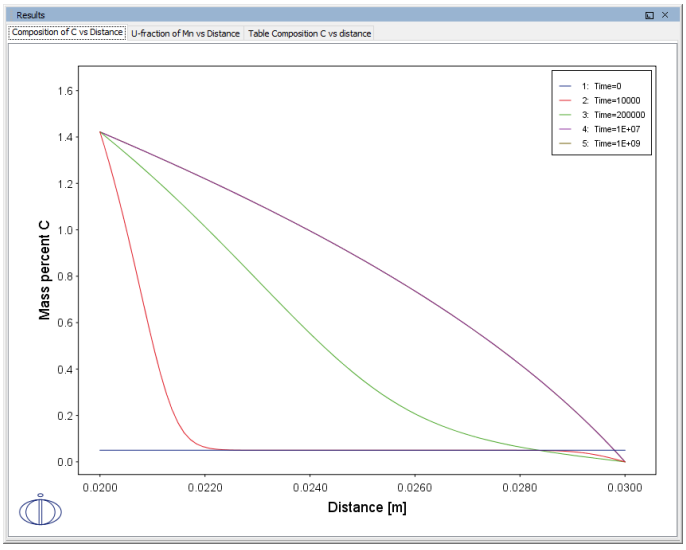


Figure 71: Composition of C vs Distance.

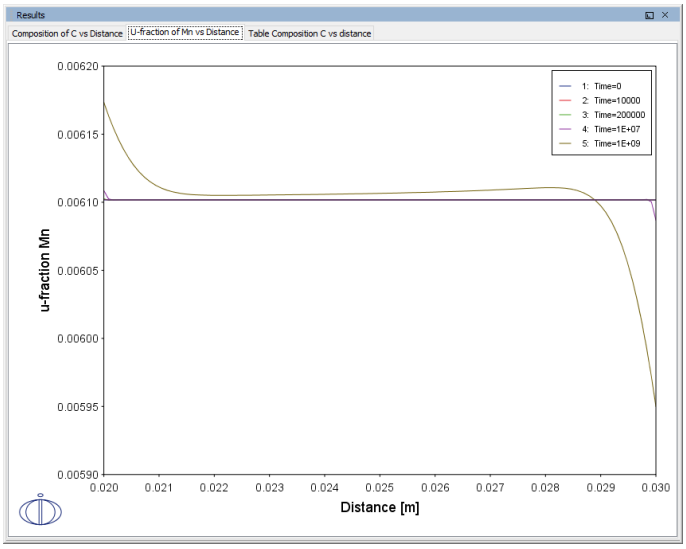


Figure 72: U-fraction of Mn vs Distance.

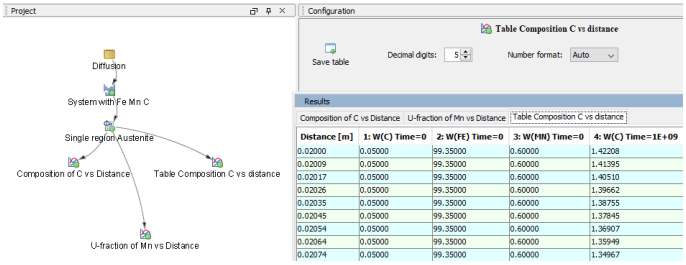


Figure 73: Table: Composition C vs Distance.

D_07: Multiphase Carburization of an Alloy

This example is based on Engström et al. [1994Eng] and is about carburization of a Ni-25Cr-0.0001C alloy. In this case the M7C3 and M3C2 carbides are entered as spheroid phases in an FCC_A1 matrix. It is similar to Graphical Mode example D_06 except the default simulation condition is automatically set to use the homogenization model.

The isothermal calculation is run for 1000 hours at a temperature of 1123 K using the mixed zero flux and activity left boundary condition. Results are plotted using two Plot Renderers and a Table Renderer.

This example is included as a Diffusion Module (DICTRA) tutorial on our website and as part of the playlist on our YouTube channel.

Open the example project file 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: Diffusion Module - DICTRA
- File name: *D_07_Diffusion_Carburization_Multiphase.tcu*

This example is based on Console Mode exd1b. When in Console Mode, you can open the example from Thermo-Calc (**File → Examples Files → Diffusion Module**).

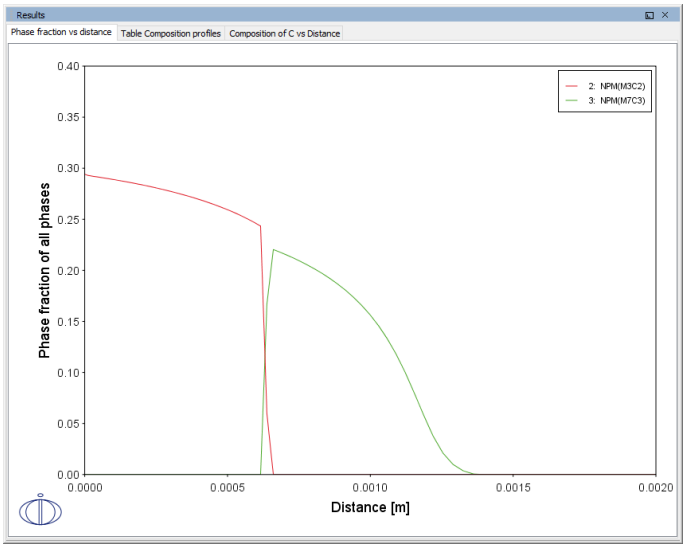
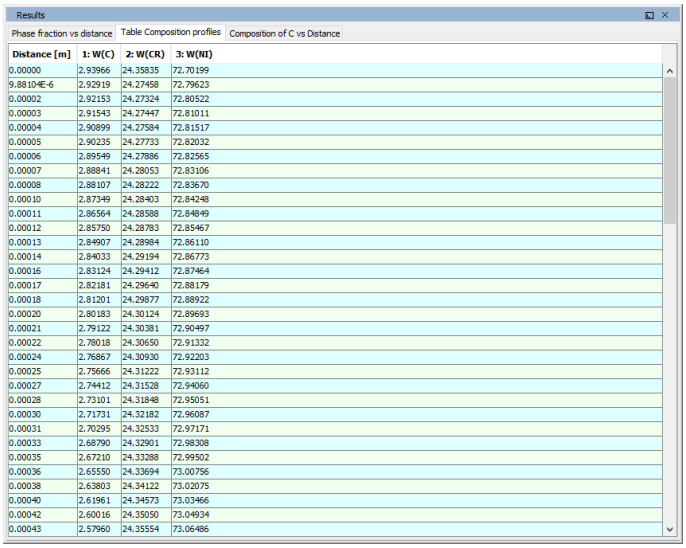


Figure 74: Phase fraction vs distance.


Results

Phase fraction vs distance | Table Composition profiles | Composition of C vs Distance

Distance [m]	1: W(C)	2: W(CR)	3: W(NI)
0.00000	2.93966	24.35835	72.70199
9.88104E-6	2.92919	24.27458	72.79623
0.00002	2.92153	24.27324	72.80522
0.00003	2.91543	24.27447	72.81011
0.00004	2.90899	24.27584	72.81517
0.00005	2.90235	24.27733	72.82032
0.00006	2.89549	24.27886	72.82565
0.00007	2.88841	24.28053	72.83106
0.00008	2.88107	24.28222	72.83670
0.00010	2.87349	24.28403	72.84248
0.00011	2.86564	24.28588	72.84849
0.00012	2.85750	24.28783	72.85467
0.00013	2.84907	24.28984	72.86110
0.00014	2.84033	24.29194	72.86773
0.00016	2.83124	24.29412	72.87464
0.00017	2.82181	24.29640	72.88179
0.00018	2.81201	24.29877	72.88922
0.00020	2.80183	24.30124	72.89693
0.00021	2.79122	24.30381	72.90497
0.00022	2.78018	24.30650	72.91332
0.00024	2.76867	24.30930	72.92203
0.00025	2.75666	24.31222	72.93112
0.00027	2.74412	24.31528	72.94060
0.00028	2.73101	24.31848	72.95051
0.00030	2.71731	24.32182	72.96087
0.00031	2.70295	24.32533	72.97171
0.00033	2.68790	24.32901	72.98308
0.00035	2.67210	24.33288	72.99502
0.00036	2.65550	24.33694	73.00756
0.00038	2.63803	24.34122	73.02075
0.00040	2.61961	24.34573	73.03466
0.00042	2.60016	24.35050	73.04934
0.00043	2.57960	24.35554	73.06486

Figure 75: Table of Composition profiles.

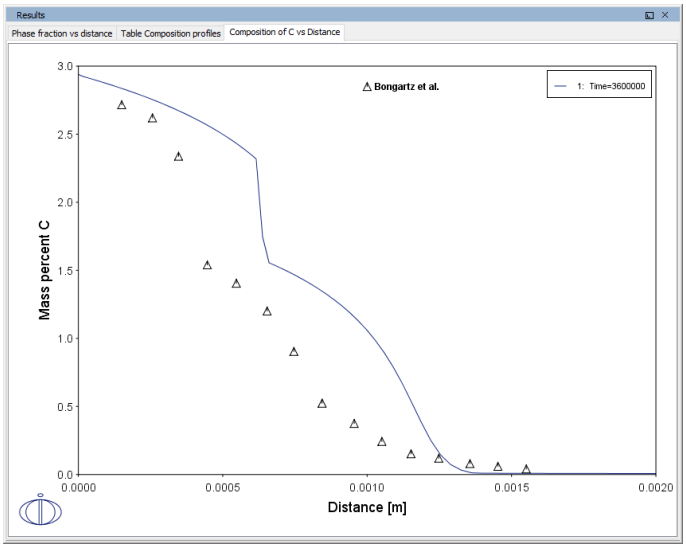


Figure 76: Composition of C vs distance.

Reference

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

D_08: Microsegregation During Solidification

This application example, which is showcased on our website, shows how Thermo-Calc together with the Diffusion Module (DICTRA) can be used to investigate and predict microsegregation during solidification, also known as solute redistribution during solidification. The example uses a steel with composition Fe – 0.8% Mn – 0.7%Si – 0.03%P – 0.4%C.

The example is based on a real case where the elemental distribution of a continuously cast steel was measured revealing the concentration of the elements Si, Mn, and P. The profile results from the well-known segregation across secondary dendrite arms. The interesting point is that the elements Si and Mn show the expected positive segregation (higher concentrations) in the interdendritic regions. The peak of the P content, on the other hand, is shifted compared to Si and Mn, and, in fact, shows negative segregation in the interdendritic region. This is unexpected and counterintuitive.

The example also touches on some very basic concepts for metallurgy and using Thermo-Calc, such as stable and meta-stable phase diagrams, Scheil and para- or partial-equilibrium Scheil solidification simulations.

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: Diffusion Module - DICTRA
- File name: *D_08_Diffusion_Microsegregation_During_Solidification.tcu*

Running this calculation requires licenses for the Add-on Diffusion Module (DICTRA) plus the steels thermodynamic database (TCFE9 or newer) and mobility database (MOBFE4 or newer).

The resulting plots and details related to setting up this example are available via the dedicated web page, or you can read the more in depth step-by-step documentation as a PDF, also available via our website.

Precipitation Module (TC-PRISMA) Graphical Mode Examples

Examples that use up to three elements are available to all users. The other examples require a Precipitation Module (TC-PRISMA) license to calculate and plot results.

All examples use demonstration database packages included with your installation. You can open the examples from the main menu: **File →** or **Help → Examples Files**.

Unless specified in tables for each example, all the numerical parameters are assumed default values.

In this section:

P_01: Isothermal Precipitation of Al_3Sc

This example simulates the kinetics of precipitation of Al_3Sc from an FCC_A1 solution phase. The simulation results can be compared with experimental data collected from Marquis and Seidman [2001Mar] and Novotny and Ardell [2001Nov].

This example also includes a plot using the **Yield strength** Property Model. This demonstrates how you can use the results from a Precipitation Module (TC-PRISMA) simulation as input to the Yield Strength Model, i.e. the calculated precipitate radius/radii for each time step is used to calculate the precipitation strengthening, and similarly, the matrix composition for each time step is used to calculate the solid solution strengthening when this is selected in the **Configuration** on the Plot Renderer. The experimental data for the Yield Strength Model is from Seidman et al. [2002Sei]. In this example, the *Precipitation strengthening model* used is **Seidman model (Al-base)**. This is selected on the Plot Renderer configuration panel that is connected to the Property Model.

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*.	

Results

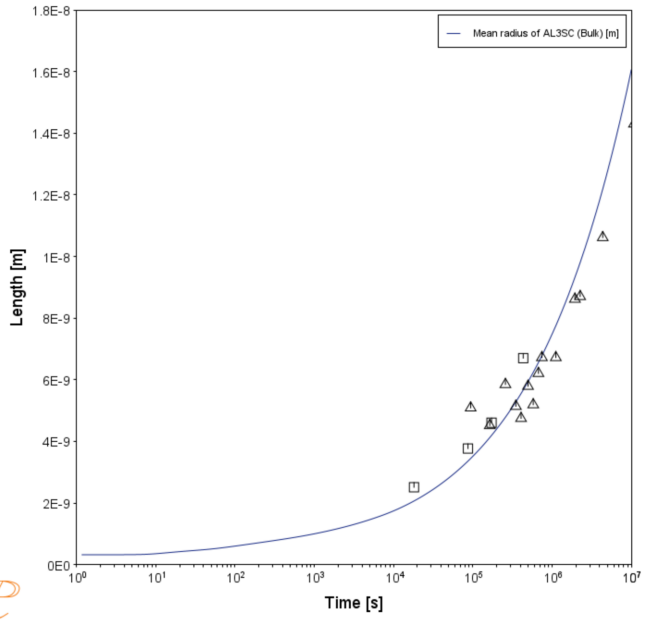


Figure 77: The mean radius of the AL3SC precipitate as a function of time.

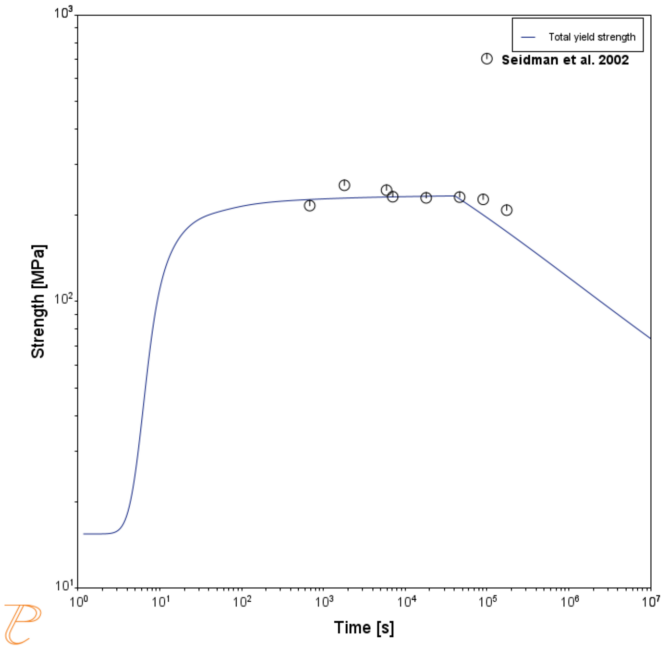


Figure 78: The total yield strength of the AL3SC precipitate as a function of time compared to experimental data from Sieldmen et al. [2002Sei].

References

[2001Mar] E. A. Marquis, D. N. Seidman, Nanoscale structural evolution of Al3Sc precipitates in Al(Sc) alloys. Acta Mater. 49, 1909–1919 (2001).

[2001Nov] G. M. Novotny, A. J. Ardell, Precipitation of Al3Sc in binary Al–Sc alloys. Mater. Sci. Eng. A Struct. Mater. Prop. Microstruct. Process. 318, 144–154 (2001).

[2002Sei] D. N. Seidman, E. A. Marquis, D. C. Dunand, Precipitation strengthening at ambient and elevated temperatures of heat-treatable Al(Sc) alloys. Acta Mater. 50, 4021–4035 (2002).

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

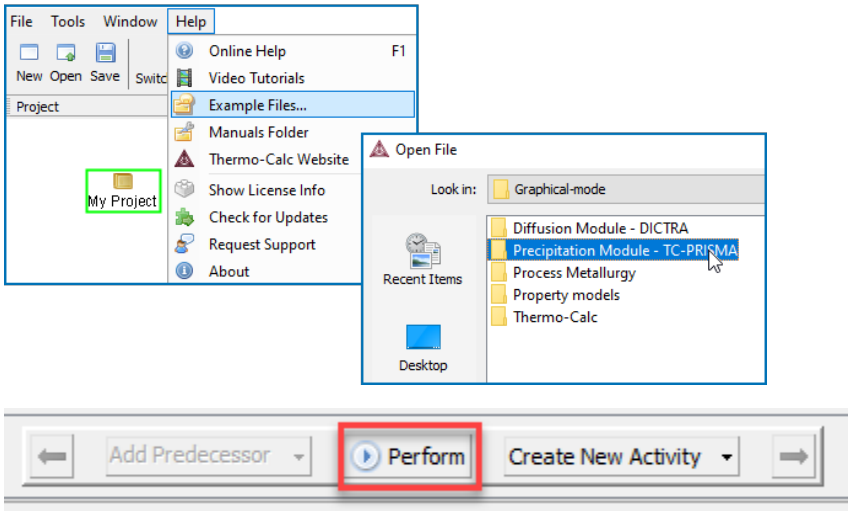
This example shows you how to set up an isothermal precipitation calculation for the formation of AL_3SC in an aluminium-scandium alloy at 350° using the Precipitation Module (TC-PRISMA).

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. To run the example file, open Thermo-Calc and select **Help > Examples Files**. Open the *Precipitation Module (TC-PRISMA)* folder. Double-click the example file and click **Perform** at the bottom center of the **Configuration** window in Thermo-Calc.

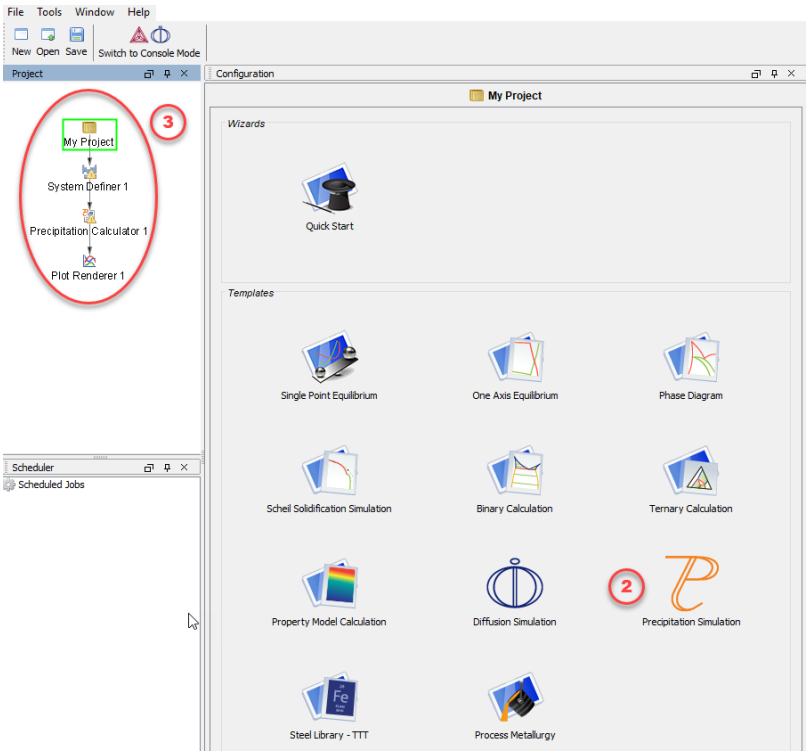


ABOUT THE EXAMPLE

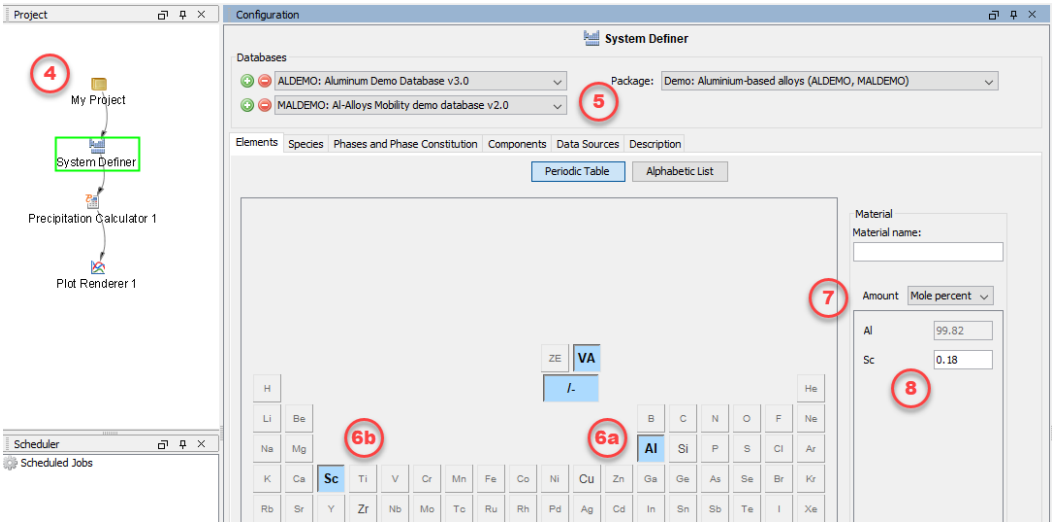
This example simulates the kinetics of precipitation of Al_3Sc from an FCC_A1 solution phase. The results of the simulation are also used to model yield strength.

SETTING UP THE SYSTEM

1. Open Thermo-Calc in Graphical Mode.
2. Under *Templates*, click **Precipitation Simulation**.
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 as follows. 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.

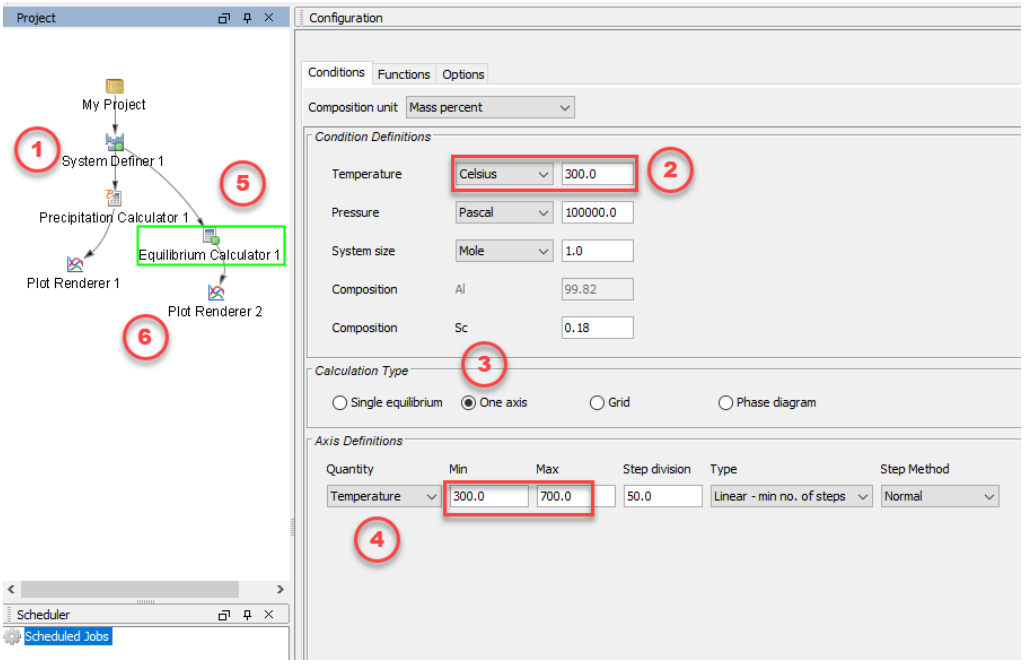
ONE AXIS CALCULATION

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.

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*, select **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, right-click the **Plot Renderer 2** node you just created and select **Perform Now**. Or click **Perform** at the bottom of the **Configuration** window.



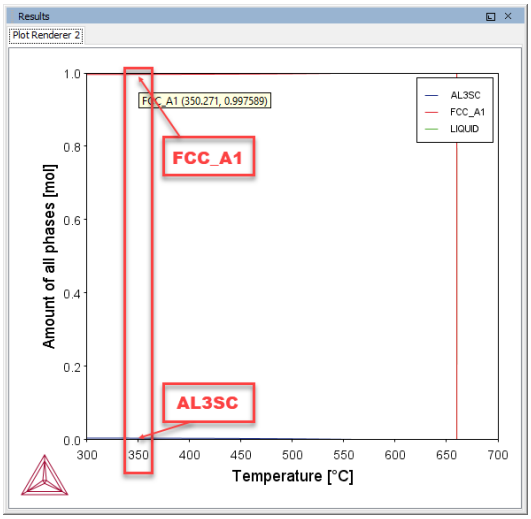
Interpreting the Results of the One Axis Calculation

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 Al_3SC, 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.



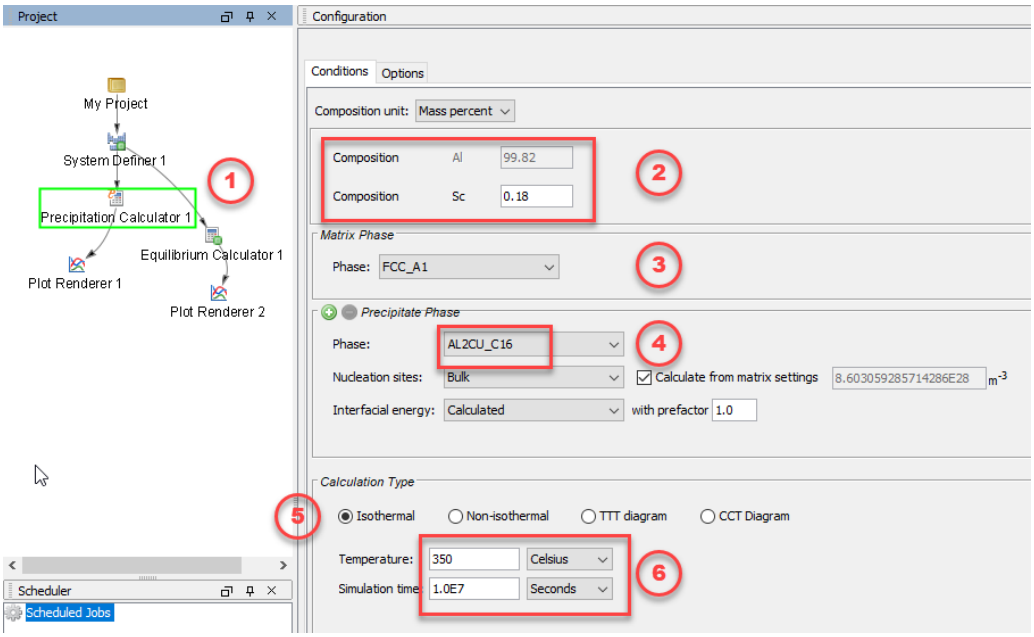
PRECIPITATION CALCULATION

Setting up the Precipitation Calculation

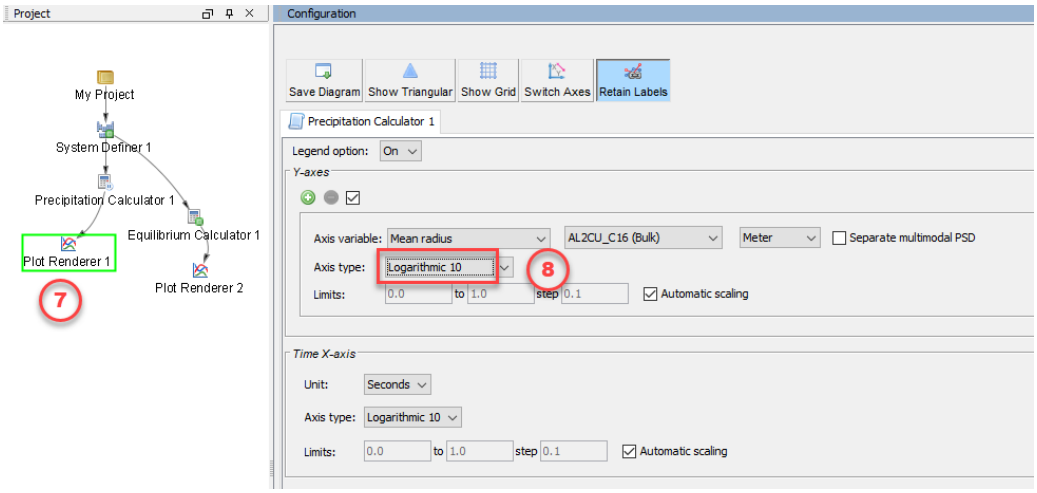
1. In the **Project** window, click the **Precipitation Calculator 1** node.
2. Notice that the *Composition* set in the *System Definer* auto-populated here.
3. Under *Matrix Phase*, the *Phase* defaults to **FCC_A1**, which is the primary phase present in the one axis calculation.

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 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.

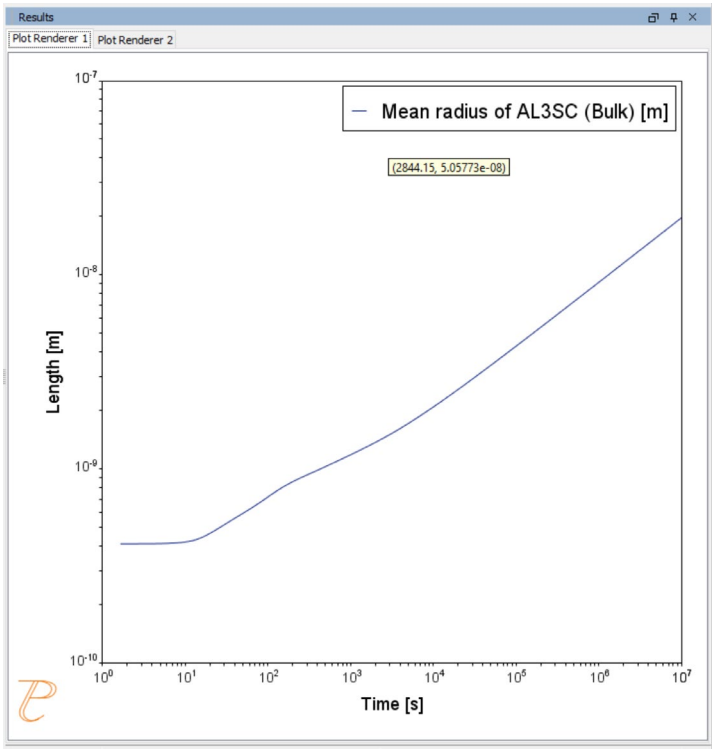


8. In the **Project** window, click the **Plot Renderer 1** node.
9. Under *Y-axes*, from the *Axis type* menu select **Logarithmic 10** for a better view of the plot.
10. Click **Perform** at the bottom, center of the **Configuration** window.



Interpreting the Results of the Precipitation Calculation

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



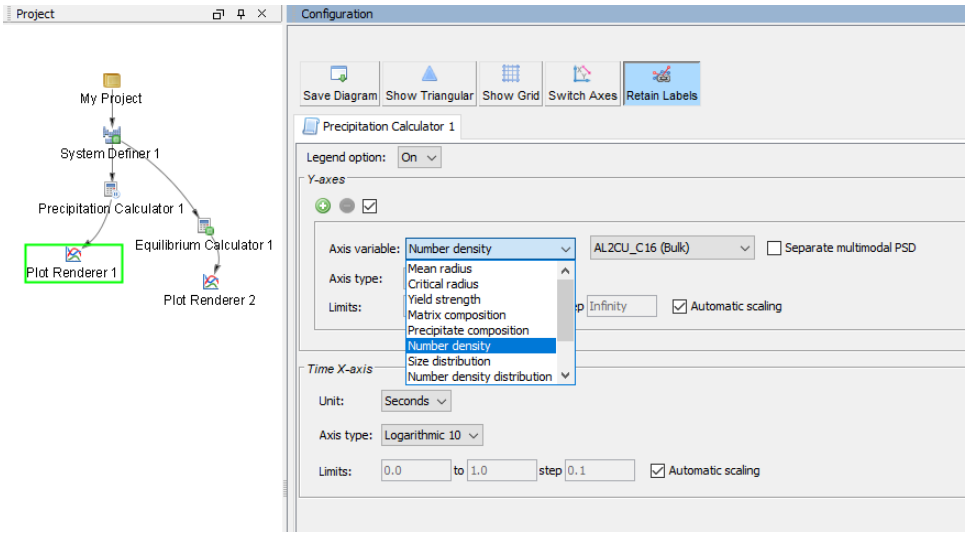
This plot shows the Mean radius of the AL3SC precipitate as a function of time.

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.

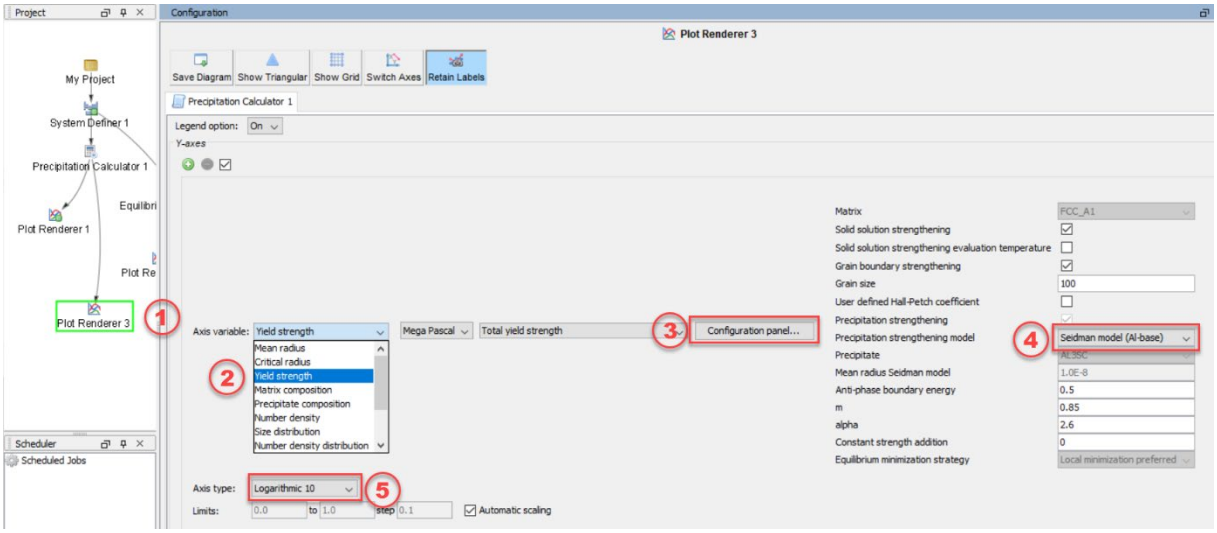


Model Yield Strength

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.

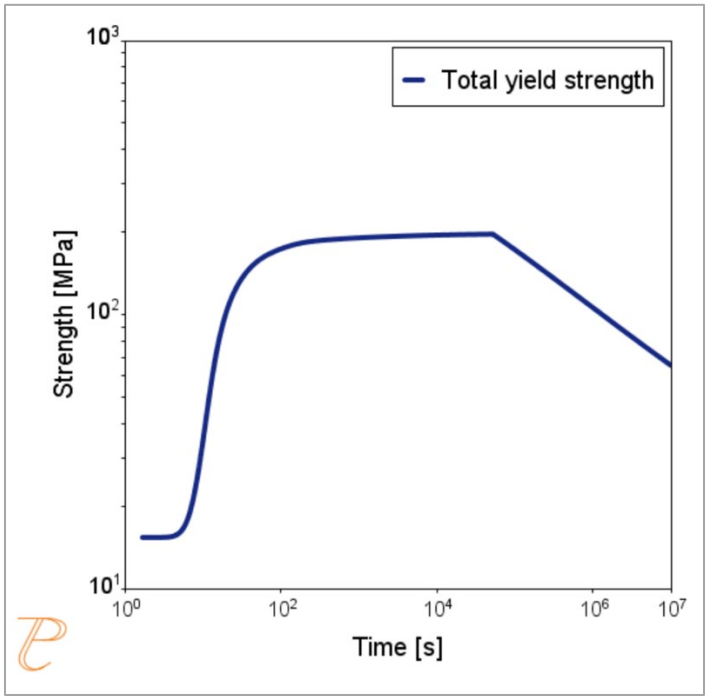
1. Right click the **Precipitation Calculator 1** node and select **Create New Successor > Plot Renderer**.
2. Under *Y-axes*, from the *Axis variable* menu, select **Yield strength**.
3. Click the *Configuration panel* button.
4. If required, expand the Plot Renderer Configuration window. Then from 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 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 setting)	1.0E-4 m
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Grain boundaries
Interfacial energy	Cementite 0.167 J/m^2, M23C6 0.252 J/m^2, M7C3 0.282 J/m^2
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	1053 K
Simulation time	400 000 seconds

Results

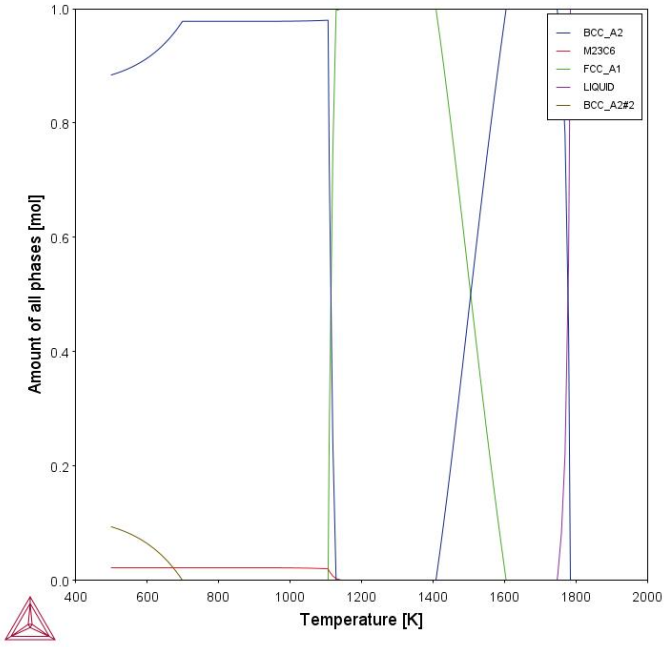


Figure 79: The Equilibrium Calculator and a one axis calculation is used to determine how the phases change with temperature.

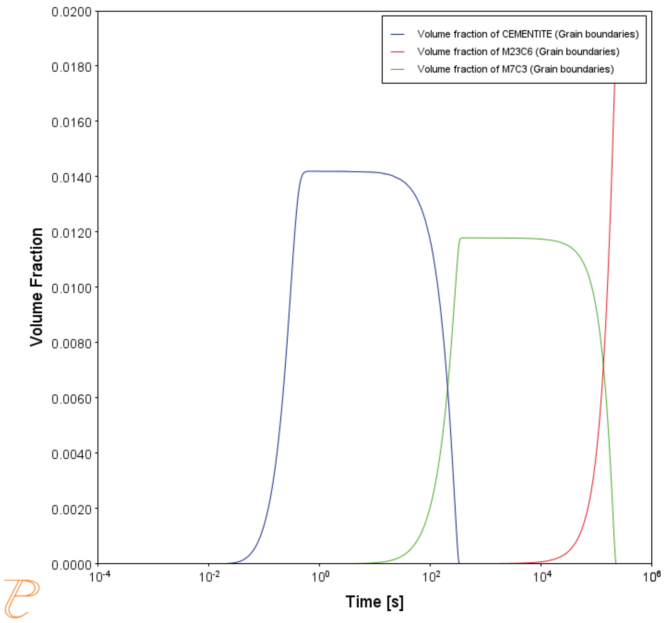


Figure 80: The Precipitation Calculator is used to do an isothermal calculation of the three phases (cementite, M23C6, and M7C3) where cementite and M7C3 are metastable phases.

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 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

Results

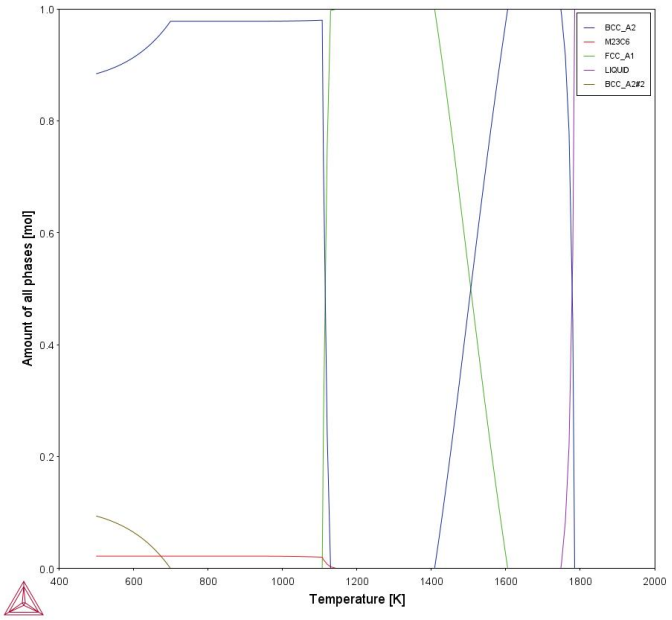


Figure 81: The Equilibrium Calculator is used to show how the phases change with temperature.

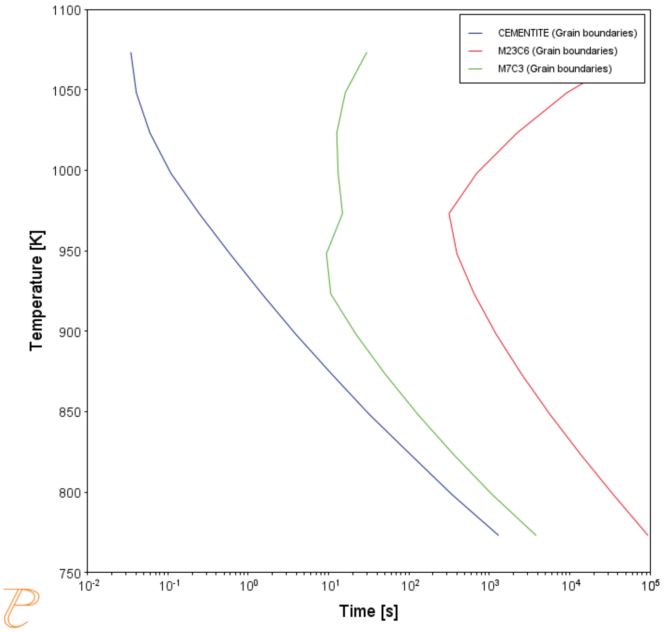


Figure 82: The Precipitation Calculator is used to do a TTT (Time-Temperature-Transformation) diagram calculation of the three phases (cementite, M23C6 and M7C3) at the grain boundaries.

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 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

Results

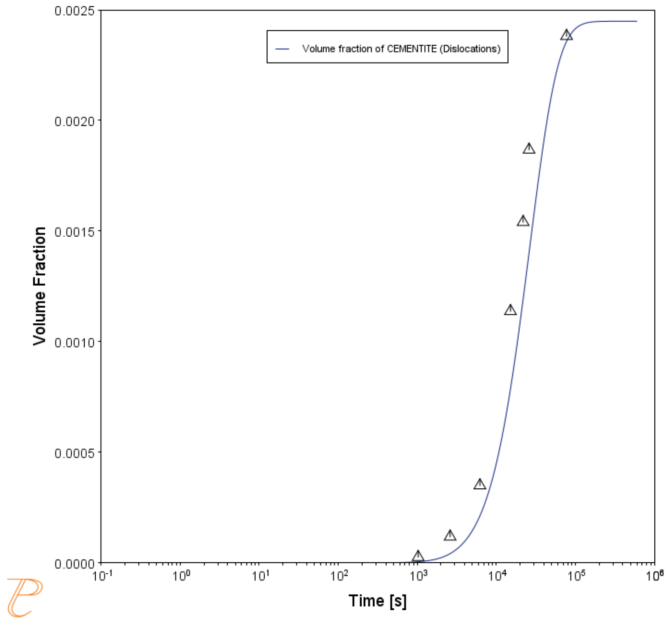


Figure 83: Volume fraction of the cementite phase.

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 primate (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.

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 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
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

Results

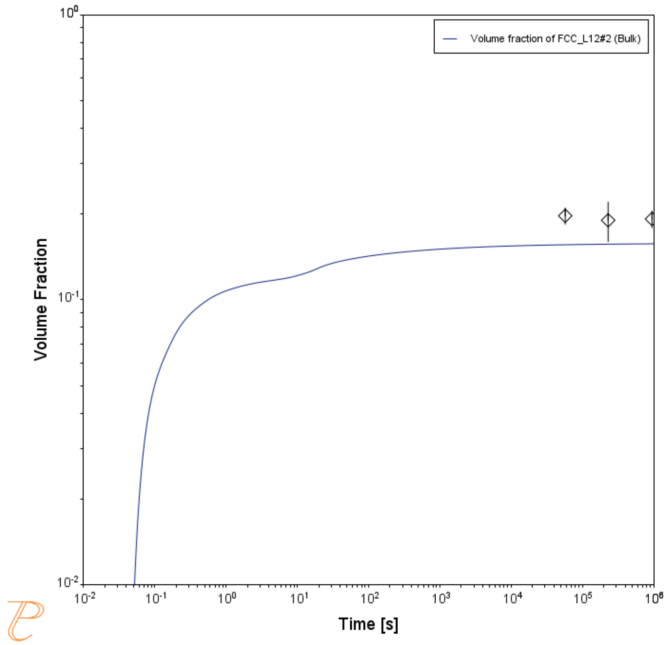


Figure 84: The results of an isothermal calculation to plot the volume fraction of the cementite phase.

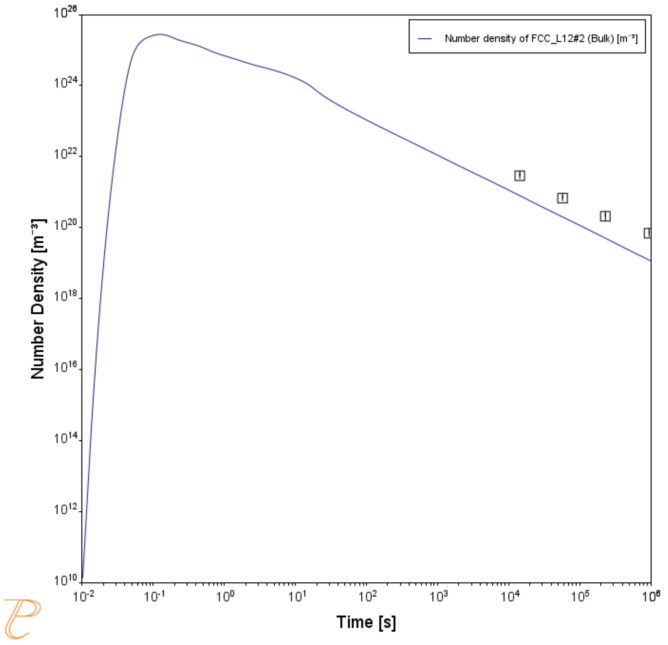


Figure 85: The results of an isothermal calculation to plot the number density of the cementite phase.

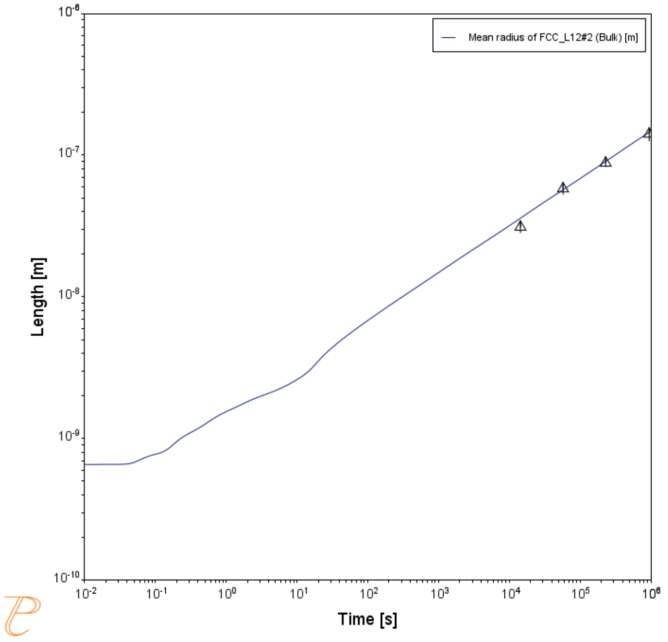


Figure 86: The results of an isothermal calculation to plot the mean radius of the cementite phase.

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.

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 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
Precipitate phase	FCC_L12#2
Matrix Phase Data Parameters (Precipitation Calculator)	
Mobility enhancement prefactor (click **Show details** to display this	5.0

setting)	
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.

Results

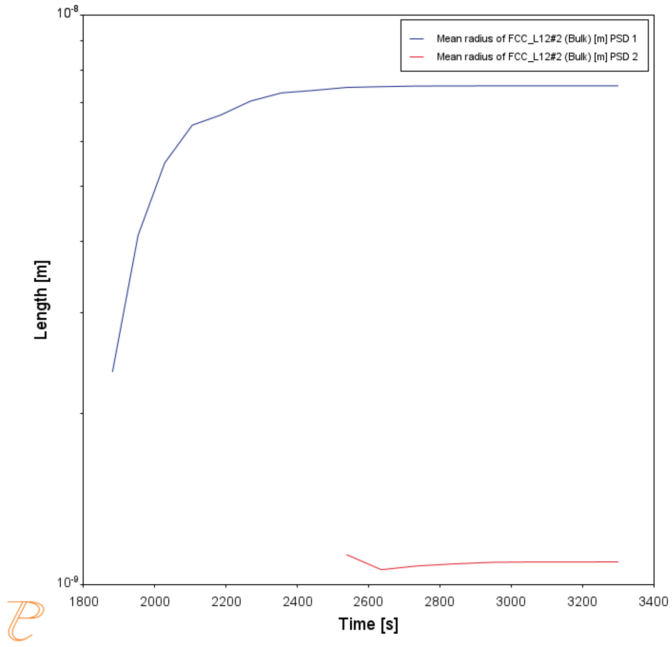


Figure 87: Mean radius Ni-8Al-8Cr.

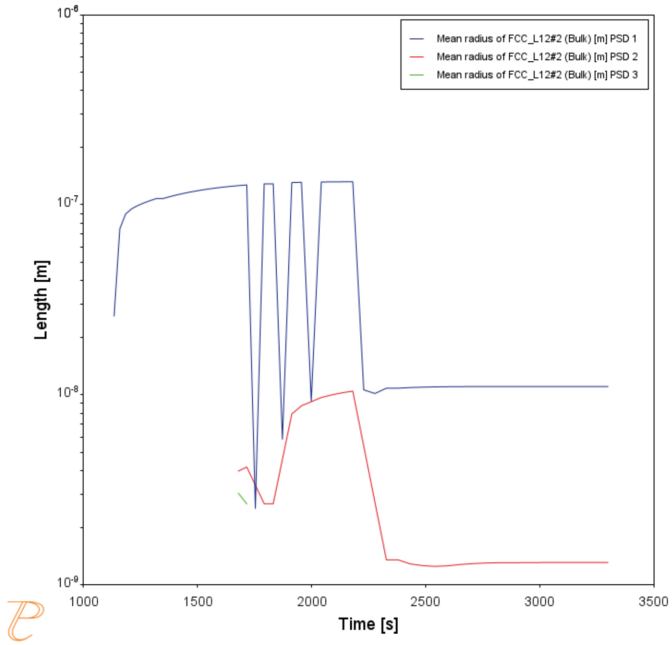


Figure 88: Mean radius Ni-10Al-10CR.

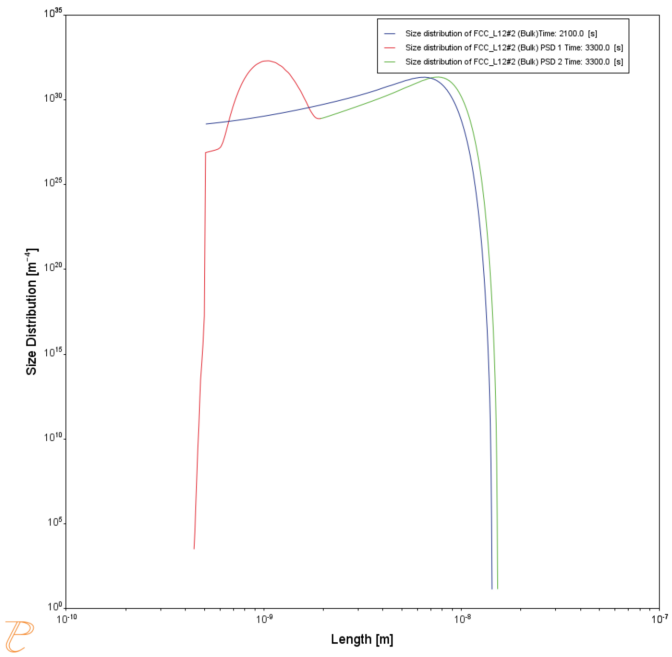


Figure 89: Preexisting Size Distribution (PSD) Ni-8Al-8Cr.

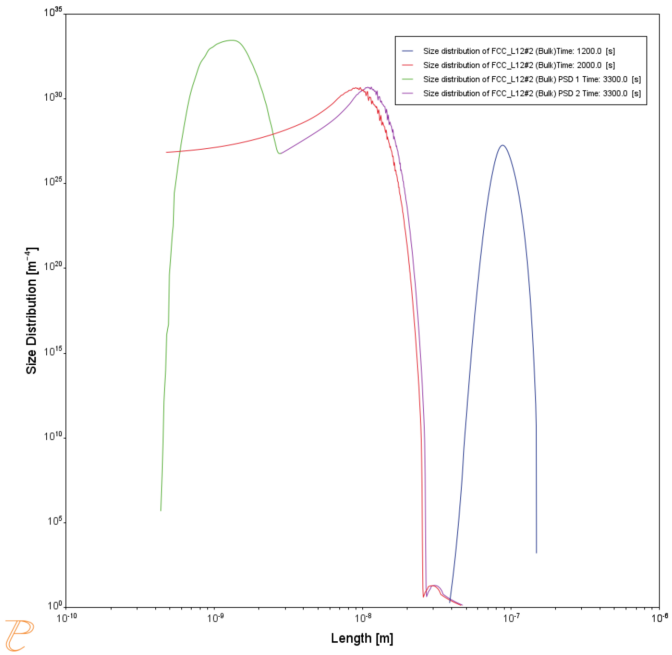


Figure 90: Preexisting Size Distribution (PSD) Ni-10Al-10Cr.

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.

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

Results

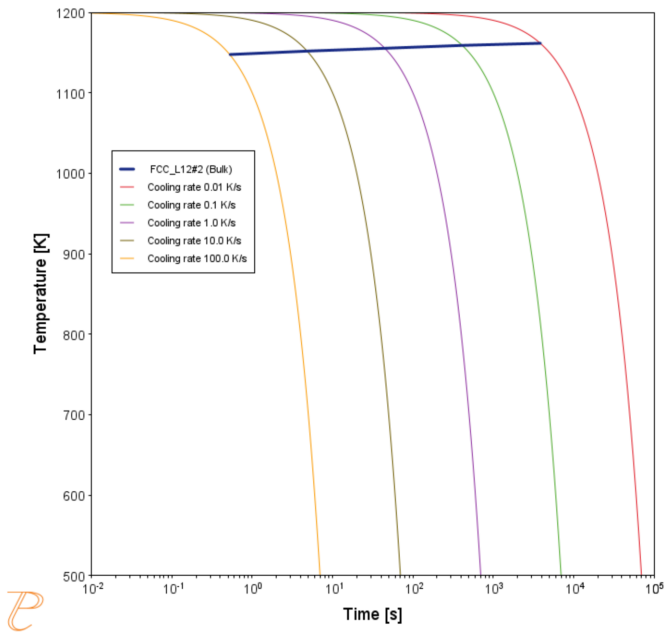


Figure 91: In this plot, the blue horizontal line shows the time it takes for γ' to transform at each of the cooling rates according to the stop criteria, which is set as 1e-4 volume fraction. The cooling rates are represented by the multicoloured curved lines.

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.

Results

Plot Renderer 1 | Table Renderer 1

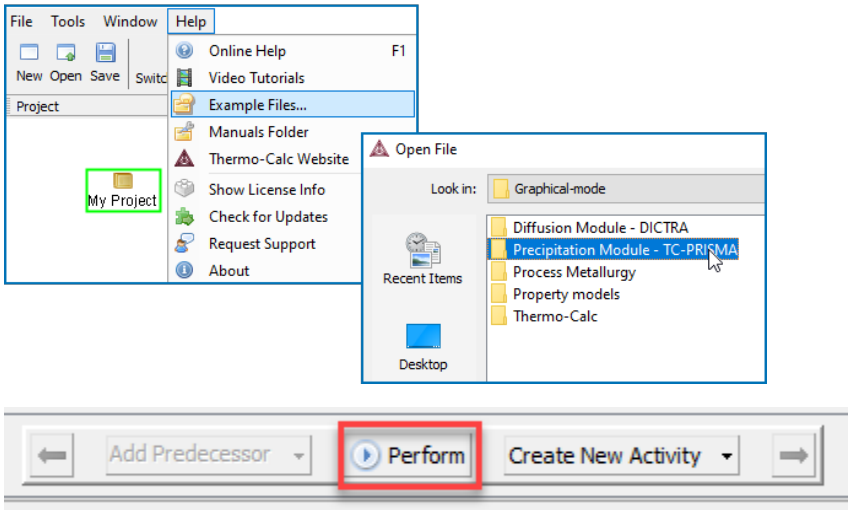
Temperature [K]	FCC_L12#2 (Bulk)
1147.52034	0.53291
1151.74192	4.83553
1155.24636	44.76534
1158.85368	411.49173
1161.48750	3851.47779

Figure 92: An example of the table shown in the Results 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. To run the example file, open Thermo-Calc and select **Help > Examples Files**. Open the *Precipitation Module (TC-PRISMA)* folder. Double-click the example file and click **Perform** at the bottom center of the **Configuration** window in Thermo-Calc.



ABOUT THE EXAMPLE

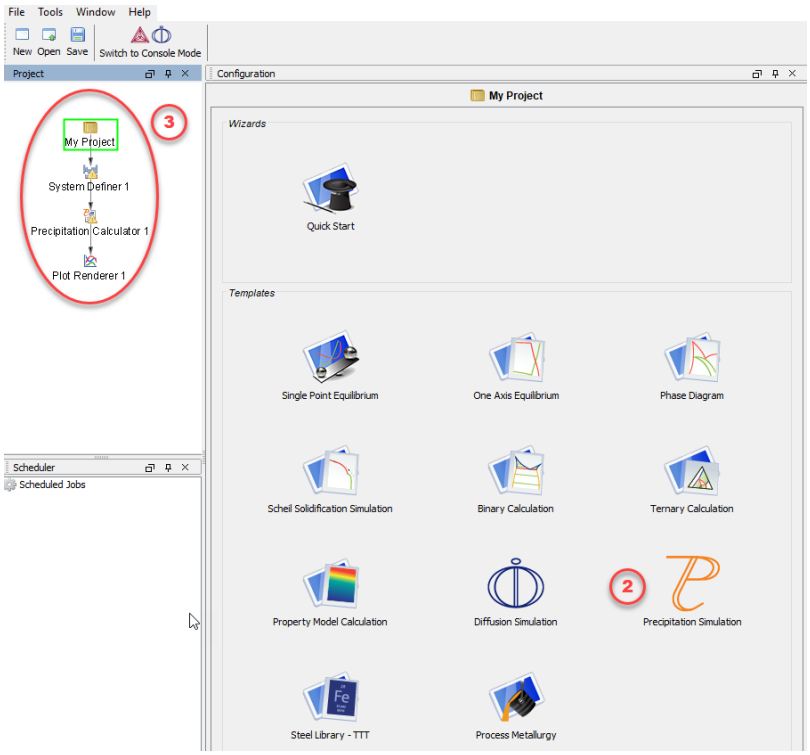
This example shows you how to simulate a CCT diagram for gamma prime (γ') precipitation in a Ni-Cr-Al alloy using the Precipitation Module known as TC-PRISMA.

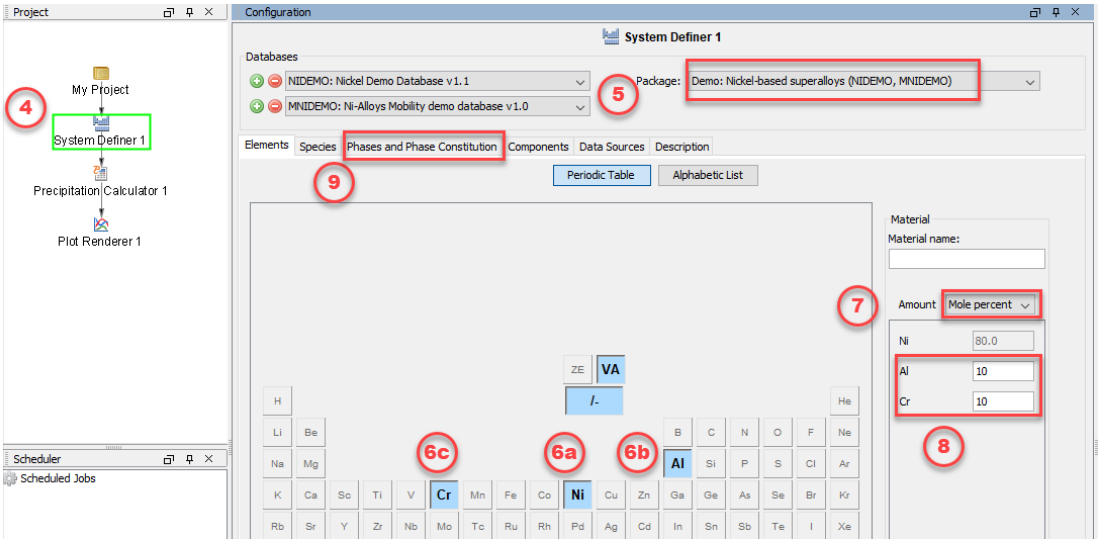
CCT stands for Continuous Cooling Transformation and is a calculation that maintains the same cooling rate the entire time.

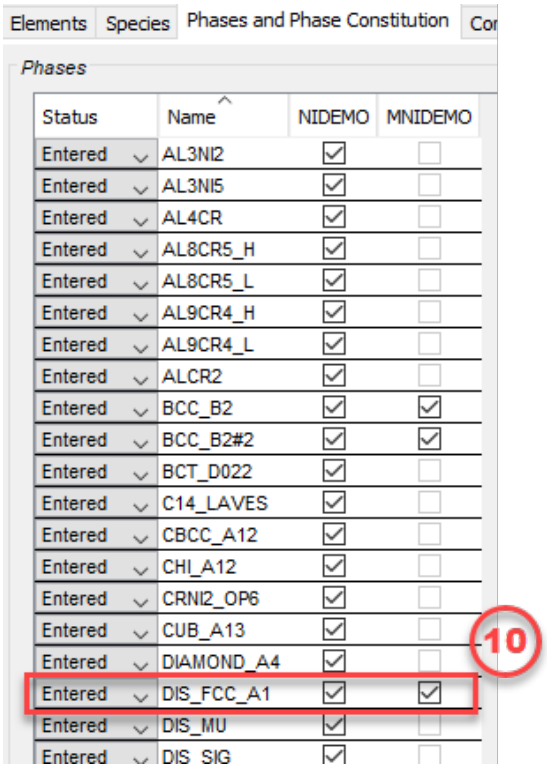
The system is a Ni-10Al-10Cr γ - γ' alloy and it is calculated and plotted with superimposition of the cooling rate values using the Precipitation Module (TC-PRISMA).

SETTING UP THE SYSTEM

1. Open Thermo-Calc in Graphical Mode.
2. Under *Templates*, click **Precipitation Simulation**.
3. All the nodes for a precipitation calculation are added to the **Project** window:



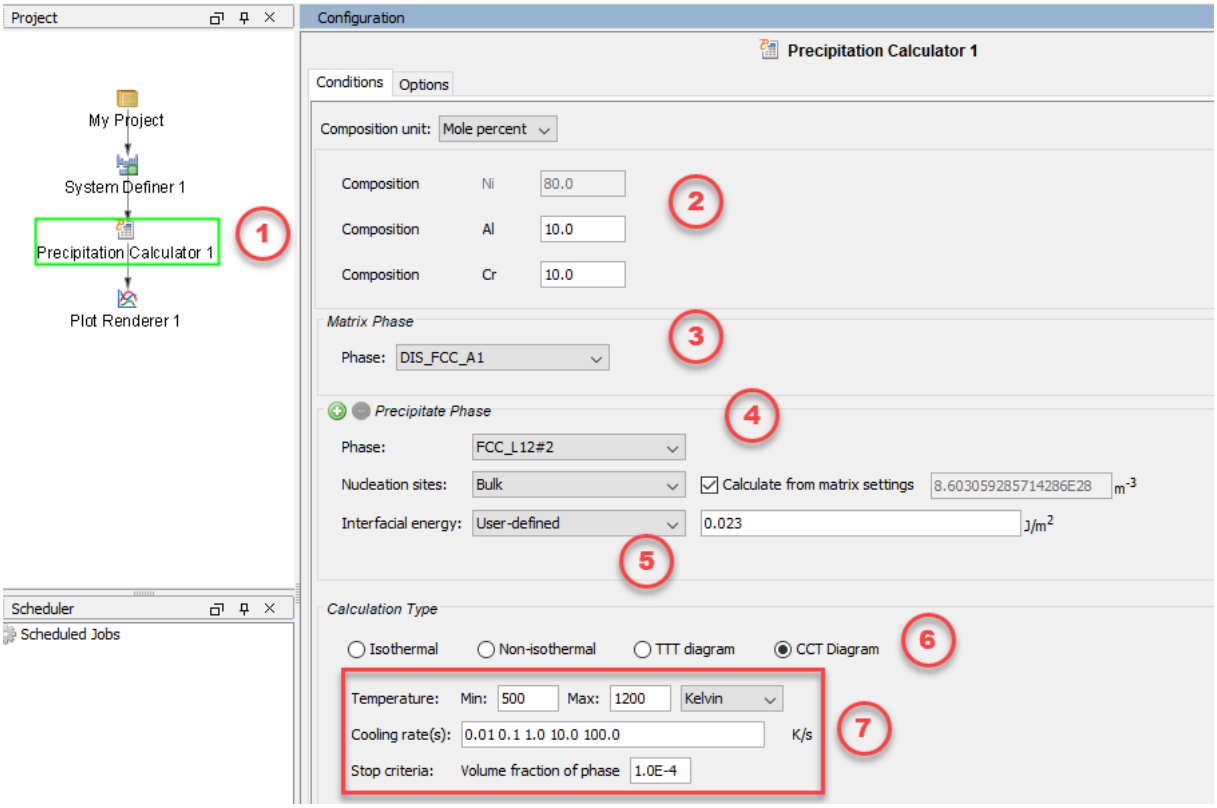
4. In the **Project** window, click the **System Definer 1** node.
5. Set the database *Package* to **Demo: Nickel-based alloys (NIDEMO, MNIDEMO)**, which loads both thermodynamic and kinetic demonstration nickel databases.
6. From the **Periodic Table**, select the elements as follows. Select Ni first 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. Click to select both check boxes next to the disordered FCC phase, **DIS_FCC_A1**.
11. 



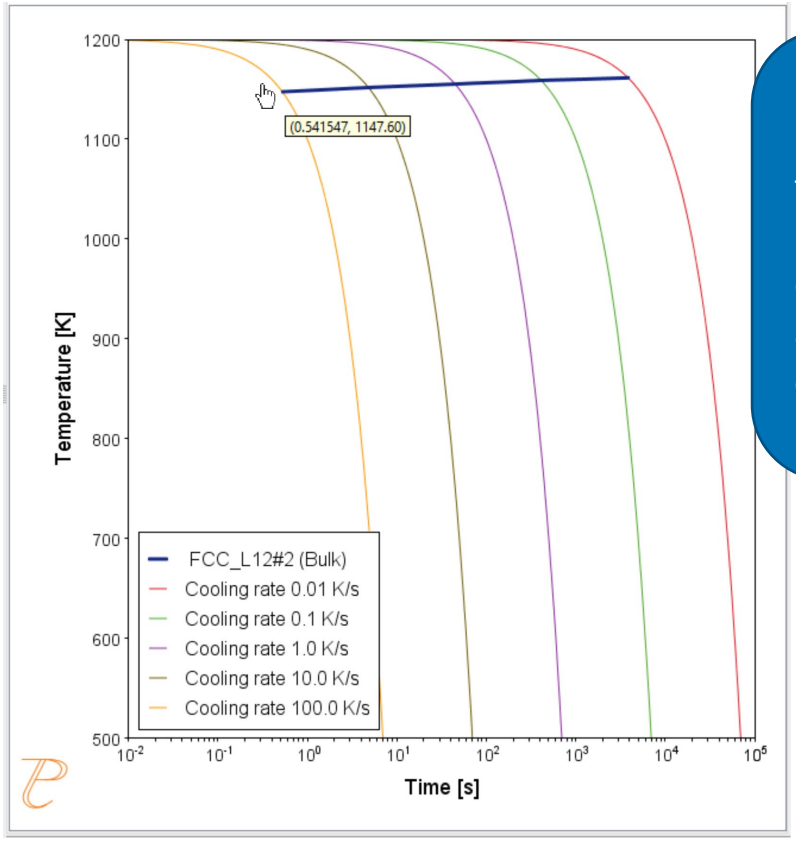
The system is now defined. Now set up the precipitation calculations.

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 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. Choose **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. Click **Perform CCT Diagram Simulation** at the bottom, center of the **Configuration** window.



INTERPRETING THE RESULTS OF THE PRECIPITATION CALCULATION



In this plot, the blue, horizontal line shows the time it takes for gamma prime 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 0.54147 seconds and a temperature of 1147.60 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**.

Time [s]	FCC_L12#2 (Bulk)
0.53291	1147.52034
4.83553	1151.74192
44.76534	1155.24636
411.49174	1158.85368
3851.40881	1161.48822

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.

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].

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.

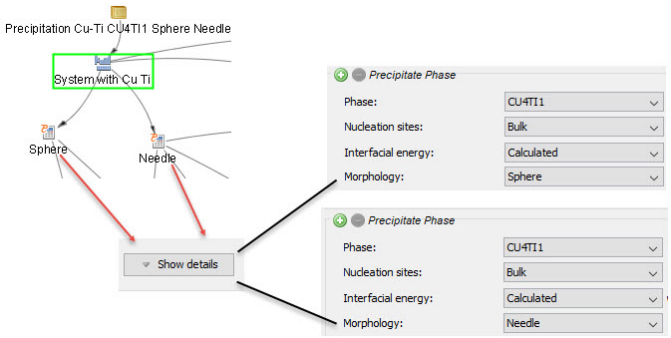
Project File Information

- 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 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 enhancement prefactor (click **Show details** to display this setting)	100
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.

Results

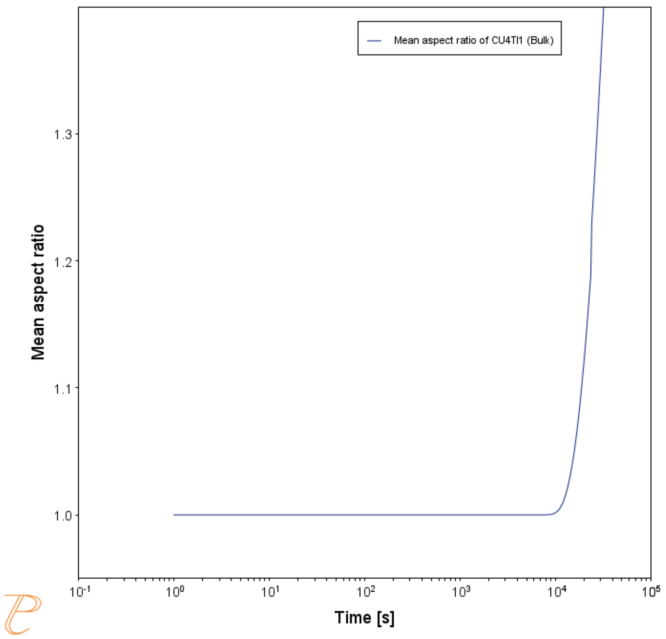


Figure 93: Mean Aspect Ratio.

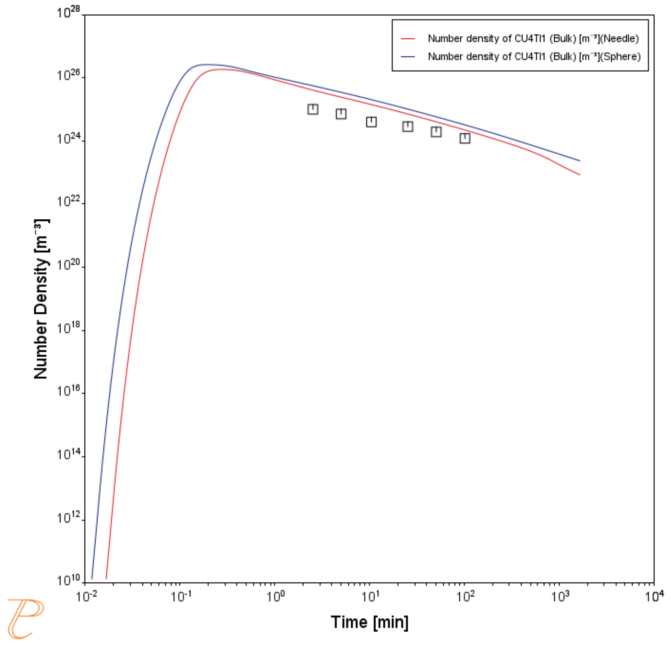


Figure 94: Number Density.

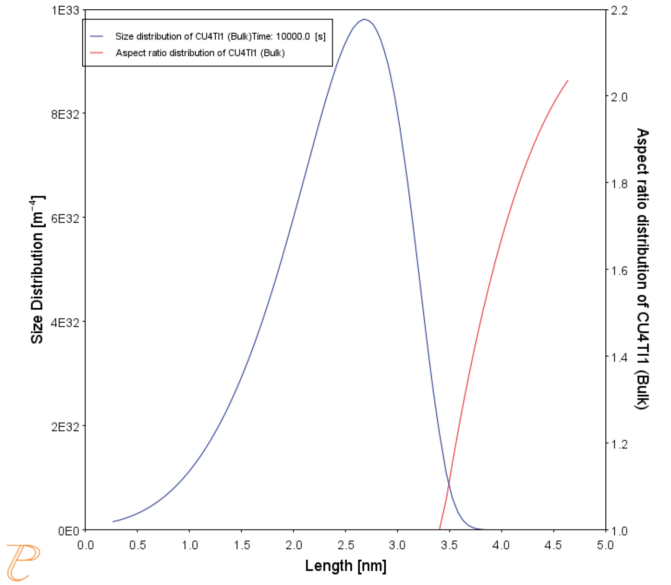


Figure 95: PSD and ASD.

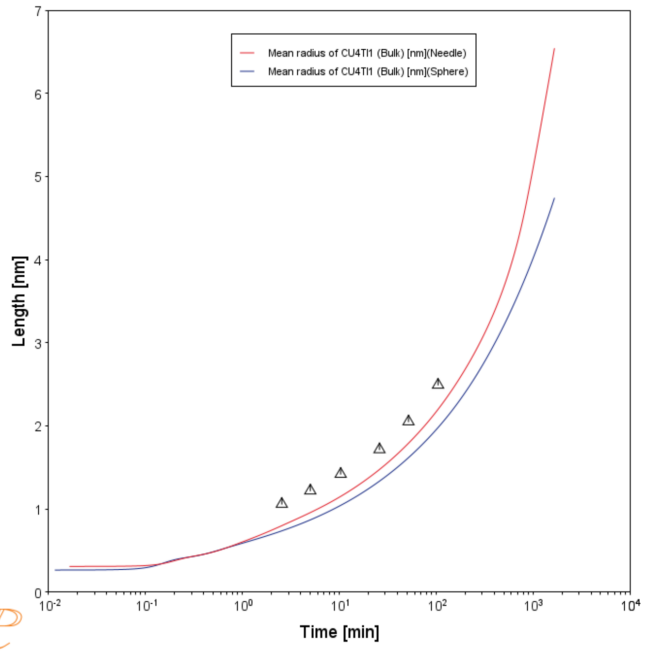


Figure 96: Mean Radius.

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.

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.

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.

Results

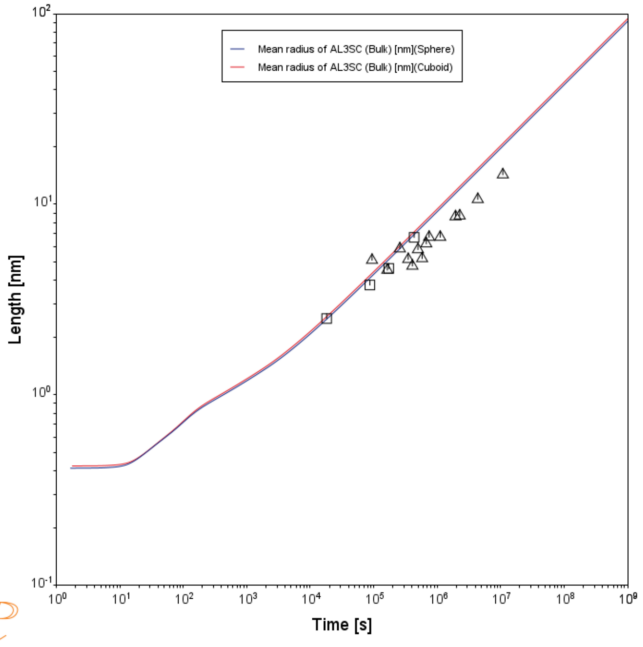


Figure 97: Mean Radius

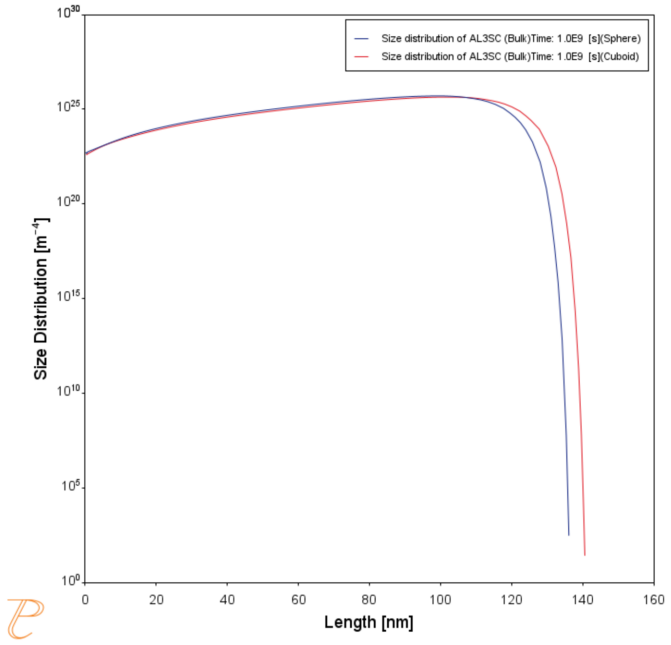


Figure 98: Particle size distribution (PSD).

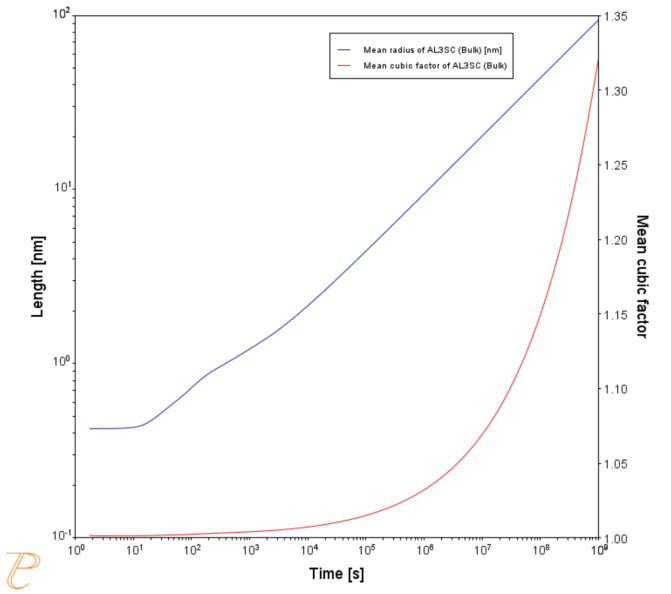


Figure 99: Mean Radius and Cubic Factor

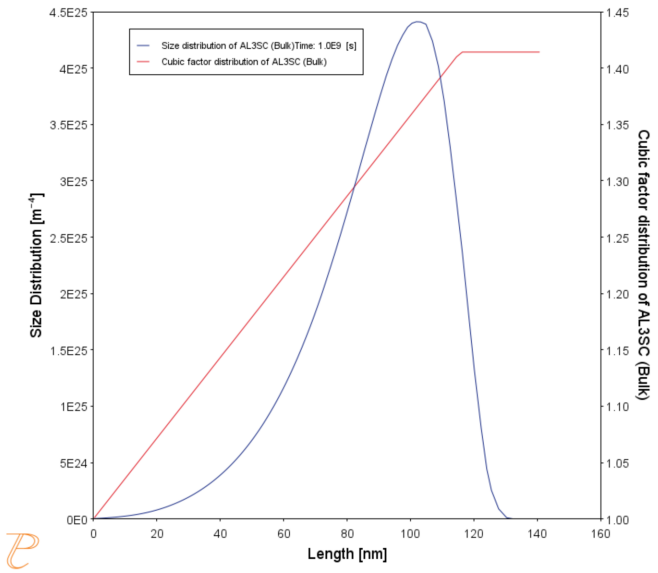


Figure 100: Particle size distribution (PSD) and cubic factor.

References

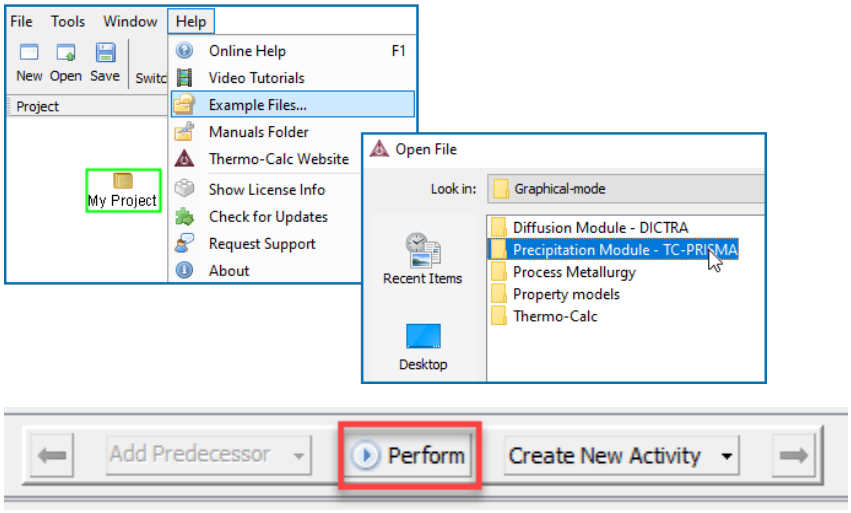
[2001Mar] E. A. Marquis, D. N. Seidman, Nanoscale structural evolution of Al3Sc precipitates in Al(Sc) alloys. Acta Mater. 49, 1909–1919 (2001).

[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

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. To run the example file, open Thermo-Calc and select **Help > Examples Files**. Open the *Precipitation Module (TC-PRISMA)* folder. Double-click the example file and click **Perform** at the bottom center of the **Configuration** window in Thermo-Calc.



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).

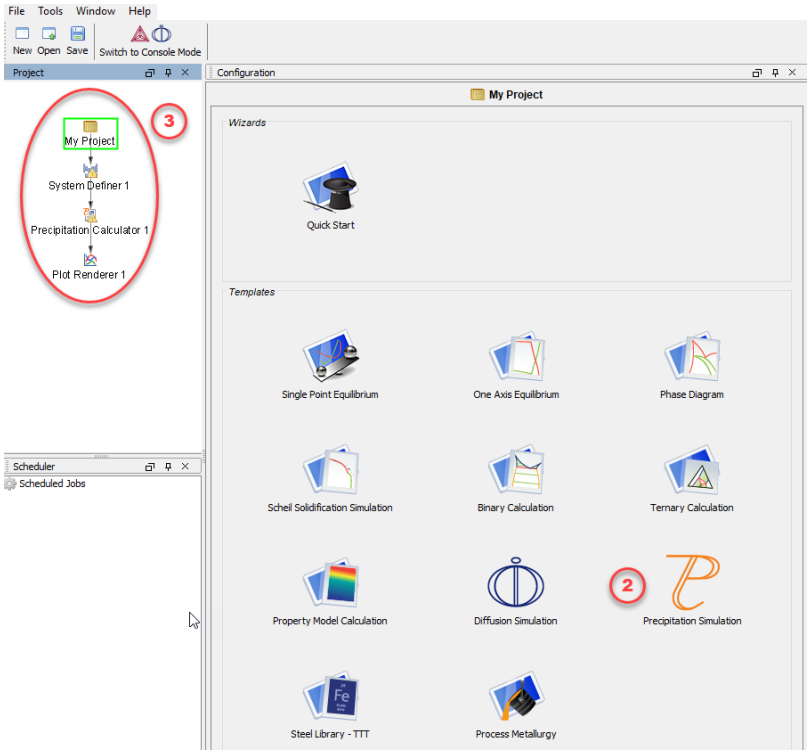
Two separate calculations are performed so you can make a comparison of the results, one assuming spherical morphology without elastic strain energy, and the other assuming cuboid morphology whose shape is determined by competition between interfacial energy and elastic strain energy.

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

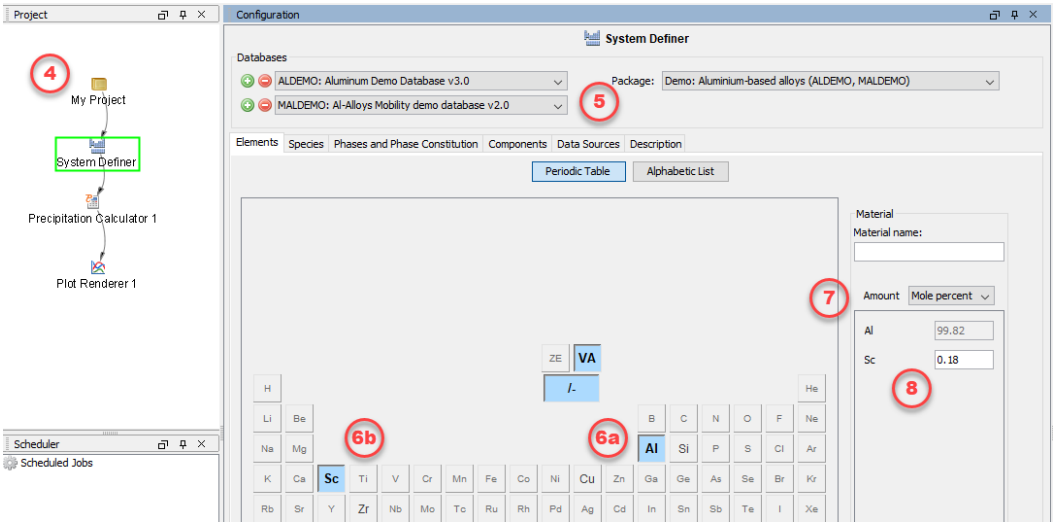
If you run the example file included in your software, the simulation results are compared with experimental data collected from Marquis and Seidman (2001) and Novotny and Ardell (2001).

SETTING UP THE SYSTEM

1. Open Thermo-Calc in Graphical Mode.
2. Under *Templates*, click **Precipitation Simulation**.
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 as follows. 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.



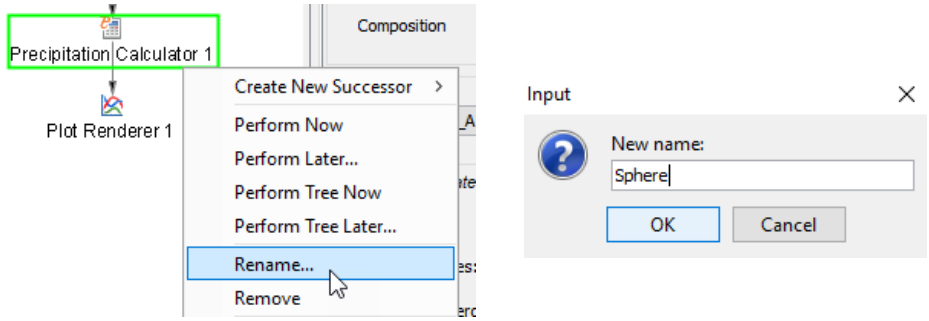
Our system is now defined. Now set up the precipitation calculations.

SETTING UP THE PRECIPITATION CALCULATIONS

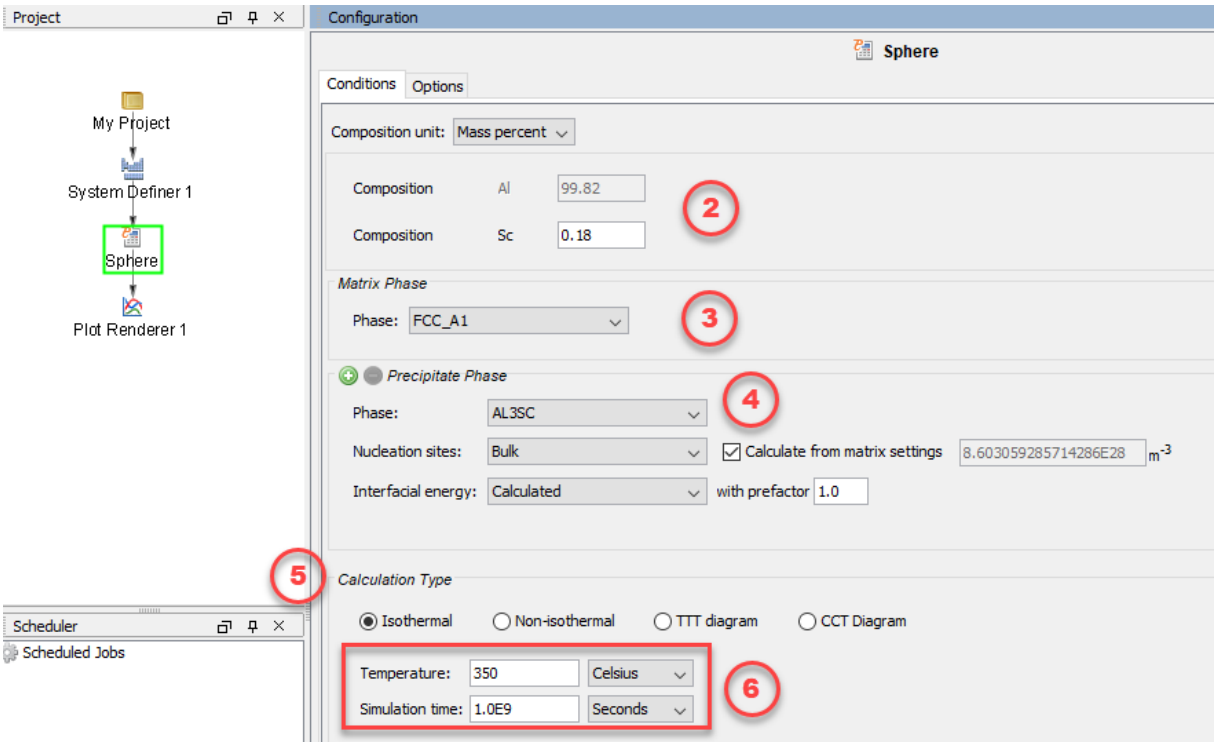
There are two precipitation calculations in this example, one assuming spherical morphology without elastic strain energy, and the other assuming cuboid morphology whose shape is determined by competition between interfacial energy and elastic strain energy. The results are then compared for both calculations.

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**.



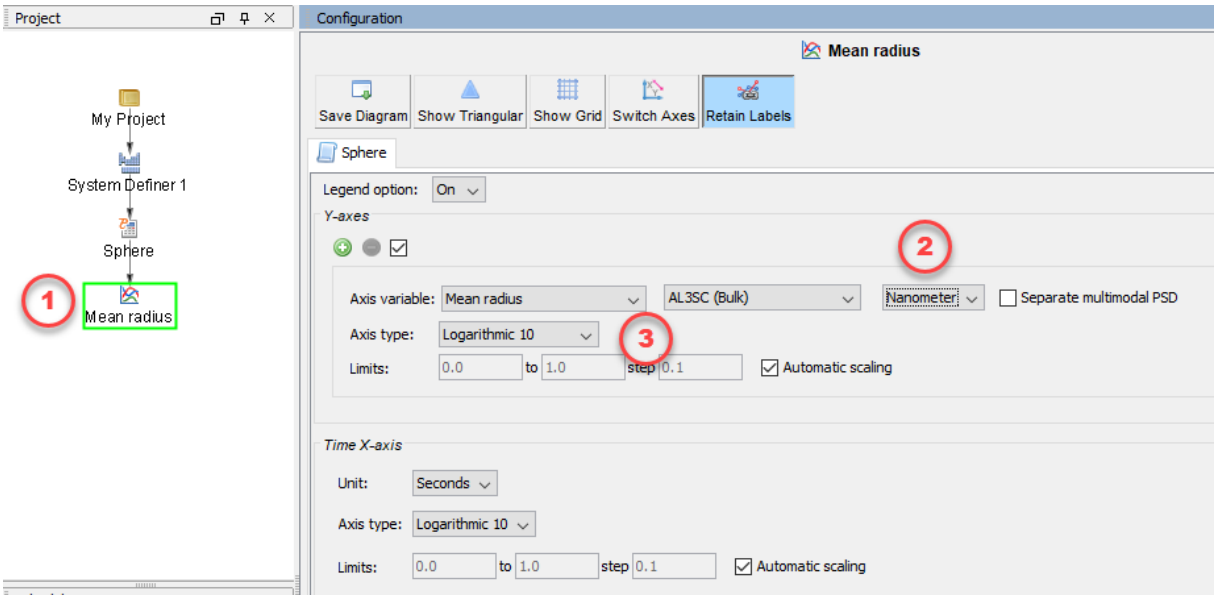
2. Notice that the composition set in the *System Definer* auto-populated on the Precipitation Calculator.
3. Under *Matrix Phase* from the *Phase* list it defaults to **FCC_A1**.
4. Under *Precipitate Phase* from the *Phase* list select **AL3SC**.
5. Under *Calculation Type*, make sure **Isothermal** is selected, which means that the same temperature is maintained throughout the calculation.
6. Enter
    a. `350` as the *Temperature* and select **Celsius**.
    b. `1.0E9` as the *Simulation time* and select **Seconds**.



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

Configuring the Plot

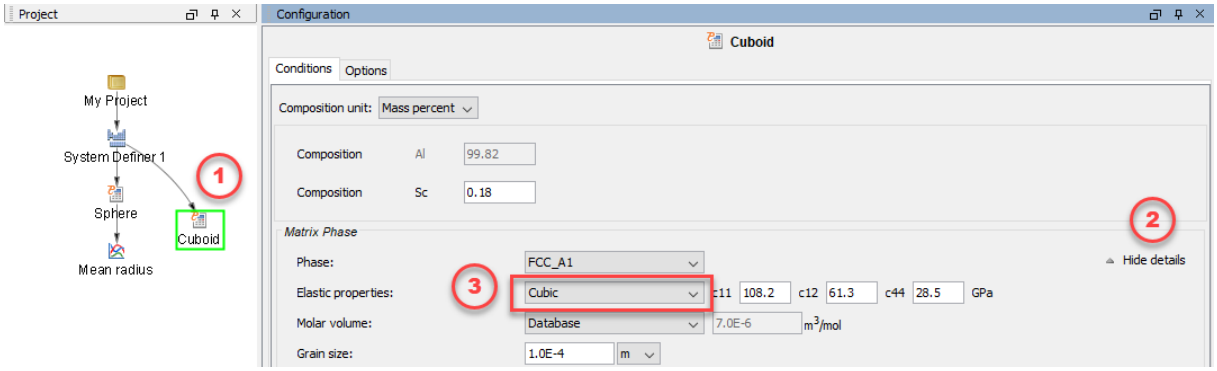
1. In the **Project** window, right-click **Plot Renderer 1** and select **Rename**. Name the plot `Mean radius` then press Enter or click **OK**.
2. Under *Y-axes* change the units to **Nanometer** (nm).
3. From the *Axis type* list select **Logarithmic 10**.



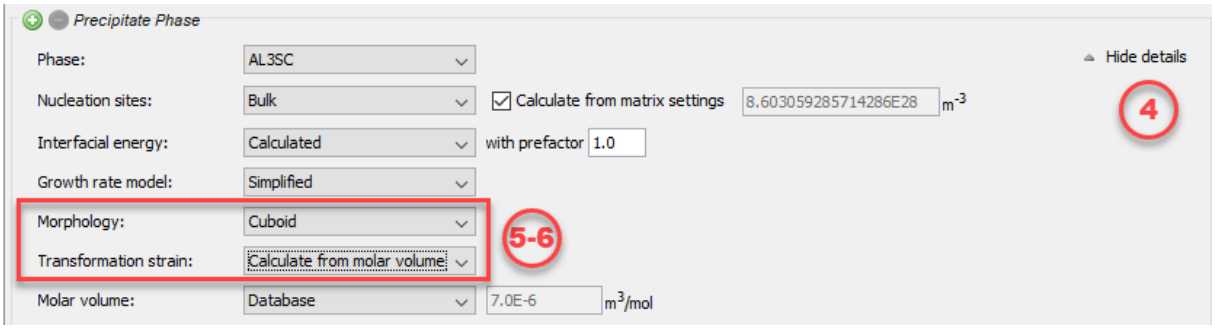
The plot is now set, but before running the simulation you set up another calculation and link it to the same Plot Renderer.

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**.
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**.

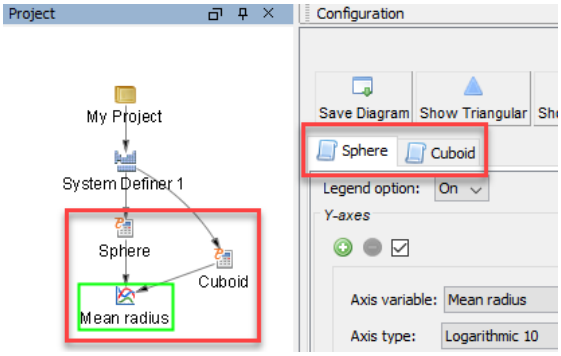


The second calculation is now set up, so now link it to the Plot Renderer node.

Linking the Plot to the Calculation with Cuboid Morphology

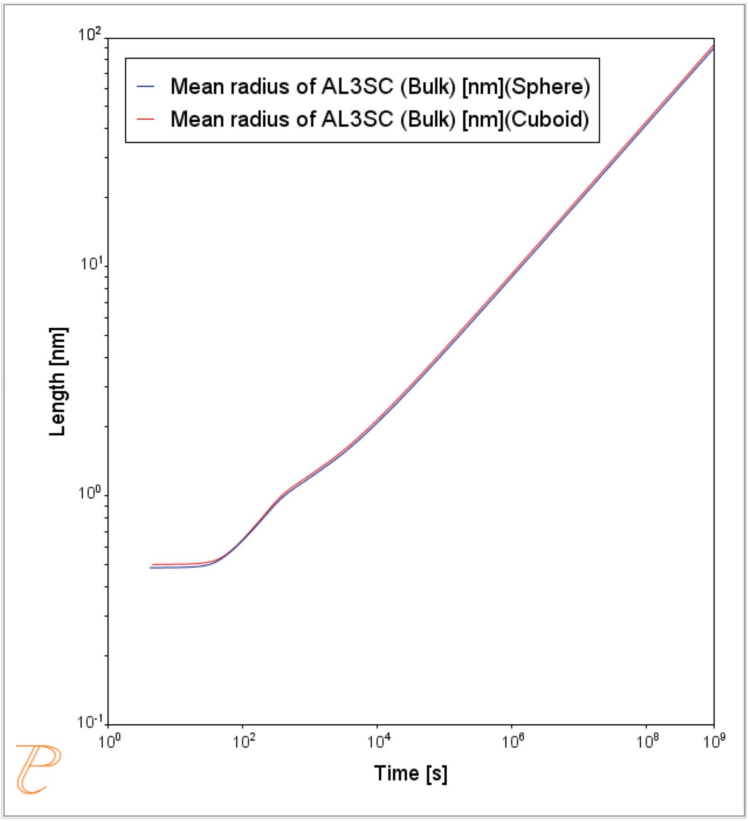
1. In the **Project** window, right-click the **Mean radius** node and select **Add Predecessor >Cuboid**.
2. Notice that in the **Configuration** window there are two tabs associated with this plot, one for **Sphere** and one for **Cuboid**. The Sphere settings are already configured, so you just need 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.

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.

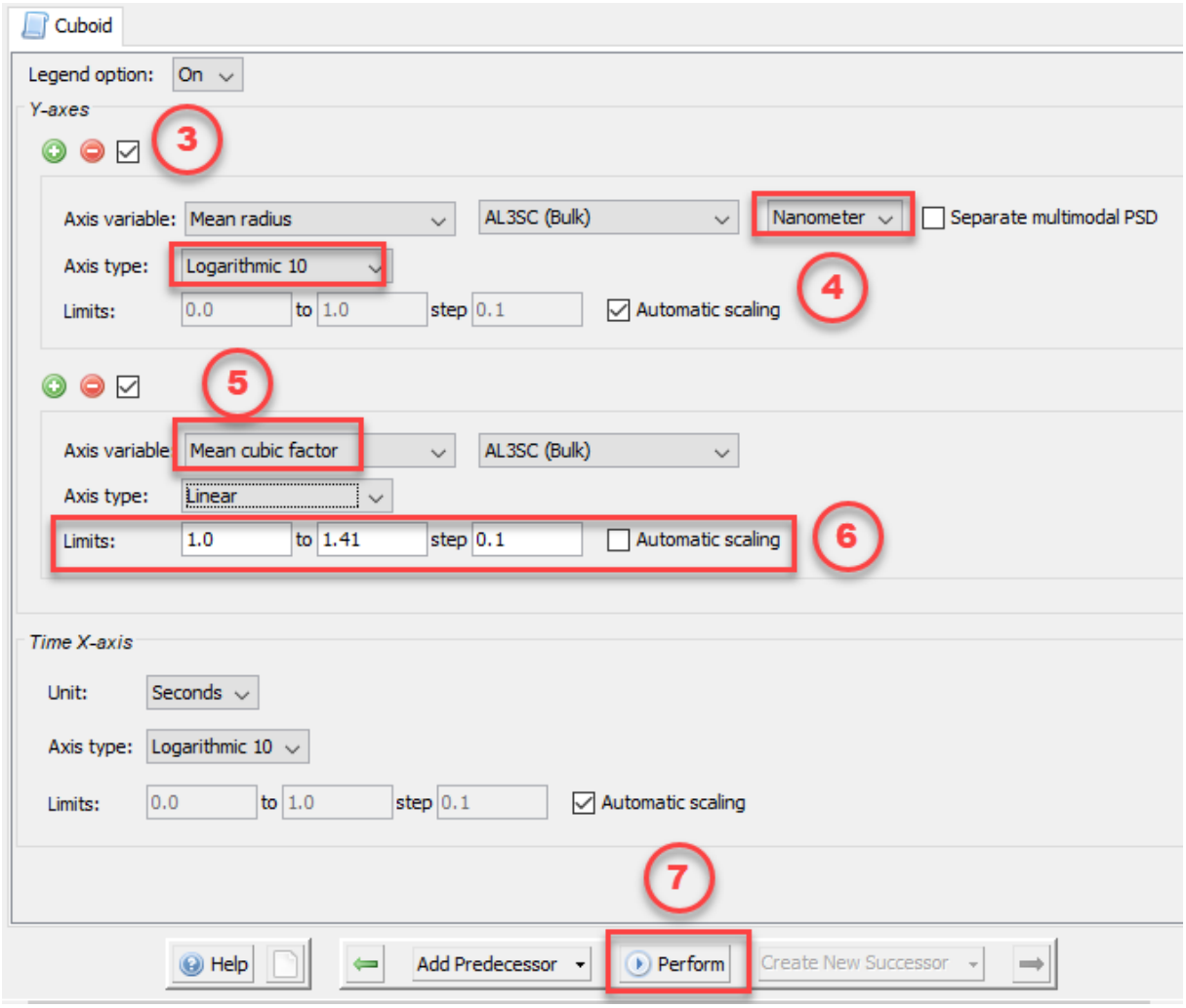
PLOTTING ADDITIONAL VARIABLES

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

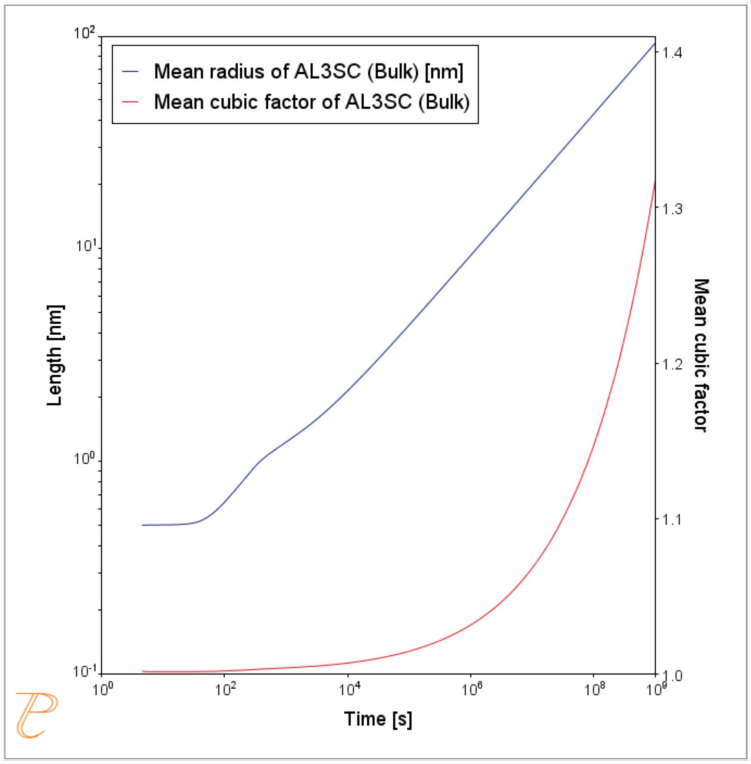
Plotting Mean Radius and Cuboid Factor

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 green plus sign to add another axis.
4. Keep *Mean radius* as the first axis variablebut change the units to **Nanometers** (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**.



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.

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.

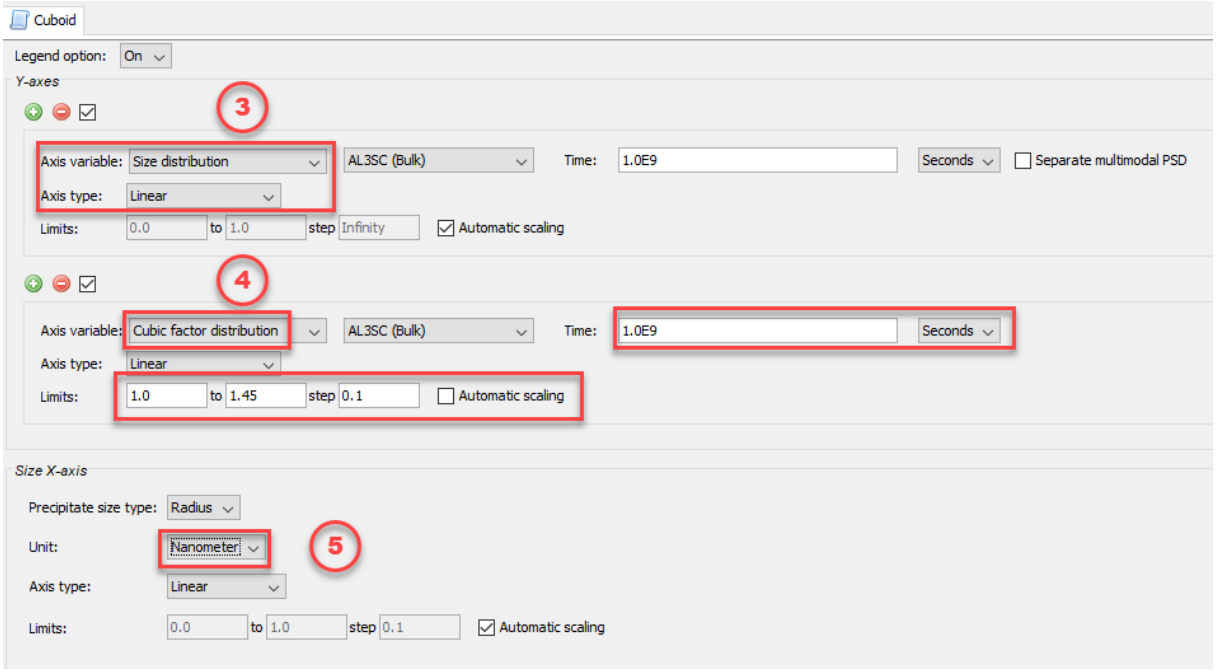
Plotting Particle Size and Cubic Factor Distribution

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

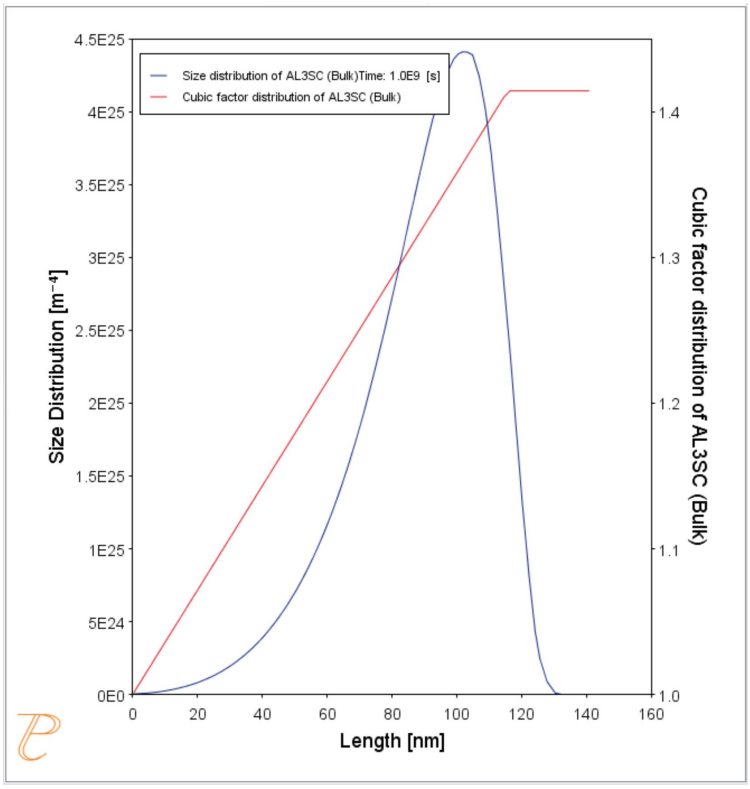
This plot also has two Y-axes, so you can clone the previous plot.

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.



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 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.

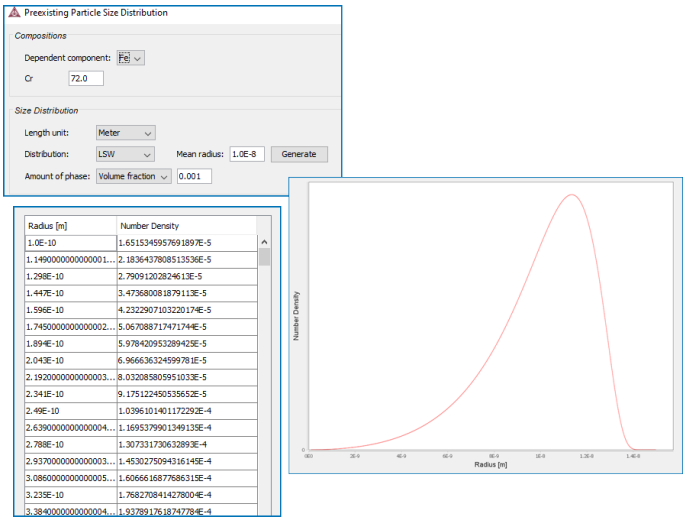


Figure 101: The Preexisting Particle Size Distribution (PSD) settings window for example P_10.

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 check box 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

Results

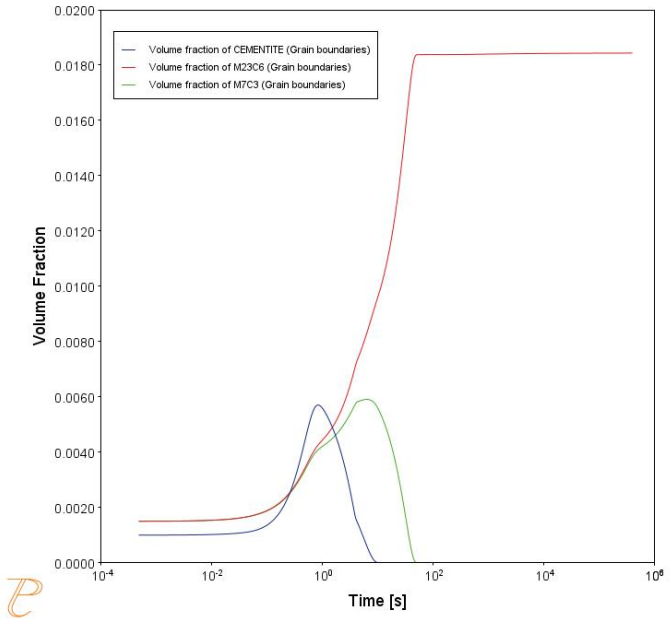


Figure 102: Volume fraction with initial particle size distribution (PSD).

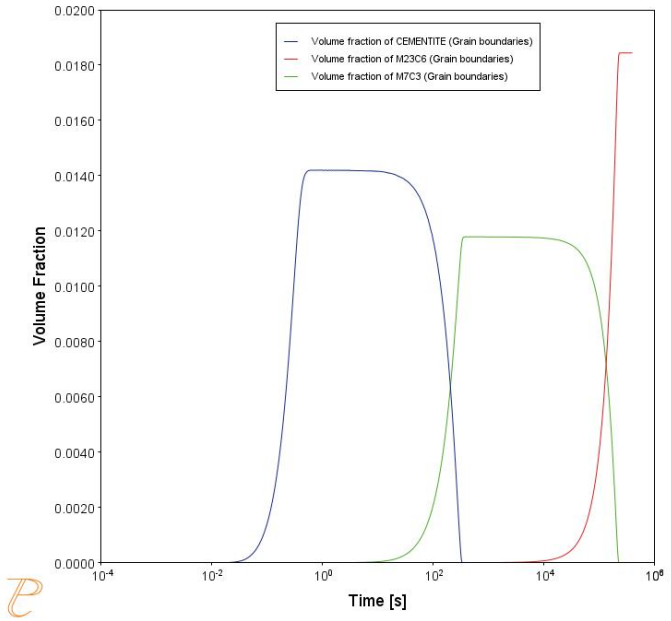


Figure 103: Volume fraction with no initial particle size distribution (PSD).

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.

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 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.

Results

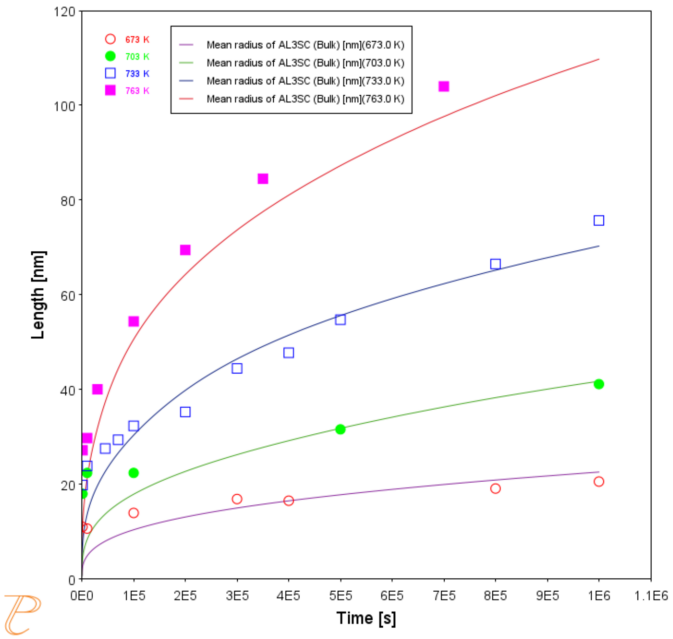


Figure 104: The results of an isothermal calculation to examine the mean radius of an Al-0.12Sc system with experimental data from [2004Iwa].

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.

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 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.

Results

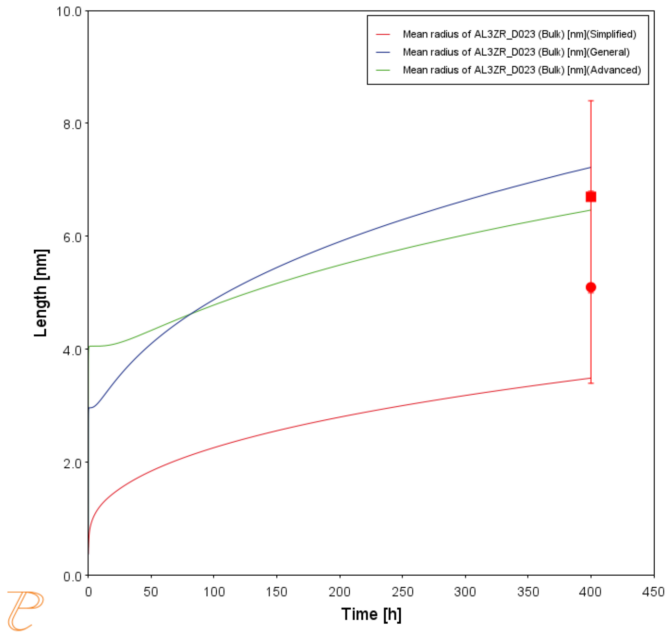


Figure 105: Result comparing the mean radius of the spheres for each AL3ZR_D023 precipitate phase calculated for each type of growth rate model.

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.

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 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.

Results

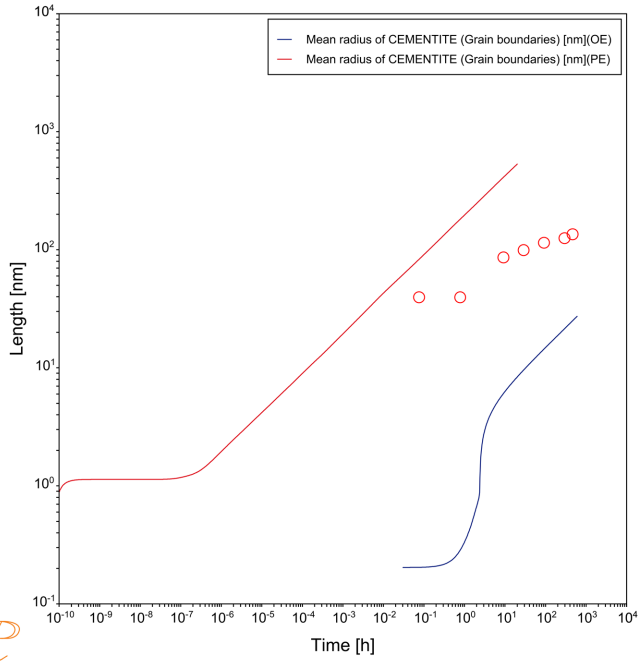


Figure 106: Comparing results from Para-eq (PE) and Simplified (OE) growth models.

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.

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.

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 adjusted interfacial energy 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 107).

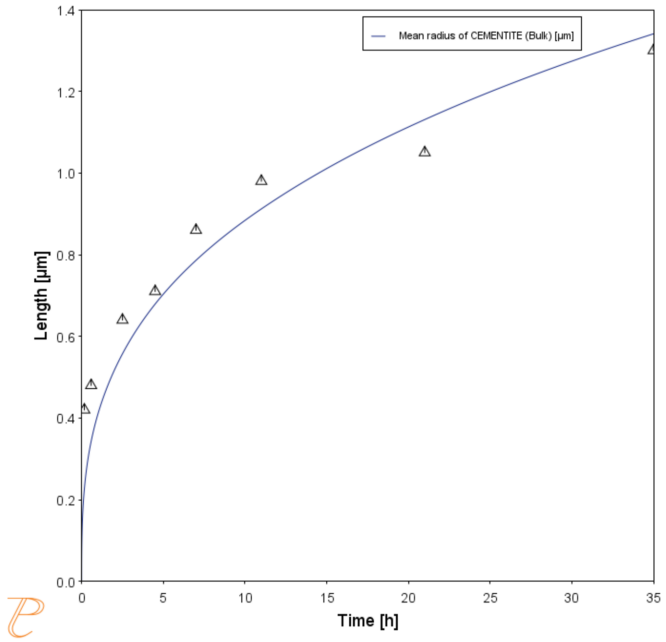


Figure 107: Result comparing the cementite mean radius to experimental data from [1975Hel].

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. The experimental grain growth data from Hellman and Hillert [1975Hel] indicates that for this commercial alloy, the grain boundary mobility should be in the magnitude of 10^{-16} m^4/Js. The closet match was from Malow and Koch [1997Mal], though their data, obtained from nanocrystalline structures, which reduce the grain boundary mobility, are underestimated for the micron scale grains. Therefore, the activation energy of 242 000 J/mol is adopted from their work, while increased the grain boundary mobility prefactor to 4 x 10^{-3} m^4/Js, which gives a grain boundary mobility of 7.9432 x 10^{-16} m^4/Js at 722 °C.

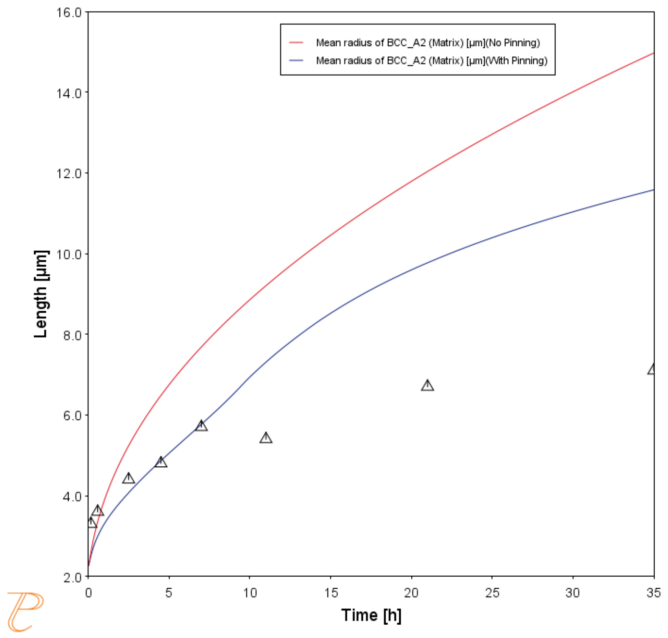


Figure 108: Result comparing the ferrite mean grain radius with and without pinning for the BCC-A2 phase and compared to experimental data [1975Hel].

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): 0.004 • Grain boundary mobility: Activation energy (J/mol): 242000 • Initial grain size distribution: Lognormal distribution with average radius 2.0 x 10^{-6} m

Precipitate phase	CEMENTITE Interfacial energy: Calculated with Prefactor 0.15
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.

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).

[1997Mal] T. R. Malow, C. C. Koch, Grain growth in nanocrystalline iron prepared by mechanical attrition. Acta Mater. 45, 2177–2186 (1997).

[1998Man] P. A. Manohar, M. Ferry, T. Chandra, Five Decades of the Zener Equation. ISIJ Int. 38, 913–924 (1998).