Graphical Mode Examples Guide

Thermo-Calc Version 2019b

Thermo-Calc Software

Thermo-Calc Software AB

Råsundavägen 18, SE-169 67 Solna, Sweden

+46 8 545 959 30

documentation@thermocalc.com

www.thermocalc.com

Contents

Graphical Mode Examples

About the Examples

This guide includes descriptions of the following examples.

Category	Example number
"Thermo-Calc Graphical Mode Examples Collection" on the next page includes binary and ternary system examples, Scheil, the Equilibrium Calculator, plus more	T_01 to T_09
"Thermo-Calc Property Model Examples Collection" on page 26: General and Steel models	General models: PM_G_01 to PM_G_03 Steel models: PM_Fe_01 to PM_Fe_03
"Process Metallurgy Examples Collection" on page 41	PMET_01 to PMET_02
"Diffusion Module (DICTRA) Graphical Mode Examples" on page 55	D_01, D_02, D_03 (the Quick Start Guide Examples) D_04 to D_07
"Precipitation Module (TC-PRISMA) Graphical Mode Examples" on page 77	P_01 to P_13

Thermo-Calc Graphical Mode Examples Collection

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 101325 Pa
- **System size** is 1 mole
- **Mass percent carbon** is 0.1%

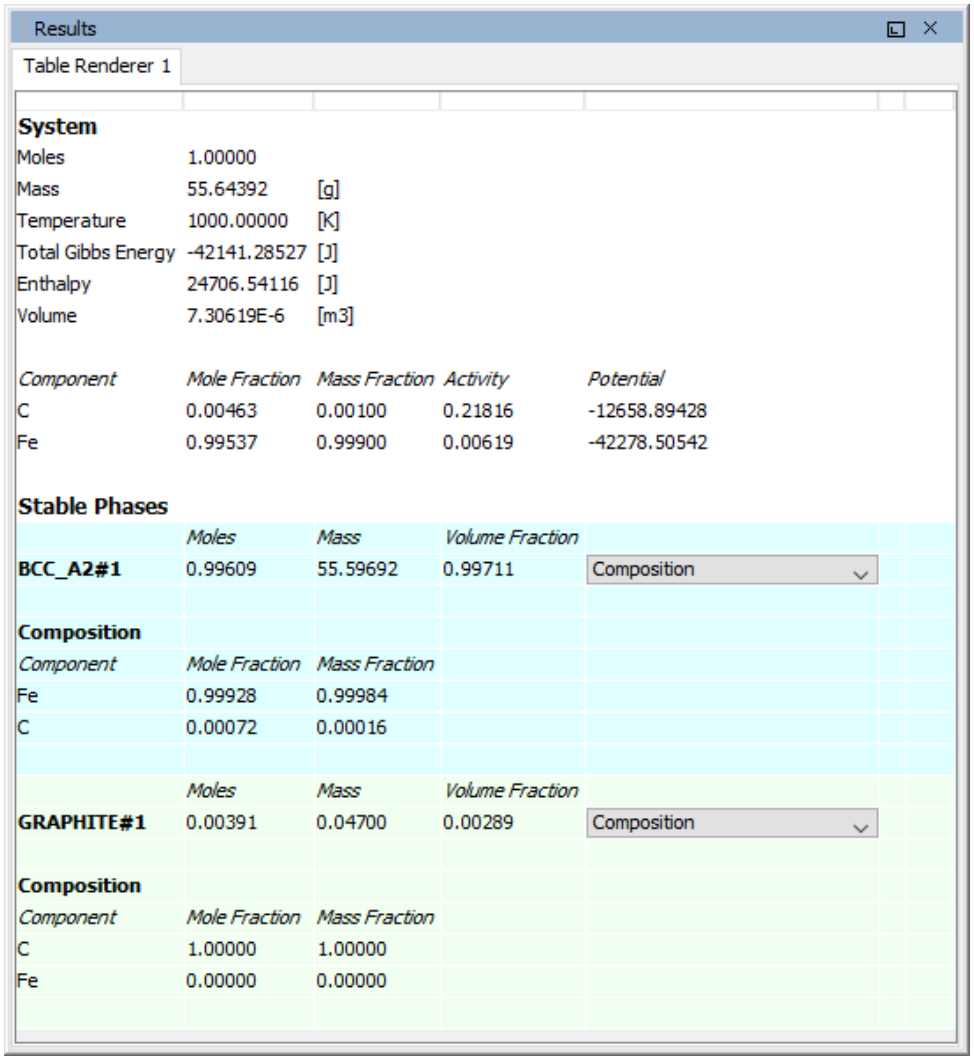
Project File and Video Tutorial Information

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

This example is included as a tutorial on our website and our YouTube channel.

TABLE RESULT

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.

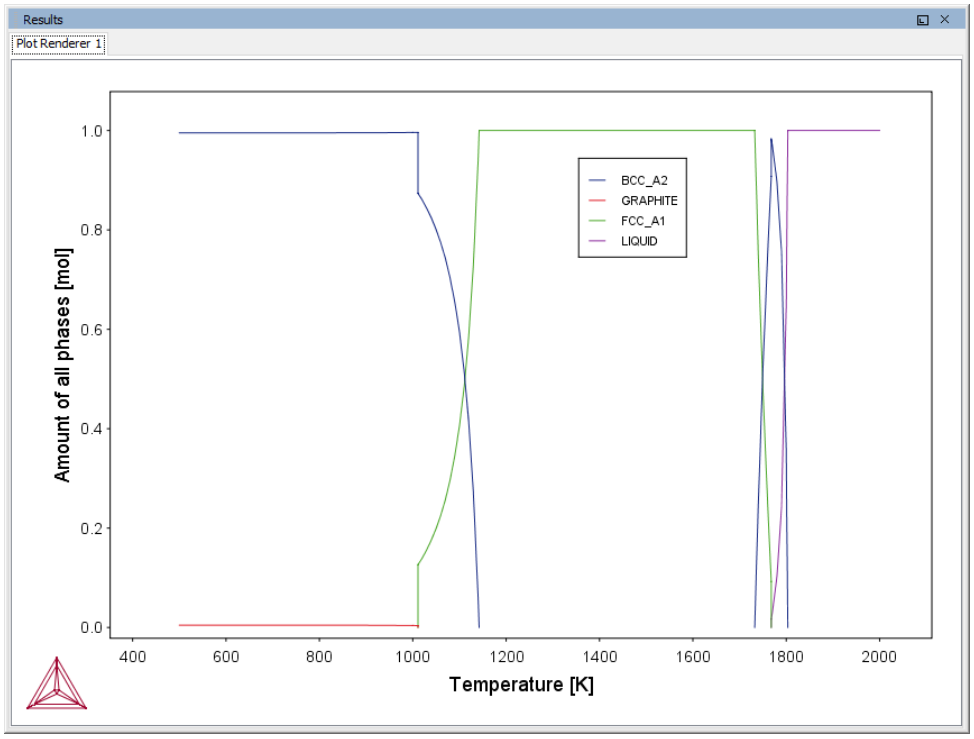
Project File and Video Tutorial Information

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

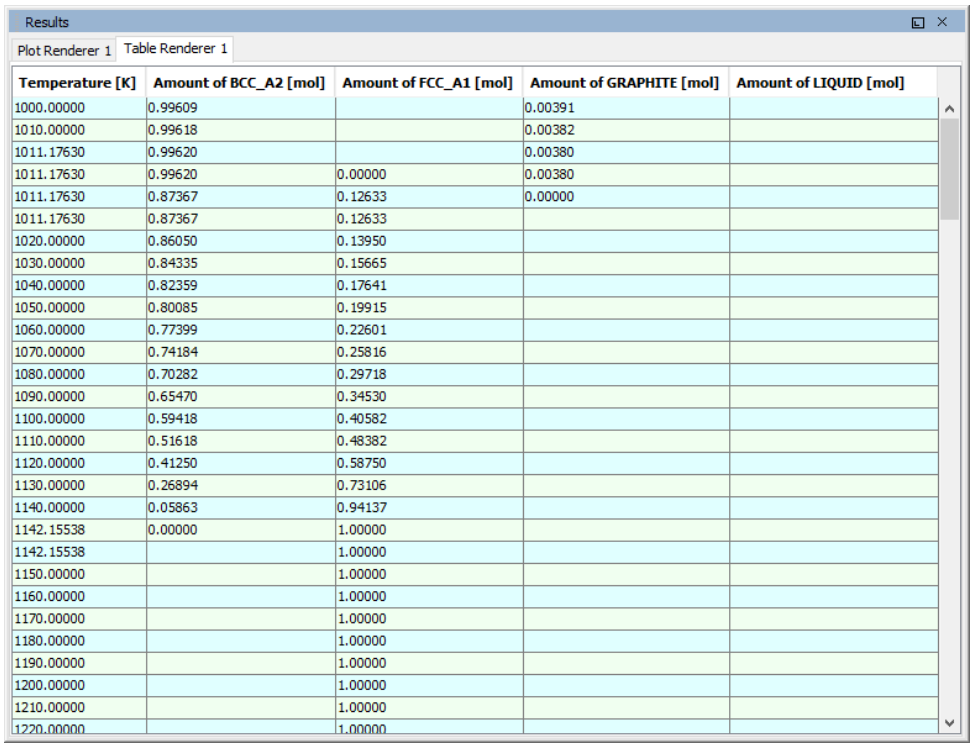
This example is included in the tutorial on our website and YouTube channel.

PLOT RESULT

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.

Project File and Video Tutorial Information

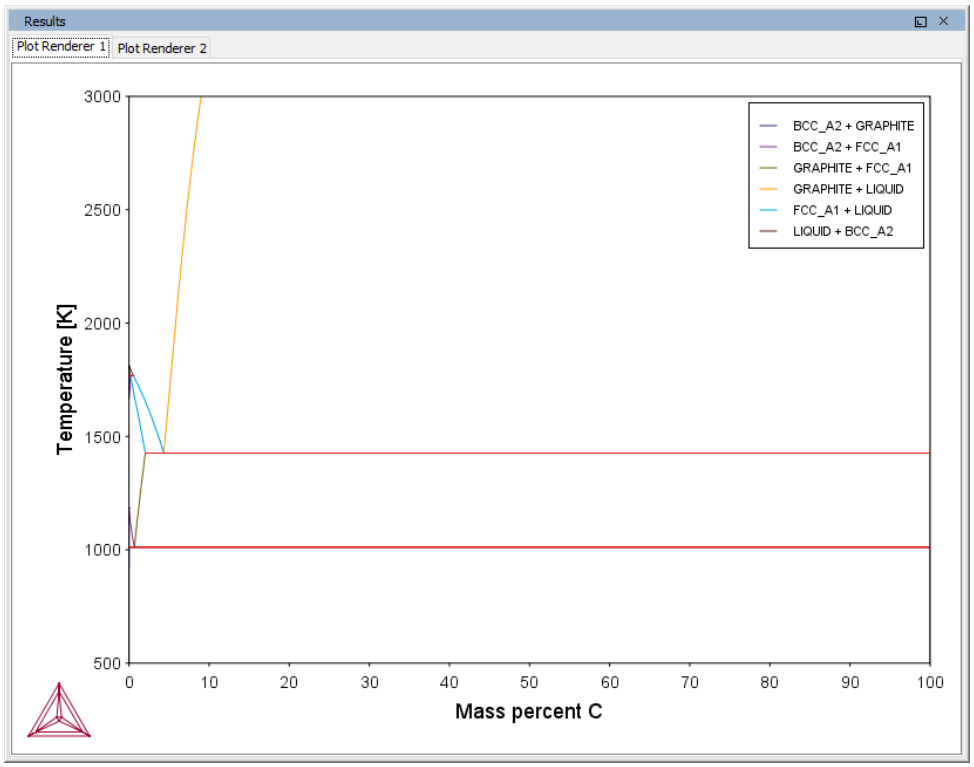
- Folder: Thermo-Calc
- File name: *T_03_Fe-C_phase_diagram.tcu*

This example is included as a tutorial on our website and our YouTube channel.

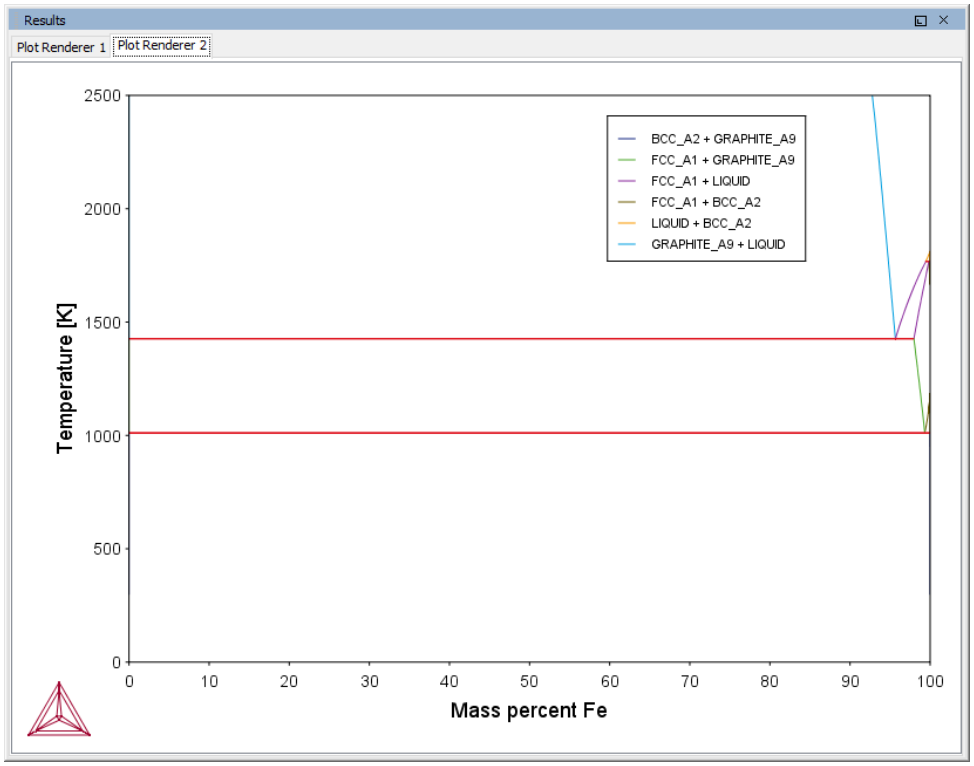
PLOT RESULTS

Equilibrium Calculator Results

This shows the plot result of the System Definer and Equilibrium Calculator system.



Binary Calculator Results



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" on page 10, the same diagram is calculated using a Ternary Calculator and then using a System Definer and Equilibrium Calculator. Two Plot Renderer activities are added to create two plots.

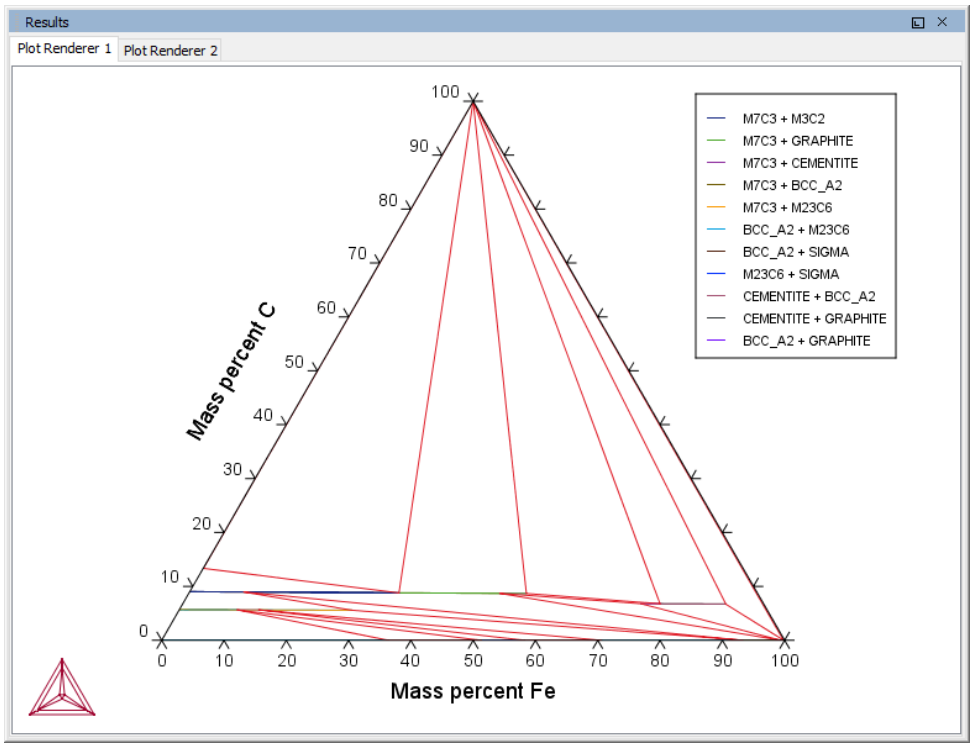
Project File and Video Tutorial Information

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

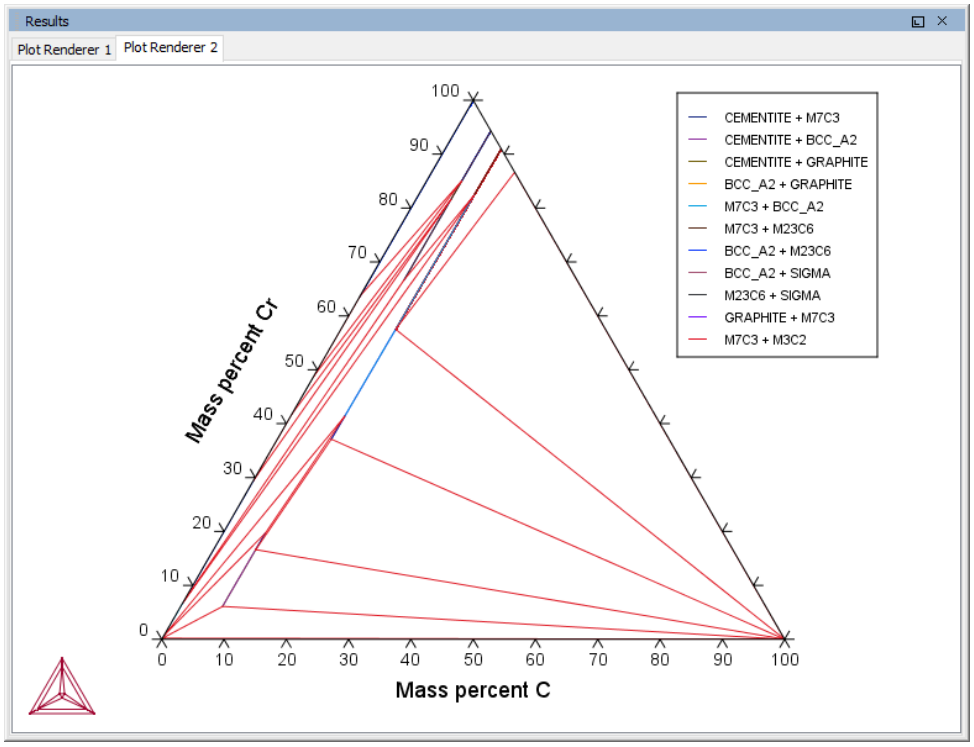
This example is included as a tutorial on our website and our YouTube channel.

PLOT RESULTS

Ternary Calculator



Equilibrium Calculator

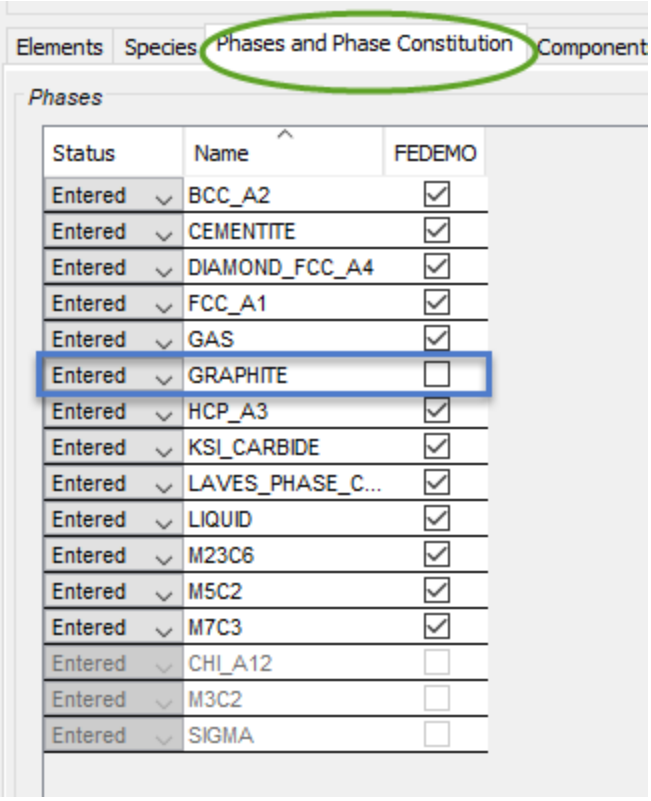


Try practicing with two features on the Plot Renderer Configuration window. To toggle between a triangular and a rectangular diagram, click the **Show Triangular** button then click **Perform** to see what happens. To toggle the X and Y axis variables, click the **Switch Axes** button and then click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

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.

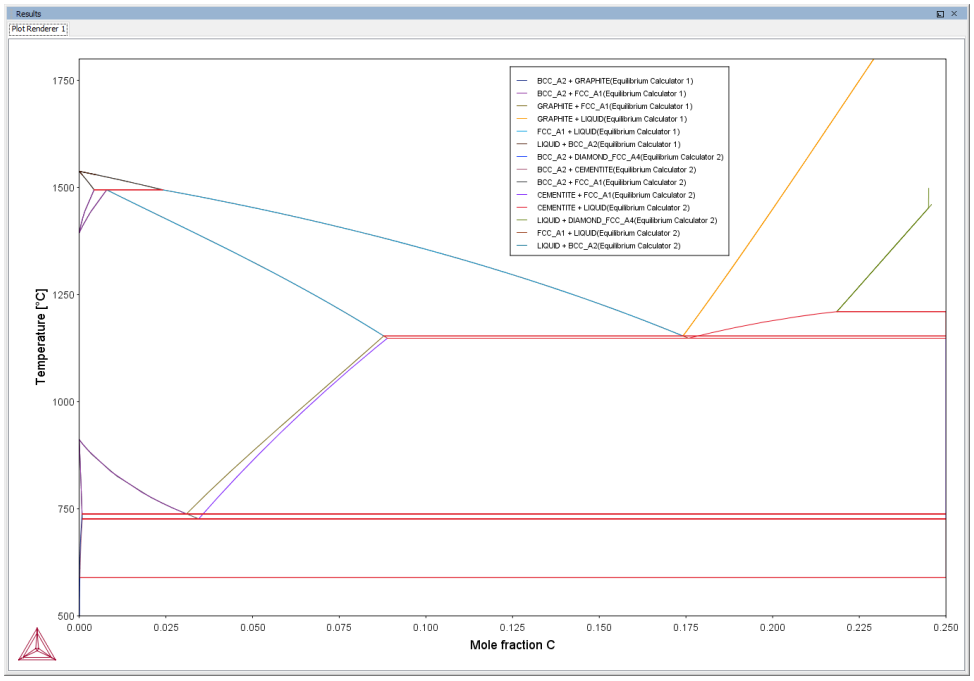
1. The Plot Renderer activity is first created as a successor to Equilibrium Calculator 1.
2. Then right-click the Plot Renderer node and select **Add predecessor** and the results from both equilibrium calculators are in the same plot. In *Equilibrium Calculator 1* the stable phase diagram is calculated 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.



Project File Name

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

PLOT RESULT



T_06: Serially Coupled Equilibrium Calculators

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

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

PROJECT FILE NAME

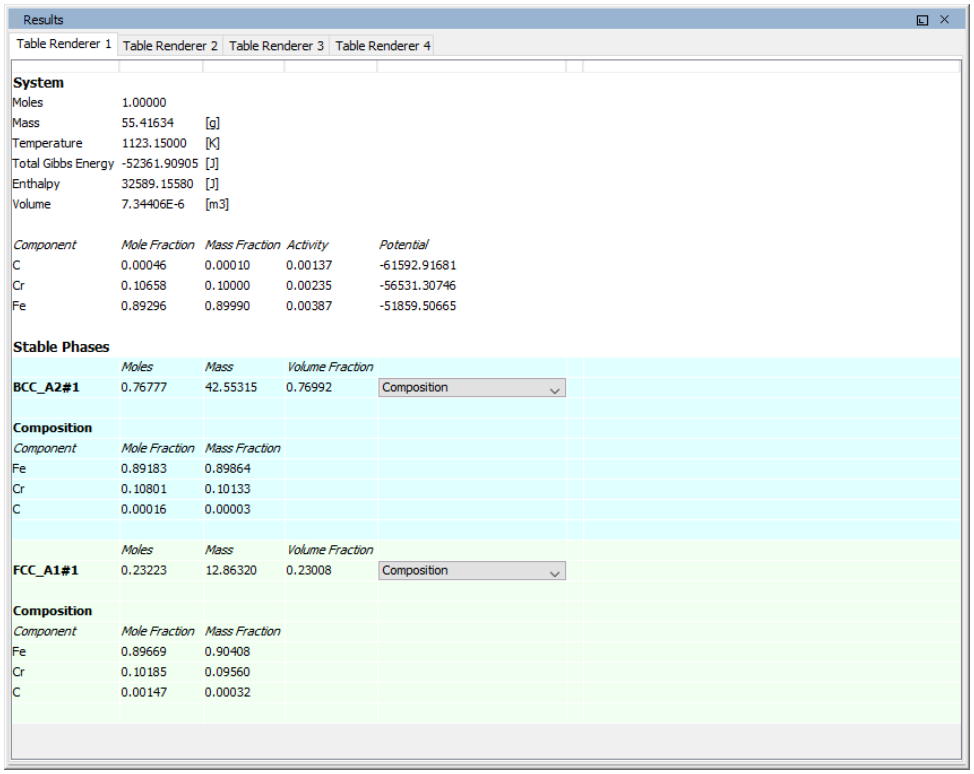
- Folder: Thermo-Calc
- File name: *T_06_Serial_equilibrium_calculators.tcu*

Table Renderer Results

Equilibrium Calculator 1

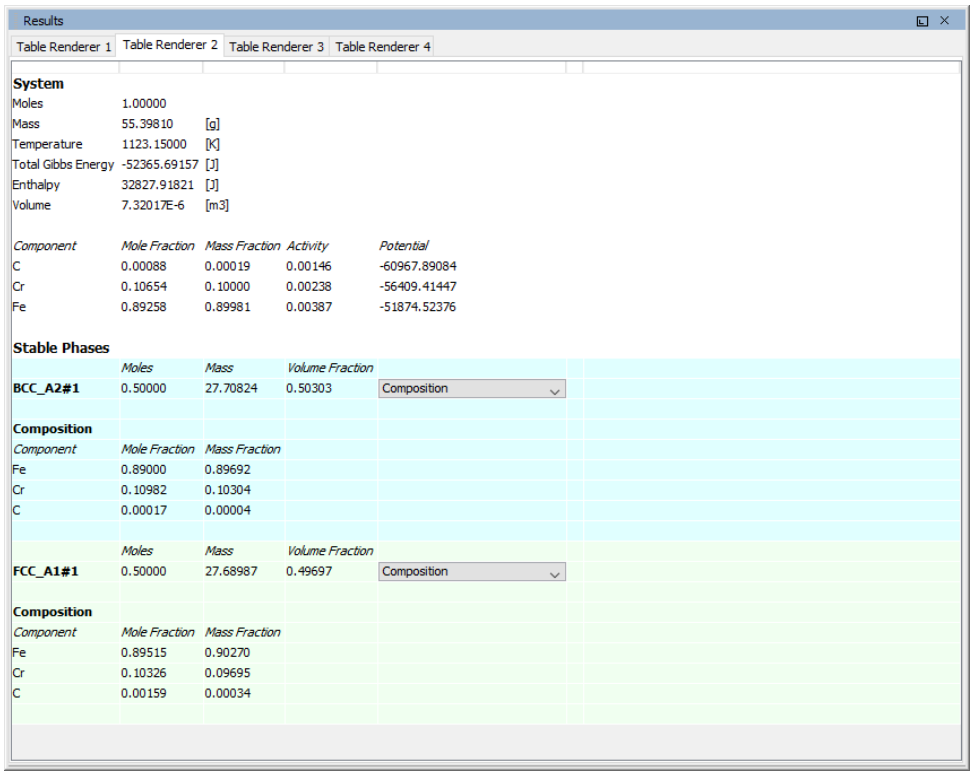
In the first example, the objective is to calculate the equilibrium at 850° C where the mole

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.



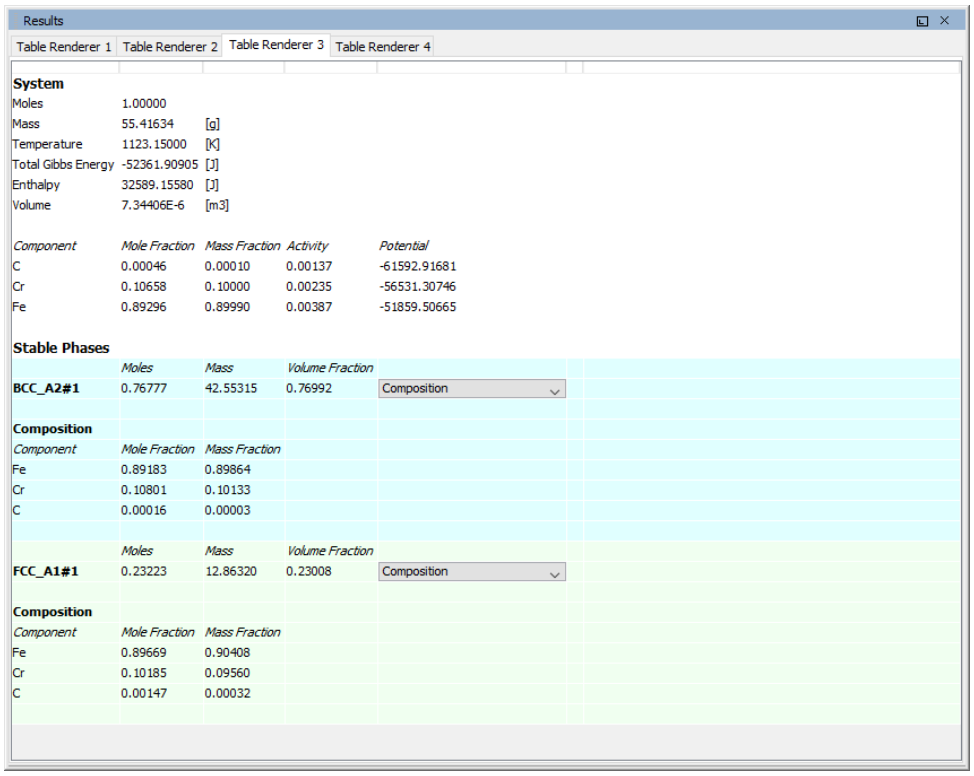
Equilibrium Calculator 2

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.



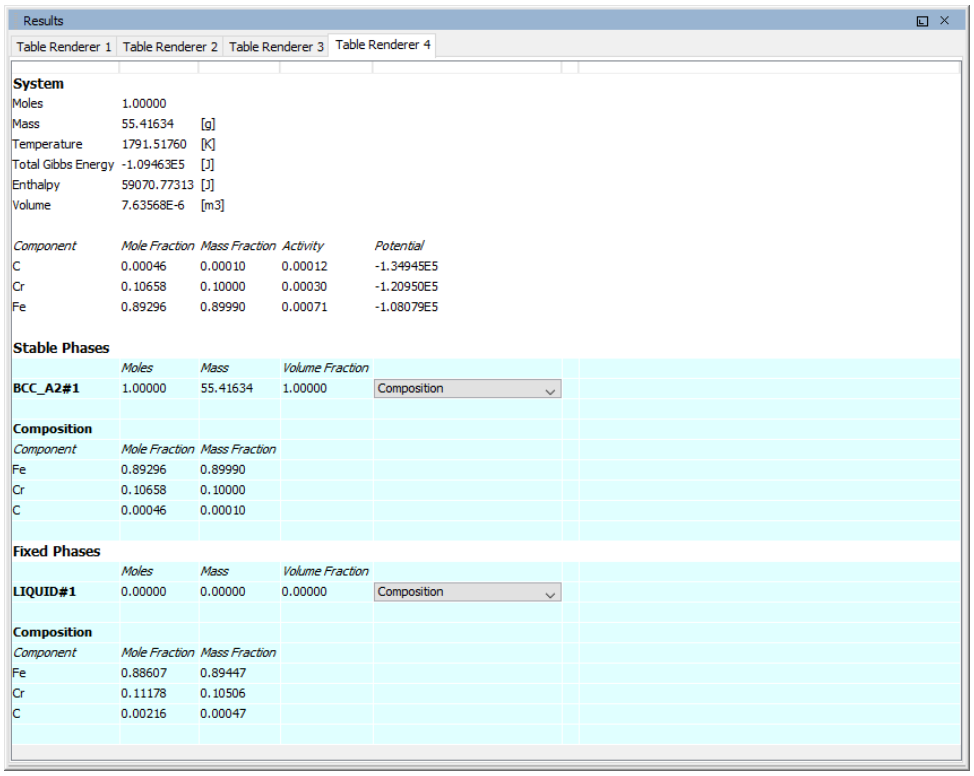
Equilibrium Calculator 3

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.

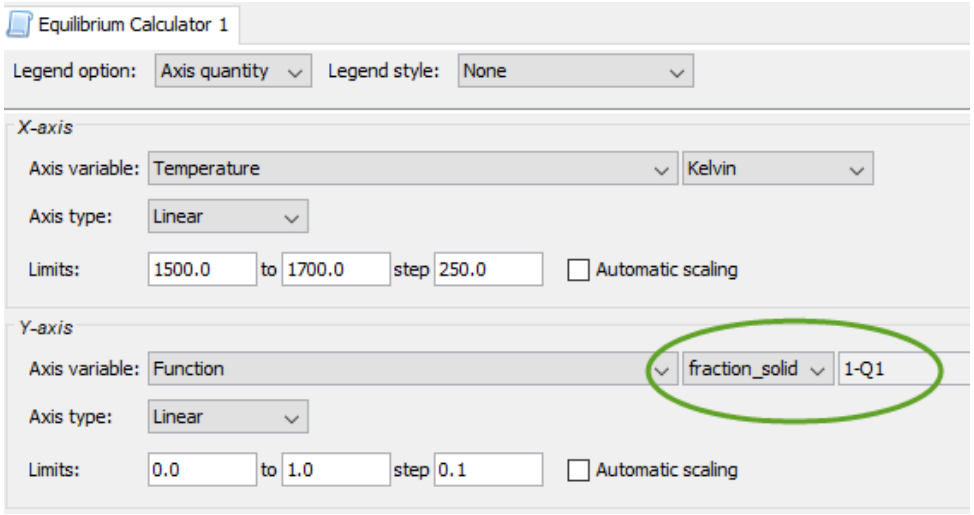
A series of equilibria for an Fe-Cr-C alloy are calculated by varying temperature between 500 and 3000 K. In the configuration window of the Equilibrium Calculator under the **Functions** tab, two identically meaning functions are defined, *fraction solid* and *f solid*, the values of which are plotted 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.

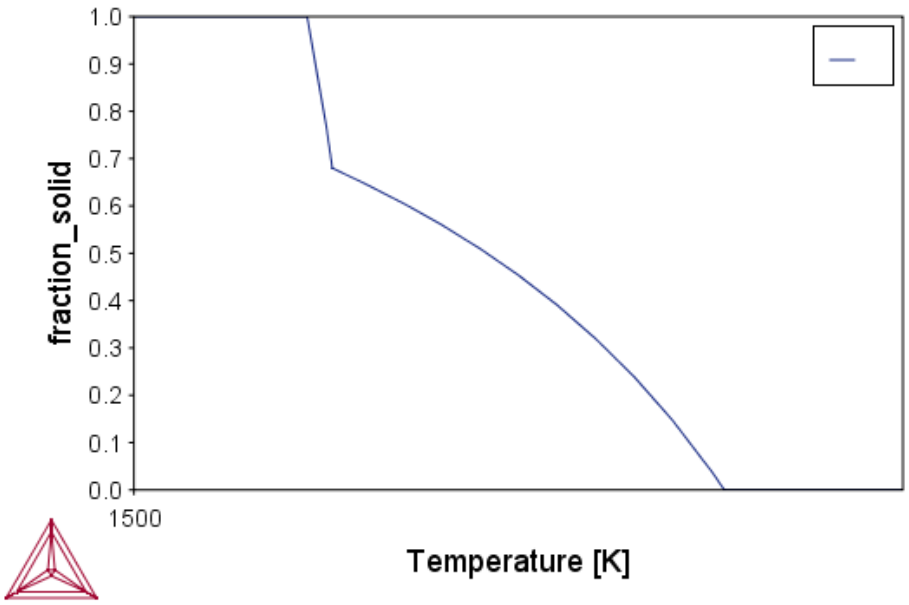
Project File Information

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

PLOT RESULT

This plot example shows the result of the fraction 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.

Project File and Video Tutorial Information

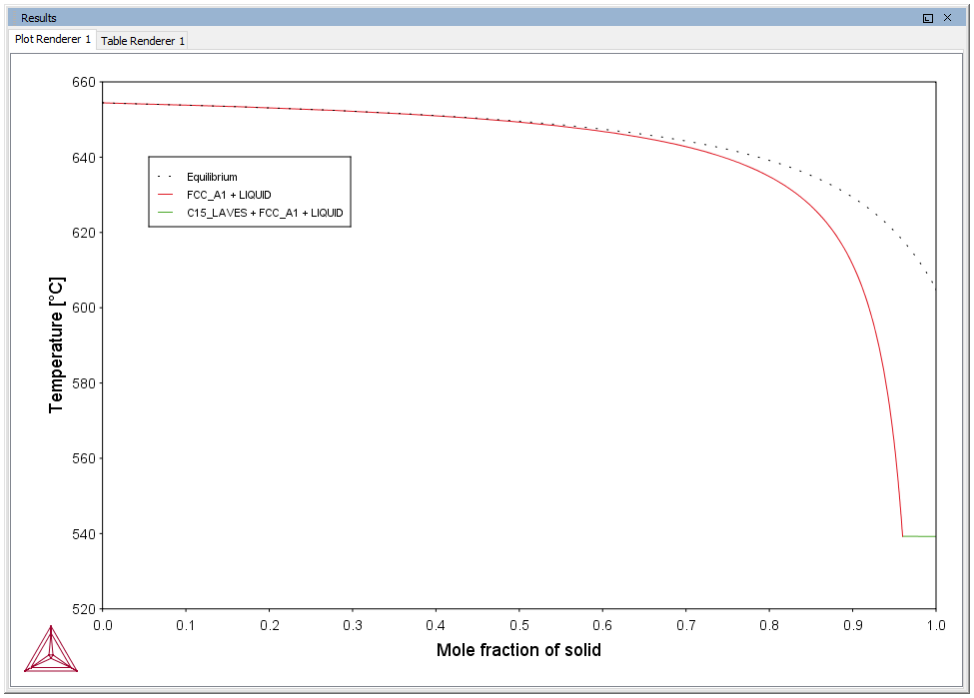
- Folder: Thermo-Calc
- File name: *T_08_Scheil_and_equilibrium_solidification.tcu*.

For other examples of using Scheil, see our website and YouTube channel:

- Modified Austenitic Stainless Steel 18/8 Scheil Solidification Simulation
- Applications to Welding and Joining with Bonus Scheil Example

TABLE AND PLOT RESULTS

The plot compares the mole fraction of a solid vs temperature. The table provides the data, which you can also export.



Results

Plot Renderer 1 | Table Renderer 1

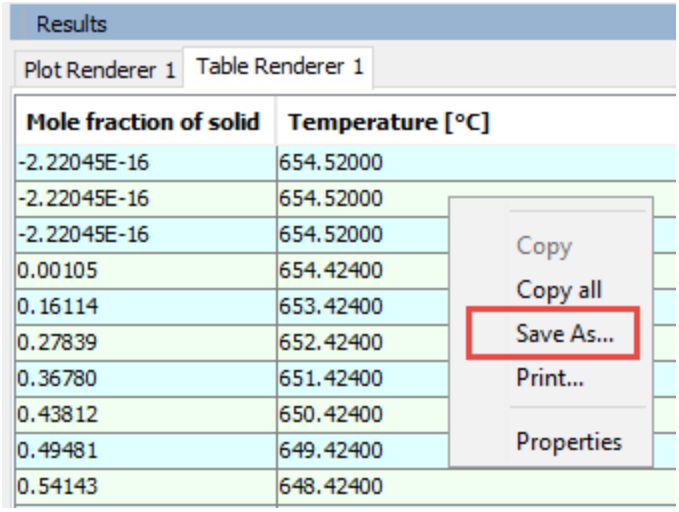
Mole fraction of solid	Temperature [°C]
-2.22045E-16	654.52000
-2.22045E-16	654.52000
-2.22045E-16	654.52000
0.00105	654.42400
0.16114	653.42400
0.27839	652.42400
0.36780	651.42400
0.43812	650.42400
0.49481	649.42400
0.54143	648.42400

To Save the Table

There are two ways to save the table.

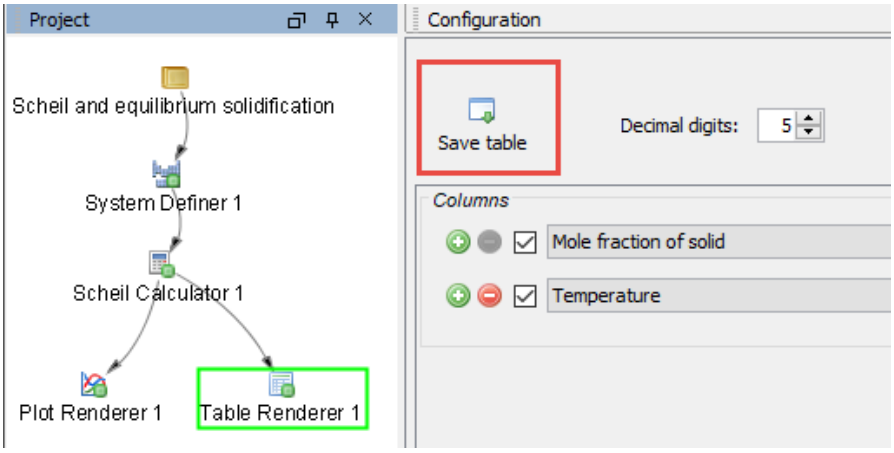
Method 1

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



Method 2

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



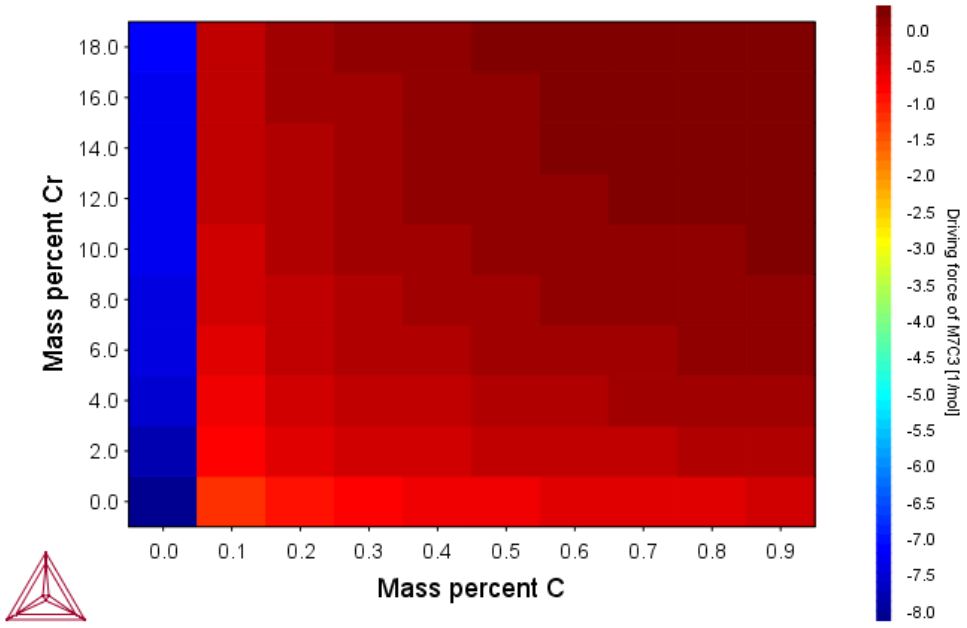
T_09: Carbide Driving Force Heat Map

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. The final plot can be either a heat map or a contour plot.

Project File Name

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

Plot Result



Thermo-Calc Property Model Examples Collection

The **General models** are available to all users. To run calculations with the **Steel models** (martensite and pearlite) requires a valid maintenance license plus licenses for both the TCFE9 and MOBFE4 databases.

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

About the Examples

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* or *probability* plot.

Phase Transition Model in the *Thermo-Calc User Guide*.

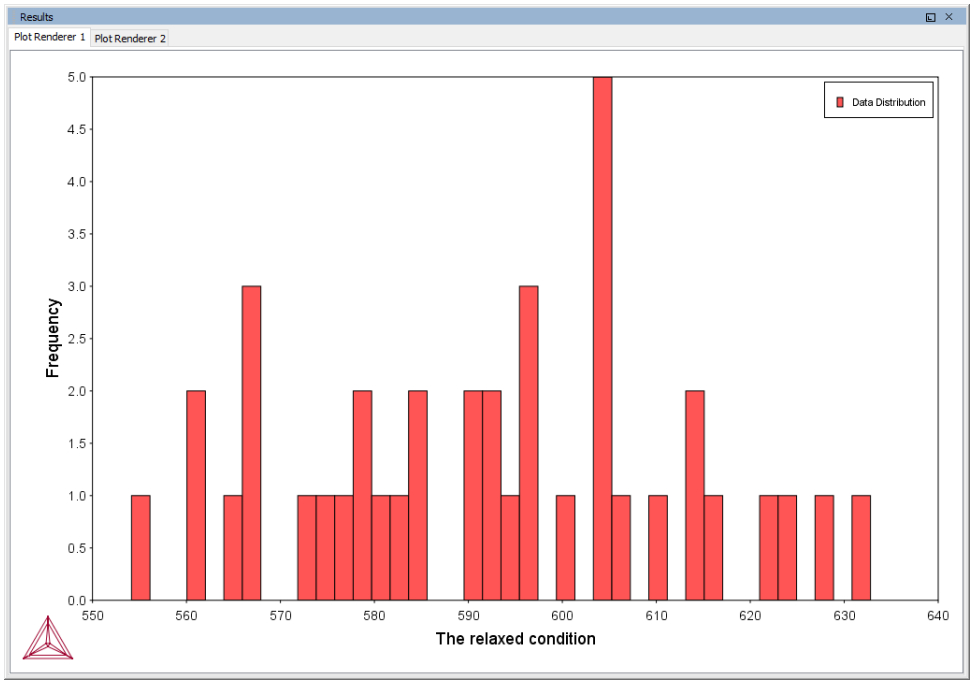
Project File and Video Tutorial Information

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

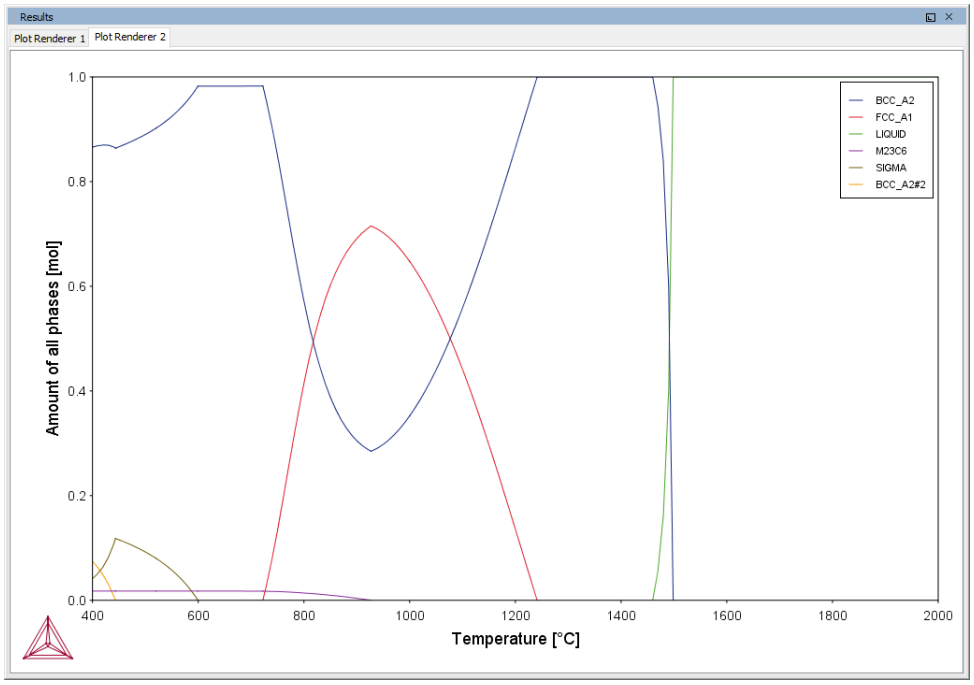
This example is included as a tutorial on our website and our YouTube channel.

PLOT RESULTS

Histogram plot



Probability plot



Experienced users can also create custom property models for use with the Property Model Calculator.

Search for Property Model Calculator and Development Framework in the help.

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.

Coarsening Model and Interfacial Energy Model

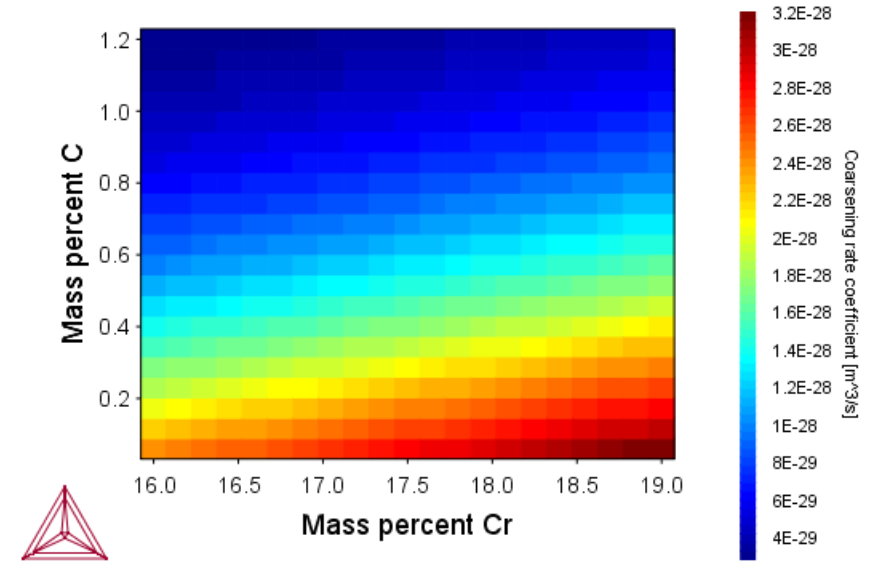
Project File and Video Tutorial Information

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

This example is included as a tutorial on our website and our YouTube channel.

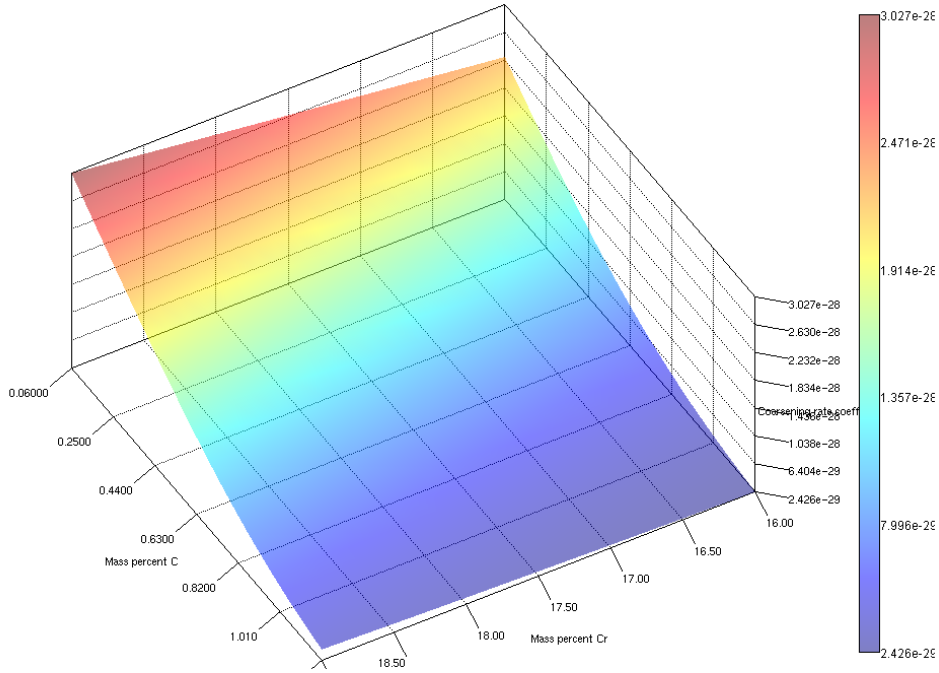
Plot Results

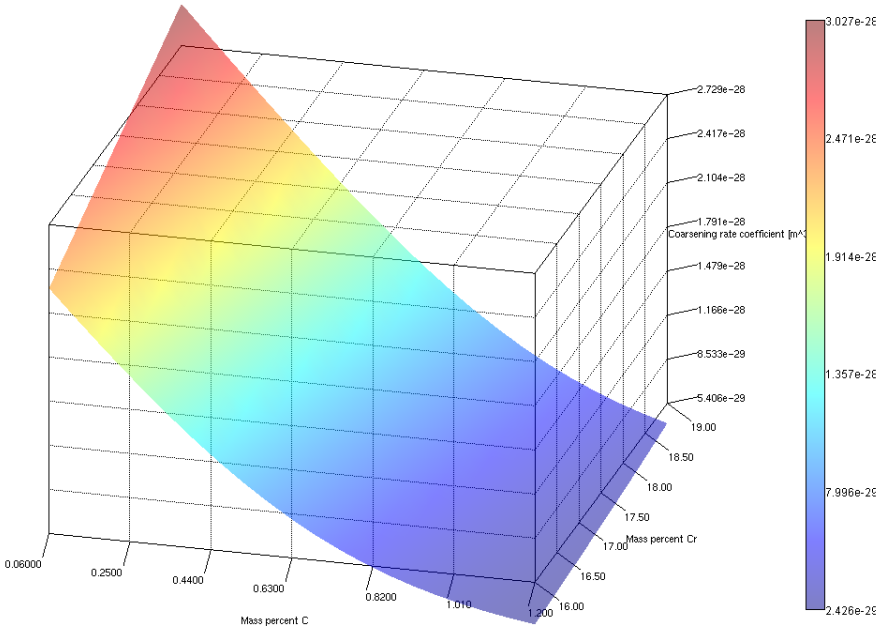
Coarsening rate coefficient (heat map)



Coarsening rate coefficient (3D plot)

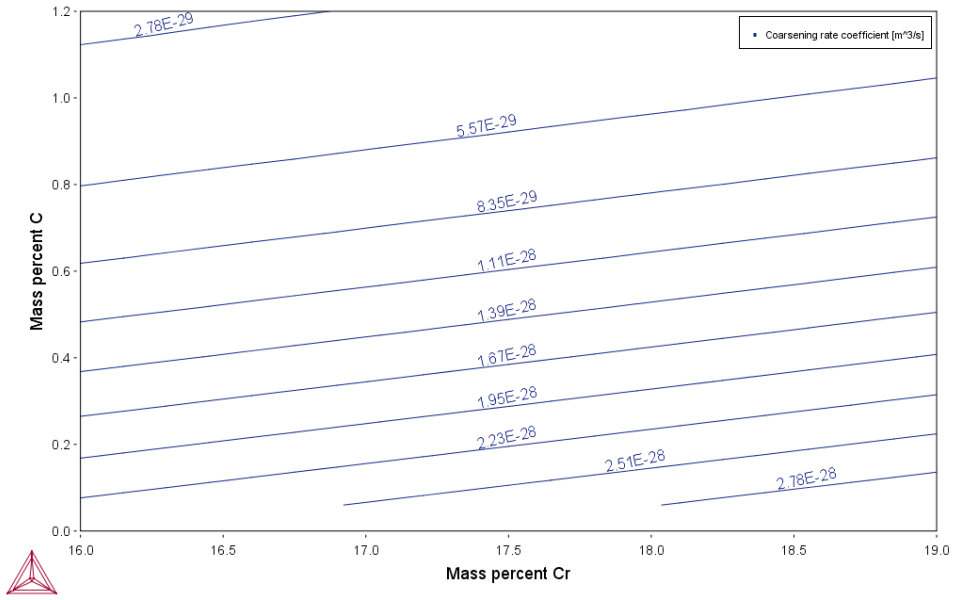
Two different rotation angles. When viewing in Thermo-Calc you can rotate the plot.



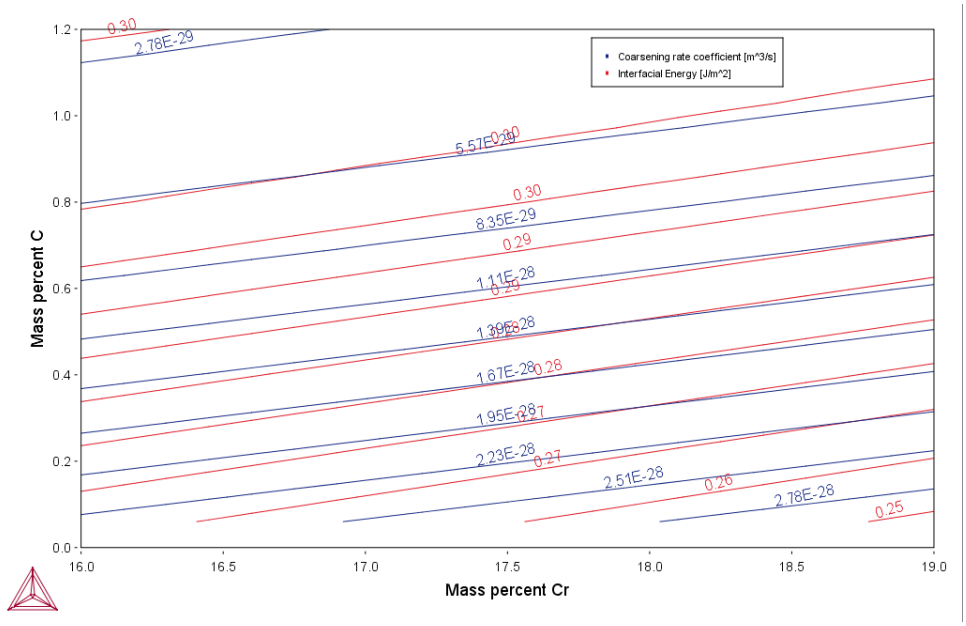


Coarsening rate coefficient (contour plot)

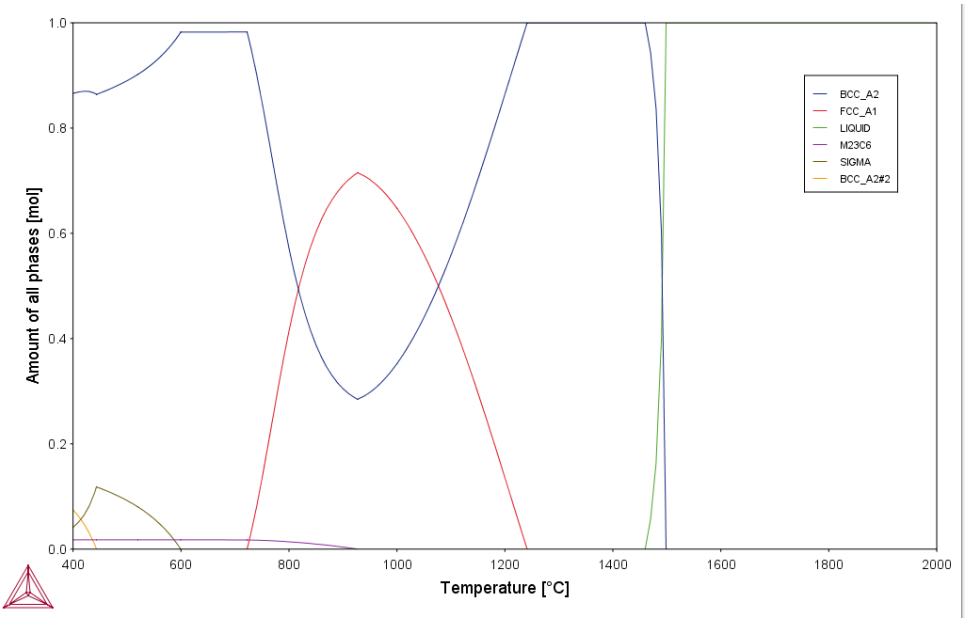
Coarsening rate coefficient



Coarsening rate coefficient and Interfacial energy (overlayed plots)



Phase fractions vs T (One axis)



Experienced users can also create custom property models for use with the Property Model Calculator.

Search for Property Model Calculator and Development Framework in the help.

PM_G_03: Driving Force and Interfacial Energy

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

Driving Force Model and Interfacial Energy Model in the *Thermo-Calc User Guide*.

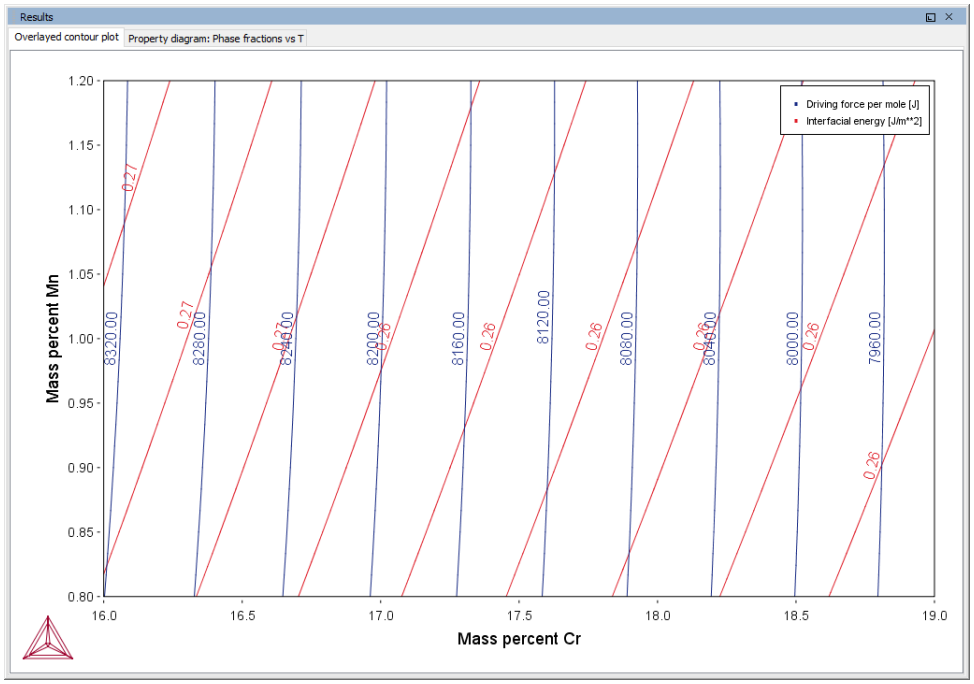
Project File and Video Tutorial Information

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

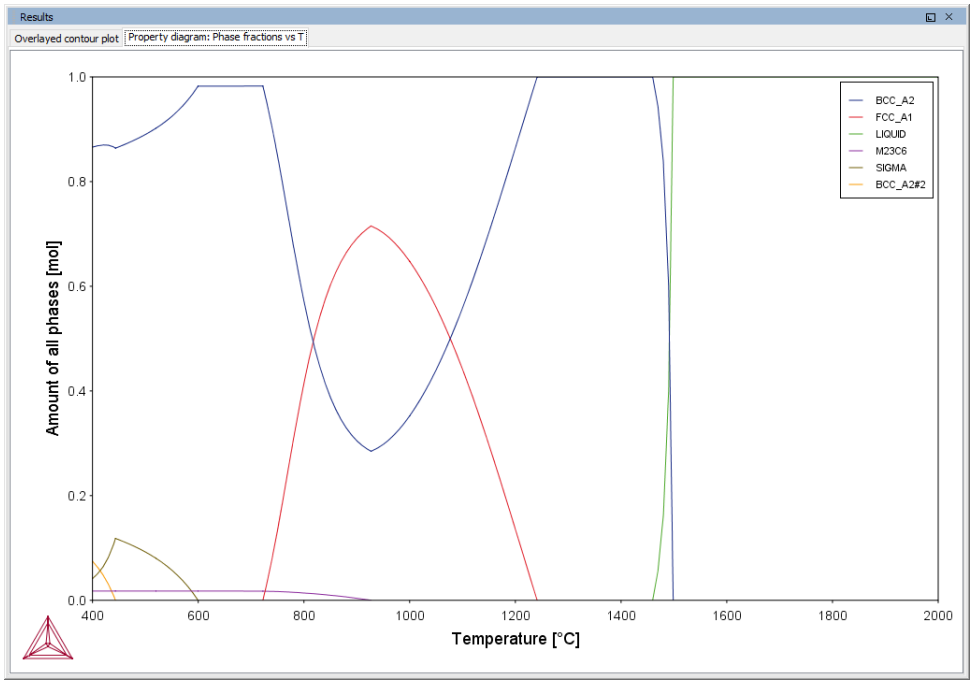
This example is included as a tutorial on our website and our YouTube channel.

PLOT RESULT

A contour plot



Phase Fraction



Experienced users can also create custom property models for use with the Property Model Calculator.

Search for Property Model Calculator and Development Framework in the help.

PM_Fe_01: Fe-Cr-C Martensite with Intercritical Annealing

To run calculations with the **Steel models** (martensite and pearlite) requires a valid maintenance license plus licenses for both the TCFE9 and MOBFE4 databases.

The example uses the Property Model Calculator with the **Martensite Fractions** and **Martensite Temperatures** models.

The example shows how 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.

Reference

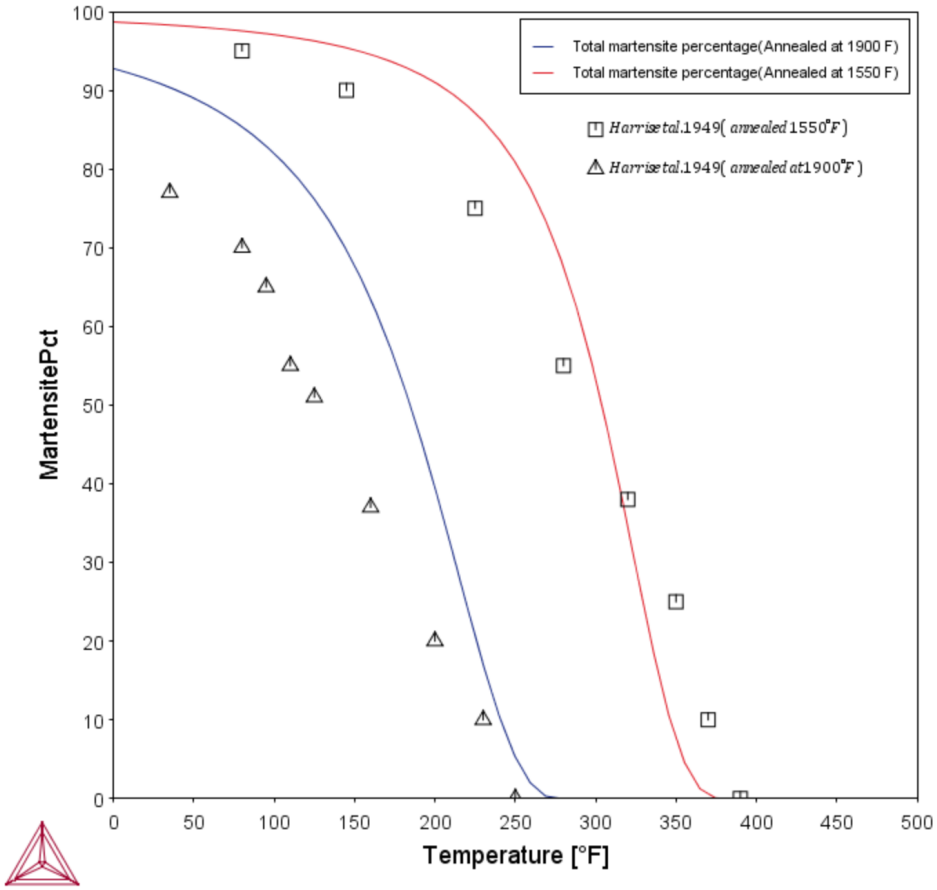
Harris, William J, and Morris Cohen. 1949. “Stabilization Of The Austenite-Martensite Transformation.” *Transactions of the American Society for Metals, AIME* 180: 447–70.

Project File Information

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

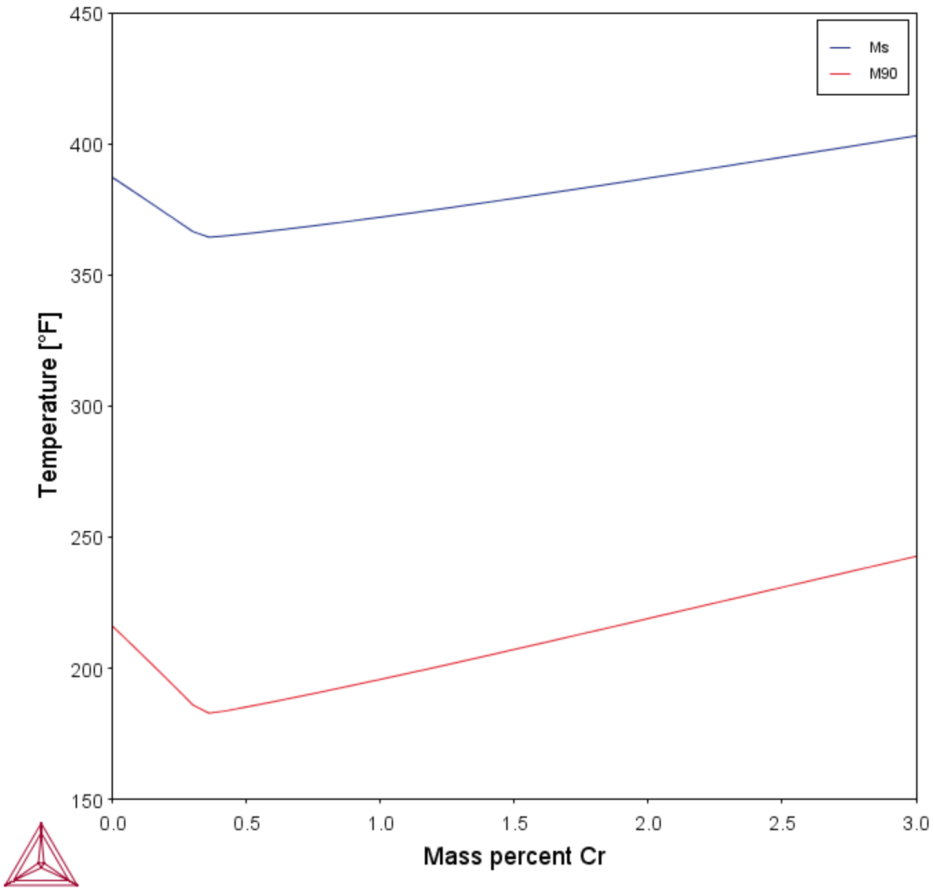
Plot Results

Transformation curves



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

Ms-Mf



PM_Fe_02: Fe-Mn Martensite Morphologies

To run calculations with the **Steel models** (martensite and pearlite) requires a valid maintenance license plus licenses for both the TCFE9 and MOBFE4 databases.

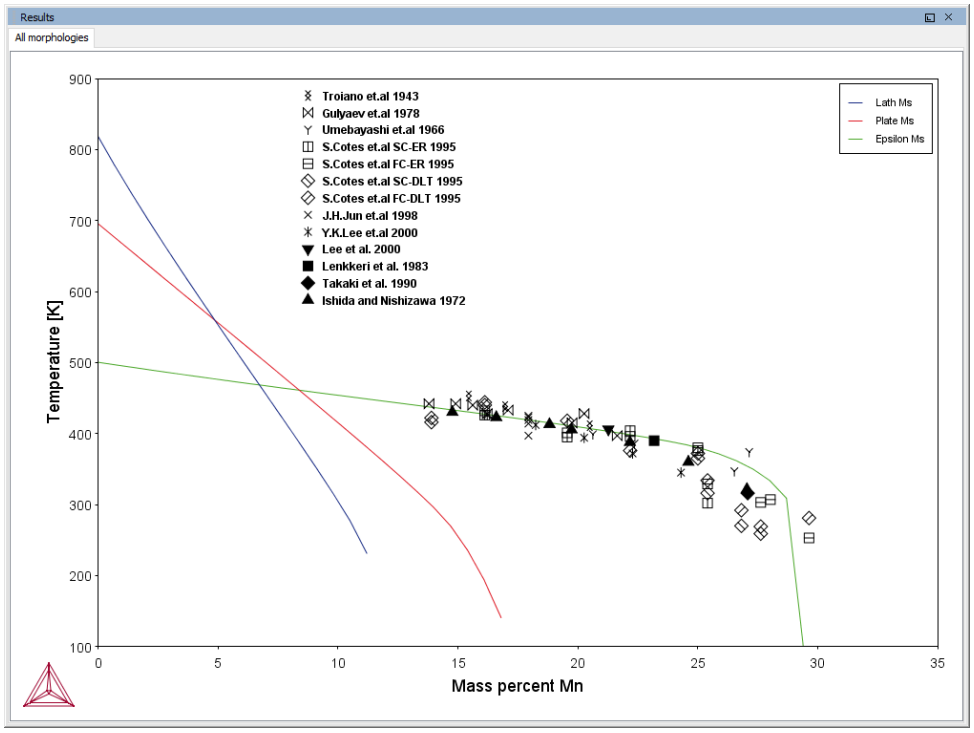
The example uses the Property Model Calculator with the **Martensite Temperatures** model. It shows the Ms temperatures of different types of martensites: lath, plate, and ε (hcp), compared with experimental ε Ms values.

Project File Information

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

Plot Result

All morphologies



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

To run calculations with the **Steel models** (martensite and pearlite) requires a valid maintenance license plus licenses for both the TCFE9 and MOBFE4 databases.

The example uses the Property Model Calculator with the **Pearlite** model.

The example 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.

Reference

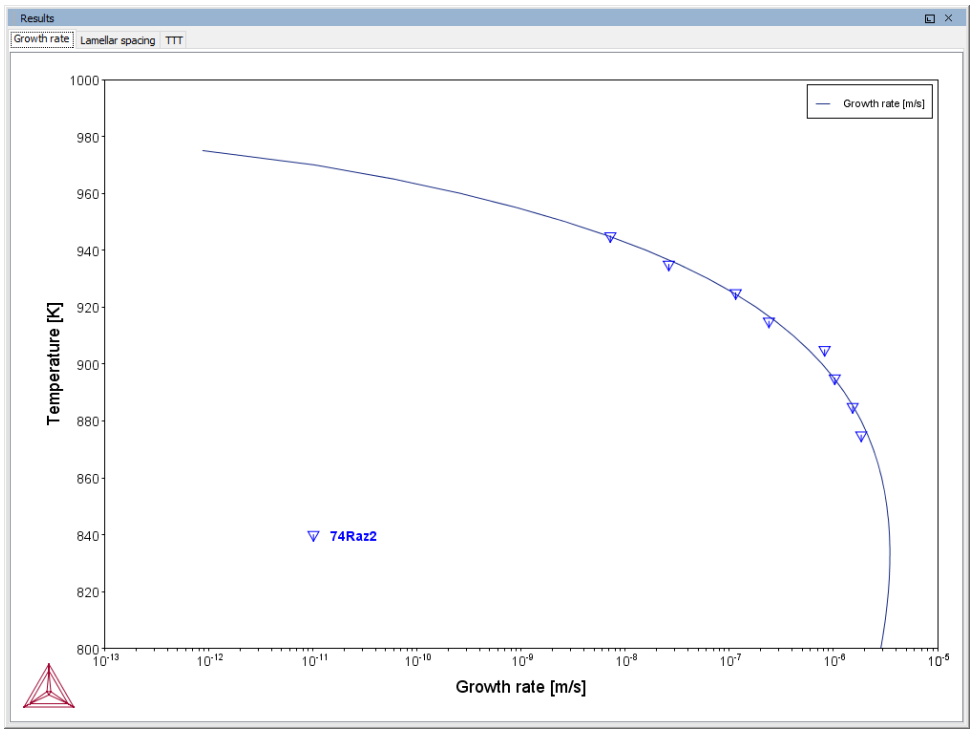
Razik, N.A, G.W. Lorimer, and N Ridley. 1974. “An Investigation of Manganese Partitioning during the Austenite-Pearlite Transformation Using Analytical Electron Microscopy.” Acta Metallurgica 22 (10): 1249–58. doi:10.1016/0001-6160(74)90138-2.

Project File Information

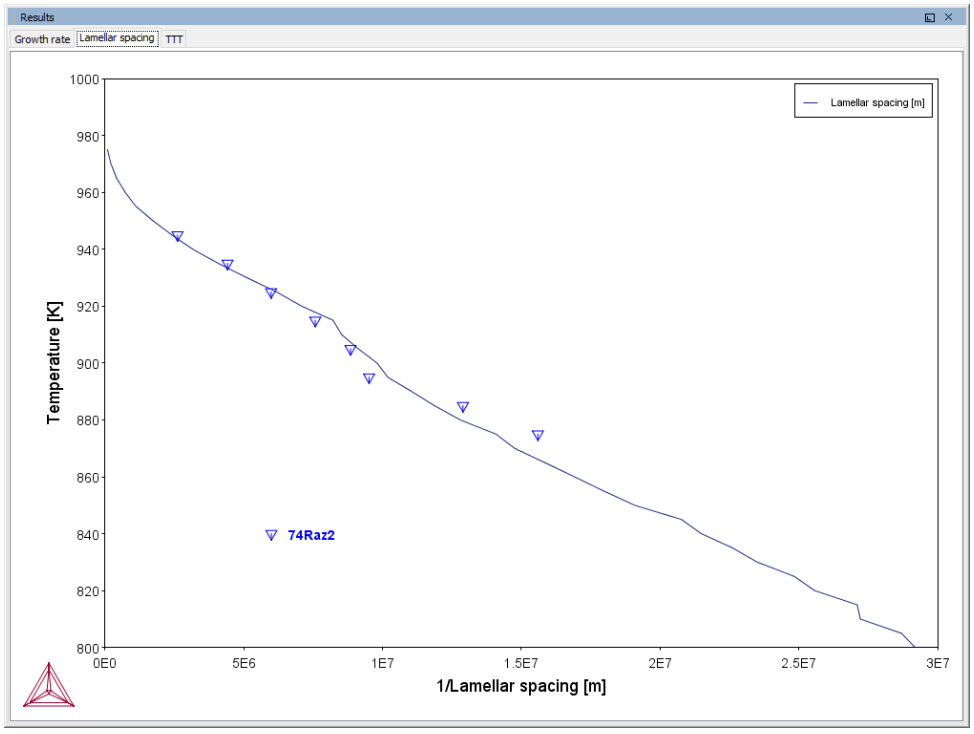
- Folder: Property Models>Steel
- File name: *PM_Fe_03_Fe-C-Mn_Pearlite.tcu*

Plot Results

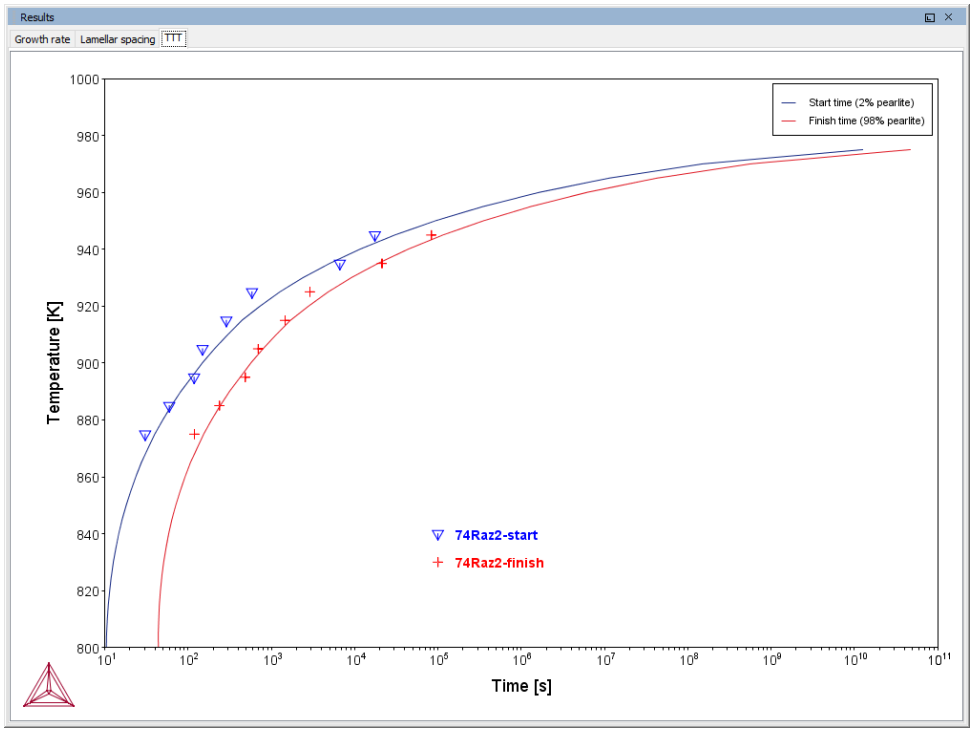
Growth Rate



Lamellar Spacing



TTT



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 %).

Process Metallurgy Examples Collection

The Process Metallurgy Module works with TCOX8 and newer versions of the database. The current version of the database is TCOX9.

All other users can test the 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.

About the Examples

PMET_01: Basic Oxygen Furnace (BOF)

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 9 and newer) as well as the free OXDEMO database.

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

The real-world BOF process is highly exothermic and needs adiabatic calculations. These are not available with the current version of the Process Metallurgy Module.

It is recommended you open the example project file and watch the companion video. The video walks you through setting up the material groups as well as analyzing the results.

You can open the example project file from Thermo-Calc **Help → Example Files → Process Metallurgy → PMET_01_Basic_Oxygen_Furnace.tcu**.

This example is included as a tutorial on our website and our YouTube channel.

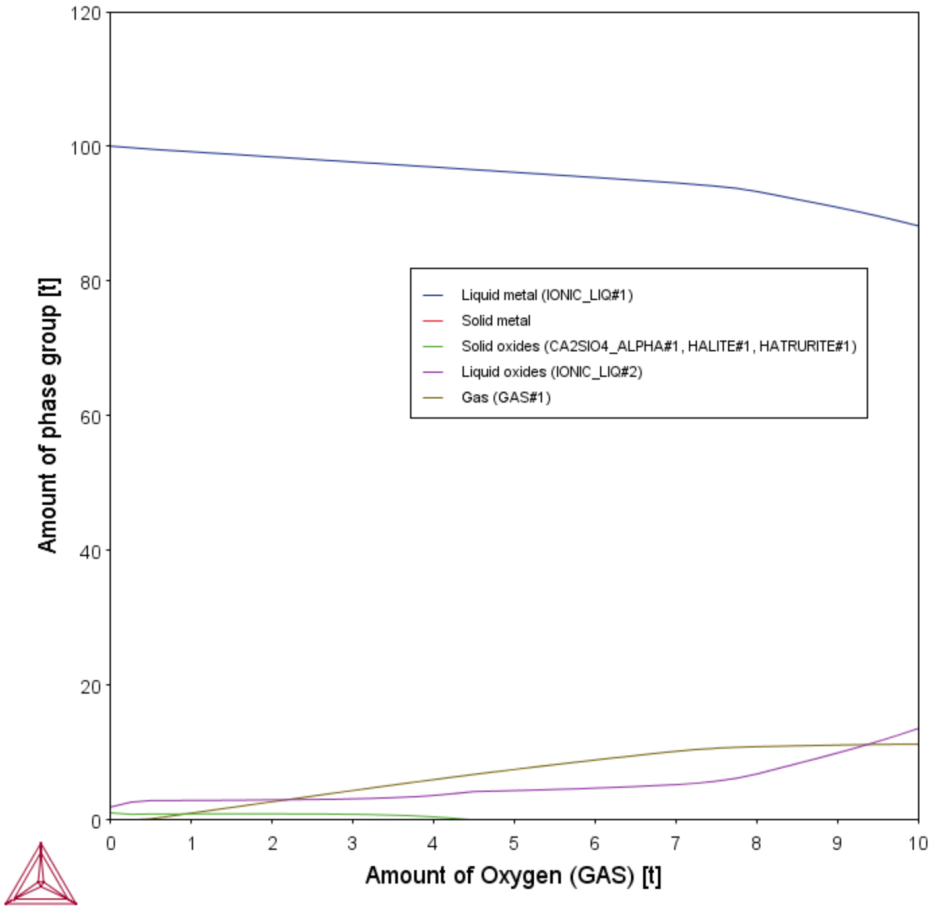
In general, the steps to set up this simulation are described in Defining the Process Metallurgy Calculator. After setting up the steel, slag and gas system, you can generate various plots to analyze the results. Below is a brief summary of this analysis.

See Phase Groups for details about how the Process Metallurgy Module plot labels are grouped into the *liquid metal*, *solid metal*, *solid oxides*, *liquid oxides* and *gas* phases.

For this example, a **One axis** calculation type is used for all plots. The *Grid Definition* settings for these plots are also set on the Process Metallurgy Calculator:

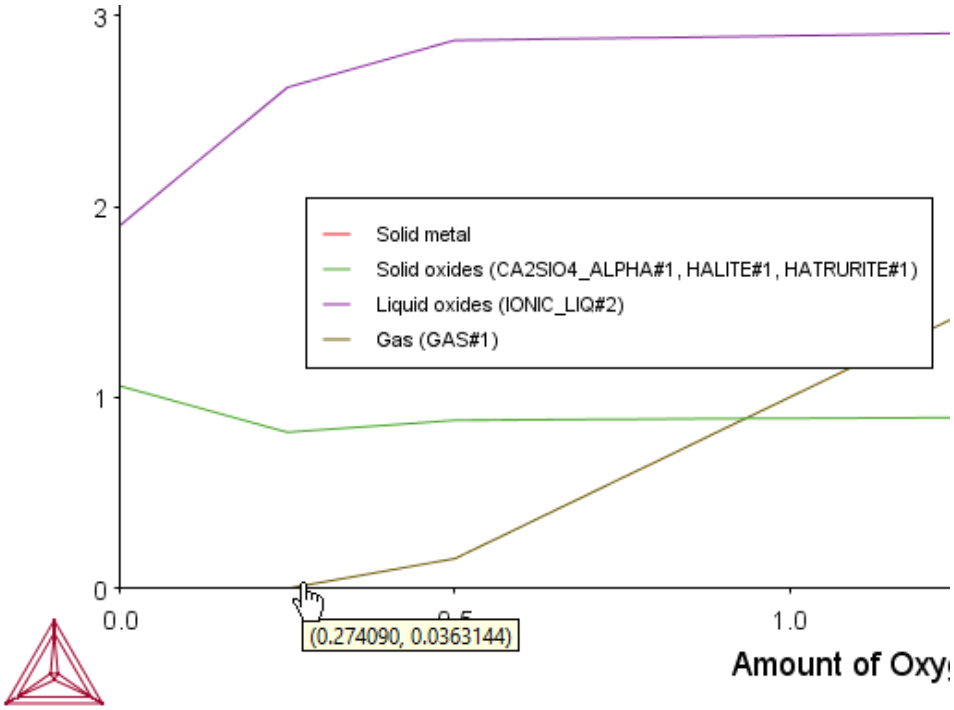
- Quantity: Amount of Oxygen (GAS)
- Stepping 0 min to 10 max with 40 steps

Amount of Phase Groups



After the plot is generated, by default you can see the **Amount of phase group** is plotted on the Y-axis as a function of the quantity plotted on the X-axis, in this case the **Amount of Oxygen (GAS)**.

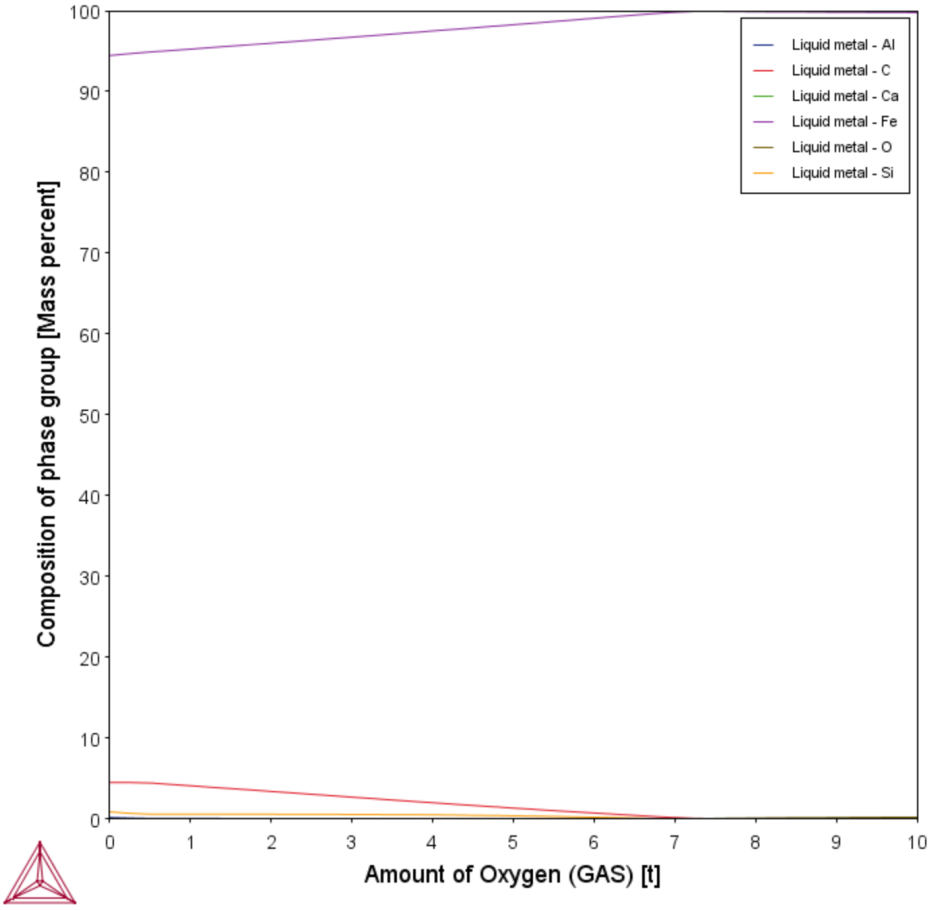
Zooming into the low gas amount (see below), it can be seen that the evolution of the gas phase is retarded. The reason is that the oxygen gas first oxidizes some of the silicon dissolved in the steel to form silicon dioxide (SiO_2). Only when the silicon content in the steel has dropped below a certain level can the oxygen gas burn away the carbon dissolved in the steel to form a carbon monoxide (CO)-rich gas phase.



These reactions can be investigated in more detail with different plots, so we will do that.

Composition of Liquid Metal

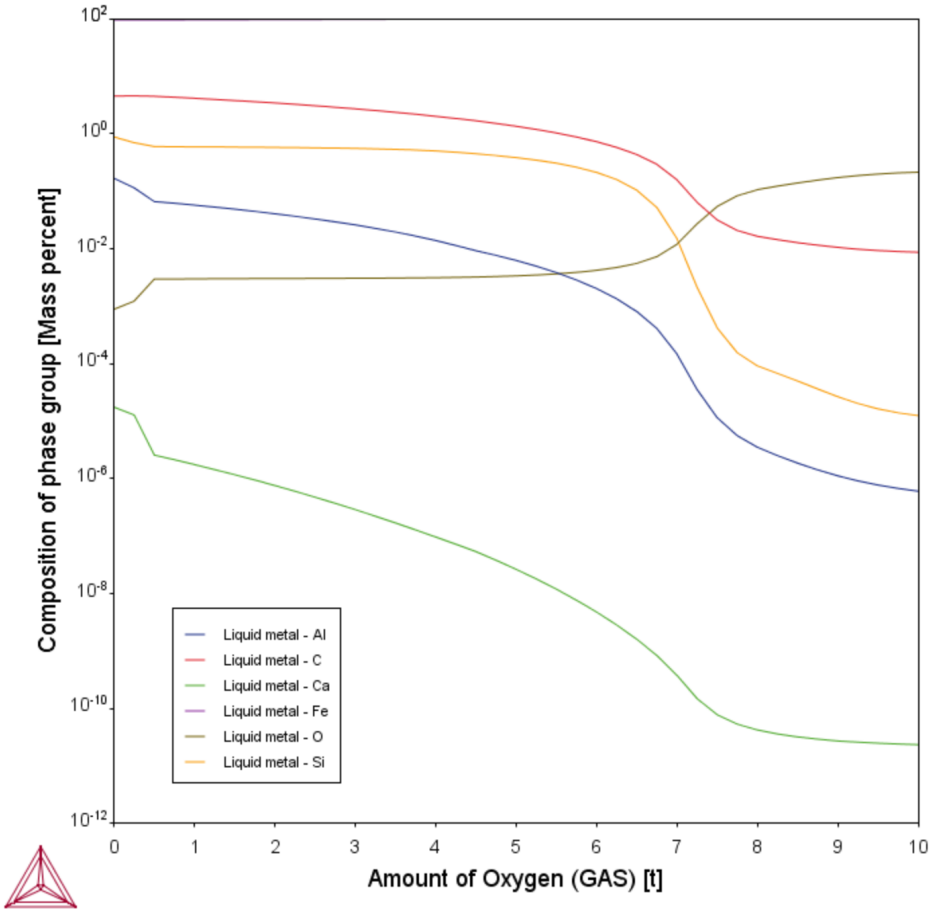
For the next plot, you define the following on a Plot Renderer, which you add to the Process Metallurgy Calculator. Keep the X-axis setting. For the Y-axis, choose **Composition of a phase group**, **Liquid Metal**, **All elements**.



In the plot (that uses a linear axis) the reduction of the carbon content can be clearly seen. This reduction of the carbon content is what is termed “steelmaking”. The hot metal coming from the blast furnace has a very high carbon content of typically 4.5 wt%. If it is left to solidify without lowering the carbon content, it will be extremely brittle and be unfit for rolling or forging.

Other changes in steel chemistry occurring in the BOF can be made visible by changing the Y-axis type from linear to logarithmic.

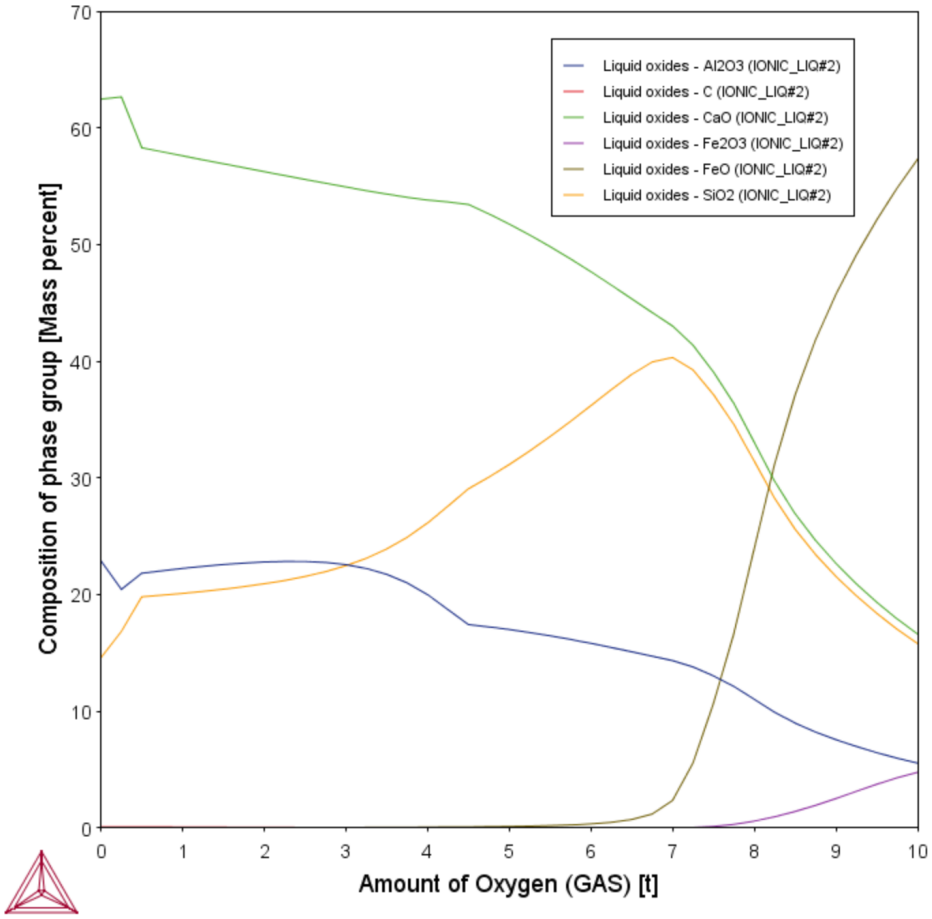
In the example project file only the logarithmic 10 version of the plot is included.



Now you can see the removal of the elements from the liquid steel in the following order: first calcium, then aluminium, then silicon and finally carbon (Ca, Al, Si and C) according to their position on the Ellingham diagram.

Composition of Liquid Slag

Add another Plot Renderer and define the following. Keep the X-axis setting. For the Y-axis, choose **Composition of a phase group**, **Liquid Oxides**, **All components**.



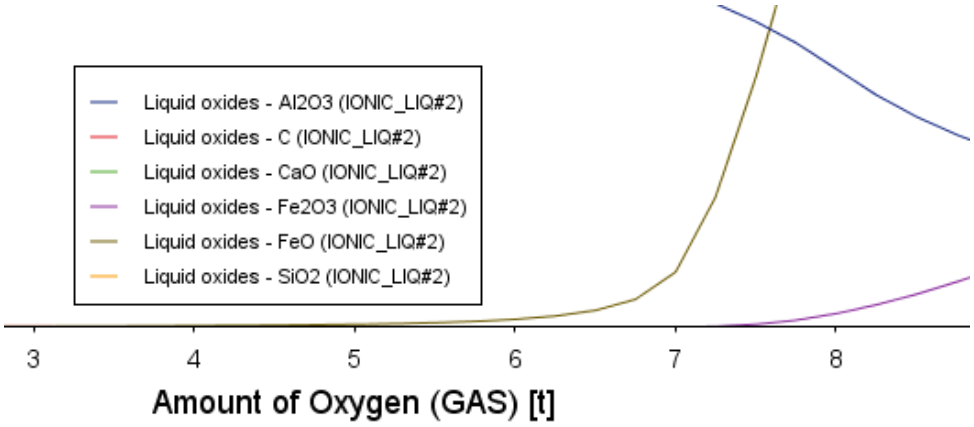
This plot shows how the liquid slag composition changes as a function of the amount of oxygen added to the BOF.

At first, the SiO_2 content of the slag rises sharply. This is due to the initial oxidation of the silicon dissolve in the hot metal. The SiO_2 that is formed combines with the slag and increases its SiO_2 content.

This increased SiO_2 content reduces the liquidus temperature of the slag and, as you can see in the first plot, thereby increases the amount of liquid slag and reduces the amount of solid oxides. This is also exactly what happens in reality.

On further addition of oxygen to the liquid steel, the silicon dioxide (SiO2) content in the slag increases further and further as more silicon is oxidized and combines with the slag. At the same time the oxygen partial pressure in the steel slowly increases. After about 6 tonnes of oxygen have been added to the system, the oxygen pressure is high enough to start oxidizing the steel itself.

The slag quickly becomes rich in iron oxide (FeO). When this starts happening, the steelmaking process is complete and the steel is ready to be tapped into a ladle for further steel refining.



PMET_02: Ladle Furnace

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 9 and newer) as well as the free OXDEMO database.

The example uses the **Process Metallurgy Calculator** to represent a simplified steel refining process in a ladle furnace (LF). It introduces you to the workflow of the Process Metallurgy Module. It is recommended you open the example project file and watch the companion video. The video walks you through setting up the material groups as well as analyzing the results.

You can open the example project file from Thermo-Calc **Help → Example Files → Process Metallurgy → PMET_02_Ladle_Furnace.tcu**.

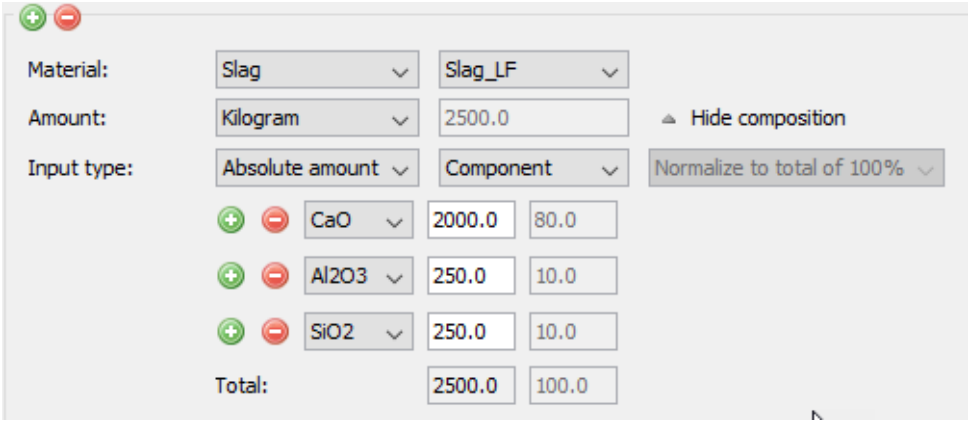
This example is included as a tutorial on our website and our YouTube channel.

In general, the steps to set up this simulation are described in Defining the Process Metallurgy Calculator. After setting up the steel, slag and gas system, you can generate various plots to analyze the results. Below is a brief summary of this analysis.

See Phase Groups for details about how the Process Metallurgy Module plot labels are grouped into the *liquid metal*, *solid metal*, *solid oxides*, *liquid oxides* and *gas* phases.

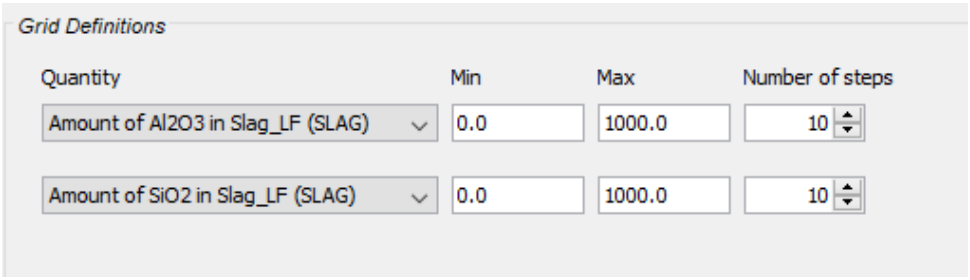
The material saved for this example, *Steel_LF*, could be a typical, but simplified composition of a fully killed SAE 1040 grade steel. The sulfur content, however, is too high for most final applications and must be reduced. Sulfur is usually removed from liquid steel in a ladle furnace using a calcium oxide-rich slag.

In this example, we want to find a slag composition that efficiently desulphurizes the steel. For this particular calculation we choose not to define a constant amount of slag but instead use absolute amounts of components. To do this, we set the **Input type** for the **Slag** material group to use **Absolute amount**. After saving this composition, it becomes the slag material for this example, *Slag_LF*.



For this example, the gas phase is not considered, which is why the Gas material group has been removed in the example project. This does not mean that no gas phase is allowed to form; it simply means that no gas phase is used to set the calculation conditions.

For this example, a **Grid** calculation type is used for all plots. The *Grid Definition* settings for these plots are also set on the Process Metallurgy Calculator:

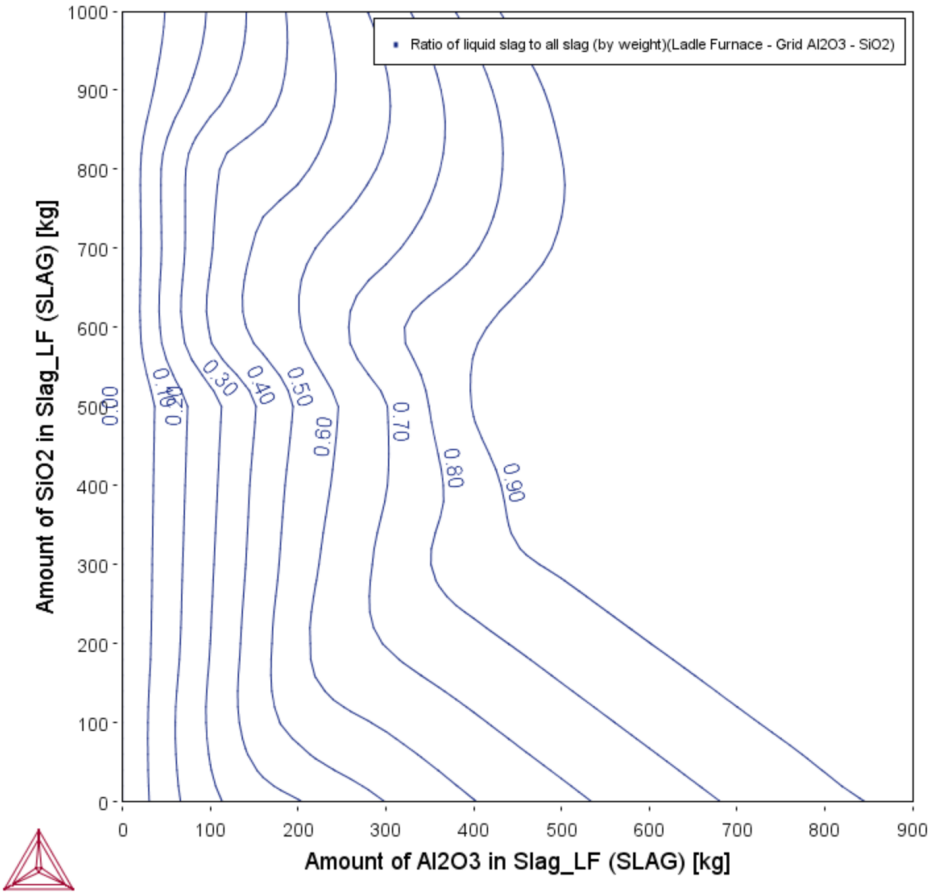


Leave the number of calculation steps at 10 for both axes in order to shorten the calculation time. With this setting, the calculation should be completed in just under one minute. The number of steps could be increased to maybe 30 x 30 for higher resolution of the results, but this increases the calculation time significantly.

Fraction of Liquid Slag

In the example project file only the *Ratio of liquid slag and sulfur in liquid steel* contour plot is included.

We want to understand whether our slag phase is liquid or not. To create the plot below, add a Plot Renderer node with a **Contour** plot and choose **Fraction of liquid slag** as the **Z-axis variable**. Set the interpolation as **50 x 50** and click **Perform**.



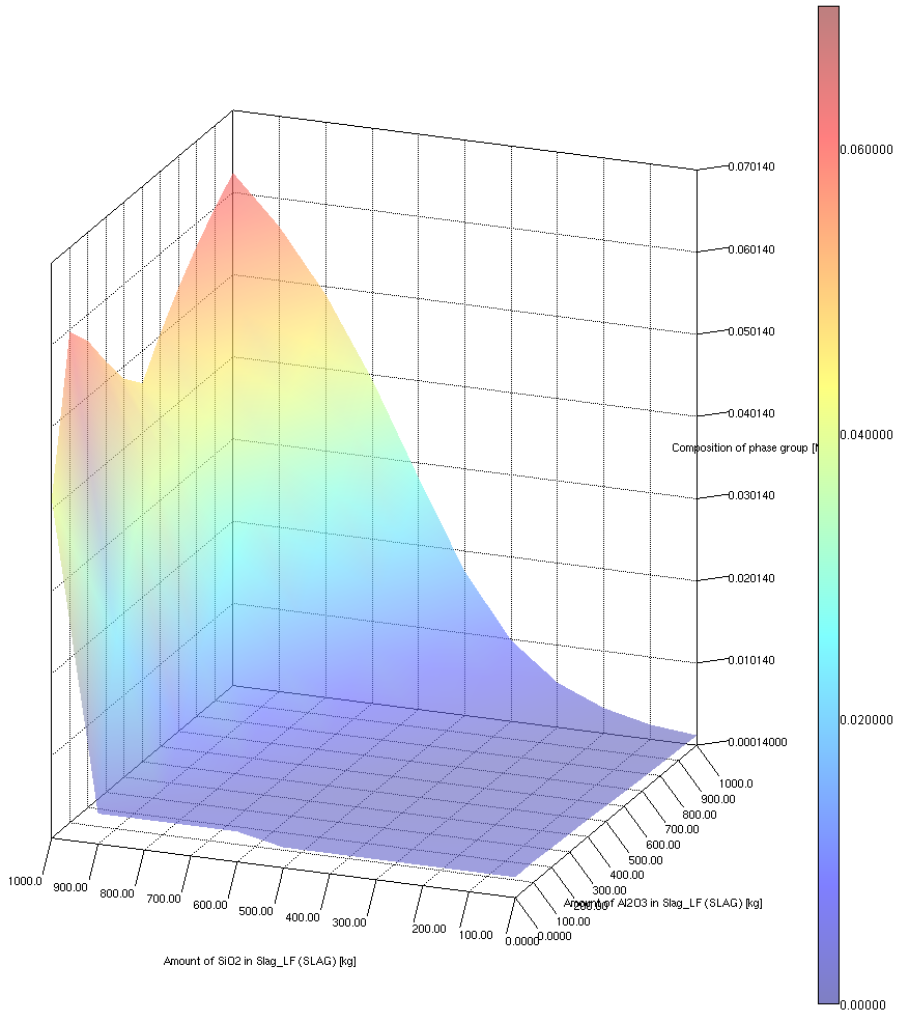
The plot shows that for low amounts of aluminium oxide (Al_2O_3) and silicon dioxide (SiO_2), almost no liquid slag is present. Process metallurgists refer to this as a *hard slag*.

Such a hard slag is in fact just solid oxide phases that passively float on the liquid steel. It does not react with the liquid steel for kinetic reasons and therefore does not desulfurize the steel.

Practical slag compositions are limited to the top, right field above the “fraction liquid slag = 0.9” contour line. Only here a liquid slag phase is present that can flow and can mix and react with the steel.

Next we are interested in the ability of the slag phase to remove sulfur (s) from the liquid steel.

Sulfur in Liquid Steel



Refer to the *Sulfur in liquid steel* 3D plot included with the example. The red colors in the upper right-hand corner at high SiO_2 and Al_2O_3 content show that the steel contains high amounts of sulfur.

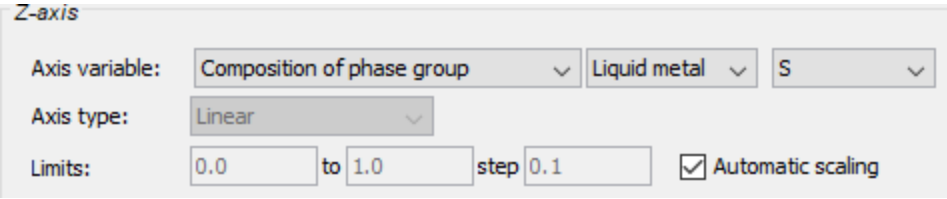
This means that only a little of the sulfur in the liquid steel partitioned into the slag phase and the slag phase has a poor capacity to take up sulfur.

The blue colors in the lower left-hand corner indicate that the liquid steel contains only very low amounts of sulfur, so this indicates a slag composition that is effective at removing sulfur, or in other words, has a high sulfur capacity.

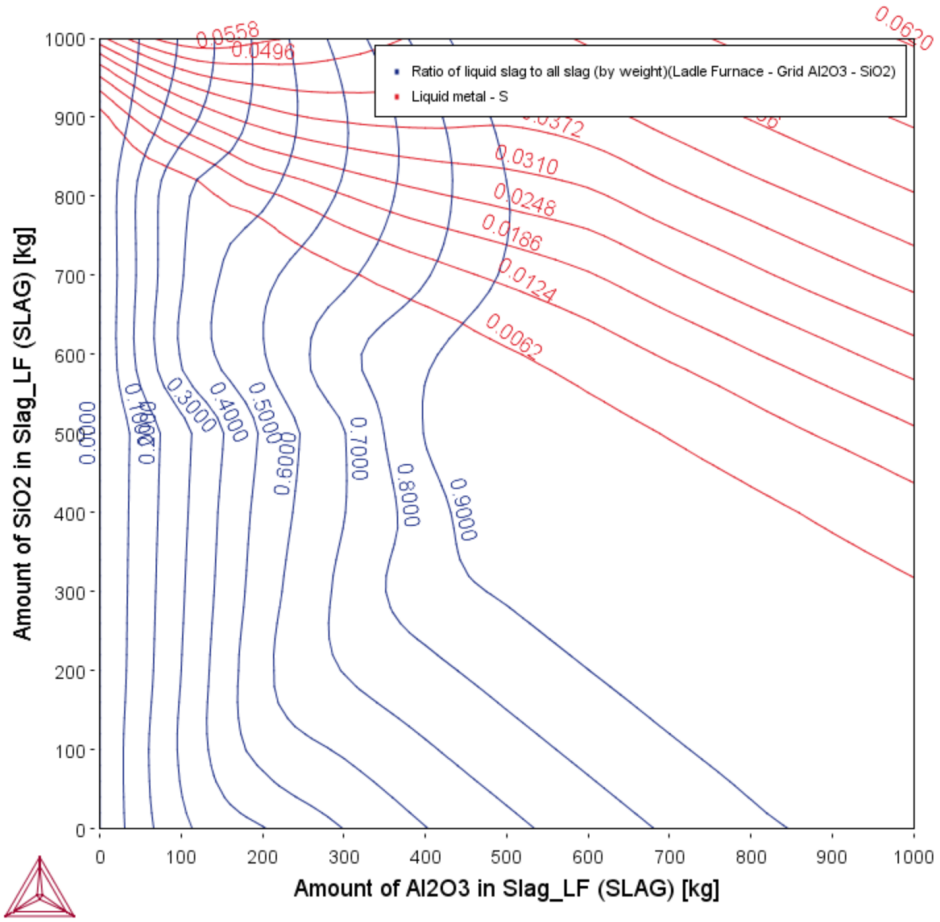
The performed calculations assume thermodynamic equilibrium. As shown in the previous plot, there is almost no liquid slag phase present in the lower left corner at low SiO_2 and Al_2O_3 content. This means that thermodynamic equilibrium would not be achieved due to the very slow kinetics of the reaction between the liquid steel and the solid oxides.

Ratio of Liquid Slag and Sulfur in Liquid Steel

Refer to the *Ratio of liquid slag and sulfur in liquid steel* contour plot included with your example. This is two plots combined into one contour plot. If you created the above *Fraction of Liquid Slag* contour plot, this plot is created simply by adding another set of axes and then defining the Z-axis.



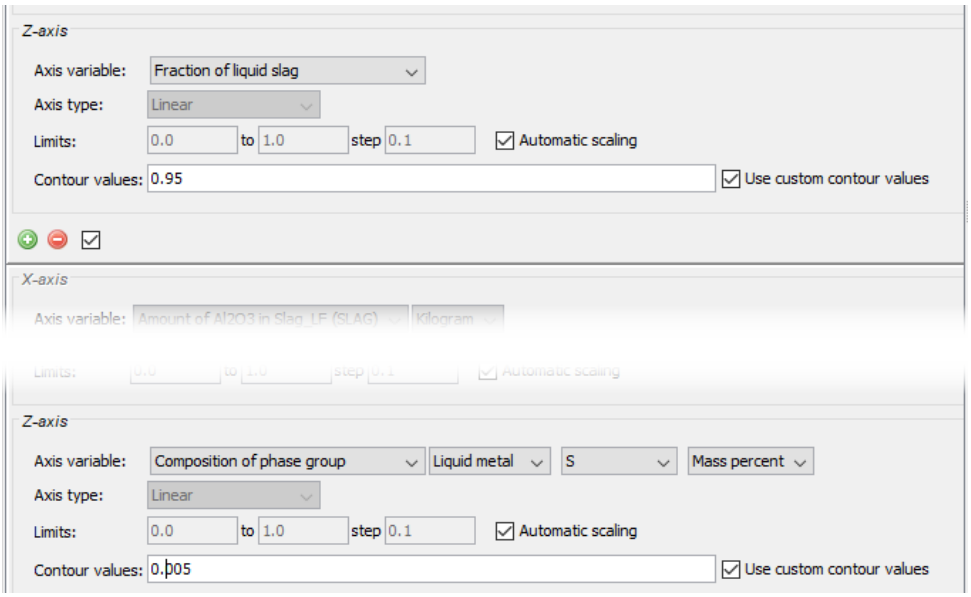
Combining the information contained in the two plots results in an optimum slag composition in a narrow composition band. To smooth the contours, Set the interpolation as **50 x 50**.

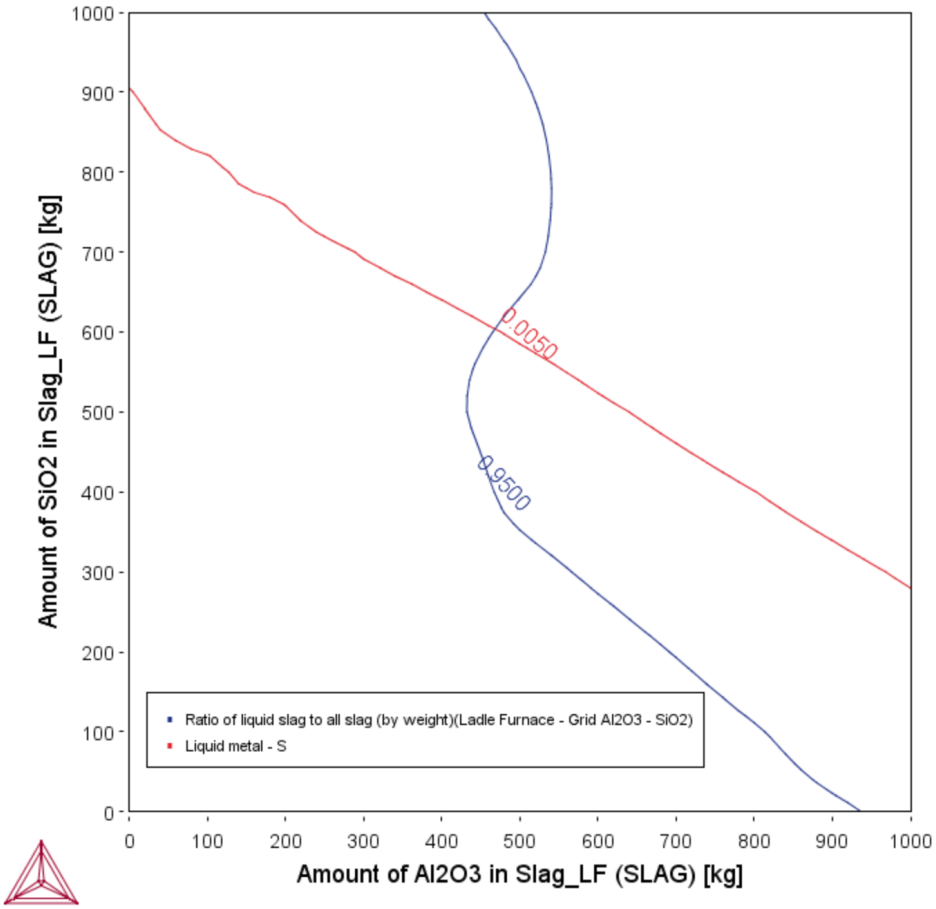


To map this optimal composition field one more plot can be generated by superimposing contour plots of sulfur content in the liquid steel and fraction of liquid slag.

Since we want to have at least 95% liquid slag, in the set of axis variables for **Fraction of liquid slag**, click to select the check box next to **Use custom contour values** and enter `0.95` in the field.

We also want to have less than 0.005% sulfur in the liquid metal, so also select the same check box for the other Z-axes and set the value of sulfur to `0.005` . Click **Perform**.


Z-axis
Axis variable: Fraction of liquid slag
Axis type: Linear
Limits: 0.0 to 1.0 step 0.1 Automatic scaling
Contour values: 0.95 Use custom contour values
X-axis
Axis variable: Amount of Al2O3 in Slag_LF (SLAG) Kilogram
Limits: 0.0 to 1.0 step 0.1 Automatic scaling
Z-axis
Axis variable: Composition of phase group Liquid metal S Mass percent
Axis type: Linear
Limits: 0.0 to 1.0 step 0.1 Automatic scaling
Contour values: 0.005 Use custom contour values


Amount of SiO2 in Slag_LF (SLAG) [kg]
Amount of Al2O3 in Slag_LF (SLAG) [kg]
0.0050
0.9500
Ratio of liquid slag to all slag (by weight)(Ladle Furnace - Grid Al2O3 - SiO2)
Liquid metal - S

The optimal slag has a composition delimited by these two contour lines, so below the contour line for sulfur content in the liquid steel and above the contour line for fraction of liquid slag will be both fully liquid and effectively desulfurizes the steel.

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.

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

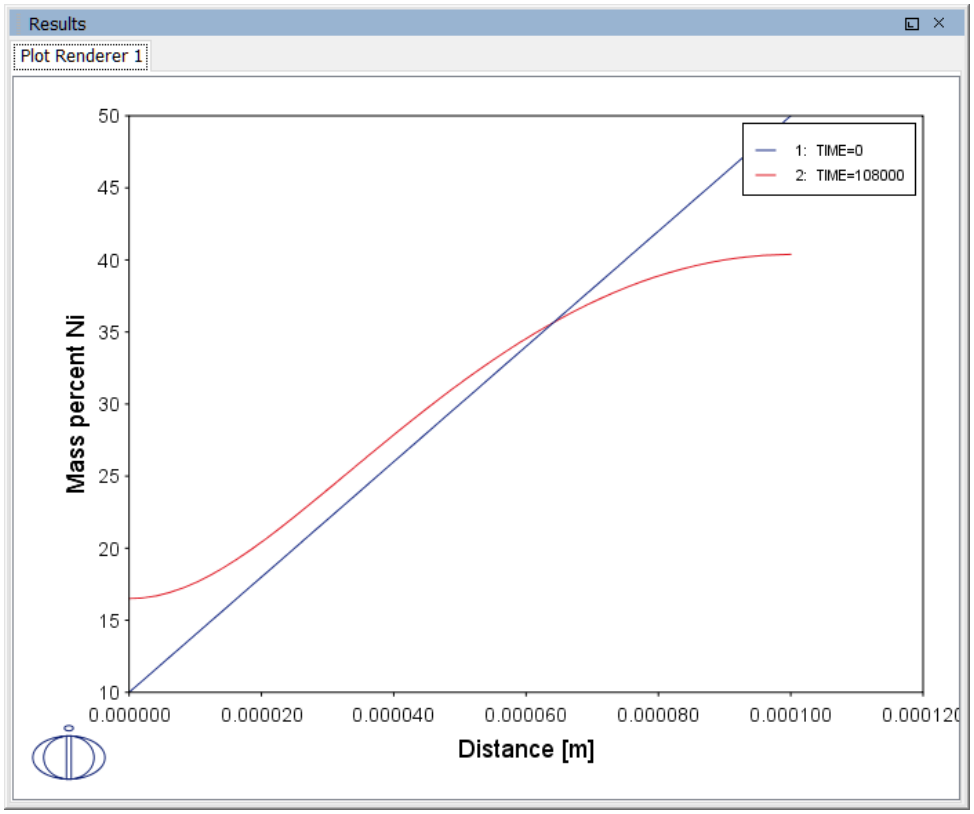
About the Examples

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 available as a video tutorial on our website and YouTube channel. In previous versions of the software (prior to 2017b) it is example 19.

Composition of Ni vs Distance



PROJECT FILE NAME

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

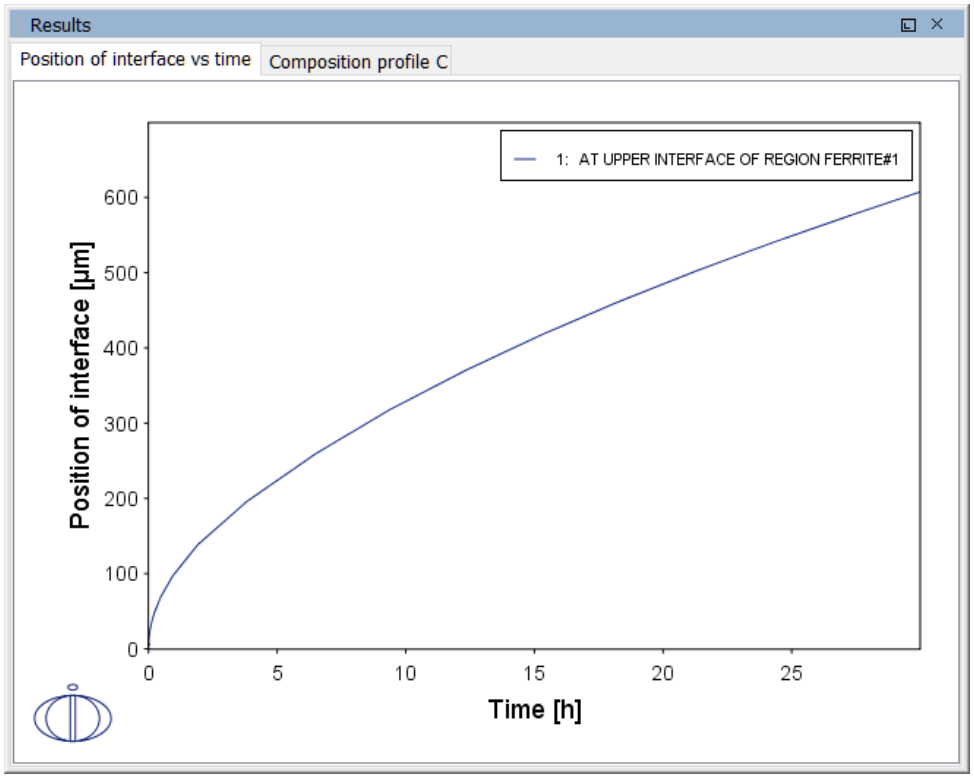
This example is part of the *Diffusion Module (DICTRA) Quick Start Guide* available to all users. A version of the example is also available for Console Mode.

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

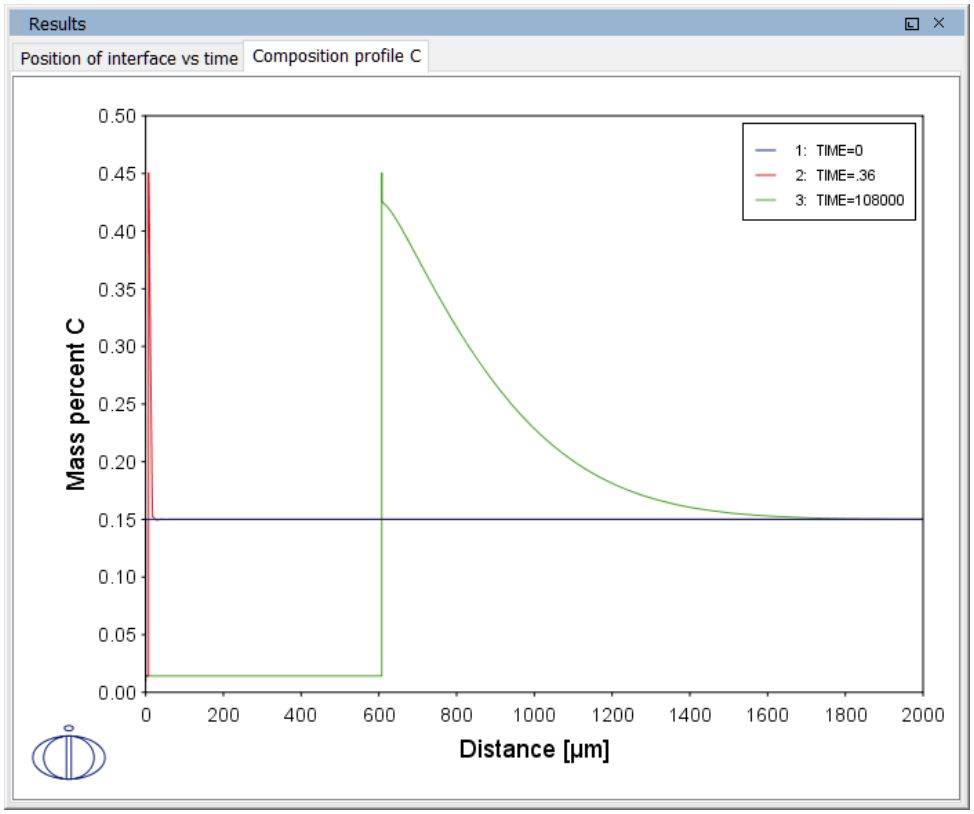
The moving phase boundary example simulates the growth of ferrite (bcc) into austenite (fcc). The austenite is assumed to be initially homogeneous with the composition Fe-0.15 mass-% C. The transformation temperature is 1050 K. The initial thickness of the austenite is 2 mm and an initially very thin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

This example is available as a video tutorial on our website and YouTube channel.

Position of interface vs time



Composition profile C



PROJECT FILE NAME

- 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.

D_03 Evolution of an Fe-Cr-Ni Diffusion Couple

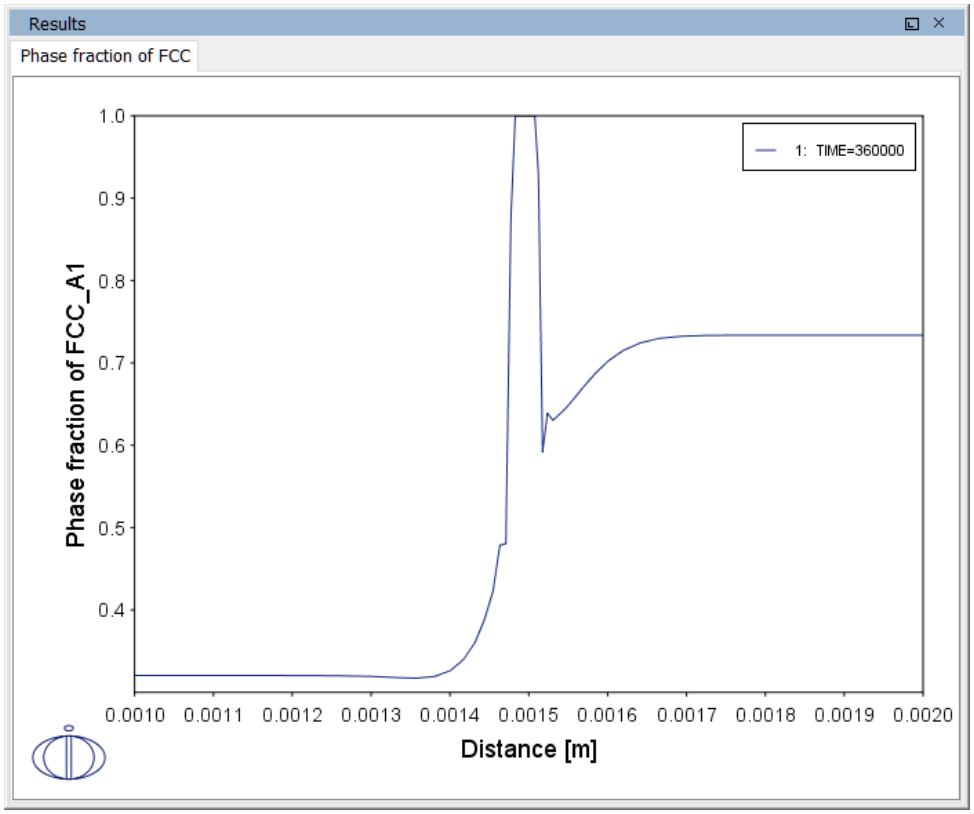
The multiphase example simulates the evolution of an Fe-Cr-Ni diffusion couple during a 100 hour heat treatment at 1100° C (1373.15 K). Both end members of the diffusion couple are duplex ferrite plus austenite, but the majority phase is ferrite on the left-hand side and austenite on the right.

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 (2006)[1.] and Larsson and Höglund (2009)[2.] . Experimental data is from Engström (1995)[3.] .

1. "A homogenization approach to diffusion simulations applied to α + γ Fe–Cr–Ni diffusion couples", *Acta Mater.*, 54 (9), pp. 2431–2439.
2. "Multiphase diffusion simulations in 1D using the DICTRA homogenization model", *Calphad*, 33 (3), pp. 495–501.
3. "Interdiffusion in multiphase, Fe-Cr-Ni diffusion couples", *Scand. J. Metall.*, 24(1), 12–20.

Phase fraction of FCC



PROJECT FILE NAME

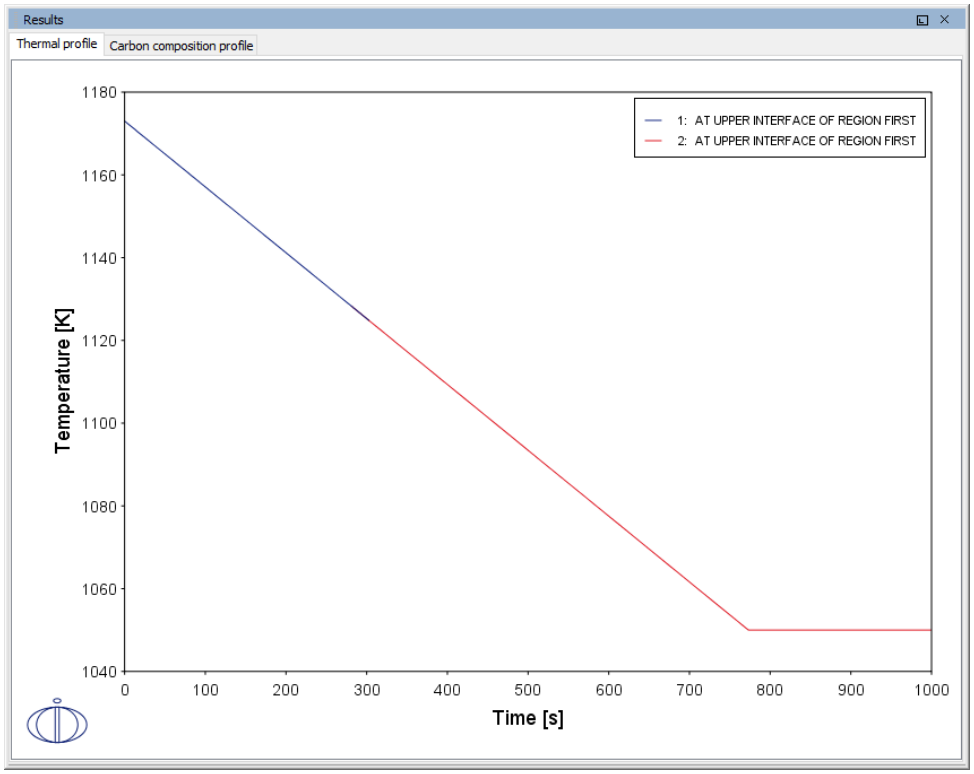
- Folder: Diffusion Module - DICTRA
- File name: *D_03_Diffusion_Multiphase.tcu*

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.

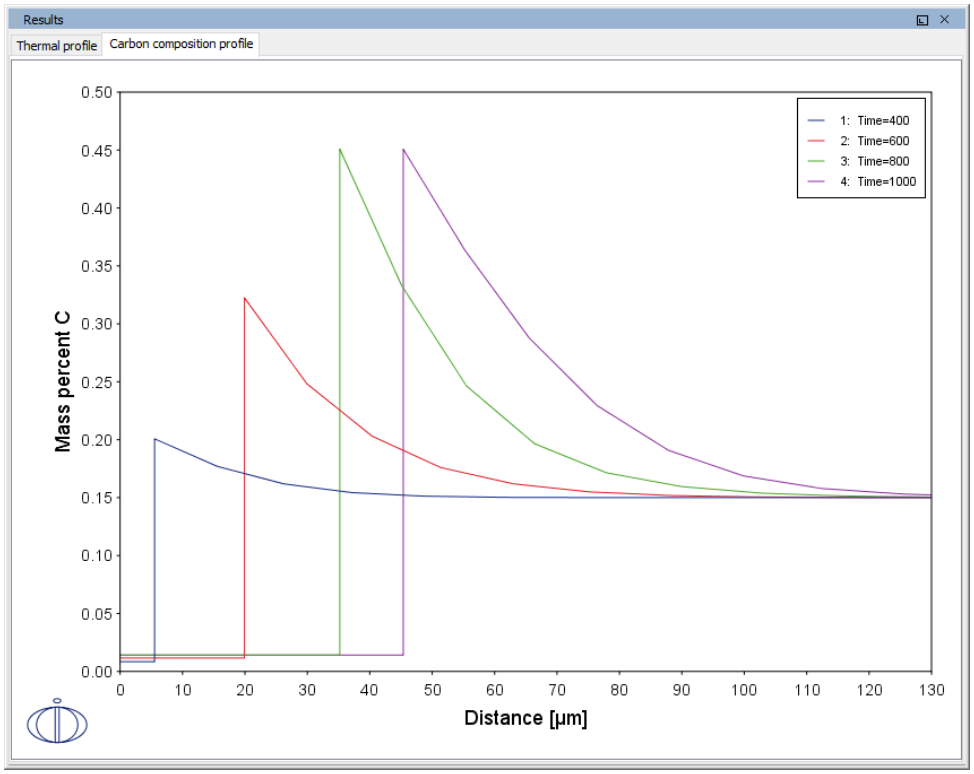
D_04 Fe-C Moving Boundary: Austenite to Ferrite

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.

Thermal profile



Carbon composition profile



PROJECT FILE NAME

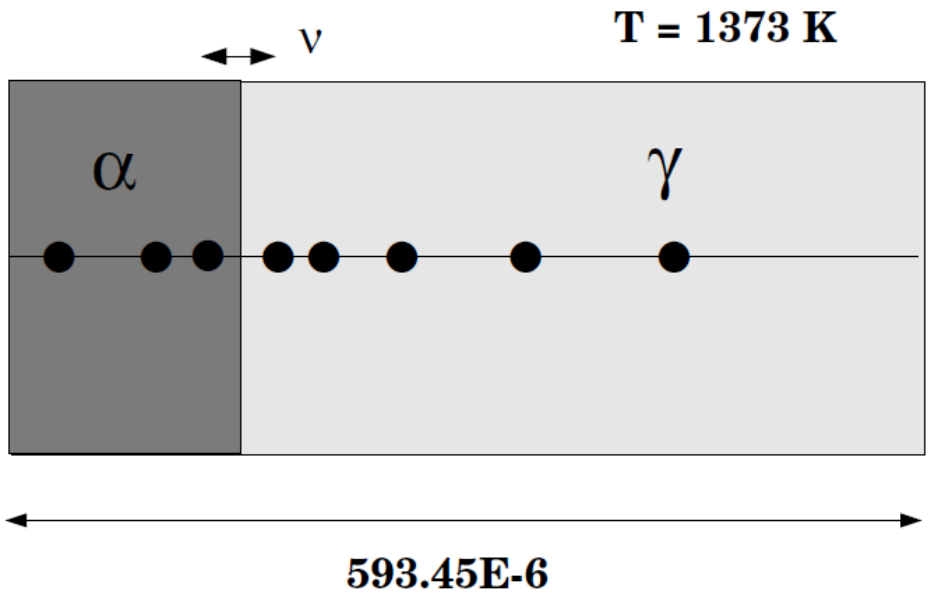
- Folder: Diffusion Module - DICTRA
- File name: *D_04_Diffusion_Fe-C_Moving_Boundary_Austenite_to_Ferrite.tcu*

This example is available to all users.

D_05 γ/α/γ Diffusion couple of Fe-Ni-Cr alloys

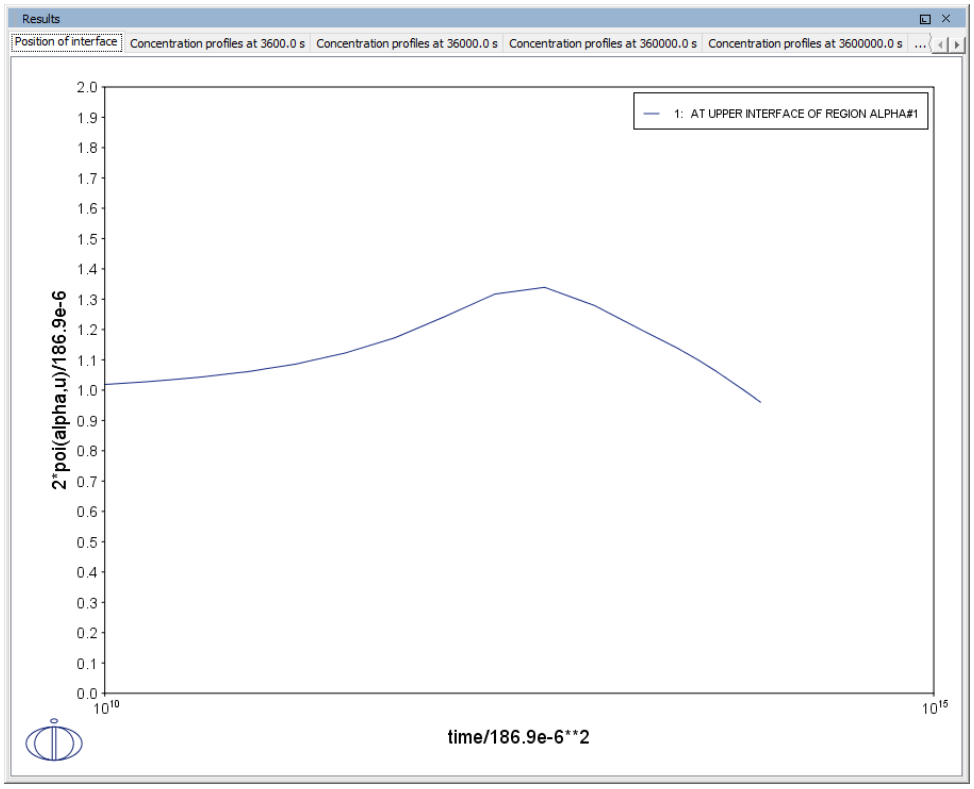
This example demonstrates the evolution of a ternary Fe-Cr-Ni diffusion couple. A thin slice of ferrite (α phase) (38%Cr,0%Ni) is clamped between two thicker slices of austenite (γ phase) (27%Cr, 20%Ni). The assembly is subsequently heat treated at 1373 K.

This set up corresponds to diffusion couple in Kajihara, Lim, and Kikuchi (1993)[1.] . Also see Kajihara and Kikuchi (1993)[2.] .

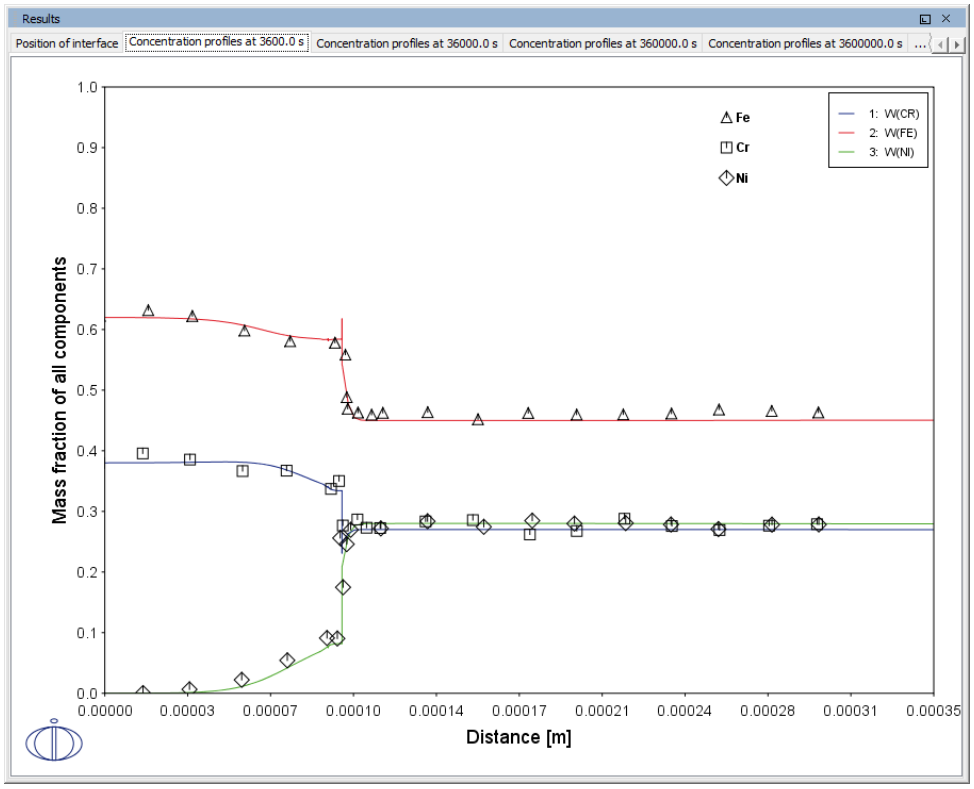


1. "Experimental Study on Dissolution of ALPHA Phase in GAMMA/ALPHA/GAMMA Diffusion Couples of the Fe-Cr-Ni System", *ISIJ Int.*, 33(4), 498–507.
2. "Numerical analysis of dissolution of α phase in γ/α/γ diffusion couples of the Fe-Cr-Ni system", *Acta Metall. Mat.*, 41 (7), 2045–2059.

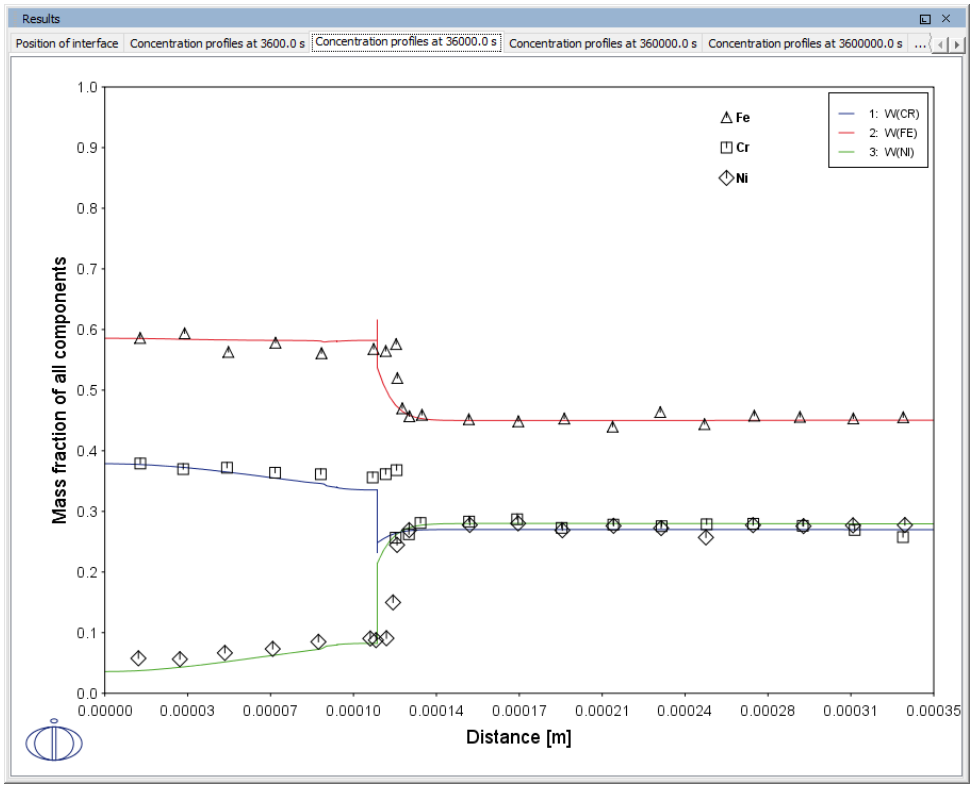
Interface Position



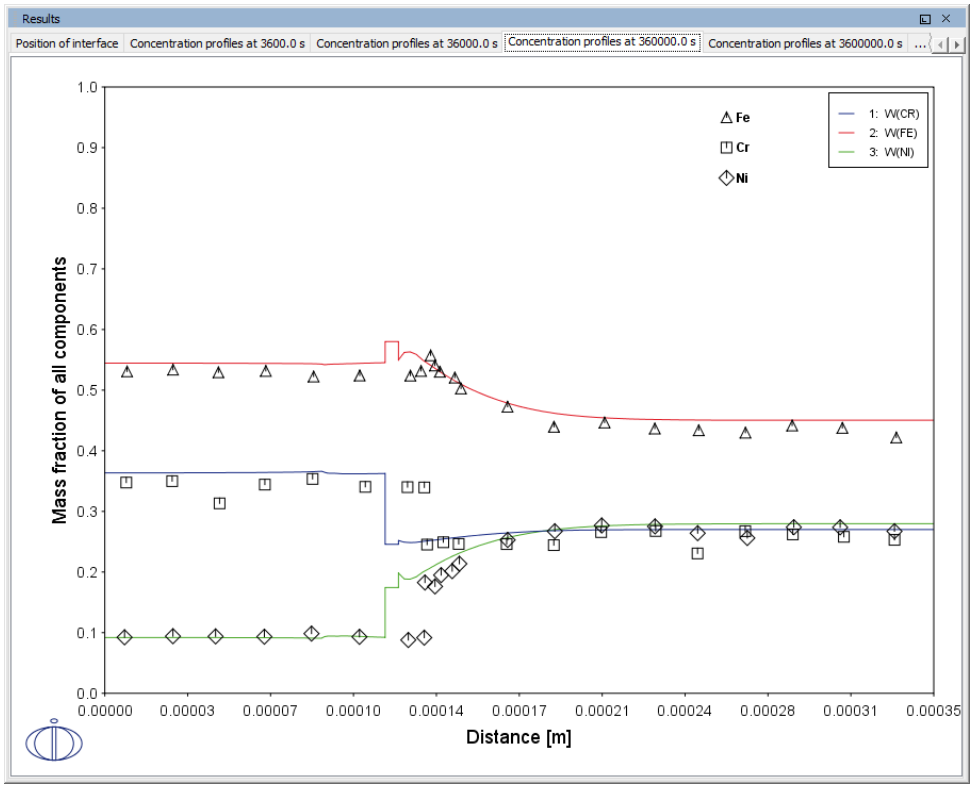
Concentration profiles at 3600 s



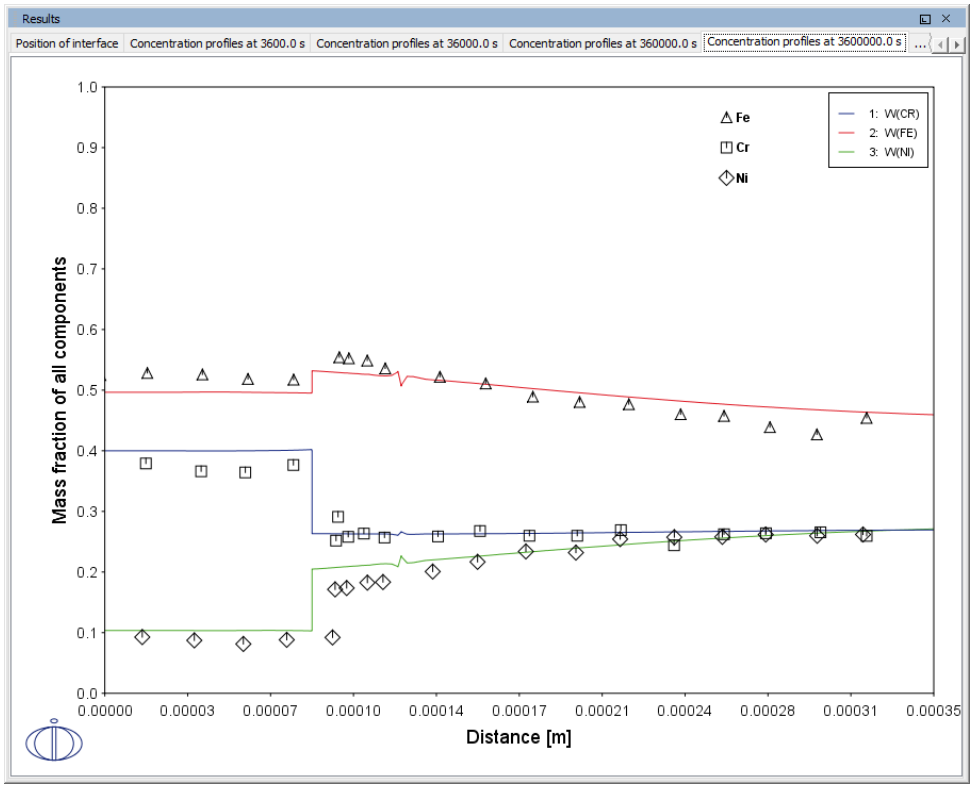
Concentration profiles at 36000 s



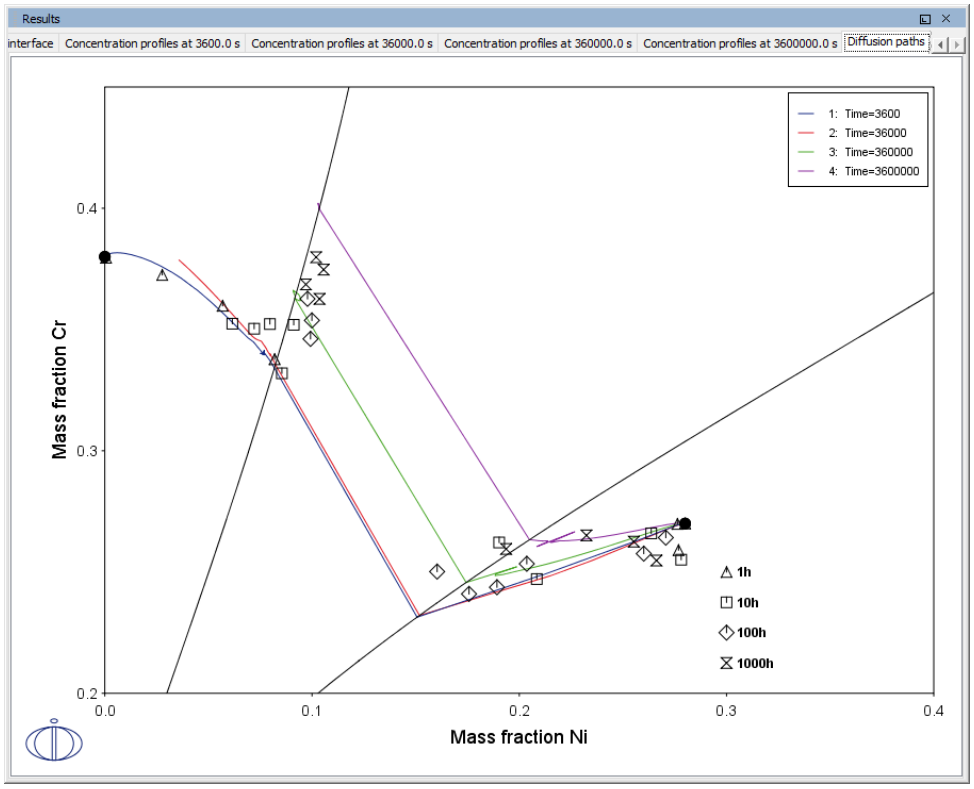
Concentration profiles at 36 0000 s



Concentration profiles at 3 600 000 s



Diffusion paths



PROJECT FILE NAME

- Folder: Diffusion Module - DICTRA
- File name: *D_05_Diffusion_Fe_Ni_Cr_Moving_Boundary_Diffusion_Couple.tcu*

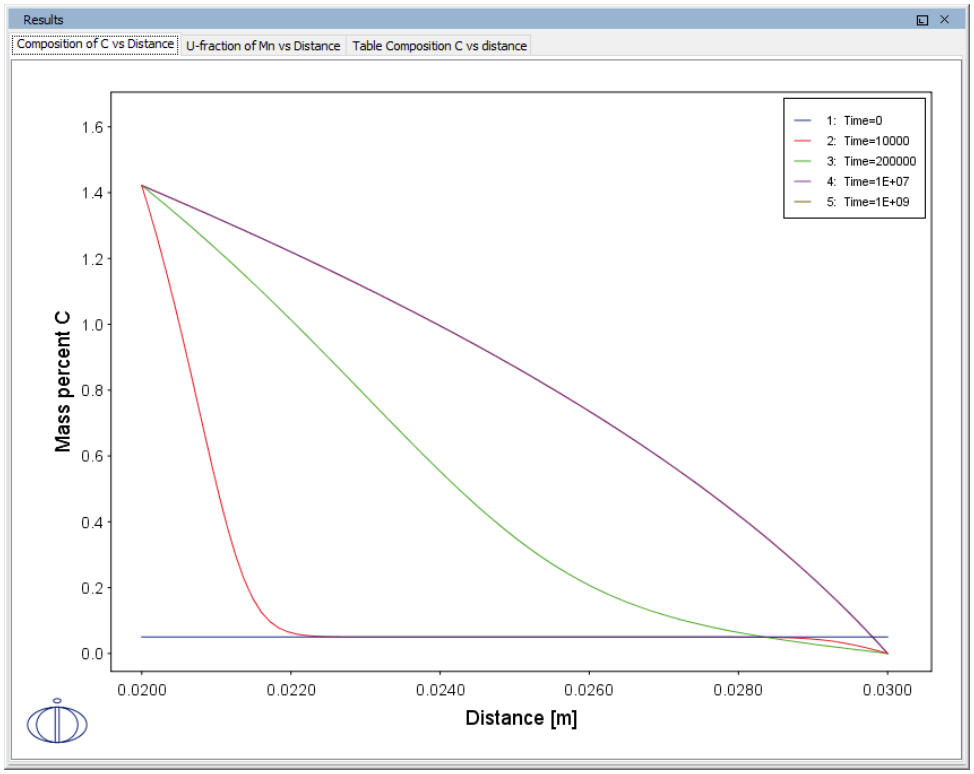
D_06 Diffusion Through a Tube Wall

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.

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**).

Composition of C vs Distance



U-fraction of Mn vs Distance

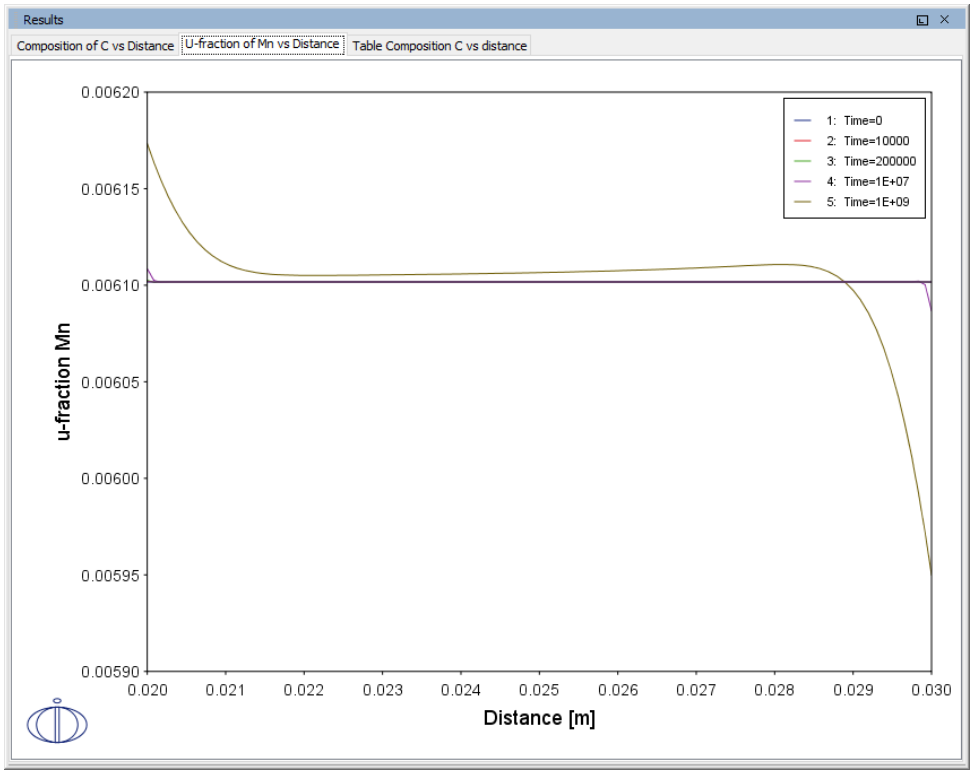
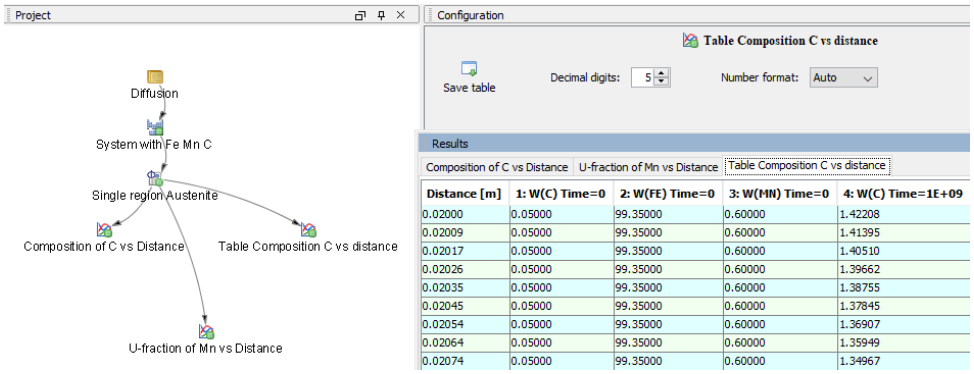


Table Composition C vs Distance



Distance [m]	1: W(C) Time=0	2: W(FE) Time=0	3: W(MN) Time=0	4: W(C) Time=1E+09
0.02000	0.05000	99.35000	0.60000	1.42208
0.02009	0.05000	99.35000	0.60000	1.41395
0.02017	0.05000	99.35000	0.60000	1.40510
0.02026	0.05000	99.35000	0.60000	1.39662
0.02035	0.05000	99.35000	0.60000	1.38755
0.02045	0.05000	99.35000	0.60000	1.37845
0.02054	0.05000	99.35000	0.60000	1.36907
0.02064	0.05000	99.35000	0.60000	1.35949
0.02074	0.05000	99.35000	0.60000	1.34967

Project File Name

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

D_07 Multiphase Carburization of a Ni-25Cr-0.0001C alloy

This example 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 case is from Engström, Höglund, and Ågren (1994), "Computer simulation of diffusion in multiphase systems", *Met. Mat. Trans. A*, 25(6), 1127–1134.

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**).

This example is available as a video tutorial on our website and YouTube channel.

Phase fraction vs distance

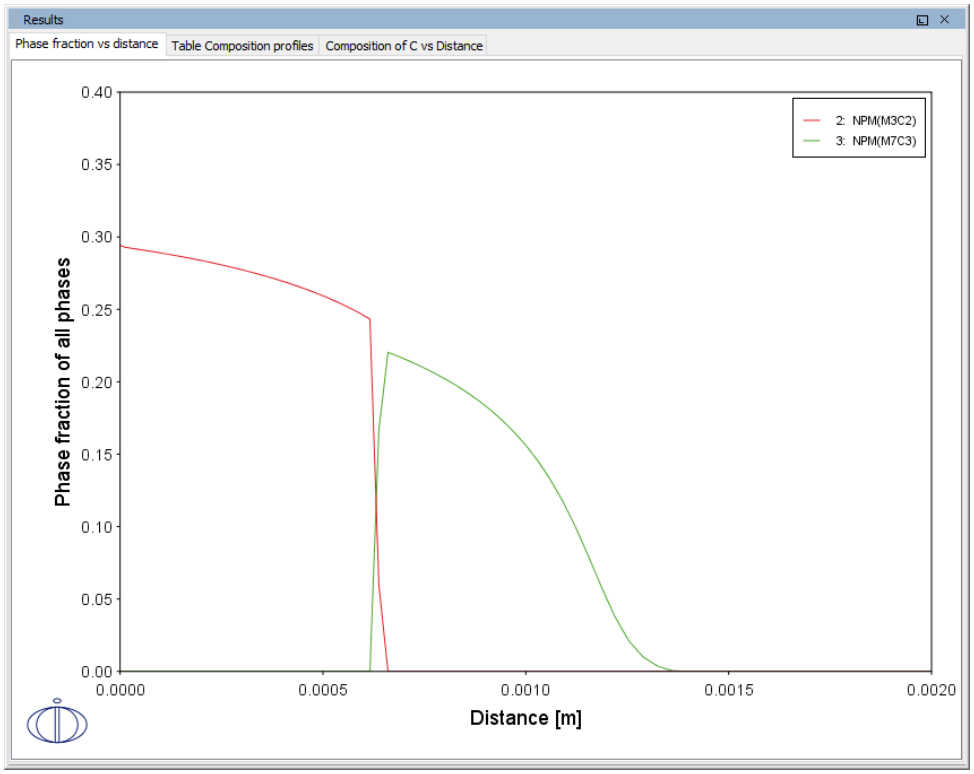
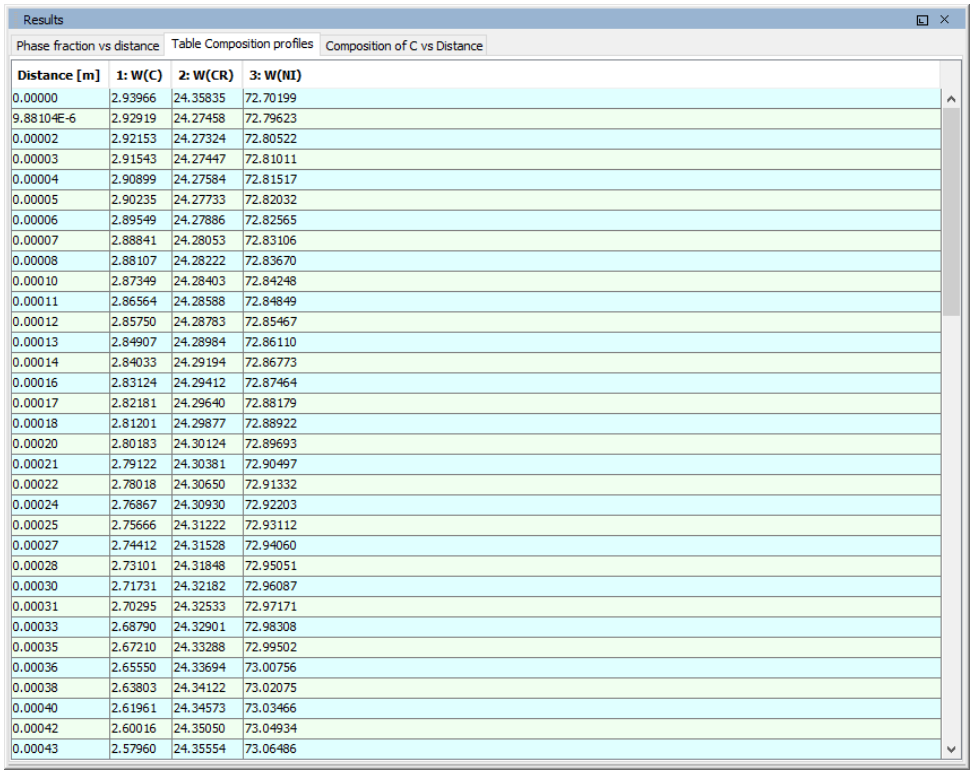
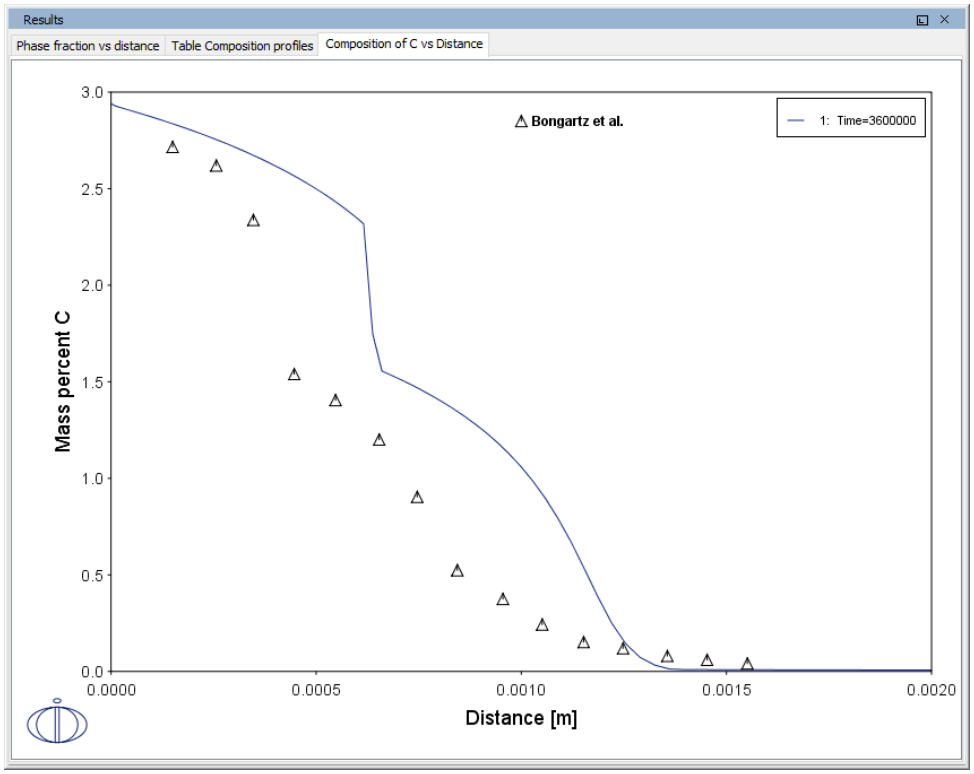


Table of Composition profiles



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

Composition of C vs Distance



PROJECT FILE NAME

- Folder: Diffusion Module - DICTRA
- File name: *D_07_Diffusion_Carburization_Multiphase.tcu*

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.

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[1.] and Novotny and Ardell (2001)[2.] .

Project File, Step-By Step Instructions and Video Information

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

This example is available as a video tutorial on our website and 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.

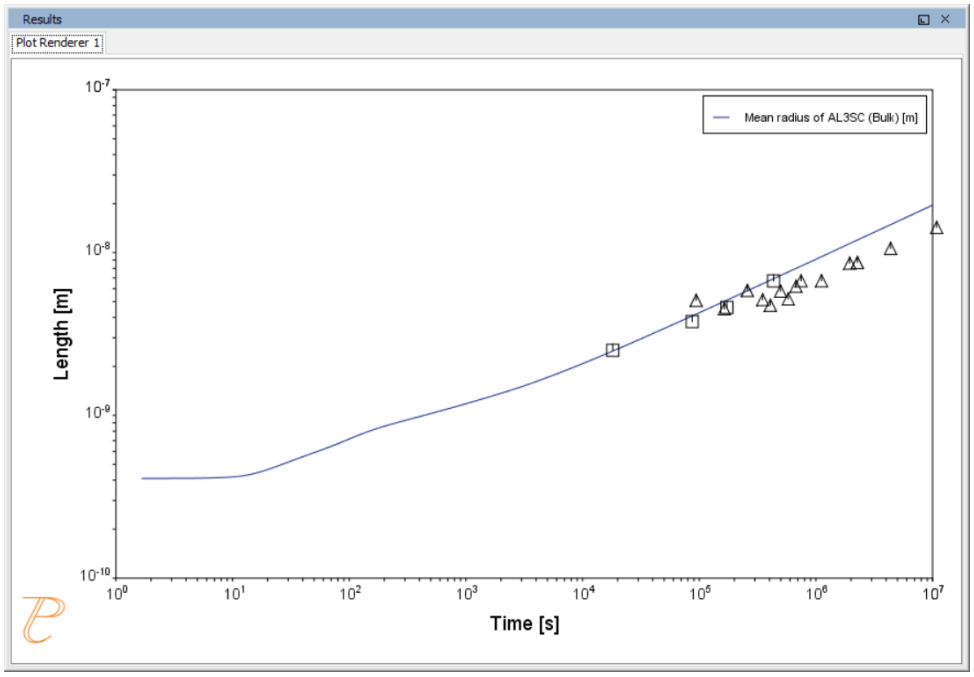
Example Settings

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.

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

PLOT RESULTS

Mean radius


Results
Plot Renderer 1
Mean radius of AL3SC (Bulk) [m]
Length [m]
Time [s]
10-7
10-8
10-9
10-10
100
101
102
103
104
105
106
107

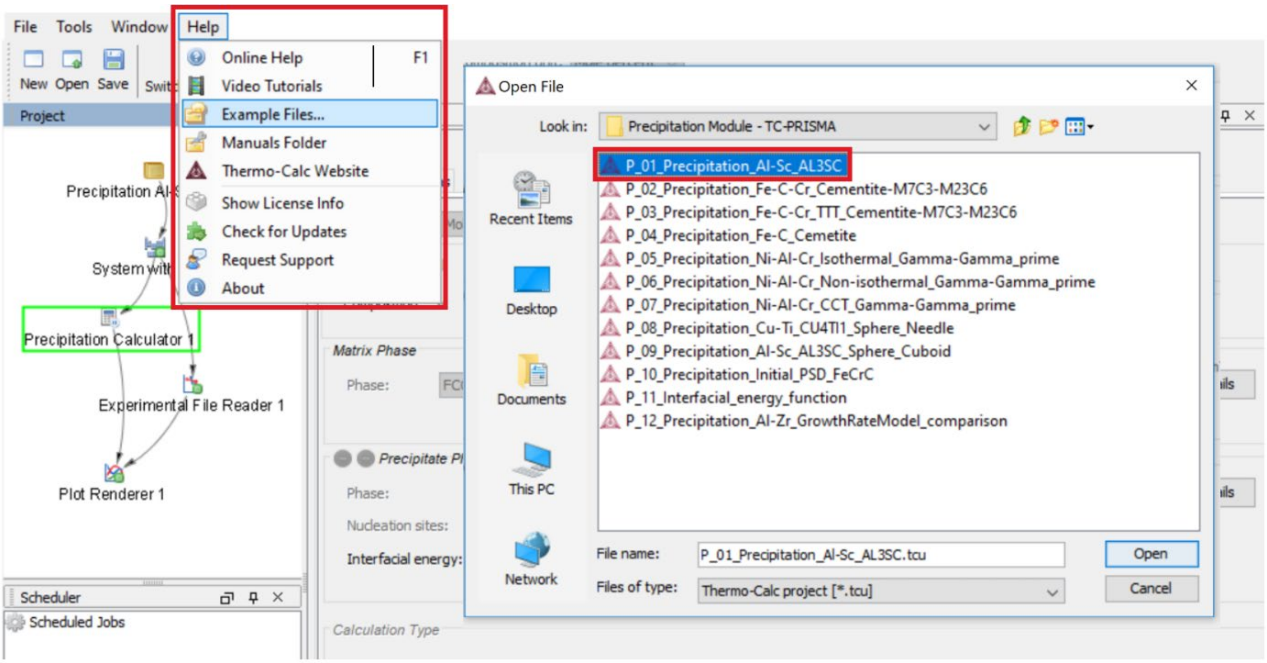
Isothermal Precipitation Calculation: Example P_01 – Precipitation Al-Sc AL3SC

This example shows you how to set up an isothermal precipitation calculation for the formation of AL3SC in an aluminium-scandium alloy at 350° using the Precipitation module (TC-PRISMA).

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 centre of the **Configuration** window in Thermo-Calc.

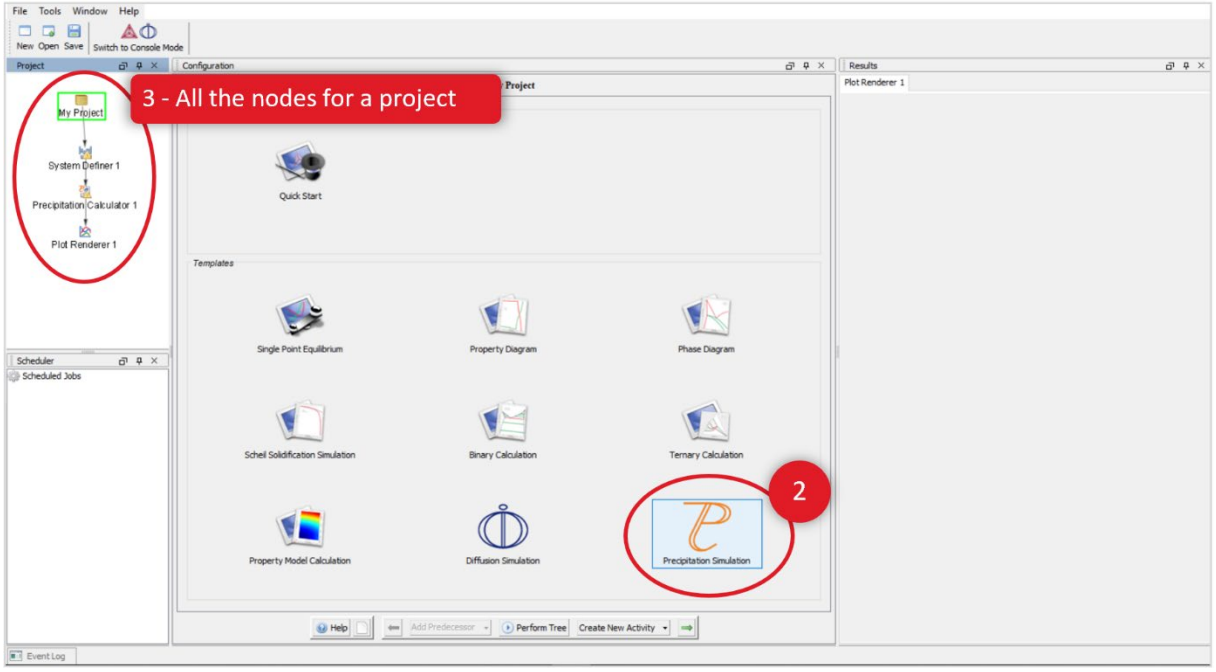


ABOUT THE EXAMPLE

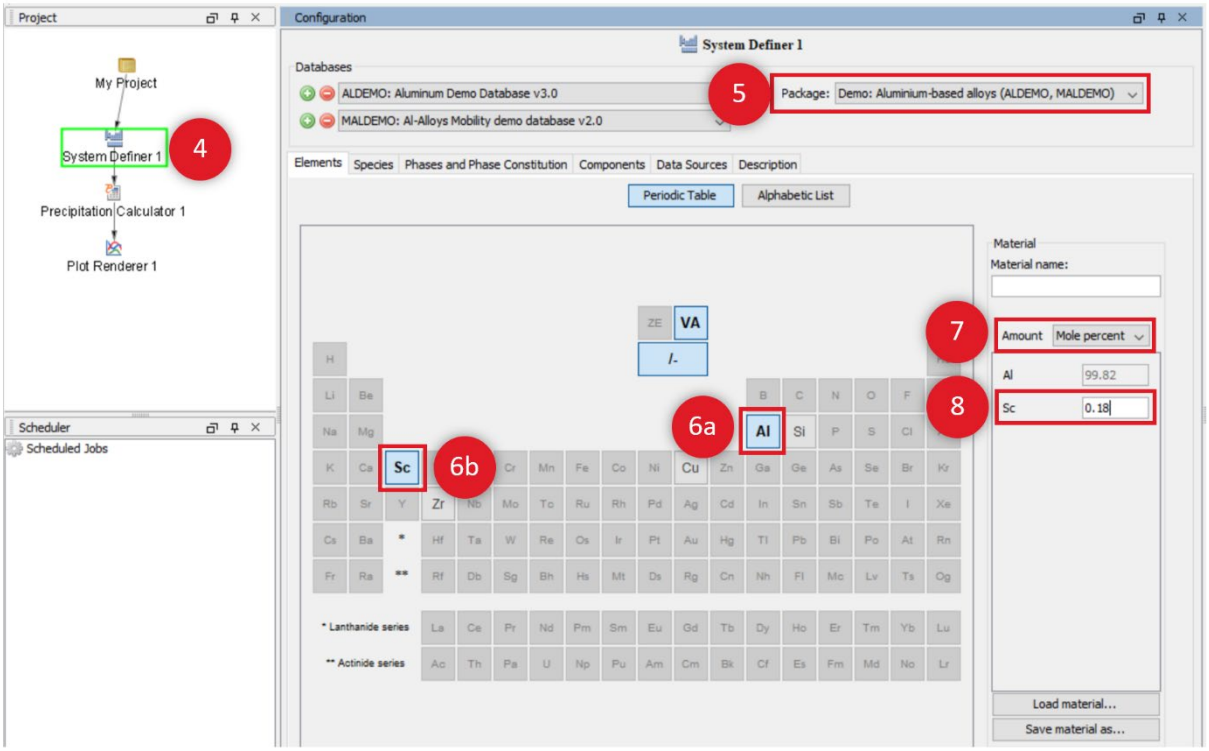
This example simulates the kinetics of precipitation of Al_3Sc from an FCC_A1 solution phase.

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. Click the **System Definer 1** node.
5. Set the database package to **DEMO: Aluminium based alloys**, which loads both thermodynamic and kinetic demonstration aluminium databases.
6. From the periodic table, select the elements **Al** (aluminium) then **Sc** (scandium). Be sure to select Al first so that it is the dependant element.
7. Just to the right of the periodic table, select **Mole Percent** as the **Amount**.
8. Enter `0.18` for **Sc**. This automatically sets **Al** to 99.82.



Our system is now defined, but before we start the precipitation calculation, we will do a quick one axis calculation to find the phases present around 350°.

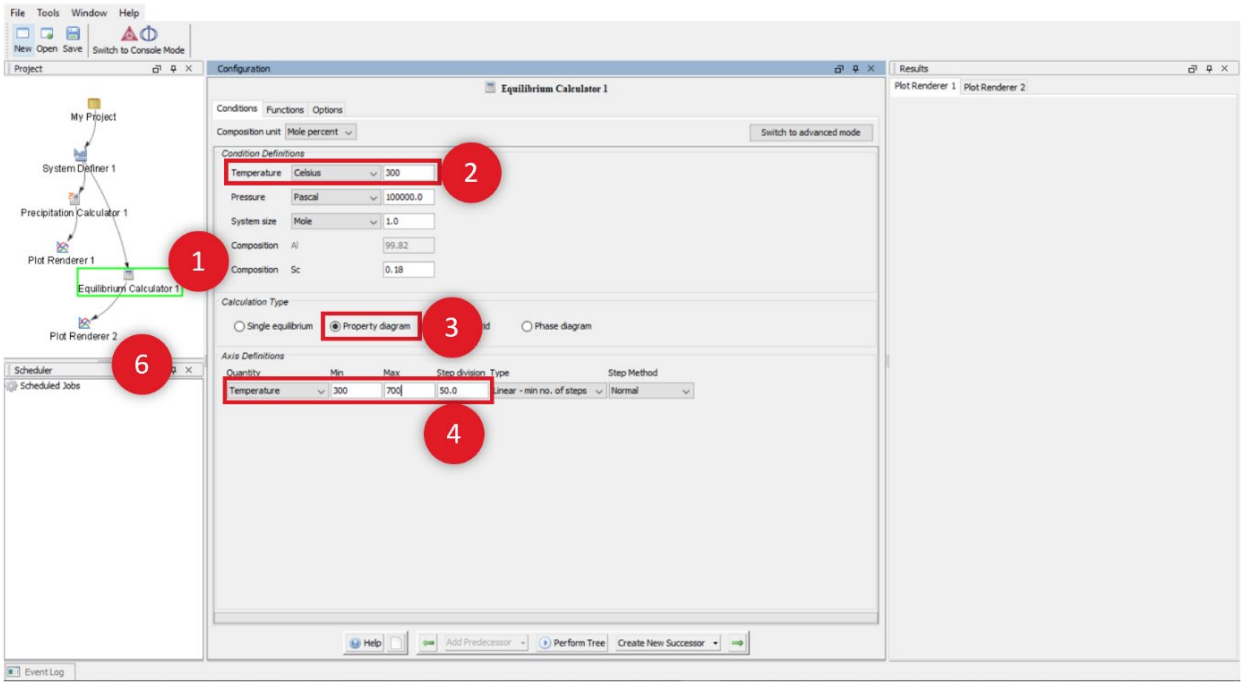
ONE AXIS CALCULATION

Why We Do This

In order to set up an isothermal precipitation calculation, we need to know which phases are present at 350°. A *one axis* calculation gives us this information.

Setting up a One Axis Calculation

1. In the **Project** window, right-click the **System Definer 1** node, and from the **Create New Successor** menu select **Equilibrium Calculator**.
2. In the **Configuration** window, select a **Temperature** in **Celsius** and enter 300.
3. Under *Calculation Type*, select **One axis**.
4. We are looking for the phases present around 350 degrees, so under *Axis Definitions* enter the **Temperature** range from **Min** 300 to **Max** 700 to capture the temperature wanted.
5. Keep the default values for everything else.
6. Our system is now defined.



7. Right-click the **Equilibrium Calculator** node and select **Create New Successor>Plot Renderer**.
8. In the **Project** window, right-click the **Plot Renderer 2** node you just created and select **Perform Now**.

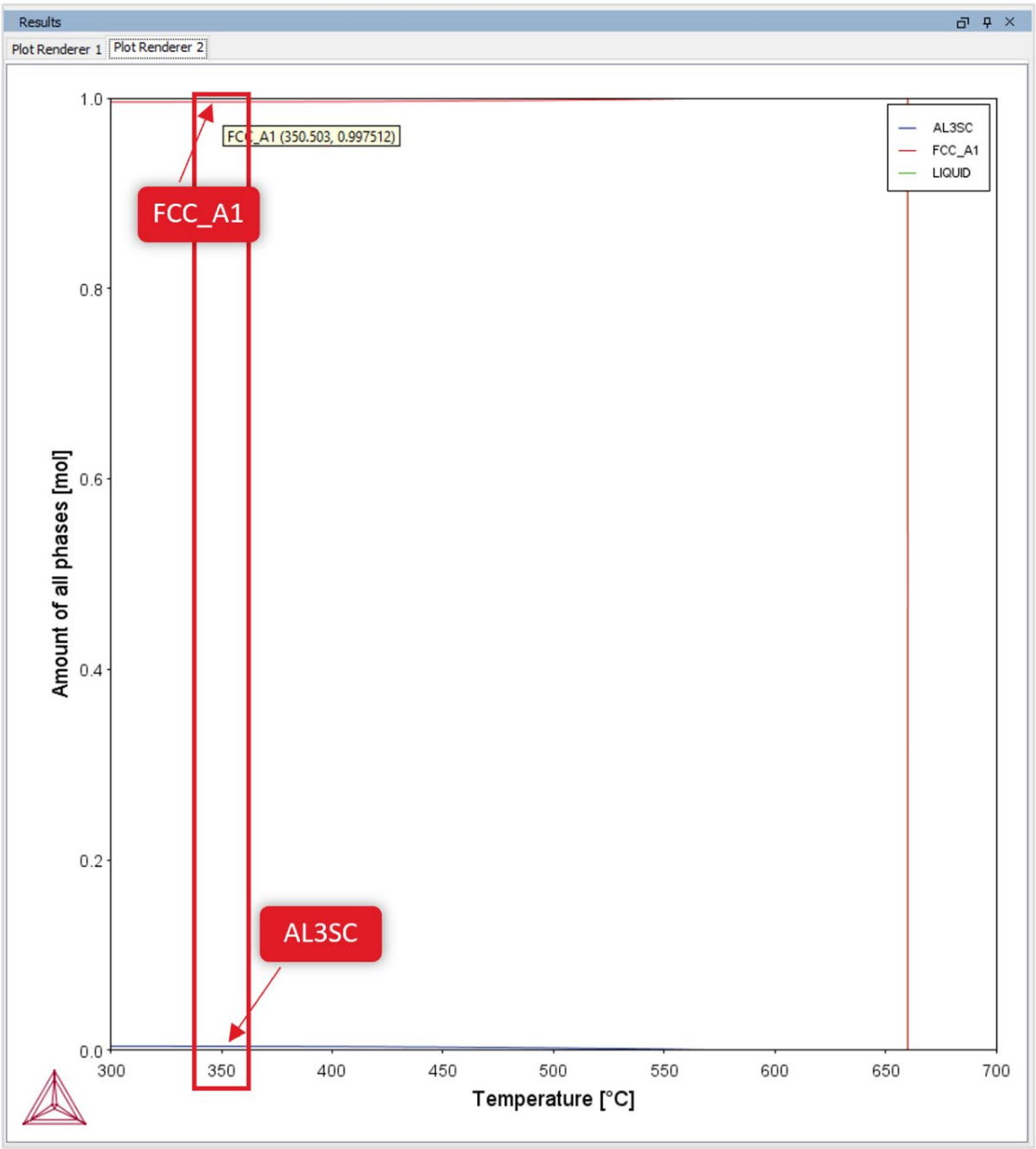
Interpreting the Results of the One Axis Calculation

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 we will use them in our precipitation calculation.



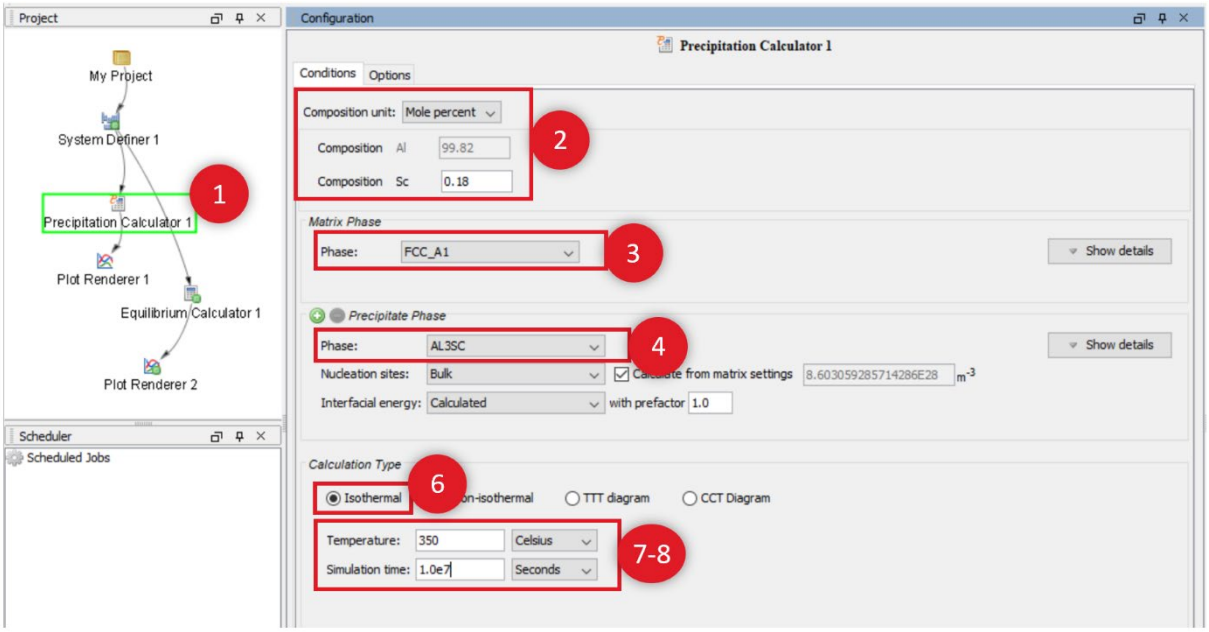
PRECIPITATION CALCULATION

Setting up the Precipitation Calculation

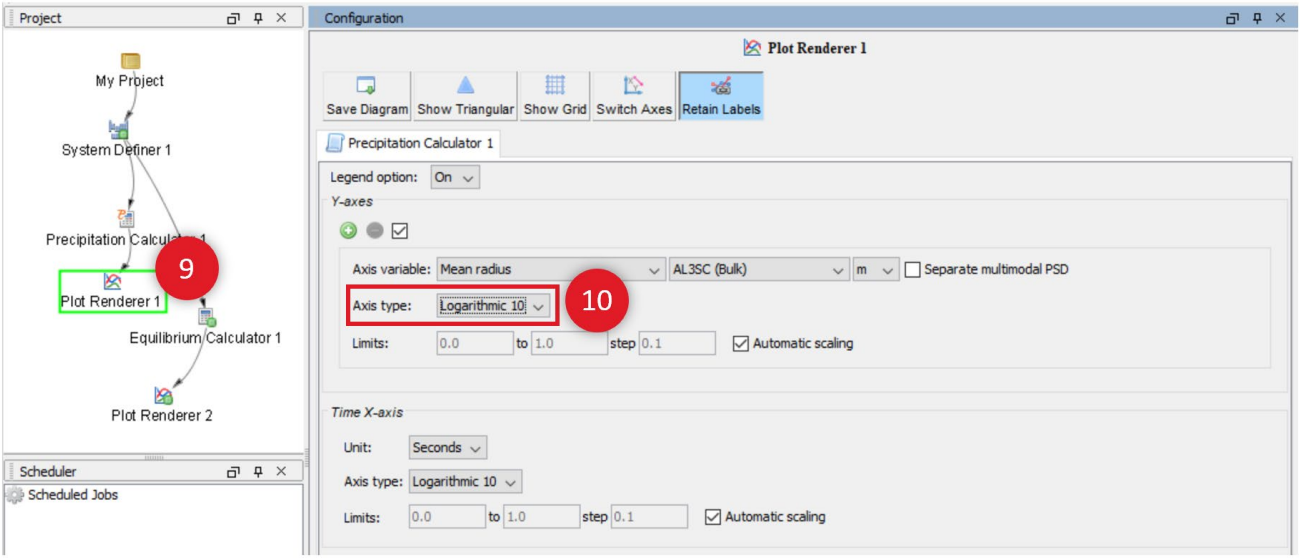
1. In the **Project** window, click the **Precipitation Calculator 1** node.
2. Notice that the composition we set in the *System Definer* auto-populated here.
3. Under *Matrix Phase*, select **FCC_A1**, which is the primary phase we saw present in the one axis calculation.

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

4. Under *Precipitate Phase* select **AL3SC** from the **Phase** menu because that is the other phase present around 350°, 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 `350` as the **Temperature** and select **Celsius**.
8. Enter `1.0E7` as the **Simulation time** and select **Seconds**, which is ten million seconds.

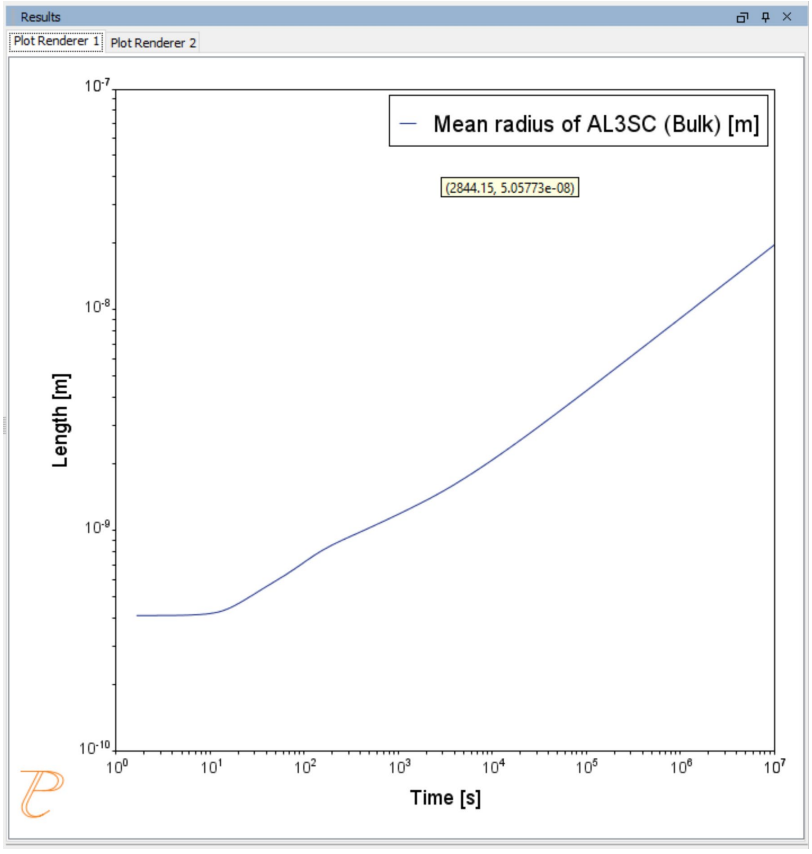


9. In the **Project** window, click the **Plot Renderer 1** node.
10. Under *Y-axes*, from the **Axis type** menu select **Logarithmic 10** for a better view of the plot.
11. Click **Perform** at the bottom, centre of the **Configuration** window.



Interpreting the Results of the Precipitation Calculation

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



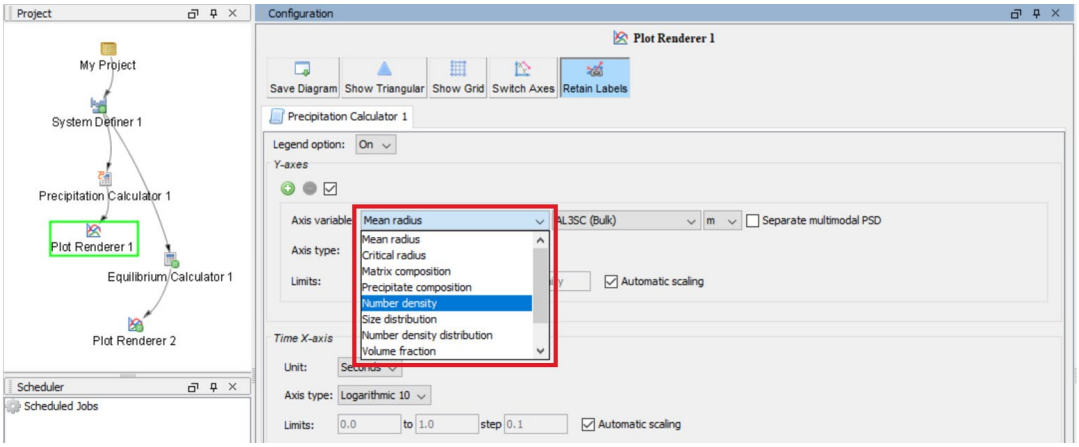
This plot shows the Mean radius of the AL3SC precipitate as a function of time.

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. In the *Y-axes* section, select the **Axis variable** menu to see what other options are available.
3. Once you have made your selection, click **Perform** at the bottom, centre of the **Configuration** window to create a new plot.



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 1053K where only the carbide M23C6 is stable according to the equilibrium calculation. The Precipitation Calculator is used to do an isothermal calculation of the three phases (cementite, M23C6 and M7C3) where cementite and M7C3 are metastable phases.

Project File Information

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

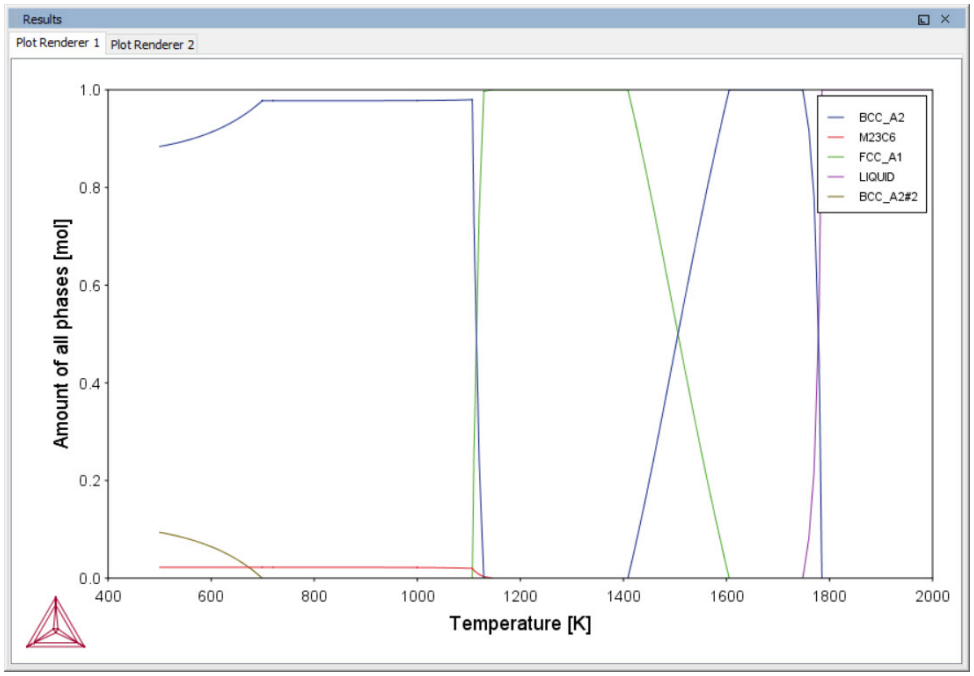
Example Settings

System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO,MFEDEMO)
Elements	Fe, C, Cr
Conditions (Precipitation Calculator)	
Composition	Fe-0.1C-12Cr Mass percent
Matrix phase	BCC_A2
Precipitate phases	Cementite, M23C6 and M7C3
Matrix Phase Data Parameters (Precipitation Calculator)	
Grain size (click **Show details** to display this setting)	1.0E-4 m
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Grain boundaries
Interfacial energy	Cementite 0.167 J/m^2, M23C6 0.252 J/m^2, M7C3 0.282

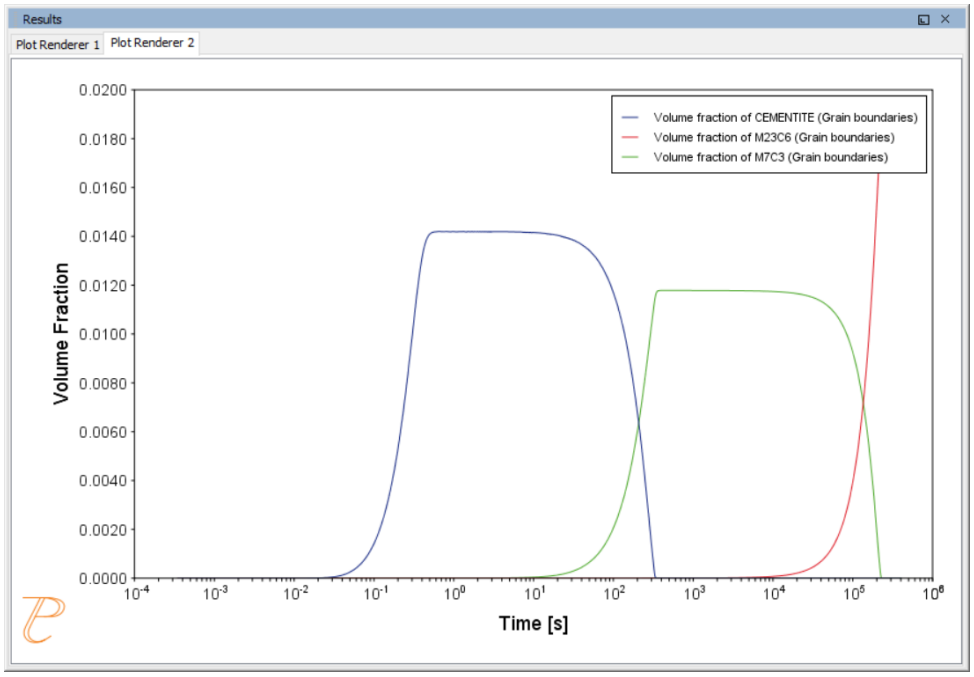
	J/m^2
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	1053 K
Simulation time	400 000 seconds

PLOT RESULTS

Equilibrium Calculator: How the phases change with temperature



Precipitation Calculator: Volume fractions



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.

Project File Information

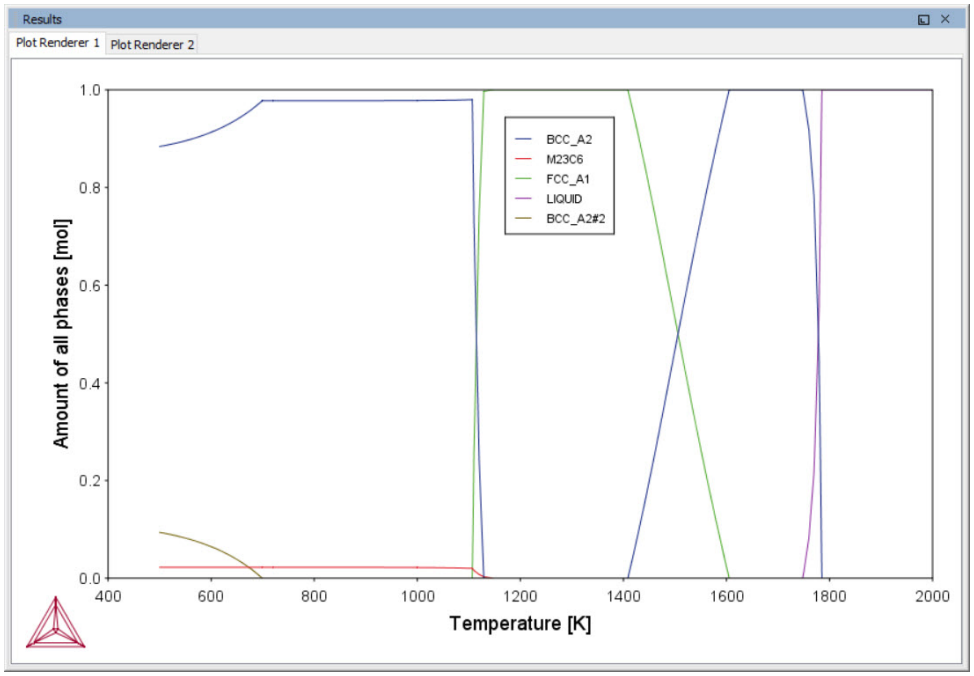
- Folder: Precipitation Module - TC-PRISMA
- File name: *P_03_Precipitation_Fe-C-Cr_TTT_Cementite-M7C3-M23C6.tcu*

Example Settings

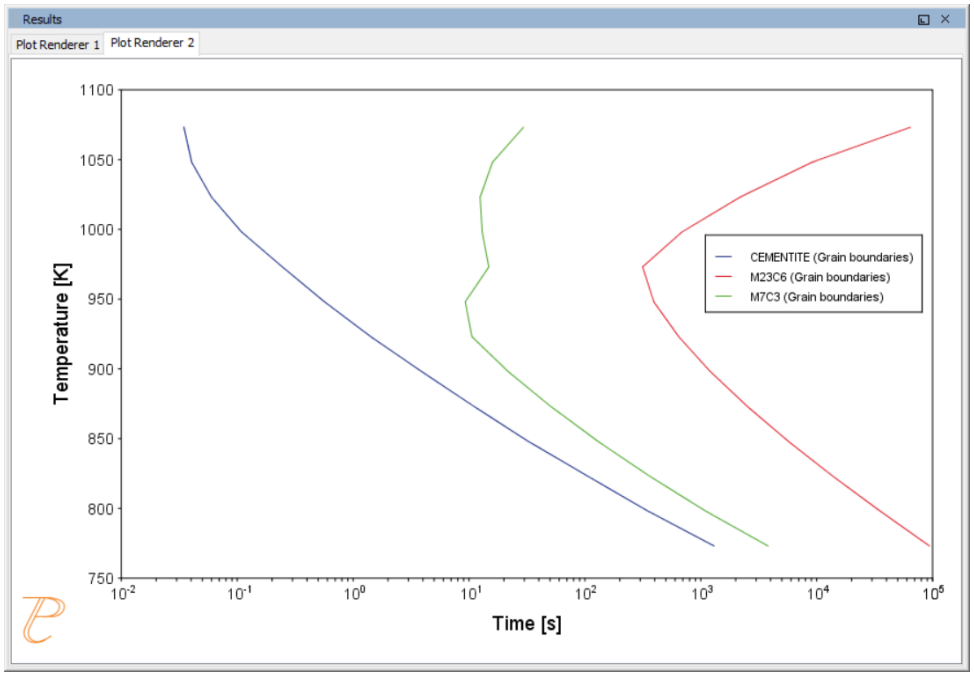
System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO)
Elements	Fe, C, Cr
Conditions (Precipitation Calculator)	
Composition	Fe-0.1C-12Cr Mass percent
Matrix phase	BCC_A2
Precipitate phases	Cementite, M23C6 and M7C3
Matrix Phase Data Parameters (Precipitation Calculator)	
Grain size (click **Show details** to display this setting)	1.0E-4 m
Precipitate Phase Data Parameters	
Nucleation sites	Grain boundaries
Interfacial energy	Cementite 0.167 J/m^2, M23C6 0.252 J/m^2, M7C3 0.282 J/m^2
Calculation Type (Precipitation Calculator)	
Calculation type	TTT diagram
Temperature	500° to 800° C with 25° C steps
Max. annealing time	1.0E8 seconds
Stop criteria	Volume fraction of phase is set to 0.0001
Options > Numerical Parameters	
No. of grid points over one order of magnitude in radius	150
Max no. of grid points over one order of magnitude in radius	200
Min no. of grid points over one order of magnitude in radius	100

PLOT RESULTS

Equilibrium Calculator: How the phases change with temperature



Precipitation Calculator: TTT diagram



P_04: Precipitation of Iron Carbon Cementite

Simulate the kinetics of precipitation of carbides from a BCC Fe solution phase. This example is based on Wert (1949)[1].

This example uses two Experimental File Reader activities with the Precipitation Calculator and an isothermal calculation, to plot the volume fraction of the cementite phase.

Project File Information

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

Example Settings

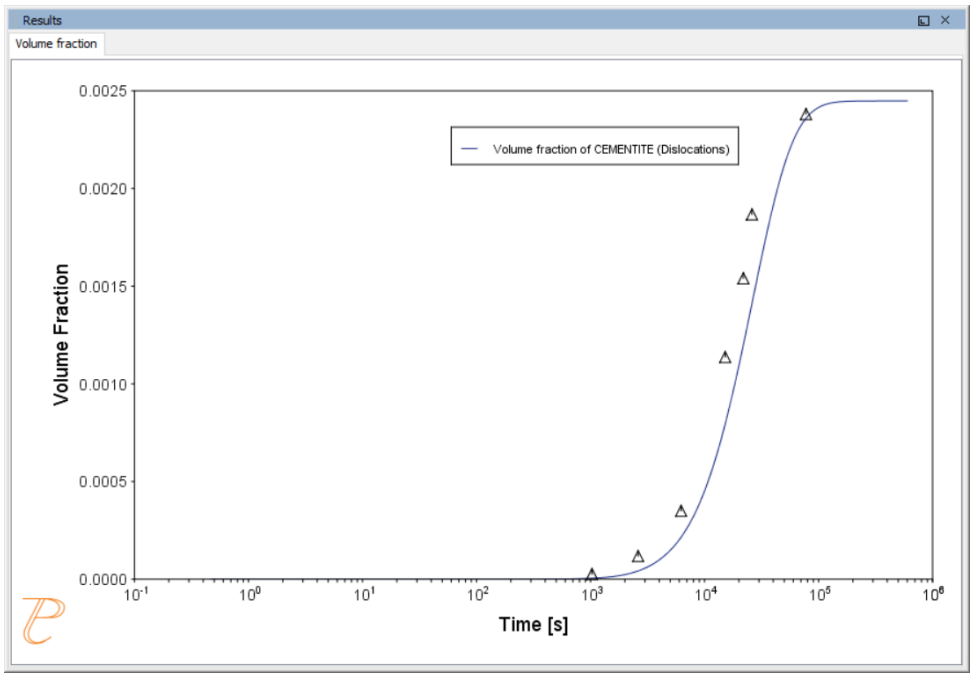
System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO)
Elements	Fe, C
Conditions (Precipitation Calculator)	
Composition	Fe-0.016C mass percent
Matrix phase	BCC_A2
Precipitate phase	Cementite
Matrix Phase Data Parameters (Precipitation Calculator)	
Grain aspect ratio (click **Show details** to display this setting)	1.0

1. Wert, Charles A. 1949. "Precipitation from Solid Solutions of C and N in α-Iron." Journal of Applied Physics 20 (10). AIP Publishing: 943.

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

PLOT RESULTS

Volume Fraction



P_05: Precipitation of γ' in Ni Superalloys - Isothermal

This example simulates the kinetics of precipitation of γ' phase from γ phase. The simulation results can be compared with experimental data collected from Sudbrack et al. (2008)[1].

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.

PROJECT FILE INFORMATION

- Folder: Precipitation Module - TC-PRISMA

1. Sudbrack, Chantal K., Tiffany D. Ziebell, Ronald D. Noebe, and David N. Seidman. 2008. "Effects of a Tungsten Addition on the Morphological Evolution, Spatial Correlations and Temporal Evolution of a Model Ni–Al–Cr Superalloy." Acta Materialia 56 (3): 448–63.

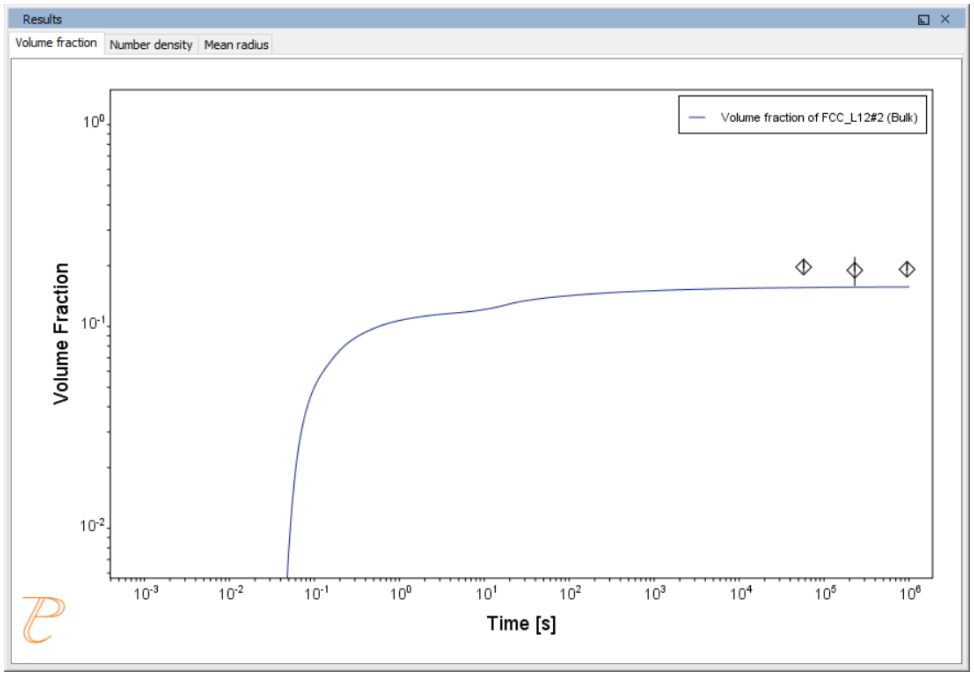
- File name: *P_05_Precipitation_Ni-Al-Cr_Isothermal_Gamma-Gamma_prime.tcu*

EXAMPLE SETTINGS

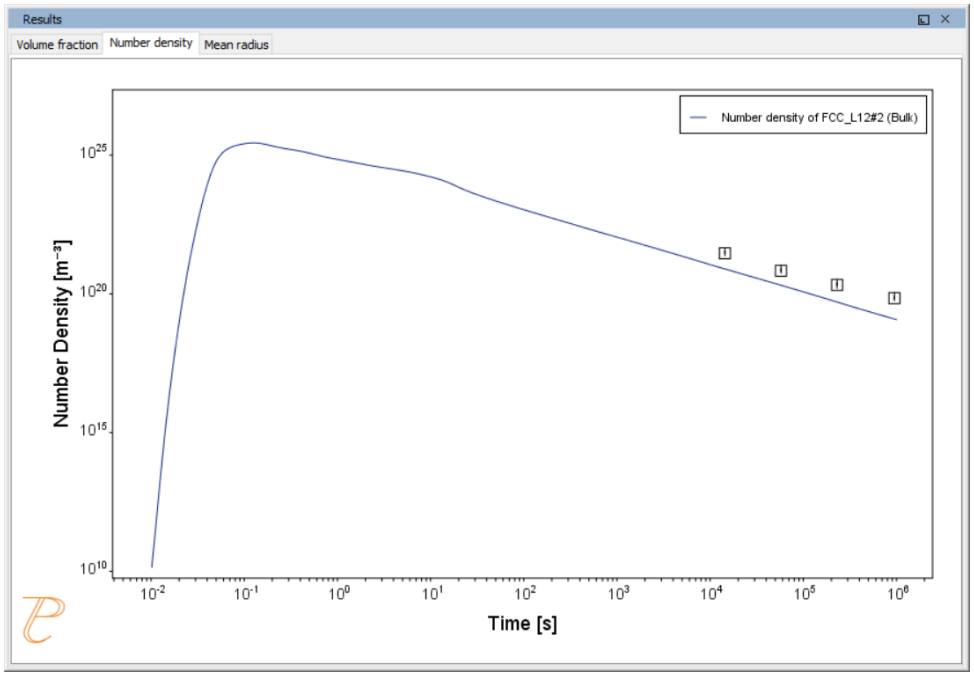
System (System Definer)	
Database package	Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO)
Elements	Ni, Al Cr
Conditions (Precipitation Calculator)	
Composition	Ni-9.8Al-8.3Cr Mole percent
Matrix phase	DIS-FCC_A1 (see note above about how to select this phase)
Precipitate phase	FCC_L12#2
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk
Interfacial energy	0.012 J/m^2
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	800° C
Simulation time	1 000 000 seconds

PLOT RESULTS

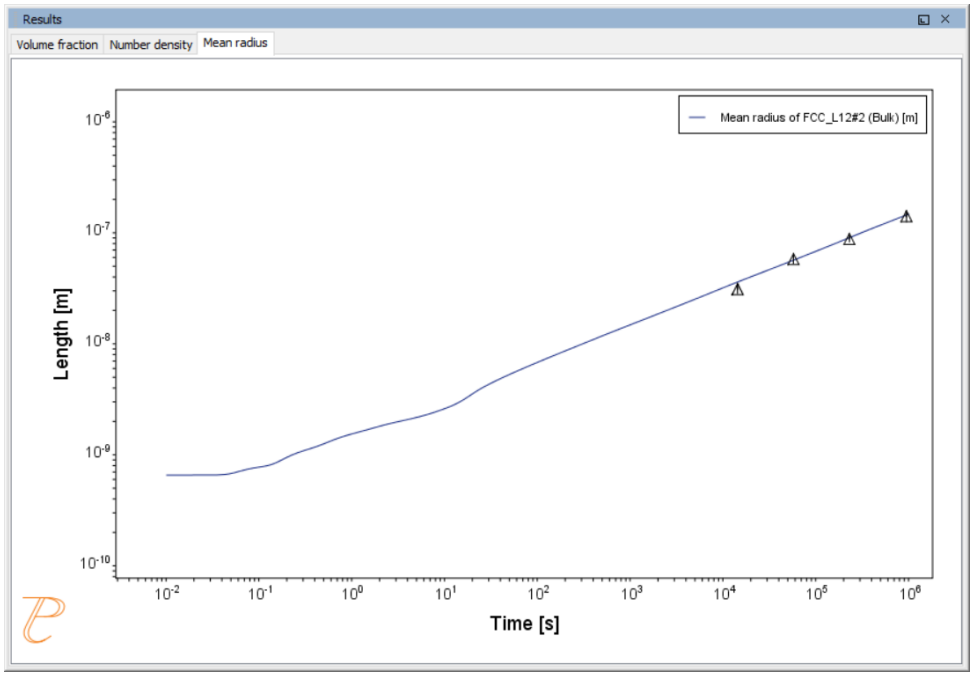
Volume Fraction



Number Density



Mean Radius



P_06: Precipitation of γ' in Ni Superalloys - Non-isothermal

This example simulates the kinetics of precipitation of γ' phase from 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. (2013)[1].

When you run (Perform) this example, it takes about 10 minutes for the calculations to complete.

DIS_FCC_A1 needs to be selected on the System Definer.

1. Rojhirunsakool, Tanaporn, S. Meher, J. Y. Hwang, S. Nag, J. Tiley, and Rajarshi Banerjee. 2013. "Influence of Composition on Monomodal versus Multimodal Γ' Precipitation in Ni–Al–Cr Alloys." Journal of Materials Science 48 (2): 825–31.

Project File Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_06_Precipitation_Ni-Al-Cr_Non-isothermal_Gamma-Gamma_prime.tcu*

Example Settings

In these examples a linear, continuously cooling condition is set up. This is done on the Precipitation Calculator settings window in the **Calculation Type** section:

1. Select a **Non-Isothermal**.
2. Select a **Temperature Unit** and **Time Unit** from the lists.
3. Click **Thermal Profile**, where **Time-Temperature** profile points are entered to describe the stepwise heat treatment schedule with linear segments. Up to 999 rows of data points can be entered.

   In these examples two rows of data points are needed for starting time 0s and temperature 1150° C, as well as end time 3300s and temperature 380° C.

4. Click the **Plot Renderer** node to select the **Separate multimodal PSD** check box.

   Plotting the size distribution from the final simulation time of 3300 seconds, you can see there are several peaks, although these are not completely separated. As above, select the **Separate multimodal PSD** check box to separate the peaks.

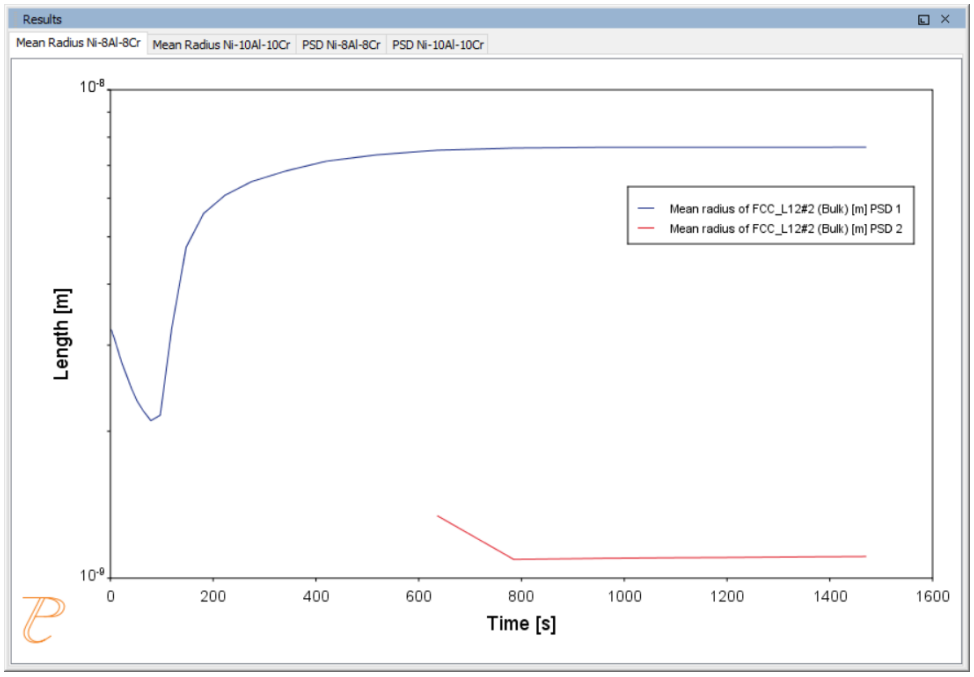
5. Adjust the **Valley depth ratio** setting to 0.05 to separate into two peaks as shown in the Ni-10Al-10Cr plot example. You can experiment with this setting to see how the size distribution evolves with time, for example, try entering several values as plot times **400 600 3300**.

System (System Definer)	
Database package	Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO)
Elements	Ni, Al, Cr
Conditions (Precipitation Calculator)	
Composition (Ni-8Al-8Cr)	Ni-8Al-8Cr Mole percent
Composition (Ni-10Al-10Cr)	Ni-10Al-10Cr Mole percent

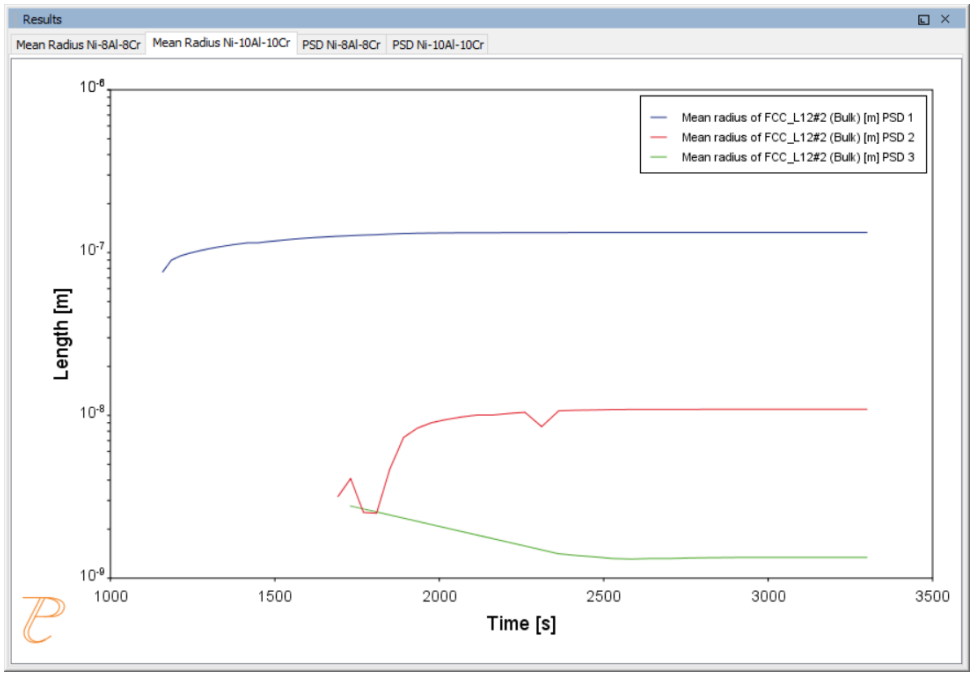
Matrix phase	DIS_FCC_A1 (see note above about how to select this phase)
Precipitate phase	FCC_L12#2
Matrix Phase Data Parameters (Precipitation Calculator)	
Mobility enhancement prefactor (click **Show details** to display this setting)	5.0
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk
Interfacial energy	0.023 J/m^2
Calculation Type (Precipitation Calculator)	
Calculation type	Non-isothermal
Temperature unit	Celsius
Time unit	Seconds
Simulation time (Ni-8Al-8Cr)	1470 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. 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.

PLOT RESULTS

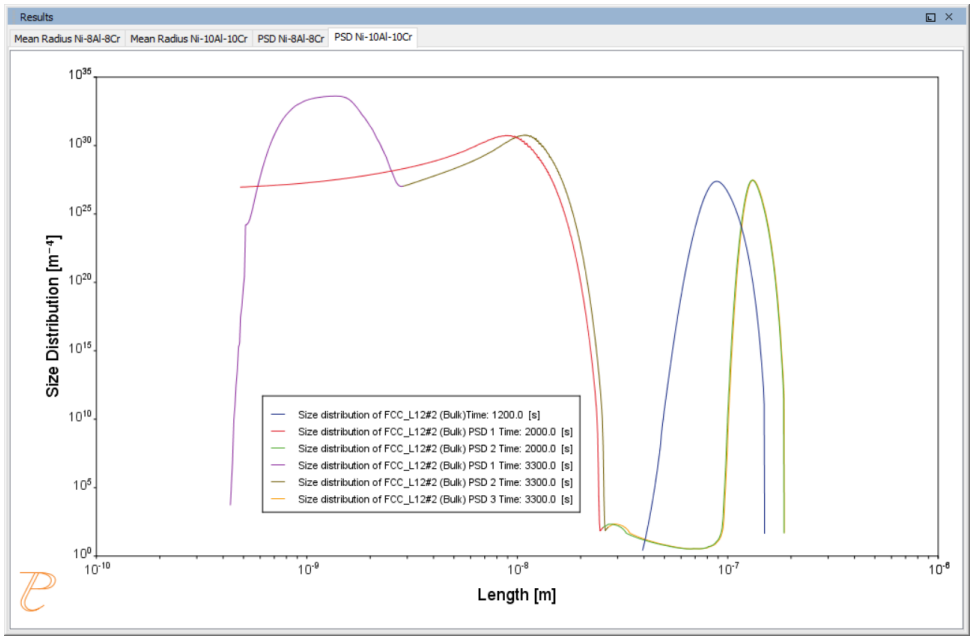
Mean Radius Ni-8Al-8Cr



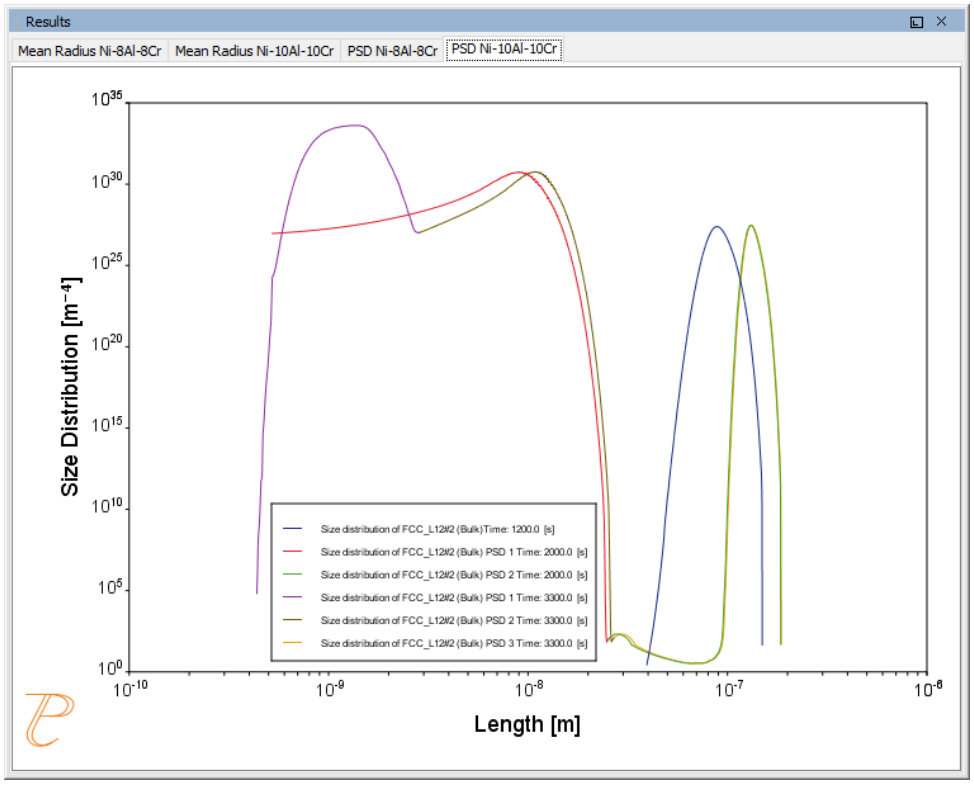
Mean Radius Ni-10Al-10CR



Size Distribution (PSD) Ni-8Al-8Cr



Size Distribution (PSD) Ni-10Al-10Cr



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

In this example, a Continuous Cooling Transformation (CCT) diagram for a Ni-10Al-10Cr γ-γ' alloy is calculated and plotted with superimposition of the cooling rate values.

Project File, Step-By Step Instructions and Video Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_07_Precipitation_Ni-Al-Cr_CCT_Gamma-Gamma_prime.tcu*

This example is available as a video tutorial on our website and YouTube channel.

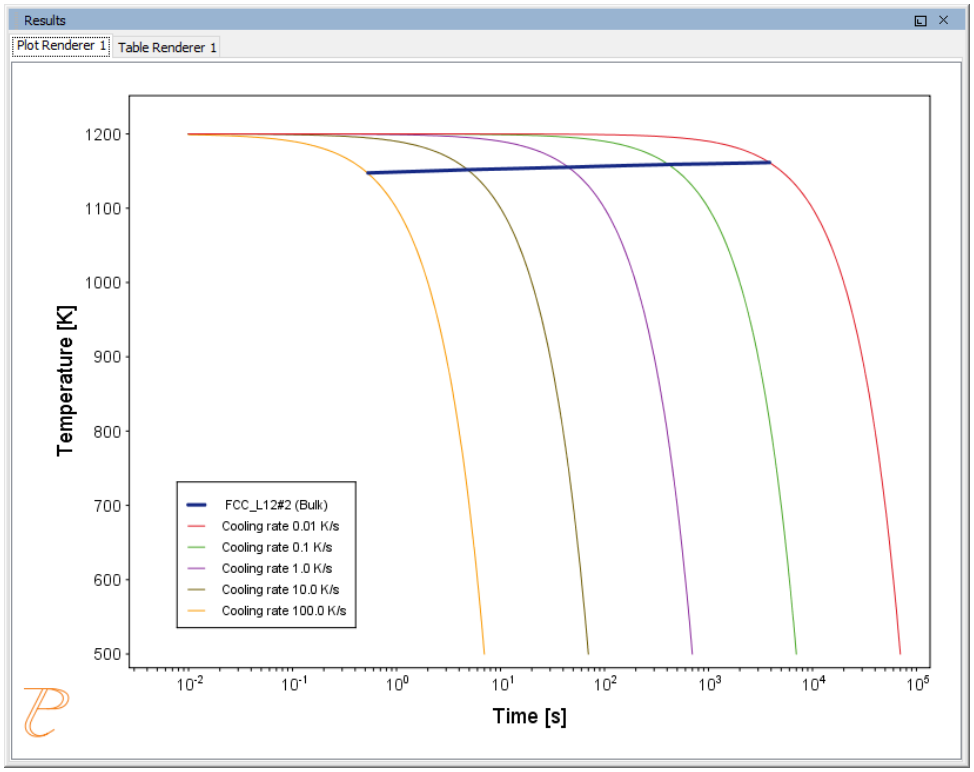
You can also use the step-by-step instructions included in a PDF to follow the video or compare to the project file in Thermo-Calc.

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

Plot and Table Results



Results

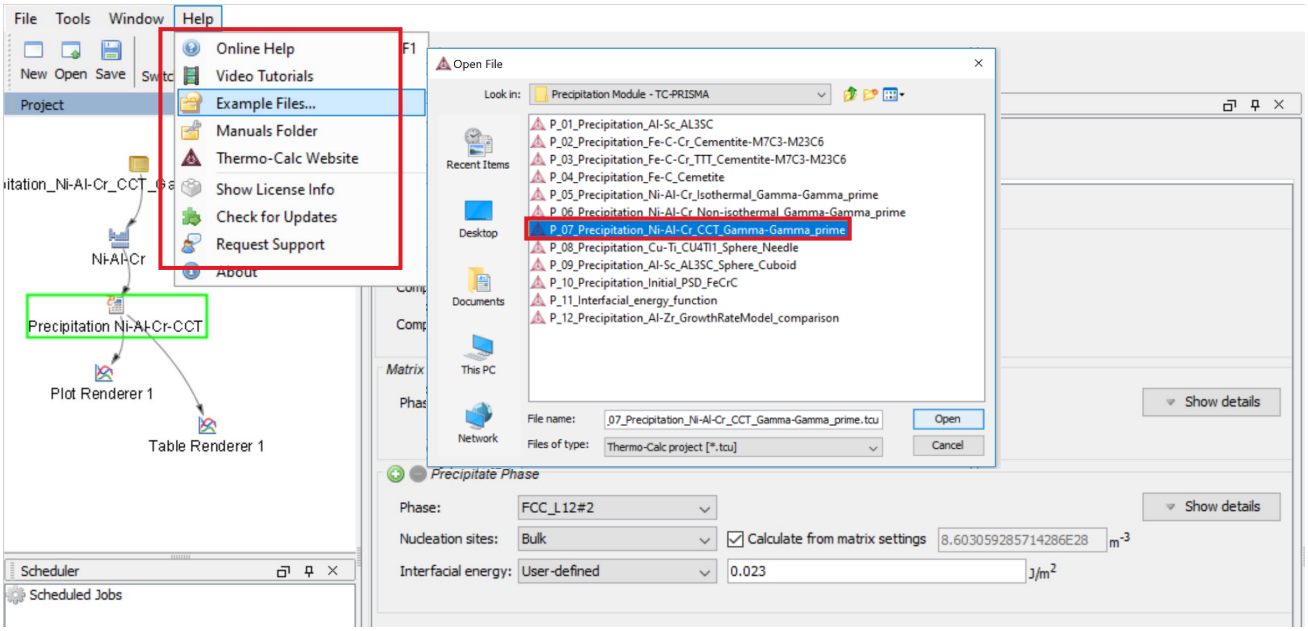
Plot Renderer 1 | Table Renderer 1

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

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 centre of the **Configuration** window in Thermo-Calc.



ABOUT THE EXAMPLE

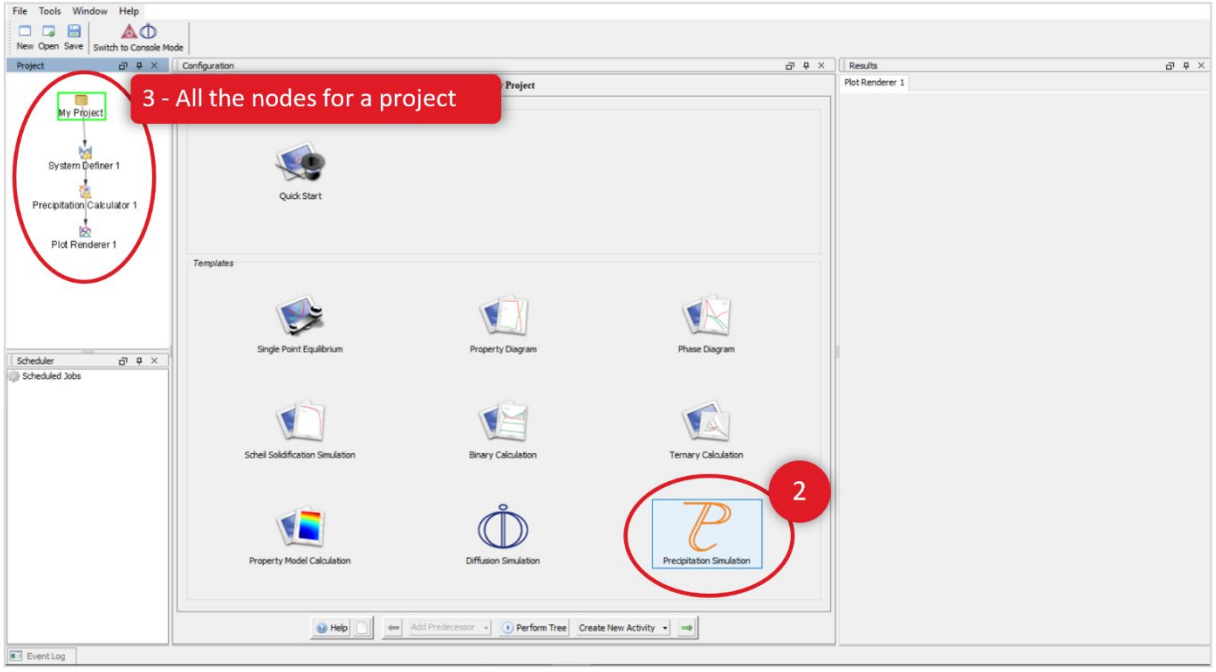
This example shows you how to simulate a CCT diagram for gamma prime (γ') precipitation in a Ni-Cr-Al alloy using the Precipitation module known as TC-PRISMA.

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

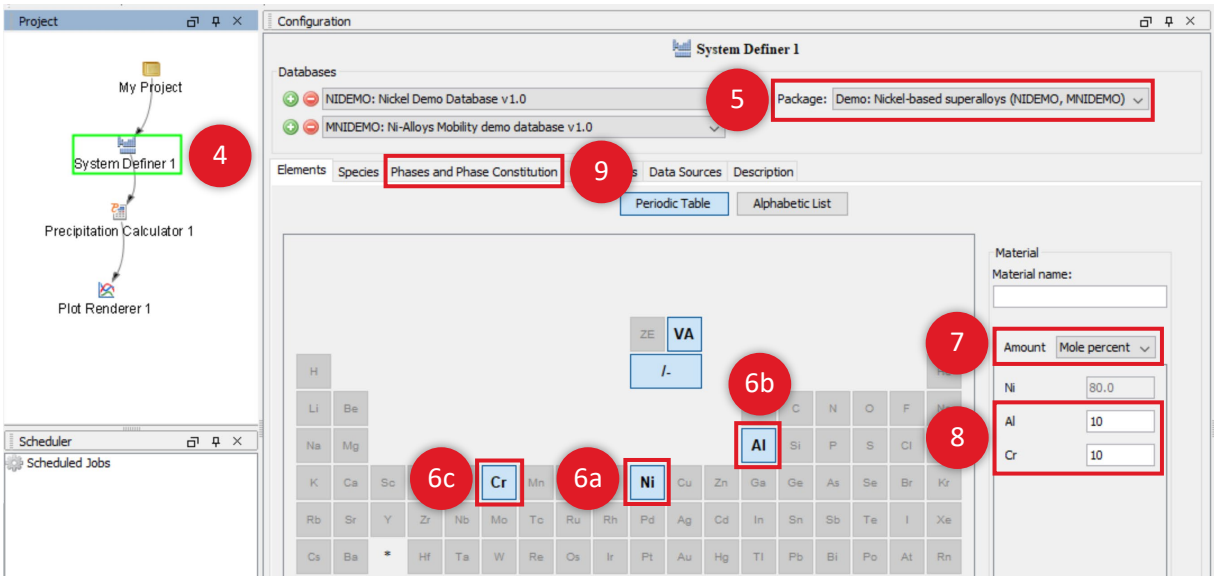
The system is a Ni-10Al-10Cr γ - γ' alloy and it is calculated and plotted with superimposition of the cooling rate values using the Precipitation module (TC-PRISMA).

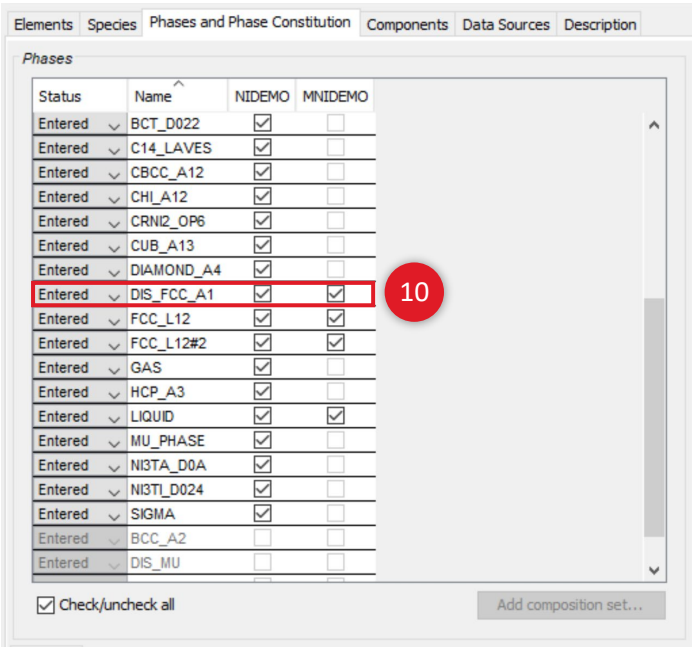
SETTING UP THE SYSTEM

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. Click the **System Definer 1** node.
5. Set the database package to **DEMO: Nickel based superalloys**, which loads both thermodynamic and kinetic demonstration nickel databases.
6. From the periodic table, select the elements **Ni** (nickel), **Al** (aluminium) then **Cr** (chromium). Be sure to select Ni first so that it is the dependant element.
7. Just to the right of the periodic table, select **Mole Percent** as the **Amount**.
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.



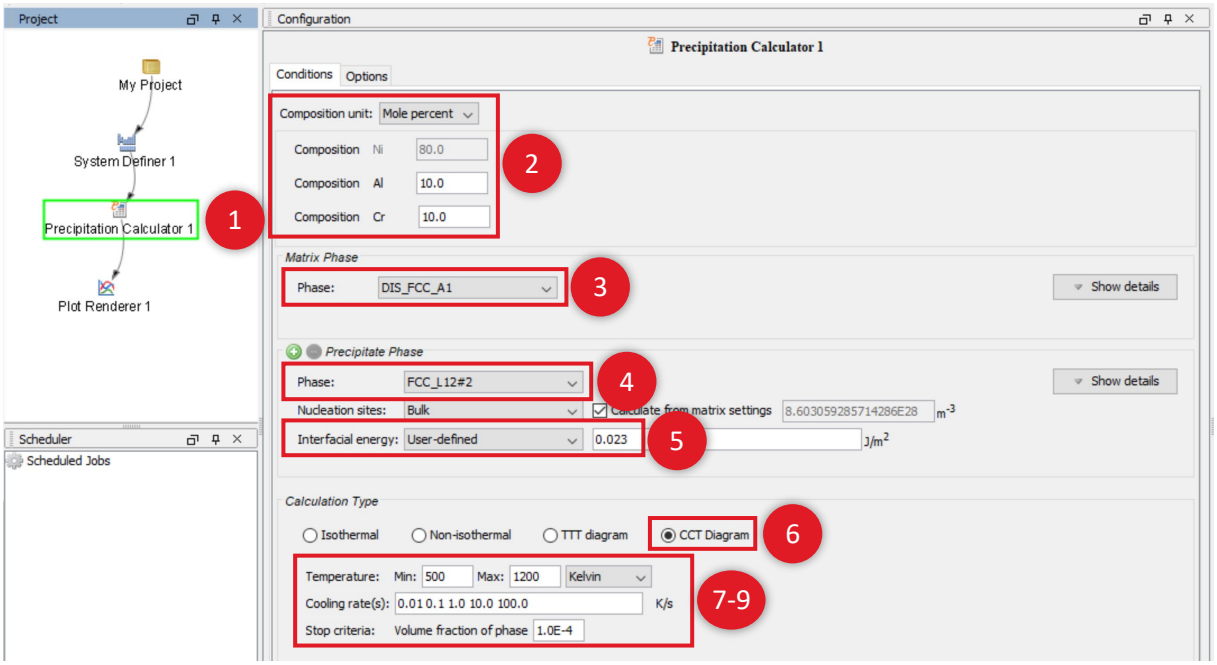


10. Click to select both check boxes next to the disordered FCC phase, **DIS_FCC_A1**.

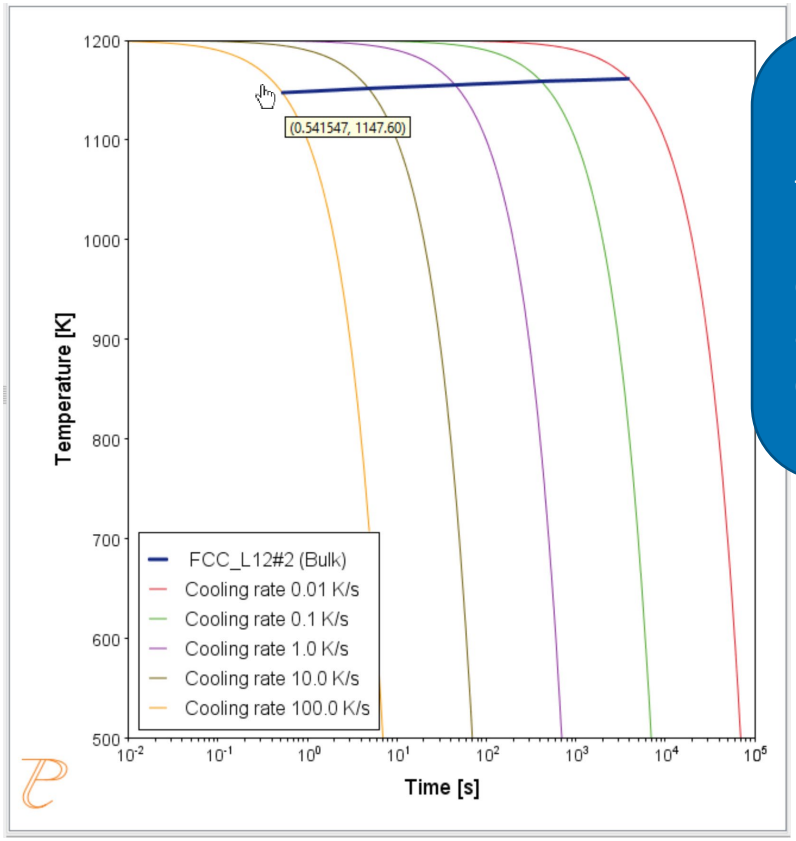
Our system is now defined, so we will set up the precipitation calculation.

SETTING UP THE PRECIPITATION CALCULATION

1. In the **Project** window, click the **Precipitation Calculator 1** node.
2. Notice that the composition we 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*, select **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 the **Min** (minimum) **Temperature** to `500` and the **Max** (maximum) to `1200` and choose **Kelvin** as the temperature unit.
8. We will enter several cooling rates for our calculation. The rates are separated by a space, so enter these values as shown: `.01 .1 1 10 100`.
9. Keep the default **Stop criteria** of `1E-4` volume fraction of the γ' phase.
10. The calculation is now set, so click **Perform CCT Diagram Simulation** at the bottom, centre 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 we 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, we 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

Your 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[1]. The results are compared with experiment results from Kampmann et al[2].

This example takes a few minutes to run.

Project File Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_08_Precipitation_Cu-Ti_CU4TI1_Sphere_Needle.tcu*

Example Settings

To ensure that the settings are done on the correct Precipitation Calculators, the **Sphere** and **Needle** nodes are renamed from **Precipitation Calculator** to match their morphology. The morphology is set in the **Precipitate Phase** section when you click **Show details**.

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

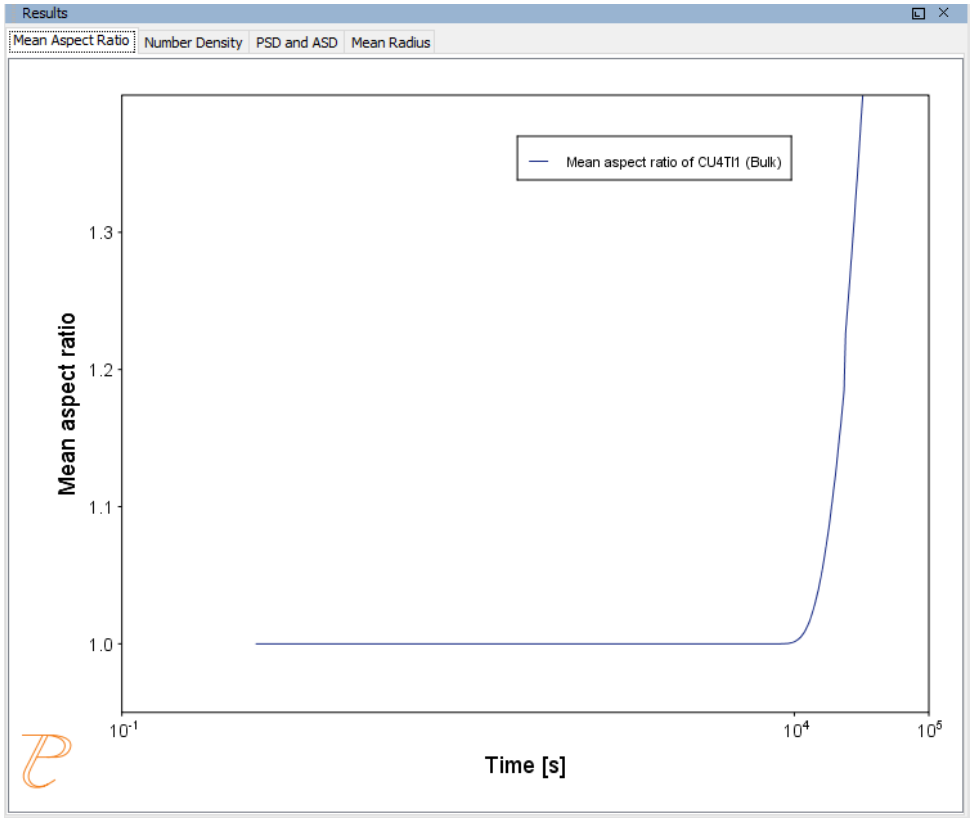
1. Borchers C. 1999. "Catastrophic Nucleation during Decomposition of Cu-0.9at.%Ti." Phil. Mag. A 79(3):537-547

2. Kampmann R., Eckerlebe H., and Wagner R. 1987. "Precipitation Kinetics in Metastab le Solid Solutions - Theoretical Considerations and Application to Cu-Ti Alloys." Mat. Res. Soc. Symp. Proc. 57: 525-542.

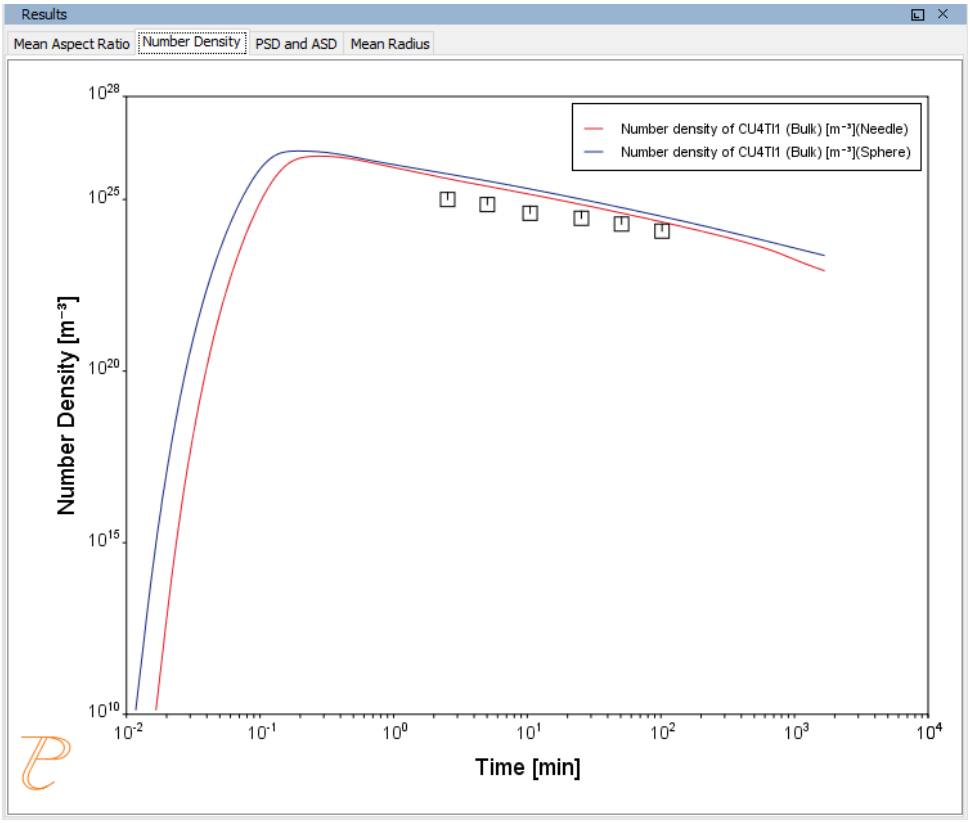
Precipitate phase	CU4TI1
Matrix Phase Data Parameters (Precipitation Calculator)	
Mobility enhancement prefactor (click **Show details** to display this setting)	100
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk
Interfacial energy	The default
Morphology (click **Show 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.

PLOT RESULTS

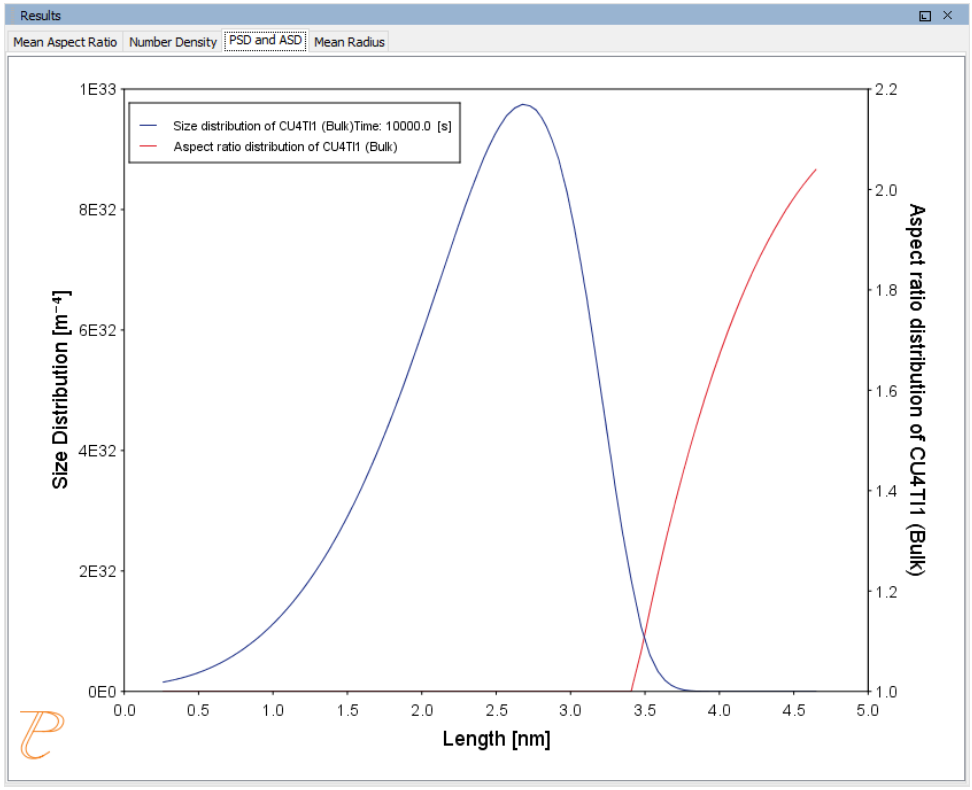
Mean Aspect Ratio



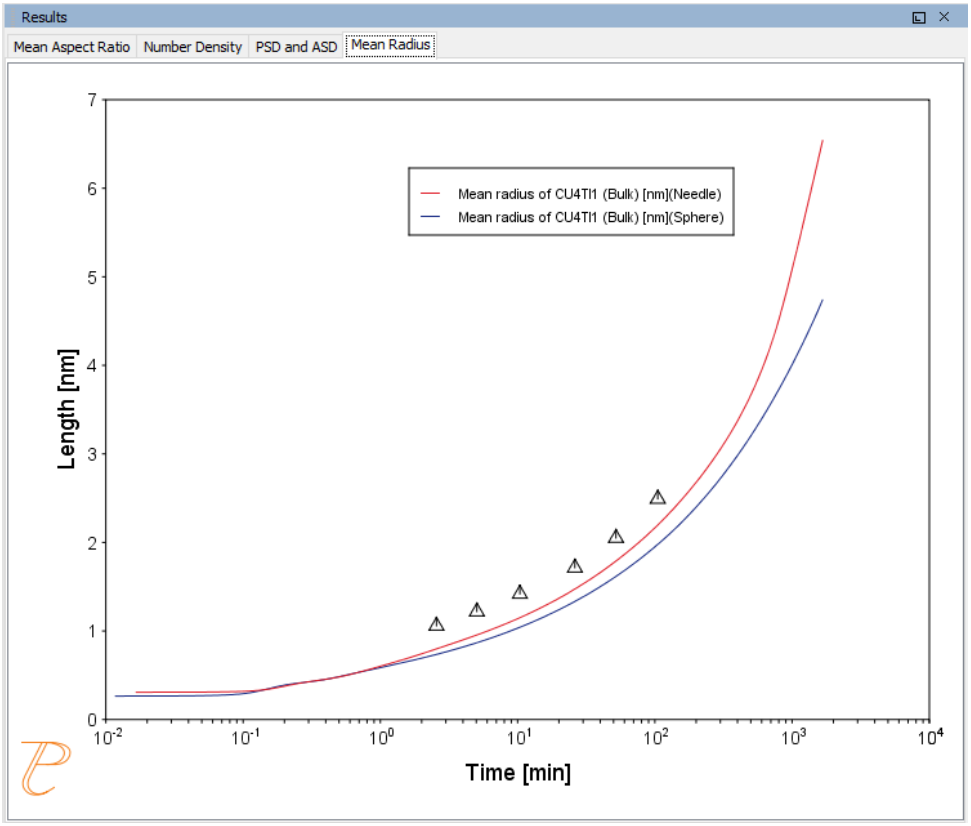
Number Density



PSD and ASD


Results
Mean Aspect Ratio
Number Density
PSD and ASD
Mean Radius
Size distribution of CU4TI1 (Bulk)Time: 10000.0 [s]
Aspect ratio distribution of CU4TI1 (Bulk)
Size Distribution [m⁻⁴]
Aspect ratio distribution of CU4TI1 (Bulk)
Length [nm]
1E33
8E32
6E32
4E32
2E32
0E0
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0

Mean Radius



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[1.] and Novotny and Ardell (2001)[2.]. In addition, mean cubic factor and cubic factor distribution are also plotted for cuboid shape to illustrate the spherical-cuboidal transition during precipitation.

PROJECT FILE, STEP-BY STEP INSTRUCTIONS AND VIDEO INFORMATION

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.

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_09_Precipitation_Al-Sc_AL3SC_Sphere_Cuboid.tcu*

This example is available as a video tutorial on our website and 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

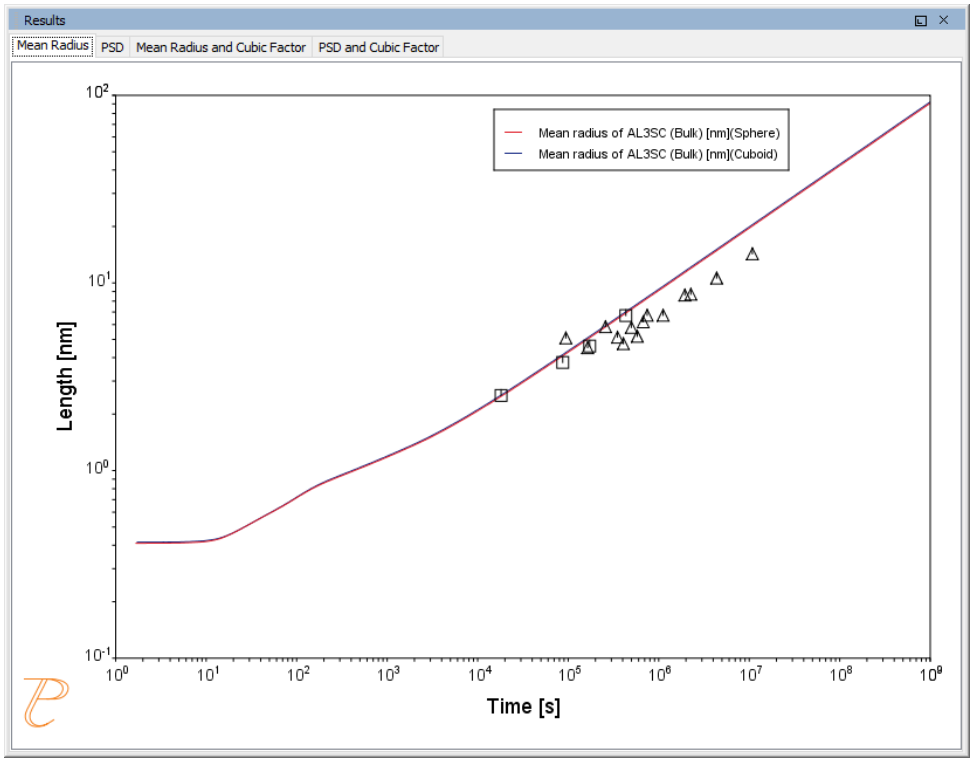
To ensure that the settings are done on the correct Precipitation Calculators, the **Sphere** and **Cuboid** nodes are renamed from **Precipitation Calculator** to match their morphology. The morphology is set in the **Precipitate Phase** section when you click **Show details**. See P_08 for an example 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

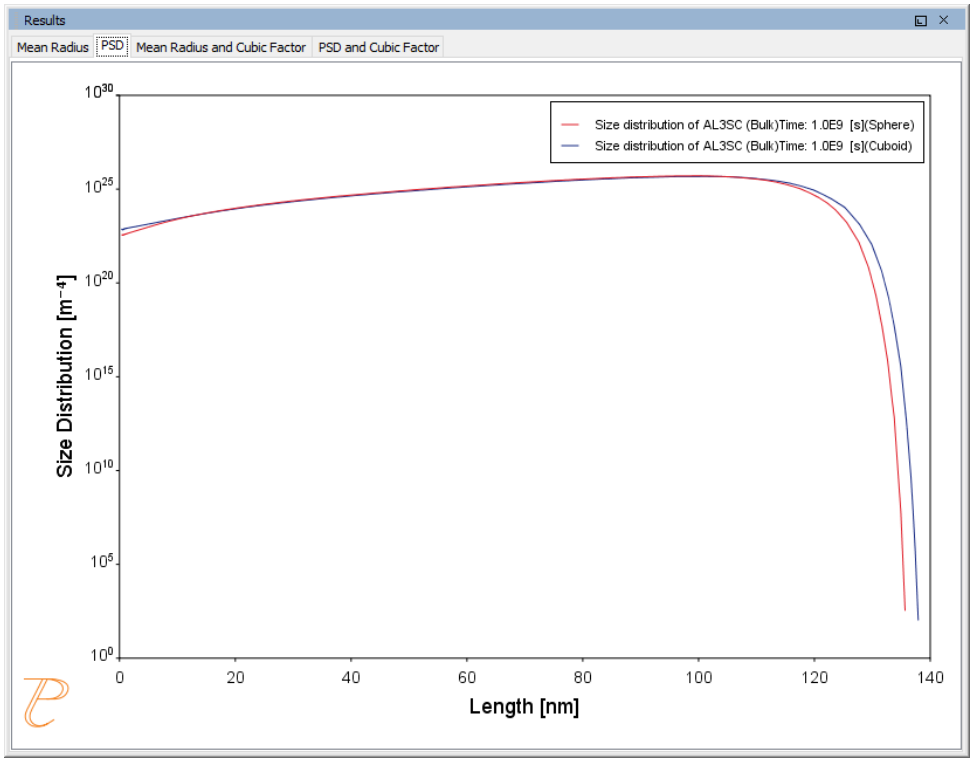
Precipitate phase	AL3SC
Matrix Phase Data Parameters (Precipitation Calculator)	
Elastic properties (click **Show details** to display this setting)	For the **Sphere** node (renamed from Precipitation Calculator), the default, **Disregard** is kept. For the **Cuboid** node (renamed from Precipitation 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.

PLOT RESULTS

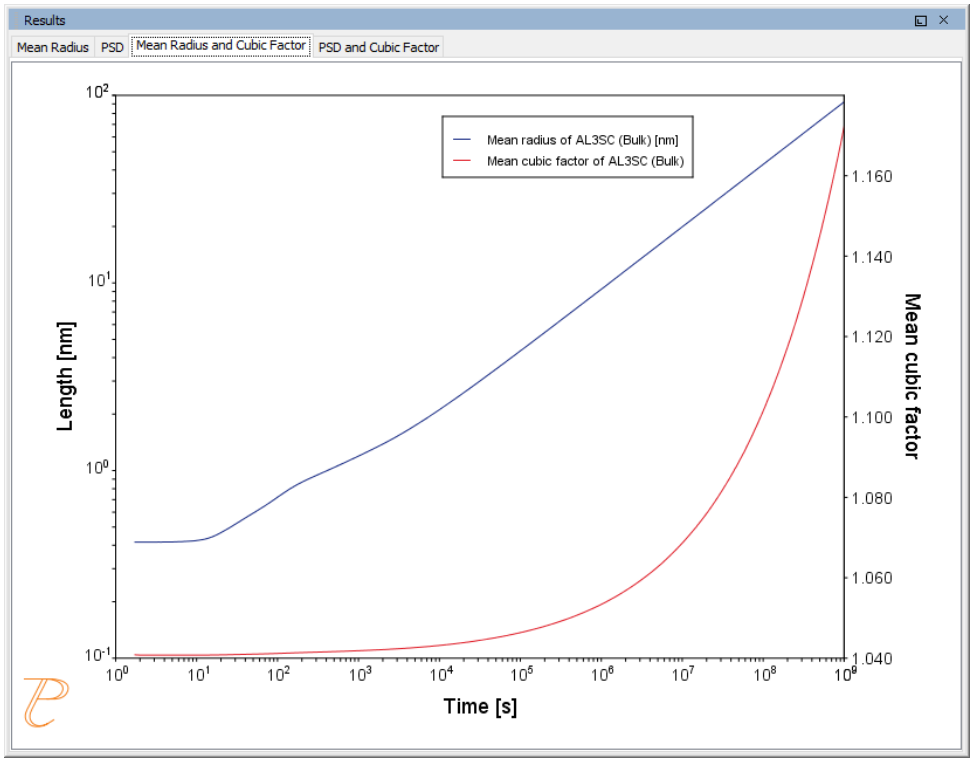
Mean Radius


Results
Mean Radius
PSD
Mean Radius and Cubic Factor
PSD and Cubic Factor
Mean radius of AL3SC (Bulk) [nm](Sphere)
Mean radius of AL3SC (Bulk) [nm](Cuboid)
Length [nm]
Time [s]

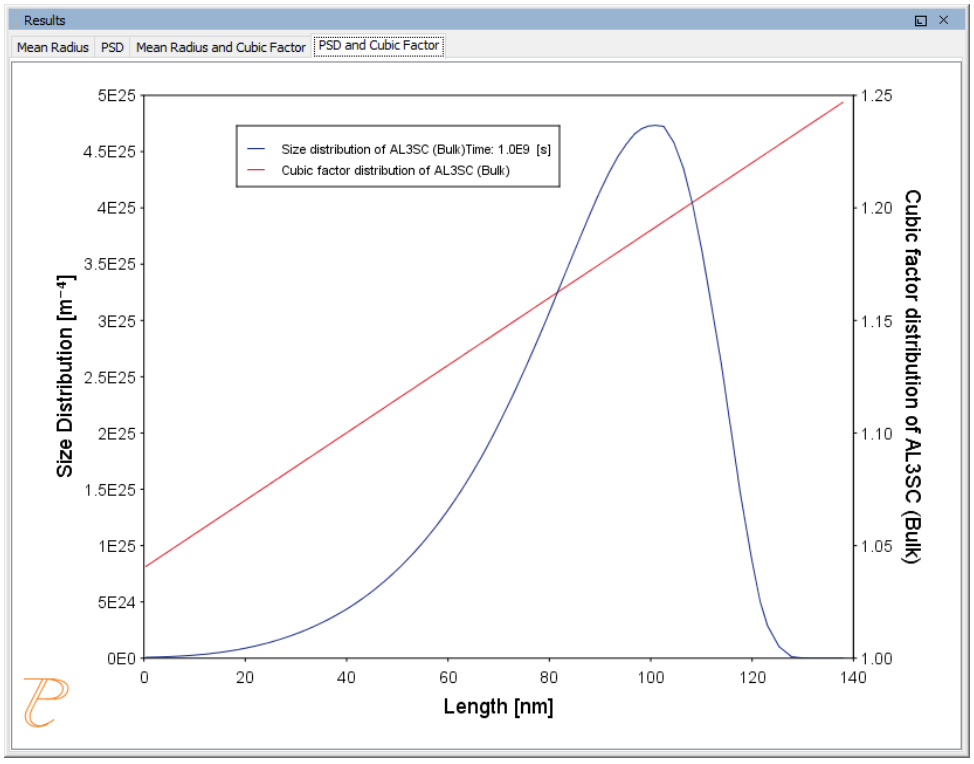
PSD


Results
Mean Radius
PSD
Mean Radius and Cubic Factor
PSD and Cubic Factor
Size distribution of AL3SC (Bulk)Time: 1.0E9 [s](Sphere)
Size distribution of AL3SC (Bulk)Time: 1.0E9 [s](Cuboid)
Size Distribution [m⁻⁴]
Length [nm]
10^30
10^25
10^20
10^15
10^10
10^5
10^0
0
20
40
60
80
100
120
140

Mean Radius and Cubic Factor



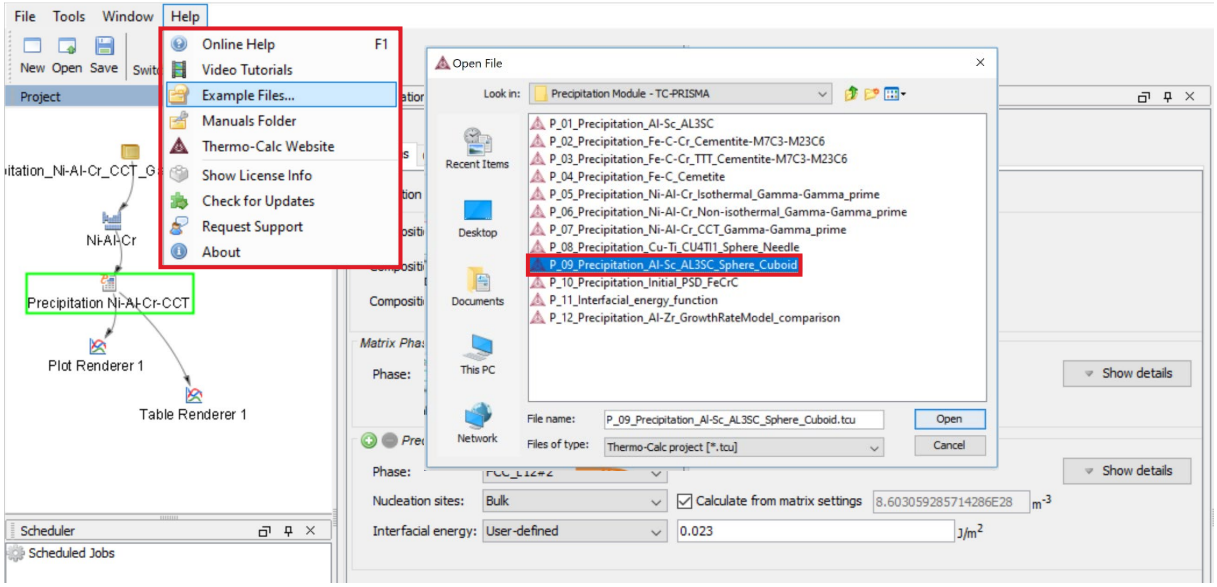
PSD and Cubic Factor



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 centre 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).

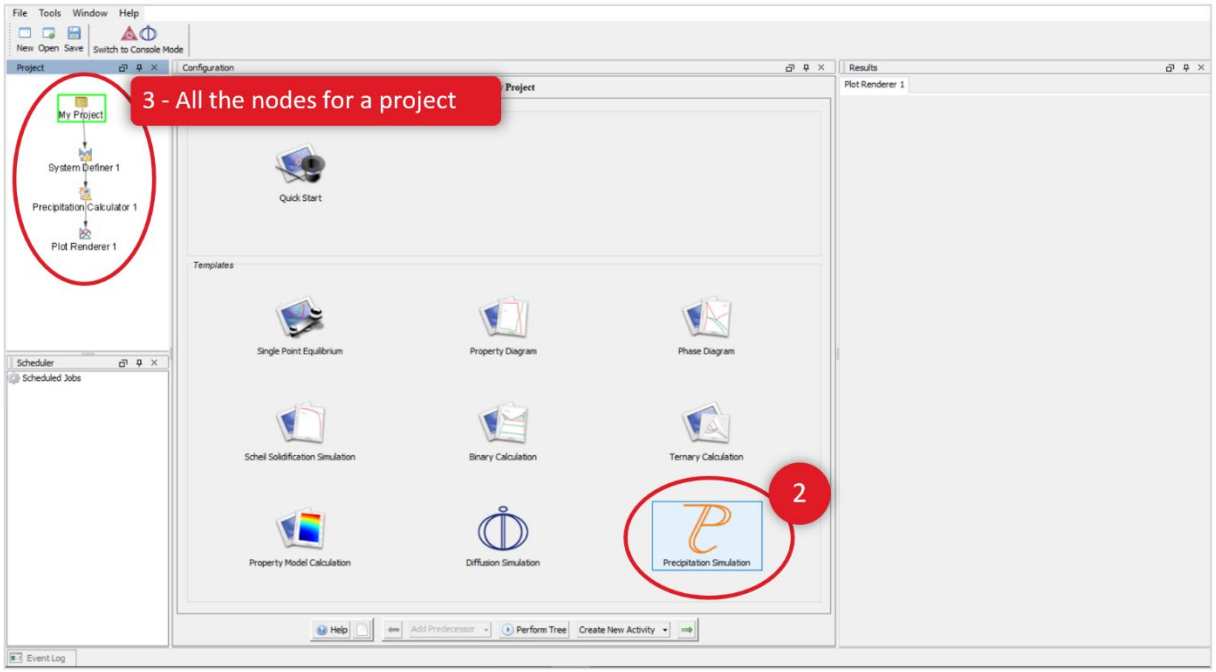
Two separate calculations are performed so you can make a comparison of the results, one assuming spherical morphology without elastic strain energy, and the other assuming cuboid morphology whose shape is determined by competition between interfacial energy and elastic strain energy.

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

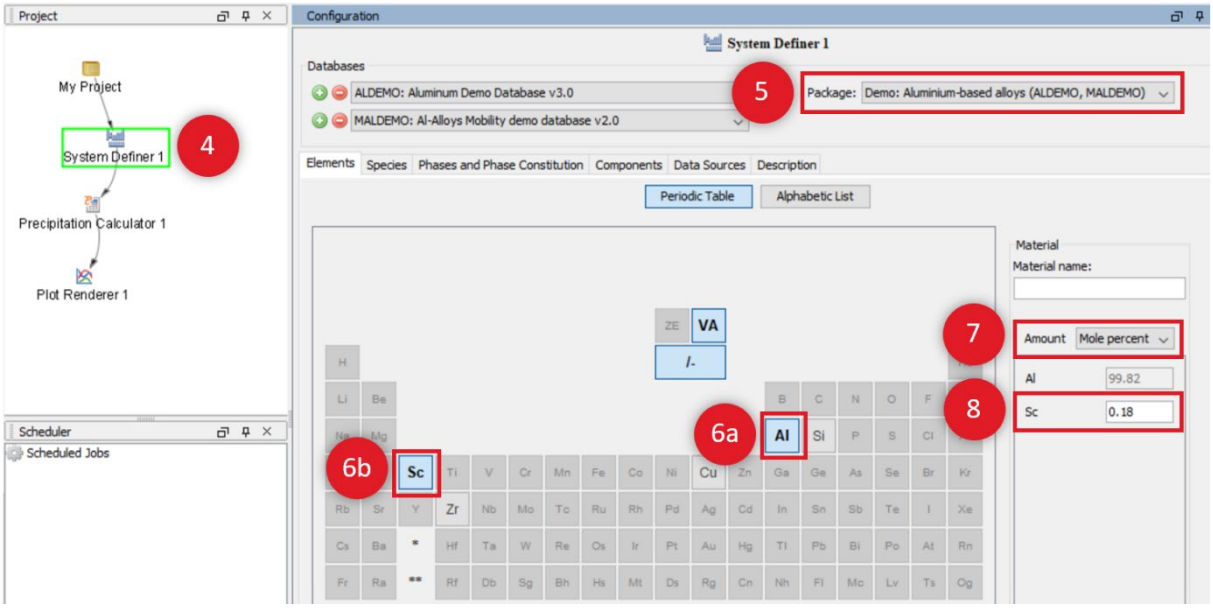
If you run the example file included in your software, the simulation results are compared with experimental data collected from Marquis and Seidman (2001) and Novotny and Ardell (2001).

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. Click the **System Definer 1** node.
5. Set the database package to **DEMO: Aluminium based alloys**, which loads both thermodynamic and kinetic demonstration aluminium databases.
6. From the periodic table, select the elements **Al** (aluminium) then **Sc** (scandium). Be sure to select Al first so that it is the dependant element.
7. Just to the right of the periodic table, select **Mole Percent** as the **Amount**.
8. Enter `0.18` for **Sc**. This automatically sets **Al** to 99.82.



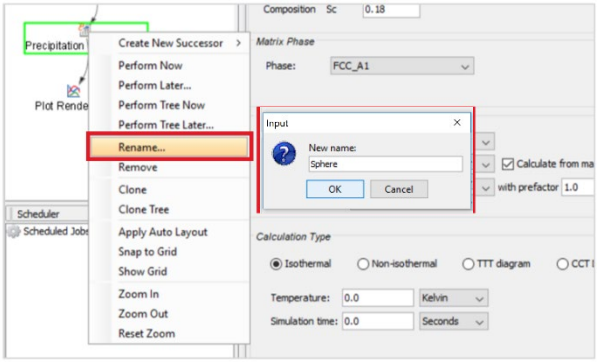
Our system is now defined, so we will set up the precipitation calculations.

SETTING UP THE PRECIPITATION CALCULATIONS

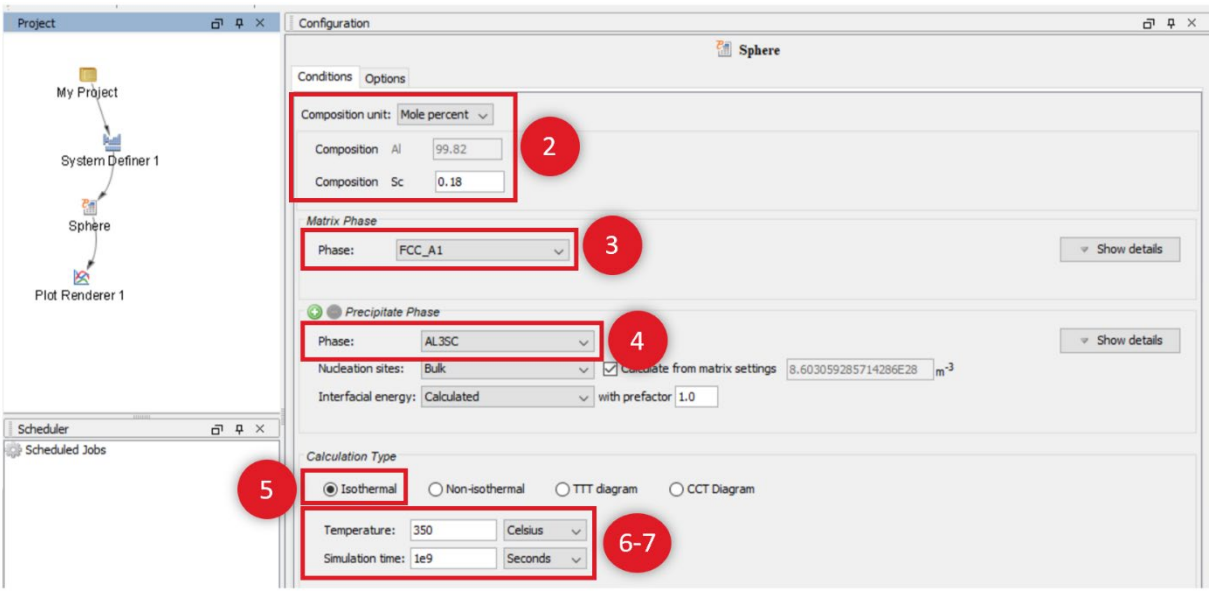
We will have two precipitation calculations in this example, one assuming spherical morphology without elastic strain energy, and the other assuming cuboid morphology whose shape is determined by competition between interfacial energy and elastic strain energy. We will then compare the results of the two 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**.



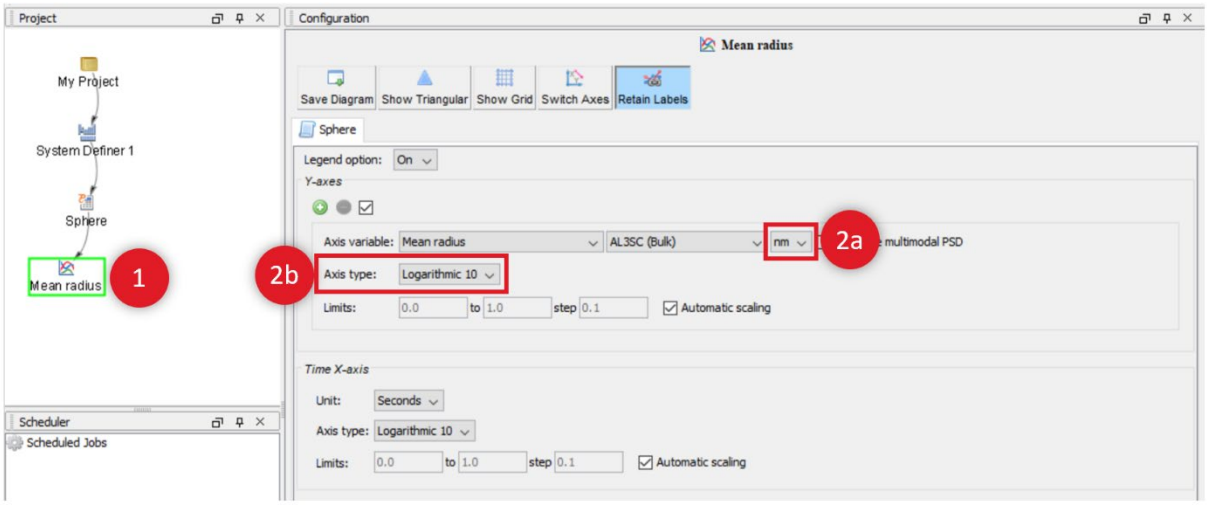
2. Notice that the composition we set in the **System Definer** auto-populated here.
3. Under *Matrix Phase* from the **Phase** list select **FCC_A1**.
4. Under *Precipitate Phase* from the **Phase** list select **AL3SC**.
5. Under *Calculation Type*, select **Isothermal**, which means that the same temperature is maintained throughout the calculation.
6. Enter `350` as the **Temperature** and select **Celsius**.
7. Enter `1.0E9` as the **Simulation time** and select **Seconds**.



Our first calculation is set, so we will configure the plot.

Configuring the Plot

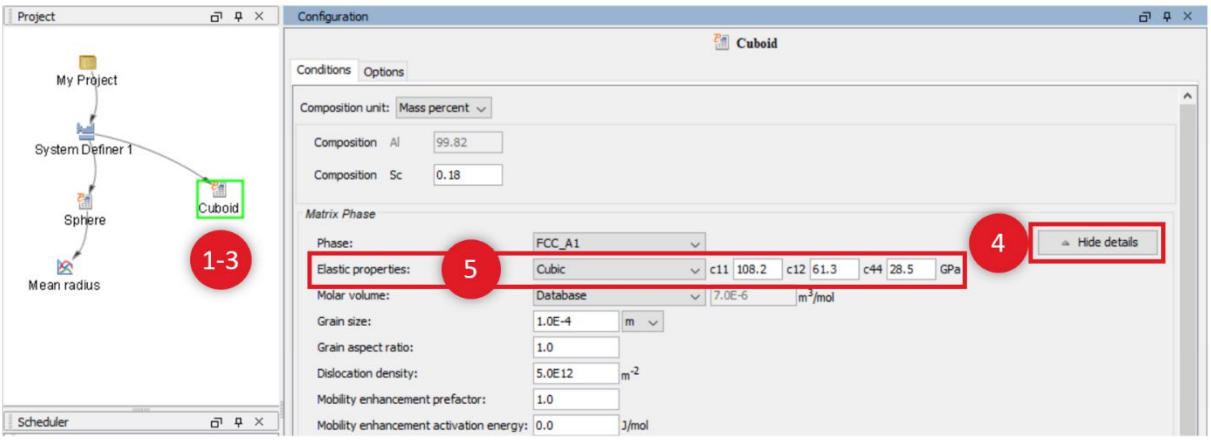
1. In the **Project** window, right-click **Plot Renderer 1** and select **Rename**. Name the plot `Mean radius` then press enter or click **OK**.
2. Under *Y-axes,* change the units to **nm** (nanometres) and from the **Axis type** list select **Logarithmic 10**.



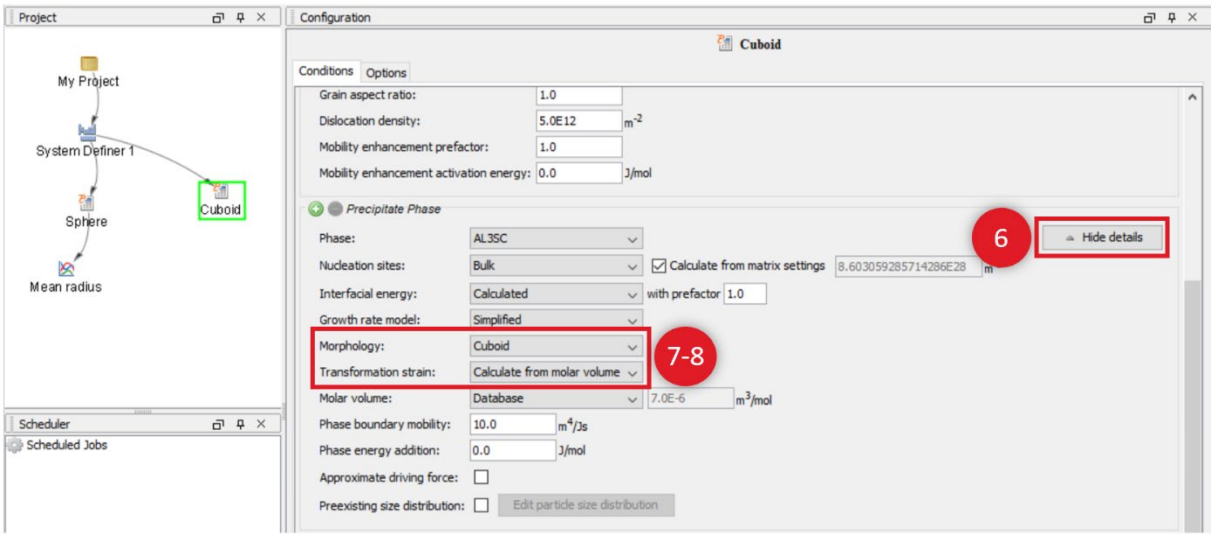
The plot is now set, but we will set up another calculation and link it to the same plot renderer before we run the simulation.

Setting up the Precipitation Calculation with Cuboid Morphology

1. In the **Project** window, right-click the **Sphere** node and select **Clone**.
2. Right-click the new calculator node and select **Rename**.
3. Name the node `Cuboid` and click **OK**.
4. On the **Configuration** window to the right of *Matrix Phase* click **Show Details**.
5. From the **Elastic Properties** list select **Cubic**. The program automatically suggests a good set of default values, so we will leave them as they are.



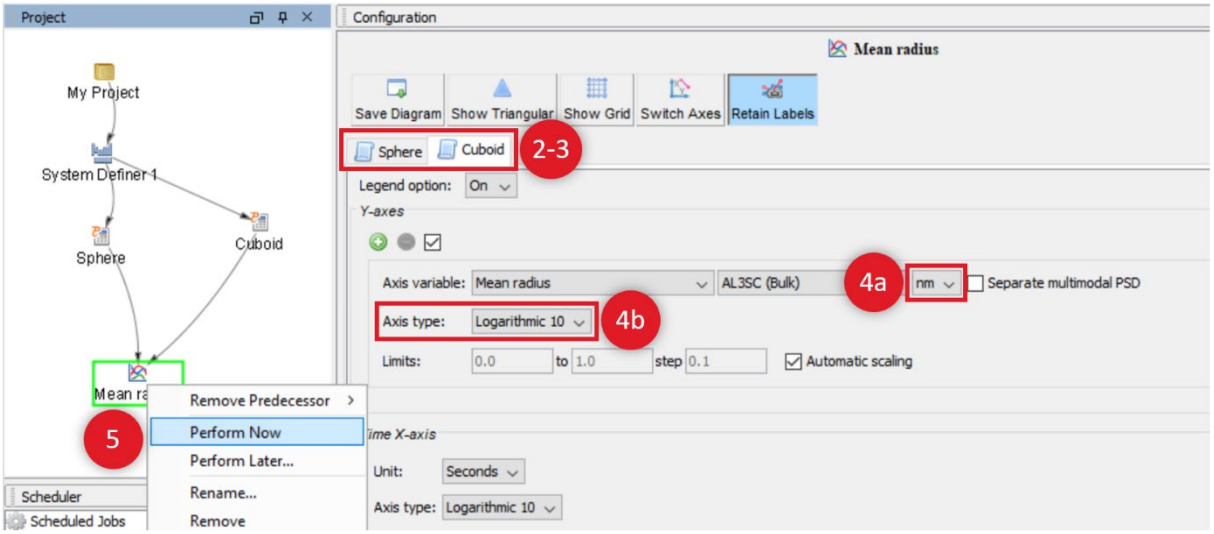
6. To the right of *Precipitate Phase*, click **Show Details**.
7. From the **Morphology** list select **Cuboid**.
8. From the **Transformation strain** list select **Calculate from molar volume**.



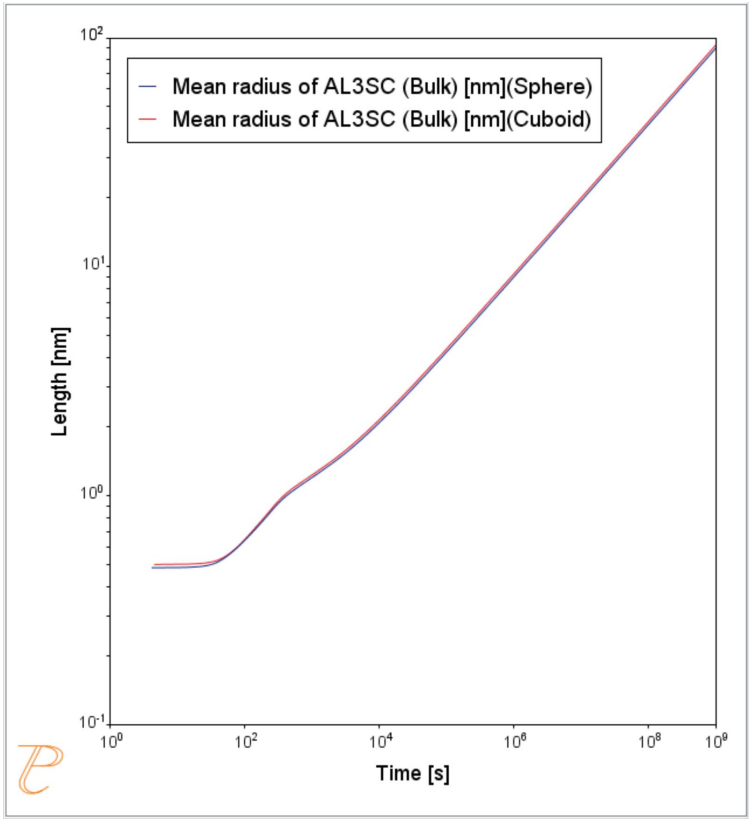
The second calculation is now set up, so we will link it to the Plot Renderer node.

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**. We already configured the Sphere settings, so we just need to set up the Cuboid tab.
3. Click the **Cuboid** tab.
4. Under *Y-axes*, change the unit to **nm** (nanometers) and from the **Axis type** list select **Logarithmic 10**.
5. Our calculation is now ready, so right-click the **Mean radius** node and select **Perform Now**.



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, they are almost identical.

By 'radius for non-spherical particles' we mean 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

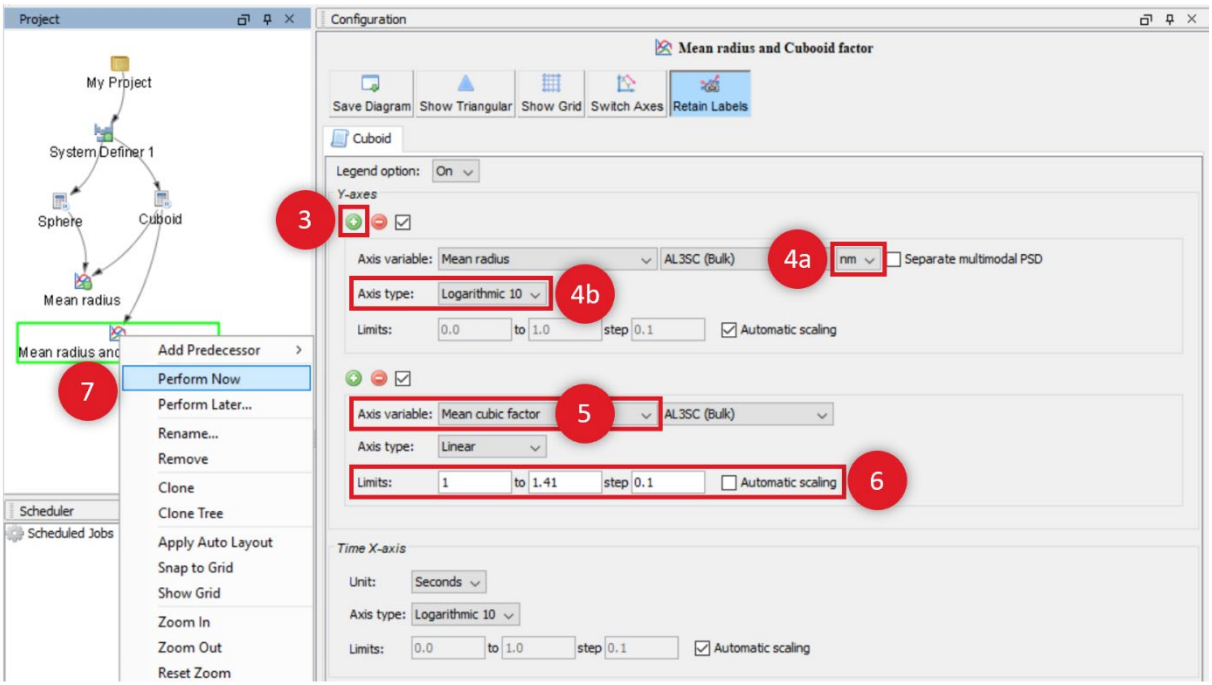
We will now use the same calculation to set up additional plots using the many plot variables that are available in the program. The examples below include two Y-axes each.

Plotting Mean Radius and Cuboid Factor

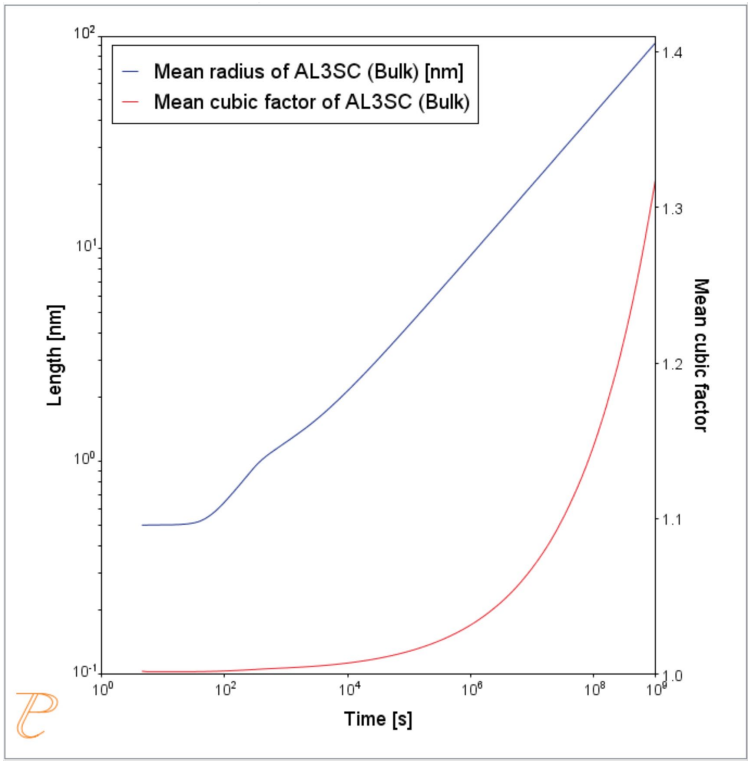
This plot will have two Y-axes: Mean radius and Cuboid factor.

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. Leave the first axis variable as *Mean radius*, but change the units to **nm** (nanometers) 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, so right-click the **Mean radius and Cuboid factor** node and select **Perform Now**.



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.

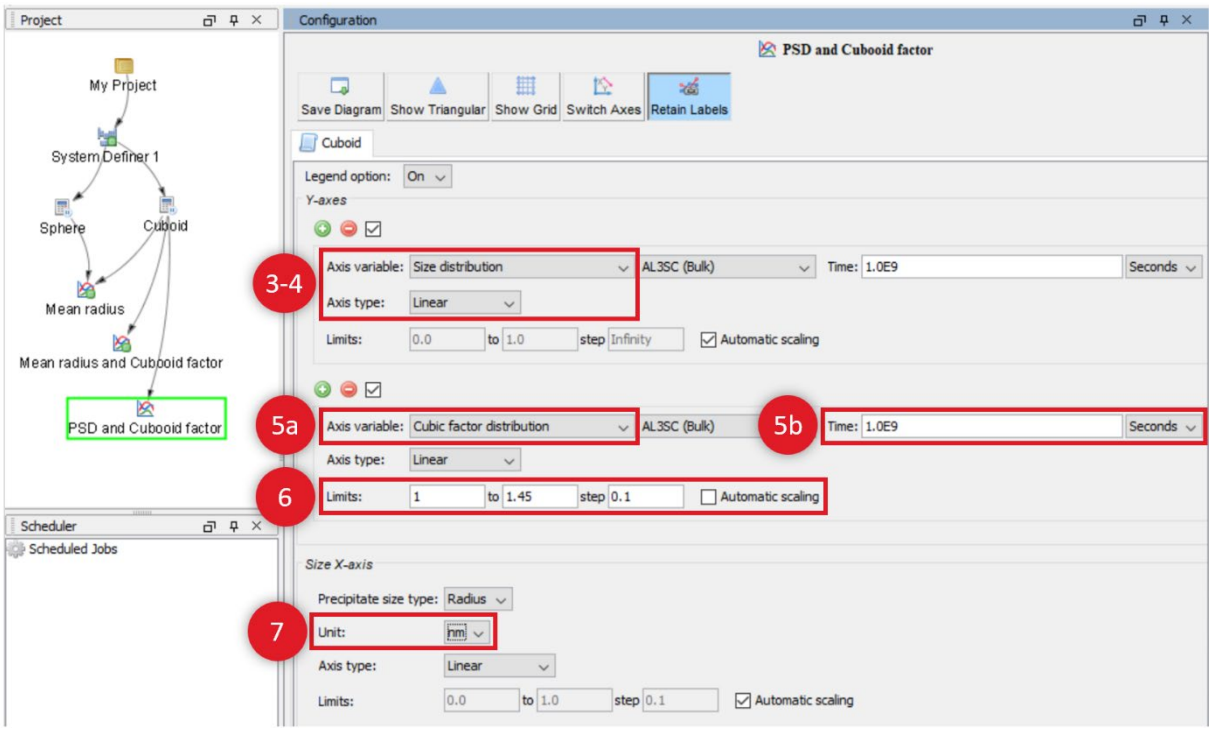
At large sizes the elastic energy dominates and it is therefore more favourable with a non-spherical shape. We can see that the particles get a more cubic form at later times when they grow to larger sizes.

Plotting Particle Size and Cubic Factor Distribution

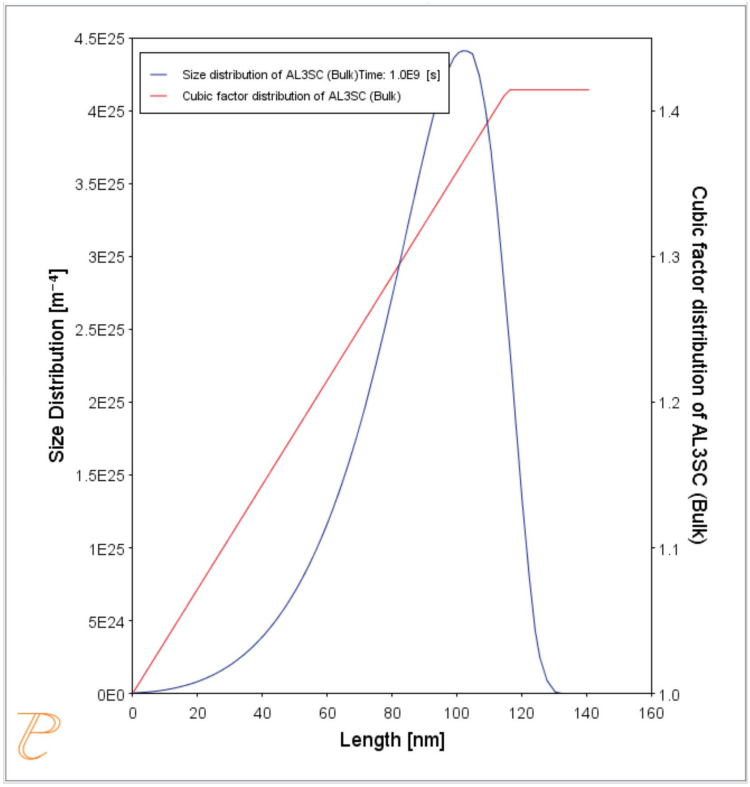
This final plot will show the particle size and cubic factor distribution at the end of the simulation.

This plot will also have two Y-axes, so we will 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*, select **Size Distribution** as the first **Axis variable**.
4. Change the **Axis type** to **Linear**.
5. Set the second Y-axis to **Cubic factor distribution** and enter a **Time** of `1e9` **Seconds**.
6. Click to clear the **Automatic Scaling** check box. Enter the **Limits** from `1` to `1.45` and the **step** to `0.1`.
7. Under *Size X-axis*, change the unit to **nm** (nanometers).
8. Click **Perform** at the bottom centre 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 we would have 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.

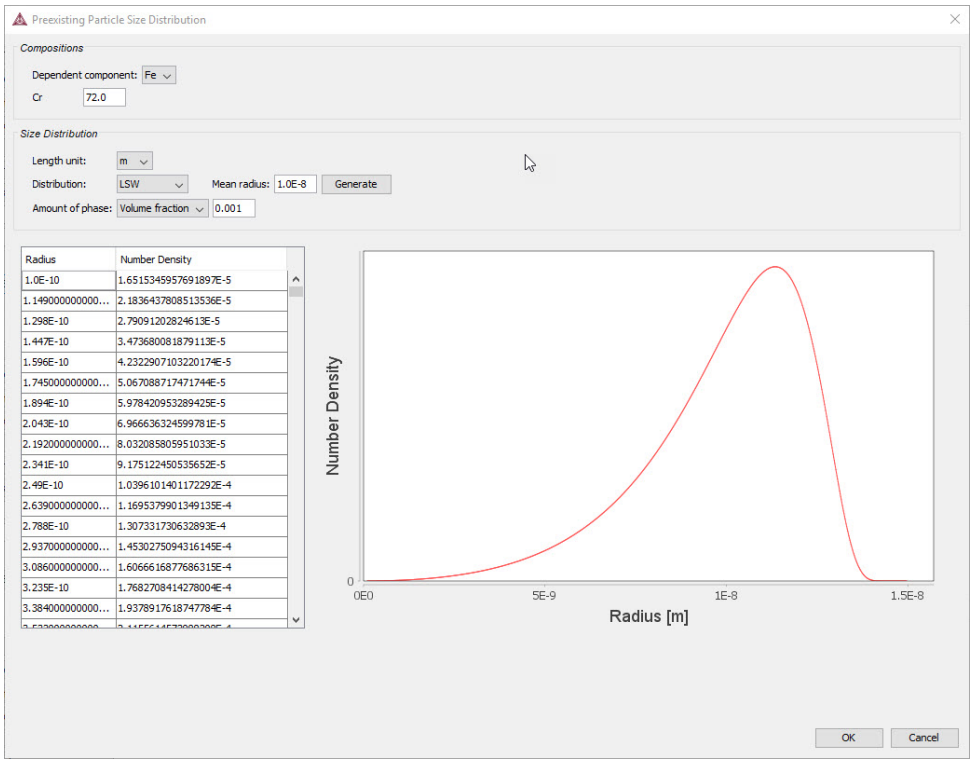
References

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 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.

The example illustrates the use of the particle size distribution 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.



Project File Information

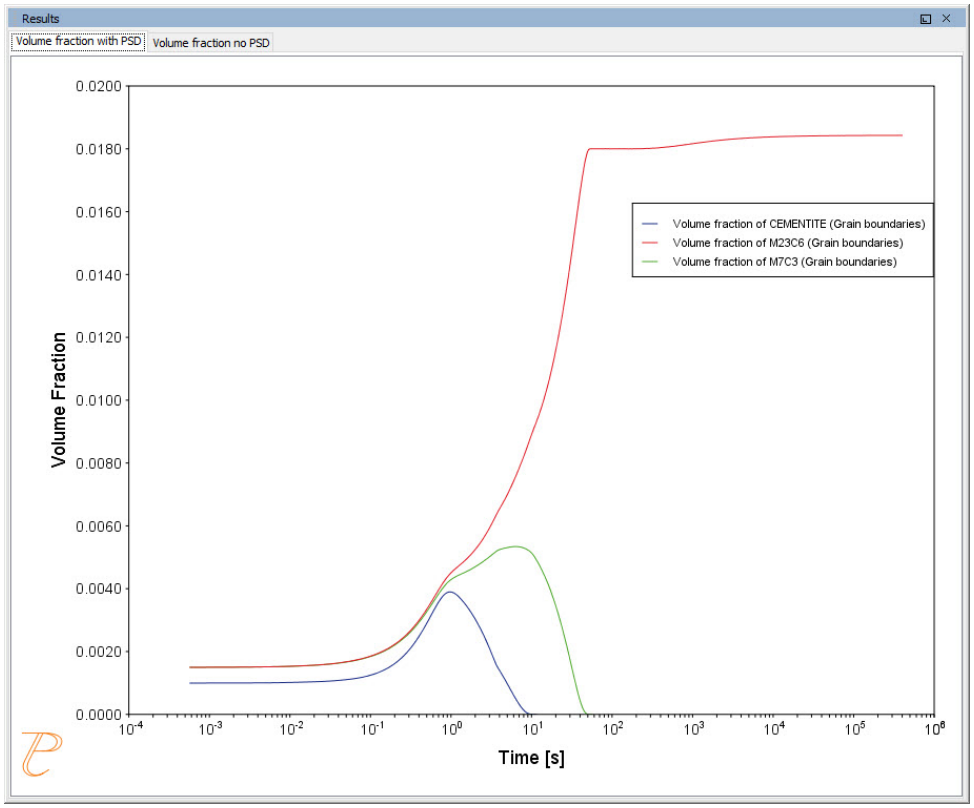
- Folder: Precipitation Module - TC-PRISMA
- File name: *P_10_Precipitation_Initial_PSD_FeCrC.tcu*

Example Settings

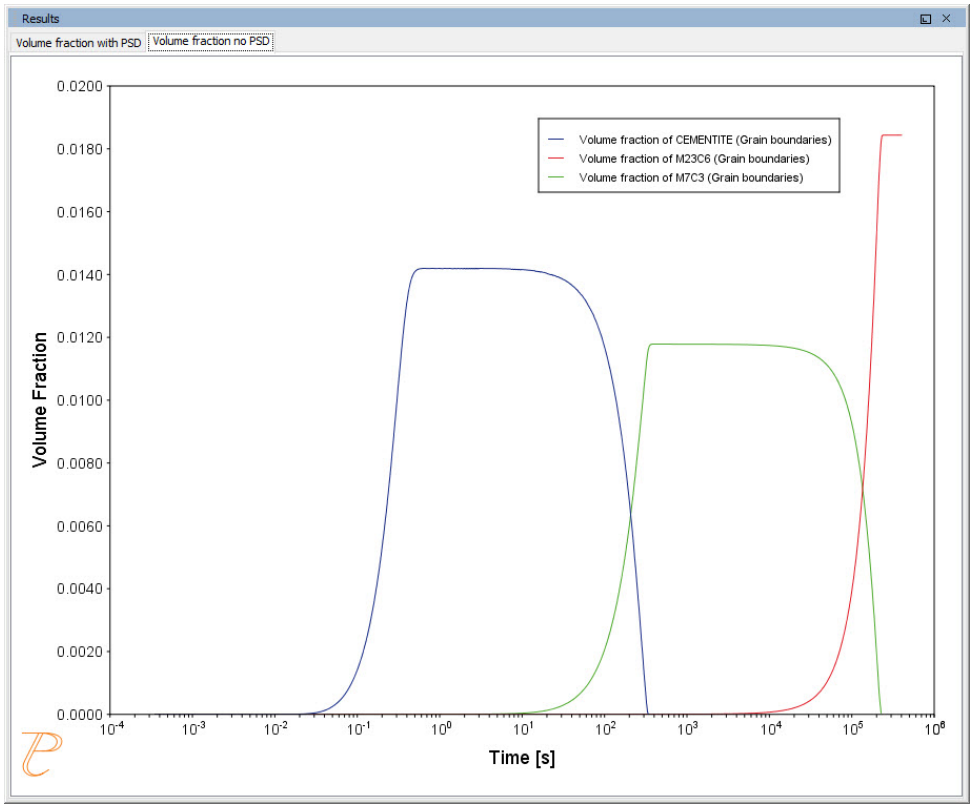
System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO)
Elements	Fe, C, Cr
Conditions (Precipitation Calculator)	
Composition	Fe-0.1C-12Cr Mass percent
Matrix phase	BCC_A2 All other defaults are kept.
Precipitate phases	CEMENTITE, M23C6 and M7C3
Precipitate Phase Data 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

PLOT RESULTS

Volume Fraction with Initial Particle Size Distribution



Volume Fraction with No Initial Particle Size Distribution



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 ([1.]) data is compared with the calculated results.

PROJECT FILE INFORMATION

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

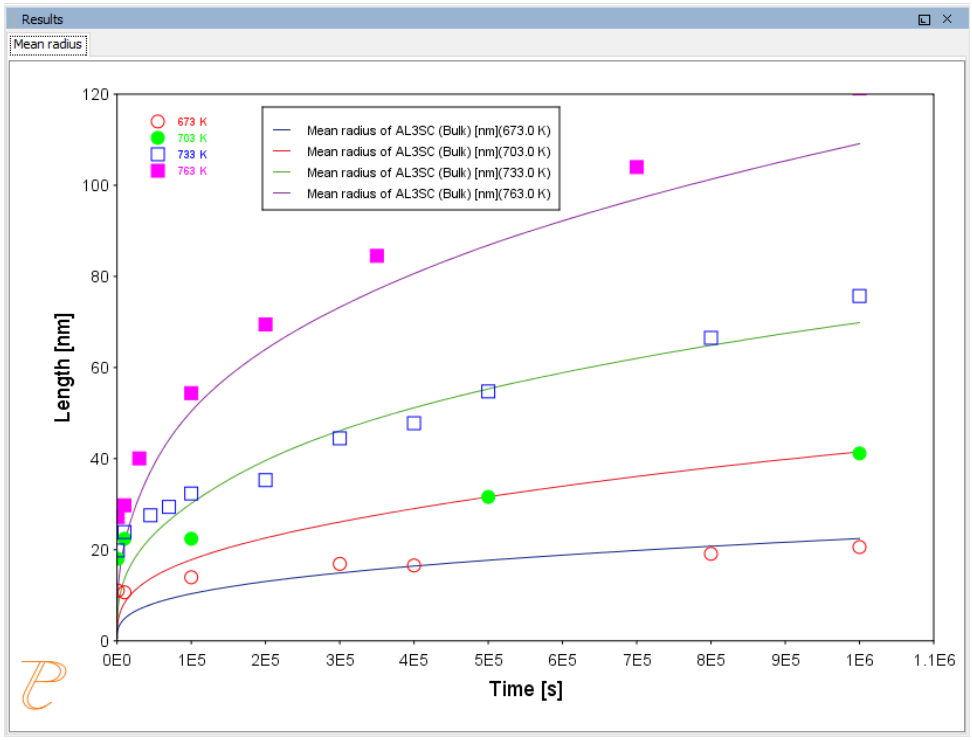
- Folder: Precipitation Module - TC-PRISMA
- File name: *P_11_Interfacial_energy_function.tcu*

EXAMPLE SETTINGS

System (System Definer)	
Database package	Demo: Aluminum-based Alloys (ALDEMO, MALDEMO)
Elements	Al, Sc
Conditions (Precipitation Calculator)	
Composition	Al-0.12Sc Mole percent
Matrix phase	FCC_A1 All other defaults are kept.
Precipitate phase	AL3SC Nucleation sites (all calculations): Bulk (6.025E28 m^{-3}) Interfacial energy (all calculations): User-defined function f(r,T): 0.075+0.011*erf ((r-3e-8)/1e-8 J/m^2)
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal (all calculations)
Temperature	Four temperature points in 30 K increments: 673 K, 703 K, 733 K, and 763 K.
Simulation time	1 000 000 seconds (all calculations)
Datasets (Experimental File Reader)	
Wamura 2004 (Dataset 1)	Data set included with this example and imported to one Experimental File Reader.

PLOT RESULTS

Mean Radius



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.

The example takes several minutes to run.

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. ([1.]) data is compared with the calculated results.

PROJECT FILE INFORMATION

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_12_Precipitation_Al-Zr_GrowthRateModel_comparison.tcu*

EXAMPLE SETTINGS

System (System Definer)	
Database package	Demo: Aluminum-based Alloys (ALDEMO, MALDEMO)
Elements	Al, Zr
Conditions (Precipitation Calculator)	
Composition	Al-0.2Zr Mole percent
Matrix phase	FCC_A1 All other defaults are kept.
Precipitate phase	AL3ZR_D023 Click **Show details** to select the **Growth rate model** (**Simplified**, **Advanced** and **General**). All other defaults are kept.
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal

1. Knipling, Keith E., David C. Dunand, and David N. Seidman. 2008. "Precipitation Evolution in Al–Zr and Al–Zr–Ti Alloys during Isothermal Aging at 375–425°C." Acta Materialia 56 (1): 114–27. doi:10.1016/j.actamat.2007.09.004.

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.

PLOT RESULTS

Mean Radius