Thermo-Calc Software

Graphical Mode Examples Guide

Thermo-Calc Version 2021a

Graphical Mode Examples

This guide includes descriptions of the following examples.

Category	Example number
Thermo-Calc Graphical Mode Examples Collection includes binary and ternary system examples, Scheil, the Equilibrium Calculator, plus more	T_01 to T_12
Thermo-Calc General Property Model Examples Collection: General Models Library	General Models: PM_G_01 to PM_G_11
Steel Model Library Examples Collection	Steel Models: PM_Fe_01 to PM_Fe_05
Process Metallurgy Module Examples Collection	PMET_01 to PMET_07
Diffusion Module (DICTRA) Graphical Mode Examples	D_01, D_02, D_03 (the Quick Start Guide Examples) D_04 to D_07
Precipitation Module (TC-PRISMA) Graphical Mode Examples	P_01 to P_13

Thermo-Calc Graphical Mode Examples Collection

In this section:

T_01: Calculating a Single-Point Equilibrium

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

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

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

Project File Information

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

Results

Table Renderer 1

System

Moles	1.00000	
Mass	55.64392	[g]
Temperature	1000.00000	[K]
Total Gibbs Energy	-42141.28527	[J]
Enthalpy	24706.54116	[J]
Volume	7.30619E-6	[m3]

Component	*Mole Fraction*	*Mass Fraction*	*Activity*	*Potential*
C	0.00463	0.00100	0.21816	-12658.89428
Fe	0.99537	0.99900	0.00619	-42278.50542

Stable Phases

	Moles	*Mass*	*Volume Fraction*	
BCC_A2#1	0.99609	55.59692	0.99711	Composition

Composition

Component	*Mole Fraction*	*Mass Fraction*
Fe	0.99928	0.99984
C	0.00072	0.00016

	Moles	*Mass*	*Volume Fraction*	
GRAPHITE#1	0.00391	0.04700	0.00289	Composition

Composition

Component	*Mole Fraction*	*Mass Fraction*
C	1.00000	1.00000
Fe	0.00000	0.00000

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

T_02: Stepping in Temperature in the Fe-C System

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

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

Project File Information

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

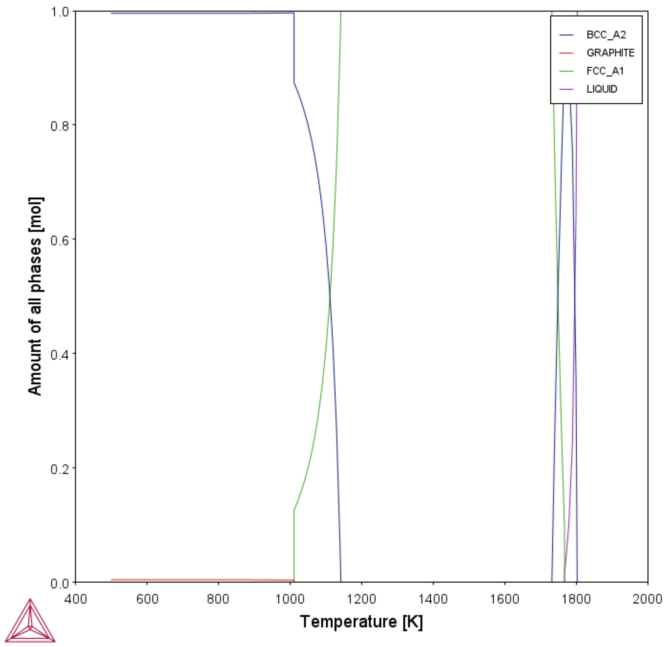


Figure 2: In this example, results are displayed graphically using a Plot Renderer activity.

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

Results

Plot Renderer 1 | Table Renderer 1

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

T_03: Fe-C Phase Diagrams

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

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

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

Project File Information

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

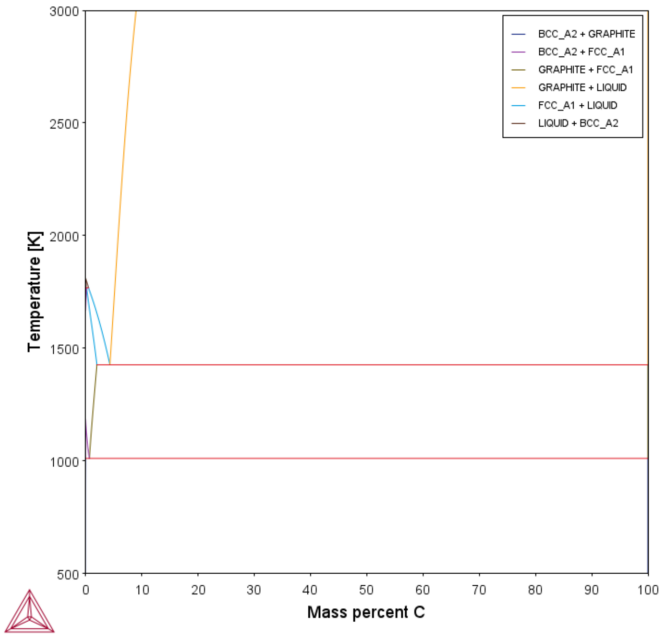


Figure 3: The plot result of the System Definer and Equilibrium Calculator.

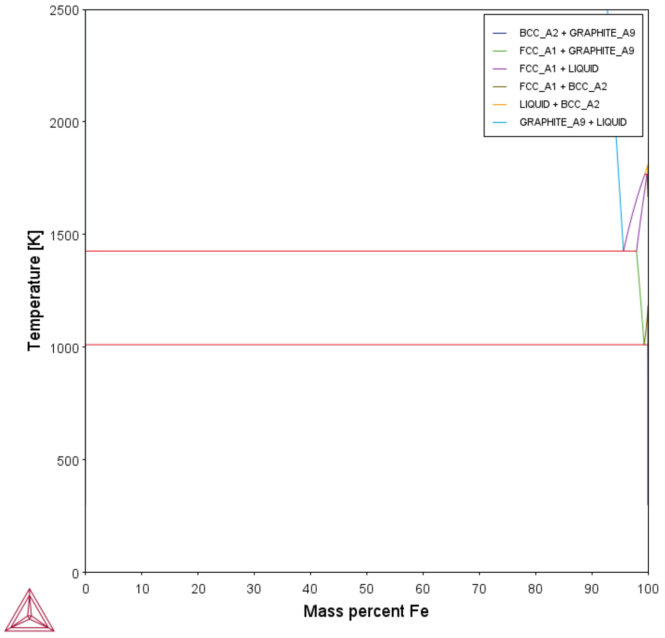


Figure 4: The plot result of the Binary Calculator simulation.

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

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

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

Project File Information

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

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

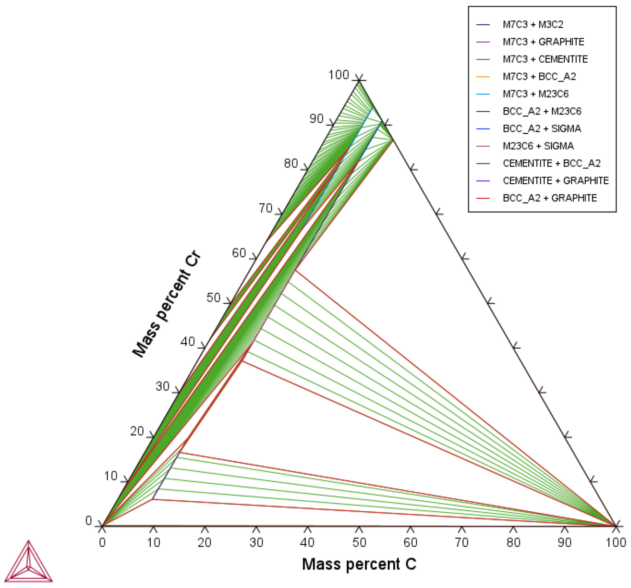


Figure 5: Ternary Calculator

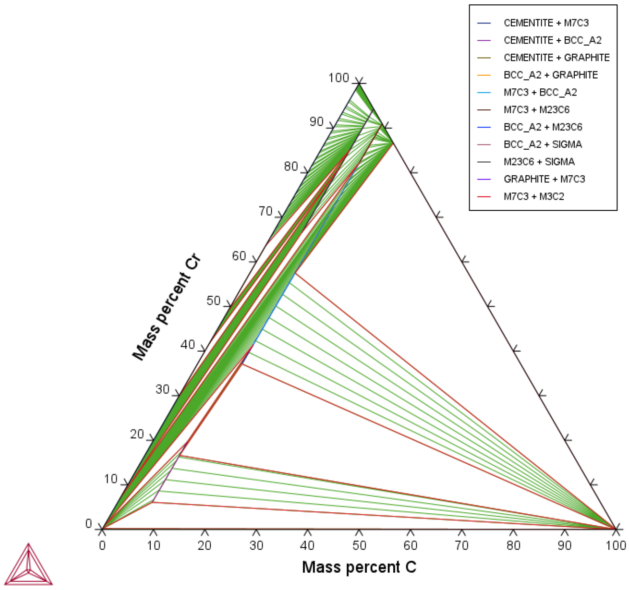
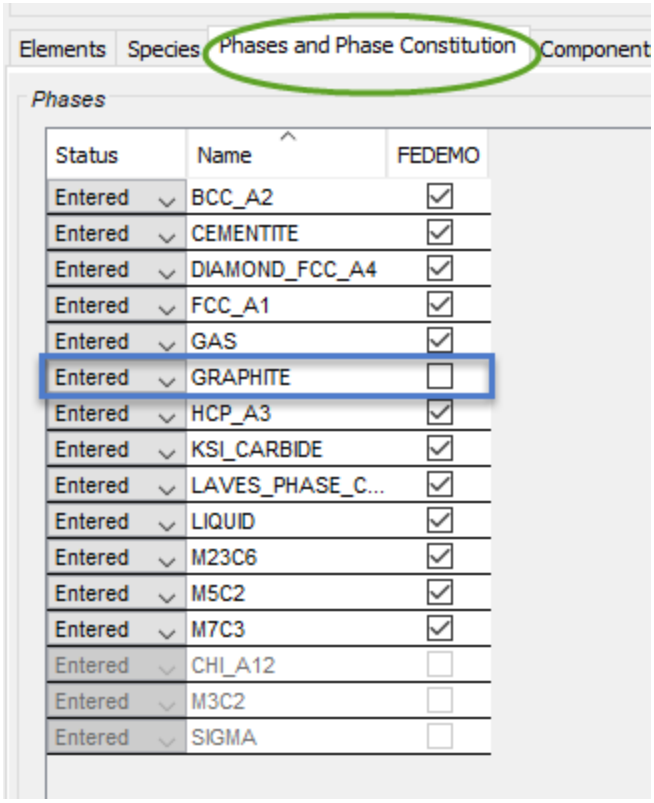


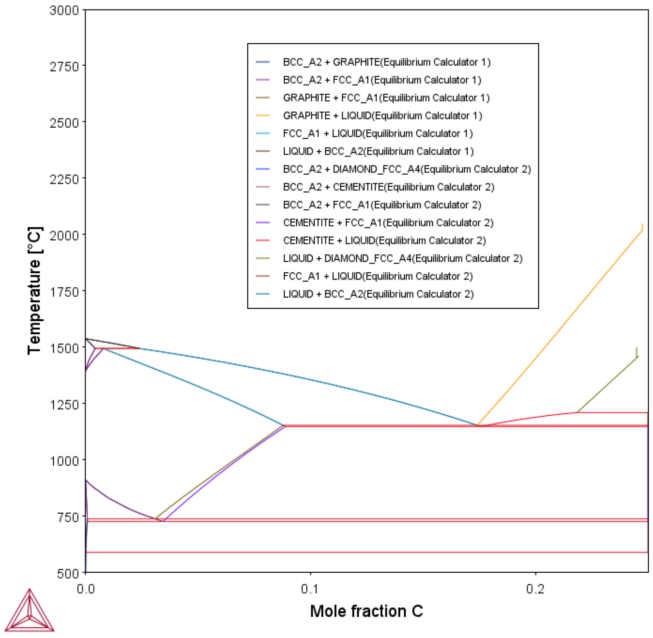
Figure 6: Equilibrium Calculator

T_05: Stable and the Metastable Fe-C Phase Diagrams

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

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 and Video Tutorial Information

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

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

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 and Video Tutorial Information

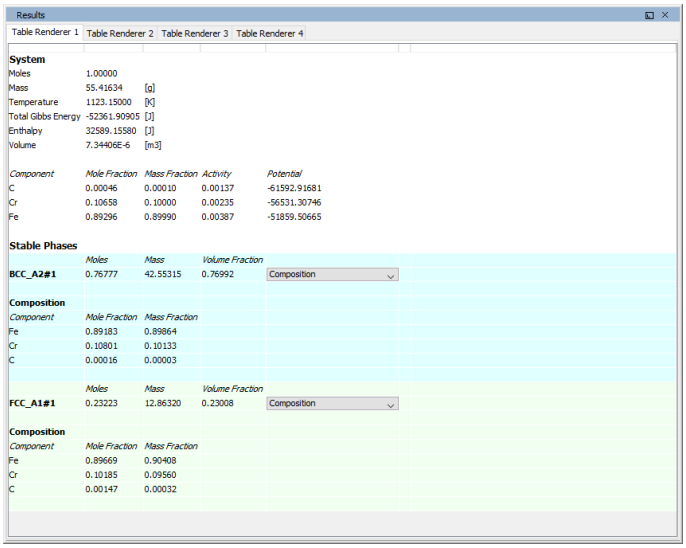
- Folder: Thermo-Calc
- File name: *T_06_Serial_equilibrium_calculators.tcu*

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

Table Renderer Results

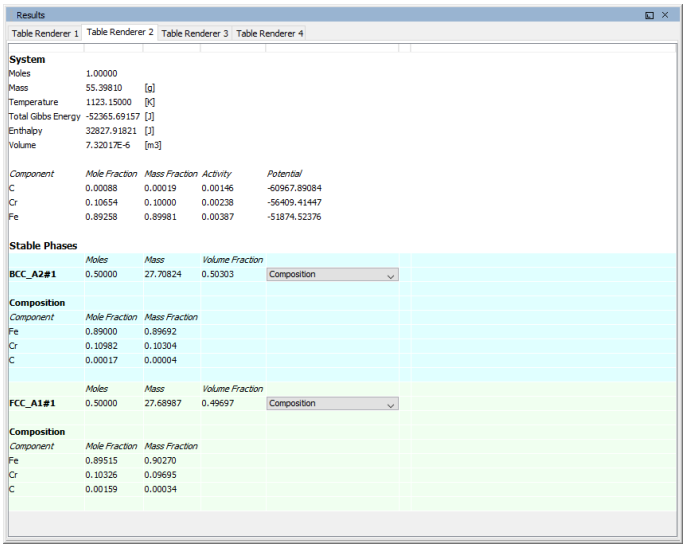
Equilibrium Calculator 1

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.



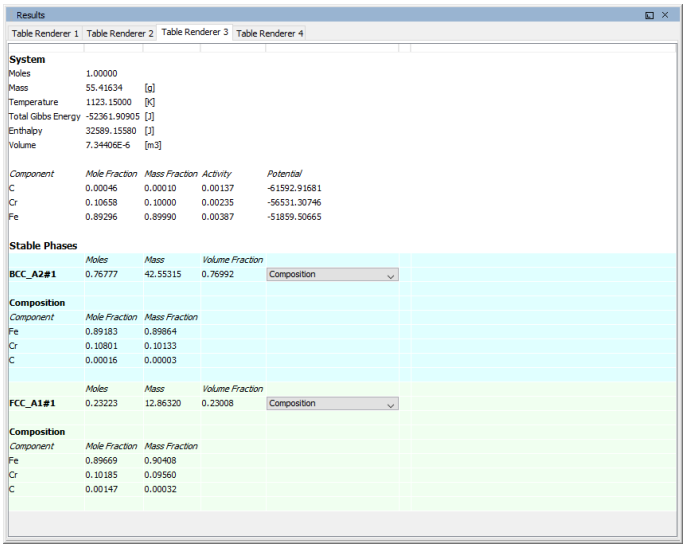
Equilibrium Calculator 2

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.



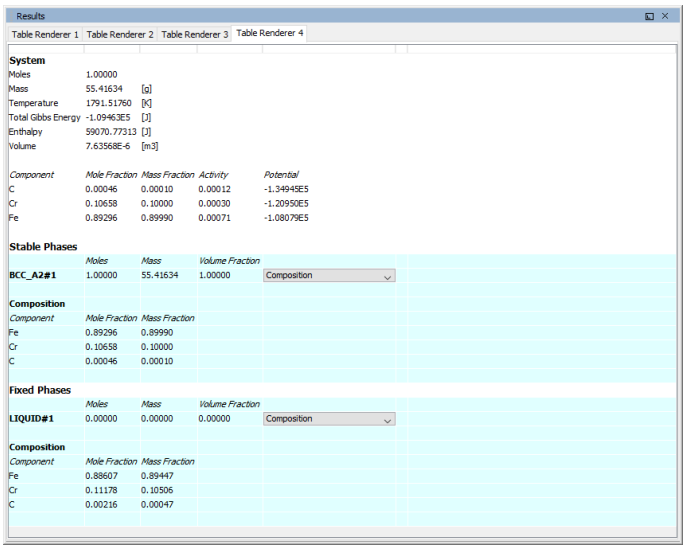
Equilibrium Calculator 3

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

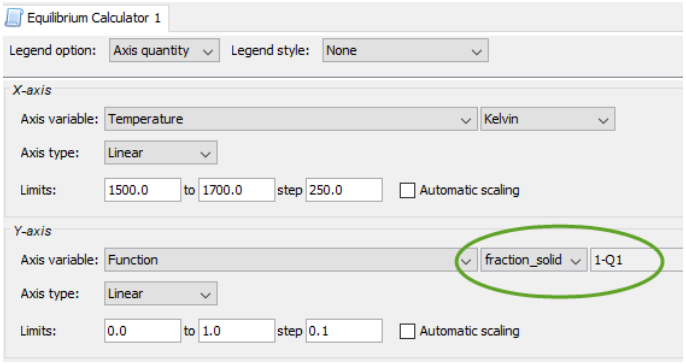
This example shows how to implement user-defined functions.

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 and Video Tutorial Information

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

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



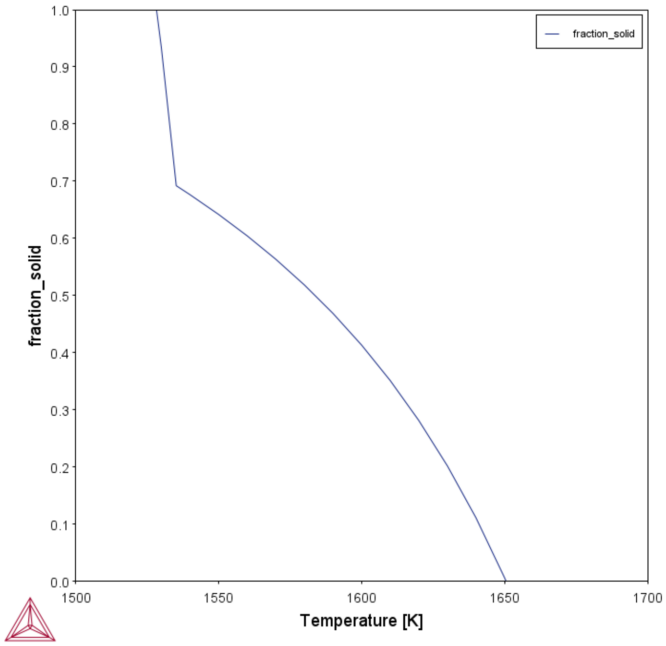


Figure 7: The result of the fraction_solid function.

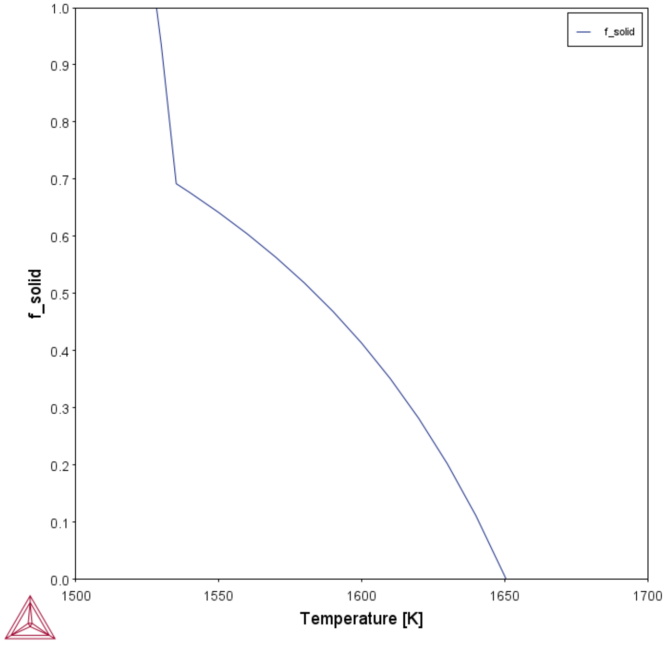


Figure 8: The result of the f_solid function.

T_08: Scheil and Equilibrium Solidification

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

- T_10: Scheil Solidification with Back Diffusion

Project File and Video Tutorial Information

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

For video tutorial examples using Scheil, see our website and YouTube channel.

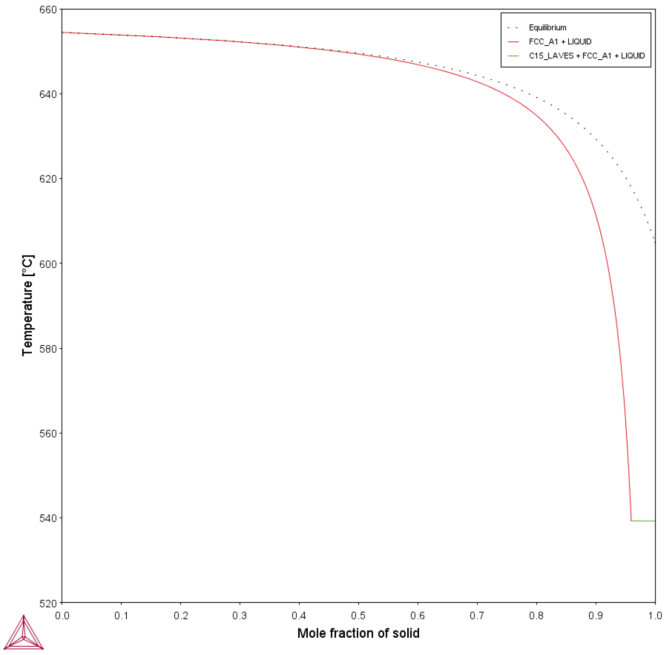
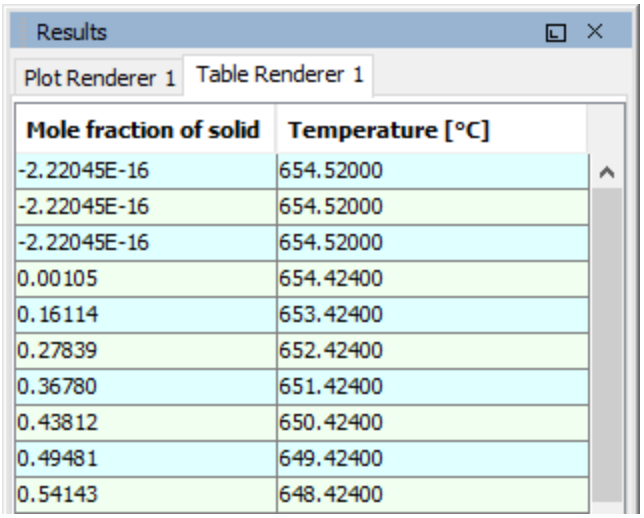


Figure 9: The plot compares the mole fraction of a solid vs temperature.



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

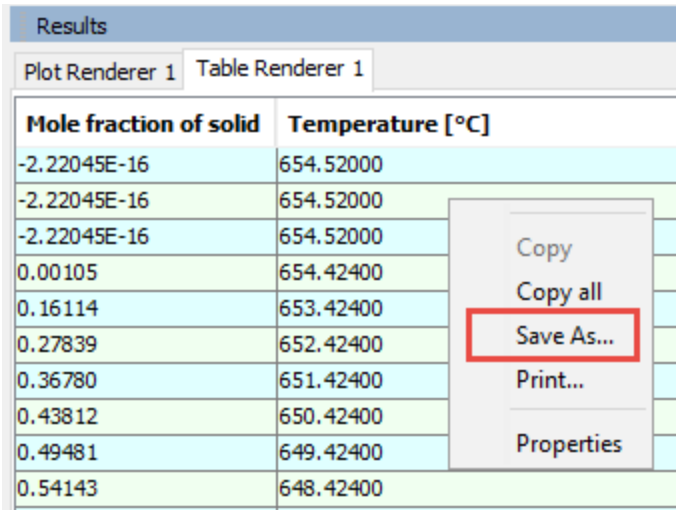
Figure 10: The table provides the data, which you can also export.

To Save the Table

There are two ways to save the table.

Method 1

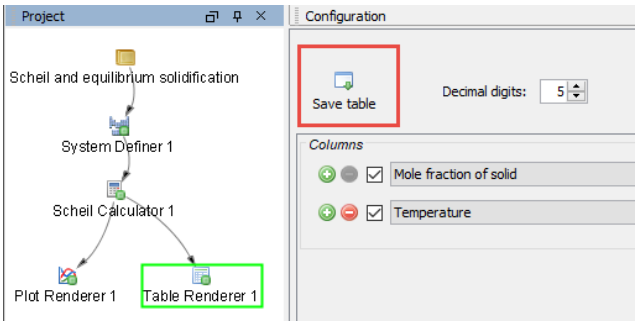
In the **Results** window, right click the table and select **Save As...**



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

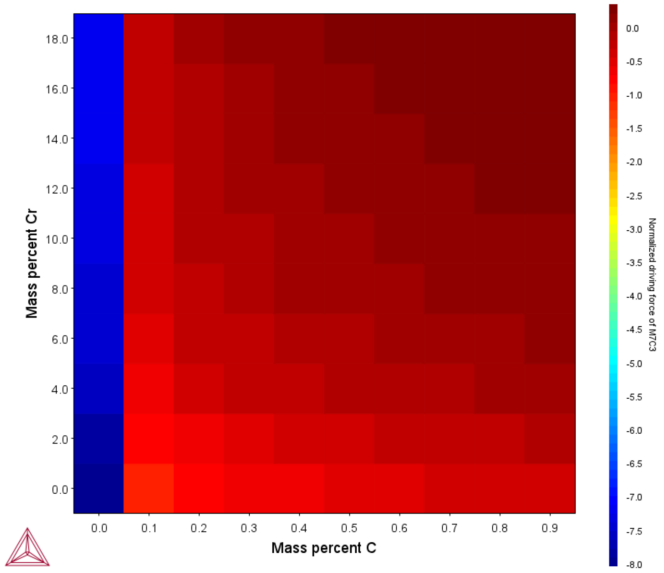
Method 2

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



T_09: Carbide Driving Force Heat Map

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



Project File and Video Tutorial Information

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

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

T_10: Scheil Solidification with Back Diffusion

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

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

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

T_08: Scheil and Equilibrium Solidification

Project File and Video Tutorial Information

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

For video tutorial examples using Scheil, see our website and YouTube channel.

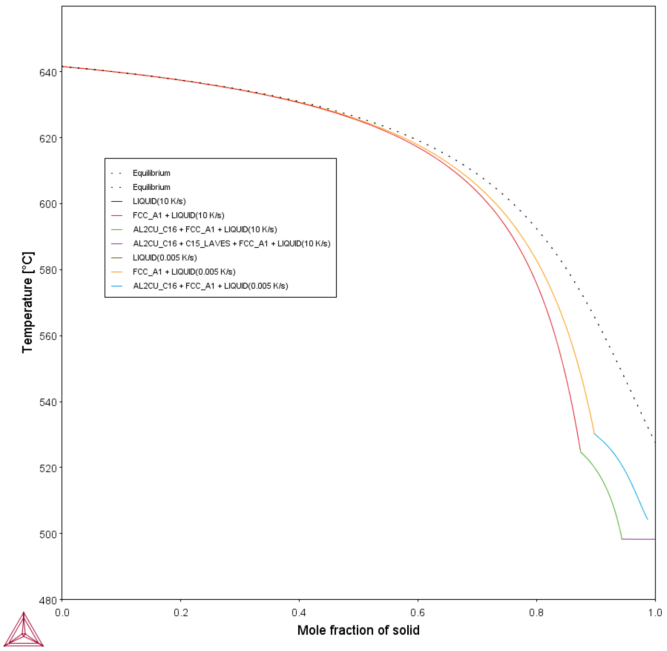


Figure 11: Scheil solidification. The lower cooling rate produces a solidification curve that is closer to the equilibrium curve .

T_11: Surface Tension in Cu-Zr

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

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

Not all databases have this property although it is being added to databases as these are updated over time. Currently it is available with the latest versions of TCNI and TCAL.

Reference

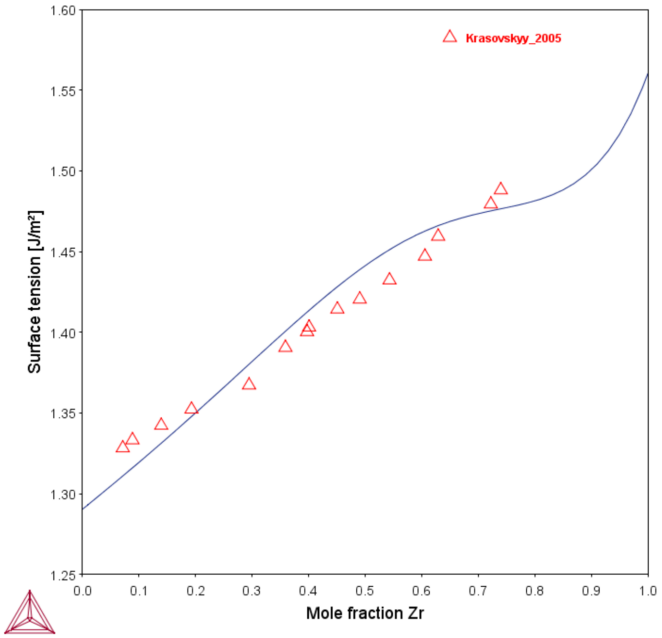
[2005, Krasovskyy] V. P. Krasovskyy, Y. V. Naidich, N. A. Krasovskaya, "Surface tension and density of copper–Zirconium alloys in contact with fluoride refractories," J. Mater. Sci. 40, 2367–2369 (2005).

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

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

Project File Information

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


Krasovskyy_2005
Surface tension [J/m²]
Mole fraction Zr
1.60
1.55
1.50
1.45
1.40
1.35
1.30
1.25
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0

T_12: Viscosity in Cr-Ni

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

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

Not all databases have this property although it is being added to databases as these are updated over time. Currently it is available with the latest versions of TCFE, TCHEA, TCNI and TCAL.

Reference

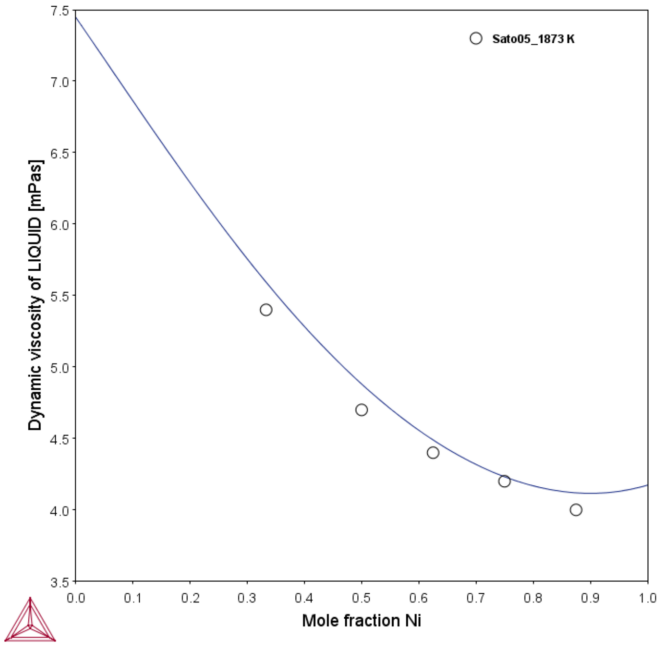
[2005, Sato] Y. Sato, K. Sugisawa, D. Aoki, T. Yamamura, "Viscosities of Fe–Ni, Fe–Co and Ni–Co binary melts," Meas. Sci. Technol. 16, 363–371 (2005).

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

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

Project File Information

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


Sato05_1873 K
Dynamic viscosity of LIQUID [mPas]
Mole fraction Ni
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0

Thermo-Calc General Property Model Examples Collection

The **General Models** are available to all users. To run calculations with the **Steel Models** (as part of the Steel Model Library) requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. See *Properties that Can Be Calculated* on our website for more information.

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

In this section:

PM_G_01: Phase Transition

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

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

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

Project File Information

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

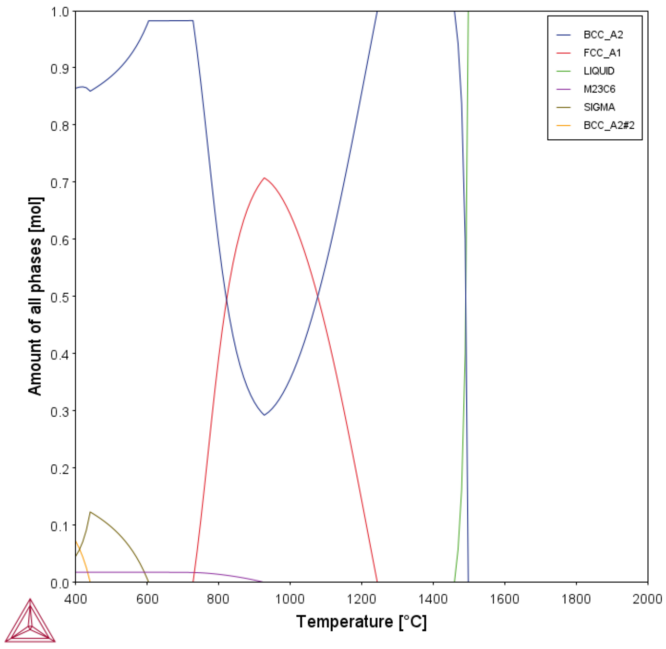


Figure 12: A property diagram as a result of using the Equilibrium Calculator with a One-axis calculation to determine a good starting temperature of the SIGMA phase.

Once you set up the Property Model Calculator, but before running a Grid calculation, it is recommended you run a Single calculation to make sure the calculation is valid. If `the subprocess completed normally` displays in the **Event Log**, it means it worked correctly. You will also see in the Log, the result "Relaxed Condition", which refers to the variable, in this case, temperature. If the calculation did not work, you will see `NAN` (not a number) display instead. Check your configurations and run it again before moving on to the more complicated calculation.

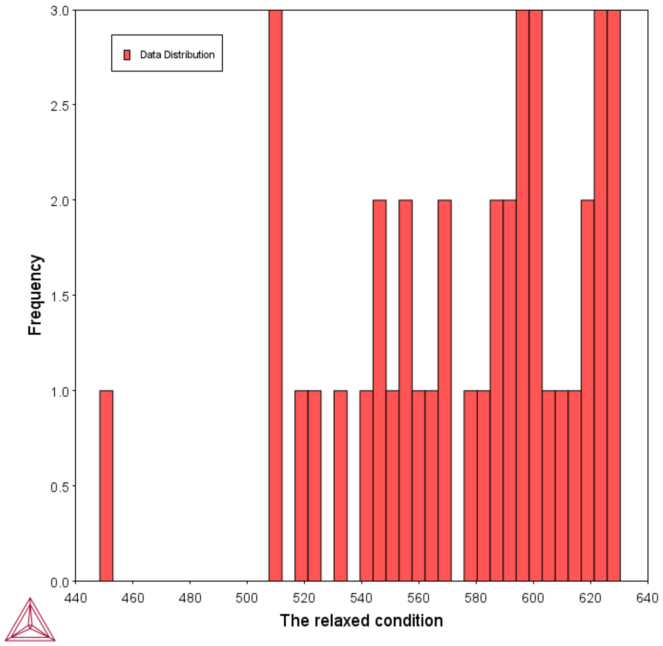


Figure 13: Using the Property Model Calculator with the Phase Transition Model to plot a histogram showing how the transition temperature of sigma varies when you vary the composition. The plot changes each time you run the calculation because it is taking a random sampling from the composition range set.

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

PM_G_02: Coarsening and Interfacial Energy

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

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

Project File Information

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

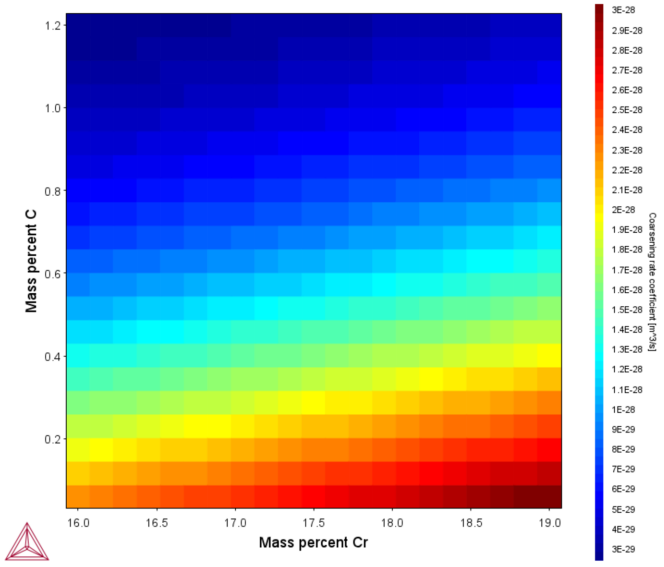


Figure 14: Coarsening rate coefficient (heat map plot).

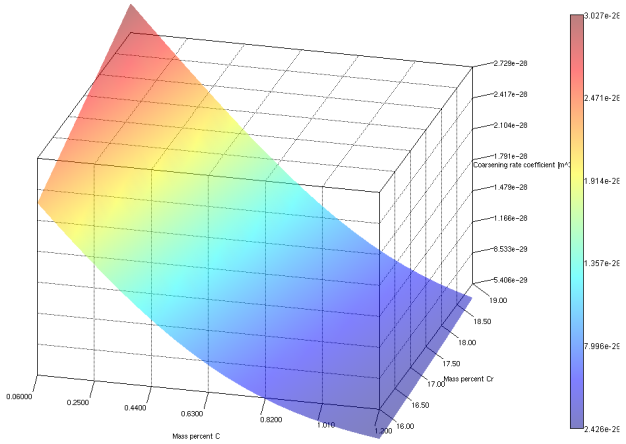


Figure 15: Coarsening rate coefficient (3D plot).

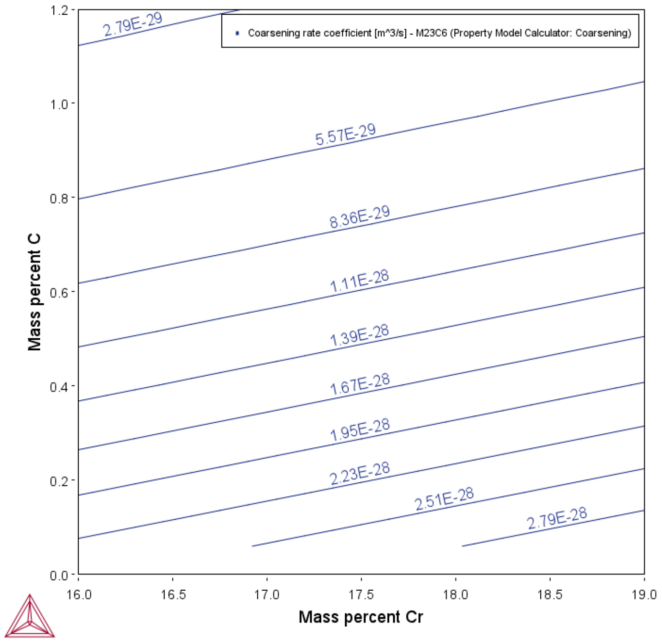


Figure 16: Coarsening rate coefficient (contour plot)

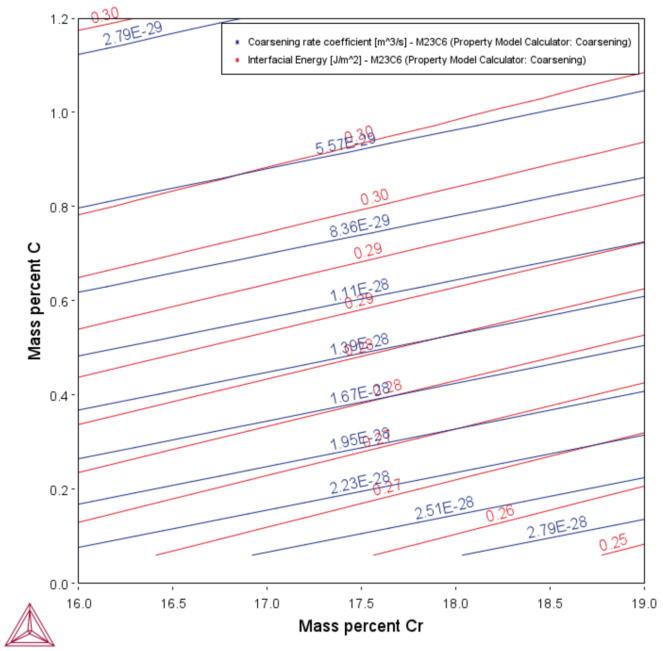


Figure 17: The coarsening rate coefficient and interfacial energy in overlayed plots.

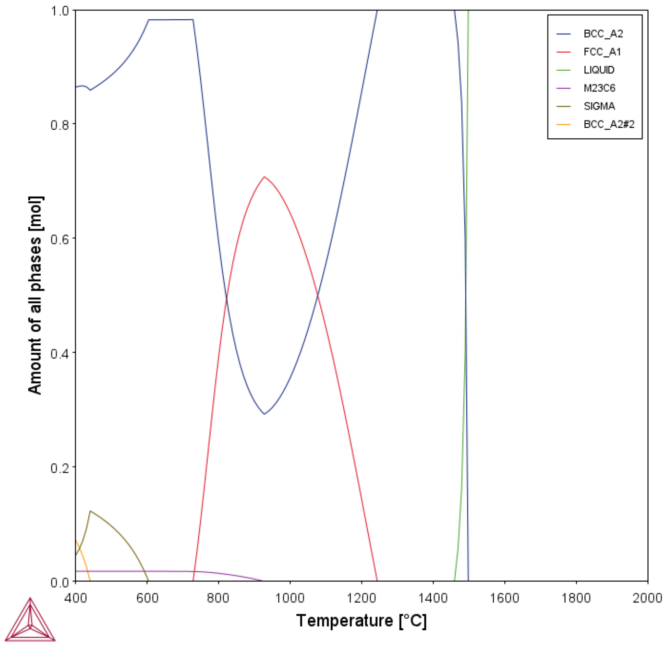


Figure 18: Phase fractions vs T (One axis).

PM_G_03: Driving Force and Interfacial Energy

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

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

Project File Information

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

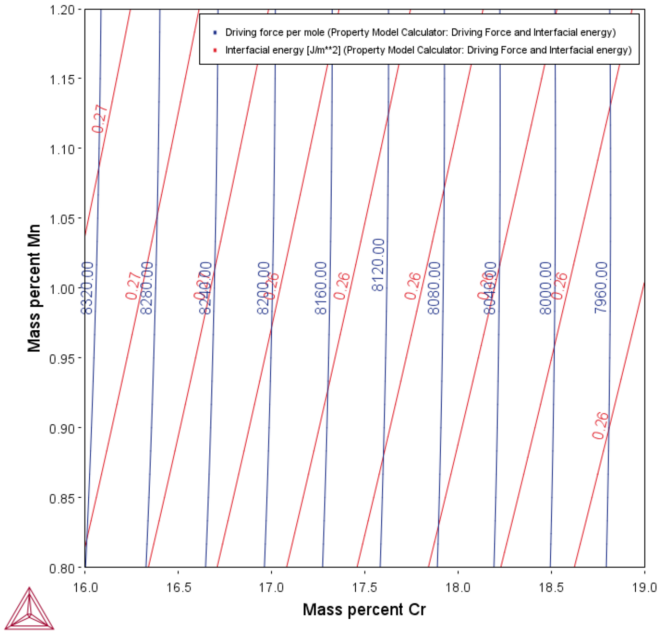


Figure 19: A contour plot.

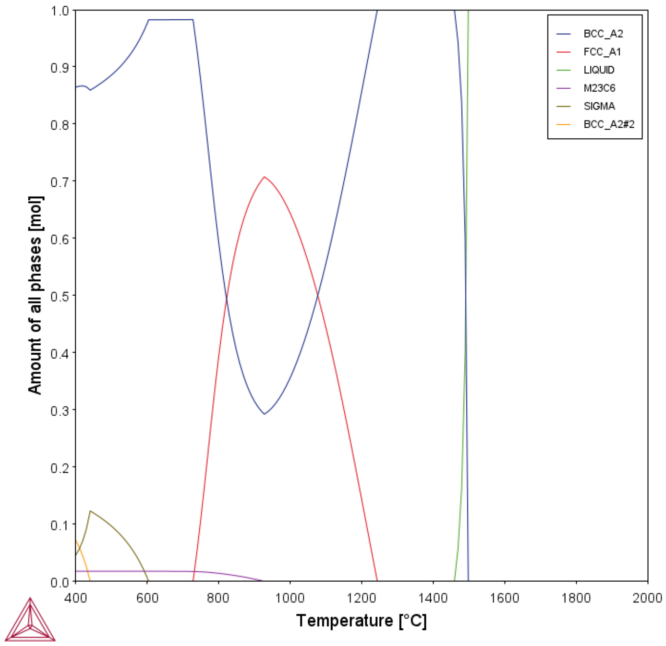


Figure 20: Phase fraction.

PM_G_04: Yield Strength

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

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

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_04_Yield_Strength.tcu*

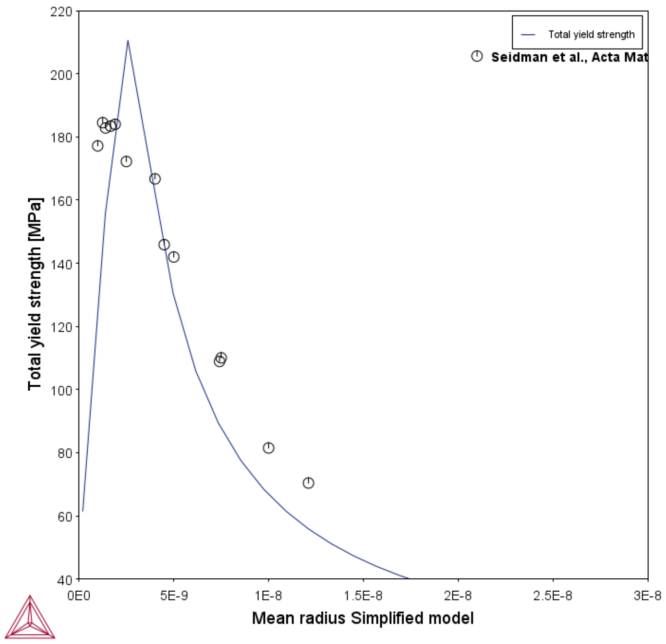


Figure 21: Strength vs Radius - Simplified.

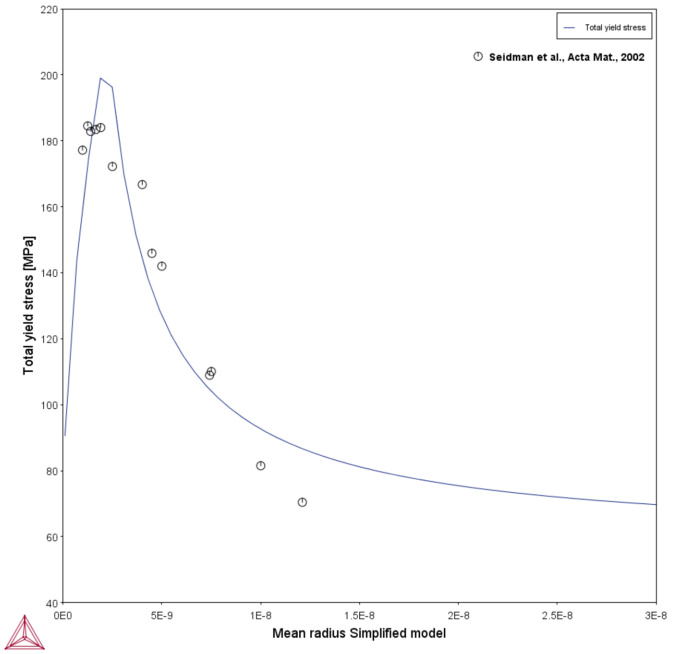


Figure 22: Strength vs Radius - Seidman.

PM_G_05: Yield Strength NiAlCr

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

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

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_05_Yield_Strength_NiAlCr.tcu*

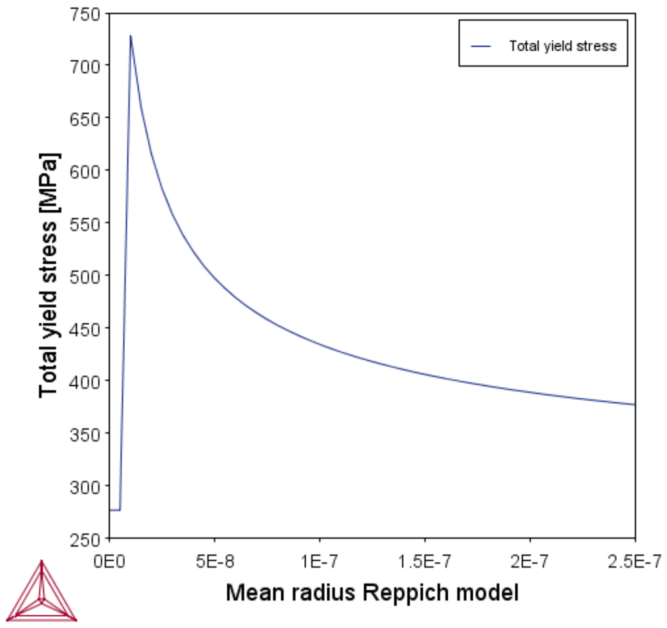


Figure 23: Reppich model plotted with results and experimental data for PE16, all data is normalized with the square root of the volume fraction of precipitate.

PM_G_06: Yield Strength HEA

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

The example uses the **Property Model Calculator** and the **Yield strength** Property Model with a thermodynamic high entropy alloy database (TCHEA). This is an example of solid solution strengthening, which is the contribution to total strength due to the elastic strains in the crystal lattice caused by alloying elements of a lattice parameter differing from the main constituent. The example shows the solid solution strengthening over the full solubility range for the Mo-Ta system as compared to experimental data.

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

Project File Information

- Folder: **Property Models>General**
- File name: *PM_G_06_Yield_Strength_HEA.tcu*

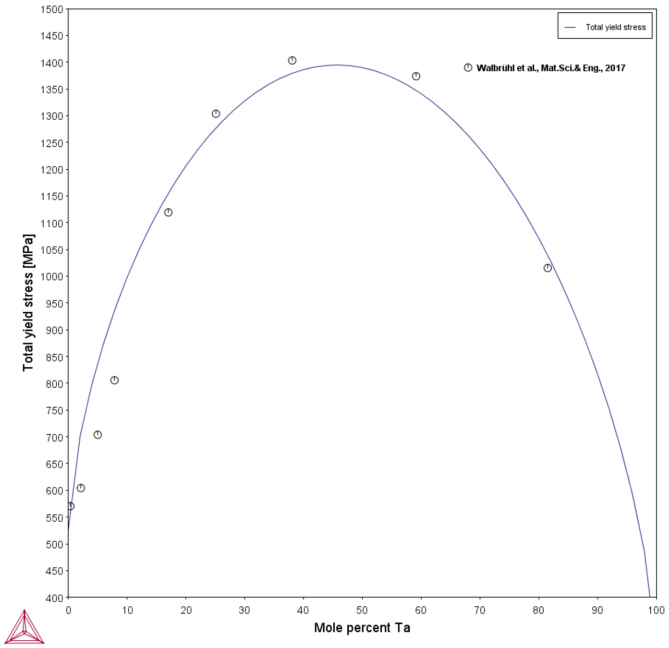


Figure 24: Strength vs at% Ta

PM_G_07: Hot Crack Susceptibility

The example uses the **Property Model Calculator** and the **Crack Susceptibility Coefficient** Property Model to calculate the hot tearing tendency during solidification for an Al-Si alloy.

The **ALDEMO: Aluminum Demo Database** is used and this example is available to all users.

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

The Model is based on the publication by Yan and Lin [2006, Yan] and uses experimental data [1955, Pumphrey; 1976, Feurer; 2004 Barnett] from this paper.

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

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

Project File Information

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

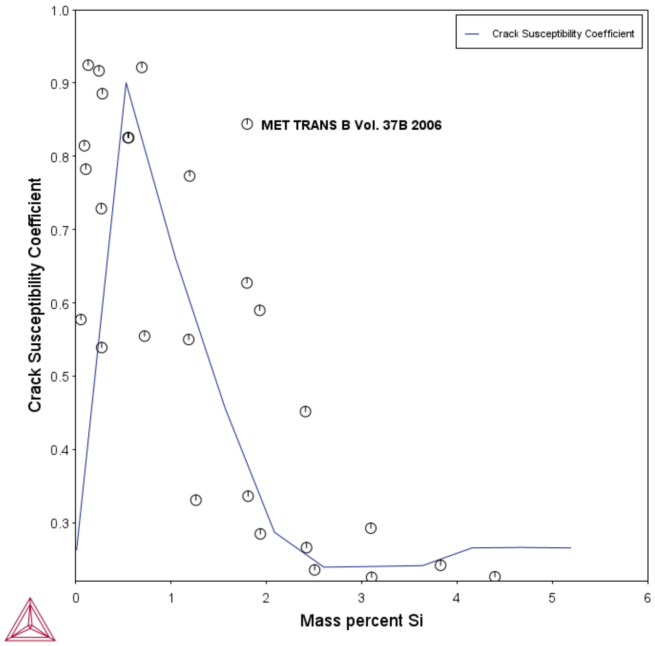


Figure 25: The plot compares the predicted cracking susceptibility/composition curve for the Al-Si system with the experimental hot tearing tendencies [1955, Pumphrey; 1976, Feurer; 2004 Barnett].

References

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

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

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

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

PM_G_08: Spinodal

The example uses the **Property Model Calculator** and the **Spinodal** Property Model to calculate the so-called spinodal curve for the BCC_A2 miscibility gap in the system Fe-Cr.

The **FEDEMO: Iron Demo Database** is used and this example is available to all users.

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

Project File and Video Tutorial Information

- Folder: **Property Models>General**
- File name: *PM_G_08_Spinodal.tcu*

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

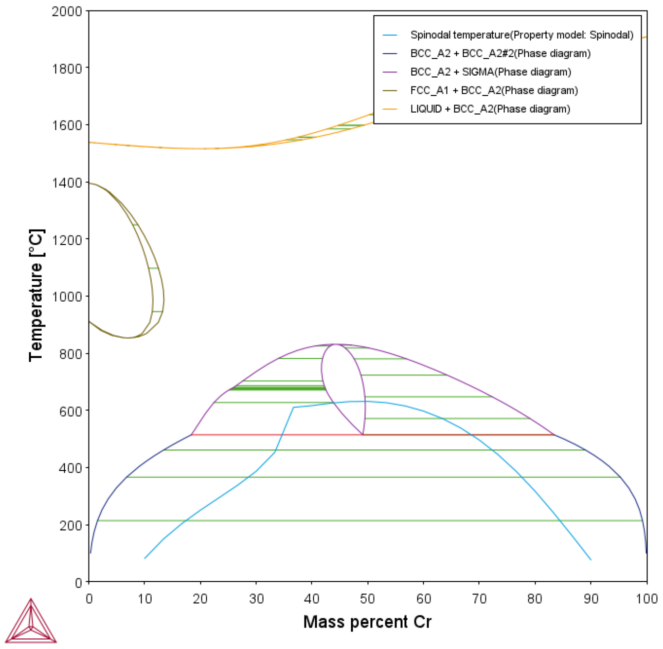


Figure 26: An Fe-Cr spinodal curve for BCC goes through the one-phase region for Sigma.

PM_G_09: T-Zero Temperature

The example uses the **Property Model Calculator** and the **T-Zero Temperature** Property Model to calculate the so-called T_0 line for the two-phase field FCC_A1 and BCC_A2 in the Fe-Ni system. The line is plotted together with the phase diagram for the same Fe-Ni system.

The **FEDEMO: Iron Demo Database** is used and this example is available to all users.

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

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

Project File and Video Tutorial Information

- Folder: **Property Models>General**
- File name: *PM_G_09_T-Zero_temperature.tcu*

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

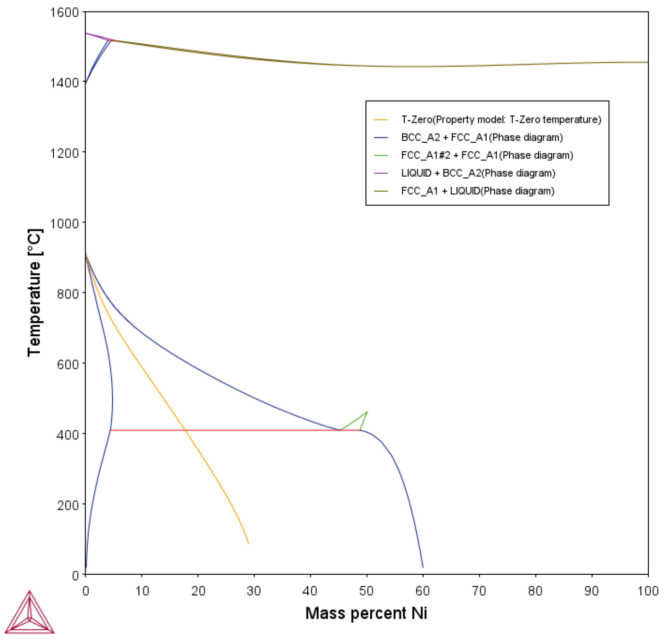


Figure 27: In this plot for the Fe-Ni system, the T_0 line for the FCC_A1 and BCC_A2 phases is located in the middle of the two-phase region. No solution for the T_0 temperature exists above about 30 mass% Ni.

PM_G_10: Freeze-in Thermal Conductivity

The **TCAL Al-Alloys** Database (version 7 and newer) is used in this example. A valid license is required to run the example.

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

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

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

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

As can be seen in Figure 28, the calculation including the approximate effect of grain boundary phase scattering is close to the experimentally measured values. Excluding the effect of grain boundary phase scattering slightly overestimates the thermal conductivity. Experimental data is from [2008, ASM].

Project File and Video Tutorial Information

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

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

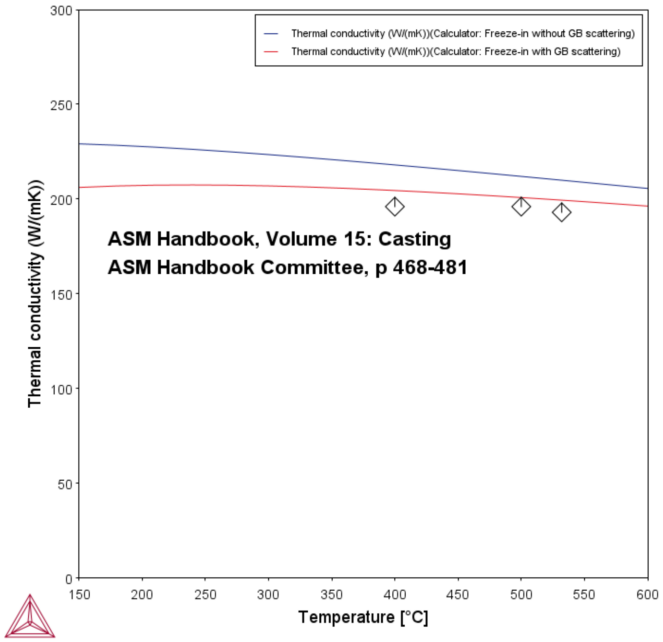


Figure 28: Comparing the freeze-in temperature for the 7075_T6 alloy with and without grain boundary (GB) scattering included in the calculations.

Reference

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

PM_G_11: Freeze-in Electric Conductivity

The **TCAL Al-Alloys** Database (version 7 and newer) is used in this example. A valid license is required to run the example.

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

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

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

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

As can be seen from Figure 29, the calculated electric resistivity at room temperature, including grain boundary phase scattering, is very close to the experientially measured value (4.3E-8) for the alloy. Excluding the grain boundary phase scattering somewhat underestimates the electric resistivity for the alloy. Experimental data is from [1993, Davis].

Project File and Video Tutorial Information

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

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

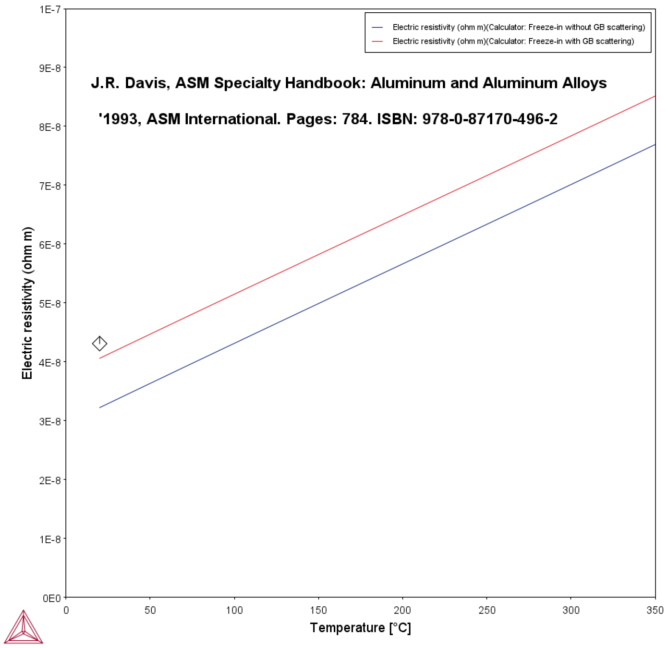


Figure 29: Comparing the freeze-in temperature for the 4032-O alloy with and without grain boundary (GB) scattering included in the calculations.

Reference

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

Steel Model Library Examples Collection

The **General Models** are available to all users. To run calculations with the **Steel Models** (as part of the Steel Model Library) requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. See *Properties that Can Be Calculated* on our website for more information.

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

In this section:

PM_Fe_01: Fe-Cr-C Martensite with Intercritical Annealing

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. See *Properties that Can Be Calculated* on our website for more information about what is available specifically with the Steel Model Library.

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

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

Project File and Video Tutorial Information

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

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

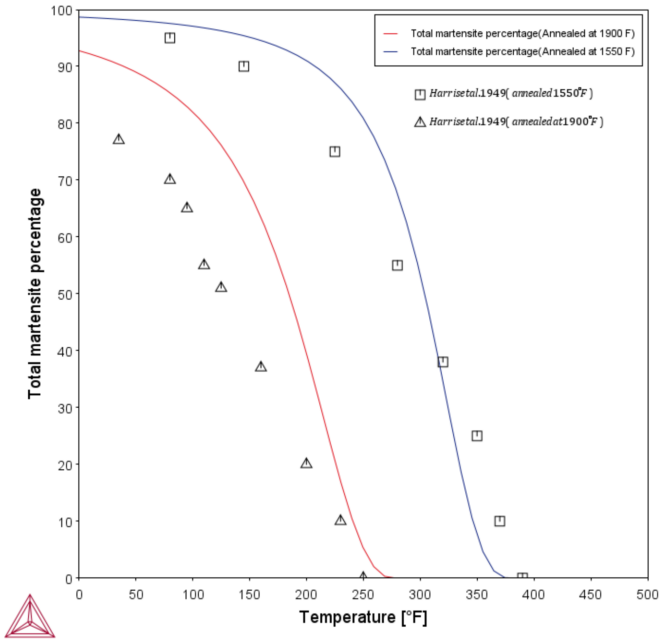


Figure 30: The transformation curves plot showing Fe-Cr-C martensite with intercritical annealing.

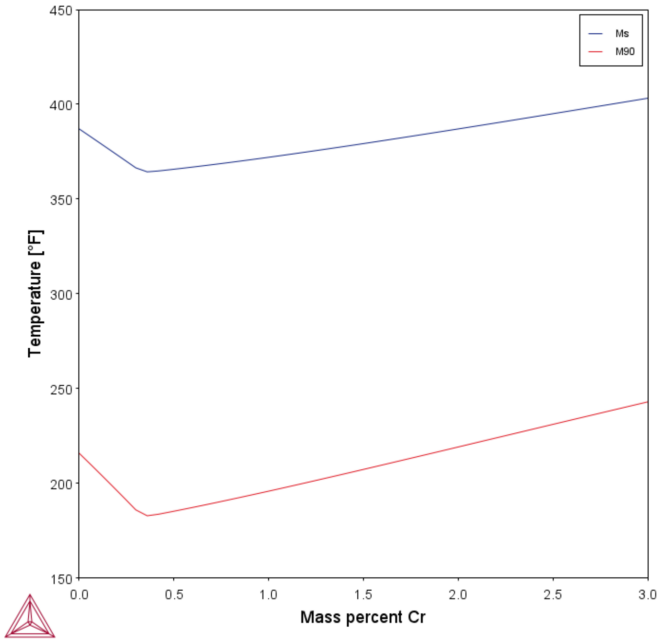


Figure 31: Comparing Martensite start (Ms) to Martensite finish (Mf).

Reference

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

PM_Fe_02: Fe-Mn Martensite Morphologies

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. See *Properties that Can Be Calculated* on our website for more information about what is available specifically with the Steel Model Library.

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

Project File and Video Tutorial Information

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

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

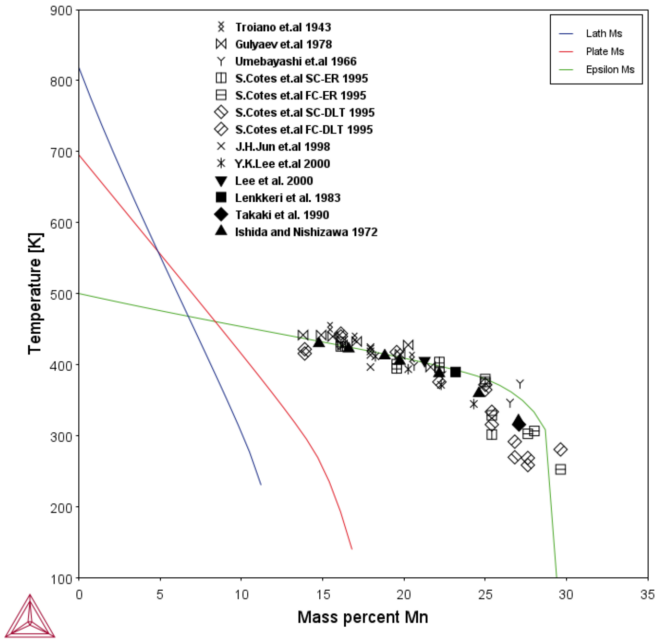


Figure 32: A diagram showing all the Ms temperatures of different types of martensite morphologies (lath, plate and epsilon (hcp) compared with experimental epsilon Ms values.

PM_Fe_03: Fe-C-Mn Pearlite

To run calculations with the **Steel Models** requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases. See *Properties that Can Be Calculated* on our website for more information about what is available specifically with the Steel Model Library.

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

Project File and Video Tutorial Information

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

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

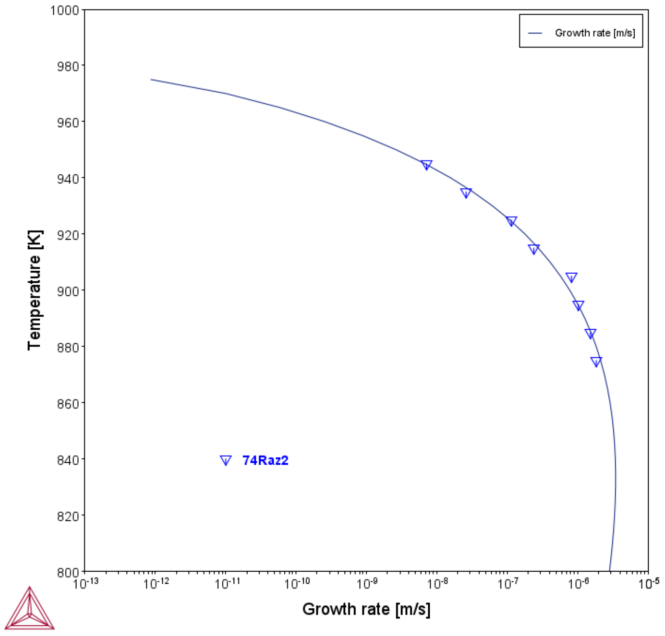


Figure 33: Growth rate as a function of temperature.

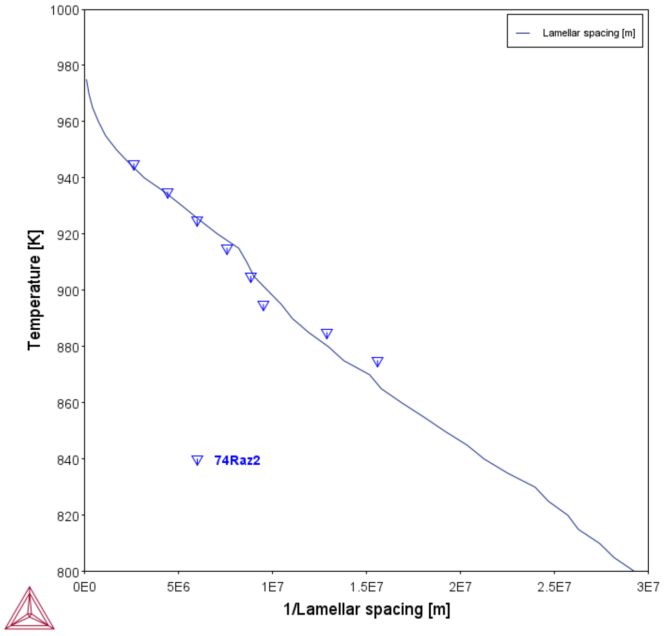


Figure 34: Lamellar spacing as a function of temperature.

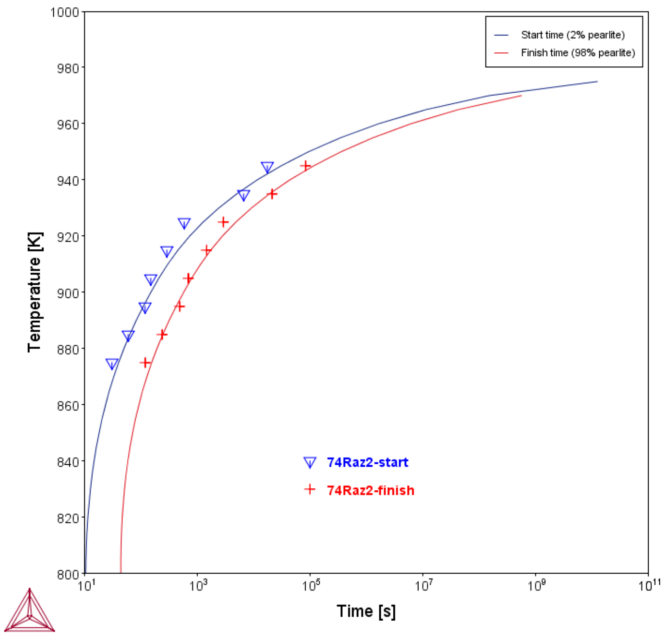


Figure 35: The TTT (time-temperature-transformation) diagram showing times of start (2% transformation) and finish (98% transformation) as functions of isothermal heat treating temperature in an Fe-0.69C-1.80Mn alloy (mass %).

Reference

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

PM_Fe_04: Critical Temperatures

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

The **FEDEMO: Iron Demo Database** is used and this example is available to all users.

In the set up of the example, the **Critical Transformation Temperatures** model is used with a Property Model Calculator **Uncertainty** calculation to plot a histogram showing the distribution of A1- and A3-temperatures (Figure 36). As a comparison, an Equilibrium Calculator, **One axis** calculation results in a property diagram showing the phase transitions for the nominal composition (Figure 37).

The phase transition temperatures are defined as:

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

Project File and Video Tutorial Information

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

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

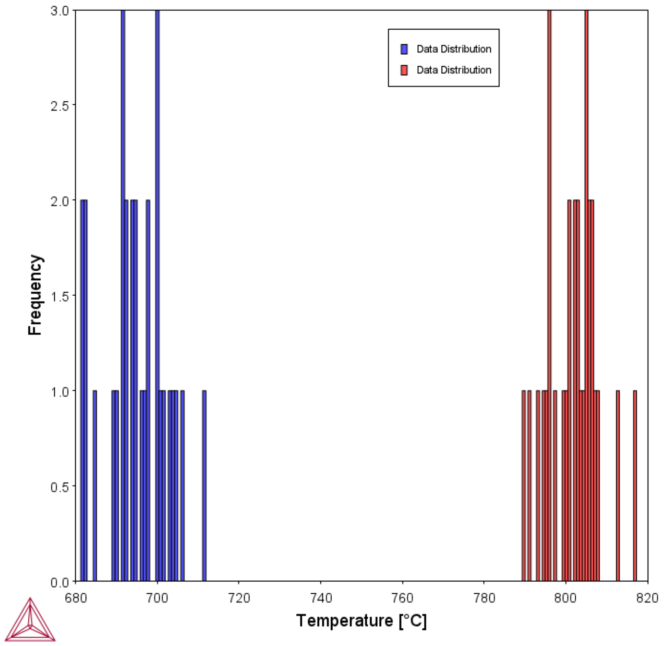


Figure 36: The distribution of the A1 and A3 phase transition temperatures for a low alloyed steel (Fe-0.3Cr-1.0Mn-0.3Mn-0.18C) when the composition is varied within the specification. This plot uses the Critical Transformation Temperatures model with the Property Model Calculator.

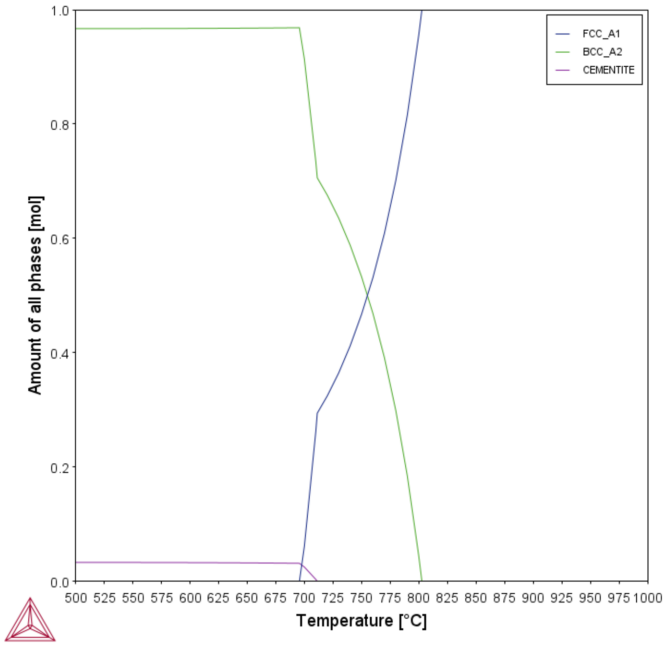


Figure 37: This plot uses an Equilibrium Calculator to show an alternate visualization of the phase transitions in a property diagram for the nominal composition.

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

A license for both TCFE and MOBFE databases are required run this example, which is part of the Steel Model Library.

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

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

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

Also see our website and YouTube channel for tutorial videos related to the Property Model Calculator.

Project File Information

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

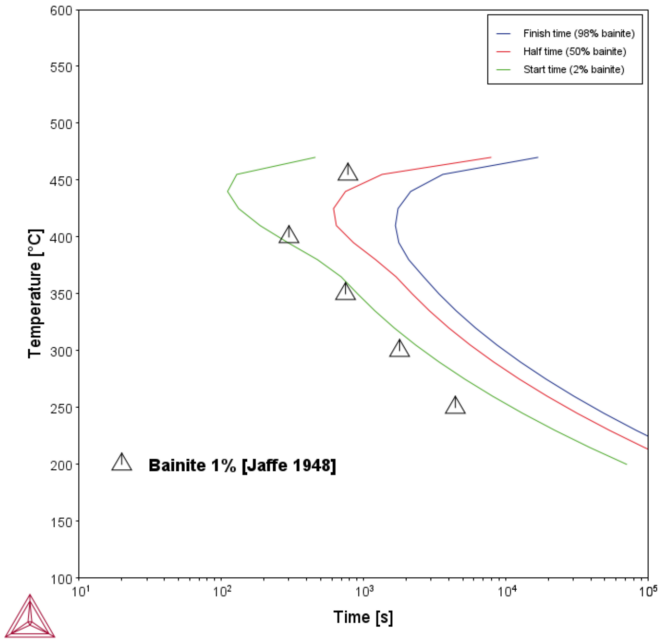


Figure 38: The bainite TTT diagram for an Fe-0.97C-0.72Mn-0.32Si-1.54Ni-0.8Cr-0.26Mo alloy.

Reference

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

Process Metallurgy Module Examples Collection

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

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

In this section:

PMET_01: Basic Oxygen Furnace (BOF)

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

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.

Open the Project File

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.

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

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

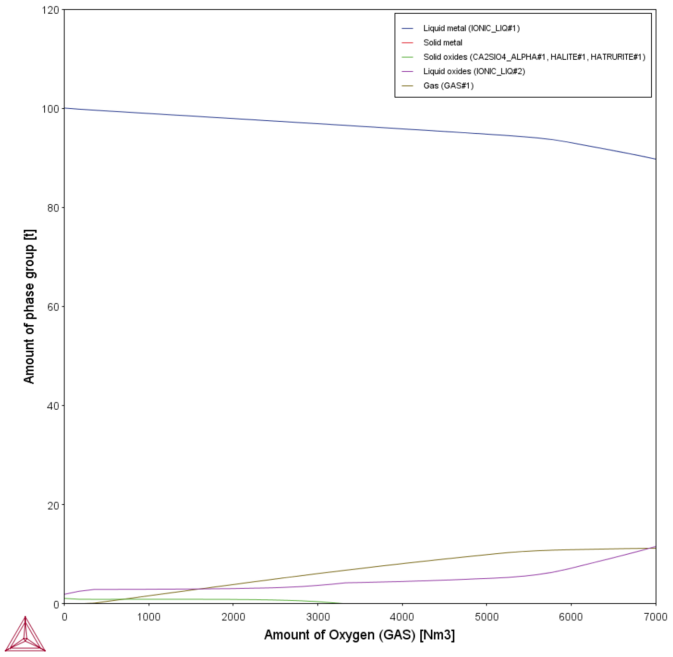
This example is included as a tutorial on our website and our YouTube channel.

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.

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:

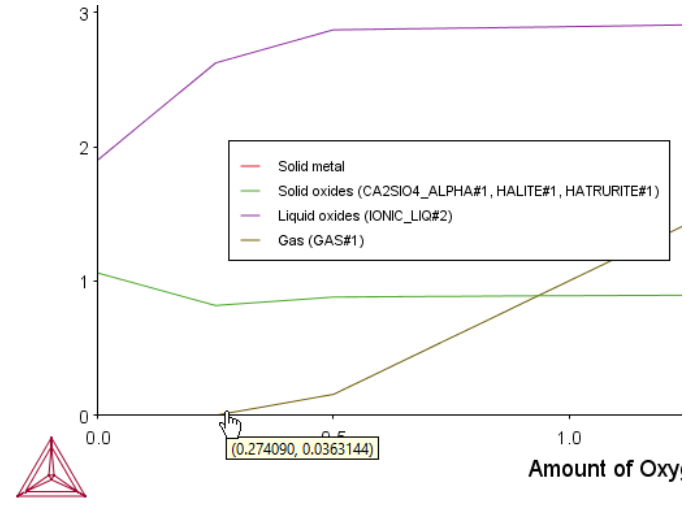
- Quantity: Amount of Oxygen (GAS)
- Stepping 0 min to 10 max with 40 steps

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)**.

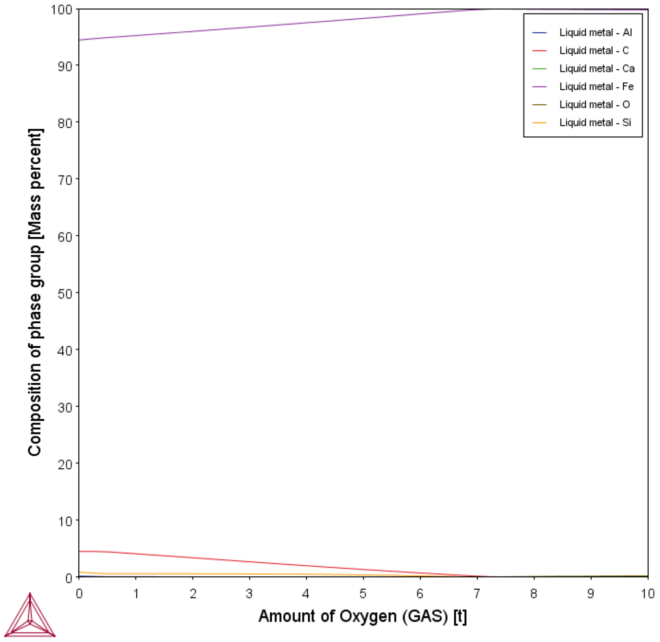
Zooming into the low gas amount (see below), it can be seen that the evolution of the gas phase is retarded. The reason is that the oxygen gas first oxidizes some of the silicon dissolved in the steel to form silicon dioxide (SiO_2). Only when the silicon content in the steel has dropped below a certain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

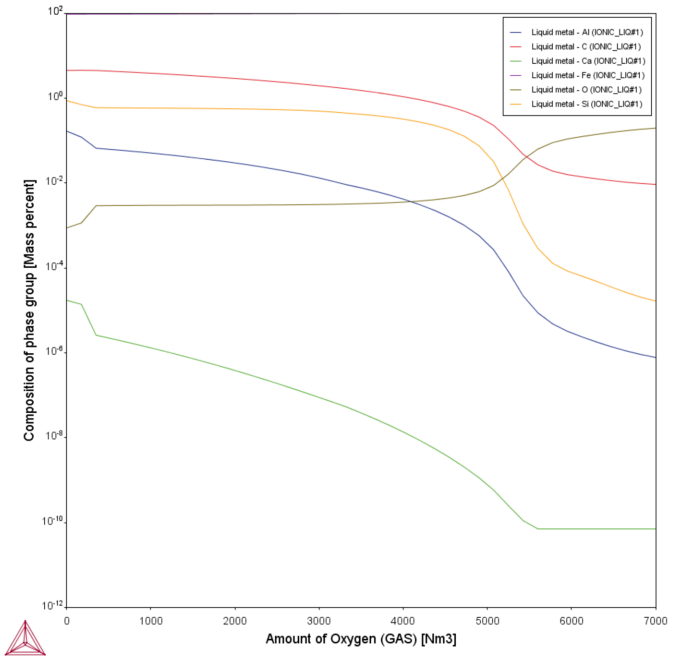
For the next plot, you define the following on a Plot Renderer, which you add to the Process Metallurgy Calculator. Keep the X-axis setting. For the Y-axis, choose **Composition of a phase group**, **Liquid Metal**, **All elements**.



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.

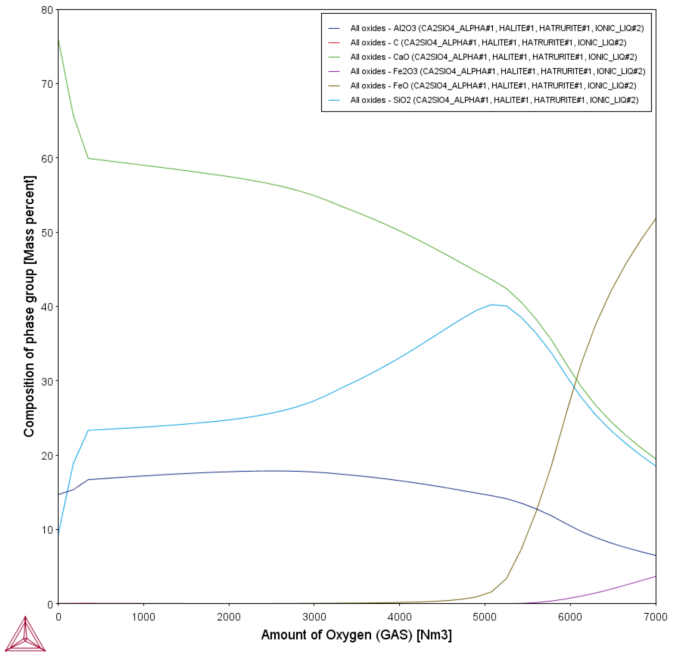
In the example project file only the logarithmic 10 version of the plot is included.



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**.



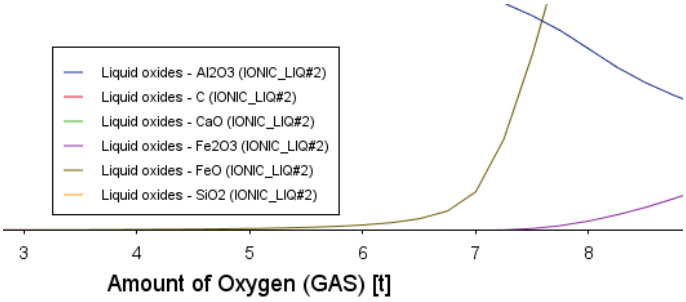
This plot shows how the liquid slag composition changes as a function of the amount of oxygen added to the BOF.

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 (LF)

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

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.

Open the Project File

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

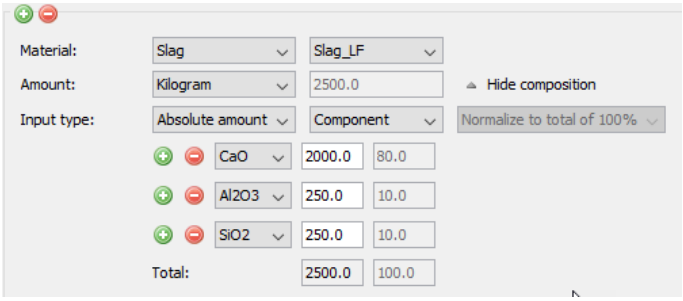
You can open the example project file from Thermo-Calc **Help** → **Example Files** → **Process Metallurgy** → **PMET_02_Ladle_Furnace.tcu**.

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

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.

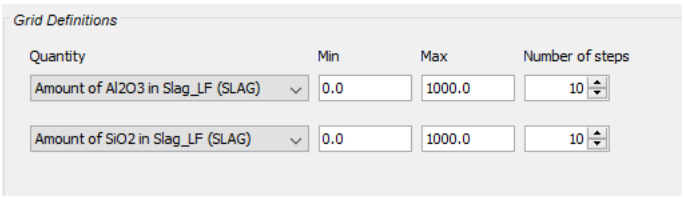
The material saved for this example, *Steel_LF*, could be a typical, but simplified composition of a fully killed SAE 1040 grade steel. The sulfur content, however, is too high for most final applications and must be reduced. Sulfur is usually removed from liquid steel in a ladle furnace using a calcium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

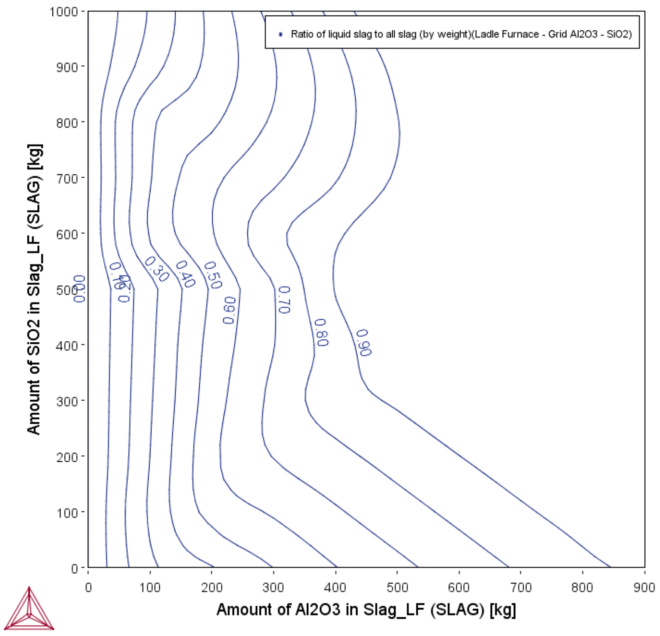


Leave the number of calculation steps at 10 for both axes in order to shorten the calculation time. With this setting, the calculation should be completed in just under one minute. The number of steps could be increased to maybe 30 x 30 for higher resolution of the results, but this increases the calculation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



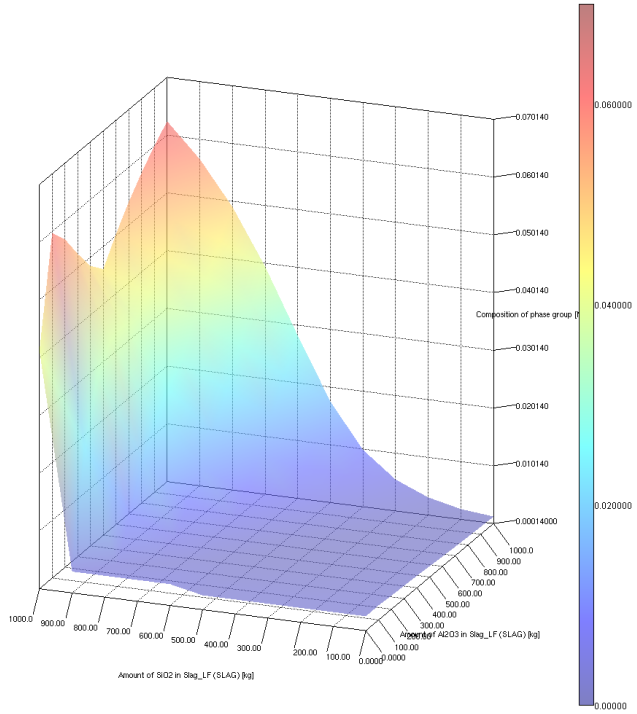
The plot shows that for low amounts of aluminium oxide (Al_2O_3) and silicon dioxide (SiO_2), almost no liquid slag is present. Process metallurgists refer to this as a *hard slag*.

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.

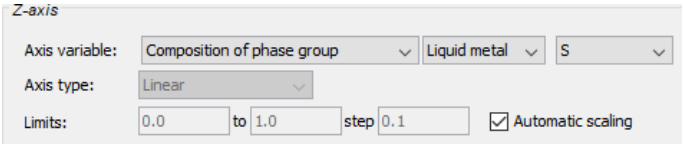
This means that only a little of the sulfur in the liquid steel partitioned into the slag phase and the slag phase has a poor capacity to take up sulfur.

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.

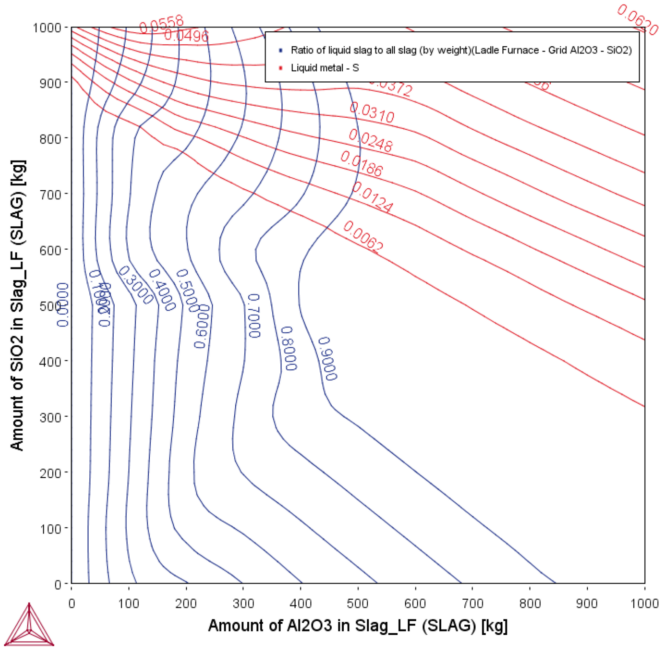
The performed calculations assume thermodynamic equilibrium. As shown in the previous plot, there is almost no liquid slag phase present in the lower left corner at low SiO_2 and Al_2O_3 content. This means that thermodynamic equilibrium would not be achieved due to the very slow kinetics of the reaction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



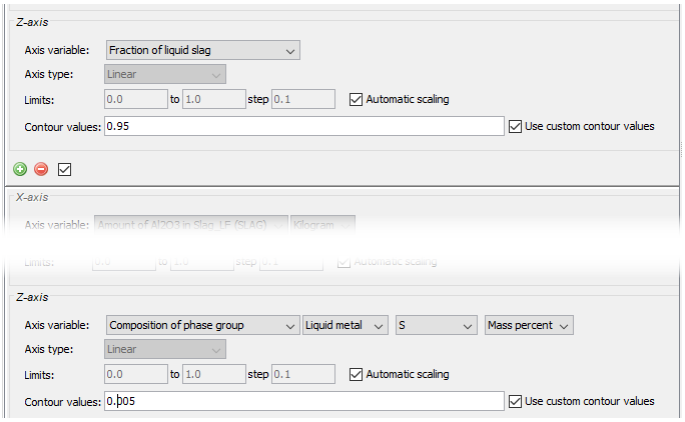
Combining the information contained in the two plots results in an optimum slag composition in a narrow composition band. To smooth the contours, Set the interpolation as **50 x 50**.

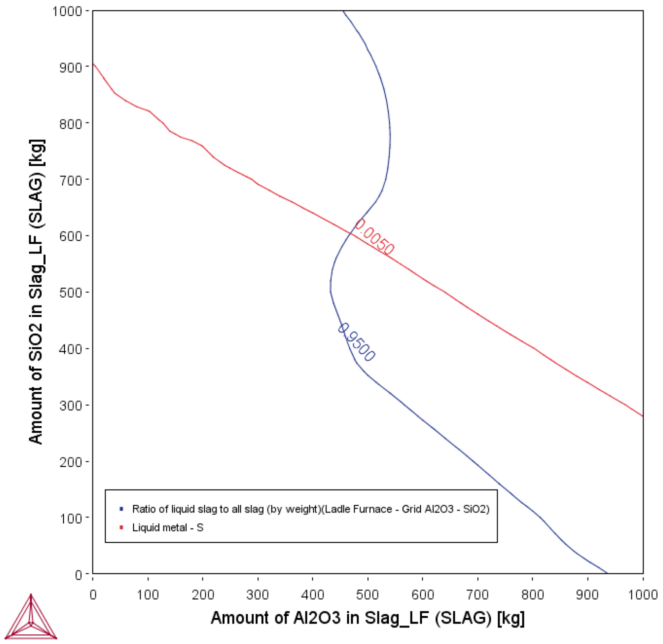


To map this optimal composition field one more plot can be generated by superimposing contour plots of sulfur content in the liquid steel and fraction of liquid slag.

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**.





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.

PMET_03: Argon Oxygen Decarburization (AOD)

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

The example uses the **Process Metallurgy Calculator**.

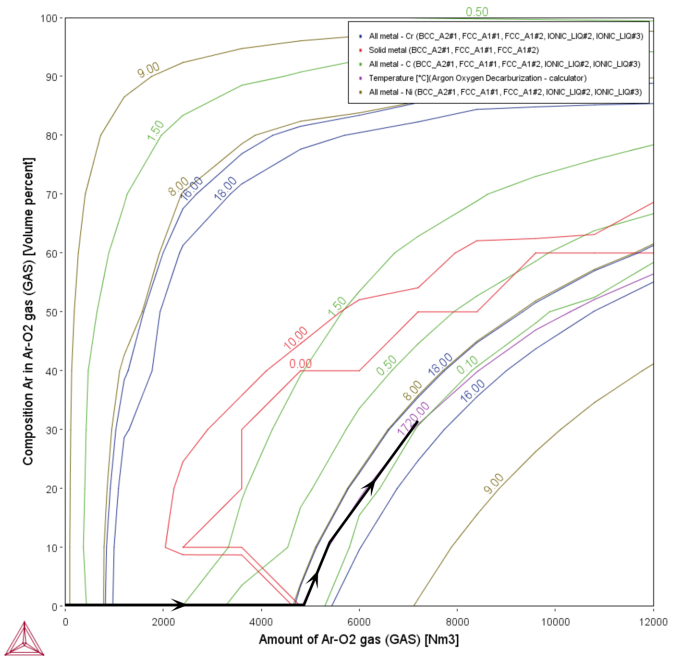
Open the Project File

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

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

The example takes several minutes to run.

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



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

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

Slag Basicity

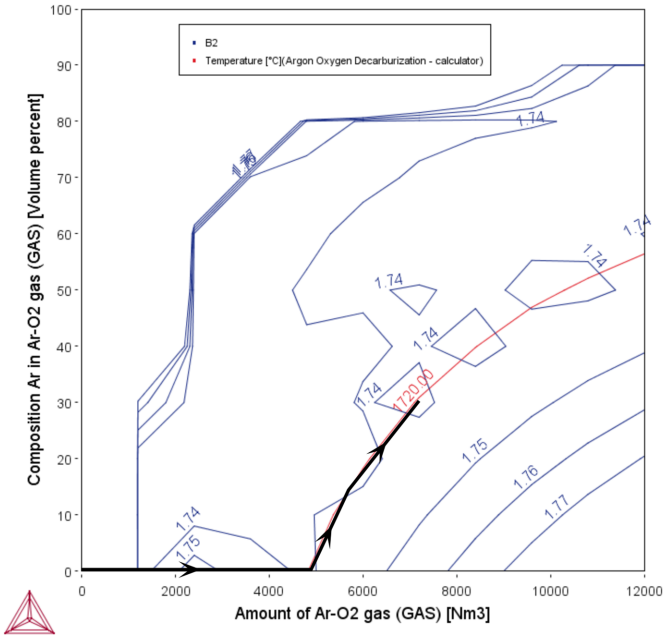


Figure 39: The Slag Basicity plot shows the basicity of the slag (which is a measure for the sulphur capacity of the slag). The process achieves a final basicity of 1.74 which is typical for an AOD-process. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

S Content in Steel

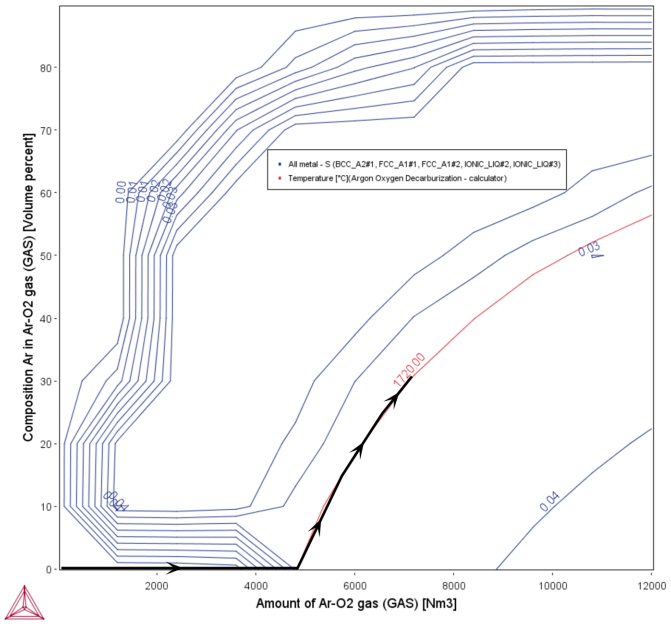


Figure 40: In the S Content in Steel plot, the sulphur content in the steel melt is slightly reduced during the process from 0.056% in the initial steel scrap to finally ca. 0.035%. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

Cr Content in Slag

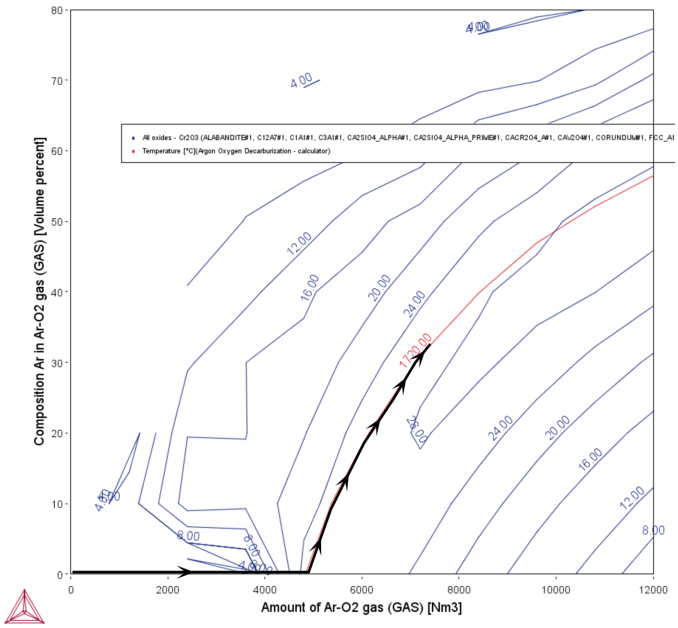


Figure 41: In the Cr Content in Slag plot, the Cr2O3-content in the slag reaches at the end of the process ca. 26 wt-%. This is typical for the AOD-process and requires an additional Cr-recovery step after the conversion to reduce the loss of chromium. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

Amount of Slag

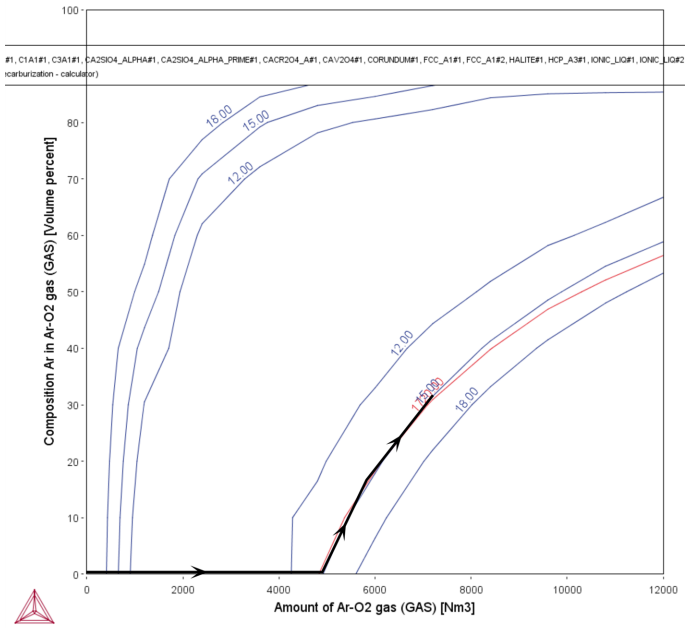


Figure 42: In the Amount of Slag plot, you can see that the process generates about 15 tons of slag in the total. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

Liquid Slag Fraction

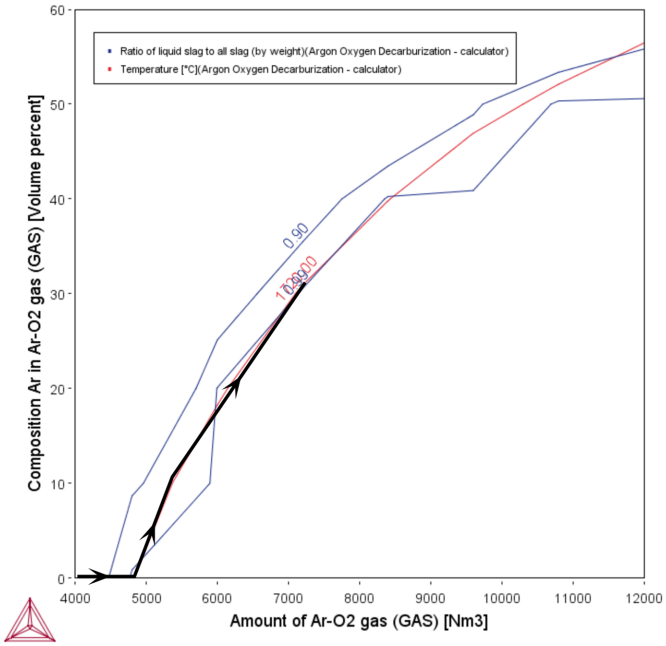


Figure 43: In the Liquid Slag Fraction plot, you can see that towards the end of the process the slag is calculated to be mostly liquid. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

PMET_04: Basic Oxygen Furnace (BOF) Kinetics

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

Open the Project File

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

One way to learn how to work with the Process Metallurgy Calculator is to use the project files as templates to help you set up your own simulation. For example, you can examine the settings available on the **Configuration** window and that are described in Conditions Tab (Process) and the Options Tab.

To open this project file, from the Thermo-Calc menu, go to **Help** → **Example Files** → **Process Metallurgy** → **PMET_04_Basic_Oxygen_Furnace_Kinetics.tcu**.

Once you open the project file, click **Perform Tree** at the bottom center of the **Configuration** window. It takes a few minutes to run the simulation.

Setting Up the BOF Process Simulation

Using the **Process Metallurgy Calculator** and the **Process simulation** branch, this example sets up a kinetic simulation of a simplified basic oxygen furnace (BOF) process applying the effective equilibrium reaction zone (EERZ) to simulate the kinetics of the process.

What follows is a general overview of the three basic steps required to set up a kinetic simulation.

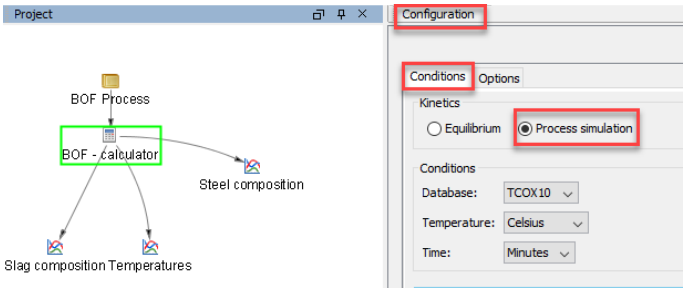


Figure 44: The Process Metallurgy Calculator for this example is renamed BOF - Calculator in the Project window. To the right is the Configuration window where you choose to define a Process simulation.

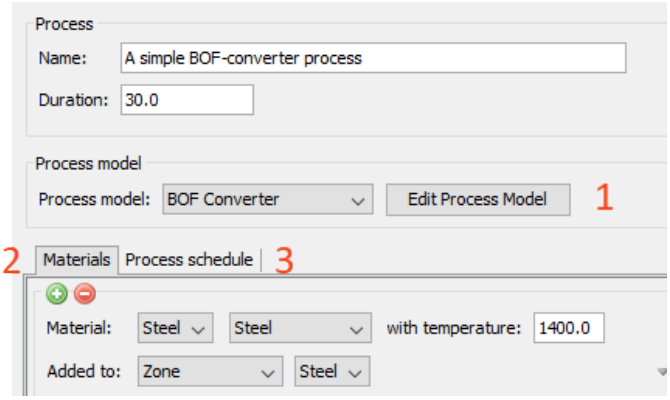


Figure 45: The settings you need to access are on the Process Metallurgy Calculator Configuration window. From here, you perform three steps to set up a kinetic simulation. (1) Edit the Process Model, (2) Define the Materials, and then (3) Define the Process Schedule.

Step 1: Edit the Process Model

Click **Edit Process Model** to open the settings window. This is where general kinetic parameters are defined that depend on the type of process to be simulated as well as the equipment size and shape to be used. The reaction zone area is the area of the interface between the steel and the slag in the crucible. This is where the steel and slag react with each other. The kinetics of the reaction is limited by the mass transfer to and from the interface.

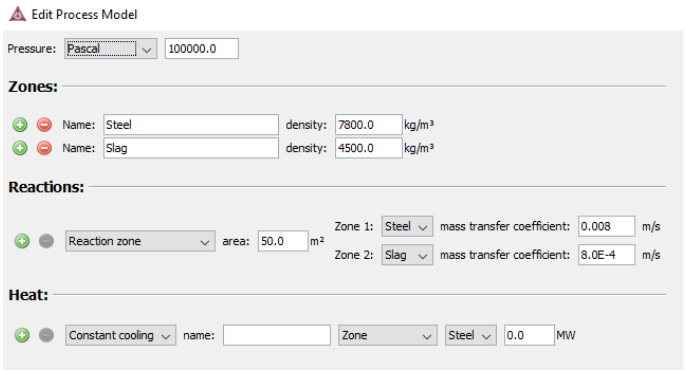


Figure 46: The Edit Process Model window for a Process Metallurgy Calculator using the Process simulation branch.

Step 2: Define Materials

On the **Materials** tab all the compositions of the materials that are to be used during the process are defined. Also, the temperature at which they are added and the zone to which they are added is defined.

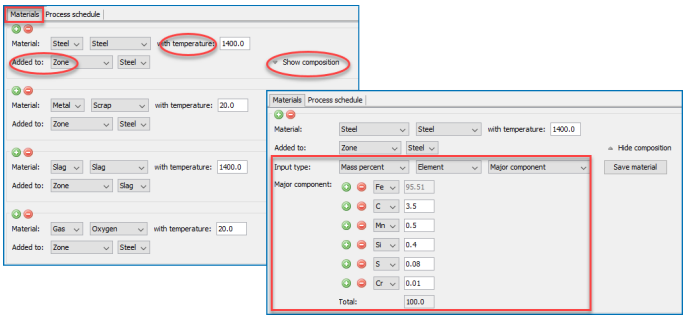


Figure 47: The Materials tab for a Process Metallurgy Calculator where you can define the composition, temperature and zone.

Step 3: Define the Process Schedule

On the **Process schedule** tab the steelmaking recipe is entered, which defines at what times how much of which materials is added. The process schedule in this example is not meant to closely represent a real process; it is intended only to show the general principles.

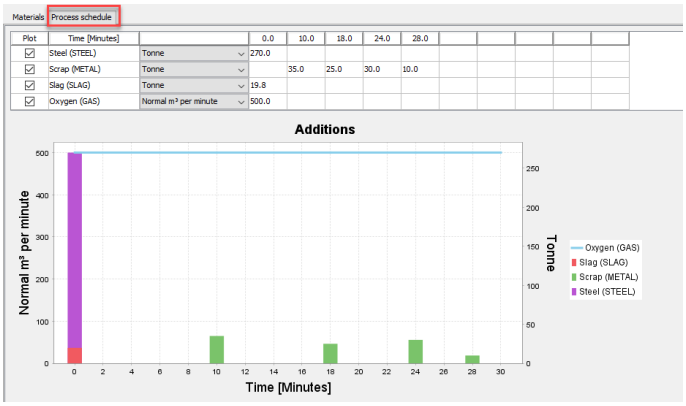


Figure 48: The Process schedule tab for a Process Metallurgy Calculator where you enter your steelmaking recipe.

Plot Results

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

A variety of video tutorials are available for many of our products and features on our website and our YouTube channel. The library keeps growing so be sure to check back on a regular basis.

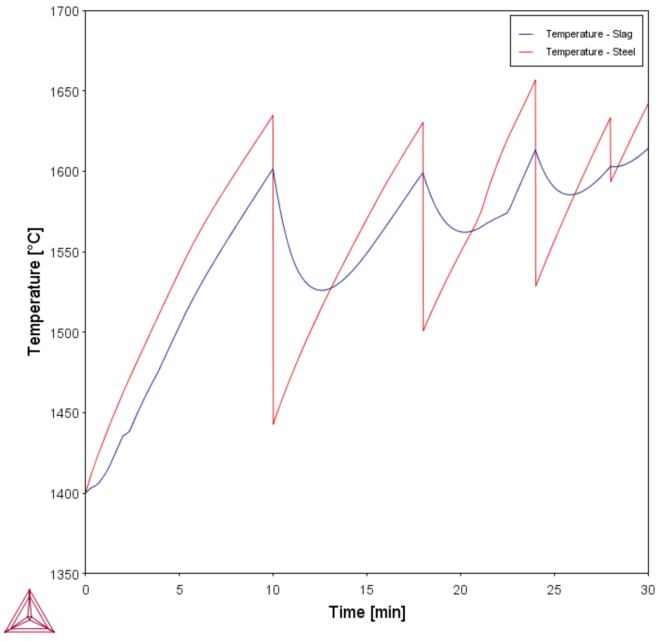


Figure 49: The temperatures of the steel and slag bulk zones.

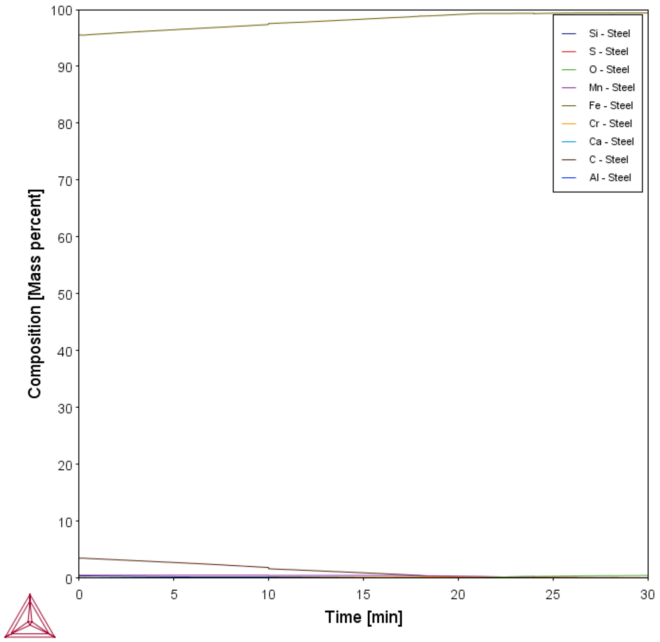


Figure 50: The steel composition in the bulk zone.

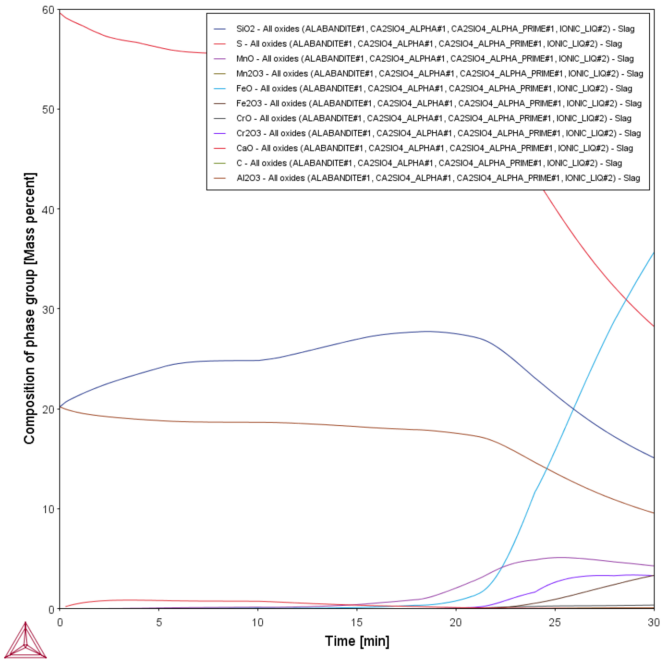


Figure 51: The slag composition in the bulk zone.

PMET_05: Lab Scale Ladle Furnace (LF) Kinetics

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

Open the Project File

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

One way to learn how to work with the Process Metallurgy Calculator is to use the project files as templates to help you set up your own simulation. For example, you can examine the settings available on the **Configuration** window and that are described in Conditions Tab (Process) and the Options Tab.

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

Once you open the project file, click **Perform Tree** at the bottom center of the **Configuration** window.

About the Plot Results

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

Setting Up the LF Process Simulation

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

- Setting Up a Process Metallurgy Simulation

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

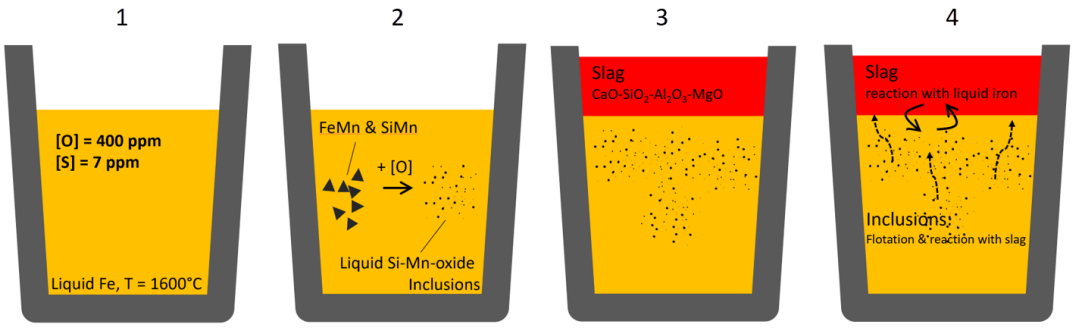


Figure 52: Diagram of the experiment performed by Piva et al. [2017]. The sequence as described in the text is: (1) liquid Fe with dissolved oxygen; (2) FeMn and SiMn added to deoxidize Fe; (3) top slag added after 360s; and (4) gradual reaction between steel, slag and inclusions.

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

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

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

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

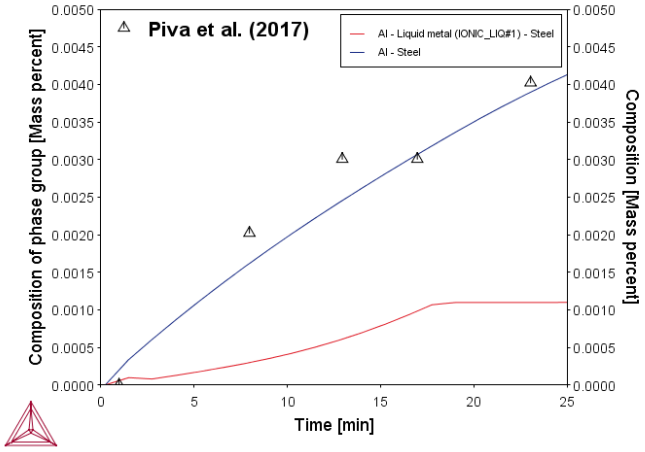
Results and Experimental Analysis

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

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

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

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



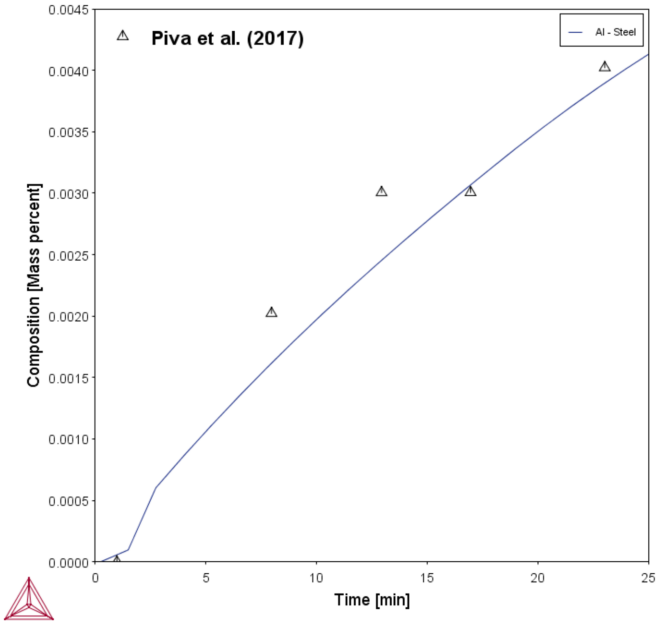


Figure 53: Total Al in the steel compared with experimental data (blue/top curve). If only the fraction of dissolved Al is to be plotted (red/bottom curve), this is done by selecting "Composition of phase group" and "Liquid metal". The bottom figure is available with the example.

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

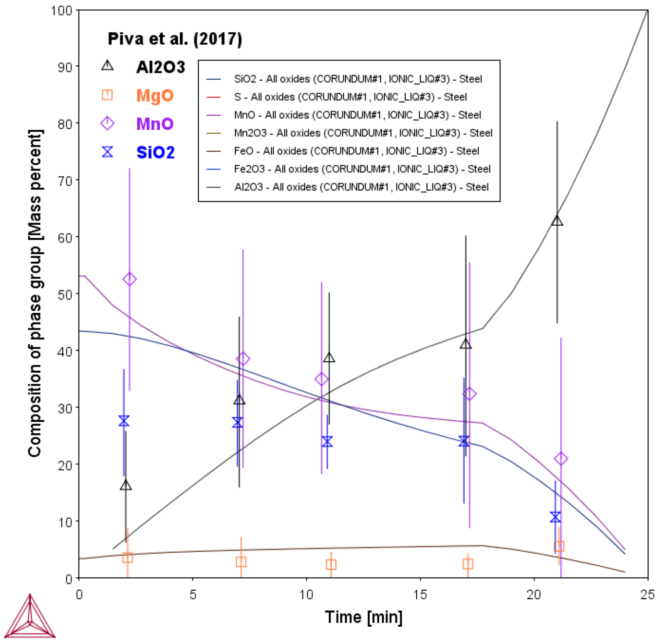


Figure 54: Calculated composition of non-metallic inclusions in function of processing time compared to experimental data [2017, Piva].

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

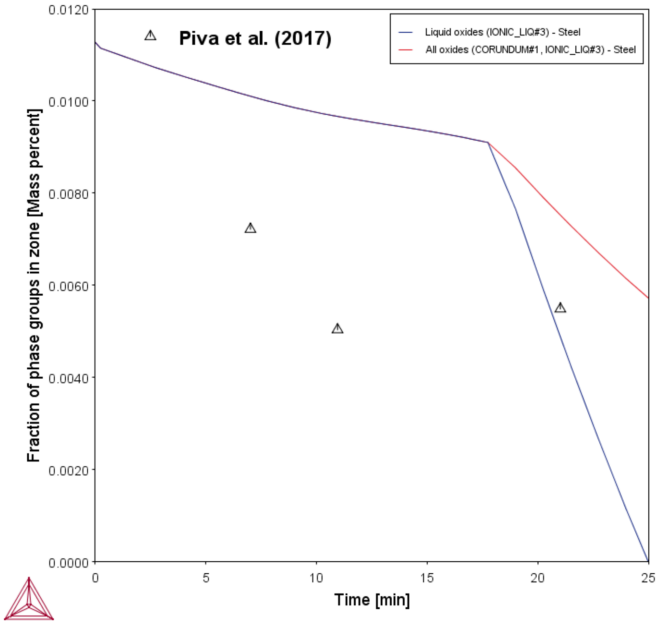


Figure 55: Amount of inclusions in the liquid steel in function of processing time. The total amount of inclusions (red line) and liquid oxide inclusions (blue line) are plotted. Up to about 20 min all inclusions are liquid oxide type, then they are replaced by solid corundum (Al_2O_3) inclusions. Experimental data from Piva et al. [2017].

Reference

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

PMET_06: Ladle Furnace (LF) Kinetics

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

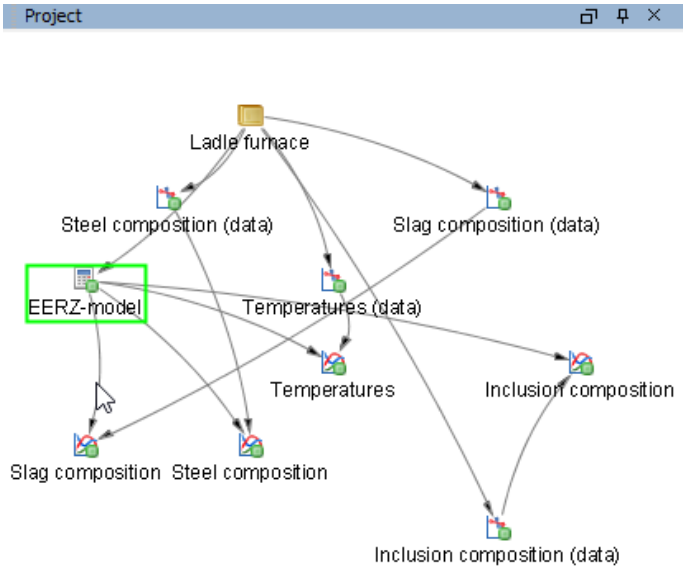
Open the Project File

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

One way to learn how to work with the Process Metallurgy Calculator is to use the project files as templates to help you set up your own simulation. For example, you can examine the settings available on the **Configuration** window and that are described in Conditions Tab (Process) and the Options Tab.

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

Once you open the project file, click **Perform Tree** at the bottom center of the **Configuration** window. It takes several minutes to run the simulation.



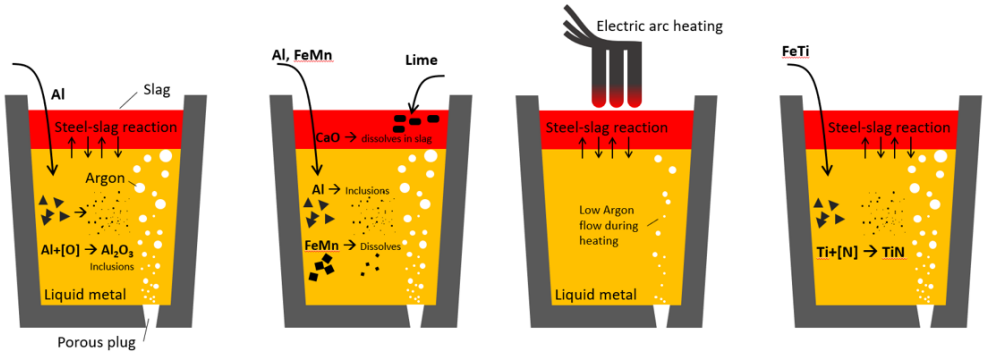
The nodes in the Project window for this example. The Process Metallurgy Calculator is renamed to EERZ model. If you click this node the Configuration window opens, which is where all the settings for the process simulation are located. This advanced example also uses three Experimental Data Reader nodes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

About the Plot Results

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

Setting Up the LF Process Simulation Kinetics

The example uses the **Process Metallurgy Calculator** and the **Process simulation** branch to show how a full kinetic simulation of the LF refining process is set up as shown in the diagram below. The simulation is based on an LF process described in an article by Graham and Irons [2009, Graham] and the results of the simulation are compared to their experimentally determined steel, slag, and inclusion composition in function of processing time. Only some plotting results and analysis are presented, discussed and compared to the experimental data from Graham and Irons [2009].



Time = 1	Time = 20 min	Time = 27 min	Time = 39 min
105 kg Al added to	140 kg Al added	Heating by electric arc	46 kg of FeTi added
165 t liquid steel	50 kg FeMn added		
4.95 t slag	100 kg Lime added		
Ar bubbling	Ar bubbling	Ar bubbling	Ar bubbling

Figure 56: Overview of the LF process to be simulated.

Process Schedule

The process schedule shows how this LF process is implemented in the Process Metallurgy Module.

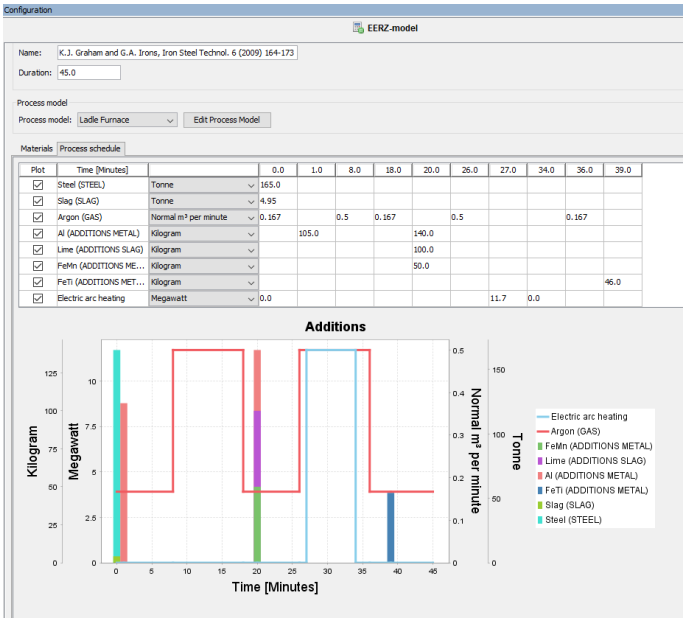


Figure 57: The Process schedule set up for this example. If you have the project open in Thermo-Calc , click the Process schedule tab to view this. You can then click the check boxes in the Plot column to include or exclude materials to better visualize the process schedule on this tab. This is based on the LF steel refining process schedule as published by Graham and Irons [2009, Graham].

Temperature

The experimentally determined temperature of the steel can easily be reproduced to within experimental uncertainty. In addition many more details of the temperature evolution in the different zones of the ladle furnace can be resolved by the simulation. For example, the addition of Al to the liquid steel results in a temperature increase due to the exothermal oxidation of the Al by the dissolved oxygen. The addition of CaO to the slag phase on the other hand results in a significant cooling of the slag due to the heat required to heat up and melt the added CaO. It can also be seen that the heat added to the reaction zone during electric arc heating results in a strong temperature increase of this zone. In reality the local temperature is even much higher, but this is not resolved by this model.

A finer point to observe is that the temperature of the reaction zone is always slightly higher than both the steel zone and the slag zone. The reason for this is that the reaction between the steel and the slag is exothermic.

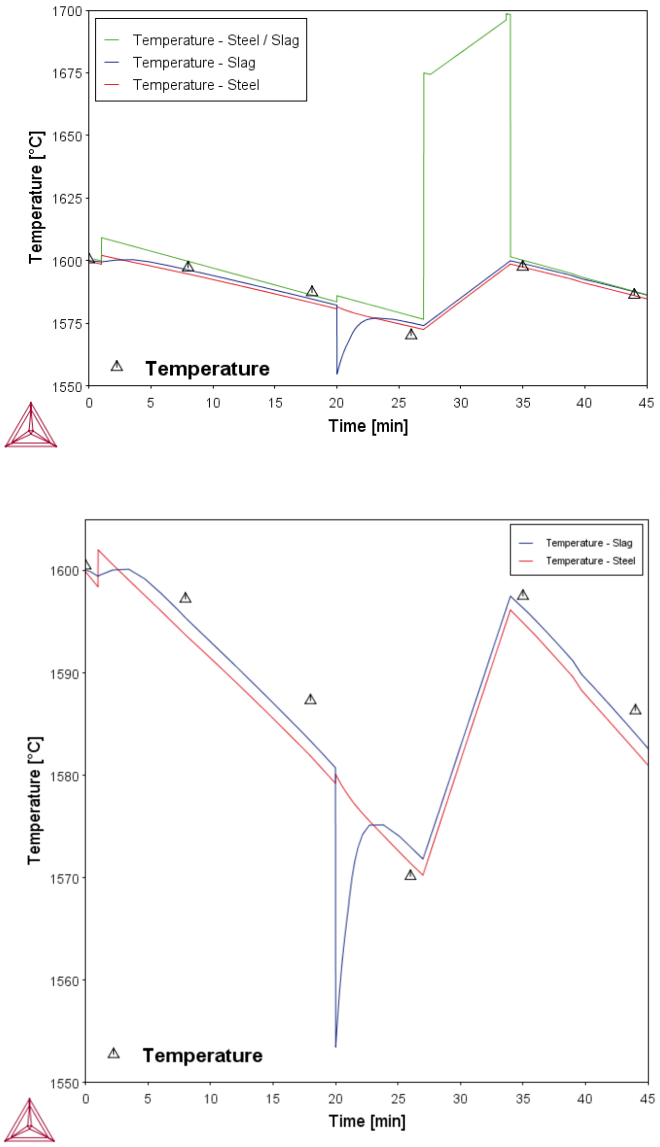


Figure 58: Temperature evolution of the steel zone, slag zone and reaction zone during the LF treatment. The temperature of the reaction zone has been added to illustrate how its temperature is increased by the heat input by the electric arc that is added to this zone (top). The bottom plot is included with the example in Thermo-Calc and shows another way you can visualize the results.

Liquid Metal Composition and Amount

Already this simple model captures the evolution of the steel chemistry in function of processing time very well. The experimentally determined S, Mn and Ti contents are reproduced to within experimental accuracy.

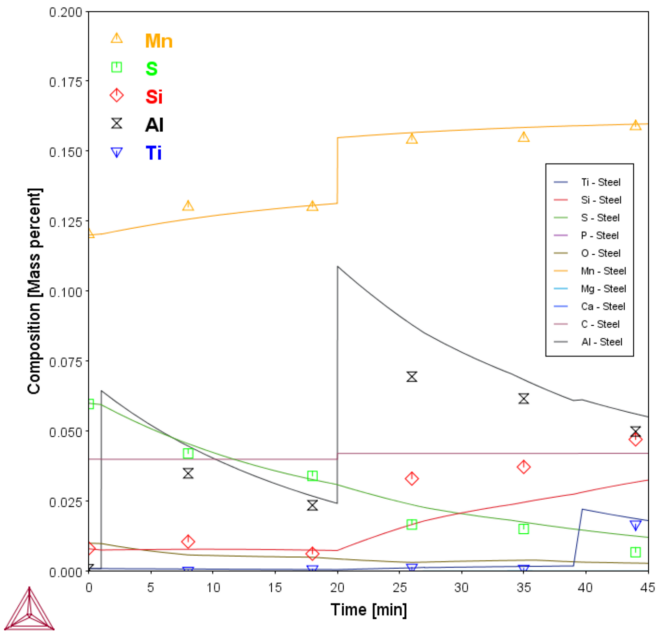


Figure 59: Evolution of the steel chemistry in function of time during ladle furnace treatment. Most of the experimentally measured datapoints are very well reproduced by this very simple model set-up demonstrating that the underlying processes are well captured. This plot is not included with the example but you can try to reproduce it yourself or go to our website to see the detailed example available there.

Slag Composition and Amount

Also the evolution of the slag chemistry is well reproduced. Some of the important changes in chemistry, such as the gradual decrease of FeO and MnO and uptake of S in function of time can only be seen after zooming into the plot somewhat

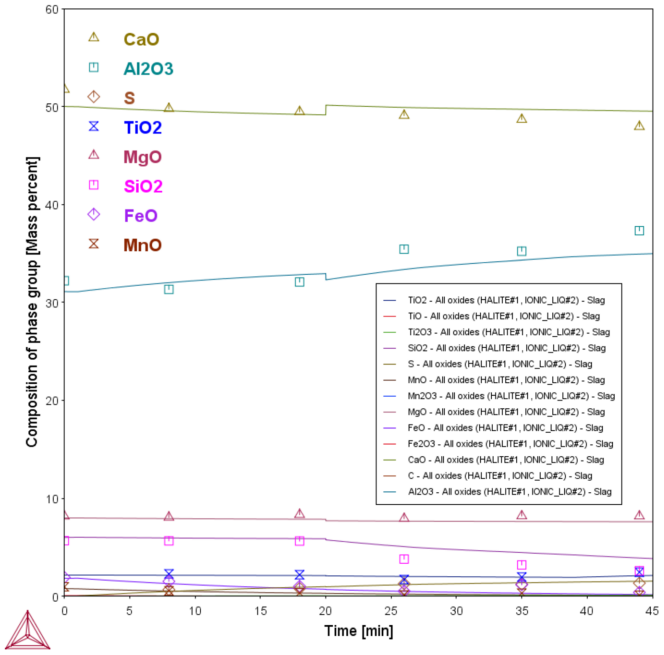


Figure 60: Evolution of the slag chemistry in function of time during ladle furnace treatment.

Inclusion Composition

Finally, also the evolution of the inclusion compositions can be calculated. Up to about 25 min into ladle furnace processing the inclusions are almost pure solid corundum (Al_2O_3), then a second population of MgO rich spinel inclusions start forming. This result captures the essence of what is experimentally observed.

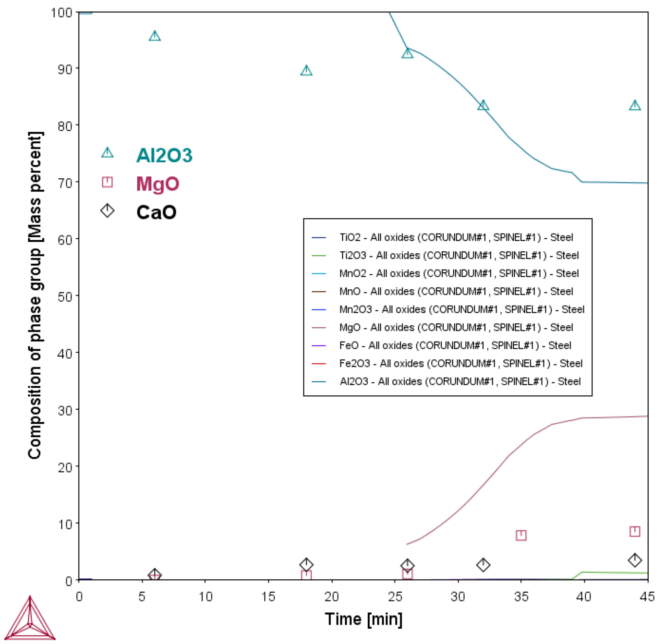


Figure 61: Evolution of the inclusion chemistry in function of time.

References

[2009, Graham] K. J. Graham, G. A. Irons, Toward integrated ladle metallurgy control. Iron Steel Technol. 6, 164–173 (2009).

[2020, Mason] P. Mason, A. N. Grundy, R. Rettig, L. Kjellqvist, J. Jeppsson, J. Bratberg, “The Application of an Effective Equilibrium Reaction Zone Model Based on CALPHAD Thermodynamics to Steel Making” in 11th International Symposium on High-Temperature Metallurgical Processing (2020; DOI: 10.1007/978-3-030-36540-0_10), pp. 101–113.

PMET_07_Vacuum_Oxygen_Decarburization_Kinetics

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

Open the Project File

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

One way to learn how to work with the Process Metallurgy Calculator is to use the project files as templates to help you set up your own simulation. For example, you can examine the settings available on the **Configuration** window and that are described in Conditions Tab (Process) and the Options Tab.

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

Once you open the project file, click **Perform Tree** at the bottom center of the **Configuration** window. It takes several minutes to run the simulation.

The example uses the **Process Metallurgy Calculator** to show how to set up the Vacuum Oxygen Decarburization (VOD) process. The example is based on data of a real VOD process published by [2000, Ding].

Only a brief outline of this example with the plot results are included here. Go the links on our website to read an overview of the VOD process, plus an in depth analysis of the results obtained when you run the example file. There are also additional results and extensions available.

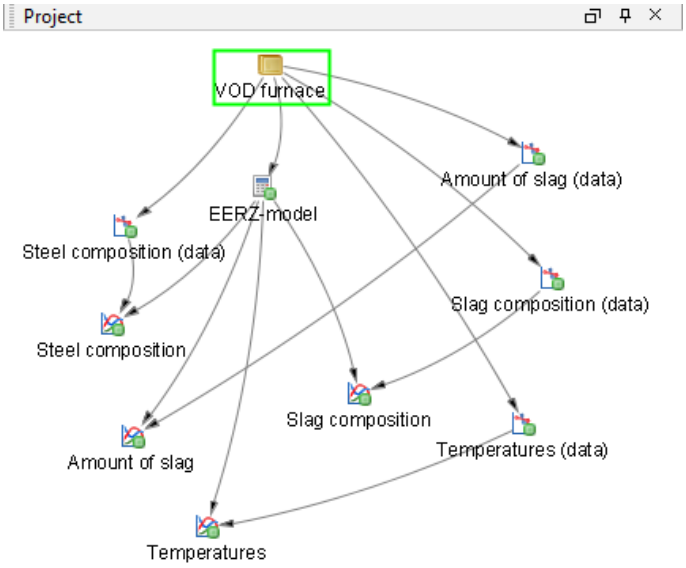


Figure 62: The set up in the Project window for this example. Go to the website to read more about how this is implemented as well as a summary of the VOD process itself as it is applied to the the use of the Process Metallurgy Module and these results.

The VOD process is split into three stages:

1. Oxygen blowing.
2. Degassing under a vacuum.
3. Reducing.

As in all kinetic simulations with the Process Metallurgy Module, three steps are required to set up the simulation:

1. **Edit Process Model** where equipment and general process dependent kinetic parameters are defined.
2. **Materials**: where all materials added during the process are defined.
3. **Process Schedule** where the timeline of the process is defined, stating what happens at which time.

During the set up of the example, the use of the following features are highlighted:

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

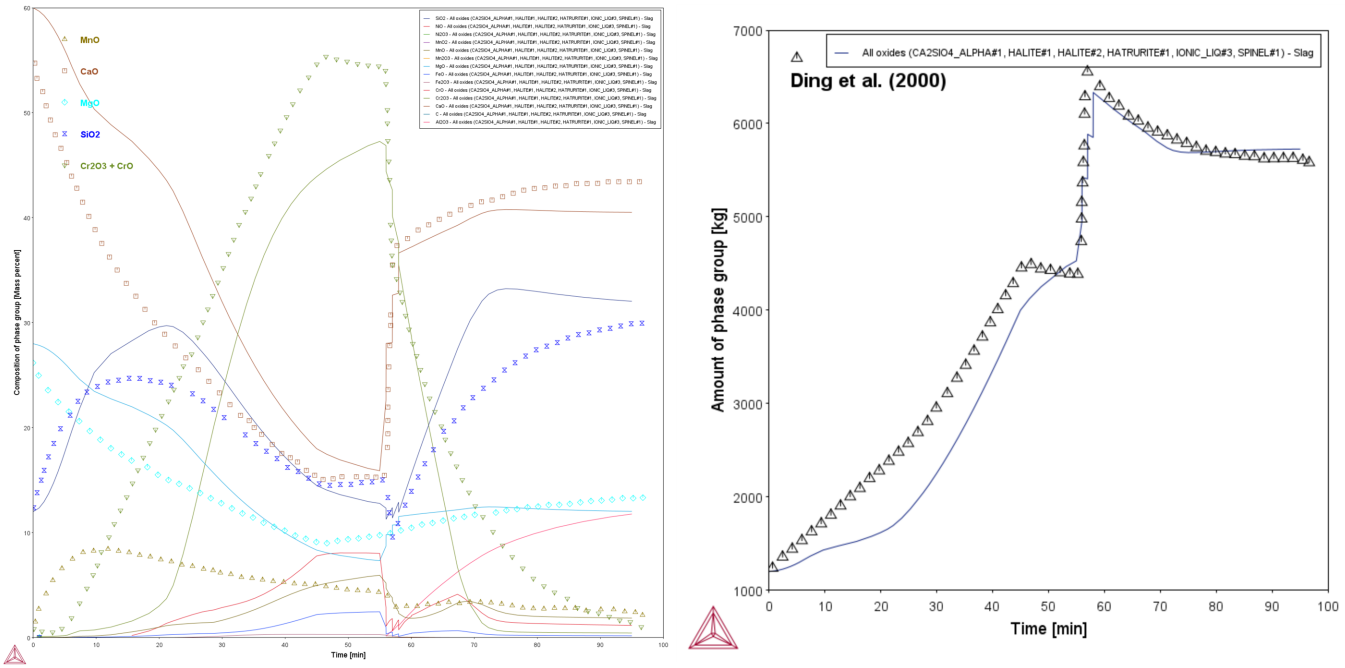


Figure 63: Evolution of the slag chemistry (left) and slag amount (right) in function of time. The comparison is made to the simulation results by [2000, Ding] (open symbols) only, as no experimental data is available.

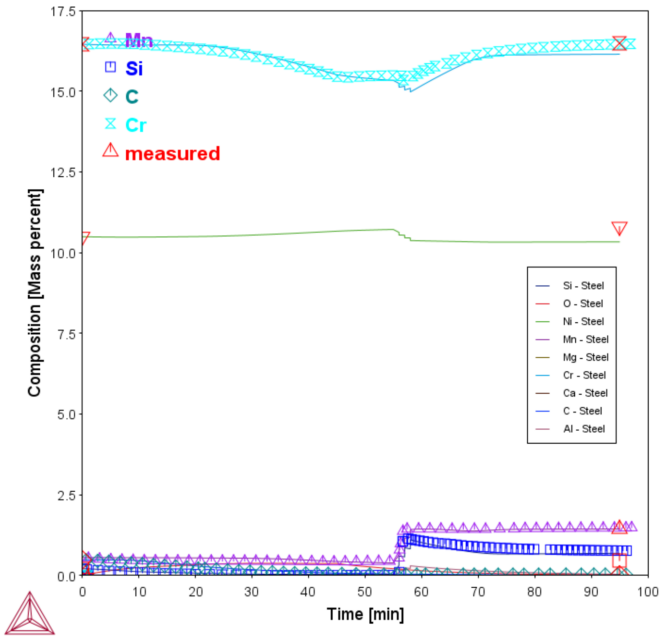


Figure 64: Comparison of the evolution of the chemical composition of the steel zone in function of processing time with the simulation results of [2000, Ding]. Note that the only experimental data available is the initial and final composition (open red symbols). All other symbols are simulation results by [2000, Ding].

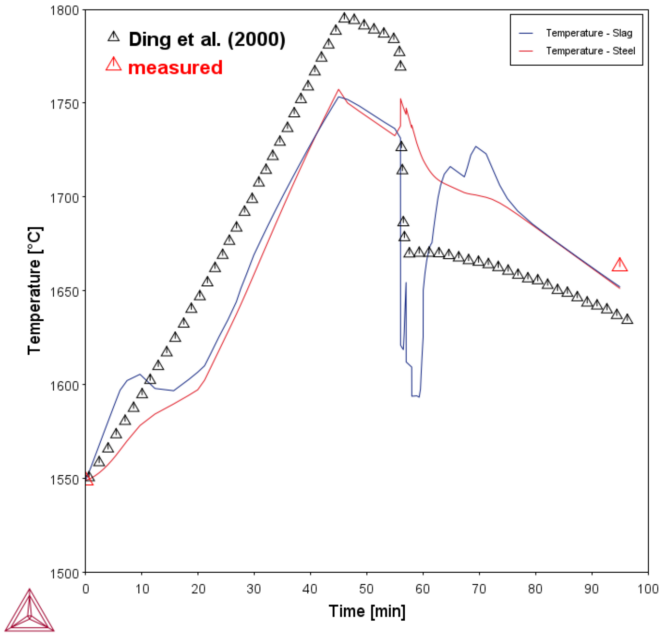


Figure 65: Calculated temperature in the steel and slag zone in function of processing time in the VOD compared to the simulation results from the publication by [2000, Ding]. Note that the only experimental data available is the initial and final temperature (red triangles). The black triangles are simulation results by [2000, Ding].

Reference

[2000, Ding] R. Ding, B. Blanpain, P. T. Jones, and P. Wollants, “Modeling of the vacuum oxygen decarburization refining process,” Metall. Mater. Trans. B, vol. 31, no. 1, pp. 197–206, Feb. 2000.

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.

In this section:

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

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.

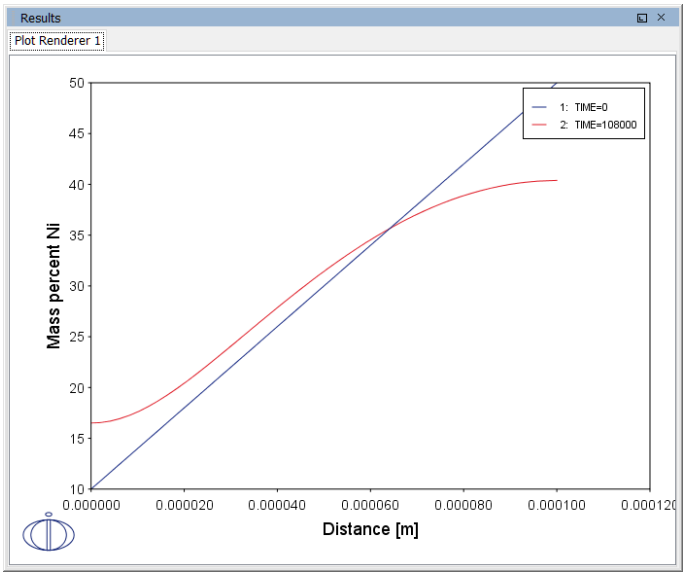


Figure 66: Composition of Ni vs Distance.

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.

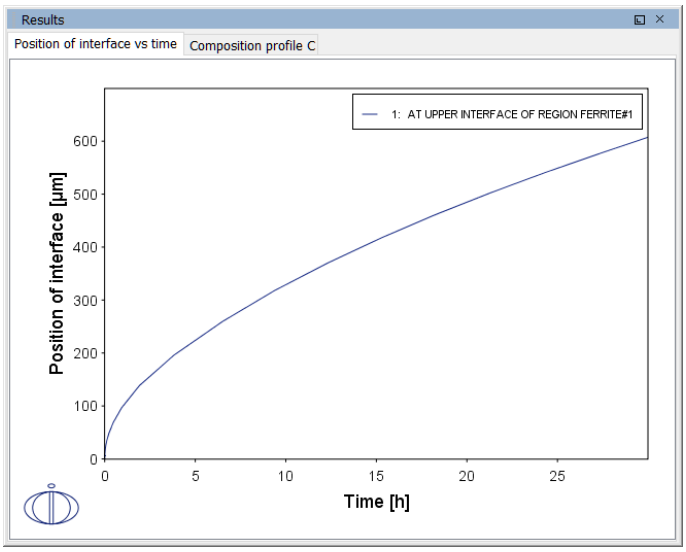


Figure 67: Position of interface vs time.

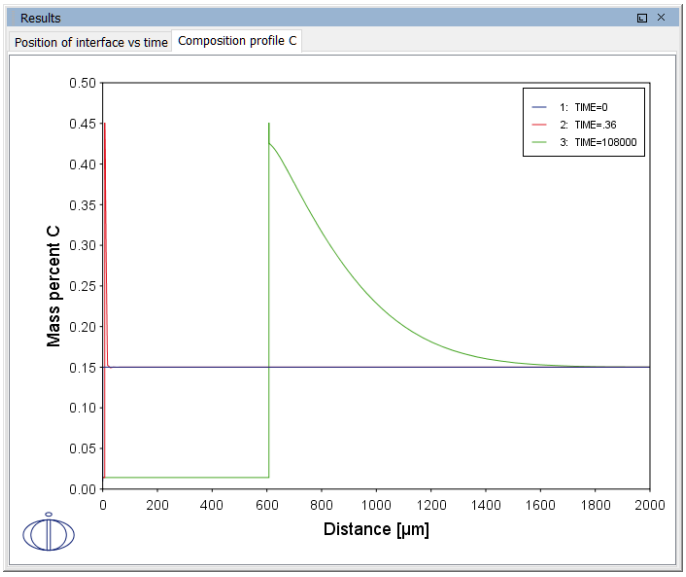


Figure 68: Composition profile C.

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] and Larsson and Höglund [2009]. Experimental data is from Engström [1995].

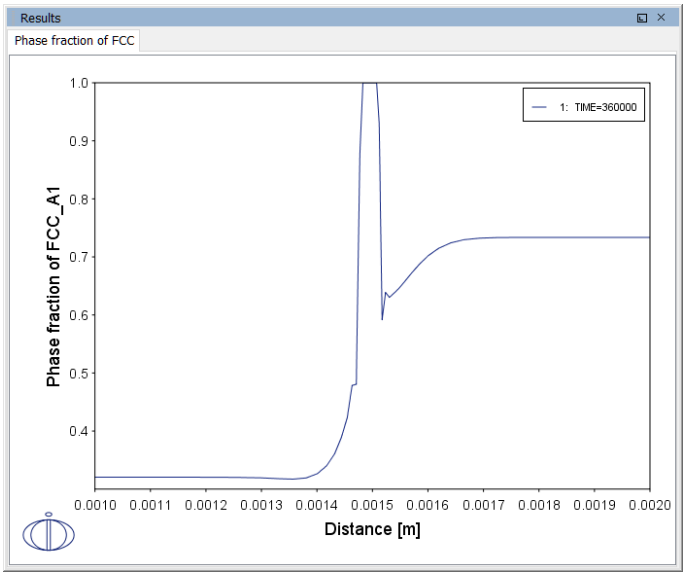


Figure 69: Phase fraction of FCC.

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.

References

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

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

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

D_04 Fe-C Moving Boundary: Austenite to Ferrite

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

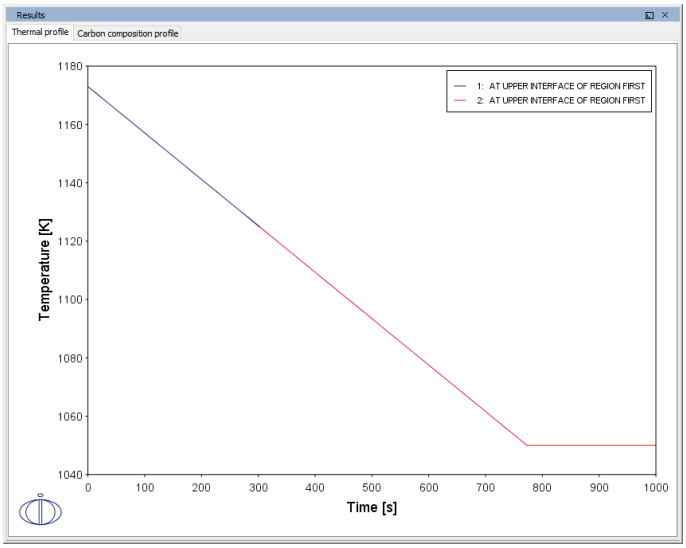


Figure 70: Thermal profile.

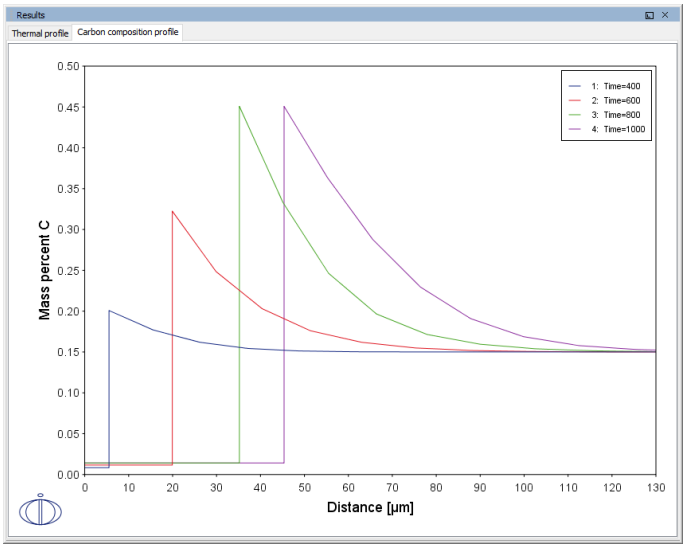


Figure 71: Carbon composition profile.

Project File Name

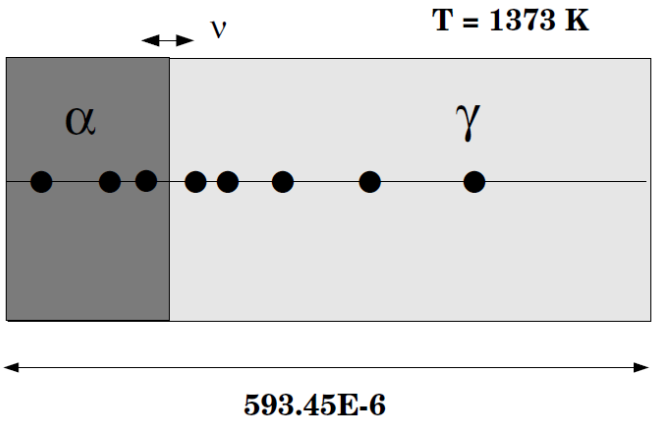
- Folder: Diffusion Module - DICTRA
- File name: *D_04_Diffusion_Fe-C_Moving_Boundary_Austenite_to_Ferrite.tcu*

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 et al. [1993a] and Kajihara and Kikuchi [1993b].



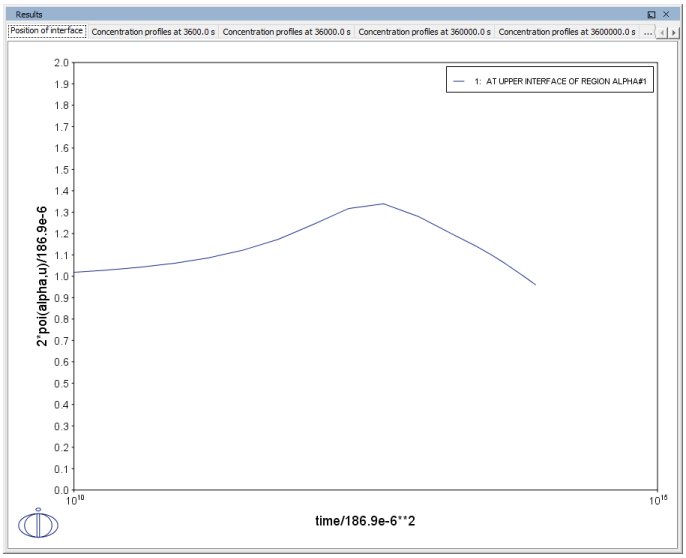


Figure 72: Interface position.

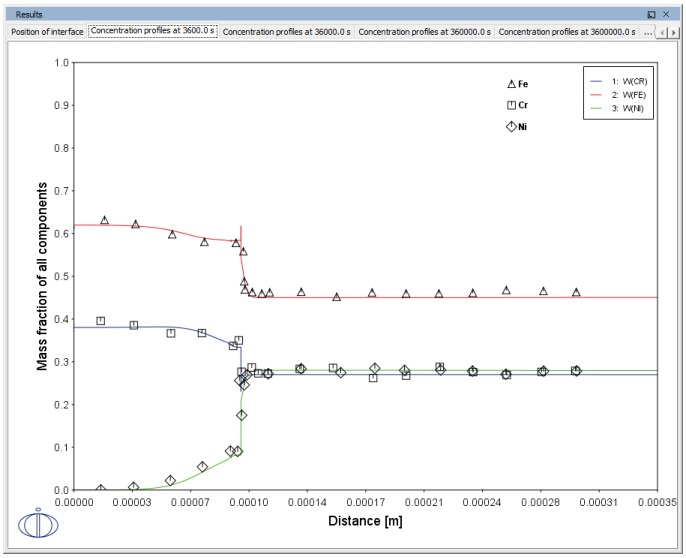


Figure 73: Concentration profiles at 3600 s.

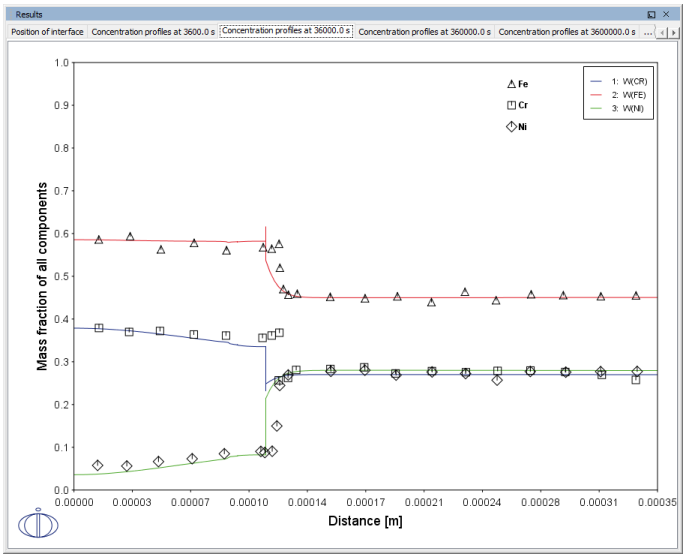


Figure 74: Concentration profiles at 36 000 s.

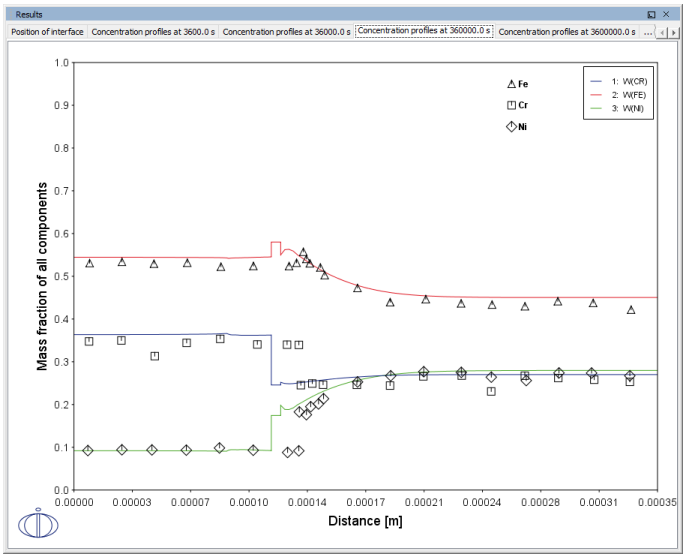


Figure 75: Concentration profiles at 360 000 s

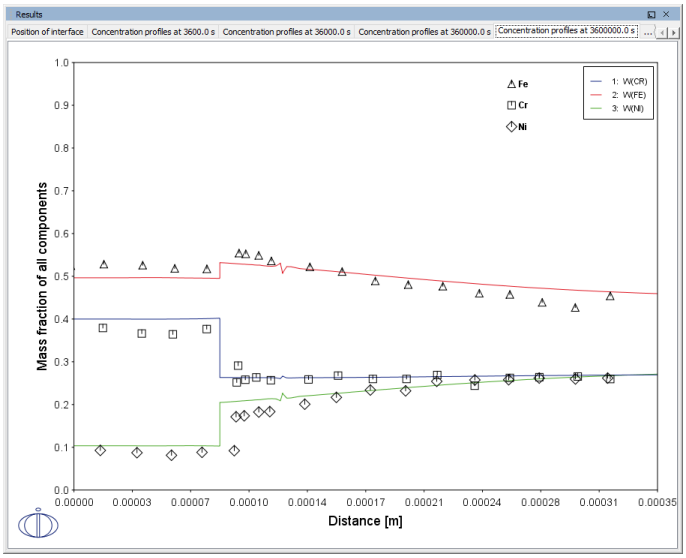


Figure 76: Concentration profiles at 3 600 000 s.

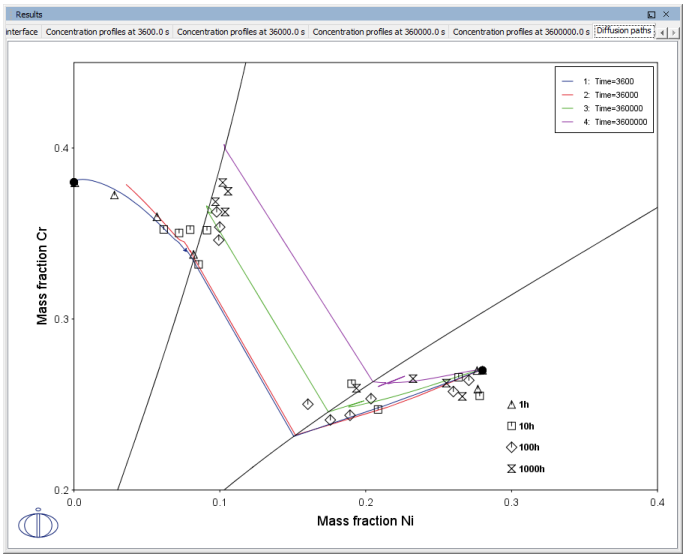


Figure 77: Diffusion paths.

Project File Name

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

References

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

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

D_06 Diffusion Through a Tube Wall

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

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

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**).

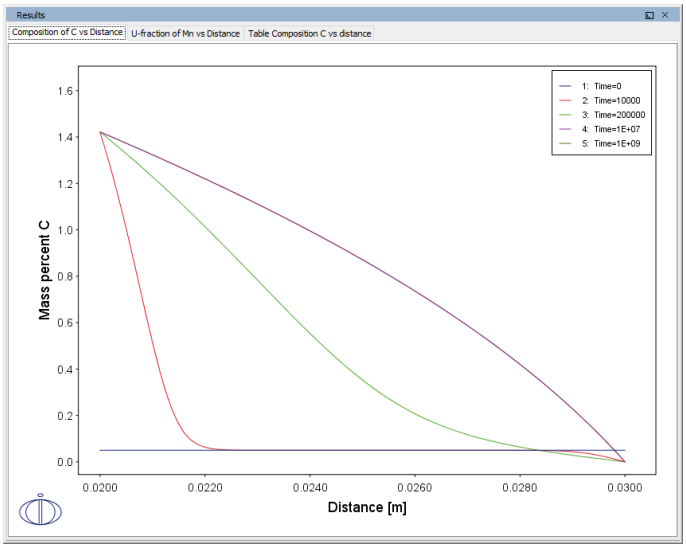


Figure 78: Composition of C vs Distance.

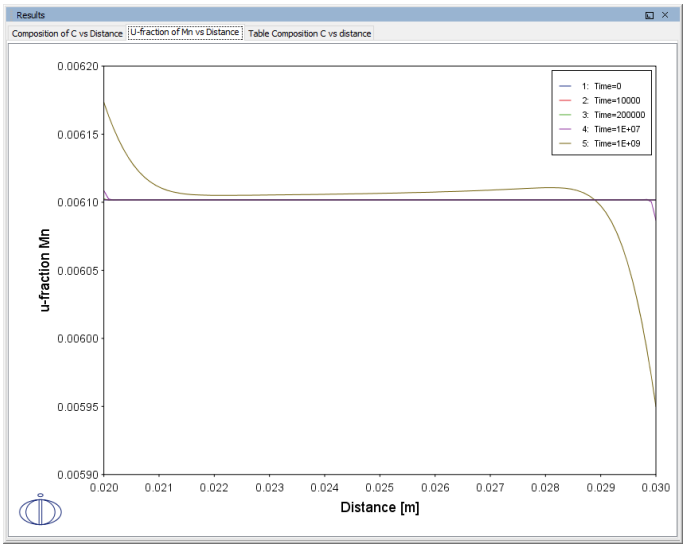


Figure 79: U-fraction of Mn vs Distance.

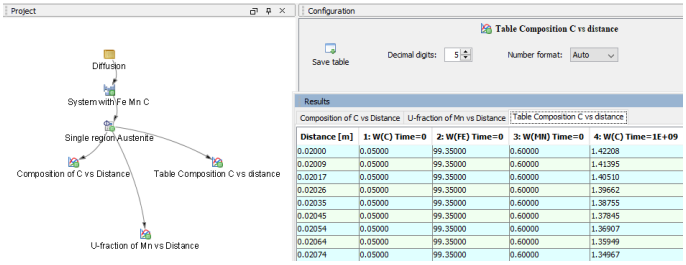


Figure 80: Table: Composition C vs Distance.

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

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

This example is 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.

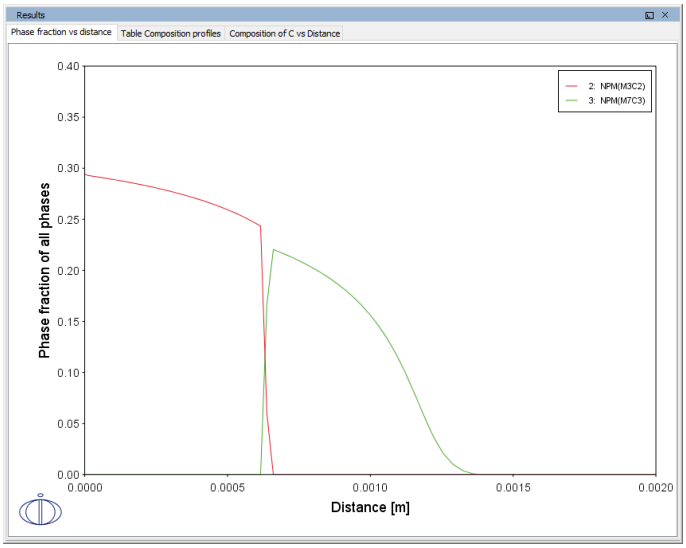
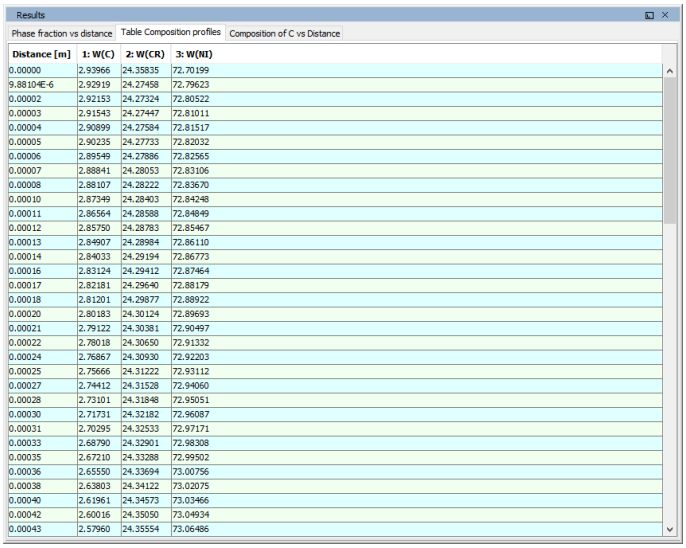


Figure 81: Phase fraction vs distance.


Results

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

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

Figure 82: Table of Composition profiles.

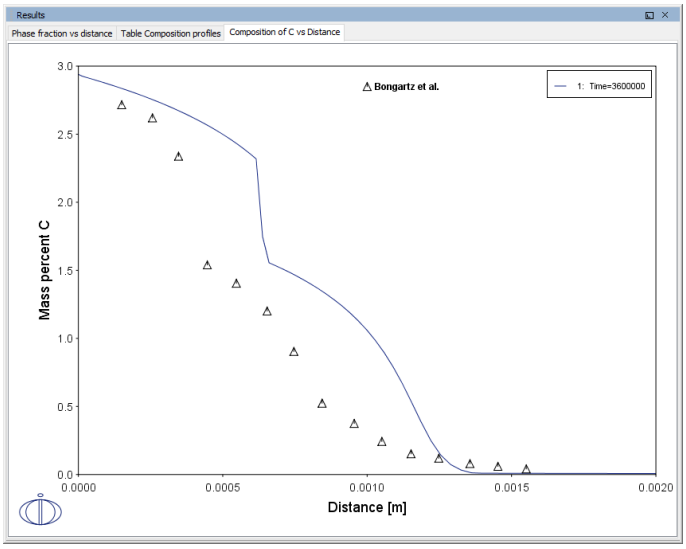


Figure 83: Composition of C vs distance.

Project File Name

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

Reference

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

Precipitation Module (TC-PRISMA) Graphical Mode Examples

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

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

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

In this section:

P_01: Isothermal Precipitation of Al_3Sc

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

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

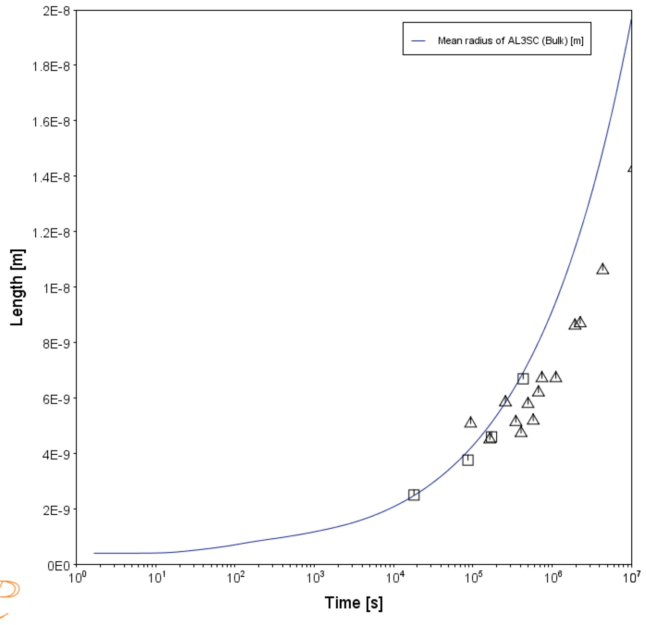


Figure 84: The mean radius of the AL3SC precipitate as a function of time.

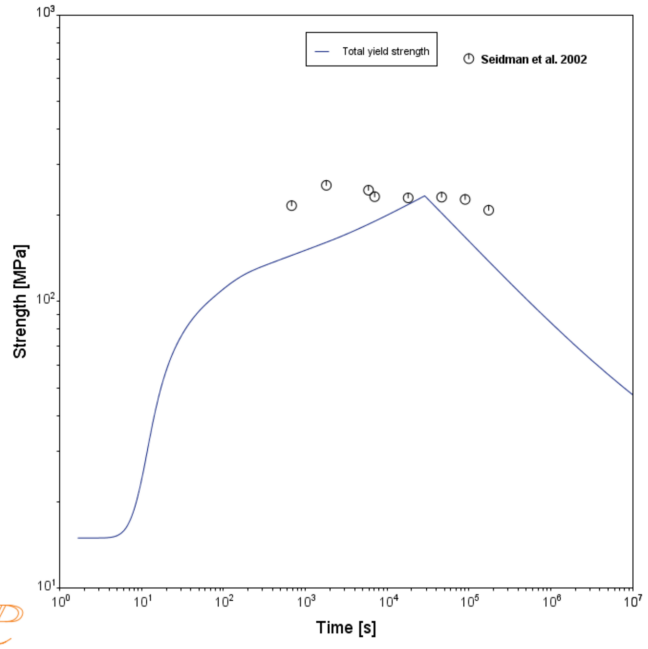


Figure 85: The total yield strength of the AL3SC precipitate as a function of time compared to experimental data from Sieldmen et al. [2002, Seidman].

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

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

This example is 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. Note that at this time, the Yield Strength Model included with this example is not specified in the step-by-step instructions.

Example Settings

System (System Definer)	
Database package	Demo: Aluminum-based alloys (ALDEMO, MALDEMO)

Elements	Al, Sc
Conditions (Precipitation Calculator)	
Composition	Al-0.18Sc Mole percent
Matrix phase	FCC_A1
Precipitate phase	AL3SC
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk
Interfacial energy	Calculated
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	350° C
Simulation time	1.0E7 seconds
Experimental File Reader 1 and 2	
There are two Experimental File Reader nodes used. One for the mean radius plot and one to demonstrate the *Yield Strength Property Model*.	

References

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

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

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

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

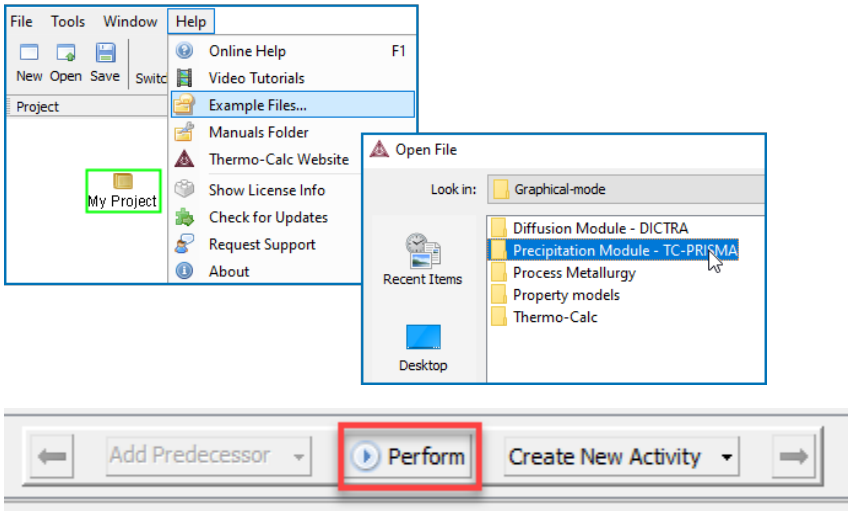
This example shows you how to set up an isothermal precipitation calculation for the formation of AL_3SC in an aluminium-scandium alloy at 350° using the Precipitation Module (TC-PRISMA).

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

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

HELPFUL INFORMATION

- **All users can run this calculation,** even those who do not have a license for the Precipitation Module (TC-PRISMA).
- **A companion video** is available for this example , which can be watched here: https://www.youtube.com/playlist?list=PLfv6McToaTGSpqvuLoY3b_UV-8xpgLUkJ
- This calculation is based on Precipitation Module example *P_01 – Precipitation Al-Sc AL3SC*, which is included in your installation. To run the example file, open Thermo-Calc and select **Help > Examples Files**. Open the *Precipitation Module (TC-PRISMA)* folder. Double-click the example file and click **Perform** at the bottom center of the **Configuration** window in Thermo-Calc.

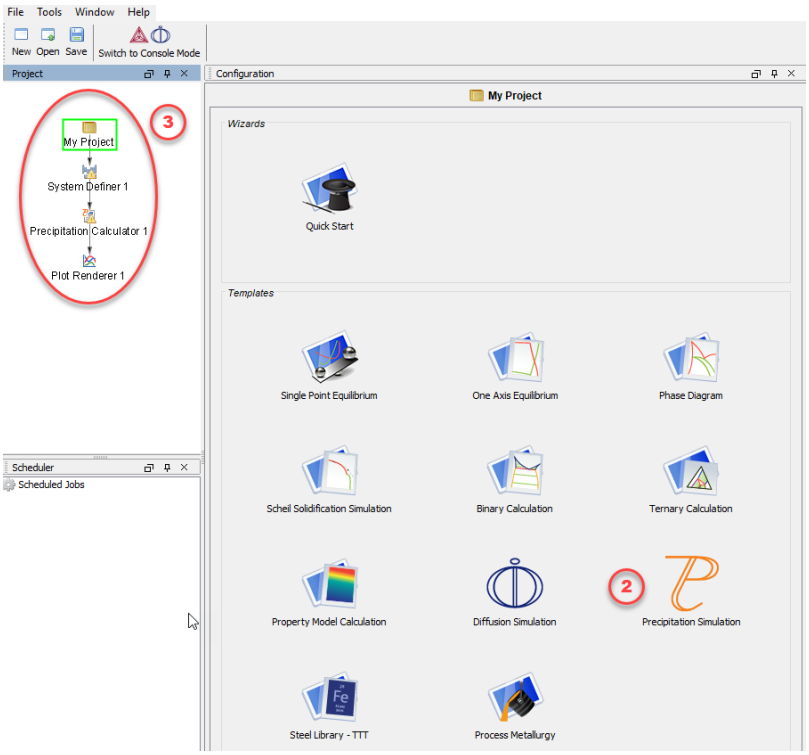


ABOUT THE EXAMPLE

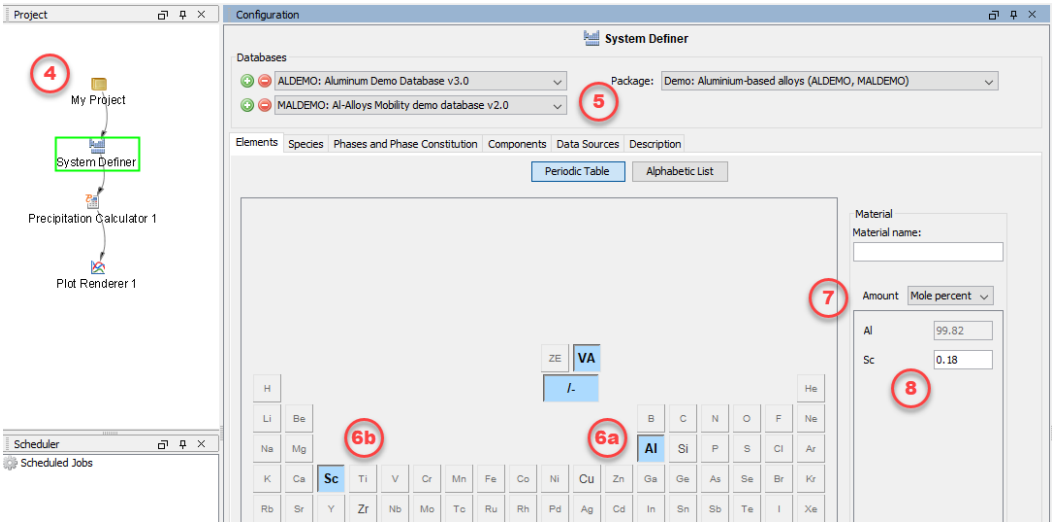
This example simulates the kinetics of precipitation of Al_3Sc from an FCC_A1 solution phase. The results of the simulation are also used to model yield strength.

SETTING UP THE SYSTEM

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



4. In the **Project** window, click the **System Definer 1** node.
5. Set the database *Package* to **Demo: Aluminium-based alloys (ALDEMO, MALDEMO)**, which loads both thermodynamic and kinetic demonstration aluminium databases.
6. From the **Periodic Table**, select the elements as follows. Select Al first so that it is the dependant element:
    a. **Al** (aluminium)
    b. **Sc** (scandium).
7. From the *Amount* list (to the right of the Periodic Table), select **Mole percent**.
8. Enter `0.18` for **Sc**. This automatically sets **Al** to 99.82.



The system is now defined. However, before starting the precipitation calculation, it is recommended to run a one axis calculation to find the phases present around 350° C.

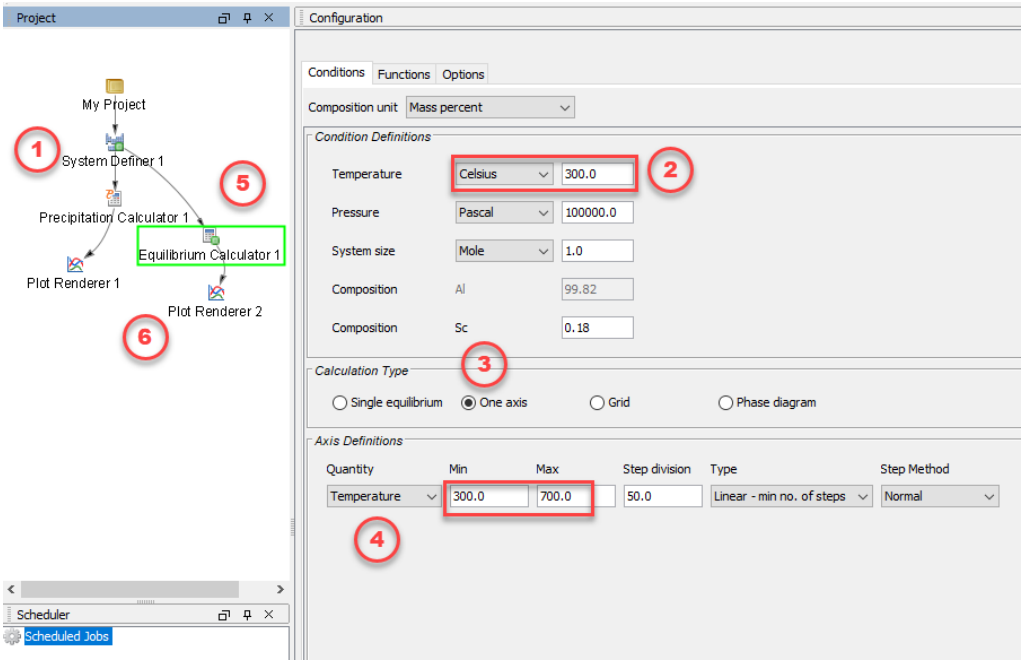
ONE AXIS CALCULATION

Why We Do This

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

Setting up a One Axis Calculation

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



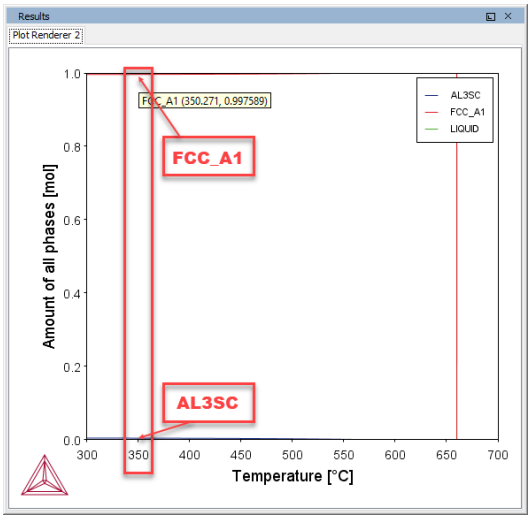
Interpreting the Results of the One Axis Calculation

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

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

We can see that there are two phases present at 350°. FCC_A1 is at the very top of the plot and makes up more than 99% of the system. The remainder of the system is made up of Al_3SC, which is near the very bottom of the plot and is the precipitate phase in the alloy we are considering.

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



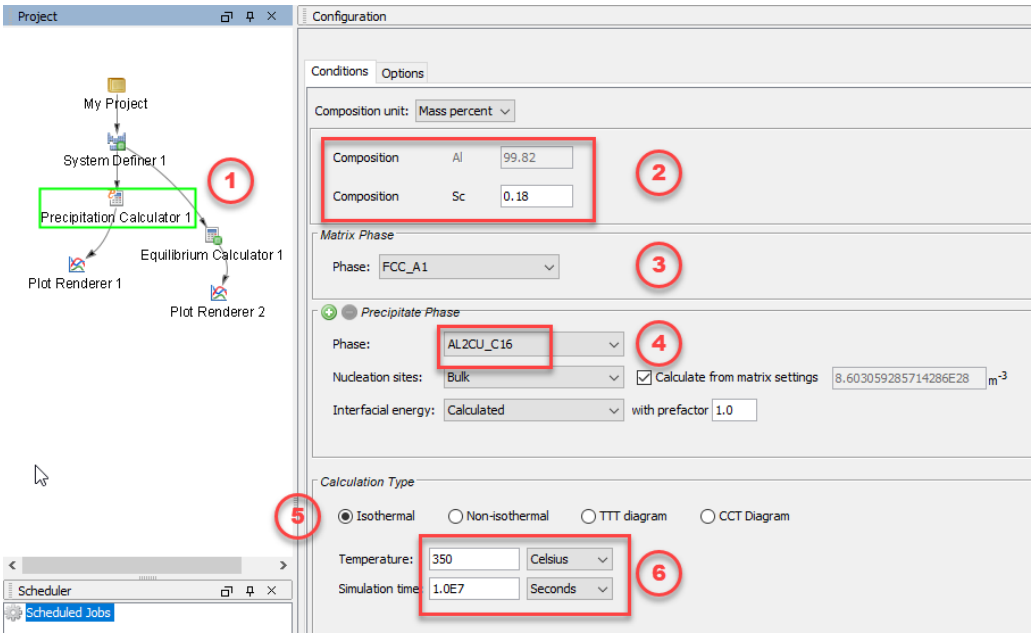
PRECIPITATION CALCULATION

Setting up the Precipitation Calculation

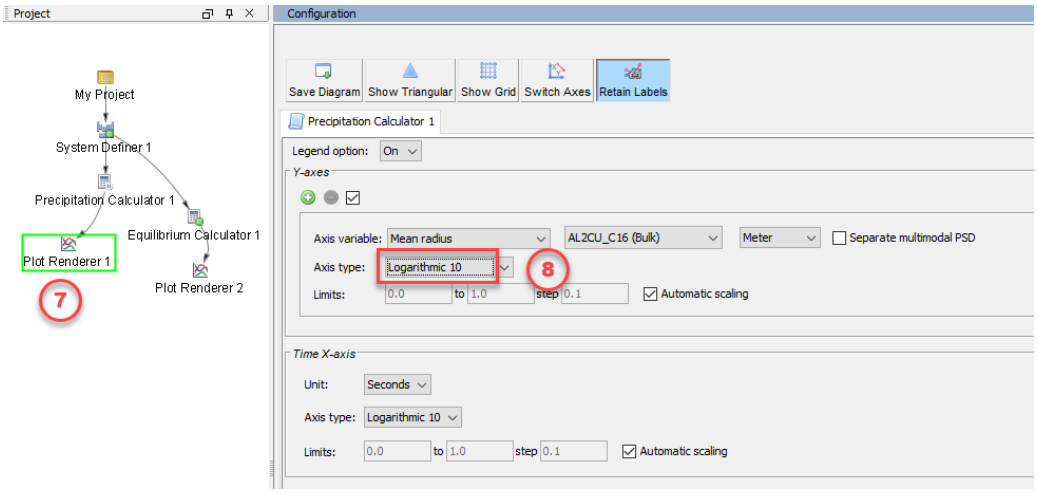
1. In the **Project** window, click the **Precipitation Calculator 1** node.
2. Notice that the *Composition* set in the *System Definer* auto-populated here.
3. Under *Matrix Phase*, the *Phase* defaults to **FCC_A1**, which is the primary phase present in the one axis calculation.

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

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

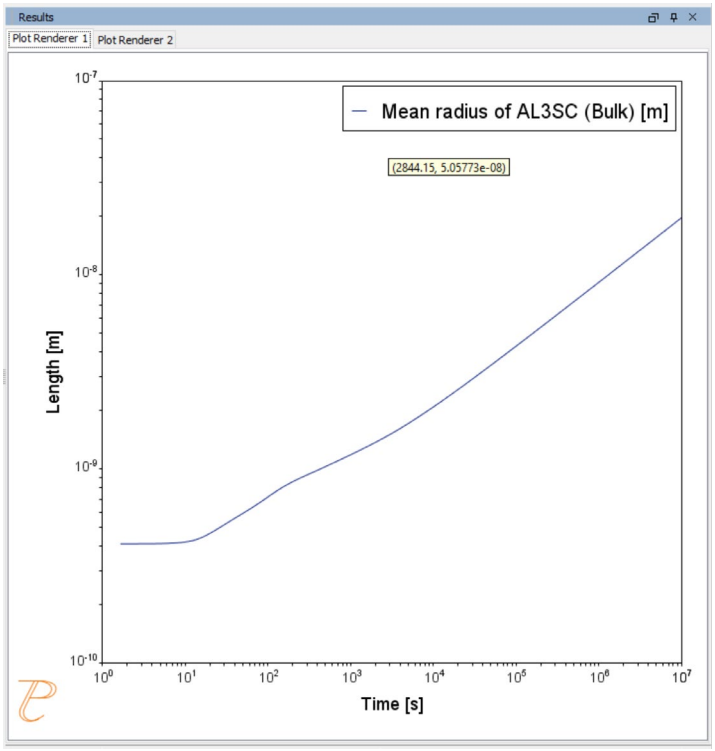


8. In the **Project** window, click the **Plot Renderer 1** node.
9. Under *Y-axes*, from the *Axis type* menu select **Logarithmic 10** for a better view of the plot.
10. Click **Perform** at the bottom, center of the **Configuration** window.



Interpreting the Results of the Precipitation Calculation

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



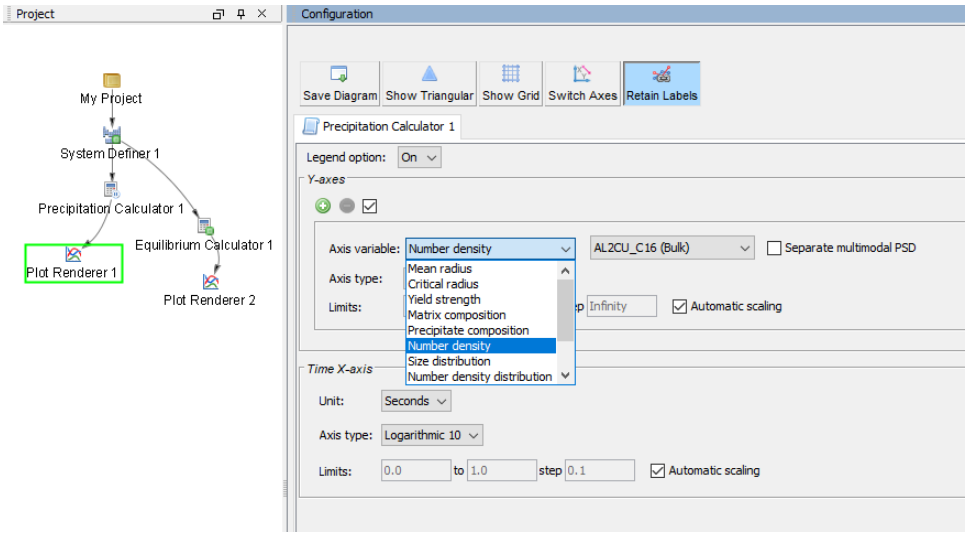
This plot shows the Mean radius of the AL3SC precipitate as a function of time.

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

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

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

1. Click the **Plot Renderer 1** node.
2. Under *Y-axes*, click the Axis variable menu to see the other available options in the list.
3. Once you have made your selection, click **Perform** at the bottom, center of the **Configuration** window to create a new plot.

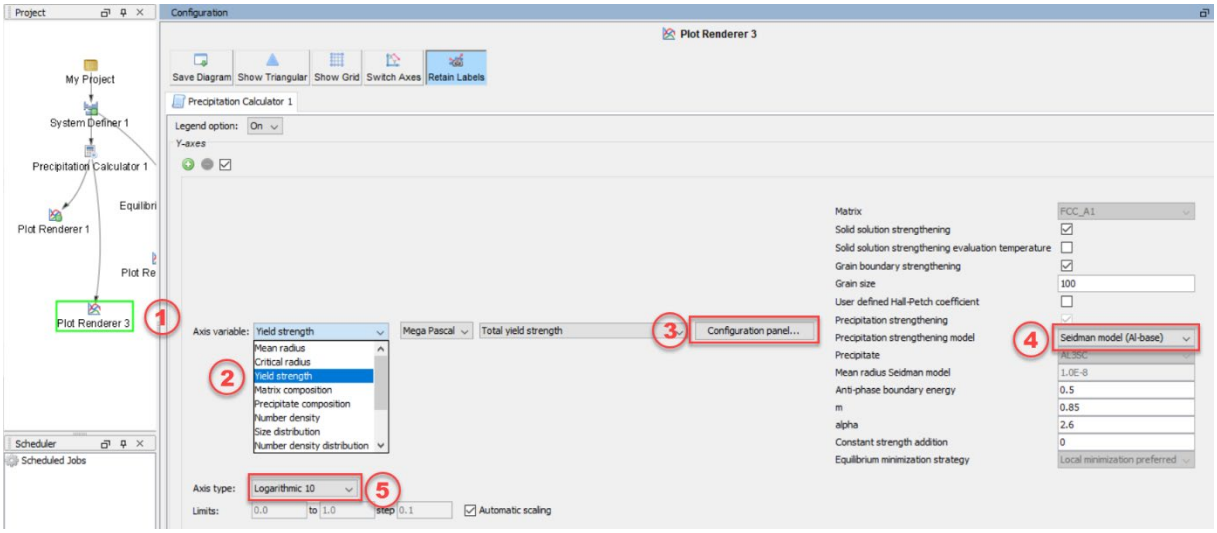


Model Yield Strength

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

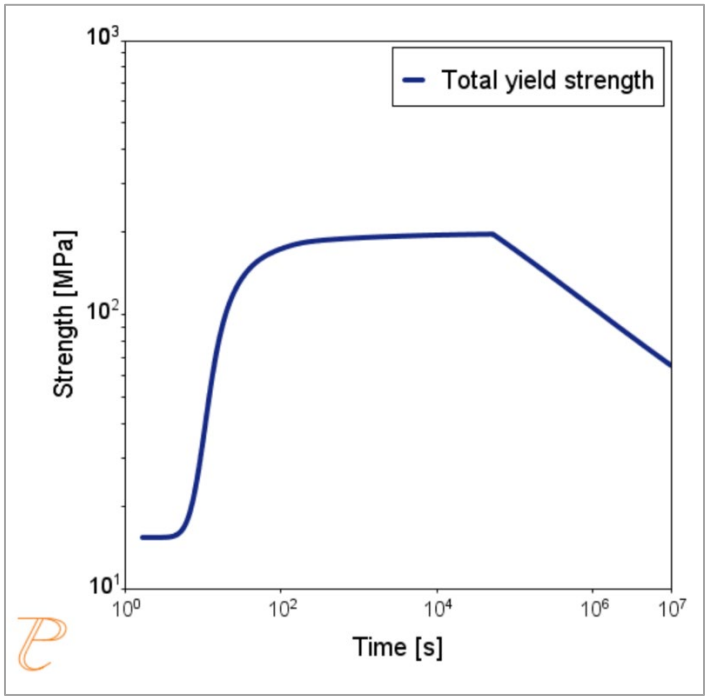
1. Right click the **Precipitation Calculator 1** node and select **Create New Successor > Plot Renderer**.
2. Under *Y-axes*, from the *Axis variable* menu, select **Yield strength**.
3. Click the *Configuration panel* button.
4. If required, expand the Plot Renderer Configuration window. Then from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

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



Interpreting the Results of the Yield Strength Model

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



This plot shows the yield strength of the AL3SC precipitate as a function of time.

P_02: Stable and Metastable Carbides - Isothermal

This example simulates the kinetics of precipitation of both stable and metastable carbides from ferrite phase. It demonstrates that metastable carbides (cementite, M7C3) may first emerge and then disappear and the stable phase (M23C6) prevails.

This example uses the Equilibrium Calculator and a one axis calculation to determine how the phases change with temperature. We are interested in the carbide precipitation at 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.

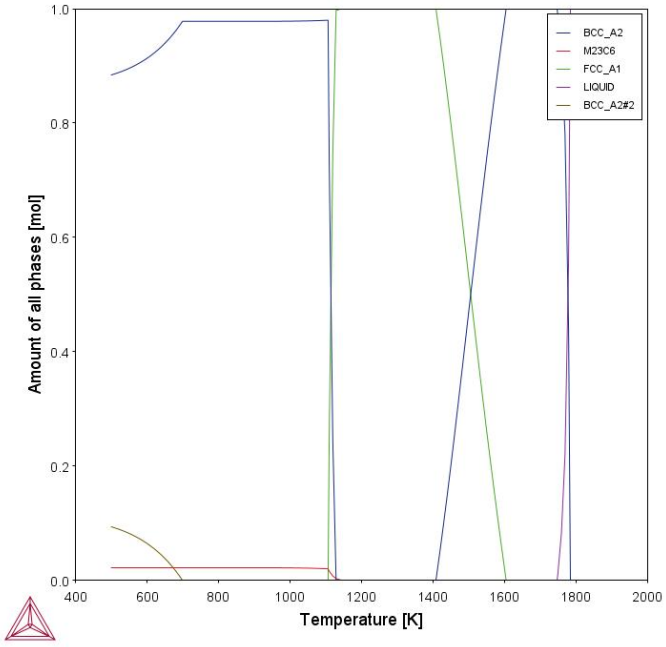


Figure 86: The Equilibrium Calculator and a One axis calculation is used to determine how the phases change with temperature.

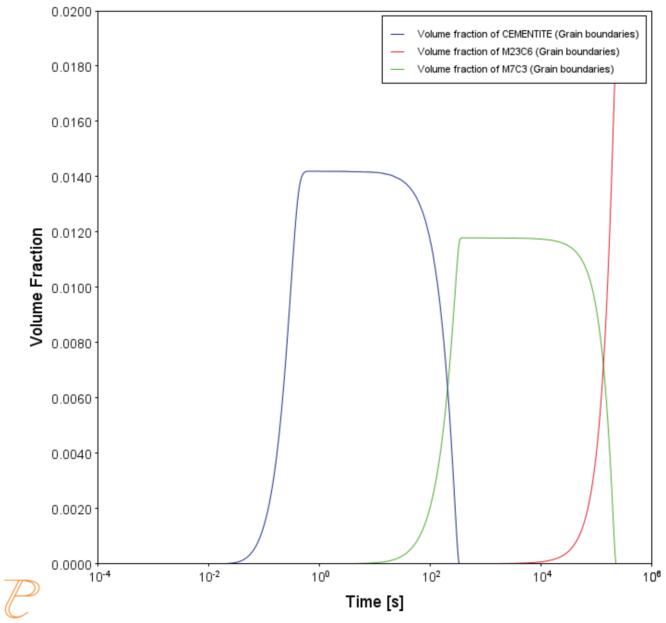


Figure 87: The Precipitation Calculator is used to do an isothermal calculation of the three phases (cementite, M23C6 and M7C3) where cementite and M7C3 are metastable phases.

Project File and Video Tutorial Information

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

Also see our website and YouTube channel for other examples of the Precipitation Module.

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

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.

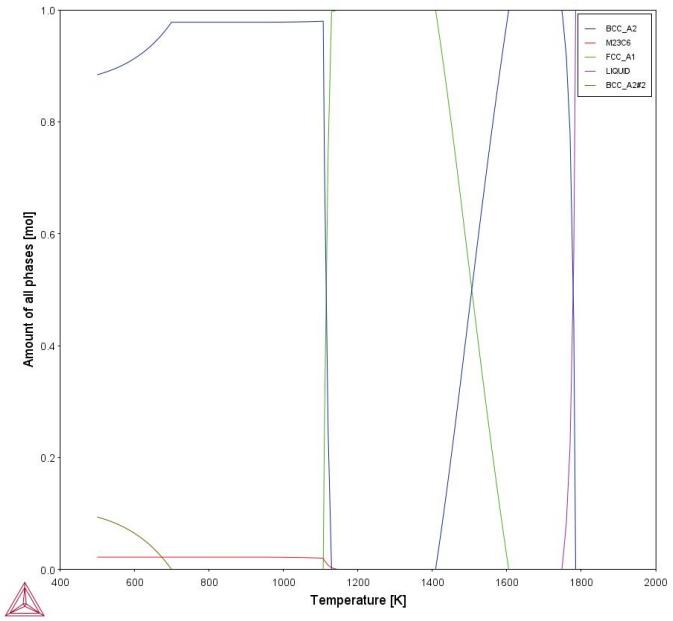


Figure 88: The Equilibrium Calculator is used to show how the phases change with temperature.

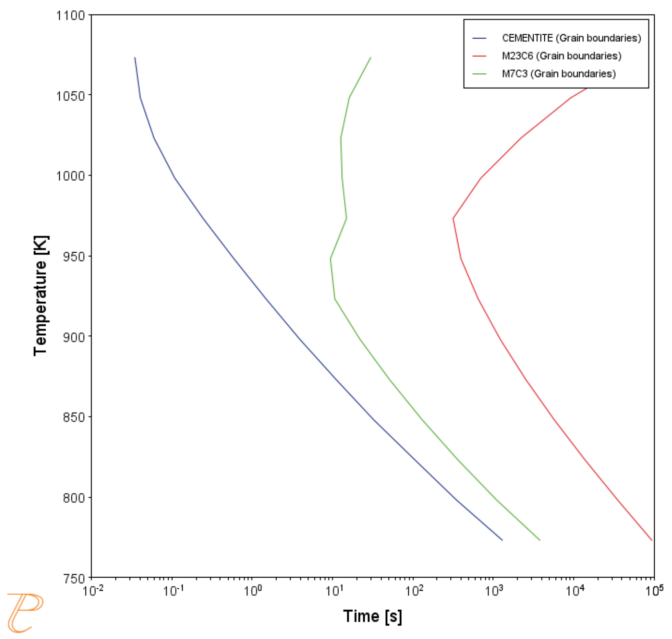


Figure 89: The Precipitation Calculator is used to do a TTT (Time-Temperature-Transformation) diagram calculation of the three phases (cementite, M23C6 and M7C3) at the grain boundaries.

Project File and Video tutorial Information

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

Also see our website and YouTube channel for other examples of the Precipitation Module.

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

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].

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.

This example takes several minutes to run.

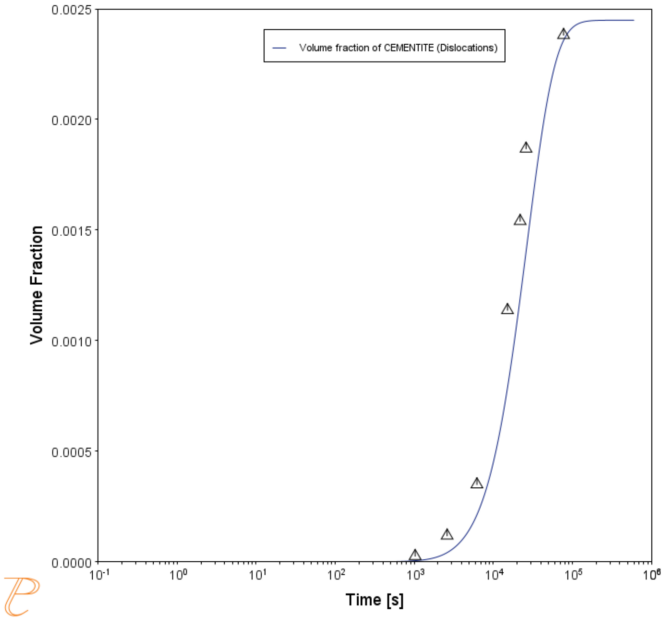


Figure 90: Volume fraction of the cementite phase.

Project File and Video Tutorial Information

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

Also see our website and YouTube channel for other examples of the Precipitation Module.

Example Settings

System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO)

Elements	Fe, C
Conditions (Precipitation Calculator)	
Composition	Fe-0.016C mass percent
Matrix phase	BCC_A2
Precipitate phase	Cementite
Matrix Phase Data Parameters (Precipitation Calculator)	
Grain aspect ratio (click **Show details** to display this setting)	1.0
Dislocation density (click **Show details** to display this setting)	$1.5e11 m^{-3}$
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

Reference

[1949,Wert] C. A. Wert, Precipitation from Solid Solutions of C and N in α-Iron. J. Appl. Phys. 20, 943 (1949).

P_05: Precipitation of γ' in Ni Superalloys - Isothermal

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

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.

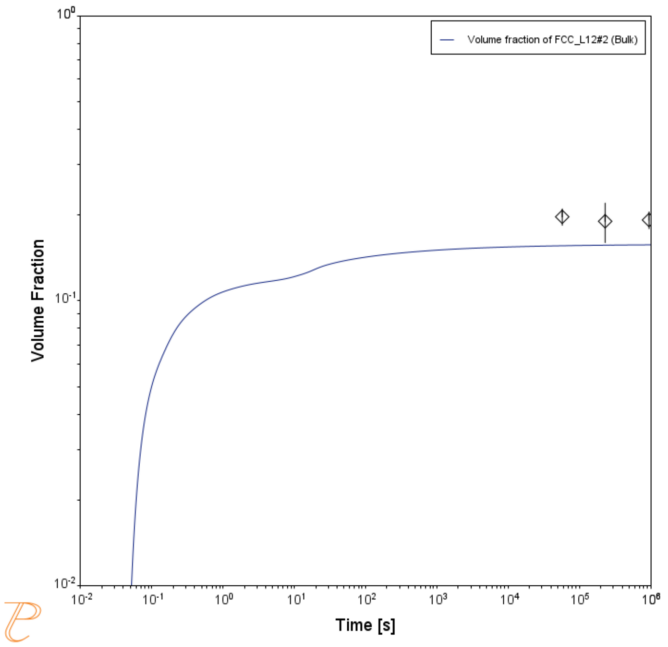


Figure 91: The results of an isothermal calculation to plot the volume fraction of the cementite phase.

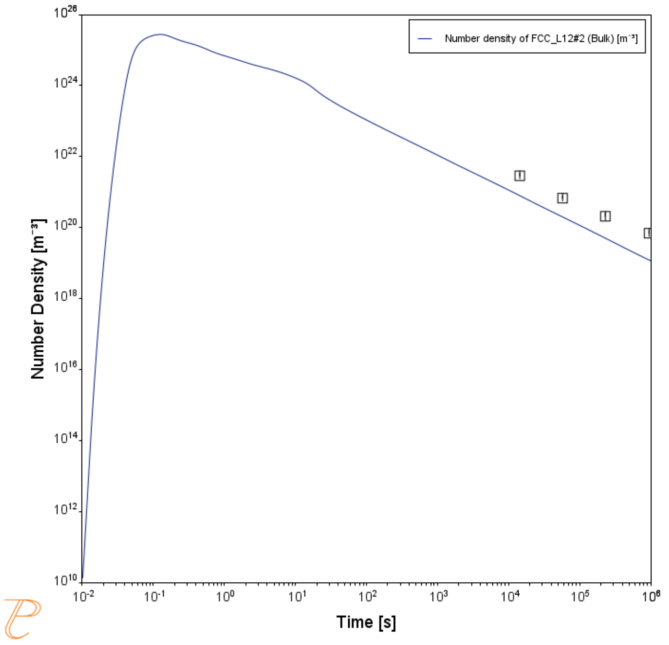


Figure 92: The results of an isothermal calculation to plot the number density of the cementite phase.

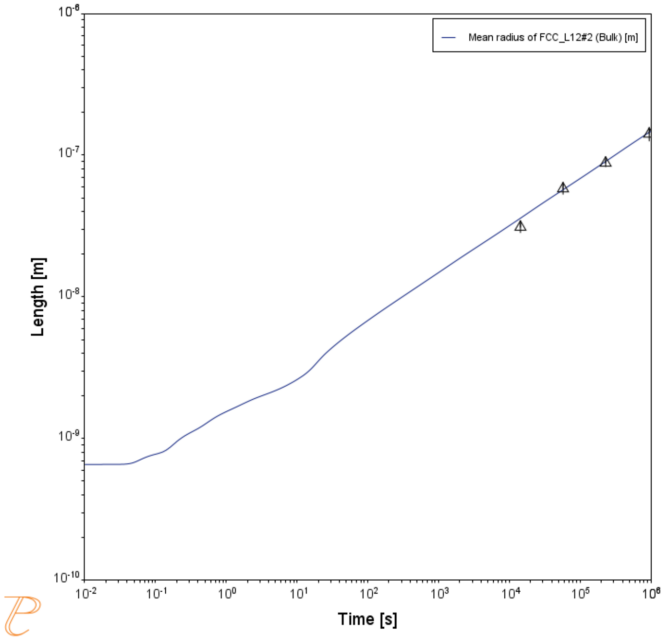


Figure 93: The results of an isothermal calculation to plot the mean radius of the cementite phase.

Project File and Video Tutorial Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_05_Precipitation_Ni-Al-Cr_Isothermal_Gamma-Gamma_prime.tcu*

Also see our website and YouTube channel for other examples of the Precipitation Module.

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

Reference

[2008, Sudbrack] C. K. Sudbrack, T. D. Ziebell, R. D. Noebe, D. N. Seidman, Effects of a tungsten addition on the morphological evolution, spatial correlations and temporal evolution of a model Ni–Al–Cr superalloy. Acta Mater. 56, 448–463 (2008).

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

This example simulates the kinetics of precipitation of 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].

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.

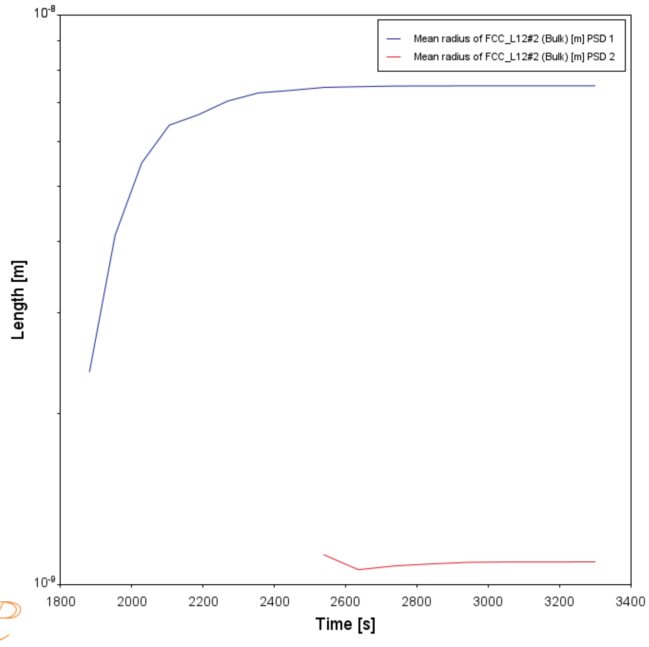


Figure 94: Mean Radius Ni-8Al-8Cr.

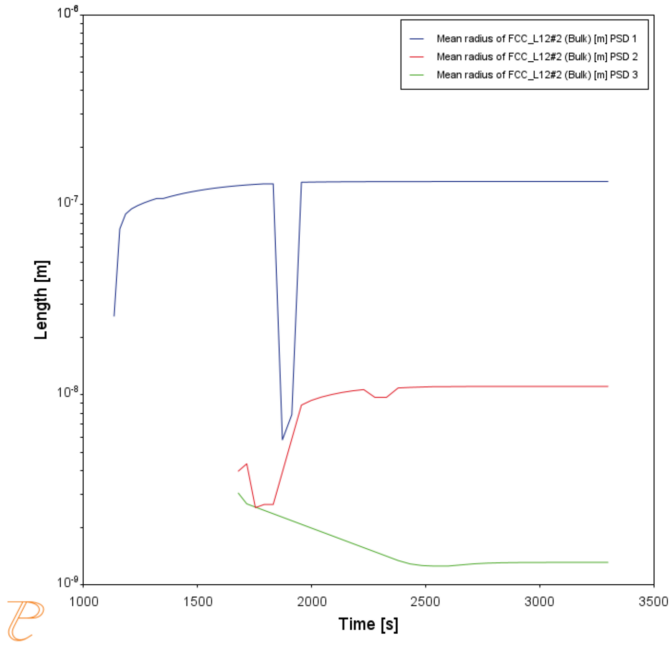


Figure 95: Mean Radius Ni-10Al-10CR.

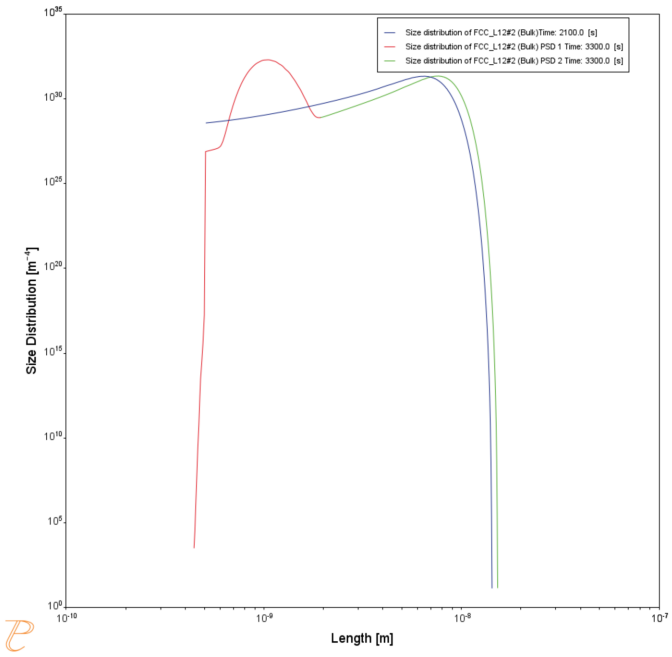


Figure 96: Size Distribution (PSD) Ni-8Al-8Cr.

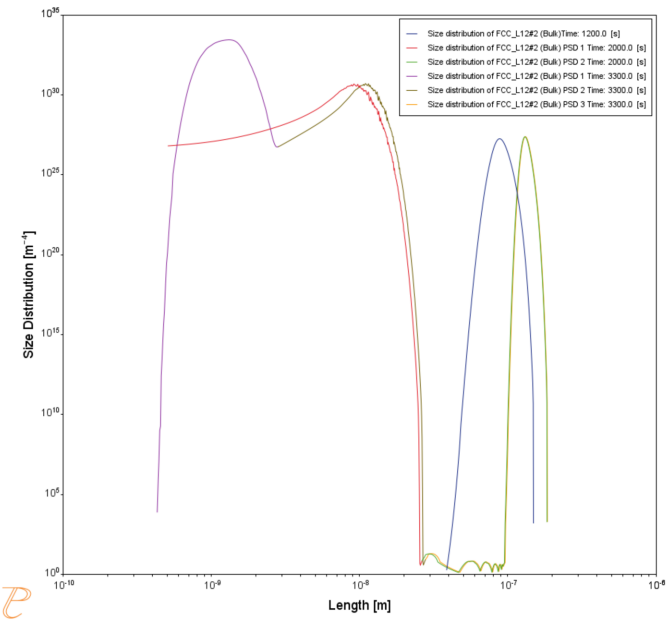


Figure 97: Size Distribution (PSD) Ni-10Al-10Cr.

Project File and Video Tutorial Information

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

Also see our website and YouTube channel for other examples of the Precipitation Module.

Example Settings

System (System Definer)	
Database package	Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO)
Elements	Ni, Al, Cr
Conditions (Precipitation Calculator)	
Composition (Ni-8Al-8Cr)	Ni-8Al-8Cr Mole percent
Composition (Ni-10Al-10Cr)	Ni-10Al-10Cr Mole percent
Matrix phase	DIS_FCC_A1 (see 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
Temperature	1150 - 380 °C Edit Thermal Profile Import... Time [s] / Temperature [°C] 0.0 / 1150.0 3300.0 / 380.0
Simulation time (Ni-8Al-8Cr)	3300 s
Simulation time (Ni-10Al-10Cr)	3300 s
Multimodal PSD (Plot Renderer)	
Separate multimodal PSD for 8Al-8Cr	The **Valley depth ratio** is set to 0.05 for both plots. 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.

Reference

[2013, Rojhirunsakool] T. Rojhirunsakool, S. Meher, J. Y. Hwang, S. Nag, J. Tiley, R. Banerjee, Influence of composition on monomodal versus multimodal γ' precipitation in Ni–Al–Cr alloys. J. Mater. Sci. 48, 825–831 (2013).

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

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.

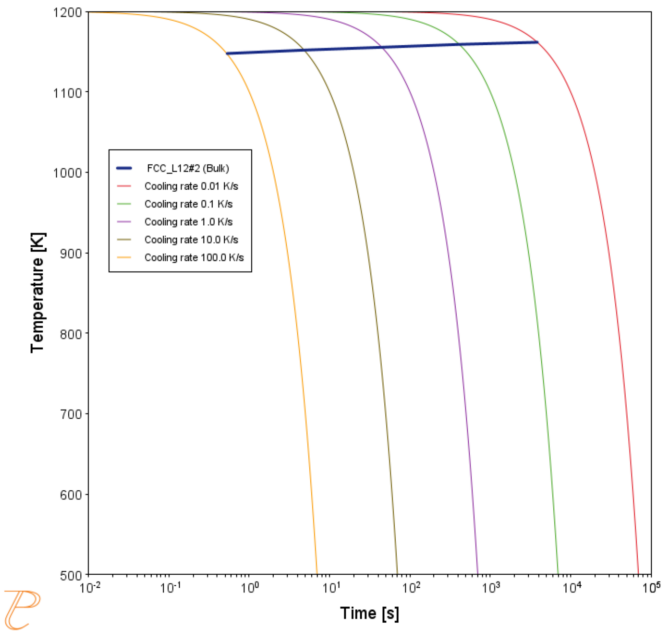


Figure 98: In this plot, the blue line shows the time it takes for γ' to transform at each of the cooling rates according to the stop criteria, which we set as 1e-4 volume fraction. The cooling rates are represented by the multi-coloured curved lines.

Results

Plot Renderer 1 | Table Renderer 1

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

Figure 99: An example of the table shown in the Results window, which shows the same information as in the plot - for each cooling rate the temperature and the time it takes for γ' to transform according to the stop criteria, which is a volume fraction of 1e-4.

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

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

This example is 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.

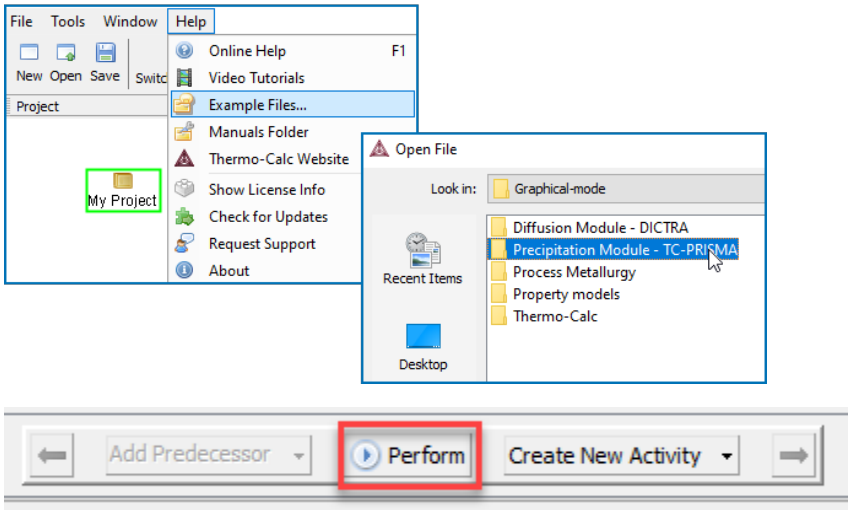
Example Settings

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

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

HELPFUL INFORMATION

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



ABOUT THE EXAMPLE

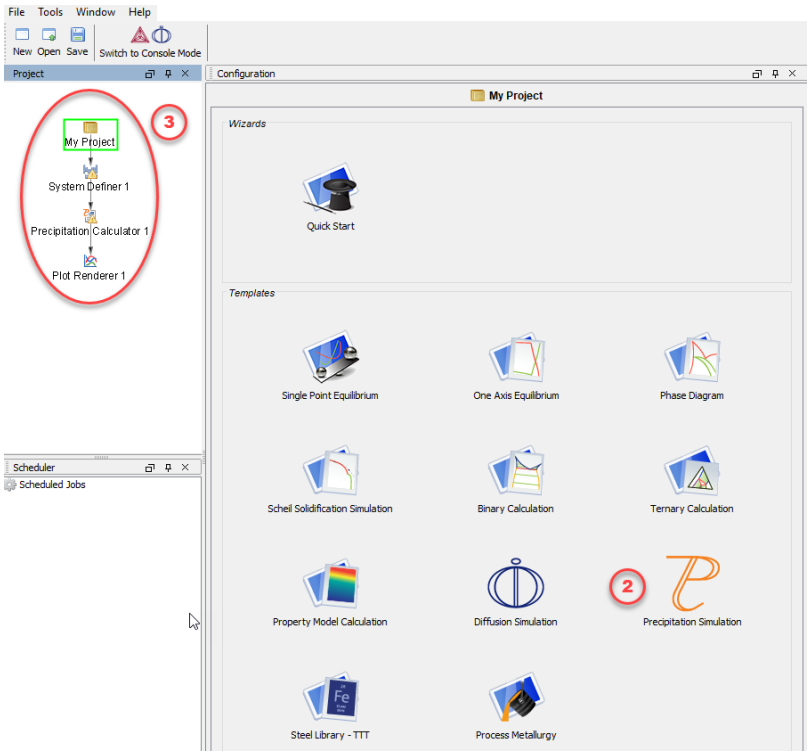
This example shows you how to simulate a CCT diagram for gamma prime (γ') precipitation in a Ni-Cr-Al alloy using the Precipitation Module known as TC-PRISMA.

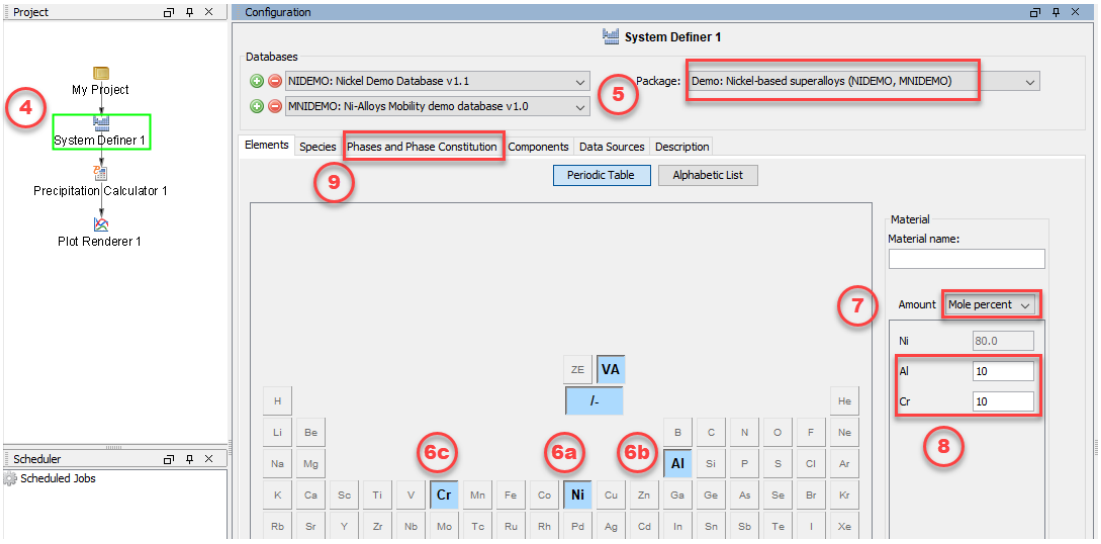
CCT stands for Continuous Cooling Transformation and is a calculation that maintains the same cooling rate the entire time.

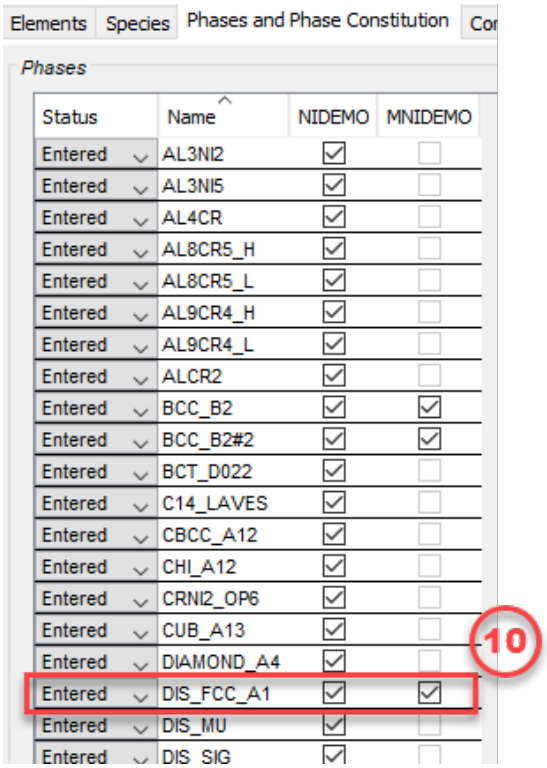
The system is a Ni-10Al-10Cr γ - γ' alloy and it is calculated and plotted with superimposition of the cooling rate values using the Precipitation Module (TC-PRISMA).

SETTING UP THE SYSTEM

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



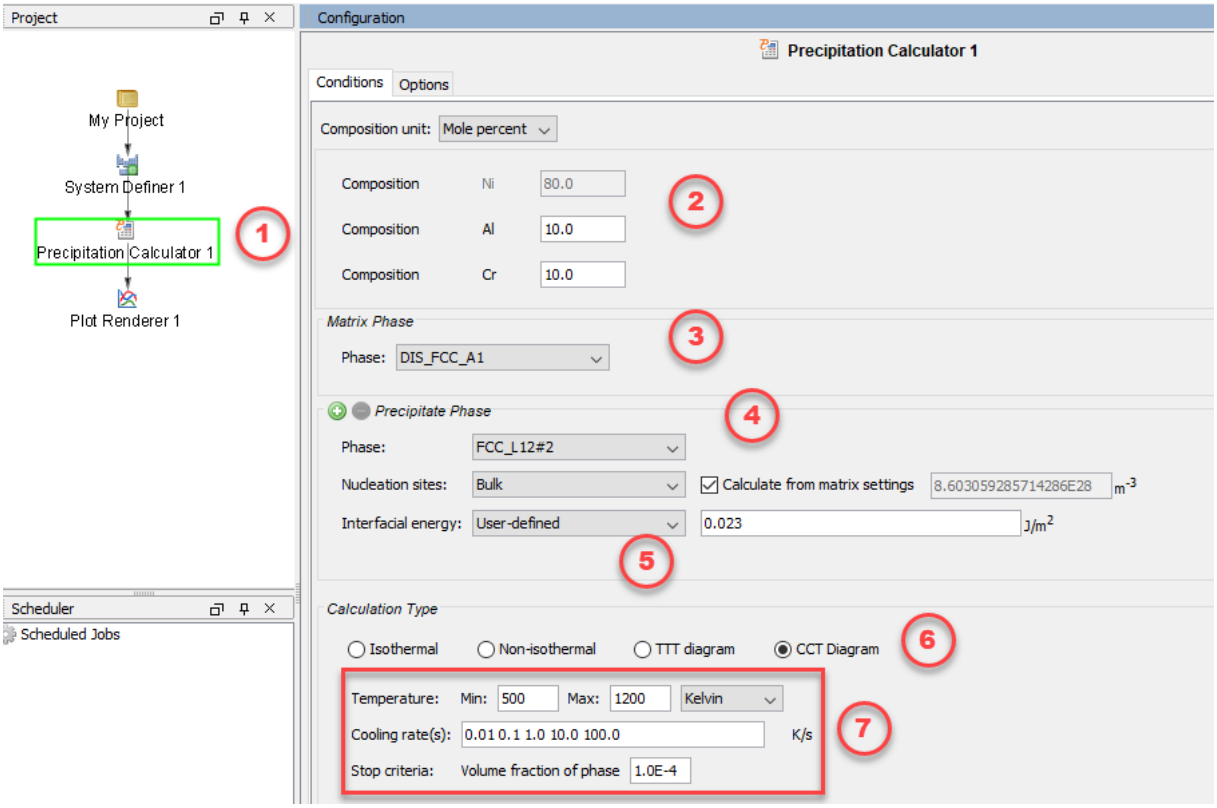
4. In the **Project** window, click the **System Definer 1** node.
5. Set the database *Package* to **Demo: Nickel-based alloys (NIDEMO, MNIDEMO)**, which loads both thermodynamic and kinetic demonstration nickel databases.
6. From the **Periodic Table**, select the elements as follows. Select Ni first so that it is the dependant element.
    a. **Ni** (nickel)
    b. **Al** (aluminium) then
    c. **Cr** (chromium).
7. From the *Amount* list (to the right of the Periodic Table), select **Mole percent**.
8. Enter `10` for **Al** and `10` for **Cr**, which automatically sets **Ni** to 80 mole percent.
9. Click the **Phases and Phase Constitution** tab.
10. Click to select both check boxes next to the disordered FCC phase, **DIS_FCC_A1**.
11. 



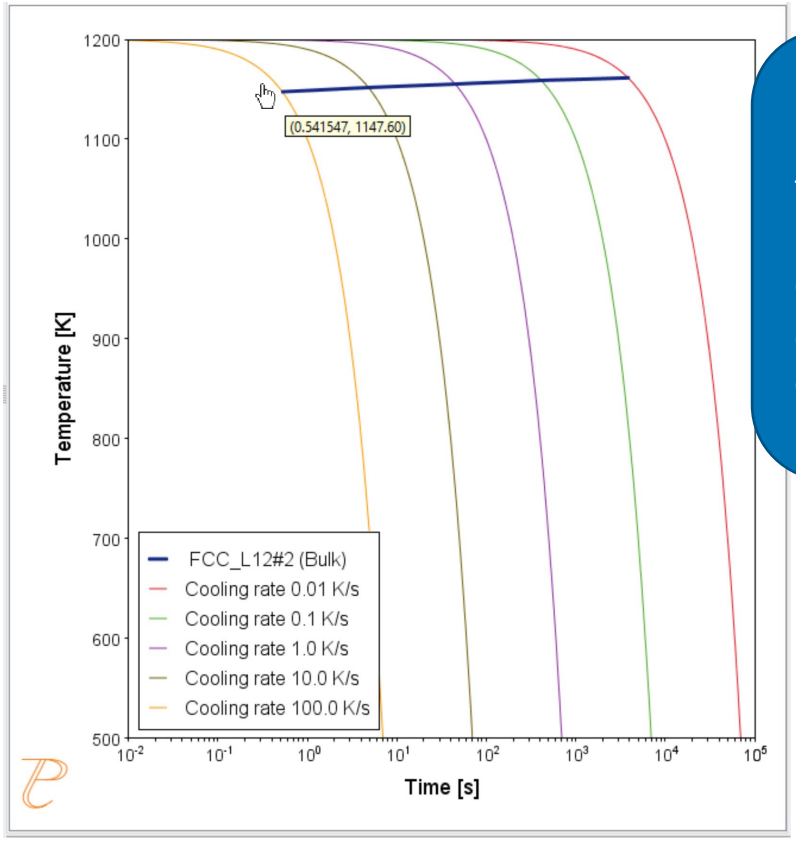
The system is now defined. Now set up the precipitation calculations.

SETTING UP THE PRECIPITATION CALCULATION

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



INTERPRETING THE RESULTS OF THE PRECIPITATION CALCULATION



In this plot, the blue, horizontal line shows the time it takes for gamma prime to transform at each of the cooling rates according to the stop criteria, which we set as 1e-4 volume fraction.

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

If you hover your mouse over the intersection of the blue line and any of the vertical lines, a yellow box shows the approximate time it takes for γ' to transform according to the stop criteria, which is a volume fraction of 1e-4, followed by the approximate temperature. In the image above, you can see a time of 0.54147 seconds and a temperature of 1147.60 Kelvin for the cooling rate of 100.0 K/s, which is represented by the yellow line.

SHOWING THE RESULTS AS A TABLE

You can also view these results in the form of a table, which gives you more precise results.

1. In the **Project** window, right-click the **Precipitation Calculator 1** node and select **Create New Successor>Table Renderer**.
2. Right-click the **Table Renderer 1** node and select **Perform Now**.

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

The table is shown in the **Results** window and shows the same information as in the plot - for each cooling rate the temperature and the time it takes for γ' to transform according to the stop criteria, which is a volume fraction of 1e-4.

P_08: Precipitation of Cu-Ti CU4TI with Assumptions of Sphere and Needle Morphologies

In this isothermal calculation example, the precipitation of Cu4Ti phase in a Cu-Ti binary alloy is calculated. To make a comparison, two separate simulations are performed, one assuming spherical morphology without elastic strain energy, and the other assuming needle morphology whose shape, determined by competition between interfacial energy and elastic strain energy, is changed during the simulation. The transformation strain is obtained from Borchers [1999]. The results are compared with experiment results from Kampmann et al. [1987].

This example takes a few minutes to run.

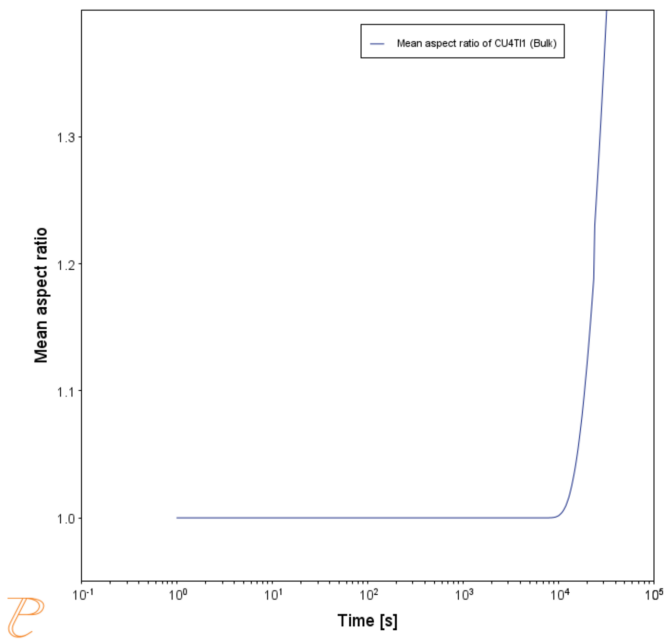


Figure 100: Mean Aspect Ratio.

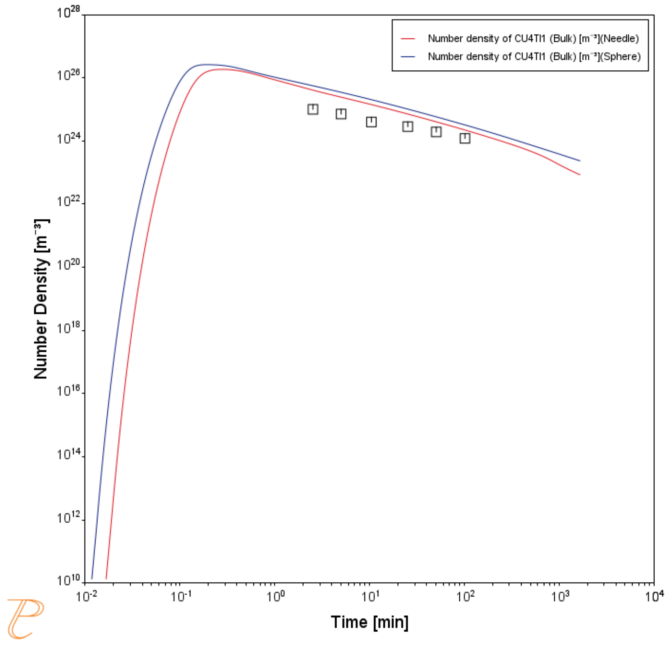


Figure 101: Number Density.

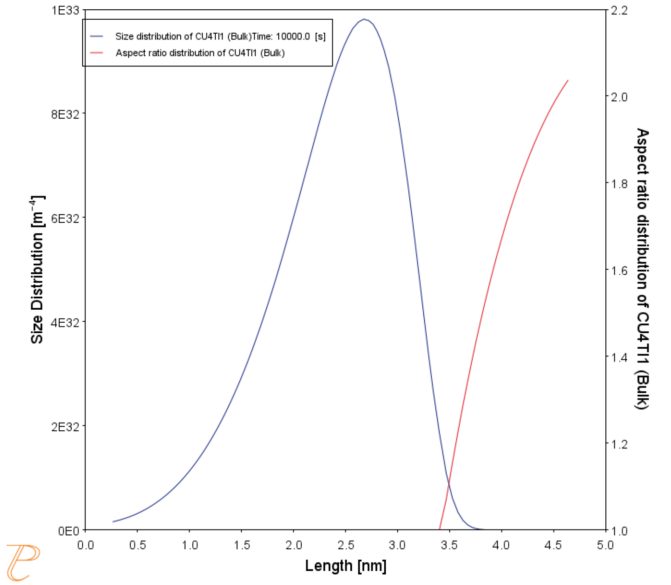


Figure 102: PSD and ASD.

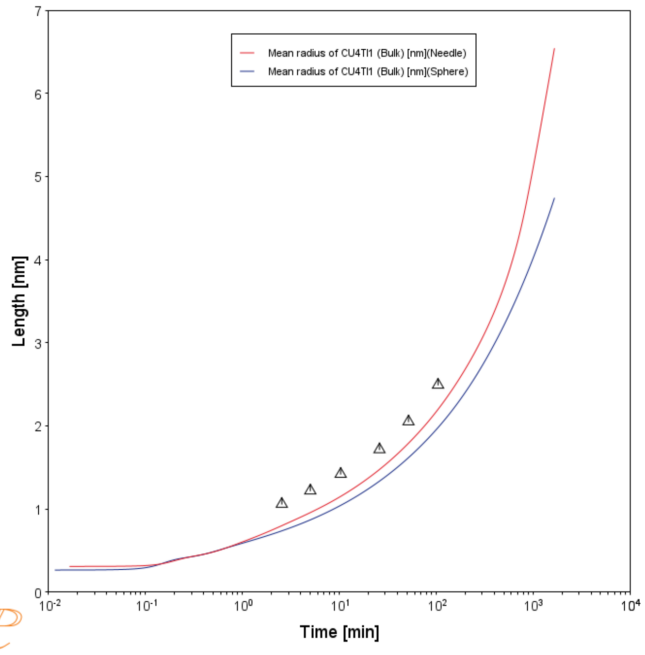


Figure 103: Mean Radius.

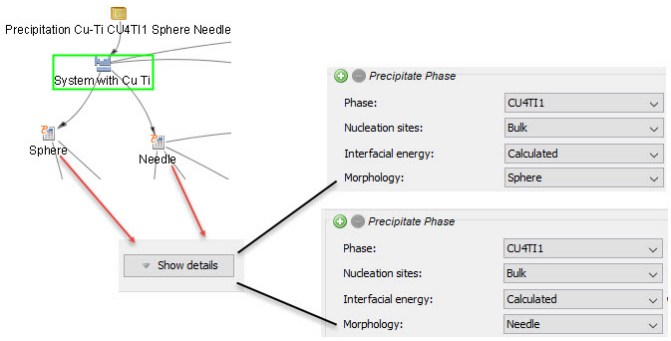
Project File and Video Tutorial Information

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

Also see our website and YouTube channel for other examples of the Precipitation Module.

Example Settings

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



System (System Definer)	
Database package	Demo: Copper-based alloys (CUDEMO and MCUDEMO)
Elements	Cu, Ti
Sphere and Needle Conditions (Precipitation Calculator)	
Composition	Cu-1.9Ti Mole percent
Matrix phase	FCC_L12
Precipitate phase	CU4TI1
Matrix Phase Data Parameters (Precipitation Calculator)	
Mobility enhancement prefactor (click **Show details** to display this setting)	100
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk
Interfacial energy	The default
Morphology (click **Show details** to display this setting)	For the **Sphere** node (renamed from Precipitation Calculator), keep the default. For the **Needle** node (renamed from Precipitation Calculator), **Needle** is selected.

Transformation strain (click **Show details** to display this setting)	For the **Sphere** node (renamed from Precipitation Calculator), keep the default. For the **Needle**node (renamed from Precipitation Calculator), **User defined** is selected. In this example, the following settings are defined: • ε11 and ε22 are set to **0.022** • ε33 is set to **0.003**
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	350° C
Simulation time	10,000 seconds
Datasets (Experimental File Reader)	
Borchers Mean radius vs Time and Borchers Number density vs Time	Data sets included with this example and imported to two Experimental File Readers. These data sets are used for the Mean Radius and Number Density plots, respectively.

References

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

[1999, Borchers] C. Borchers, Catastrophic nucleation during decomposition of Cu-0.9at.% Ti. Philos. Mag. A. 79, 537–547 (1999).

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

In this isothermal calculation example, the precipitation of Al_3Sc phase from FCC_A1 matrix phase in an Al-Sc binary alloy is simulated. To make a comparison, two separate calculations are performed, one assuming spherical morphology without elastic strain energy, and the other assuming cuboid morphology whose shape is determined by competition between interfacial energy and elastic strain energy. The simulation results are compared with experimental data collected from Marquis and Seidman [2001] and Novotny and Ardell [2001]. In addition, mean cubic factor and cubic factor distribution are also plotted for cuboid shape to illustrate the spherical-cuboidal transition during precipitation.

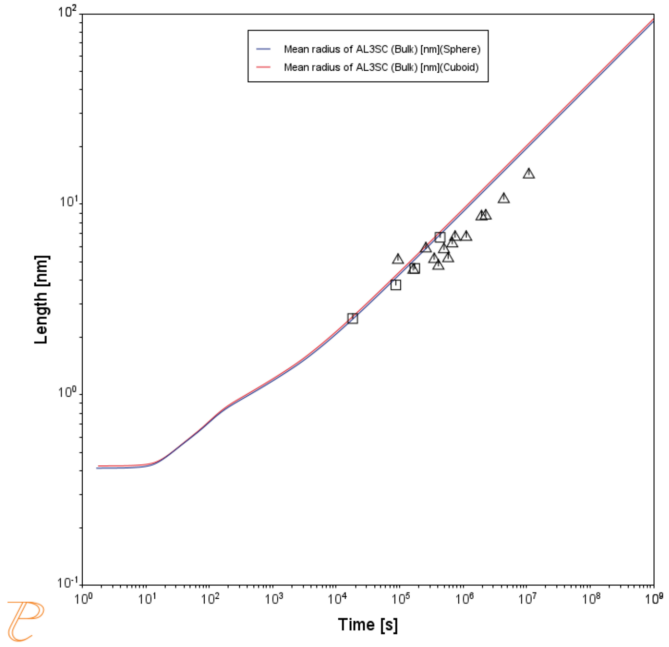


Figure 104: Mean Radius

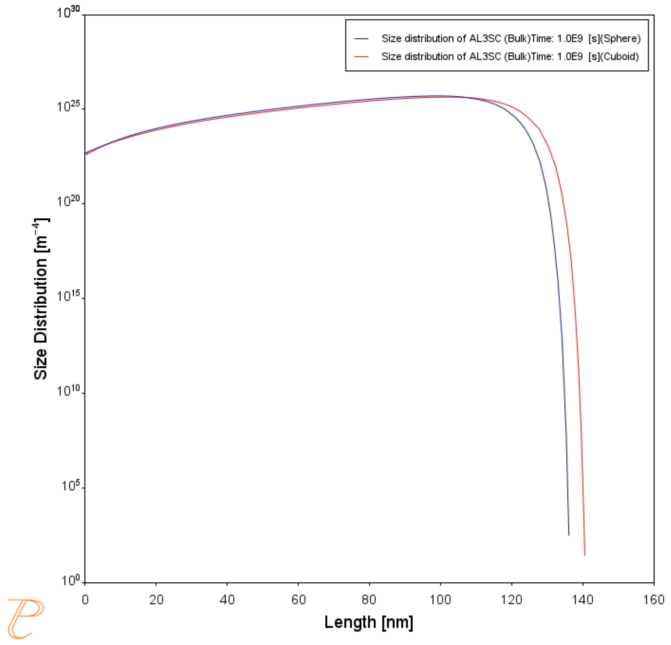


Figure 105: Particle size distribution (PSD).

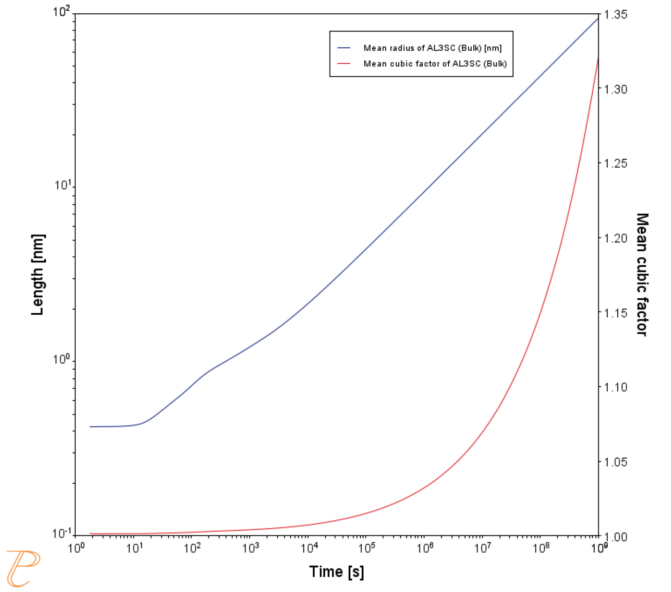


Figure 106: Mean Radius and Cubic Factor

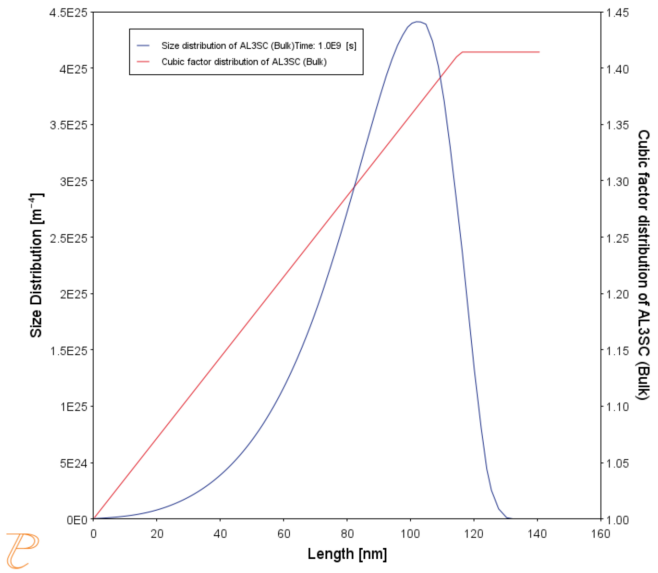


Figure 107: Particle size distribution (PSD) and cubic factor.

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

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

This example is 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.

References

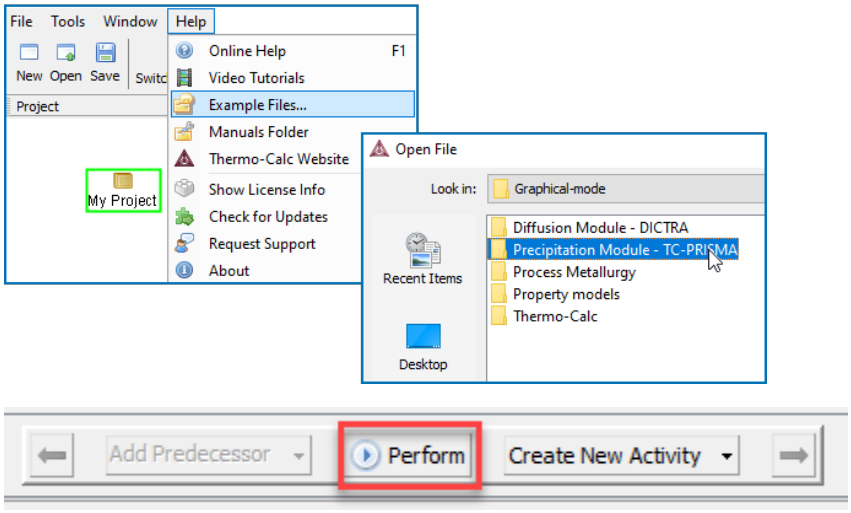
[2001, Marquis] E. A. Marquis, D. N. Seidman, Nanoscale structural evolution of Al3Sc precipitates in Al (Sc) alloys. Acta Mater. 49, 1909–1919 (2001).

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

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

HELPFUL INFORMATION

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



ABOUT THE EXAMPLE

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

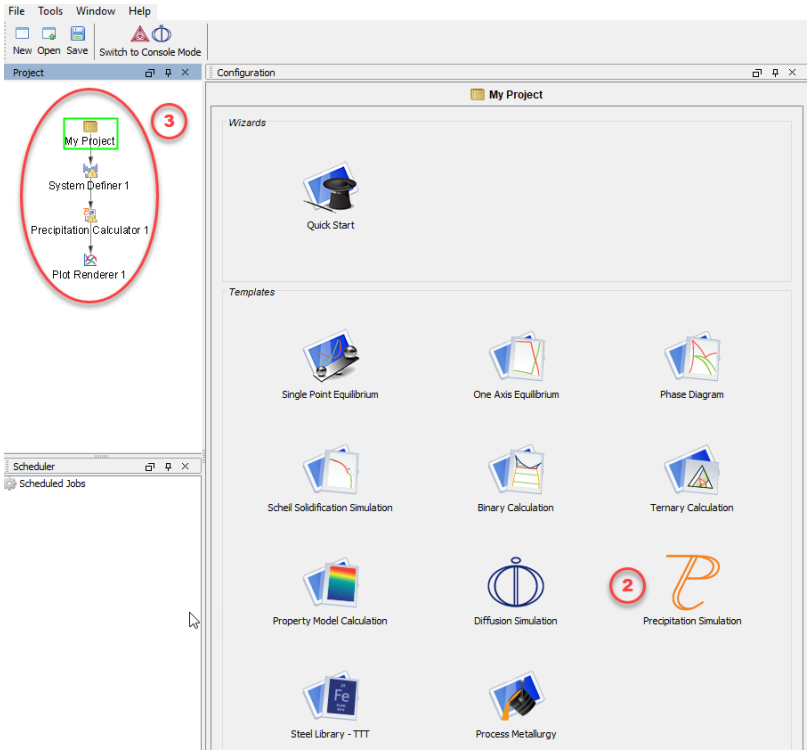
Two separate calculations are performed so you can make a comparison of the results, one assuming spherical morphology without elastic strain energy, and the other assuming cuboid morphology whose shape is determined by competition between interfacial energy and elastic strain energy.

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

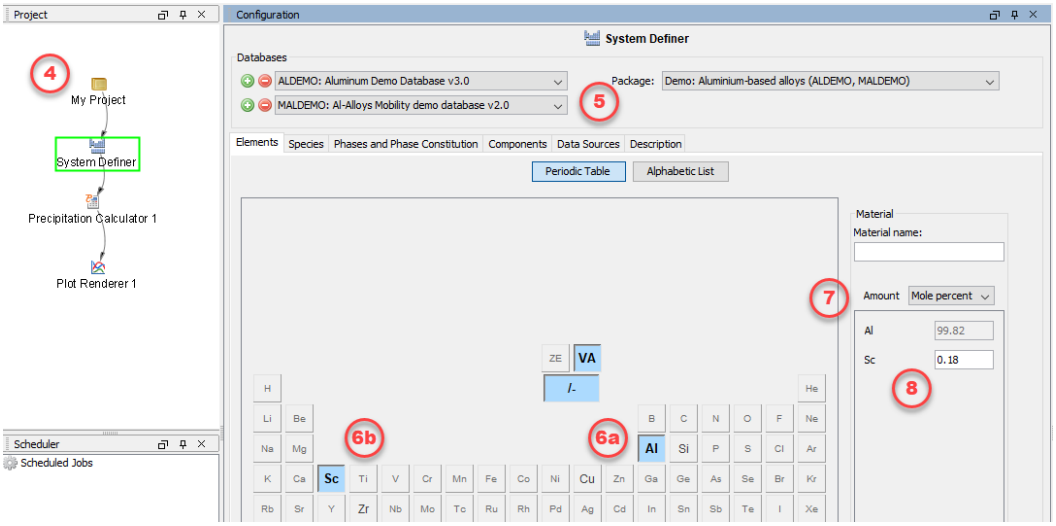
If you run the example file included in your software, the simulation results are compared with experimental data collected from Marquis and Seidman (2001) and Novotny and Ardell (2001).

SETTING UP THE SYSTEM

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



4. In the **Project** window, click the **System Definer 1** node.
5. Set the database *Package* to **Demo: Aluminium-based alloys (ALDEMO, MALDEMO)**, which loads both thermodynamic and kinetic demonstration aluminium databases.
6. From the **Periodic Table**, select the elements as follows. Select Al first so that it is the dependant element:
    a. **Al** (aluminium)
    b. **Sc** (scandium).
7. From the *Amount* list (to the right of the Periodic Table), select **Mole percent**.
8. Enter `0.18` for **Sc**. This automatically sets **Al** to 99.82.



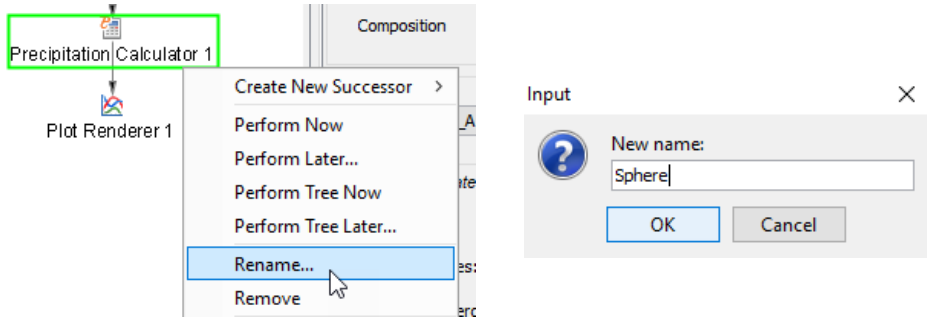
Our system is now defined. Now set up the precipitation calculations.

SETTING UP THE PRECIPITATION CALCULATIONS

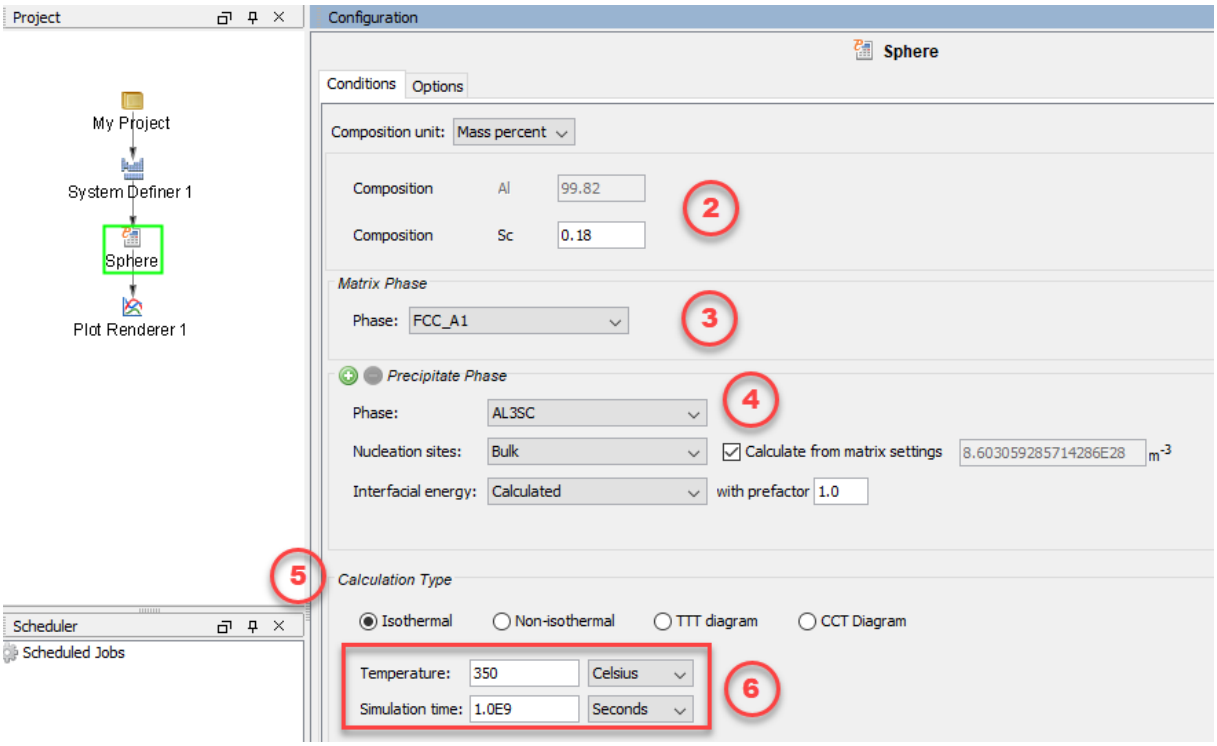
There are two precipitation calculations in this example, one assuming spherical morphology without elastic strain energy, and the other assuming cuboid morphology whose shape is determined by competition between interfacial energy and elastic strain energy. The results are then compared for both calculations.

Setting up the Precipitation Calculation with Spherical Morphology

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



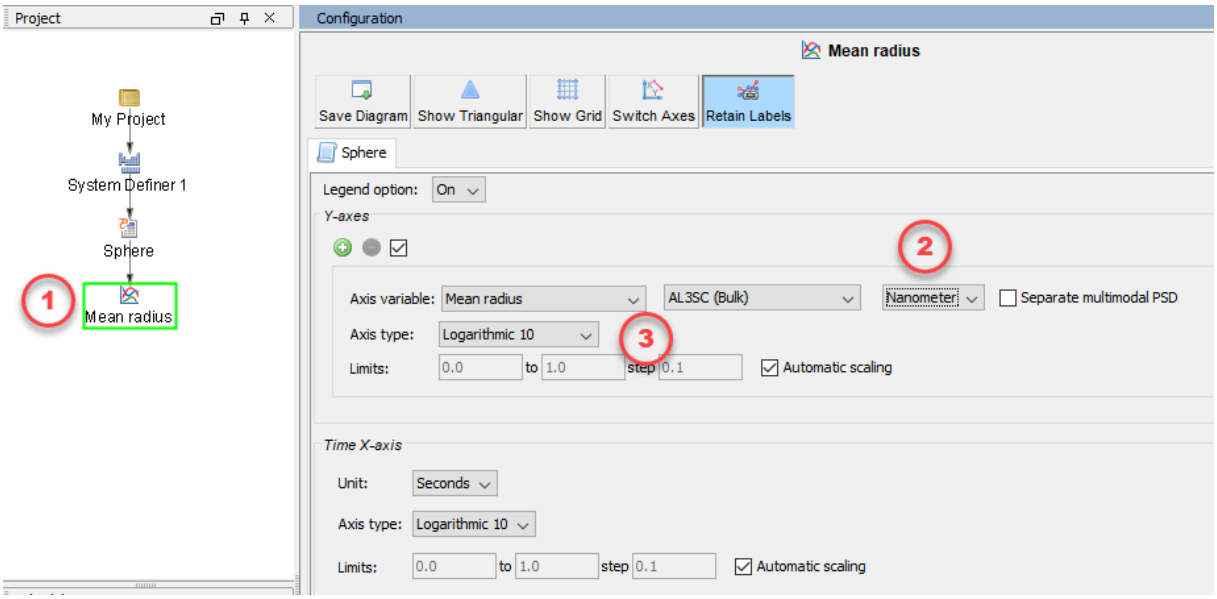
2. Notice that the composition set in the *System Definer* auto-populated on the Precipitation Calculator.
3. Under *Matrix Phase* from the *Phase* list it defaults to **FCC_A1**.
4. Under *Precipitate Phase* from the *Phase* list select **AL3SC**.
5. Under *Calculation Type*, make sure **Isothermal**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



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

Configuring the Plot

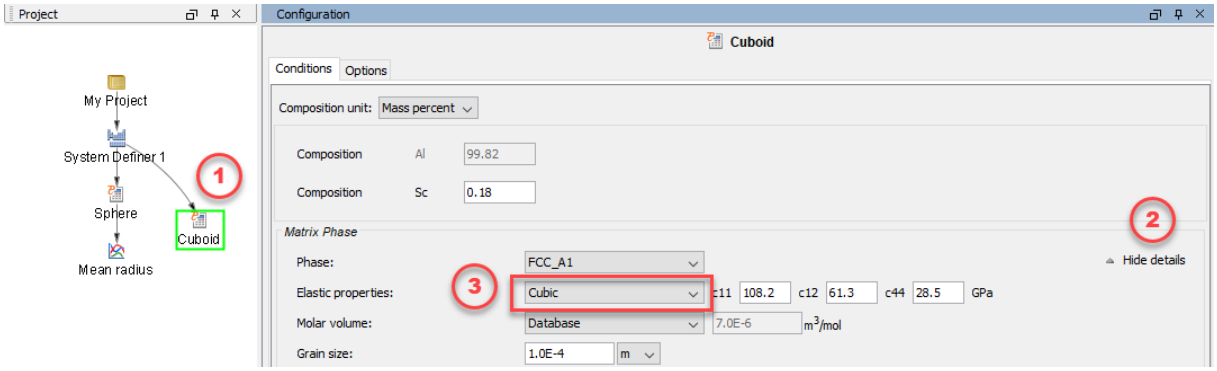
1. In the **Project** window, right-click **Plot Renderer 1** and select **Rename**. Name the plot `Mean radius` then press Enter or click **OK**.
2. Under *Y-axes* change the units to **Nanometer** (nm).
3. From the *Axis type* list select **Logarithmic 10**.



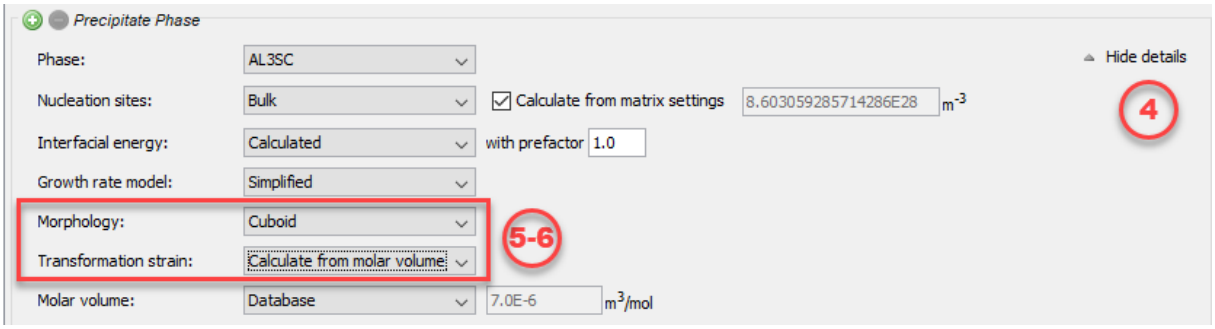
The plot is now set, but before running the simulation you set up another calculation and link it to the same Plot Renderer.

Setting up the Precipitation Calculation with Cuboid Morphology

1. In the **Project** window, right-click the **Sphere** node and select **Clone**.
   a. Right-click the **Sphere 1** node and select **Rename**.
   b. Name the node `Cuboid` and press Enter or click **OK**.
2. On the **Configuration** window to the right of *Matrix Phase* click **Show Details**.
3. From the *Elastic Properties* list select **Cubic**. Keep the suggested default values. Click **Hide details**.



4. To the right of *Precipitate Phase*, click **Show details**.
5. From the *Morphology* list select **Cuboid**.
6. From the *Transformation strain* list select **Calculate from molar volume**.

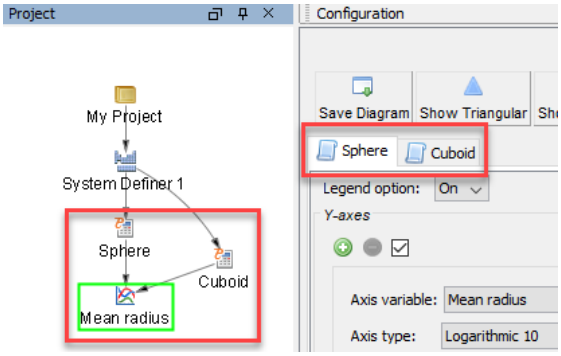


The second calculation is now set up, so now link it to the Plot Renderer node.

Linking the Plot to the Calculation with Cuboid Morphology

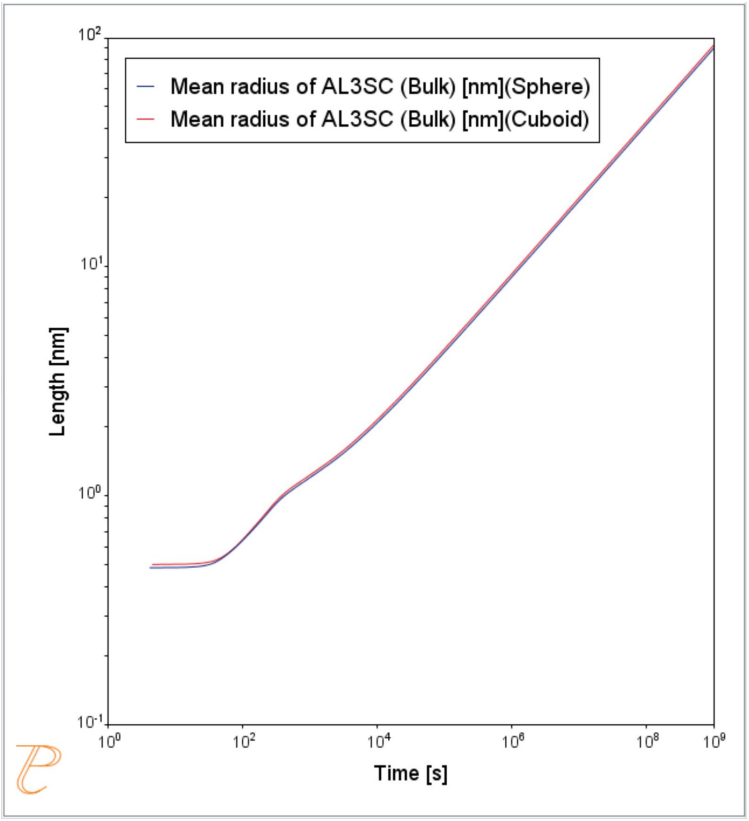
1. In the **Project** window, right-click the **Mean radius** node and select **Add Predecessor >Cuboid**.
2. Notice that in the **Configuration** window there are two tabs associated with this plot, one for **Sphere** and one for **Cuboid**. The Sphere settings are already configured, so you just need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

set up the Cuboid tab.



3. Click the **Cuboid** tab.
4. Under *Y-axes* change the units to **Nanometer** (nm).
5. From the *Axis type* list select **Logarithmic 10**.
6. The calculation is now ready to run. Right-click the **Mean radius** node and select **Perform Now** or click **Perform** on the **Configuration** window.

INTERPRETING THE RESULTS OF THE PRECIPITATION CALCULATIONS



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

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

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

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

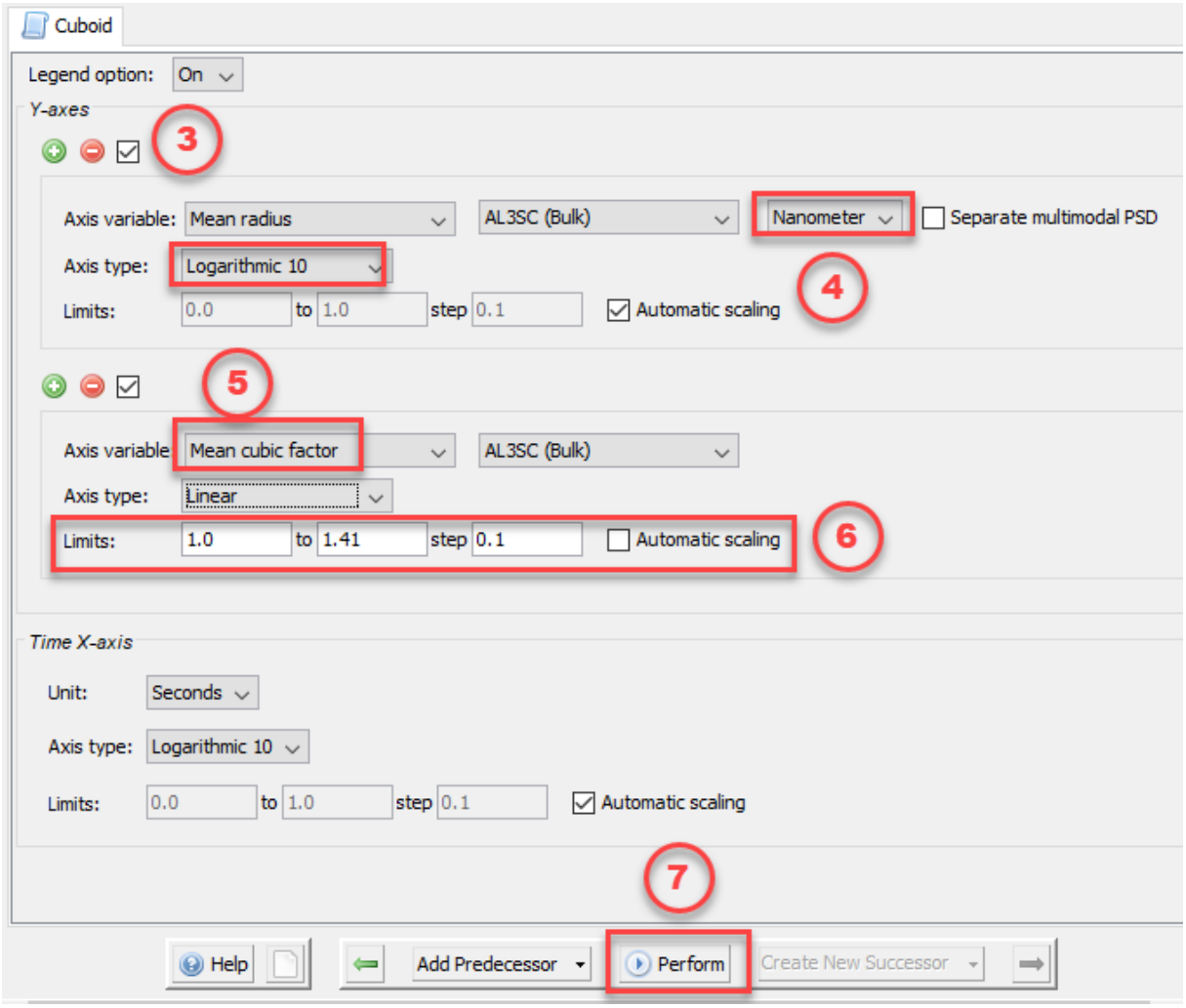
PLOTTING ADDITIONAL VARIABLES

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

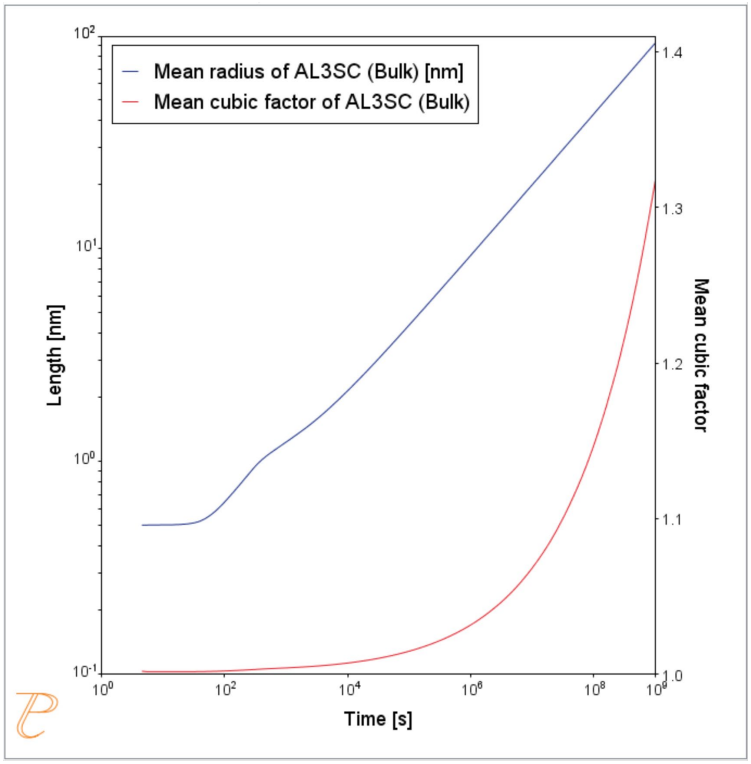
Plotting Mean Radius and Cuboid Factor

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

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



Interpreting the Results of Mean Radius and Cuboid Factor



In this plot, the blue line represents the evolution of the average radius of the cubic particles as a function of time. The red line shows the average cubic factor as a function of time.

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

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

The evolution of the shape when the particles grows is determined by competition between interfacial energy and elastic strain energy. In general, the shape is close to spherical at small particle sizes because the interfacial energy term dominates.

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

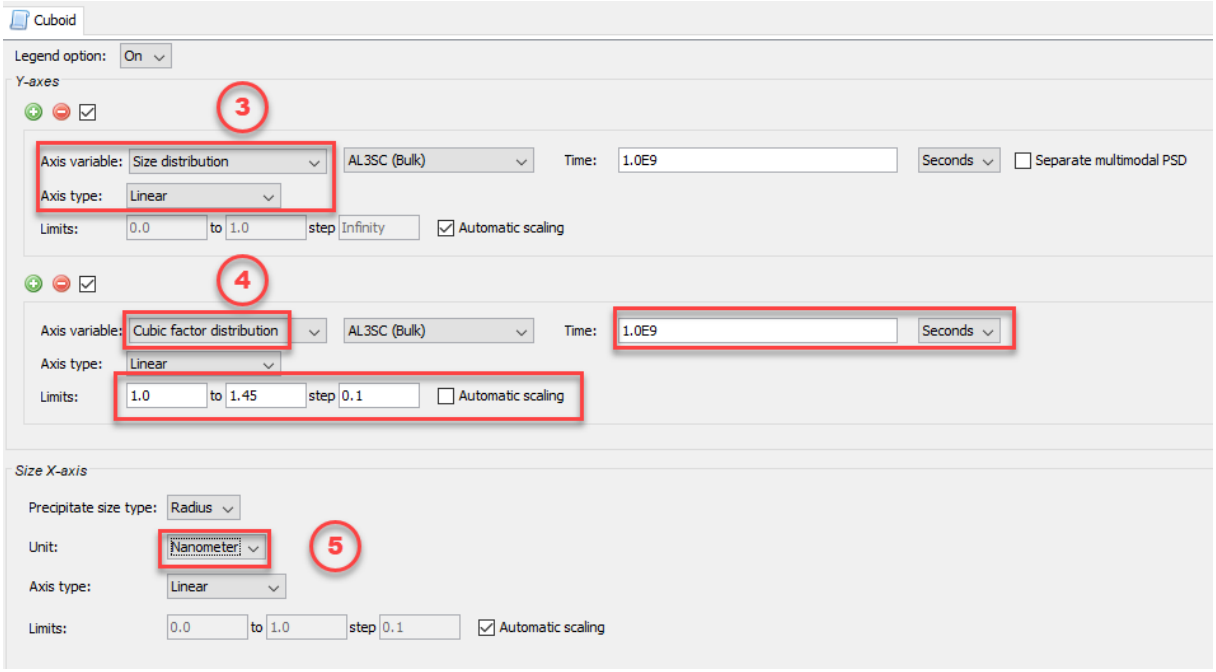
Plotting Particle Size and Cubic Factor Distribution

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

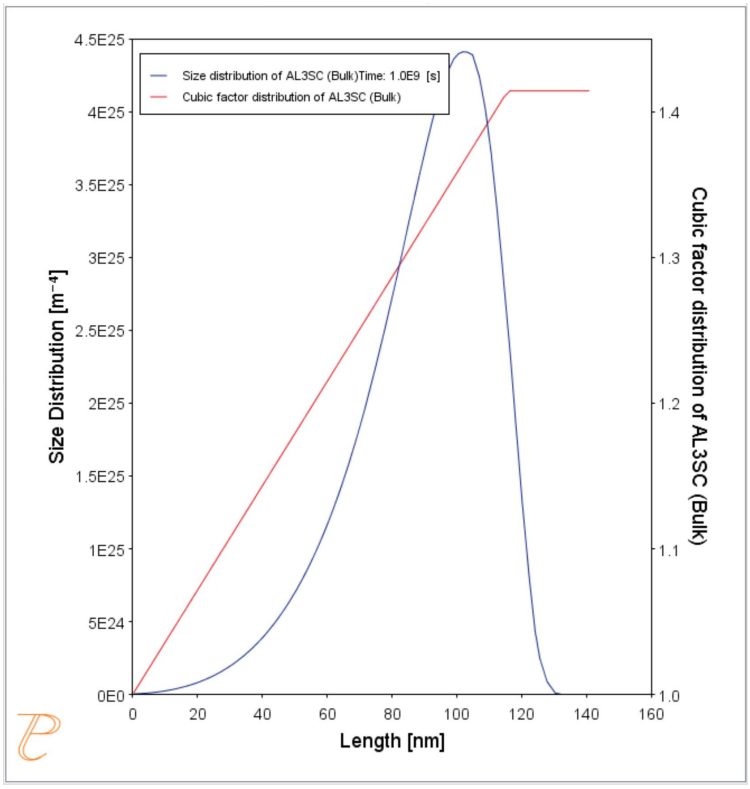
This plot also has two Y-axes, so you can clone the previous plot.

1. Right-click the **Mean radius and Cuboid factor** node and select **Clone**.
2. Right-click the new node and rename it `PSD and Cuboid factor`.
3. Under the *Y-axes*
    a. Select **Size distribution** as the first *Axis variable*.
    b. Change the *Axis type* to **Linear**.
4. Set the second Y-axis to **Cubic factor distribution** and enter a *Time* of `1e9` **Seconds**.

5. Keep the *Automatic Scaling* check box cleared. Enter the *Limits* from `1` to `1.45` and the *step* to `0.1`.
6. Under *Size X-axis*, change the unit to **Nanometer** (nm).
7. Click **Perform** at the bottom center of the **Configuration** window.



Interpreting the Results of Particle Size Distribution and Cuboid Factor



In this plot, the blue curve shows the particle size distribution and the red line shows the cubic factor distribution.

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

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

References

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

P_10: Initial Particle Size Distribution of Fe-Cr-C

This example demonstrates the effect of initial particle size distribution 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.

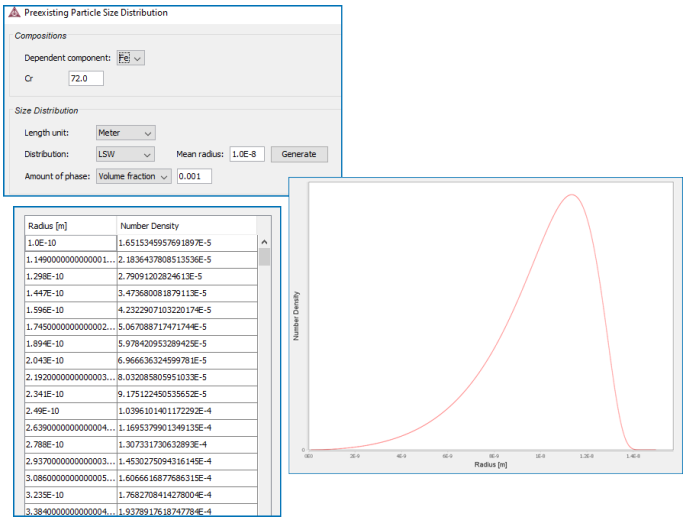


Figure 108: The Preexisting Particle Size Distribution (PSD) settings window for example P_10.

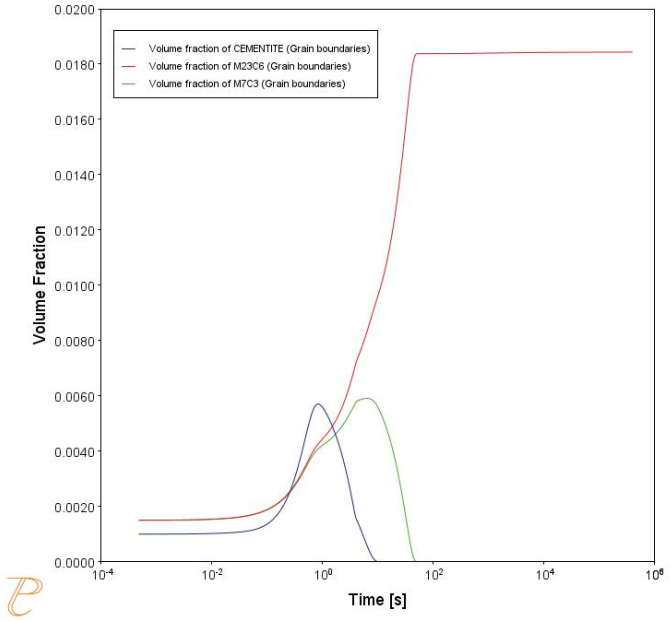


Figure 109: Volume fraction with initial particle size distribution (PSD).

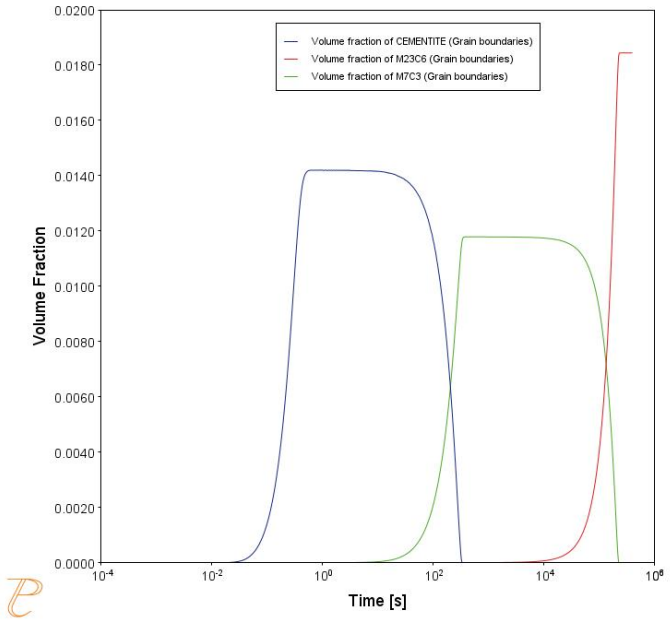


Figure 110: Volume fraction with no initial particle size distribution (PSD).

Project File and Video Tutorial Information

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

Also see our website and YouTube channel for other examples of the Precipitation Module.

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

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 (2004) data is compared with the calculated results.

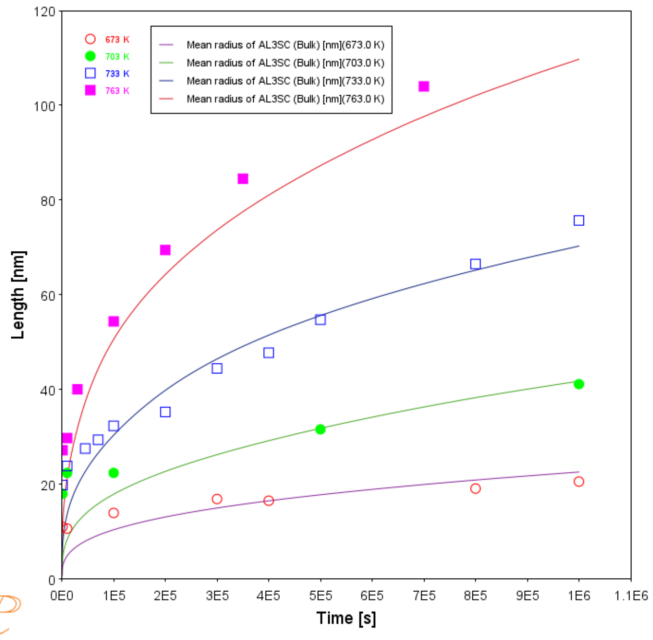


Figure 111: The results of an isothermal calculation to examine the mean radius of an Al-0.12Sc system.

Project File and Video Tutorial Information

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

Also see our website and YouTube channel for other examples of the Precipitation Module.

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.

Reference

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

P_12: Comparing Growth Rate Models for an Al-Zr System

This example compares the **Simplified**, **General** and **Advanced** growth rate models for an Al-Zr system. The resulting plot compares the mean radius of the spheres for each AL3ZR_D023 precipitate phase calculated for each type of growth rate model.

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. [2008] data is compared with the calculated results.

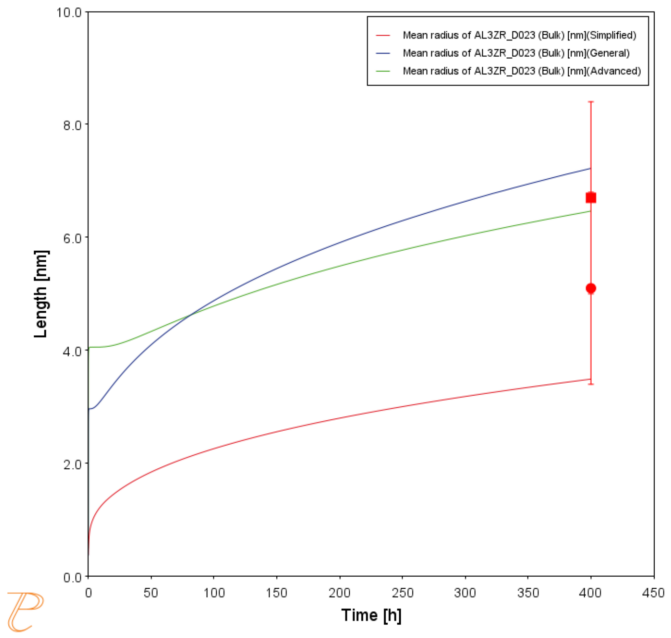


Figure 112: Result comparing the mean radius of the spheres for each AL3ZR_D023 precipitate phase calculated for each type of growth rate model.

Project File and Video Tutorial Information

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

Also see our website and YouTube channel for other examples of the Precipitation Module.

Example Settings

System (System Definer)	
Database package	Demo: Aluminum-based Alloys (ALDEMO, MALDEMO)
Elements	Al, Zr
Conditions (Precipitation Calculator)	
Composition	Al-0.2Zr Mole percent
Matrix phase	FCC_A1 All other defaults are kept.
Precipitate phase	AL3ZR_D023

	Click **Show details** to select the **Growth rate model** (**Simplified**, **Advanced** and **General**). All other defaults are kept.
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	425 Celsius
Simulation time	400 hours
Datasets (Experimental File Reader)	
2008 Knipling	Data set included with this example and imported to one Experimental File Reader.

Reference

[2008, Knipling] K. E. Knipling, D. C. Dunand, D. N. Seidman, Precipitation evolution in Al–Zr and Al–Zr–Ti alloys during isothermal aging at 375–425°C. Acta Mater. 56, 114–127 (2008).

P_13: Paraequilibrium Precipitation of Cementite Fe-C-Cr

In this example, the precipitation of cementite during tempering of a Fe-Cr-C steel is simulated considering two interface conditions: one is the usual ortho-equilibrium condition; the other is the para-equilibrium condition. The simulation results are compared with the experimental data from Sakuma et al. [1980].

The example may take over two hours to run.

This example demonstrates that the early stage of the cementite precipitation can only be accounted for by a simulation applying the para-equilibrium condition, under which the precipitation kinetics are controlled by the diffusion of C. The comparison also shows a later stage gradual transition from the para-equilibrium condition to the ortho-equilibrium condition, and if the tempering time is long enough the diffusion of Cr has a dominating effect on the coarsening of cementite.

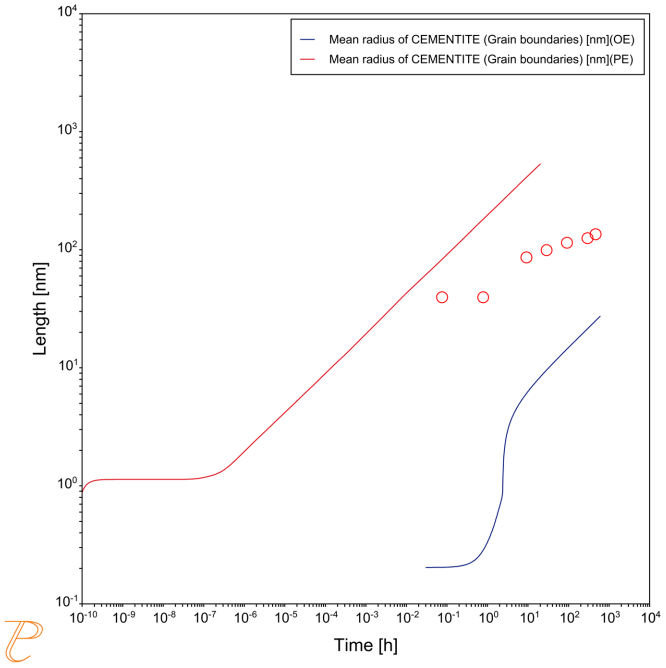


Figure 113: Comparing results from Para-eq (PE) and Simplified (OE) growth models.

Project File and Video Tutorial Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_13_Precipitation_Fe-C-Cr_Paraequilibrium_Precipitation_of_Cementite.tcu*

Also see our website and YouTube channel for other examples of the Precipitation Module.

Example Settings

System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)
Elements	Fe, Cr, C
Conditions (Precipitation Calculator)	
Composition	Fe-0.95Cr-1.065C Mass percent
Matrix phase	BCC_A2 All other defaults are kept.
Precipitate phase	CEMENTITE Click **Show details** to select the **Growth rate model** (**Simplified** and **Para-eq**). All other defaults are kept.
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	773 Kelvin
Simulation time	20 hours for the paraequilibrium model and 600 hours for the simplified model.
Datasets (Experimental File Reader)	
1980 Sakuma	Data set included with this example and imported to one Experimental File Reader.

Reference

[1980, Sakuma] T. Sakuma, N. Watanabe, T. Nishizawa, The Effect of Alloying Element on the Coarsening Behavior of Cementite Particles in Ferrite. Trans. Japan Inst. Met. 21, 159–168 (1980).