

# Graphical Mode Examples Guide

Thermo-Calc Version 2020b



## Graphical Mode Examples

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This guide includes descriptions of the following

| Category  | Example number   |
|---|--|
| <a href="#">Thermo-Calc Graphical Mode Examples Collection</a> includes binary and ternary system examples, Scheil, the Equilibrium Calculator, plus more | T_01 to T_12   |
| <a href="#">Thermo-Calc Property Model Examples Collection</a> : General Model Library and Steel Model Library  | General Models: PM_G_01 to PM_G_06<br>Steel Models: PM_Fe_01 to PM_Fe_03 |
| <a href="#">Process Metallurgy Module Examples Collection</a>   | PMET_01 to PMET_06   |
| <a href="#">Diffusion Module (DICTRA) Graphical Mode Examples</a>   | D_01, D_02, D_03 (the Quick Start Guide Examples)<br>D_04 to D_07        |
| <a href="#">Precipitation Module (TC-PRISMA) Graphical Mode Examples</a>  | P_01 to P_13   |

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## Thermo-Calc Graphical Mode Examples Collection

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## T\_01: Calculating a Single-Point Equilibrium

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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%

### Project File and Video Tutorial Information

- Folder: Thermo-Calc
- File name: *T\_01\_Single-point\_equilibrium.tcu*



This example is included as a tutorial on our [website](#) and our [YouTube](#) channel.

### Table Result

The displayed results of the calculation show that the BCC\_A2 (ferrite) and GRAPHITE phases are stable for this set of equilibrium conditions.



| Results              |                      |                      |                        |                  |
|----------------------|----------------------|----------------------|------------------------|------------------|
| Table Renderer 1     |                      |                      |                        |                  |
| <b>System</b>        |                      |                      |                        |                  |
| 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]                 |                        |                  |
| <i>Component</i>     | <i>Mole Fraction</i> | <i>Mass Fraction</i> | <i>Activity</i>        | <i>Potential</i> |
| C                    | 0.00463              | 0.00100              | 0.21816                | -12658.89428     |
| Fe                   | 0.99537              | 0.99900              | 0.00619                | -42278.50542     |
| <b>Stable Phases</b> |                      |                      |                        |                  |
|                      | <i>Moles</i>         | <i>Mass</i>          | <i>Volume Fraction</i> |                  |
| <b>BCC_A2#1</b>      | 0.99609              | 55.59692             | 0.99711                | Composition ▾    |
| <b>Composition</b>   |                      |                      |                        |                  |
| <i>Component</i>     | <i>Mole Fraction</i> | <i>Mass Fraction</i> |                        |                  |
| Fe                   | 0.99928              | 0.99984              |                        |                  |
| C                    | 0.00072              | 0.00016              |                        |                  |
|                      | <i>Moles</i>         | <i>Mass</i>          | <i>Volume Fraction</i> |                  |
| <b>GRAPHITE#1</b>    | 0.00391              | 0.04700              | 0.00289                | Composition ▾    |
| <b>Composition</b>   |                      |                      |                        |                  |
| <i>Component</i>     | <i>Mole Fraction</i> | <i>Mass Fraction</i> |                        |                  |
| C                    | 1.00000              | 1.00000              |                        |                  |
| Fe                   | 0.00000              | 0.00000              |                        |                  |

## T\_02: Stepping in Temperature in the Fe-C System

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

### Project File and Video Tutorial Information

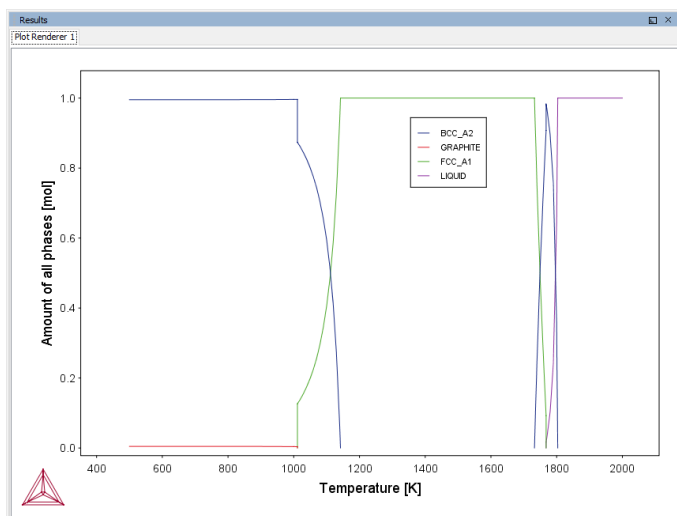
- Folder: Thermo-Calc
- File name: *T\_02\_Step\_in\_temperature\_in\_Fe-C.tcu*



This example is included in the tutorial on our [website](#) and [YouTube](#) channel.

### Plot Result

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



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

| Results                          |                        |                        |                          |                        |
|----------------------------------|------------------------|------------------------|--------------------------|------------------------|
| Plot Renderer 1 Table Renderer 1 |                        |                        |                          |                        |
| Temperature [K]                  | Amount of BCC_A2 [mol] | Amount of FCC_A1 [mol] | Amount of GRAPHITE [mol] | Amount of LIQUID [mol] |
| 1000.00000                       | 0.99609                |                        | 0.00391                  |                        |
| 1010.00000                       | 0.99618                |                        | 0.00382                  |                        |
| 1011.17630                       | 0.99620                |                        | 0.00380                  |                        |
| 1011.17630                       | 0.99620                | 0.00000                | 0.00380                  |                        |
| 1011.17630                       | 0.87367                | 0.12633                | 0.00000                  |                        |
| 1011.17630                       | 0.87367                | 0.12633                |                          |                        |
| 1020.00000                       | 0.86050                | 0.13950                |                          |                        |
| 1030.00000                       | 0.84335                | 0.15665                |                          |                        |
| 1040.00000                       | 0.82359                | 0.17641                |                          |                        |
| 1050.00000                       | 0.80085                | 0.19915                |                          |                        |
| 1060.00000                       | 0.77399                | 0.22601                |                          |                        |
| 1070.00000                       | 0.74184                | 0.25816                |                          |                        |
| 1080.00000                       | 0.70282                | 0.29718                |                          |                        |
| 1090.00000                       | 0.65470                | 0.34530                |                          |                        |
| 1100.00000                       | 0.59418                | 0.40582                |                          |                        |
| 1110.00000                       | 0.51618                | 0.48382                |                          |                        |
| 1120.00000                       | 0.41250                | 0.58750                |                          |                        |
| 1130.00000                       | 0.26894                | 0.73106                |                          |                        |
| 1140.00000                       | 0.05863                | 0.94137                |                          |                        |
| 1142.15538                       | 0.00000                | 1.00000                |                          |                        |
| 1142.15538                       |                        | 1.00000                |                          |                        |
| 1150.00000                       |                        | 1.00000                |                          |                        |
| 1160.00000                       |                        | 1.00000                |                          |                        |
| 1170.00000                       |                        | 1.00000                |                          |                        |
| 1180.00000                       |                        | 1.00000                |                          |                        |
| 1190.00000                       |                        | 1.00000                |                          |                        |
| 1200.00000                       |                        | 1.00000                |                          |                        |
| 1210.00000                       |                        | 1.00000                |                          |                        |
| 1220.00000                       |                        | 1.00000                |                          |                        |

## T\_03: Fe-C Phase Diagrams

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

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

### Project File and Video Tutorial Information

- Folder: Thermo-Calc
- File name: *T\_03\_Fe-C\_phase\_diagram.tcu*

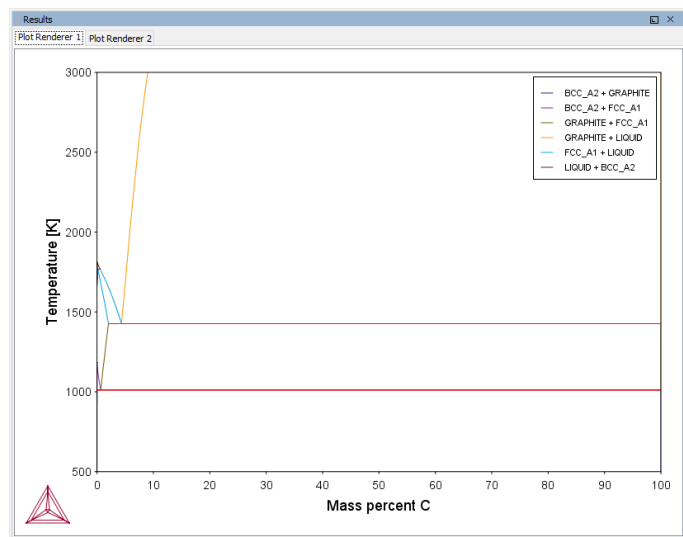


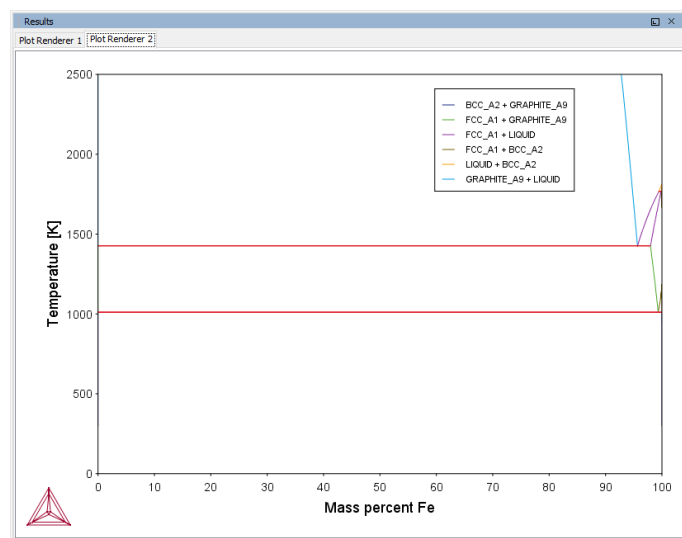
This example is included as a tutorial on our [website](#) and our [YouTube](#) channel.

### Plot Results

#### *Equilibrium Calculator Results*

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



*Binary Calculator Results*

## T\_04: Fe-Cr-C Ternary Phase Diagram at 1000 K

This example shows a ternary phase diagram in the Fe-Cr-C system at 1000 K. Similar to example [T\\_03: Fe-C Phase Diagrams](#), the same diagram is calculated using a Ternary Calculator and then using a System Definer and Equilibrium Calculator. Two Plot Renderer activities are added to create two plots.

### Project File and Video Tutorial Information

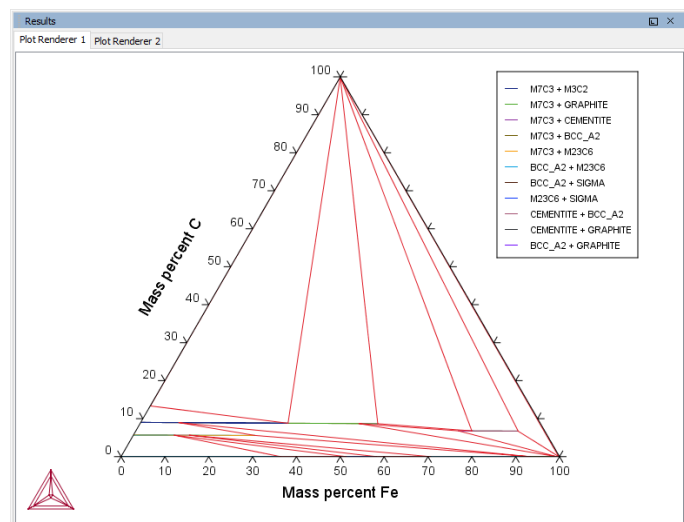
- Folder: Thermo-Calc
- File name: *T\_04\_Fe-Cr-C\_ternary\_phase\_diagram.tcu*



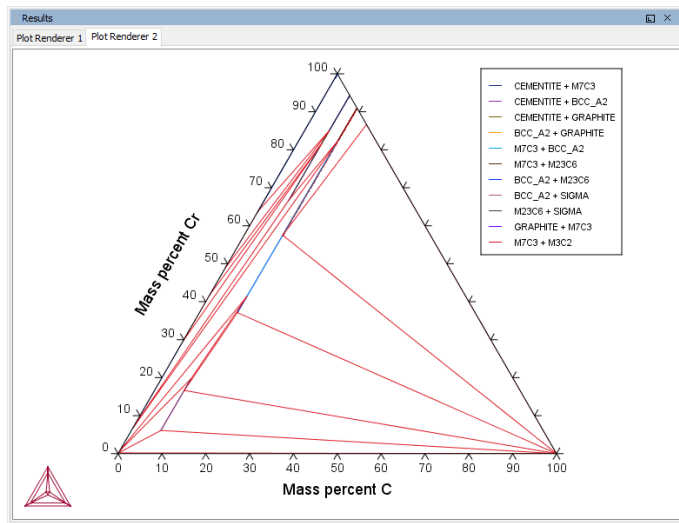
This example is included as a tutorial on our [website](#) and our [YouTube](#) channel.

### Plot Results

#### *Ternary Calculator*



## Equilibrium Calculator

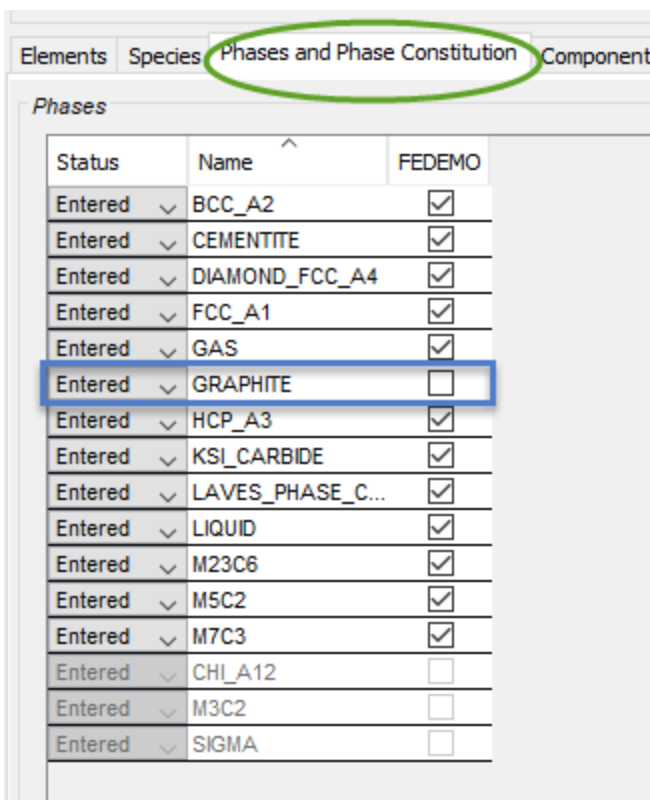


Try practicing with two features on the Plot Renderer Configuration window. To toggle between a triangular and a rectangular diagram, click the **Show Triangular** button then click **Perform** to see what happens. To toggle the X and Y axis variables, click the **Switch Axes** button and then click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

## T\_05: Stable and the Metastable Fe-C Phase Diagrams

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

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



### Project File and Video Tutorial Information

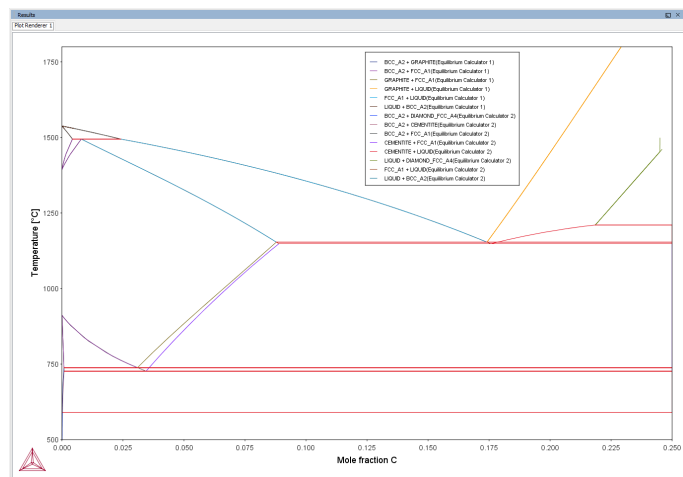
- Folder: Thermo-Calc
- File name: *T\_05\_Fe-C\_stable\_and\_metastable\_phase\_diagram.tcu*





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](#).

## Plot Result



## T\_06: Serially Coupled Equilibrium Calculators

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

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

### Project File 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.

| Results   |               |               |                 |              |
|---|---------------|---------------|-----------------|--------------|
| Table Renderer 1   Table Renderer 2   Table Renderer 3   Table Renderer 4 |               |               |                 |              |
| <b>System</b>   |               |               |                 |              |
| Moles   | 1.00000       |               |                 |              |
| Mass  | 55.41634      | [g]           |                 |              |
| Temperature   | 1123.15000    | [K]           |                 |              |
| Total Gibbs Energy  | -52361.90905  | [J]           |                 |              |
| Enthalpy  | 32589.15580   | [J]           |                 |              |
| Volume  | 7.34405E-6    | [m3]          |                 |              |
| <b>Component</b>  |               |               |                 |              |
|   | Mole Fraction | Mass Fraction | Activity        | Potential    |
| C   | 0.00046       | 0.00010       | 0.00137         | -61592.91681 |
| Cr  | 0.10658       | 0.10000       | 0.00235         | -56531.30746 |
| Fe  | 0.89296       | 0.89990       | 0.00387         | -51859.50665 |
| <b>Stable Phases</b>  |               |               |                 |              |
| <b>BCC_A2#1</b>   |               |               |                 |              |
|   | Moles         | Mass          | Volume Fraction | Composition  |
|   | 0.76777       | 42.55315      | 0.76992         |              |
| <b>Composition</b>  |               |               |                 |              |
| Component   | Mole Fraction | Mass Fraction |                 |              |
| Fe  | 0.89183       | 0.89864       |                 |              |
| Cr  | 0.10801       | 0.10133       |                 |              |
| C   | 0.00016       | 0.00003       |                 |              |
| <b>FCC_A1#1</b>   |               |               |                 |              |
|   | Moles         | Mass          | Volume Fraction | Composition  |
|   | 0.23223       | 12.86320      | 0.23008         |              |
| <b>Composition</b>  |               |               |                 |              |
| Component   | Mole Fraction | Mass Fraction |                 |              |
| Fe  | 0.89669       | 0.90408       |                 |              |
| Cr  | 0.10185       | 0.09560       |                 |              |
| C   | 0.00147       | 0.00032       |                 |              |

## 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.

| Results   |               |               |                 |              |
|---|---------------|---------------|-----------------|--------------|
| Table Renderer 1   Table Renderer 2   Table Renderer 3   Table Renderer 4 |               |               |                 |              |
| <b>System</b>   |               |               |                 |              |
| Moles   | 1.00000       |               |                 |              |
| Mass  | 55.39810      | [g]           |                 |              |
| Temperature   | 1123.15000    | [K]           |                 |              |
| Total Gibbs Energy  | -52365.69157  | [J]           |                 |              |
| Enthalpy  | 32827.91821   | [J]           |                 |              |
| Volume  | 7.32017E-6    | [m3]          |                 |              |
| <b>Component</b>  |               |               |                 |              |
|   | Mole Fraction | Mass Fraction | Activity        | Potential    |
| C   | 0.00088       | 0.00019       | 0.00146         | -40967.89084 |
| Cr  | 0.10654       | 0.10000       | 0.00238         | -56409.41447 |
| Fe  | 0.89258       | 0.89981       | 0.00387         | -51874.52376 |
| <b>Stable Phases</b>  |               |               |                 |              |
| <b>BCC_A2#1</b>   |               |               |                 |              |
|   | Moles         | Mass          | Volume Fraction | Composition  |
|   | 0.50000       | 27.70824      | 0.50303         |              |
| <b>Composition</b>  |               |               |                 |              |
| <b>Component</b>  |               |               |                 |              |
|   | Mole Fraction | Mass Fraction |                 |              |
| Fe  | 0.89000       | 0.89692       |                 |              |
| Cr  | 0.10982       | 0.10304       |                 |              |
| C   | 0.00017       | 0.00004       |                 |              |
| <b>FCC_A1#1</b>   |               |               |                 |              |
|   | Moles         | Mass          | Volume Fraction | Composition  |
|   | 0.50000       | 27.68987      | 0.49697         |              |
| <b>Composition</b>  |               |               |                 |              |
| <b>Component</b>  |               |               |                 |              |
|   | Mole Fraction | Mass Fraction |                 |              |
| Fe  | 0.89515       | 0.90270       |                 |              |
| Cr  | 0.10326       | 0.09695       |                 |              |
| C   | 0.00159       | 0.00034       |                 |              |

## Equilibrium Calculator 3

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

| Results   |               |               |                 |              |
|---|---------------|---------------|-----------------|--------------|
| Table Renderer 1   Table Renderer 2   Table Renderer 3   Table Renderer 4 |               |               |                 |              |
| <b>System</b>   |               |               |                 |              |
| Moles   | 1.00000       |               |                 |              |
| Mass  | 55.41634      | [g]           |                 |              |
| Temperature   | 1123.15000    | [K]           |                 |              |
| Total Gibbs Energy  | -52361.90905  | [J]           |                 |              |
| Enthalpy  | 32599.15580   | [J]           |                 |              |
| Volume  | 7.34405E-6    | [m3]          |                 |              |
| <b>Component</b>  |               |               |                 |              |
|   | Mole Fraction | Mass Fraction | Activity        | Potential    |
| C   | 0.00046       | 0.00010       | 0.00137         | -61592.91681 |
| Cr  | 0.10658       | 0.10000       | 0.00235         | -56531.30746 |
| Fe  | 0.89296       | 0.89990       | 0.00387         | -51859.50665 |
| <b>Stable Phases</b>  |               |               |                 |              |
| <b>BCC_A2#1</b>   |               |               |                 |              |
|   | Moles         | Mass          | Volume Fraction | Composition  |
|   | 0.76777       | 42.55315      | 0.76992         |              |
| <b>Composition</b>  |               |               |                 |              |
| <b>Component</b>  |               |               |                 |              |
|   | Mole Fraction | Mass Fraction |                 |              |
| Fe  | 0.89183       | 0.89864       |                 |              |
| Cr  | 0.10801       | 0.10133       |                 |              |
| C   | 0.00016       | 0.00003       |                 |              |
| <b>FCC_A1#1</b>   |               |               |                 |              |
|   | Moles         | Mass          | Volume Fraction | Composition  |
|   | 0.23223       | 12.86320      | 0.23008         |              |
| <b>Composition</b>  |               |               |                 |              |
| <b>Component</b>  |               |               |                 |              |
|   | Mole Fraction | Mass Fraction |                 |              |
| Fe  | 0.89669       | 0.90408       |                 |              |
| Cr  | 0.10185       | 0.09560       |                 |              |
| C   | 0.00147       | 0.00032       |                 |              |

## 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.

| Results   |                              |               |                 |             |
|---|------------------------------|---------------|-----------------|-------------|
| Table Renderer 1   Table Renderer 2   Table Renderer 3   Table Renderer 4 |                              |               |                 |             |
| <b>System</b>   |                              |               |                 |             |
| Moles   | 1.00000                      |               |                 |             |
| Mass  | 55.41634 [g]                 |               |                 |             |
| Temperature   | 1791.51760 [K]               |               |                 |             |
| Total Gibbs Energy  | -1.09463E5 [J]               |               |                 |             |
| Enthalpy  | 59070.77313 [J]              |               |                 |             |
| Volume  | 7.63568E-6 [m <sup>3</sup> ] |               |                 |             |
| <b>Component</b>  |                              |               |                 |             |
|   | Mole Fraction                | Mass Fraction | Activity        | Potential   |
| C   | 0.00046                      | 0.00010       | 0.00012         | -1.34949E5  |
| Cr  | 0.10658                      | 0.10000       | 0.00030         | -1.20950E5  |
| Fe  | 0.89296                      | 0.89990       | 0.00071         | -1.08079E5  |
| <b>Stable Phases</b>  |                              |               |                 |             |
| <b>BCC_A2#1</b>   | Moles                        | Mass          | Volume Fraction | Composition |
|   | 1.00000                      | 55.41634      | 1.00000         |             |
| <b>Composition</b>  |                              |               |                 |             |
| Component   | Mole Fraction                | Mass Fraction |                 |             |
| Fe  | 0.89296                      | 0.89990       |                 |             |
| Cr  | 0.10658                      | 0.10000       |                 |             |
| C   | 0.00046                      | 0.00010       |                 |             |
| <b>Fixed Phases</b>   |                              |               |                 |             |
| <b>LIQUID#1</b>   | Moles                        | Mass          | Volume Fraction | Composition |
|   | 0.00000                      | 0.00000       | 0.00000         |             |
| <b>Composition</b>  |                              |               |                 |             |
| Component   | Mole Fraction                | Mass Fraction |                 |             |
| Fe  | 0.88607                      | 0.89447       |                 |             |
| Cr  | 0.11178                      | 0.10506       |                 |             |
| C   | 0.00216                      | 0.00047       |                 |             |

## 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 *Quantities* *Q1*, *Q2*, *Q3* and so forth, or by using the Thermo-Calc syntax.

### Project File and Video Tutorial Information

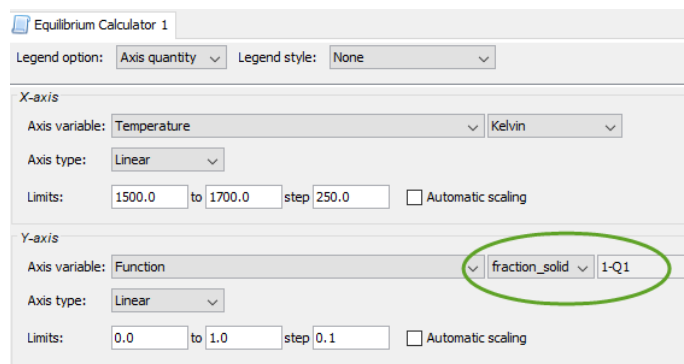
- Folder: Thermo-Calc
- File name: *T\_07\_User\_defined\_functions.tcu*



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### Plot Result

*This plot example shows the result of the fraction solid function.*



Equilibrium Calculator 1

Legend option: Axis quantity Legend style: None

**X-axis**

Axis variable: Temperature Kelvin

Axis type: Linear

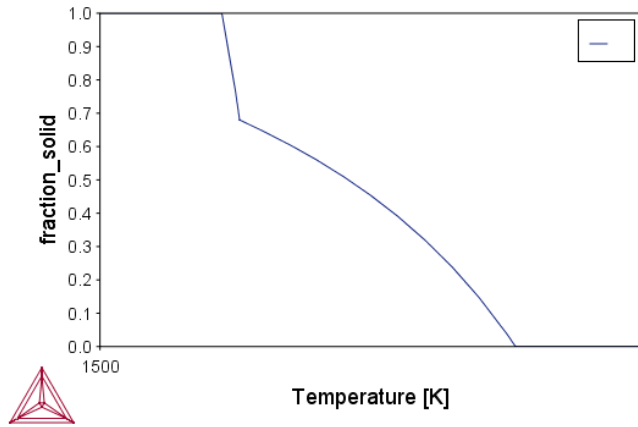
Limits: 1500.0 to 1700.0 step 250.0 ☐ Automatic scaling

**Y-axis**

Axis variable: Function **fraction\_solid** 1-Q1

Axis type: Linear

Limits: 0.0 to 1.0 step 0.1 ☐ Automatic scaling



## 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

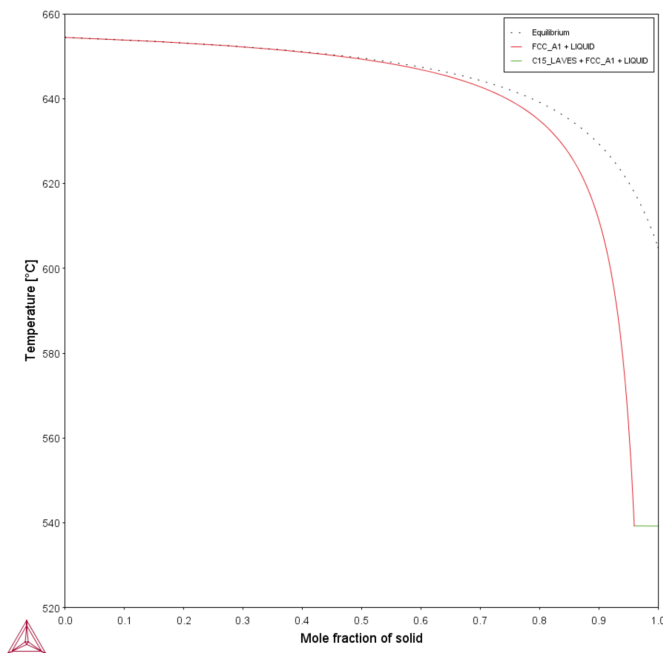
- Folder: Thermo-Calc
- File name: *T\_08\_Scheil\_and\_equilibrium\_solidification.tcu*.

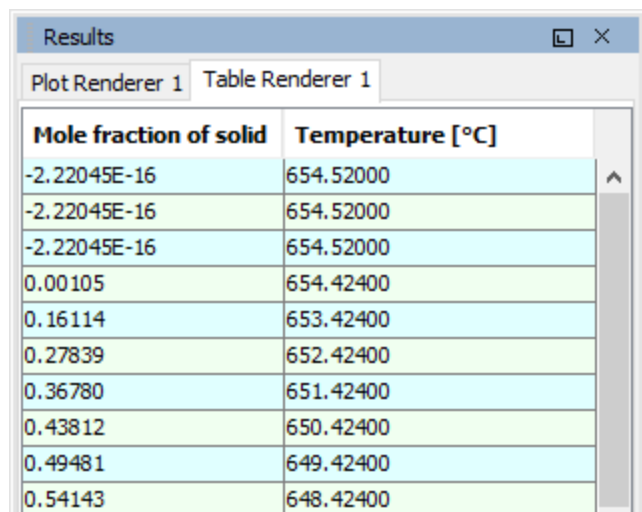


For video tutorial examples using Scheil, see our [website](#) and [YouTube channel](#).

### Table and Plot Results

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





The screenshot shows a window titled "Results" with two tabs: "Plot Renderer 1" and "Table Renderer 1". The "Table Renderer 1" tab is active, displaying a table with two columns: "Mole fraction of solid" and "Temperature [°C]". The table contains 10 rows of data, with alternating light blue and light green background colors for each row.

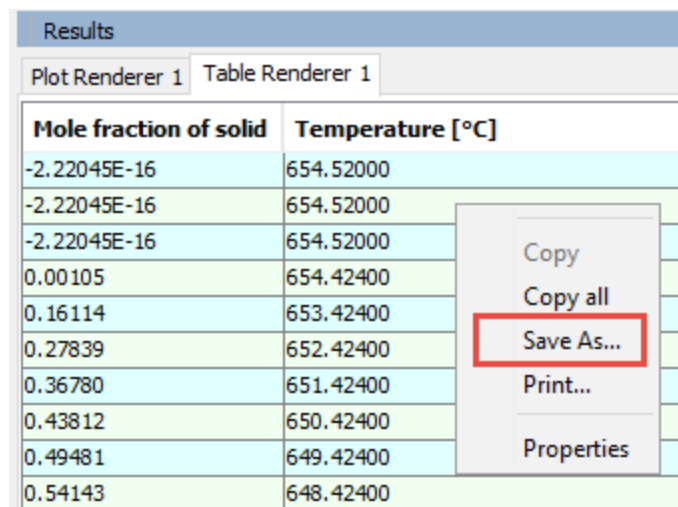
| Mole fraction of solid | Temperature [°C] |
|------------------------|------------------|
| -2.22045E-16           | 654.52000        |
| -2.22045E-16           | 654.52000        |
| -2.22045E-16           | 654.52000        |
| 0.00105                | 654.42400        |
| 0.16114               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

## To Save the Table

There are two ways to save the table.

### Method 1

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



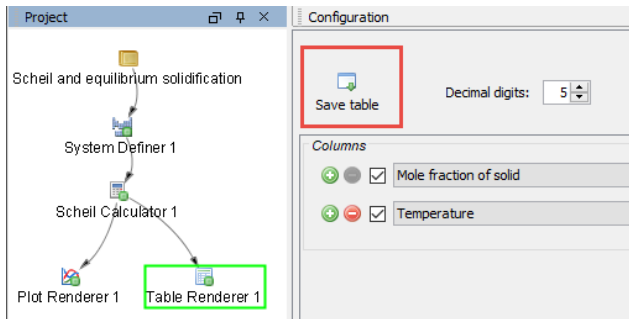
The screenshot shows the same "Results" window as before, but with a right-click context menu open over the table. The menu options are: "Copy", "Copy all", "Save As..." (highlighted with a red rectangle), "Print...", and "Properties".

| 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.

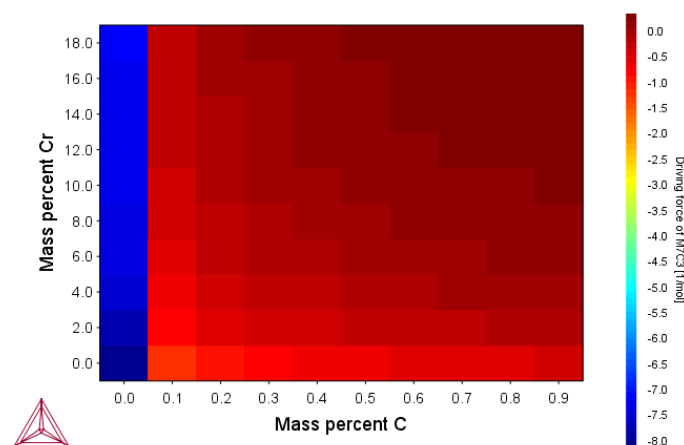
### Project File and Video Tutorial Information

- 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](#).

### Plot Result



## T\_10: Scheil Solidification with Back Diffusion

---

▶ See [Scheil Calculator](#) for an overview of the different Scheil simulation models available.



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

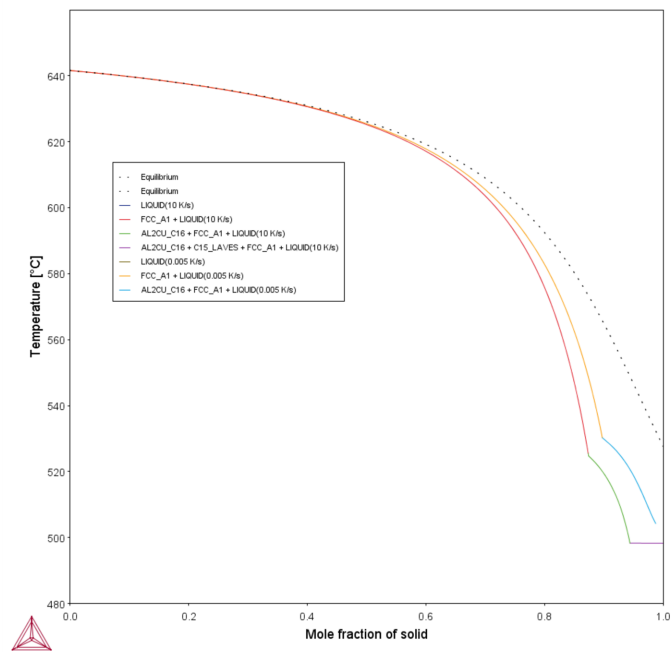
- Folder: Thermo-Calc
- File name: *T\_10\_Scheil\_with\_back\_diffusion.tcu*.



For video tutorial examples using Scheil, see our [website](#) and [YouTube channel](#).

### Plot Result

Scheil Solidification Plot



## 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 AI-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).

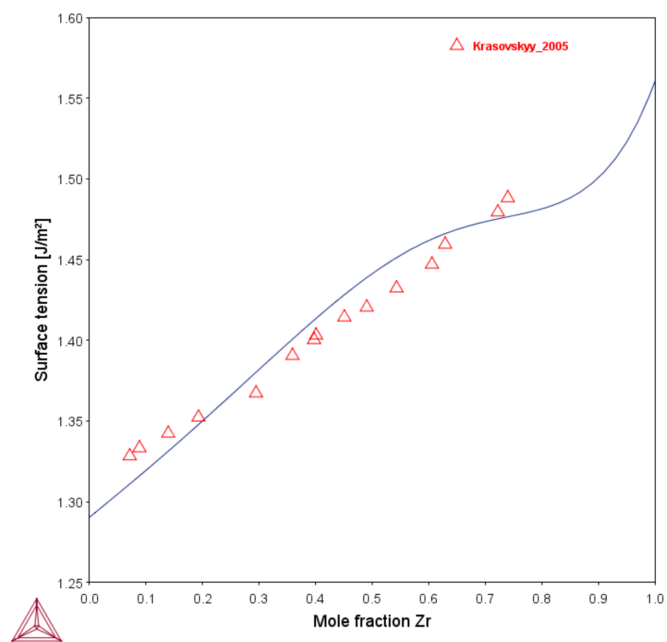


The same example is also provided in Console Mode as `tcex56`.

### Project File Information

- Folder: Thermo-Calc
- File name: *T\_11\_Surface\_tension\_in\_Cu-Zr.tcu*.

## Plot Result



## 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).

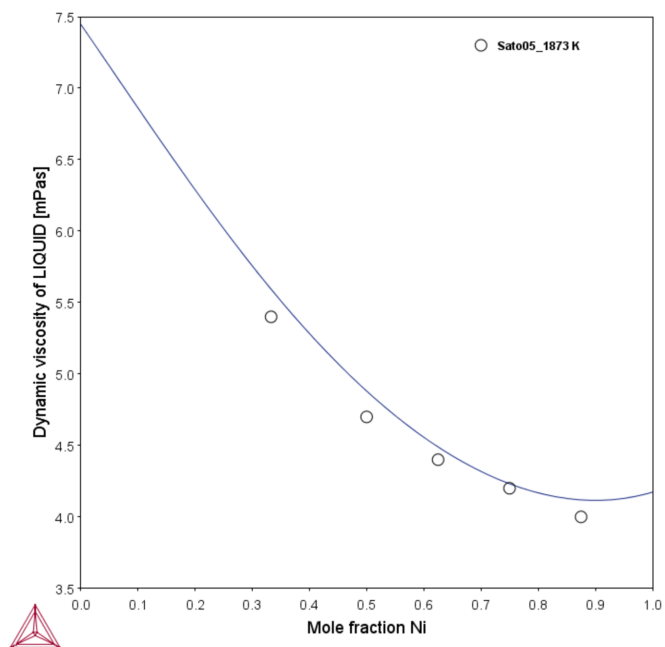


The same example is also provided in Console Mode as `tcex55`.

### Project File Information

- Folder: Thermo-Calc
- File name: *T\_12\_Viscosity\_in\_Cr-Ni.tcu*.

### Plot Result





# Thermo-Calc Property Model Examples Collection



The **General models** are available to all users. To run calculations with the **Steel models** (Martensite and Pearlite) requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases.

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

## In this section:

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## PM\_G\_01: Phase Transition

---

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

▶ [Phase Transition Model](#) in the *Thermo-Calc User Guide*.

### Project File and Video Tutorial Information

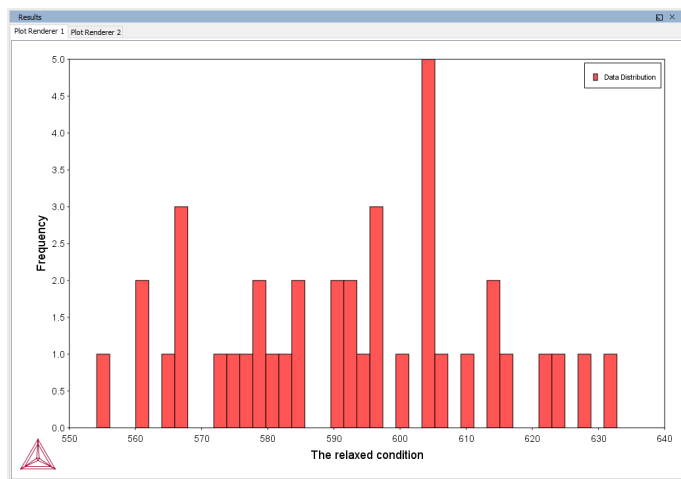
- Folder: Property models>General
- File name: *PM\_G\_01\_Phase\_Transition.tcu*



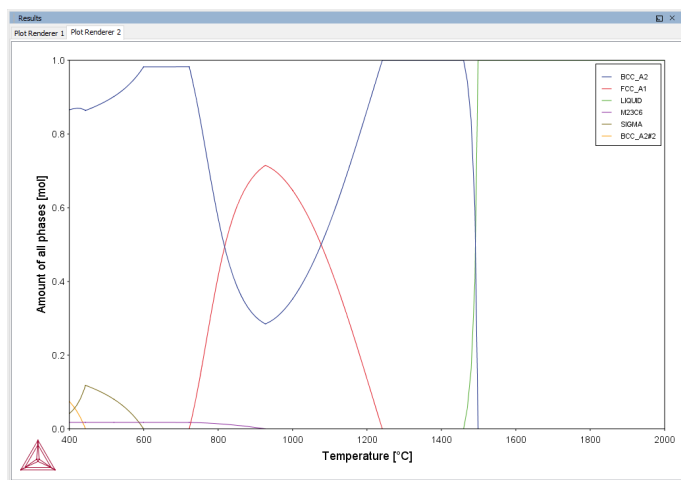
This example is included as a tutorial on our [website](#) and our [YouTube](#) channel.

## Plot Results

### Histogram plot



### Probability plot



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



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

## PM\_G\_02: Coarsening and Interfacial Energy

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

► [Coarsening Model](#) and [Interfacial Energy Model](#)

### Project File and Video Tutorial Information

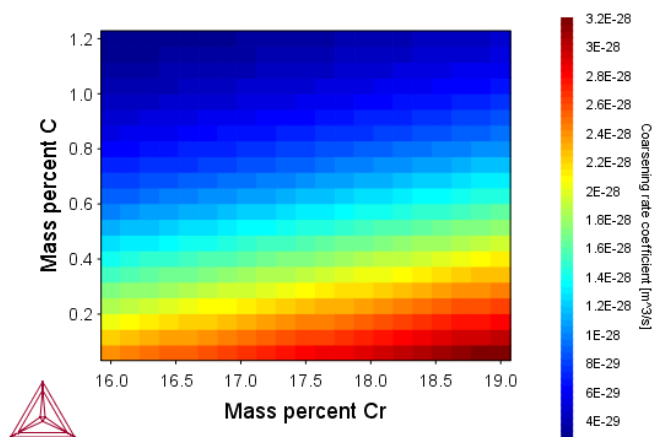
- Folder: Property models>General
- File name: *PM\_G\_02\_Coarsening\_and\_Interfacial\_energy.tcu*



This example is included as a tutorial on our [website](#) and our [YouTube](#) channel.

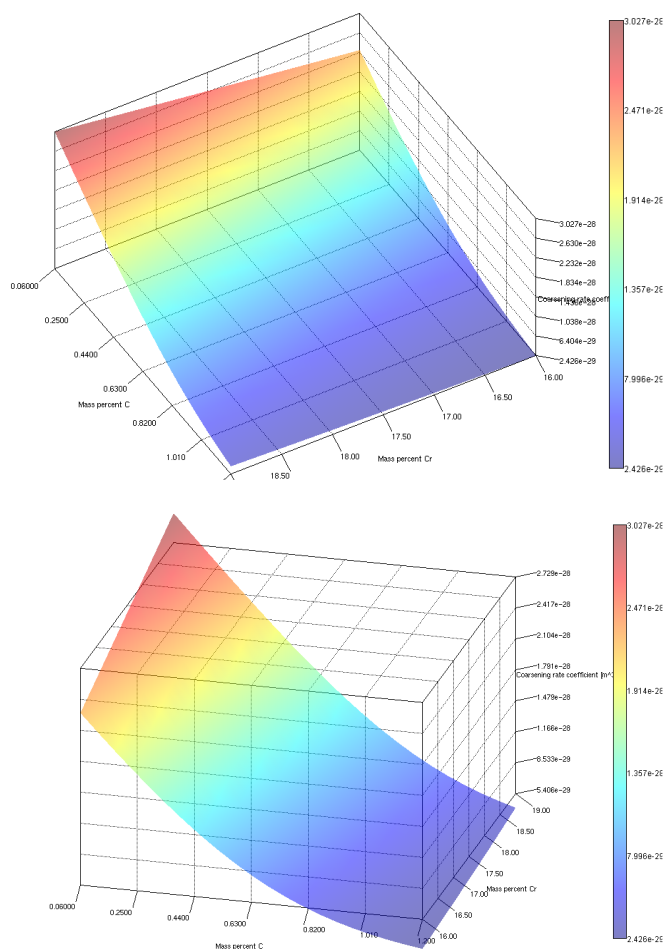
### Plot Results

#### Coarsening rate coefficient (heat map)



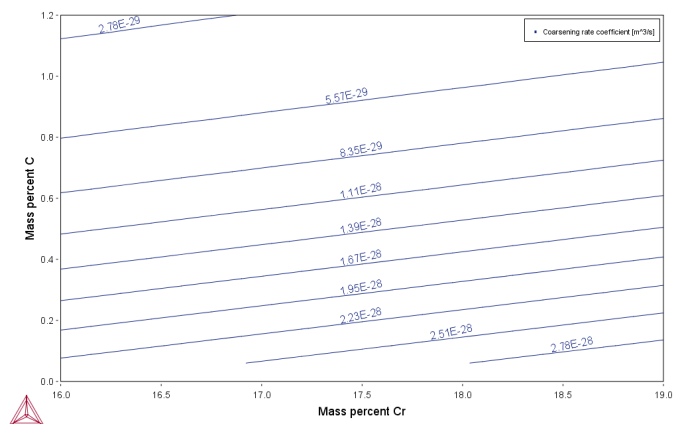
#### Coarsening rate coefficient (3D plot)

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

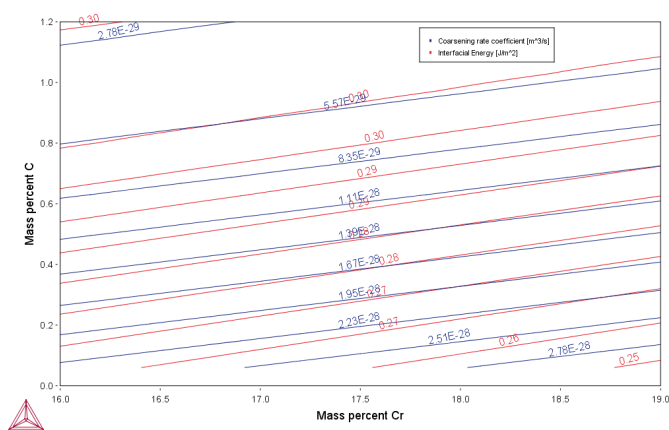


## Coarsening rate coefficient (contour plot)

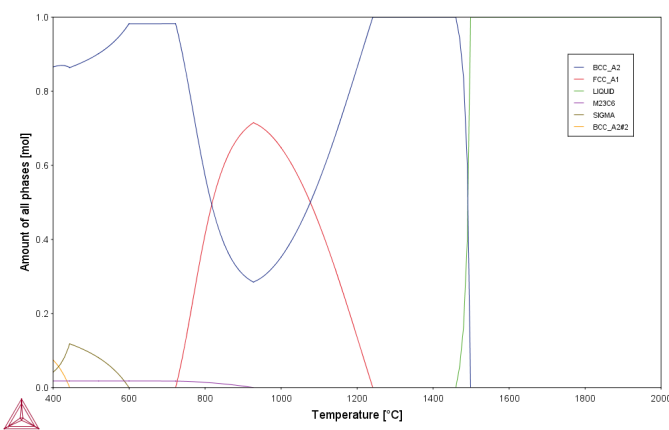
Coarsening rate coefficient



### Coarsening rate coefficient and Interfacial energy (overlaid plots)



### Phase fractions vs T (One axis)



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



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

## PM\_G\_03: Driving Force and Interfacial Energy

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

► [Driving Force Model](#) and [Interfacial Energy Model](#) in the *Thermo-Calc User Guide*.

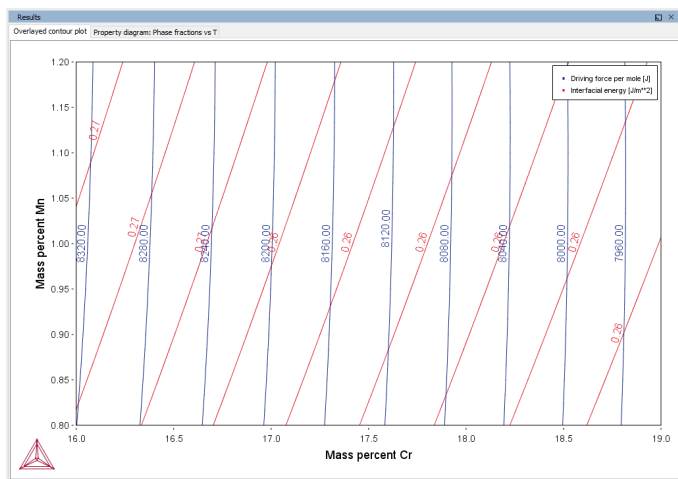
### Project File and Video Tutorial Information

- Folder: Property models>General
- File name: *PM\_G\_03\_Driving\_force\_and\_Interfacial\_energy.tcu*

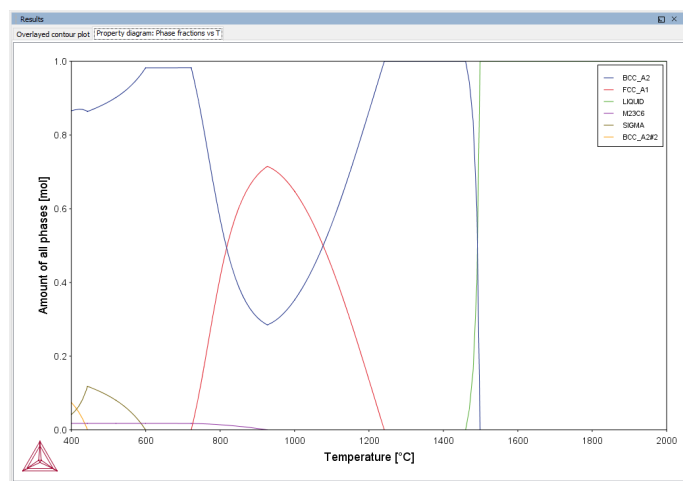


This example is included as a tutorial on our [website](#) and our [YouTube](#) channel.

### Plot Result



### A contour plot



### Phase Fraction



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



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



## PM\_G\_04\_Yield\_Strength

► [Yield Strength Model](#) and [About the Yield Strength Model](#) in the *Thermo-Calc User Guide*.

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.

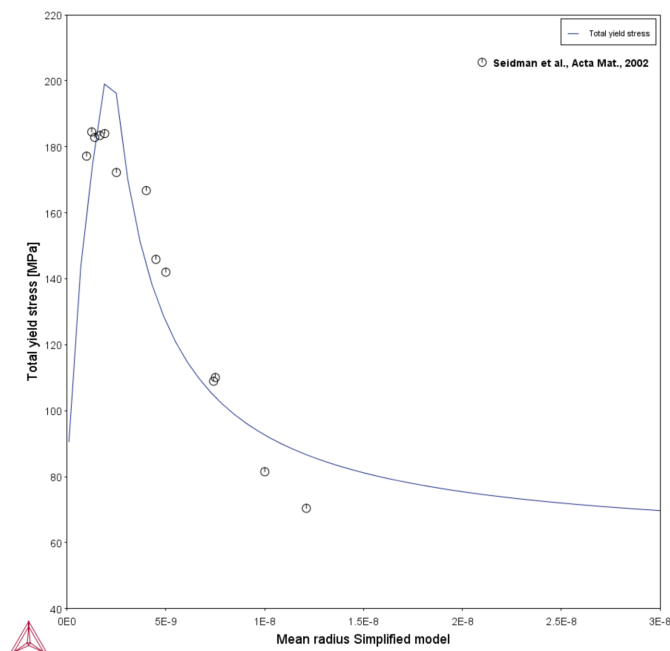
### Project File and Video Tutorial Information

- Folder: Property models>General
- File name: *PM\_G\_04\_Yield\_Strength.tcu*

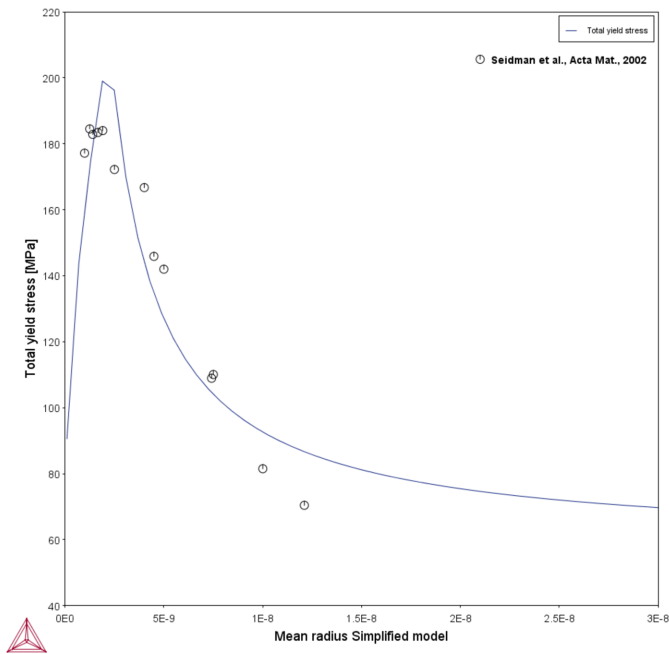


Also see our [website](#) and [YouTube channel](#) for tutorial videos related to the Property Model Calculator.

### Plot Result



### Strength vs Radius - Simplified



### Strength vs Radius - Seidman



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



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

## PM\_G\_05\_Yield\_Strength\_NiAlCr

► [Yield Strength Model](#) and [About the Yield Strength Model](#) in the *Thermo-Calc Graphical Mode User Guide*.

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.

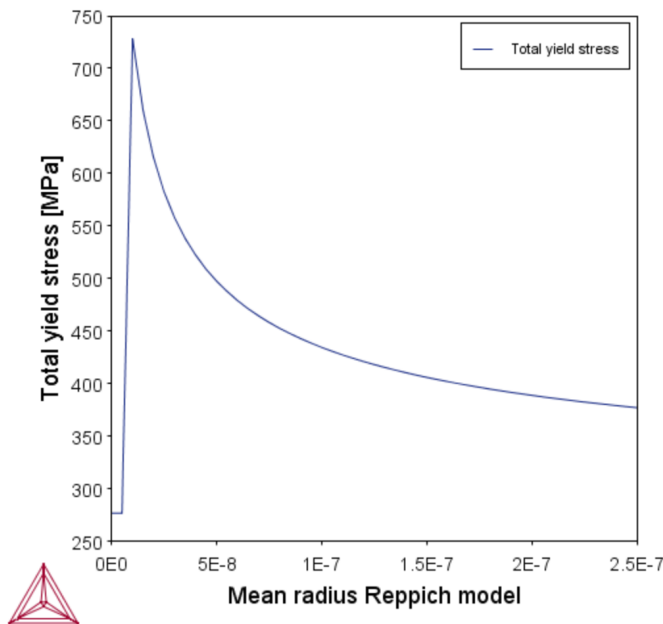
### Project File and Video Tutorial Information

- Folder: Property models>General
- File name: *PM\_G\_05\_Yield\_Strength\_NiAlCr.tcu*



Also see our [website](#) and [YouTube channel](#) for tutorial videos related to the Property Model Calculator.

### Plot Result



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



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



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

## PM\_G\_06\_Yield\_Strength\_HEA

---

▶ [Yield Strength Model](#) and [Yield Strength Model Theory](#) in the *Thermo-Calc Graphical Mode User Guide*.



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.

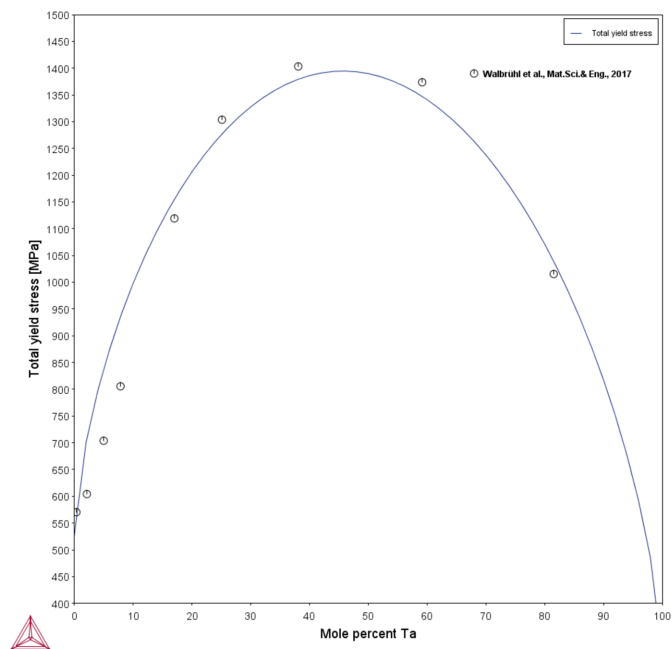
### Project File and Video Tutorial Information

- Folder: Property models>General
- File name: *PM\_G\_06\_Yield\_Strength\_HEA.tcu*



Also see our [website](#) and [YouTube channel](#) for tutorial videos related to the Property Model Calculator.

### Plot Result



### Strength vs at% Ta



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



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

## PM\_Fe\_01: Fe-Cr-C Martensite with Intercritical Annealing



To run calculations with the **Steel models** (Martensite and Pearlite) requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases.

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

The example shows how to calculate martensite fractions and martensite temperatures (martensite start,  $M_s$ , and 90% transformation temperature  $M_{90}$ ). 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  $M_s$  and  $M_{90}$  after intercritical annealing.

### Reference

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

### Project File and Video Tutorial Information

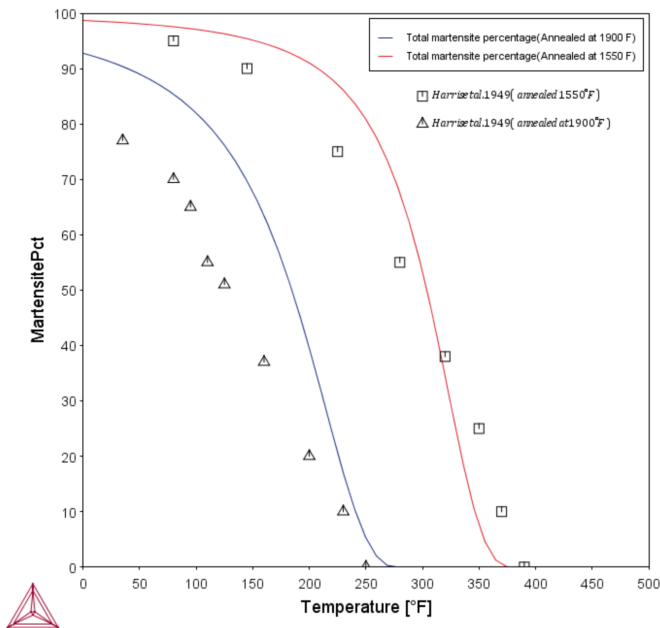
- Folder: Property models >Steel
- File name: *PM\_Fe\_01\_Fe-Cr-C\_martensite\_intercritical\_annealing.tcu*



Also see our [website](#) and [YouTube channel](#) for tutorial videos related to the Property Model Calculator.

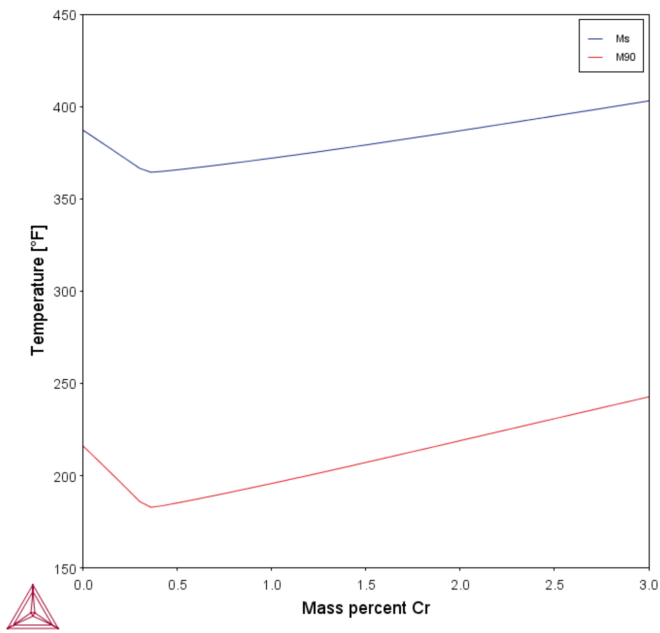
### Plot Results

*Transformation curves*



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

Ms-Mf





## PM\_Fe\_02: Fe-Mn Martensite Morphologies



To run calculations with the **Steel models** (Martensite and Pearlite) requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases.

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

### Project File and Video Tutorial Information

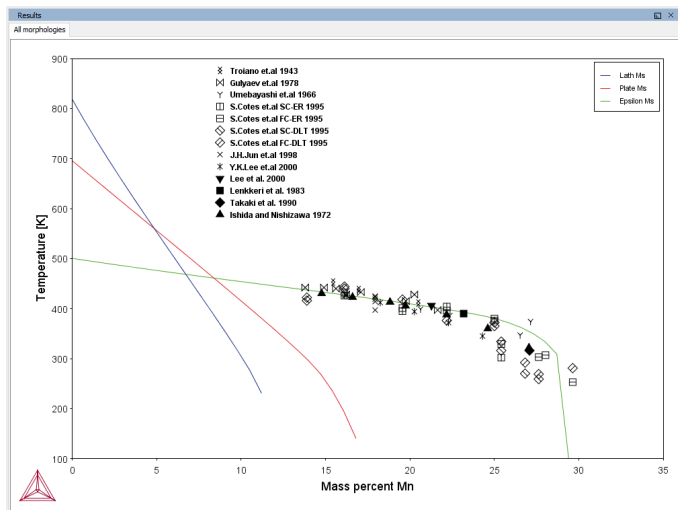
- Folder: Property Models>Steel
- File name: *PM\_Fe\_02\_Fe-Mn\_martensite\_morphologies.tcu*



Also see our [website](#) and [YouTube channel](#) for tutorial videos related to the Property Model Calculator.

### Plot Result

*All morphologies*



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

## PM\_Fe\_03: Fe-C-Mn Pearlite



To run calculations with the **Steel models** (Martensite and Pearlite) requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases.

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

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

### Reference

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

### Project File and Video Tutorial Information

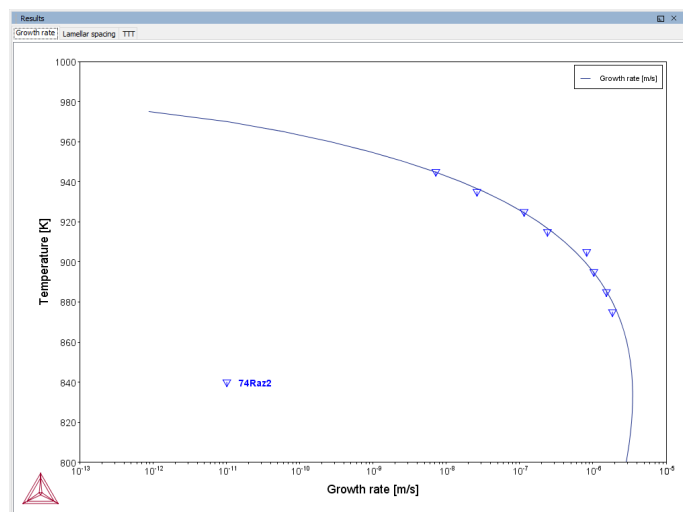
- Folder: Property Models>Steel
- File name: *PM\_Fe\_03\_Fe-C-Mn\_Pearlite.tcu*



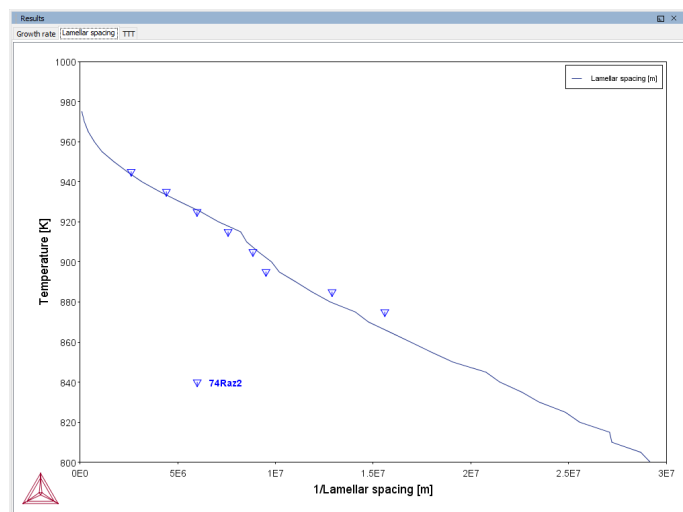
Also see our [website](#) and [YouTube channel](#) for tutorial videos related to the Property Model Calculator.

### Plot Results

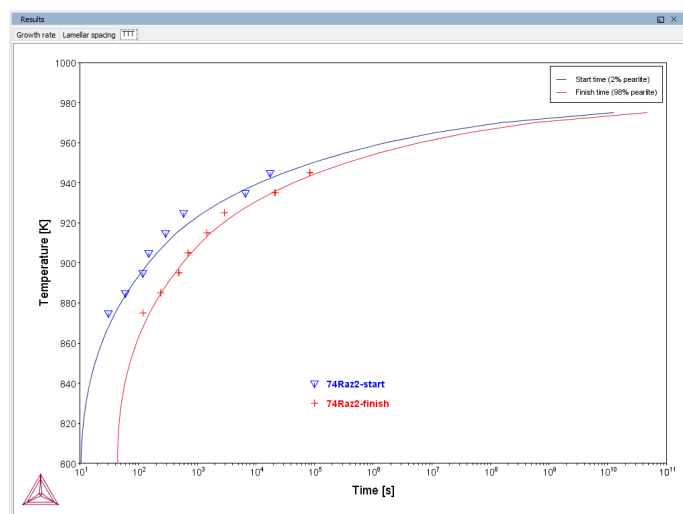
*Growth Rate*



### Lamellar Spacing



TTT



The TTT (time-temperature-transformation) diagram showing times of start (2% transformation) and finish (99% transformation) as functions of isothermal heat treating temperature in an Fe-0.69C-1.80Mn alloy (mass %).

# 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:

|  |    |
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## PMET\_01: Basic Oxygen Furnace (BOF)



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

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



The real-world BOF process is highly exothermic and needs adiabatic calculations.

### 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.



Open the example project file from Thermo-Calc **Help** → **Example Files** → **Process Metallurgy** → **PMET\_01\_Basic\_Oxygen\_Furnace.tcu**.



This example is included as a tutorial on our [website](#) and our [YouTube](#) channel.

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

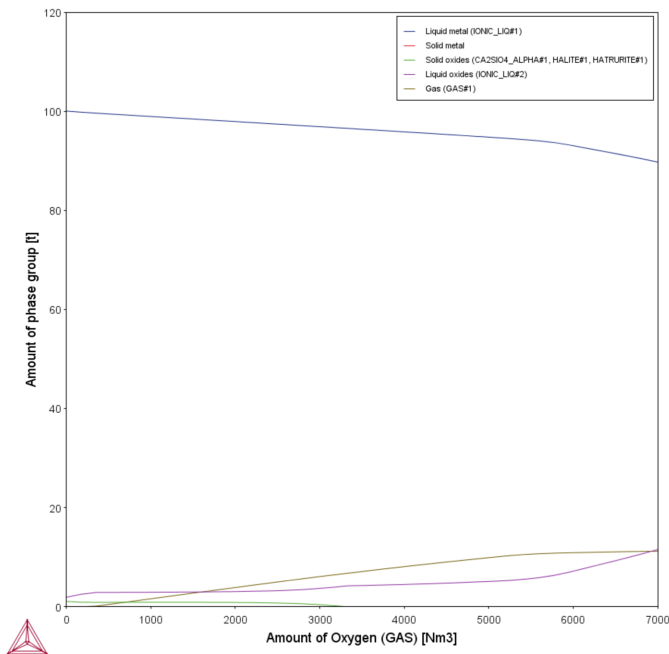


See [Phase Groups](#) for details about how the Process Metallurgy Module plot labels are grouped into the *liquid metal*, *solid metal*, *solid oxides*, *liquid oxides* and *gas* phases.

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

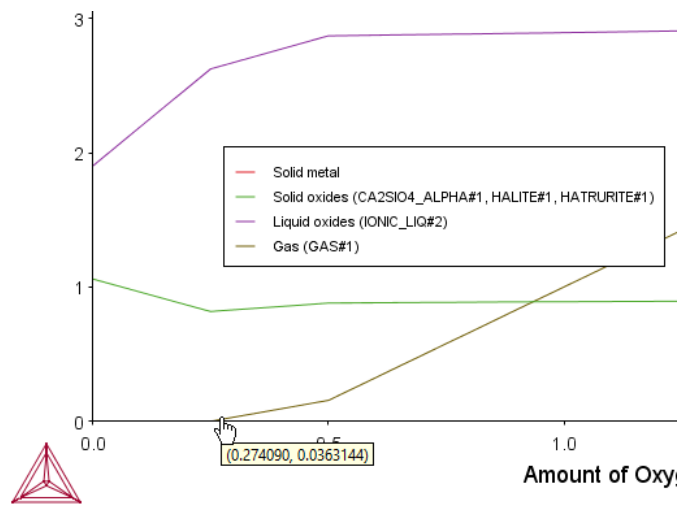
- Quantity: Amount of Oxygen (GAS)
- Stepping 0 min to 10 max with 40 steps

## Amount of Phase Groups



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

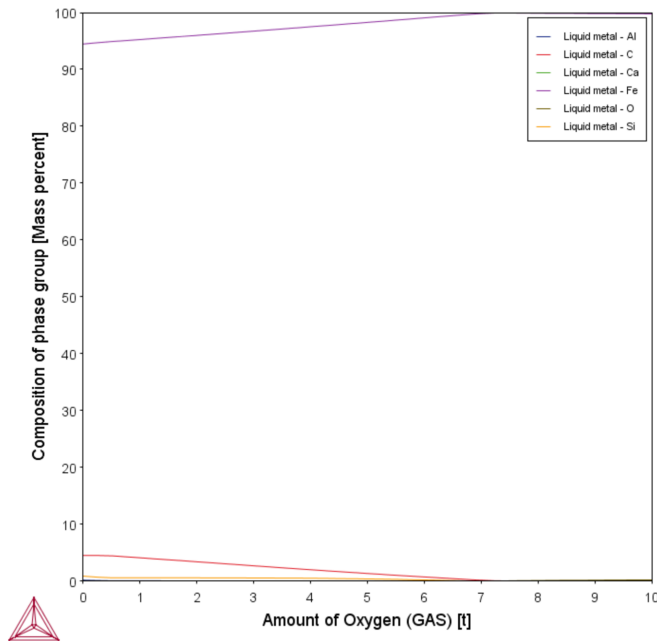
Zooming into the low gas amount (see below), it can be seen that the evolution of the gas phase is retarded. The reason is that the oxygen gas first oxidizes some of the silicon dissolved in the steel to form silicon dioxide ( $\text{SiO}_2$ ). Only when the silicon content in the steel has dropped below 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**.



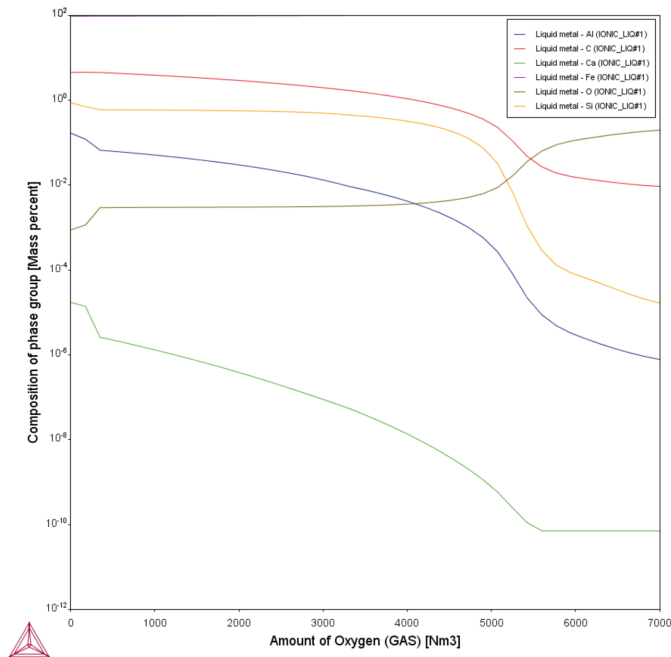
In the plot (that uses a linear axis) the reduction of the carbon content can be clearly seen. This reduction of the carbon content is what is termed “steelmaking”. The hot metal coming from the blast furnace has a very high carbon content of typically 4.5 wt%. If it is left to solidify without lowering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

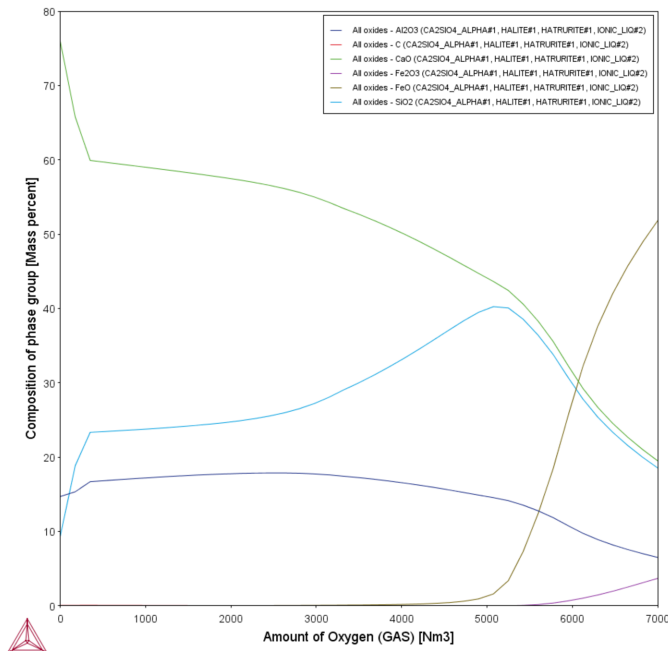




Now you can see the removal of the elements from the liquid steel in the following order: first calcium, then aluminium, then silicon and finally carbon (Ca, Al, Si and C) according to their position on the Ellingham diagram.

### 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**.



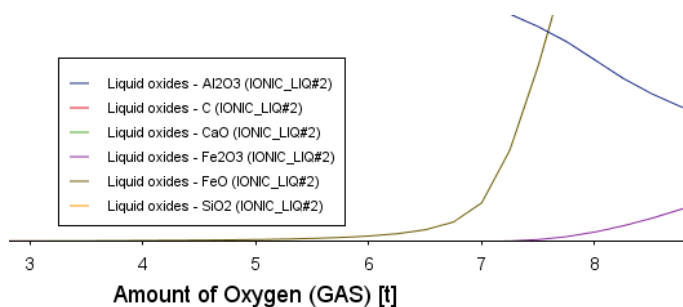
This plot shows how the liquid slag composition changes as a function of the amount of oxygen added to the BOF.

At first, the  $\text{SiO}_2$  content of the slag rises sharply. This is due to the initial oxidation of the silicon dissolve in the hot metal. The  $\text{SiO}_2$  that is formed combines with the slag and increases its  $\text{SiO}_2$  content.

This increased  $\text{SiO}_2$  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 ( $\text{SiO}_2$ ) 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 ( $\text{FeO}$ ). 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)

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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.

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



You can open the example project file from Thermo-Calc **Help** → **Example Files** → **Process Metallurgy** → **PMET\_02\_Ladle\_Furnace.tcu**.



This example is included as a tutorial on our [website](#) and our [YouTube](#) channel.

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



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

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

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

Material: Slag Slag\_LF

Amount: Kilogram 2500.0 Hide composition

Input type: Absolute amount Component Normalize to total of 100%

| Component                      | Amount        | Weight %     |
|--------------------------------|---------------|--------------|
| CaO                            | 2000.0        | 80.0         |
| Al <sub>2</sub> O <sub>3</sub> | 250.0         | 10.0         |
| SiO <sub>2</sub>               | 250.0         | 10.0         |
| <b>Total:</b>                  | <b>2500.0</b> | <b>100.0</b> |



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:

Grid Definitions

| Quantity   | Min | Max    | Number of steps |
|--|-----|--------|-----------------|
| Amount of Al <sub>2</sub> O <sub>3</sub> in Slag_LF (SLAG) | 0.0 | 1000.0 | 10              |
| Amount of SiO <sub>2</sub> in Slag_LF (SLAG)               | 0.0 | 1000.0 | 10              |



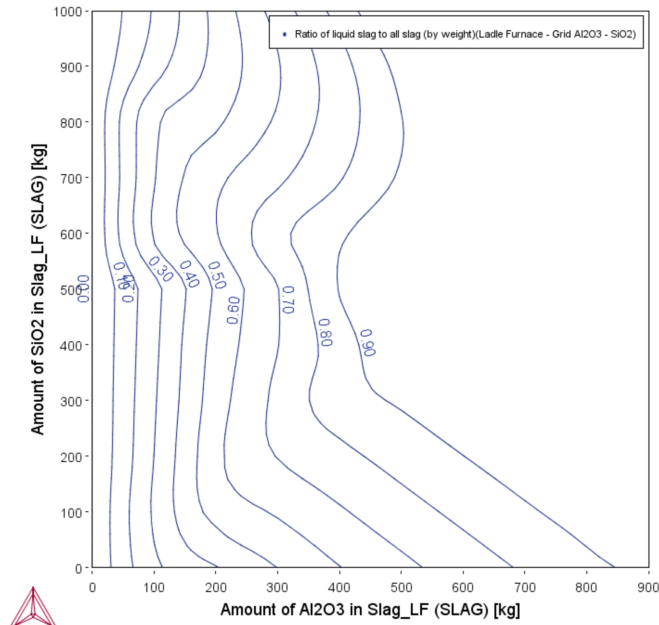
Leave the number of calculation steps at 10 for both axes in order to shorten the calculation time. With this setting, the calculation should be completed in just under one minute. The number of steps could be increased to maybe 30 x 30 for higher resolution of the results, but this increases the calculation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



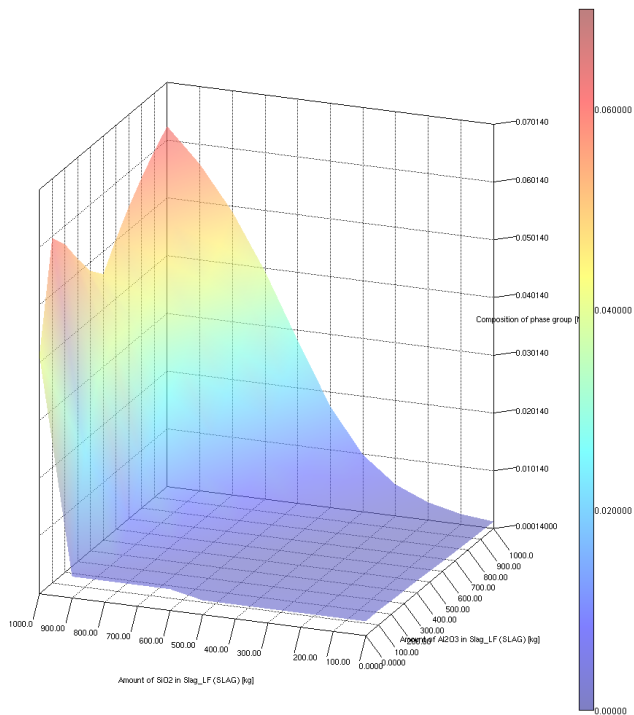
The plot shows that for low amounts of aluminium oxide (Al<sub>2</sub>O<sub>3</sub>) and silicon dioxide (SiO<sub>2</sub>), almost no liquid slag is present. Process metallurgists refer to this as a *hard slag*.

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  $\text{SiO}_2$  and  $\text{Al}_2\text{O}_3$  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  $\text{SiO}_2$  and  $\text{Al}_2\text{O}_3$  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.

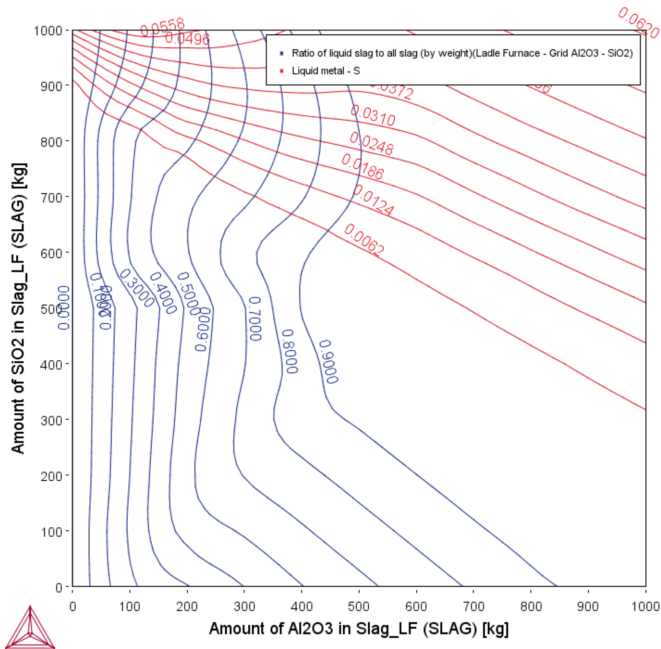
Z-axis

Axis variable: Composition of phase group   Liquid metal   S

Axis type: Linear

Limits: 0.0 to 1.0 step 0.1 ☒ Automatic scaling

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



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

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

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

**Z-axis**

Axis variable: Fraction of liquid slag

Axis type: Linear

Limits: 0.0 to 1.0 step 0.1 ☒ Automatic scaling

Contour values: 0.95 ☒ Use custom contour values

**X-axis**

Axis variable: Amount of Al<sub>2</sub>O<sub>3</sub> in Slag\_LF (SLAG) Kilogram

Limits: 0.0 to 1000 step 100 ☒ Automatic scaling

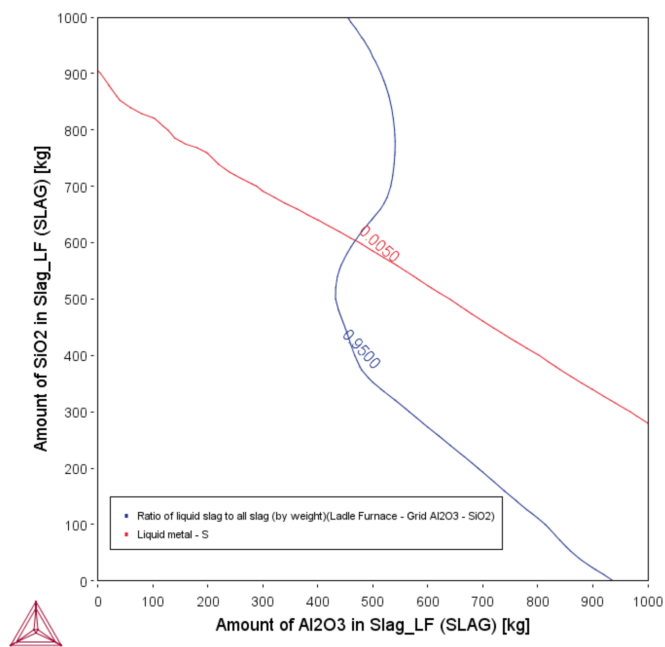
**Z-axis**

Axis variable: Composition of phase group Liquid metal S Mass percent

Axis type: Linear

Limits: 0.0 to 1.0 step 0.1 ☒ Automatic scaling

Contour values: 0.005 ☒ Use custom contour values



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)

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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.

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

### Open the Project File



You can open the example project file from Thermo-Calc **Help** → **Example Files** → **Process Metallurgy** → **PMET\_03\_Argon\_Oxygen\_Decarburization.tcu**.

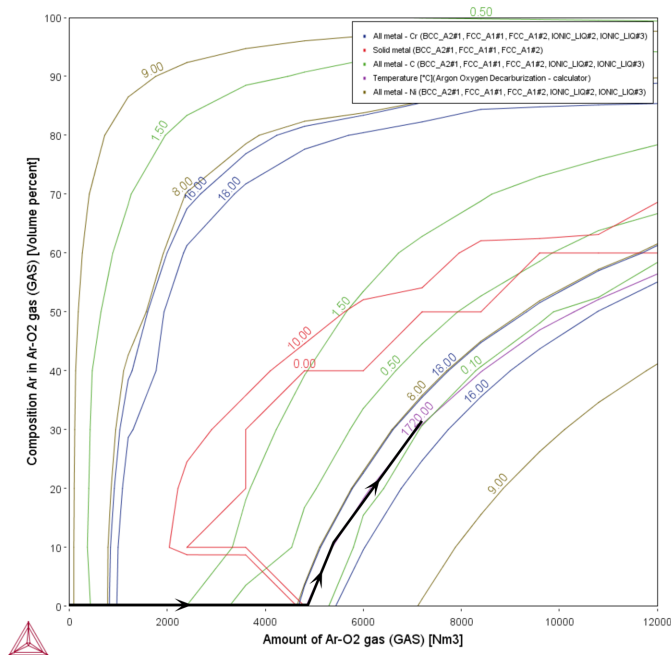


A variety of video tutorials are available for many of our products and features on our [website](#) and our [YouTube](#) channel. The library keeps growing so be sure to check back on a regular basis.



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.

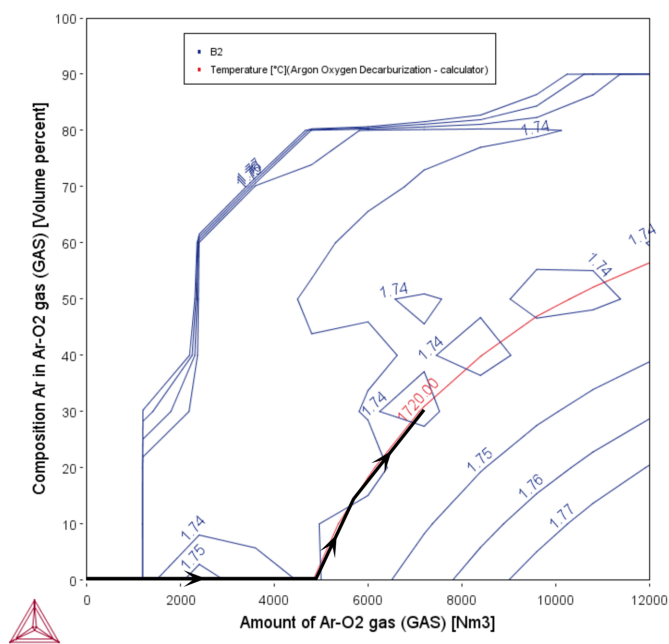


The AOD-process is characterized by an initially high O<sub>2</sub>-content of the blowing gas, which is gradually replaced by Ar. The maximum temperature of the process is typically around 1720 °C. A grid plot of an adiabatic calculation is well suited to model the required simultaneous change of amount 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.

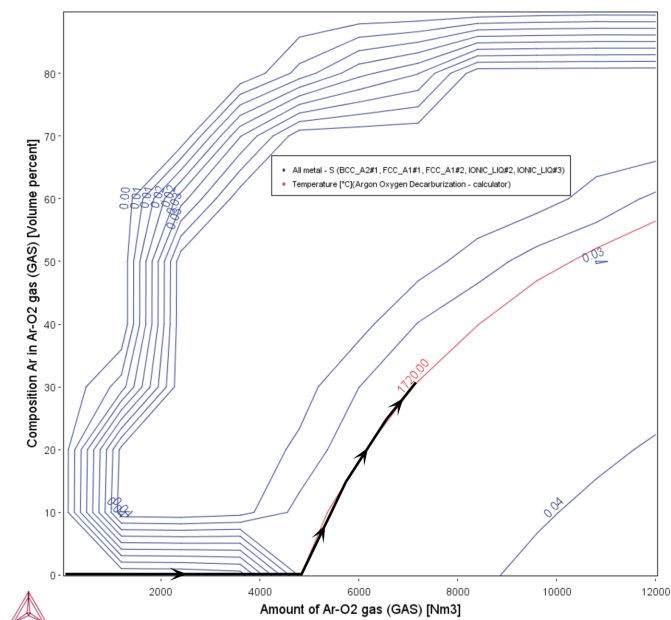
## Results

### Slag Basicity



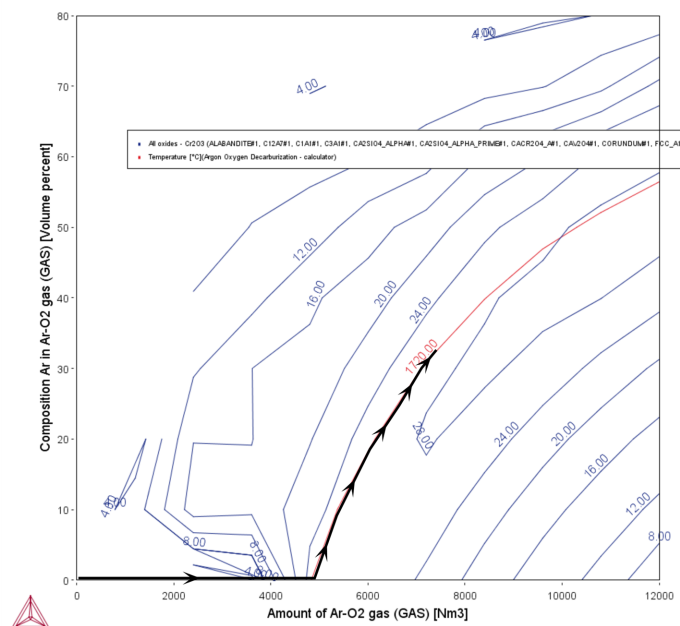
The Slag Basicity plot shows the basicity of the slag (which is a measure for the sulphur capacity of the slag). The process achieves a final basicity of 1.74 which is typical for an AOD-process. The black line in the plot indicates a possible process control path that finally leads to suitable alloy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

### S Content in Steel



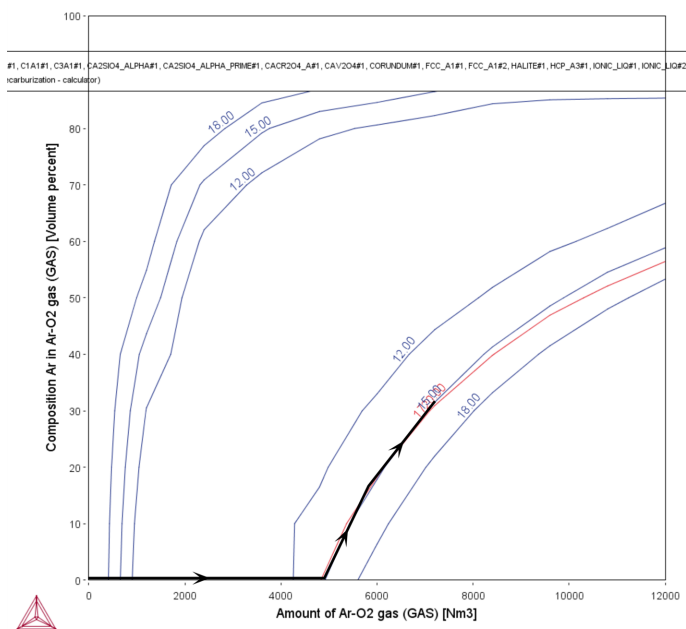
In the S Content in Steel plot, the sulphur content in the steel melt is slightly reduced during the process from 0.056% in the initial steel scrap to finally ca. 0.035%. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi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

### Cr Content in Slag



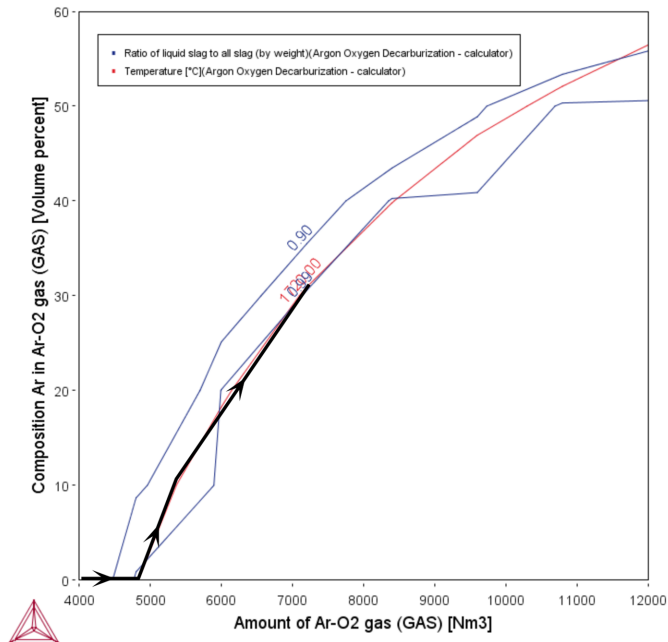
In the Cr Content in Slag plot, the Cr<sub>2</sub>O<sub>3</sub>-content in the slag reaches at the end of the process ca. 26 wt-%. This is typical for the AOD-process and requires an additional Cr-recovery step after the conversion to reduce the loss of chromium. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

### Amount of Slag



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



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



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

### Open the Project File



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.

### Visit our Website for More Information



Due to the complexity of these simulations, it is recommended that you visit our website for access to more detailed instructions related to this and the other Process Metallurgy Module examples since the details are not included in the technical help documentation.



You can find several other learning resources on the [Process Metallurgy](#) page of our website (or in Thermo-Calc, go to **Help** → **Thermo-Calc website**). You can also [subscribe to the Thermo-Calc newsletter](#) to be kept up-to-date about upcoming releases, training, examples, videos and much more.

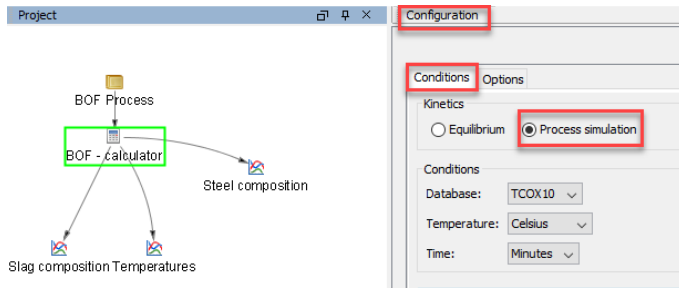
### Setting Up the BOF Process Simulation

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.

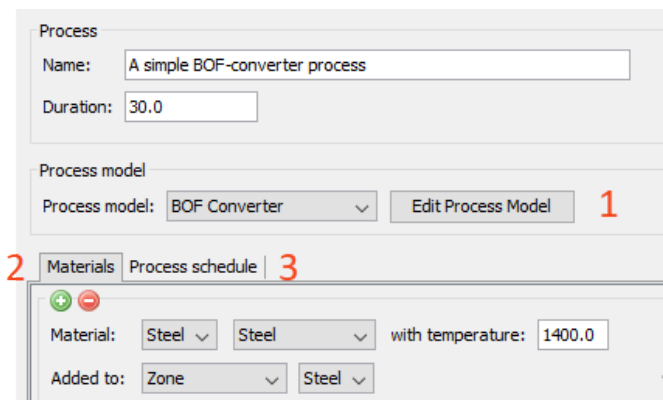
What follows is a general overview of the three basic steps required to set up a kinetic simulation.



- ▶ [Setting Up a Process Metallurgy Simulation](#)
- ▶ [Defining the Process Simulation](#)



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.



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.

**Edit Process Model**

Pressure:

**Zones:**

Name:  density:  kg/m<sup>3</sup>  
  Name:  density:  kg/m<sup>3</sup>

**Reactions:**

Reaction zone:  m<sup>2</sup> Zone 1:  mass transfer coefficient:  m/s  
 Zone 2:  mass transfer coefficient:  m/s

**Heat:**

Constant cooling:  Zone:   MW

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.

**Materials** Process schedule

Material:   with temperature:   
 Added to:

Material:   with temperature:   
 Added to:

Material:   with temperature:   
 Added to:

Material:   with temperature:   
 Added to:

**Materials** Process schedule

Material:   with temperature:   
 Added to:

Input type:

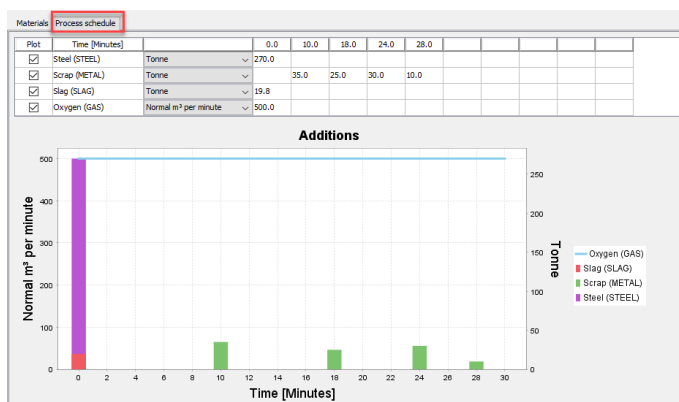
Major component:

|                                  |                                  |        |                                    |
|----------------------------------|----------------------------------|--------|------------------------------------|
| <input type="button" value="+"/> | <input type="button" value="-"/> | Fe     | <input type="text" value="95.51"/> |
| <input type="button" value="+"/> | <input type="button" value="-"/> | C      | <input type="text" value="1.5"/>   |
| <input type="button" value="+"/> | <input type="button" value="-"/> | Mn     | <input type="text" value="0.5"/>   |
| <input type="button" value="+"/> | <input type="button" value="-"/> | Si     | <input type="text" value="0.4"/>   |
| <input type="button" value="+"/> | <input type="button" value="-"/> | S      | <input type="text" value="0.08"/>  |
| <input type="button" value="+"/> | <input type="button" value="-"/> | P      | <input type="text" value="0.01"/>  |
|                                  |                                  | Total: | <input type="text" value="100.0"/> |

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.



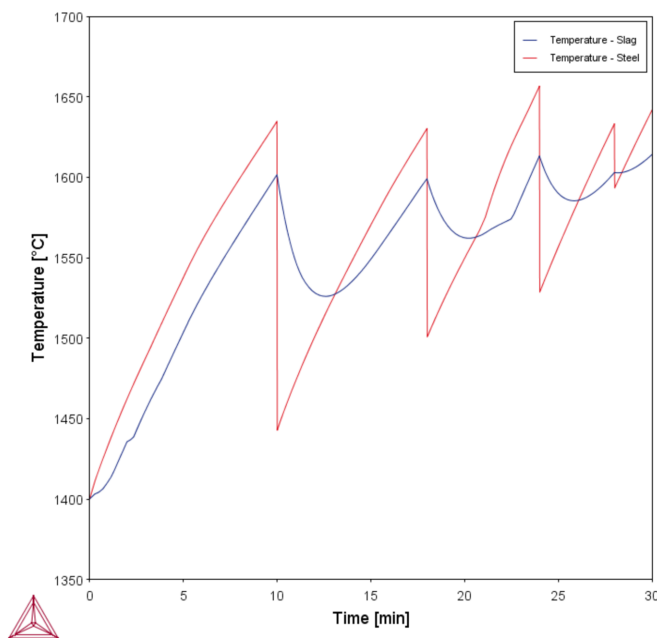
*The Process schedule tab for a Process Metallurgy Calculator where you enter your steelmaking recipe.*

## Plot Results

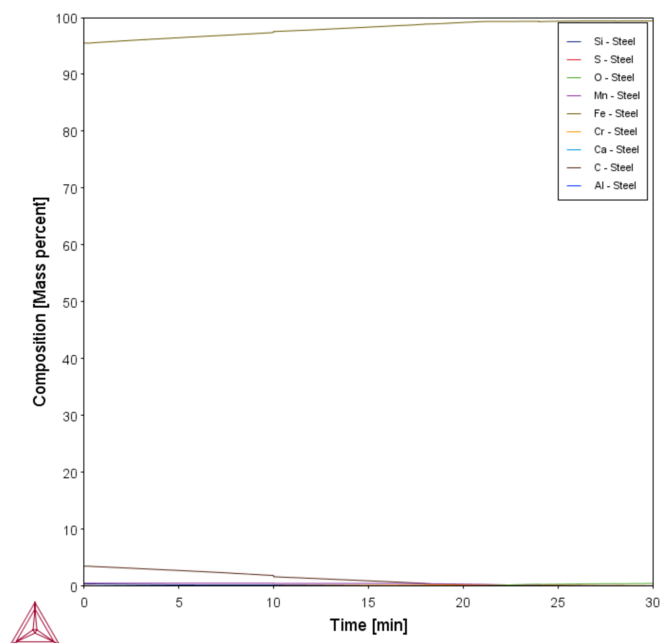
Many different aspects of the reactions taking place in the BOF can be plotted and analyzed. After you run the project file and obtain the plots, you can experiment by adjusting the settings on each Plot Renderer to see what happens in each case. There is more analysis about this and other examples available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



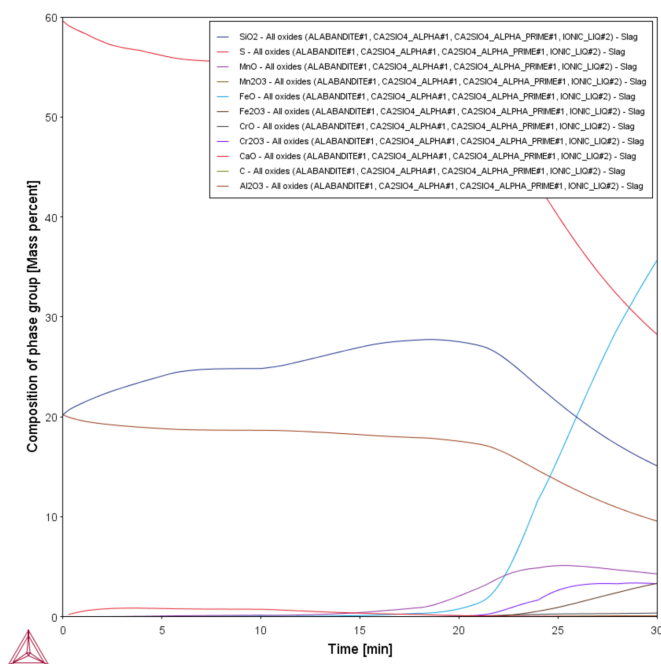
A variety of video tutorials are available for many of our products and features on our [website](#) and our [YouTube](#) channel. The library keeps growing so be sure to check back on a regular basis.



*This plot shows the temperatures of the steel and slag bulk zones.*



*This plot shows the steel composition in the bulk zone.*



*This plot shows the slag composition in the bulk zone.*

## PMET\_05: Lab Scale Ladle Furnace (LF) Kinetics



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

### Open the Project File



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.

### Visit our Website for More Information



Due to the complexity of these simulations, it is recommended that you visit our website for access to more detailed instructions related to this and the other Process Metallurgy Module examples since the details are not included in the technical help documentation.



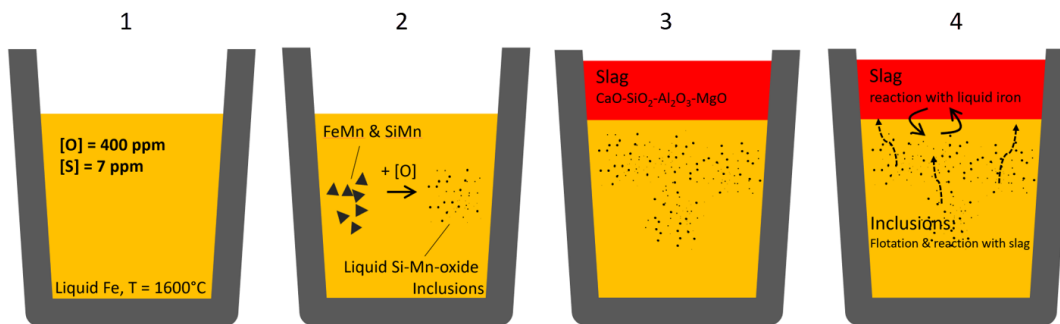
You can find several other learning resources on the [Process Metallurgy](#) page of our website (or in Thermo-Calc, go to **Help** → **Thermo-Calc website**). You can also [subscribe to the Thermo-Calc newsletter](#) to be kept up-to-date about upcoming releases, training, examples, videos and much more.

## 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](#)
- ▶ [Defining the Process Simulation](#)

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



*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

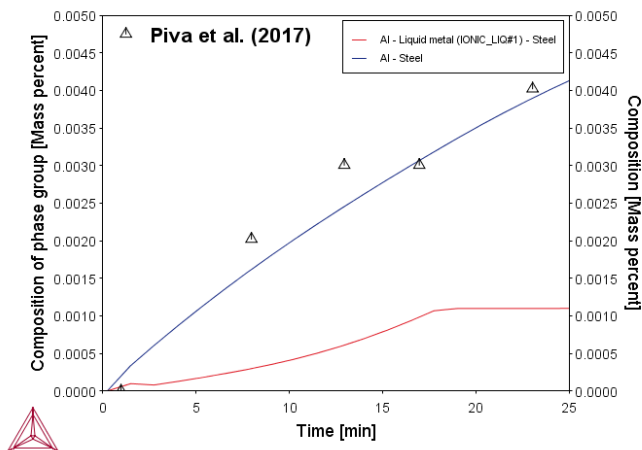
The plots below compare the Al content in the liquid steel with the experimentally determined amount. The bottom plot shows how the  $\text{Al}_2\text{O}_3$  from the slag phase is gradually reduced to metallic Al that dissolves in the liquid steel.

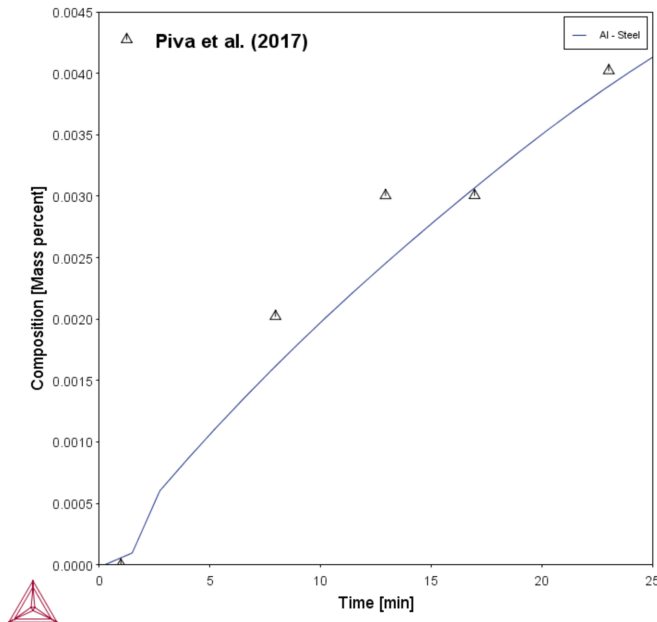


In this example, only part of the Al in the liquid steel is dissolved as metallic Al. With the Process Metallurgy Module, it is possible to plot both dissolved Al and also total Al.

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 cleanliness.

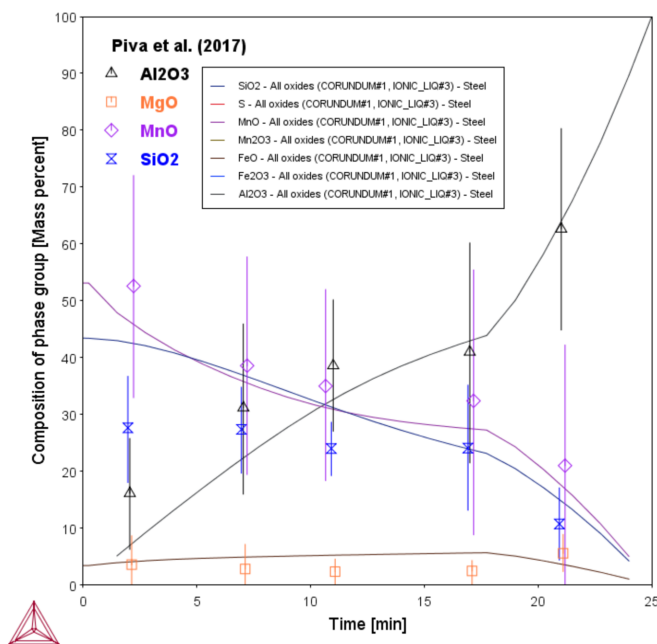
Total Al is what was measured by Piva et al. [2017] and their experimental data are compared to the calculated values below.





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.

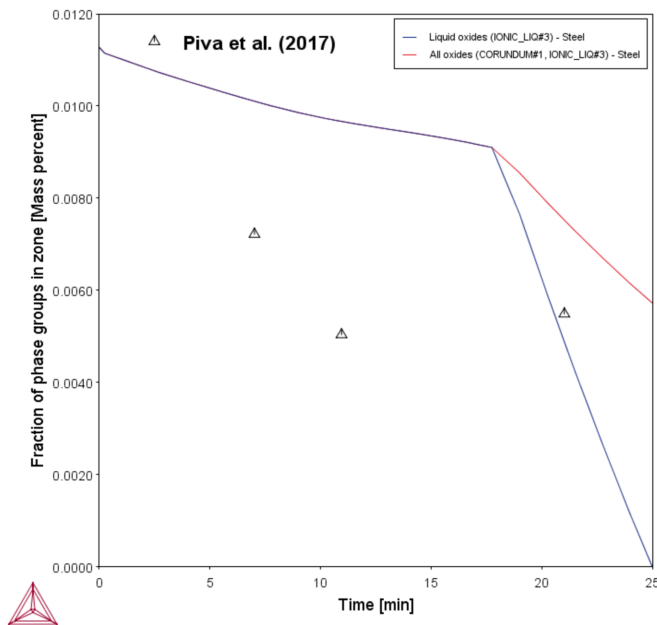
Immediately after killing the steel with SiMn and FeMn, the liquid steel contains liquid Si-Mn-oxide inclusions only. As the liquid steel picks up Al from the slag phase in function of time, the inclusions get richer and richer in Al. This experimentally verified change in inclusion chemistry is well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





*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 ( $\text{Al}_2\text{O}_3$ ) 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.



*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 ( $\text{Al}_2\text{O}_3$ ) 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



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

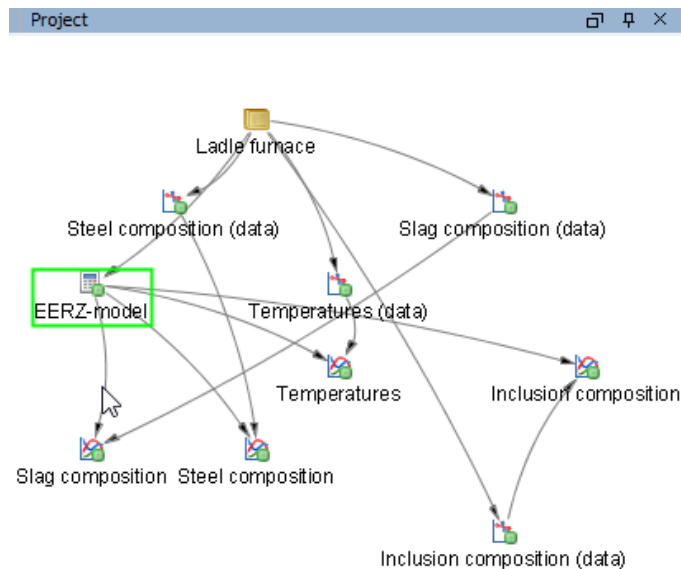
### Open the Project File



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.



Due to the complexity of these simulations, it is recommended that you visit our website for access to more detailed instructions related to this and the other Process Metallurgy Module examples since the details are not included in the technical help documentation.

## About the Plot Results

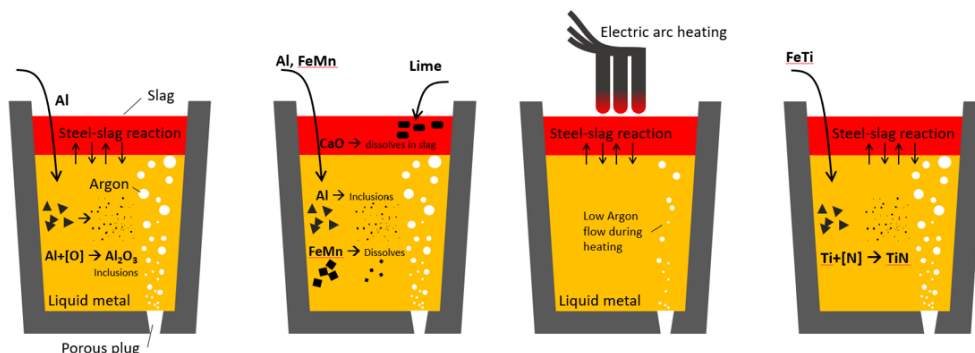
Many different aspects of the reactions taking place in the LF can be plotted and analyzed. After you run the project file and obtain the plots, you can experiment by adjusting the settings on each Plot Renderer to see what happens in each case. There is more analysis about this and other examples available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



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.

## 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

105 kg Al added to  
165 t liquid steel  
4.95 t slag  
Ar bubbling

### Time = 20 min

140 kg Al added  
50 kg FeMn added  
100 kg Lime added  
Ar bubbling

### Time = 27 min

Heating by electric arc  
Ar bubbling

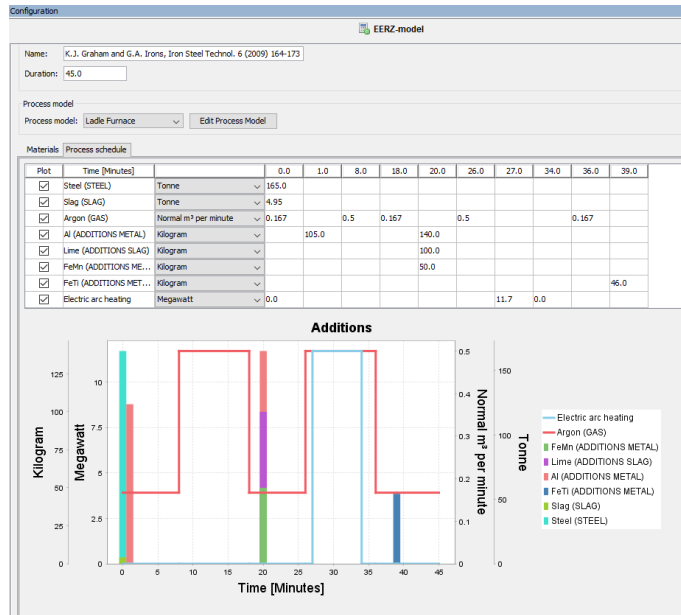
### Time = 39 min

46 kg of FeTi added  
Ar bubbling

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.

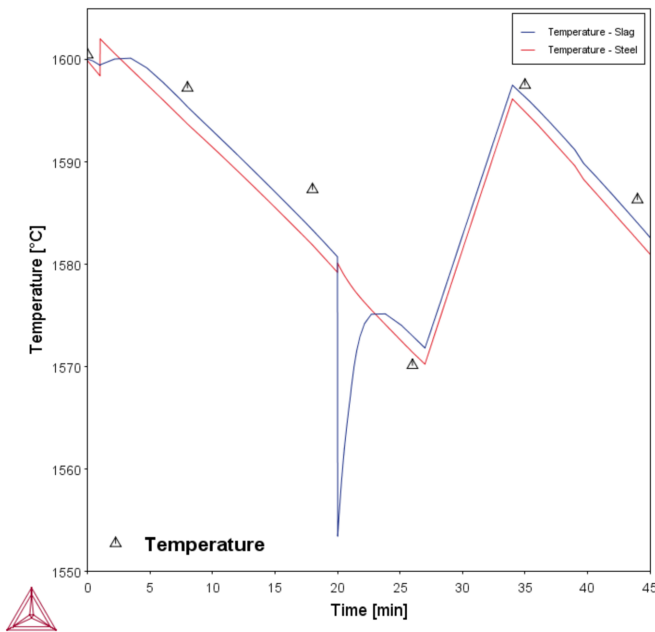
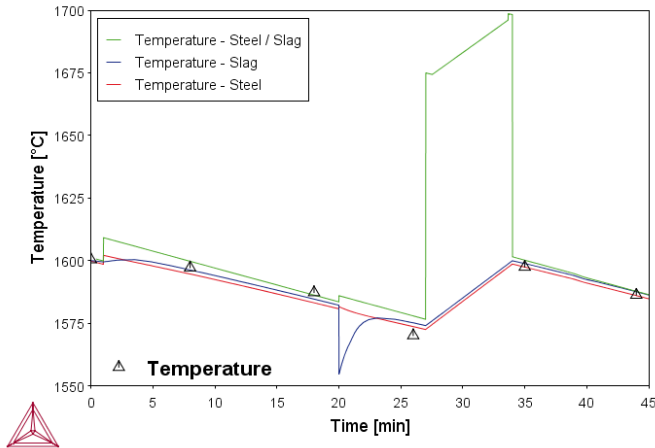


The Process schedule set up for this example. If you have the project open in Thermo-Calc, click the Process schedule tab to view this. You can then click the check boxes in the Plot column to include or exclude materials to better visualize the process schedule on this tab. This is based on the LF steel 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.

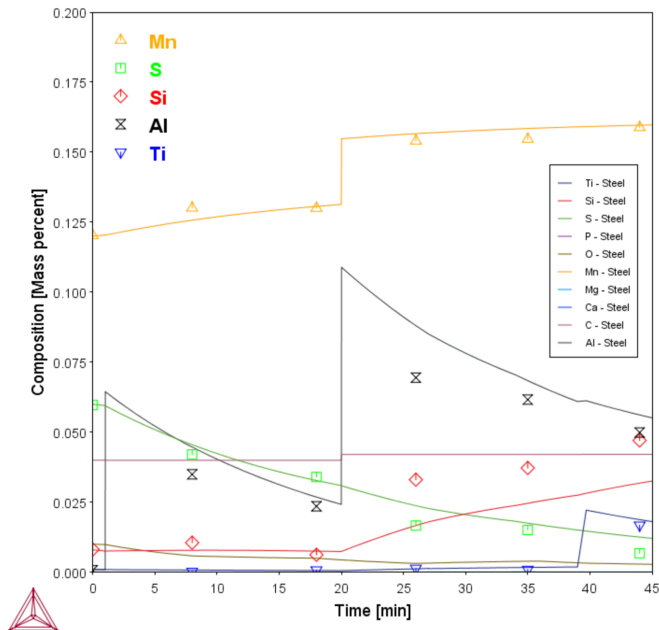
A finer point to observe is that the temperature of the reaction zone is always slightly higher than both the steel zone and the slag zone. The reason for this is that the reaction between the steel and the slag is exothermic.



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

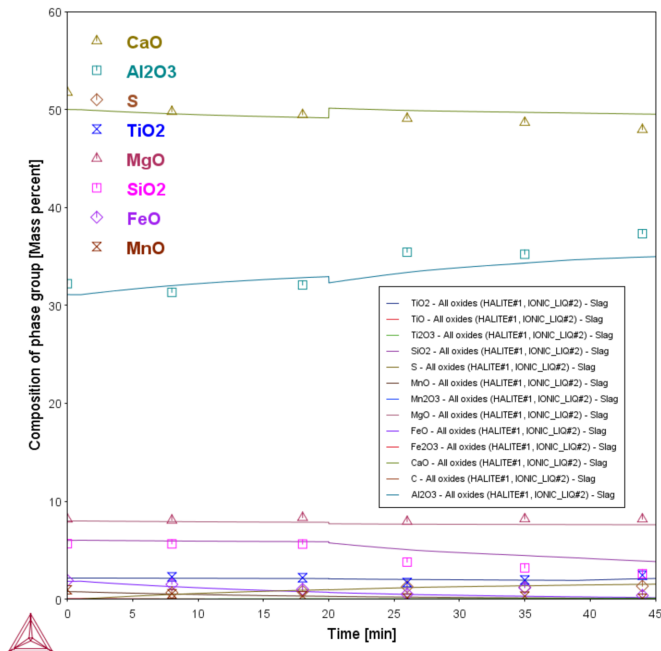
Already this simple model captures the evolution of the steel chemistry in function of processing time very well. The experimentally determined S, Mn and Ti contents are reproduced to within experimental accuracy.



*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

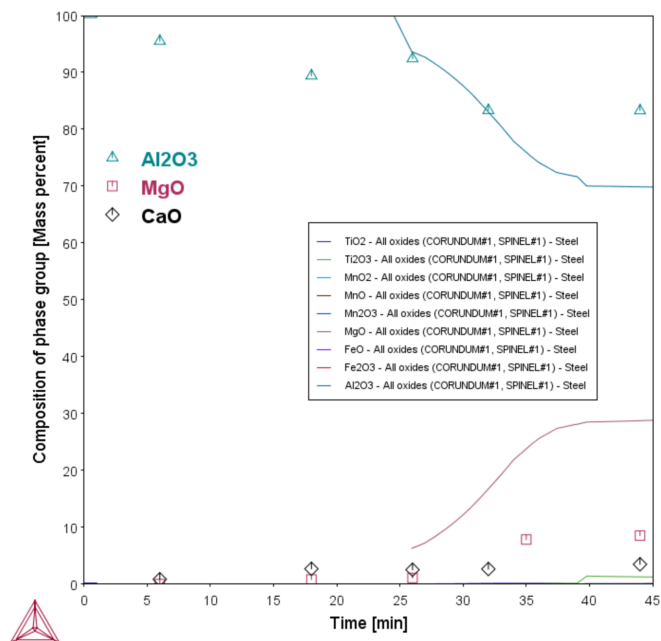
Also the evolution of the slag chemistry is well reproduced. Some of the important changes in chemistry, such as the gradual decrease of FeO and MnO and uptake of S in function of time can only be seen after zooming into the plot somewhat



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 ( $\text{Al}_2\text{O}_3$ ), then a second population of MgO rich spinel inclusions start forming. This result captures the essence of what is experimentally observed.



---

*Evolution of the inclusion chemistry in function of time.*

### Visit our Website for More Information



You can find several other learning resources on the [Process Metallurgy](#) page of our website (or in Thermo-Calc, go to **Help → Thermo-Calc website**). You can also [subscribe to the Thermo-Calc newsletter](#) to be kept up-to-date about upcoming releases, training, examples, videos and much more.

### 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.



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## Diffusion Module (DICTRA) Graphical Mode Examples

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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.

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| D_01 Homogenization of a Binary Fe-Ni Alloy .....                            | 86 |
| D_02 Ferrite(bcc)/Austenite(fcc) Transformation in a Binary Fe-C Alloy ..... | 87 |
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| D_05 $\gamma/\alpha/\gamma$ Diffusion couple of Fe-Ni-Cr alloys .....        | 93 |
| D_06 Diffusion Through a Tube Wall .....                                     | 97 |
| D_07 Multiphase Carburization of a Ni-25Cr-0.0001C alloy .....               | 99 |

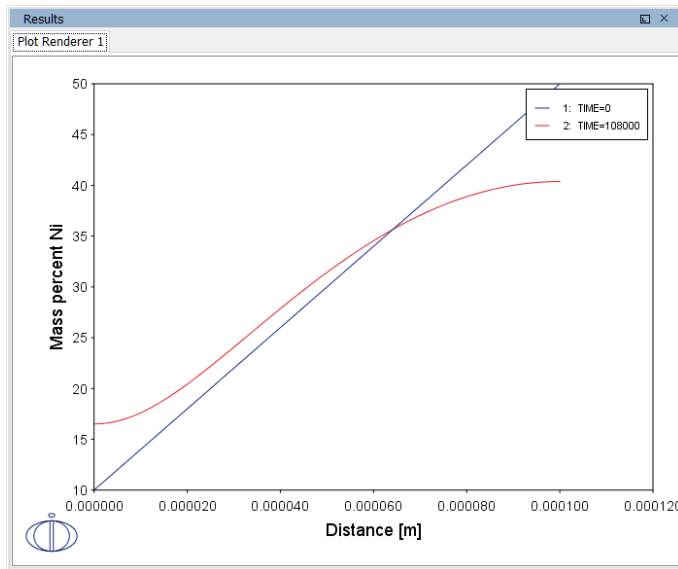
## D\_01 Homogenization of a Binary Fe-Ni Alloy

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



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

### Composition of Ni vs Distance



### Project File Name

- Folder: Diffusion Module - DICTRA
- File name: *D\_01\_Diffusion\_Single\_Phase.tcu*



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

## D\_02 Ferrite(bcc)/Austenite(fcc) Transformation in a Binary Fe-C Alloy

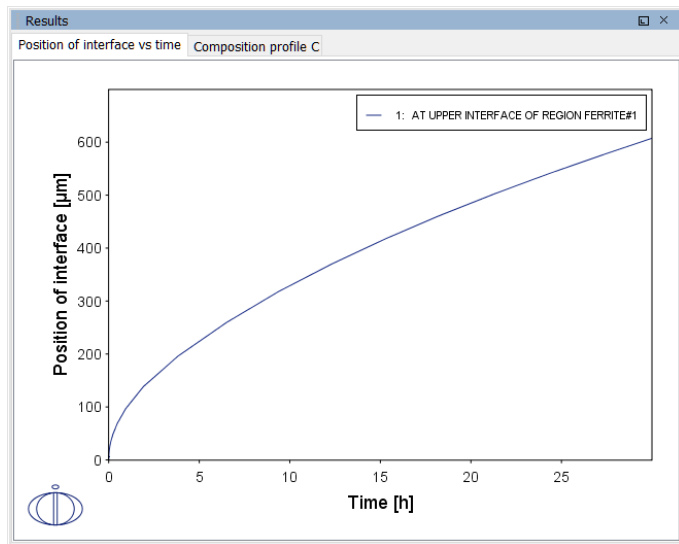
---

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

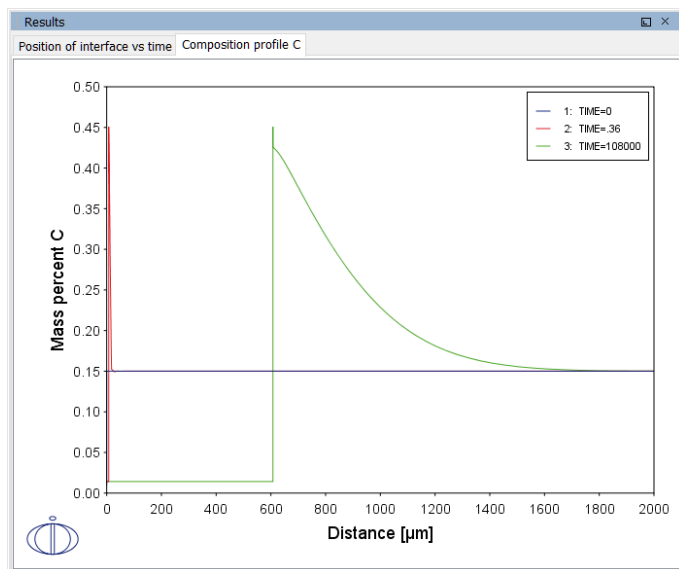


This example is available as a video tutorial on [our website](#) and [YouTube channel](#).

### Position of interface vs time



### Composition profile C



### Project File Name

- Folder: Diffusion Module - DICTRA
- File name: *D\_02\_Diffusion\_Moving\_Boundary.tcu*



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

## D\_03 Evolution of an Fe-Cr-Ni Diffusion Couple

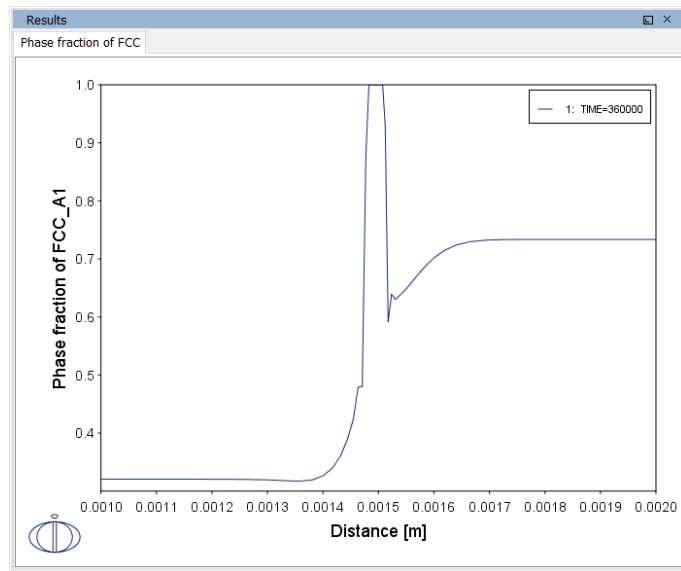
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The multiphase example simulates the evolution of an Fe-Cr-Ni diffusion couple during a 100 hour heat treatment at 1100° C (1373.15 K). Both end members of the diffusion couple are duplex ferrite plus austenite, but the majority phase is ferrite on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

### 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  $\alpha+\gamma$  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).

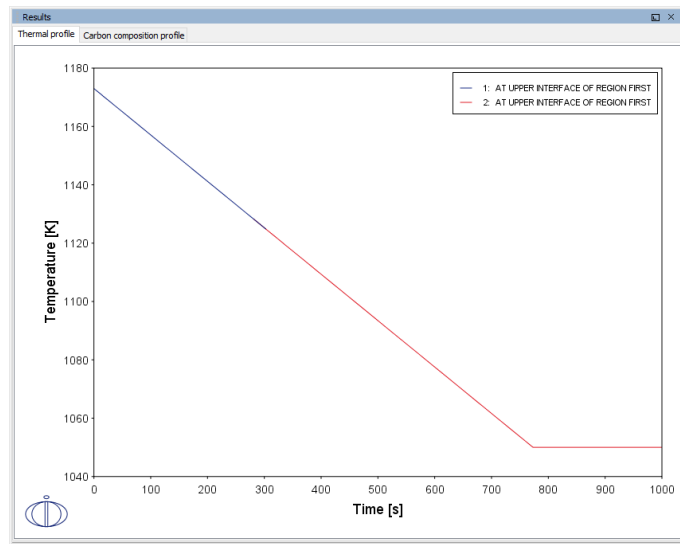
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## D\_04 Fe-C Moving Boundary: Austenite to Ferrite

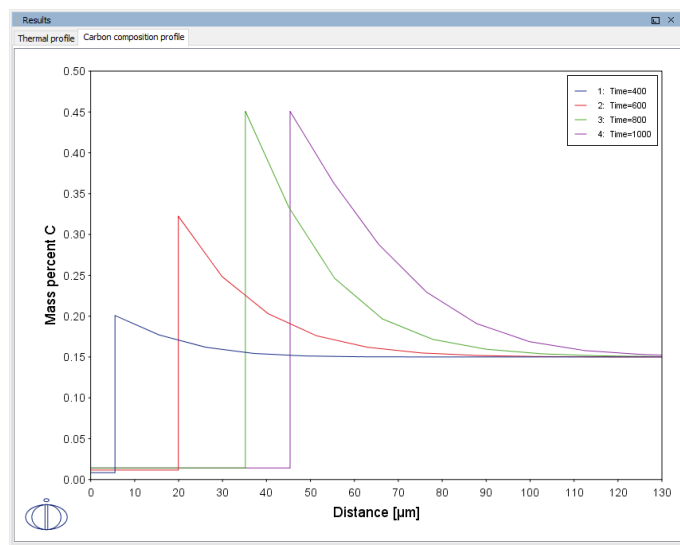
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This example simulates the austenite to ferrite transformation in a Fe-0.01 mass% C steel during continuous cooling. The simulation starts at a temperature where only austenite is stable, ferrite nucleates and grows into the austenite during cooling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

### Thermal profile



### Carbon composition profile



### Project File Name

- Folder: Diffusion Module - DICTRA
- File name: *D\_04\_Diffusion\_Fe-C\_Moving\_Boundary\_Austenite\_to\_Ferrite.tcu*



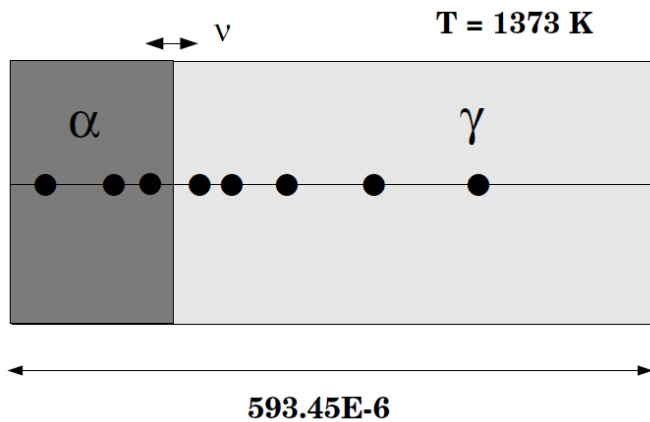
This example is available to all users.



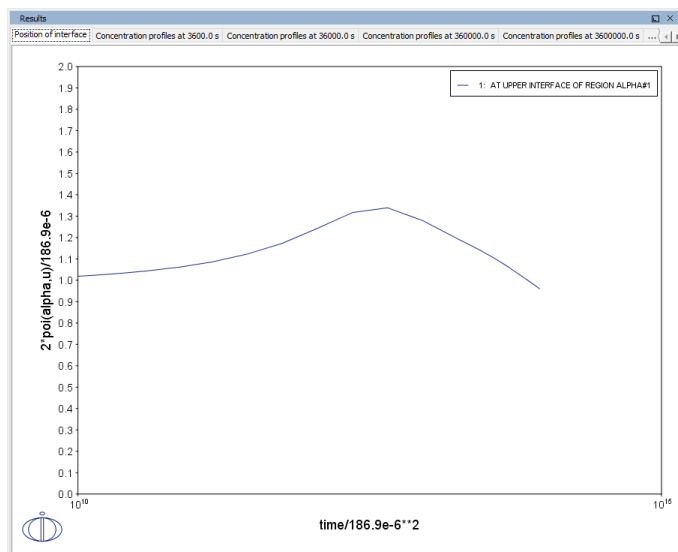
## D\_05 $\gamma/\alpha/\gamma$ Diffusion couple of Fe-Ni-Cr alloys

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

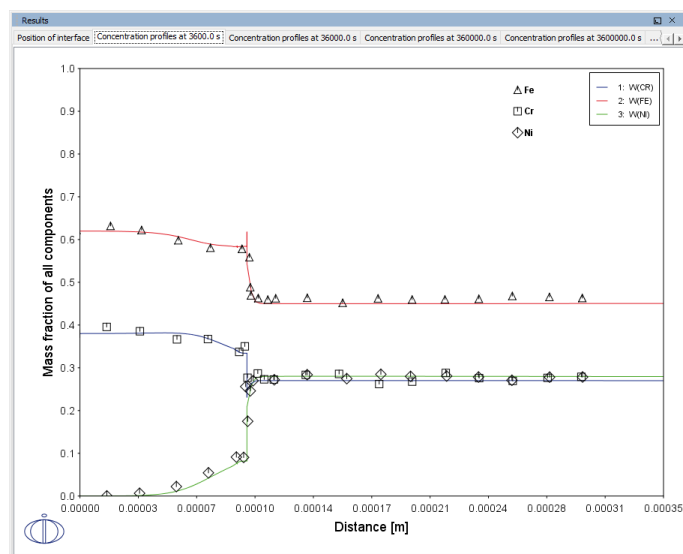
This set up corresponds to diffusion couple in Kajihara et al. [1993a] and Kajihara and Kikuchi [1993b].



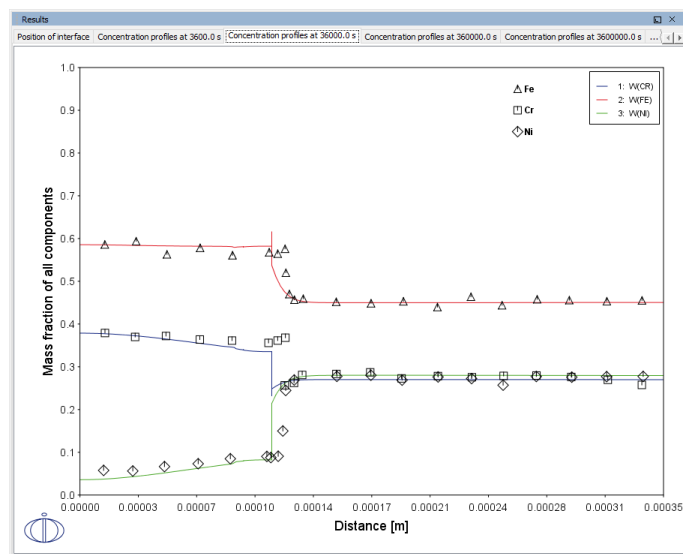
### Interface Position



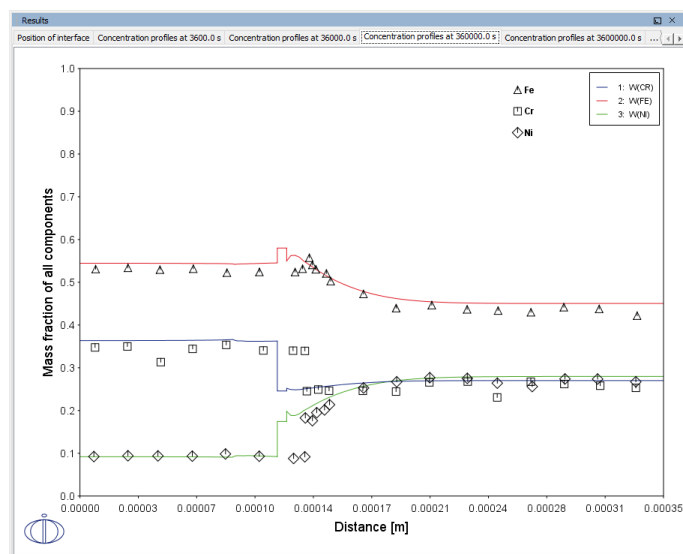
### Concentration profiles at 3600 s



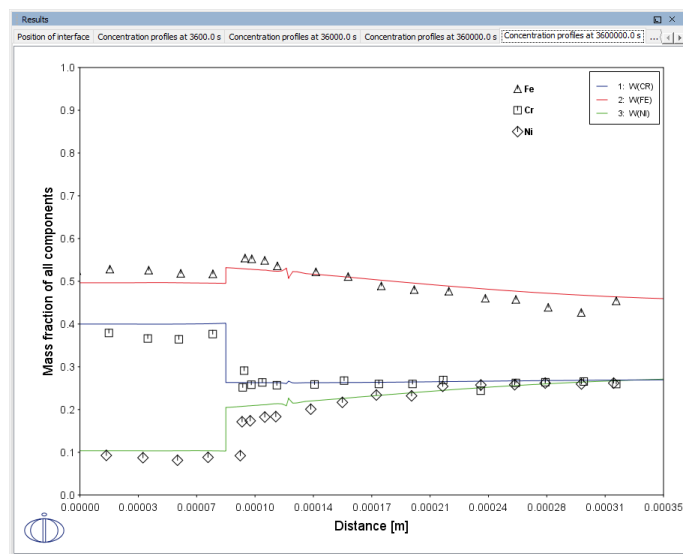
### Concentration profiles at 36 000 s



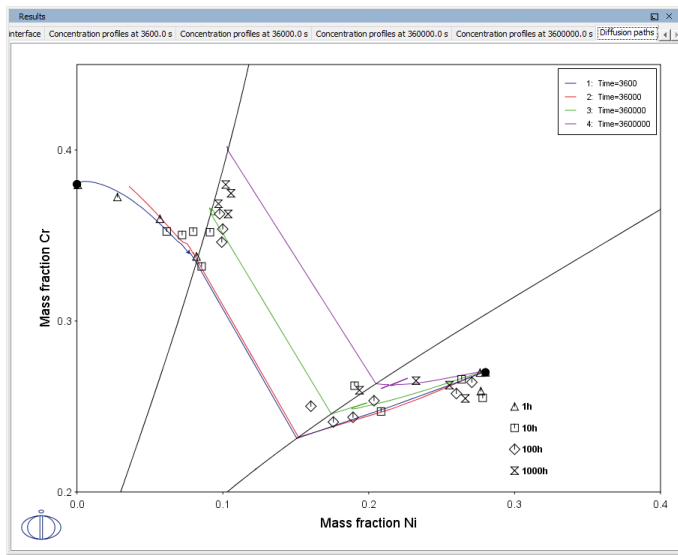
### Concentration profiles at 360 000 s



### Concentration profiles at 3 600 000 s



## Diffusion paths



## Project File Name

- Folder: Diffusion Module - DICTRA
- File name: *D\_05\_Diffusion\_Fe\_Ni\_Cr\_Moving\_Boundary\_Diffusion\_Couple.tcu*

## 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  $\alpha$  phase in  $\gamma/\alpha/\gamma$  diffusion couples of the Fe-Cr-Ni system. Acta Metall. Mater. 41, 2045–2059 (1993).

## D\_06 Diffusion Through a Tube Wall

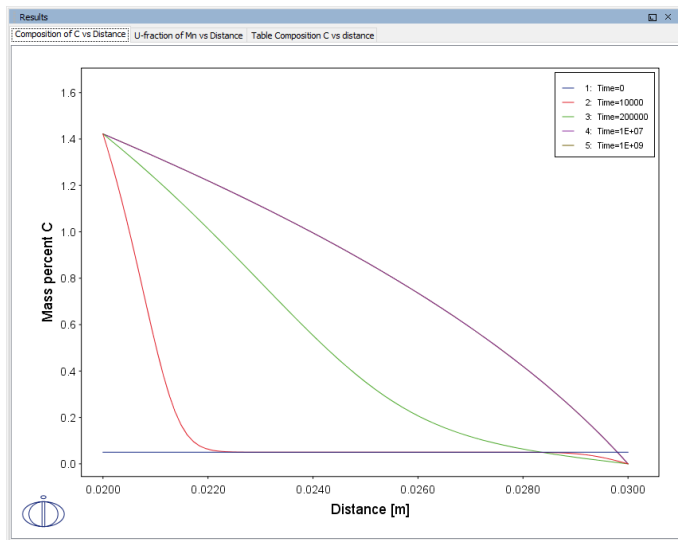
This is a simple example of diffusion through a tube wall. The tube material is an Fe-0.06Mn-0.05C alloy. Two plots comparing distance to the U-fraction of manganese and composition of carbon are generated to visualize the austenite region. A *cylindrical* geometry is used with *mixed zero flux and activity*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

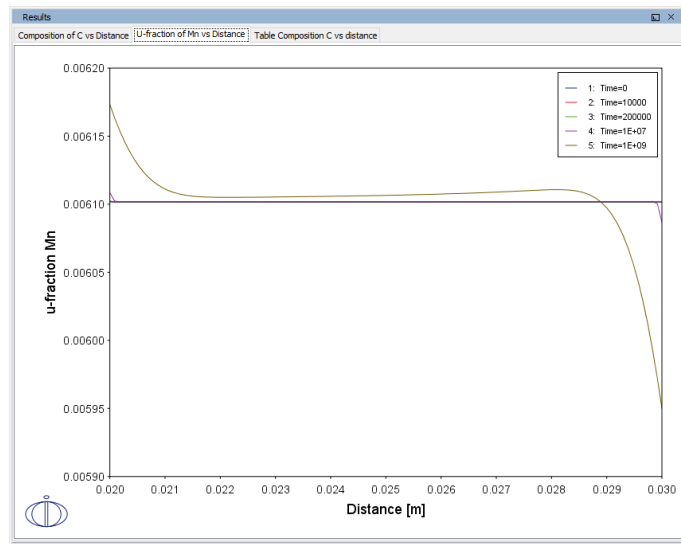


This example is based on Console Mode exab6. When in Console Mode, you can open the example from Thermo-Calc (**File** → **Examples Files** → **Diffusion Module**).

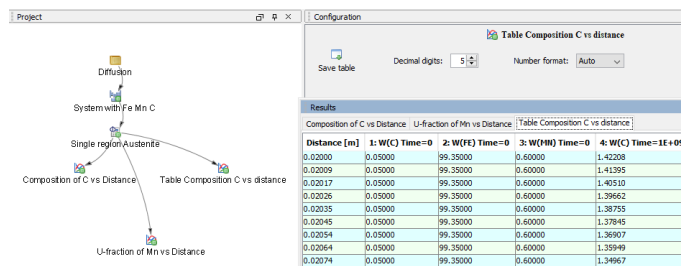
*Plot: Composition of C vs Distance*



### U-fraction of Mn vs Distance



### 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.

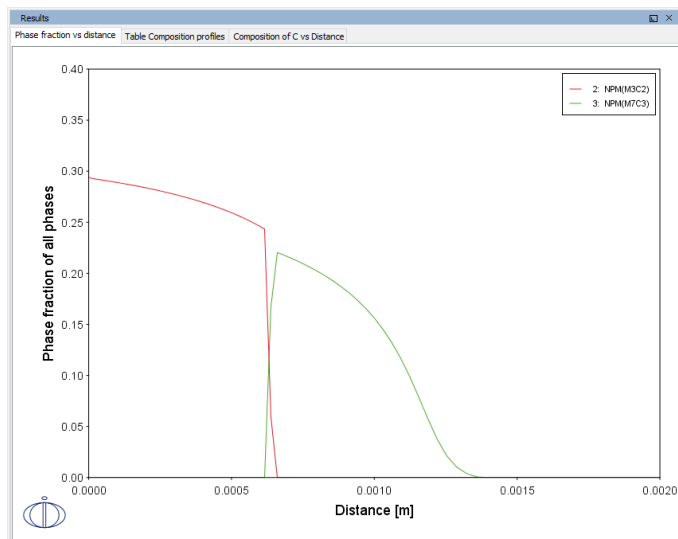


This example is based on Console Mode exd1b. When in Console Mode, you can open the example from Thermo-Calc (**File** → **Examples Files** → **Diffusion Module**).



This example is available as a video tutorial on [our website](#) and [YouTube channel](#).

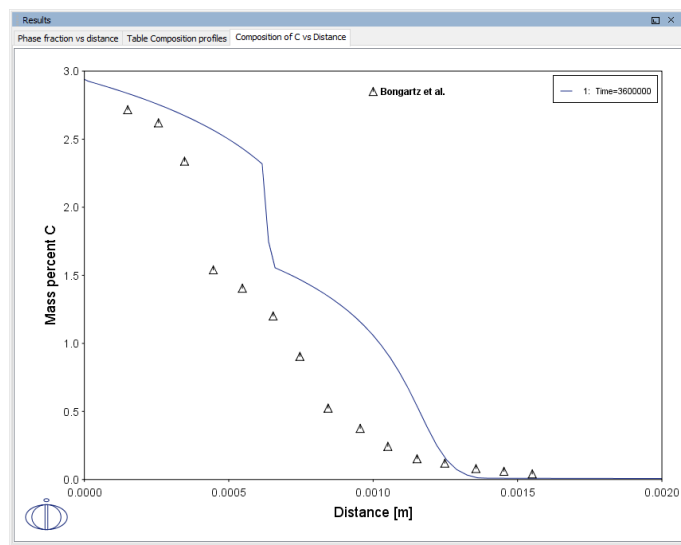
### *Phase fraction vs distance*



## Table of Composition profiles

| 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 |                              |  |
| 9.8810E-6                  | 2.92919 | 24.27408                   | 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 | 24.28463                   | 72.84248 |                              |  |
| 0.00011                    | 2.86564 | 24.28588                   | 72.84849 |                              |  |
| 0.00012                    | 2.85750 | 24.28783                   | 72.85467 |                              |  |
| 0.00013                    | 2.84907 | 24.28984                   | 72.86110 |                              |  |
| 0.00014                    | 2.84033 | 24.29194                   | 72.86773 |                              |  |
| 0.00016                    | 2.83124 | 24.29412                   | 72.87464 |                              |  |
| 0.00017                    | 2.82181 | 24.29640                   | 72.88179 |                              |  |
| 0.00018                    | 2.81201 | 24.29877                   | 72.88922 |                              |  |
| 0.00020                    | 2.80183 | 24.30124                   | 72.89693 |                              |  |
| 0.00021                    | 2.79122 | 24.30381                   | 72.90497 |                              |  |
| 0.00022                    | 2.78018 | 24.30650                   | 72.91332 |                              |  |
| 0.00024                    | 2.76867 | 24.30930                   | 72.92203 |                              |  |
| 0.00025                    | 2.75666 | 24.31222                   | 72.93112 |                              |  |
| 0.00027                    | 2.74412 | 24.31528                   | 72.94060 |                              |  |
| 0.00028                    | 2.73101 | 24.31848                   | 72.95051 |                              |  |
| 0.00030                    | 2.71731 | 24.32182                   | 72.96087 |                              |  |
| 0.00031                    | 2.70295 | 24.32533                   | 72.97171 |                              |  |
| 0.00033                    | 2.68790 | 24.32901                   | 72.98308 |                              |  |
| 0.00035                    | 2.67210 | 24.33288                   | 72.99502 |                              |  |
| 0.00036                    | 2.65550 | 24.33694                   | 73.00756 |                              |  |
| 0.00038                    | 2.63803 | 24.34122                   | 73.02075 |                              |  |
| 0.00040                    | 2.61961 | 24.34573                   | 73.03466 |                              |  |
| 0.00042                    | 2.60016 | 24.35050                   | 73.04934 |                              |  |
| 0.00043                    | 2.57960 | 24.35554                   | 73.06486 |                              |  |

## Composition of C vs Distance



## Project File Name

- Folder: Diffusion Module - DICTRA
- File name: *D\_07\_Diffusion\_Carburization\_Multiphase.tcu*

## 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:

|  |     |
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## P\_01: Isothermal Precipitation of Al<sub>3</sub>Sc

This example simulates the kinetics of precipitation of Al<sub>3</sub>Sc 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].

### 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.



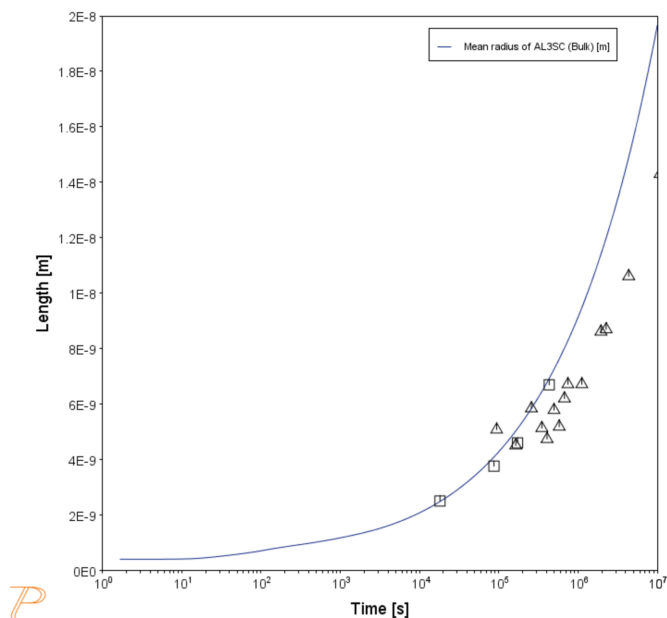
At this time, the Yield Strength Model shown with this example is not included in the step-by-step instructions.

### Example Settings

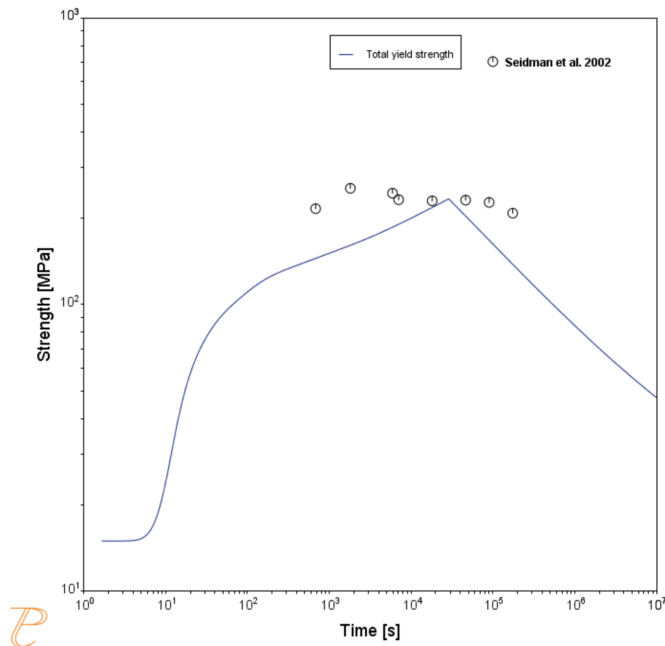
| System (System Definer)               |   |
|---------------------------------------|---|
| Database package                      | Demo: Aluminum-based alloys (ALDEMO, MALDEMO) |
| Elements                              | Al, Sc  |
| Conditions (Precipitation Calculator) |   |
| Composition                           | Al-0.18Sc Mole percent                        |
| Matrix phase                          | FCC_A1  |

|   |               |
|---|---------------|
| Precipitate phase   | AL3SC         |
| <b>Precipitate Phase Data Parameters (Precipitation Calculator)</b>   |               |
| Nucleation sites  | Bulk          |
| Interfacial energy  | Calculated    |
| <b>Calculation Type (Precipitation Calculator)</b>  |               |
| Calculation type  | Isothermal    |
| Temperature   | 350° C        |
| Simulation time   | 1.0E7 seconds |
| <b>Experimental File Reader 1 and 2</b>   |               |
| There are two Experimental File Reader nodes used. One for the mean radius plot and one to demonstrate the <i>Yield Strength Property Model</i> . |               |

## Plot Results



*This plot shows the mean radius of the  $Al_3Sc$  precipitate as a function of time.*



*This plot shows the total yield strength of the  $Al_3Sc$  precipitate as a function of time compared to experimental data from Seidman et al. [2002, Seidman].*

## References

- [2001, Marquis] E. A. Marquis, D. N. Seidman, Nanoscale structural evolution of  $Al_3Sc$  precipitates in Al (Sc) alloys. *Acta Mater.* 49, 1909–1919 (2001).
- [2001, Novotny] G. M. Novotny, A. J. Ardell, Precipitation of  $Al_3Sc$  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).

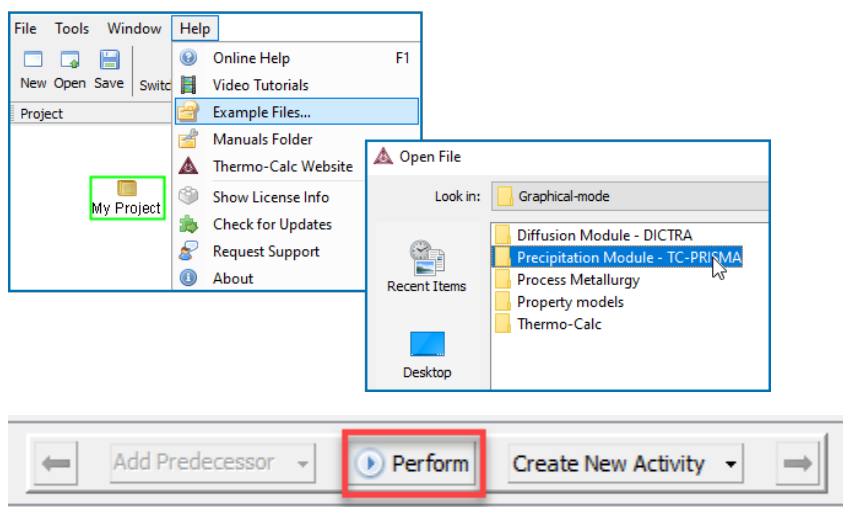
# Isothermal Precipitation Calculation: Example P\_01 – Precipitation Al-Sc AL3SC

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).

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=PLfv6McToaTGSpgvuLoY3b\\_UV-8xpgLUKj](https://www.youtube.com/playlist?list=PLfv6McToaTGSpgvuLoY3b_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.

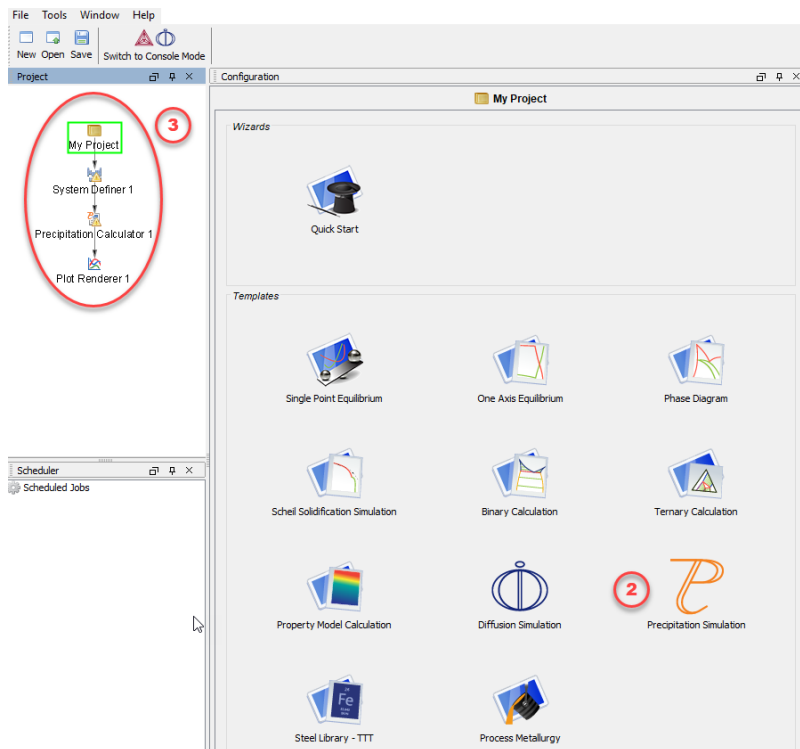


## ABOUT THE EXAMPLE

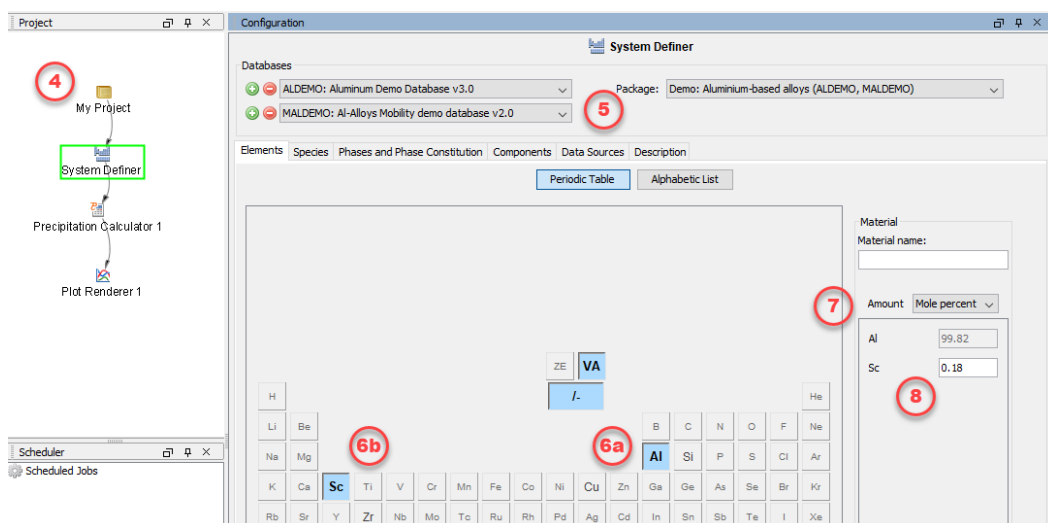
This example simulates the kinetics of precipitation of  $Al_3Sc$  from an FCC\_A1 solution phase.

## 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.

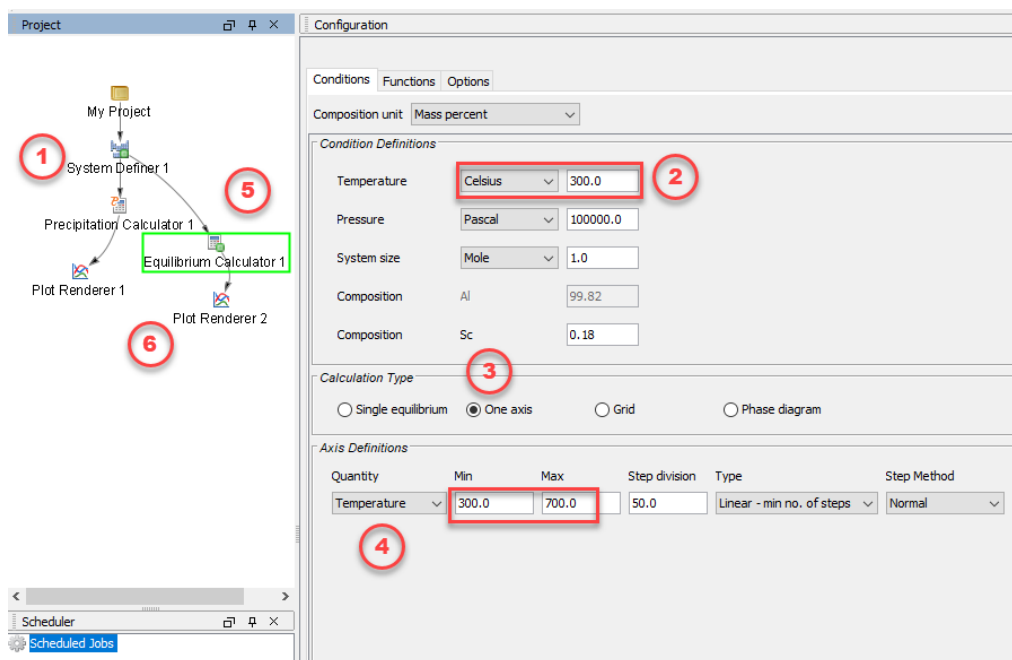
## ONE AXIS CALCULATION

### 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 from the **Create New Successor** menu select **Equilibrium Calculator**.
2. In the **Configuration** window, select a *Temperature* in **Celsius** and enter 300.
3. Under *Calculation Type*, select **One axis**.  
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

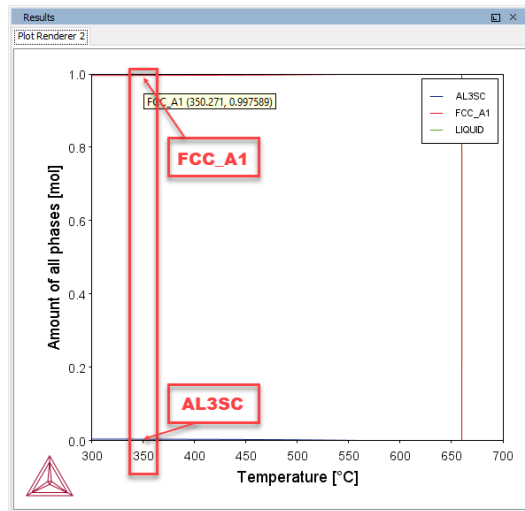
Once the calculation is complete, a plot is displayed in the **Results** window. This plot shows you which phases are present at each temperature between 300° and 700° and the amount of that phase at each temperature.

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<sub>3</sub>Sc, 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

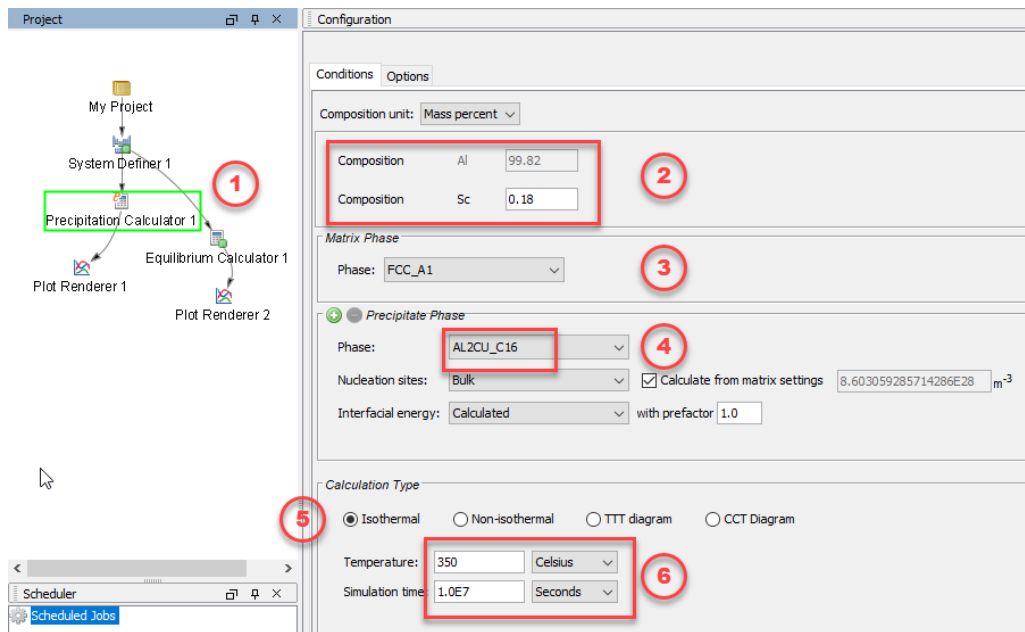
1. In the **Project** window, click the **Precipitation Calculator 1** node.
2. Notice that the *Composition* set in the *System Definer* auto-populated here.
3. Under *Matrix Phase*, the *Phase* defaults to **FCC\_A1**, which is the primary phase present in the one axis calculation.

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.

Accept the default settings in the *Precipitate Phase* section. You could choose to define your own interfacial energy settings if you have them.

5. Under *Calculation Type*, make sure **Isothermal** is selected.
6. Enter:
  - a. 350 as the *Temperature* and select **Celsius**.
  - b. 1.0E7 as the *Simulation time* and select **Seconds**, which is ten million seconds.



**Configuration**

Conditions Options

Composition unit: Mass percent

Composition Al 99.82

Composition Sc 0.18

Matrix Phase

Phase: FCC\_A1

Precipitate Phase

Phase: AL2CU\_C16

Nucleation sites: Bulk

Interfacial energy: Calculated

Calculate from matrix settings:  $8.603059285714286E28 \text{ m}^{-3}$

with prefactor 1.0

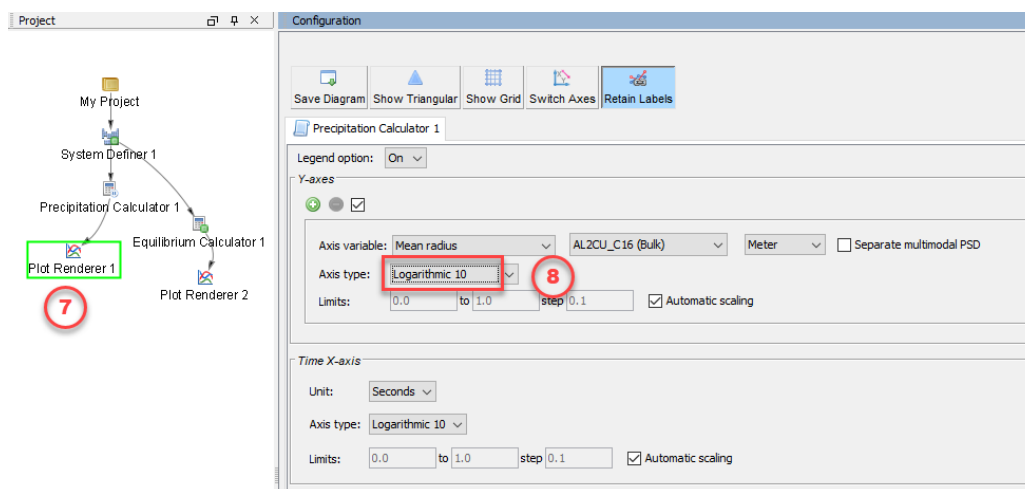
Calculation Type

☒ Isothermal ☐ Non-isothermal ☐ TTT diagram ☐ CCT Diagram

Temperature: 350 Celsius

Simulation time: 1.0E7 Seconds

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



**Configuration**

Save Diagram Show Triangular Show Grid Switch Axes Retain Labels

Precipitation Calculator 1

Legend option: On

Y-axes

Axis variable: Mean radius

Axis type: Logarithmic 10

Limits: 0.0 to 1.0 step 0.1

Automatic scaling

Time X-axis

Unit: Seconds

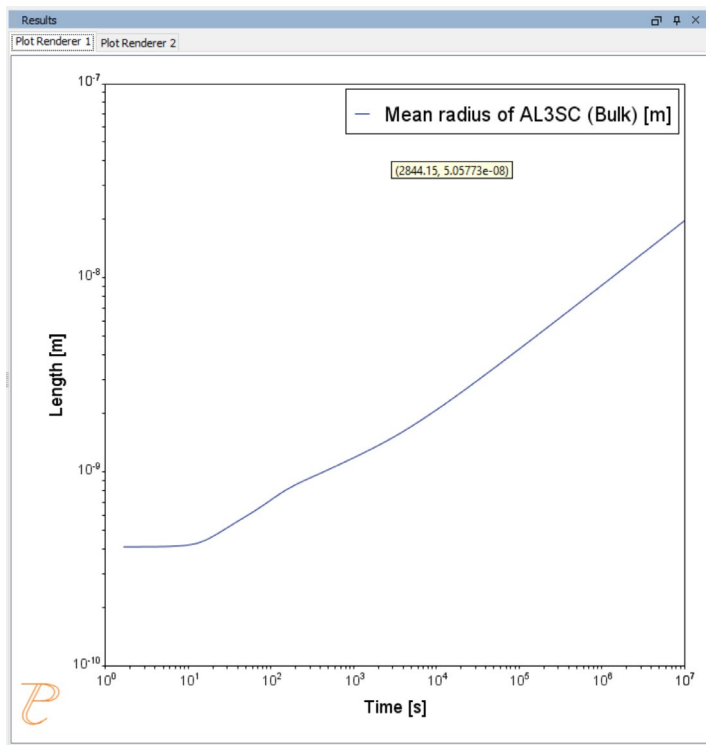
Axis type: Logarithmic 10

Limits: 0.0 to 1.0 step 0.1

Automatic scaling

### Interpreting the Results of the Precipitation Calculation

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



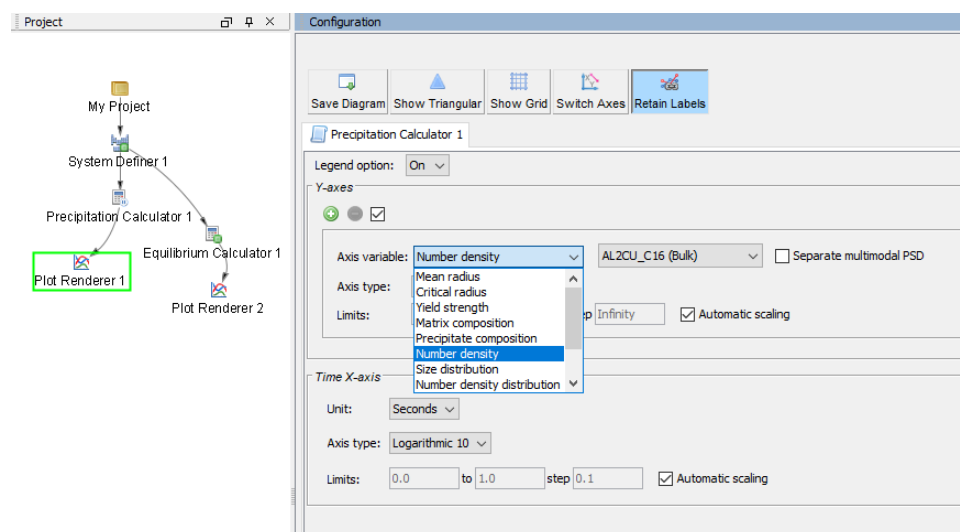
*This plot shows the Mean radius of the AL3SC precipitate as a function of time.*

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

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

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

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



## P\_02: Stable and Metastable Carbides - Isothermal

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

This example uses the Equilibrium Calculator and a one axis calculation to determine how the phases change with temperature. We are interested in the carbide precipitation at 1053K where only the carbide M23C6 is stable according to the equilibrium calculation. The Precipitation Calculator is used to do an isothermal calculation of the three phases (cementite, M23C6 and M7C3) where cementite and M7C3 are metastable phases.

### Project File 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 <b>Show details</b> 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<sup>2</sup>, M23C6 0.252 J/m<sup>2</sup>, M7C3 0.282 J/m<sup>2</sup>**Calculation Type (Precipitation Calculator)**

Calculation type

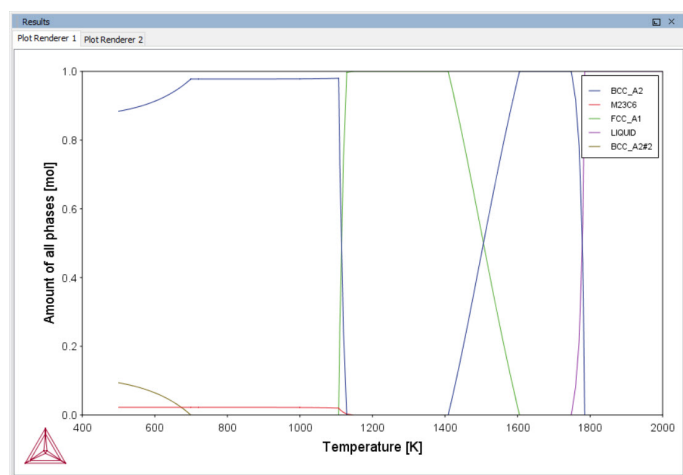
Isothermal

Temperature

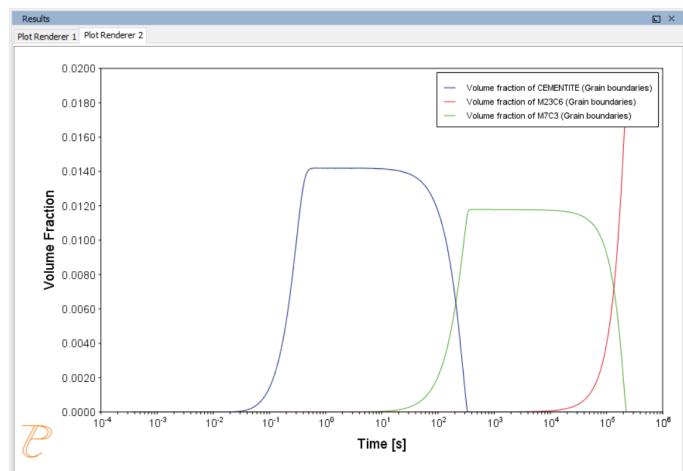
1053 K

Simulation time

400 000 seconds

**Plot Results**

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



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

## P\_03: Stable and Metastable Carbides - TTT Diagram

In this example, the kinetics of precipitation of both stable and metastable carbides is calculated from the ferrite phase. It demonstrates that metastable carbides may first emerge and then disappear and the stable phase prevails.

This example uses the Equilibrium Calculator and a one axis calculation type to determine how the phases change with temperature. Using this result, the Precipitation Calculator is used to do a TTT (Time-Temperature-Transformation) diagram calculation of the three phases (cementite, M23C6 and M7C3) at the grain boundaries.

For a TTT diagram calculation, select **TTT diagram** in **Calculation Type**, then enter **Min**, **Max**, and **Step of Temperature**, as well as **Max annealing time**. In **Stop criterion**, choose **Volume fraction of phase** and enter the value.

### Project File and Video tutorial Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P\_03\_Precipitation\_Fe-C-Cr\_TTT\_Cementite-M7C3-M23C6.tcu*



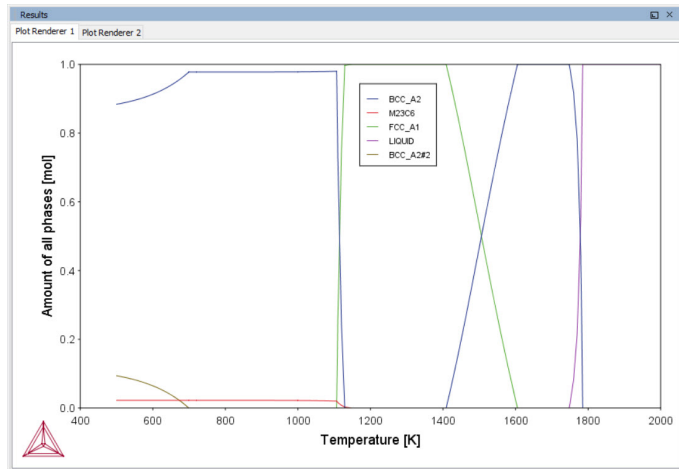
Also see [our website](#) and [YouTube channel](#) for other examples of the Precipitation Module.

### Example Settings

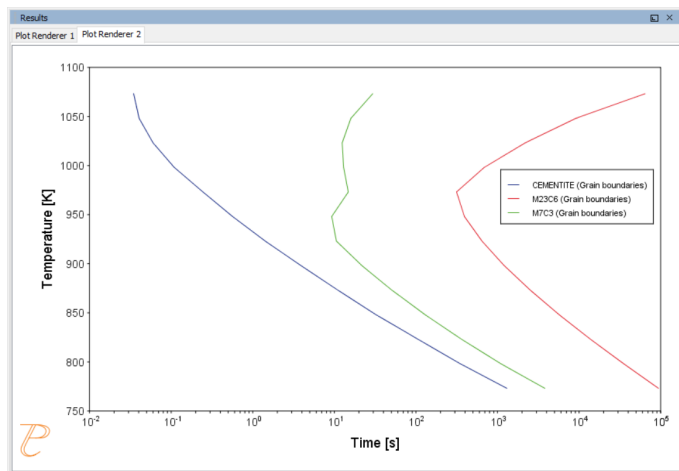
| System (System Definer)               |   |
|---------------------------------------|---|
| Database package                      | Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO) |
| Elements                              | Fe, C, Cr                                       |
| Conditions (Precipitation Calculator) |   |
| Composition                           | Fe-0.1C-12Cr Mass percent                       |
| Matrix phase                          | BCC_A2  |

|  |   |
|--|---|
| Precipitate phases   | Cementite, M23C6 and M7C3   |
| <b>Matrix Phase Data Parameters (Precipitation Calculator)</b> |   |
| Grain size (click <b>Show details</b> to display this setting) | 1.0E-4 m  |
| <b>Precipitate Phase Data Parameters</b>                       |   |
| Nucleation sites   | Grain boundaries  |
| Interfacial energy   | Cementite 0.167 J/m <sup>2</sup> , M23C6 0.252 J/m <sup>2</sup> , M7C3 0.282 J/m <sup>2</sup> |
| <b>Calculation Type (Precipitation Calculator)</b>             |   |
| 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   |
| <b>Options &gt; Numerical Parameters</b>                       |   |
| No. of grid points over one order of magnitude in radius       | 150   |
| Max no. of grid points over one order of magnitude in radius   | 200   |
| Min no. of grid points over one order of magnitude in radius   | 100   |

## Plot Results



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



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



## P\_04: Precipitation of Iron Carbon Cementite

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.

### Project File and Video Tutorial Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P\_04\_Precipitation\_Fe-C\_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 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 <b>Show details</b> to display this setting)  | 1.0   |
| Dislocation density (click <b>Show details</b> to display this setting) | 1.5e11m <sup>-3</sup>                           |
| Precipitate Phase Parameters (Precipitation Calculator)                 |   |
| Nucleation sites  | Dislocations                                    |
| Interfacial energy  | 0.24 J/m <sup>2</sup>                           |

Growth rate model (click **Show details**)

Advanced

**Calculation Type (Precipitation Calculator)**

Calculation type

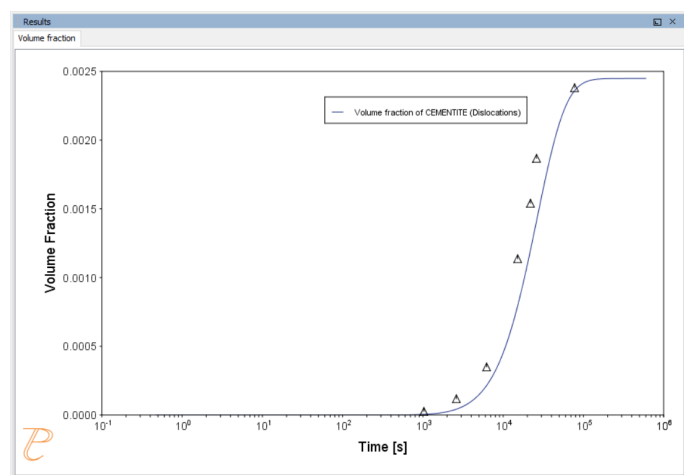
Isothermal

Temperature

102° C

Simulation time

600 000 seconds

**Plot Results***Volume fraction of the cementite phase.***Reference**

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

## P\_05: Precipitation of $\gamma'$ in Ni Superalloys - Isothermal

This example simulates the kinetics of precipitation of  $\gamma'$  phase from  $\gamma$  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.

### Project File and Video Tutorial Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P\_05\_Precipitation\_Ni-Al-Cr\_Isothermal\_Gamma-Gamma\_prime.tcu*



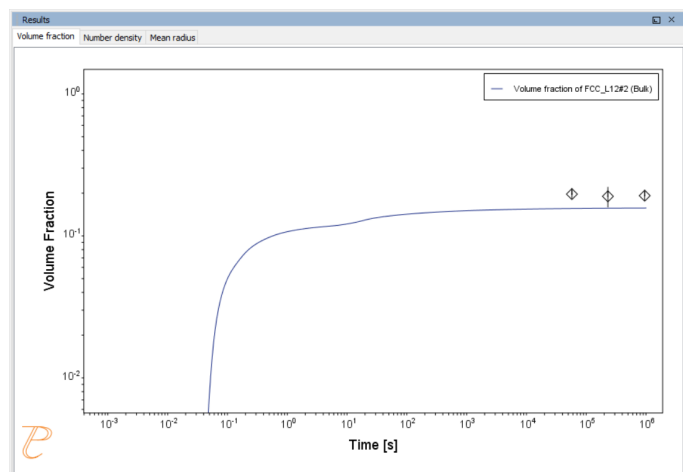
Also see [our website](#) and [YouTube channel](#) for other examples of the Precipitation Module.

### Example Settings

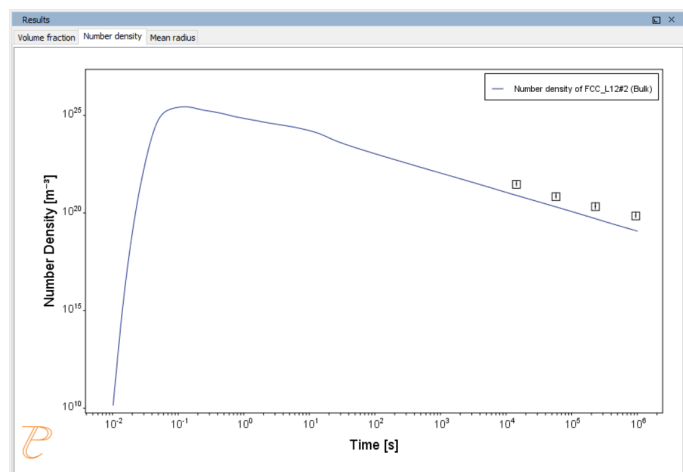
| System (System Definer)                                      |  |
|--|--|
| Database package   | Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO)       |
| Elements   | Ni, Al Cr  |
| Conditions (Precipitation Calculator)                        |  |
| Composition  | Ni-9.8Al-8.3Cr Mole percent                                |
| 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 <sup>2</sup>                                     |
| Calculation Type (Precipitation Calculator)                  |  |
| Calculation type   | Isothermal   |

|                 |                   |
|-----------------|-------------------|
| Temperature     | 800° C            |
| Simulation time | 1 000 000 seconds |

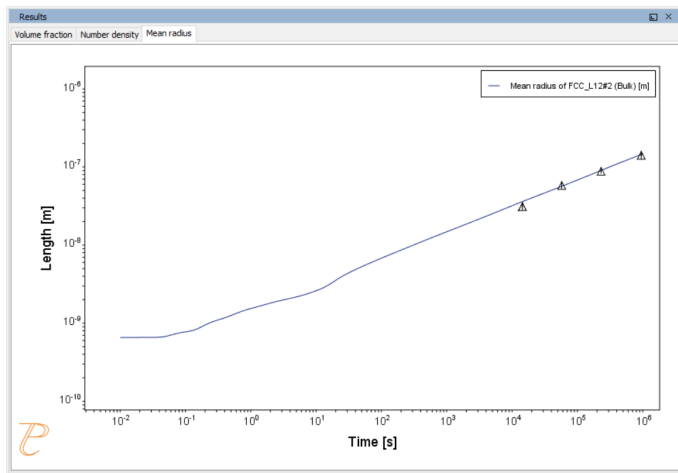
## Plot Results



*The results of an isothermal calculation to plot the volume fraction of the cementite phase.*



*The results of an isothermal calculation to plot the number density of the cementite phase.*



*The results of an isothermal calculation to plot the mean radius of the cementite phase.*

## 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 $\gamma'$ in Ni Superalloys - Non-isothermal

This example simulates the kinetics of precipitation of  $\gamma'$  phase from  $\gamma$  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.

### 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

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

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

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

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

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

5. Adjust the **Valley depth ratio** setting to 0.05 to separate into two peaks as shown in the [Ni-10Al-10Cr plot example](#). You can experiment with this setting to see how the size distribution evolves

with time, for example, try entering several values as plot times **400 600 3300**.

**System (System Definer)**

|                  |  |
|------------------|--|
| Database package | Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO) |
| Elements         | Ni, Al, Cr   |

**Conditions (Precipitation Calculator)**

|                            |  |
|----------------------------|--|
| Composition (Ni-8Al-8Cr)   | Ni-8Al-8Cr Mole percent                                    |
| Composition (Ni-10Al-10Cr) | Ni-10Al-10Cr Mole percent                                  |
| Matrix phase               | DIS_FCC_A1 (see note above about how to select this phase) |
| Precipitate phase          | FCC_L12#2  |

**Matrix Phase Data Parameters (Precipitation Calculator)**

|  |     |
|--|-----|
| Mobility enhancement prefactor (click <b>Show details</b> to display this setting) | 5.0 |
|--|-----|

**Precipitate Phase Data Parameters (Precipitation Calculator)**

|                    |                        |
|--------------------|------------------------|
| Nucleation sites   | Bulk                   |
| Interfacial energy | 0.023 J/m <sup>2</sup> |

**Calculation Type (Precipitation Calculator)**

|                  |                |
|------------------|----------------|
| Calculation type | Non-isothermal |
| Temperature unit | Celsius        |
| Time unit        | Seconds        |

1150 - 380 °C

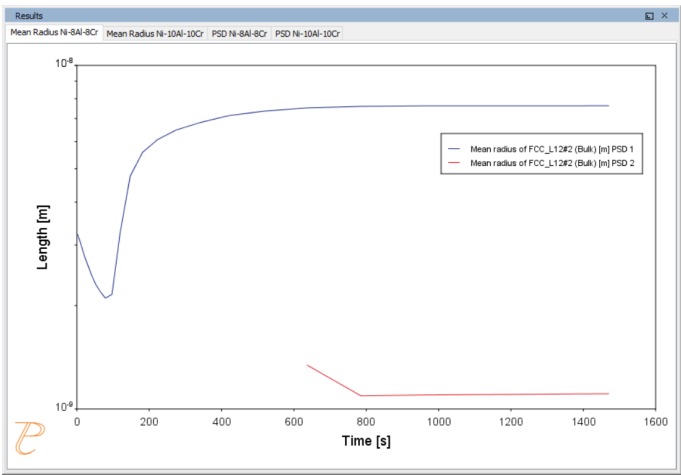
Edit Thermal Profile

Import...

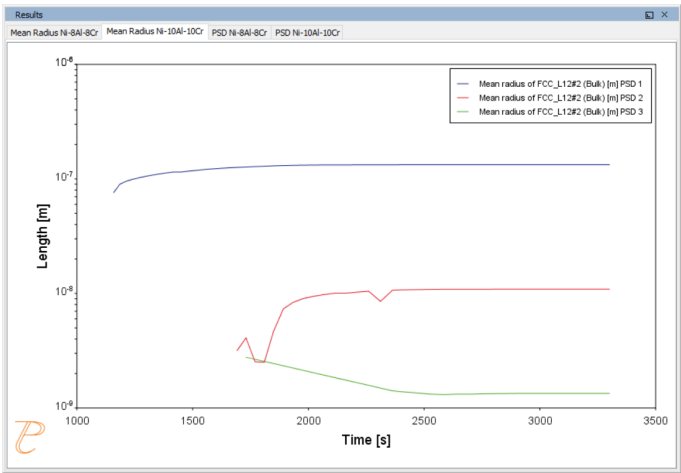
| Time [s] | Temperature [°C] |
|----------|------------------|
| 0.0      | 1150.0           |
| 3300.0   | 380.0            |

|                                       |  |
|---------------------------------------|--|
| 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 <b>Valley depth ratio</b> is set to 0.05 for both plots. The number of <b>Points</b> is increased to 200 for an average radius plot. |
| Separate multimodal PSD for 10Al-10Cr | The <b>Valley depth ratio</b> is set to 0.18 for both plots.   |

Plot Results

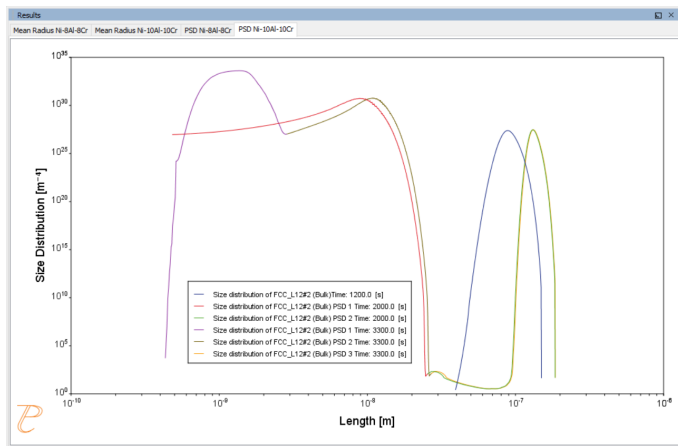


Mean Radius Ni-8Al-8Cr

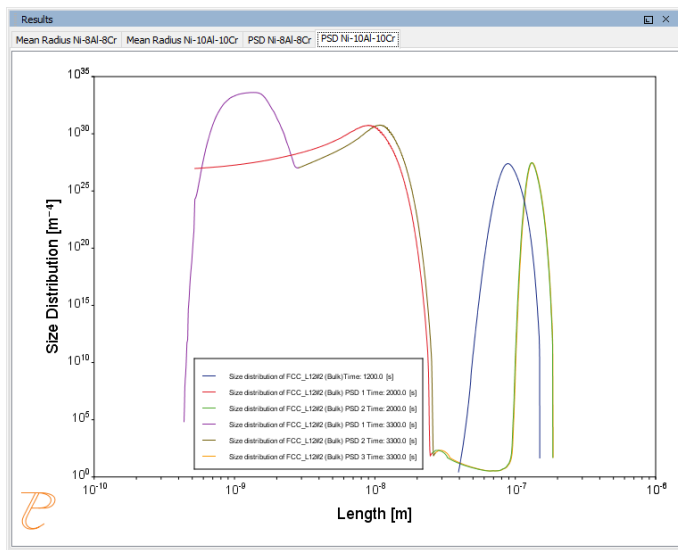




### Mean Radius Ni-10Al-10Cr



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



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

## Reference

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

## P\_07: Continuous Cooling Transformation (CCT) Diagram of Ni-Al-Cr $\gamma$ - $\gamma'$

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

### 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](#).



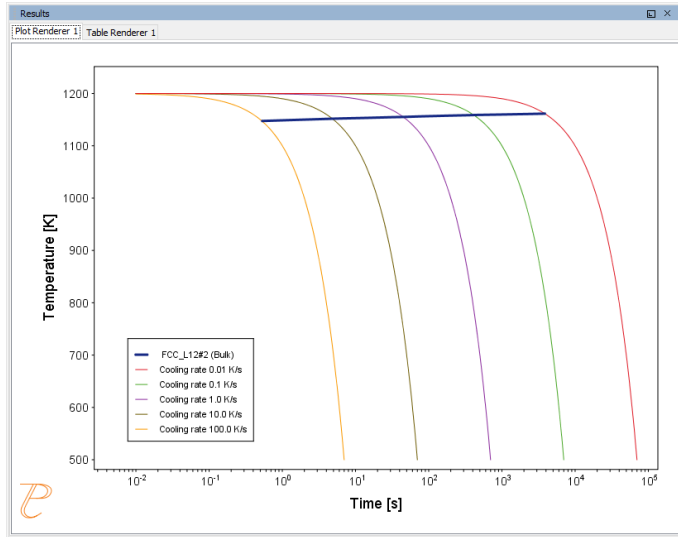
You can also use [the step-by-step instructions](#) included in a PDF to follow the video or compare to the project file in Thermo-Calc.

### 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 <sup>2</sup>                               |
| Calculation Type (Precipitation Calculator)                  |  |
| Calculation type   | CCT Diagram  |

|                        |                                 |
|------------------------|---------------------------------|
| Temperature Min to Max | 500 to 1200 Kelvin              |
| Cooling rate(s)        | .01 .1 1 10 100 K/s             |
| Stop criteria          | Volume fraction of phase 1.0E-4 |

## Plot and Table Results



In this plot, the blue line shows the time it takes for  $\gamma'$  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.

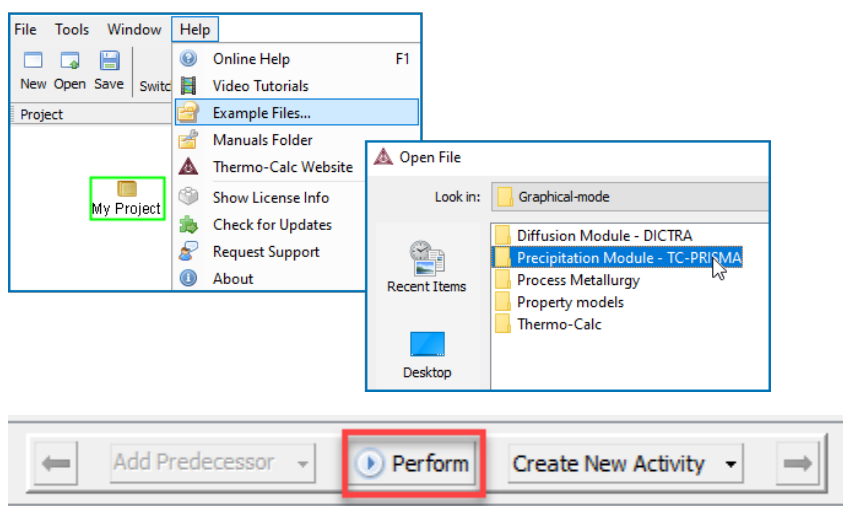
| Results         |                  |
|-----------------|------------------|
| Plot Renderer 1 | Table Renderer 1 |
| Temperature [K] | FCC_L12#2 (Bulk) |
| 1147.52034      | 0.53291          |
| 1151.74192      | 4.83553          |
| 1155.24636      | 44.76534         |
| 1158.85368      | 411.49173        |
| 1161.48750      | 3851.47779       |

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  $\gamma'$  to transform according to the stop criteria, which is a volume fraction of  $1e-4$ .

# Continuous Cooling Transformation (CCT) Diagram of Ni-Al-Cr $\gamma$ - $\gamma'$ : 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](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

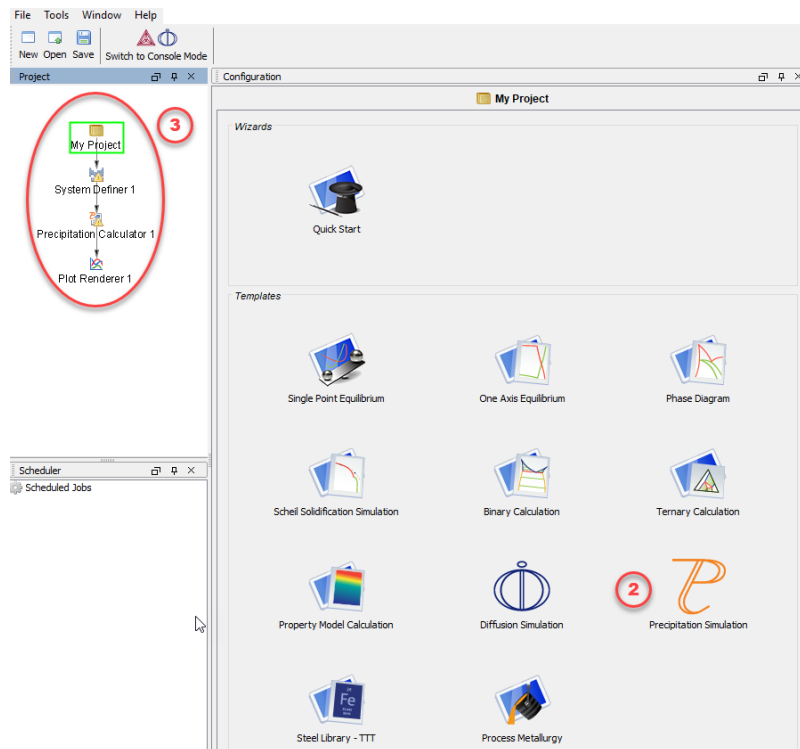
This example shows you how to simulate a CCT diagram for gamma prime ( $\gamma'$ ) precipitation in a Ni-Cr-Al alloy using the Precipitation Module known as TC-PRISMA.

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

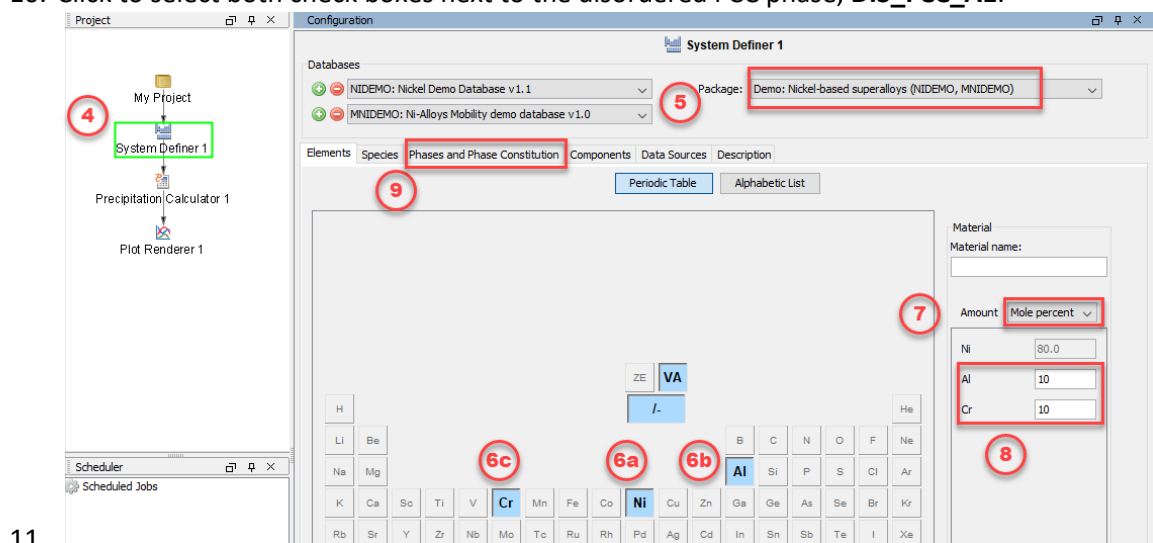
The system is a Ni-10Al-10Cr  $\gamma$  -  $\gamma'$  alloy and it is calculated and plotted with superimposition of the cooling rate values using the Precipitation Module (TC-PRISMA).

## 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**.



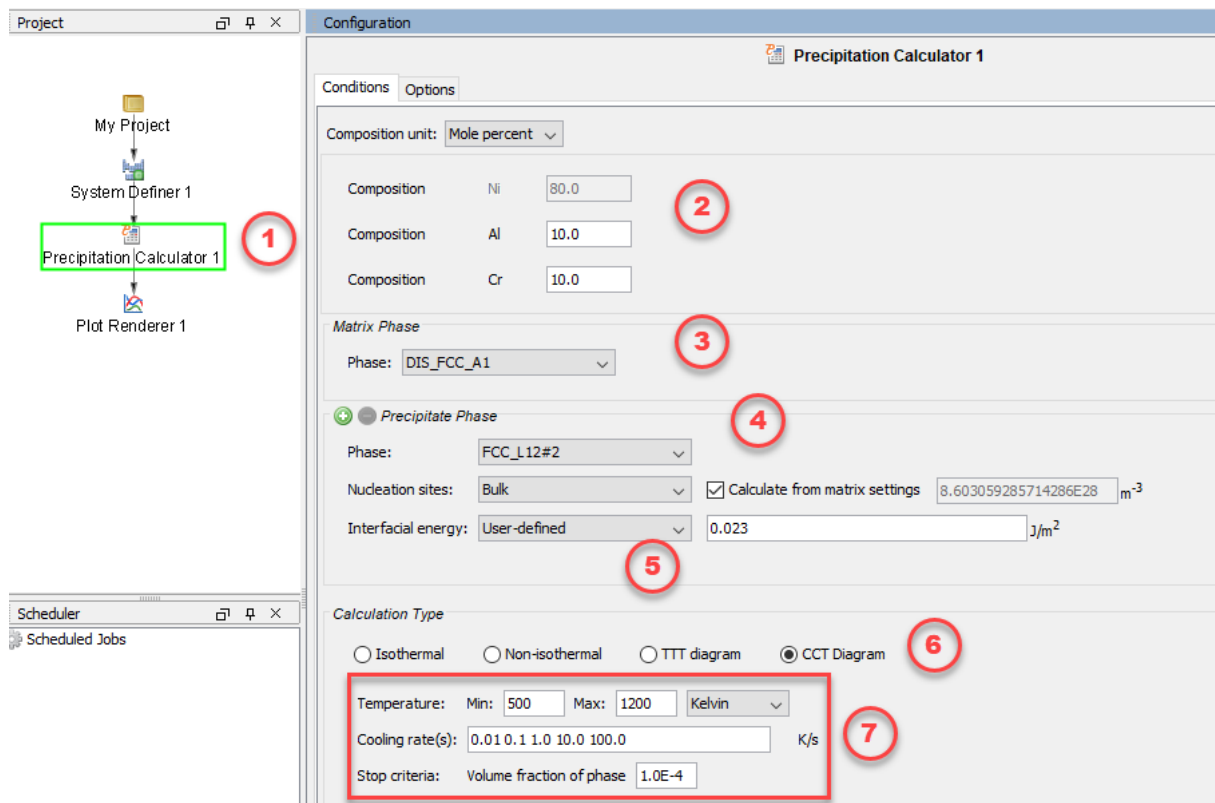
11.

| Elements      | Species    | Phases and Phase Constitution       | Cor                                 |
|---------------|------------|-------------------------------------|-------------------------------------|
| <b>Phases</b> |            |                                     |                                     |
| Status        | Name       | NIDEMO                              | MNIDEMO                             |
| Entered       | AL3NI2     | <input checked="" type="checkbox"/> | <input type="checkbox"/>            |
| Entered       | AL3NI5     | <input checked="" type="checkbox"/> | <input type="checkbox"/>            |
| Entered       | AL4CR      | <input checked="" type="checkbox"/> | <input type="checkbox"/>            |
| Entered       | AL8CR5_H   | <input checked="" type="checkbox"/> | <input type="checkbox"/>            |
| Entered       | AL8CR5_L   | <input checked="" type="checkbox"/> | <input type="checkbox"/>            |
| Entered       | AL9CR4_H   | <input checked="" type="checkbox"/> | <input type="checkbox"/>            |
| Entered       | AL9CR4_L   | <input checked="" type="checkbox"/> | <input type="checkbox"/>            |
| Entered       | ALCR2      | <input checked="" type="checkbox"/> | <input type="checkbox"/>            |
| Entered       | BCC_B2     | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Entered       | BCC_B2#2   | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Entered       | BCT_D022   | <input checked="" type="checkbox"/> | <input type="checkbox"/>            |
| Entered       | C14_LAVES  | <input checked="" type="checkbox"/> | <input type="checkbox"/>            |
| Entered       | CBCC_A12   | <input checked="" type="checkbox"/> | <input type="checkbox"/>            |
| Entered       | CHI_A12    | <input checked="" type="checkbox"/> | <input type="checkbox"/>            |
| Entered       | CRNI2_OP6  | <input checked="" type="checkbox"/> | <input type="checkbox"/>            |
| Entered       | CUB_A13    | <input checked="" type="checkbox"/> | <input type="checkbox"/>            |
| Entered       | DIAMOND_A4 | <input checked="" type="checkbox"/> | <input type="checkbox"/>            |
| Entered       | DIS_FCC_A1 | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Entered       | DIS_MU     | <input checked="" type="checkbox"/> | <input type="checkbox"/>            |
| Entered       | DIS_SIG    | <input checked="" type="checkbox"/> | <input type="checkbox"/>            |

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  $1\text{E}-4$  volume fraction of the  $\gamma'$  phase.
8. The calculation is now set. Click **Perform CCT Diagram Simulation** at the bottom, center of the **Configuration** window.



**Configuration**

**Conditions** **Options**

Composition unit: Mole percent

Composition Ni 80.0

Composition Al 10.0

Composition Cr 10.0

**Matrix Phase**

Phase: DIS\_FCC\_A1

**Precipitate Phase**

Phase: FCC\_L12#2

Nucleation sites: Bulk ☒ Calculate from matrix settings 8.603059285714286E28 m<sup>-3</sup>

Interfacial energy: User-defined 0.023 J/m<sup>2</sup>

**Calculation Type**

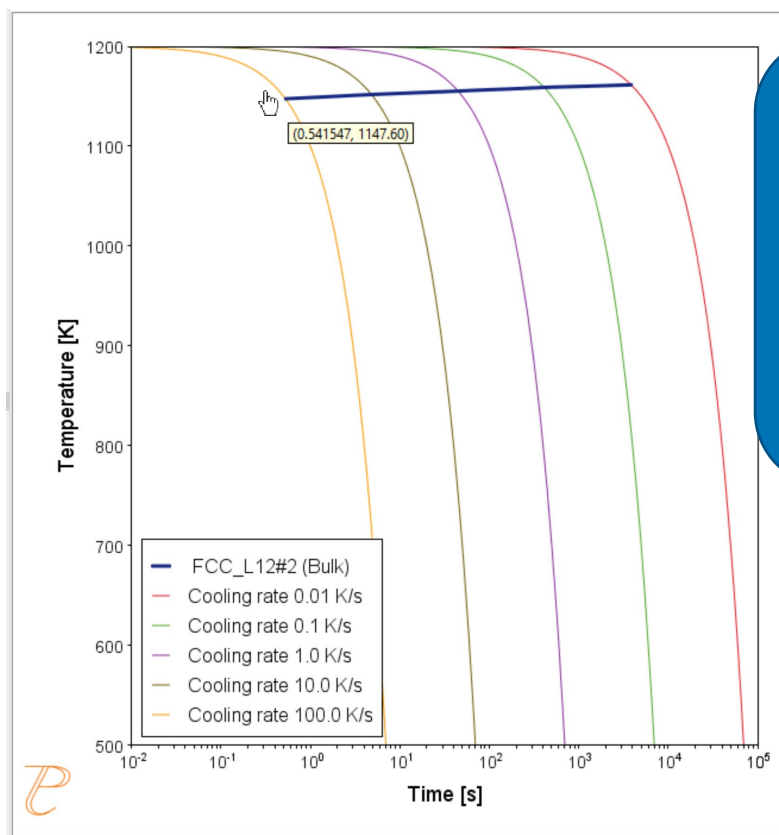
☐ Isothermal ☐ Non-isothermal ☐ TTT diagram ☒ CCT Diagram

Temperature: Min: 500 Max: 1200 Kelvin

Cooling rate(s): 0.01 0.1 1.0 10.0 100.0 K/s

Stop criteria: Volume fraction of phase 1.0E-4

## 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  $\gamma'$  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  $\gamma'$  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  $\gamma'$  to transform according to the stop criteria, which is a volume fraction of  $1e-4$ .



## P\_08: Precipitation of Cu-Ti CU<sub>4</sub>Ti with Assumptions of Sphere and Needle Morphologies

In this isothermal calculation example, the precipitation of Cu<sub>4</sub>Ti 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.

### Project File and Video Tutorial Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P\_08\_Precipitation\_Cu-Ti\_CU<sub>4</sub>Ti1\_Sphere\_Needle.tcu*

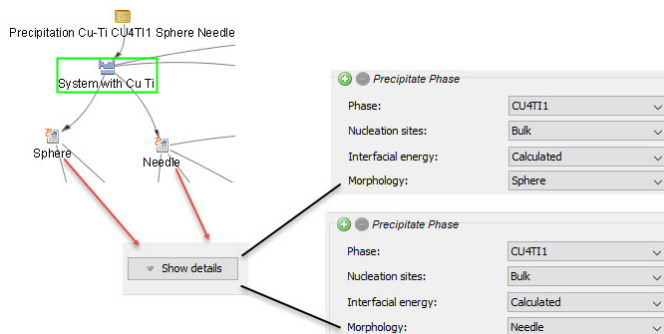


Also see [our website](#) and [YouTube channel](#) for other examples of the Precipitation Module.

### 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**.



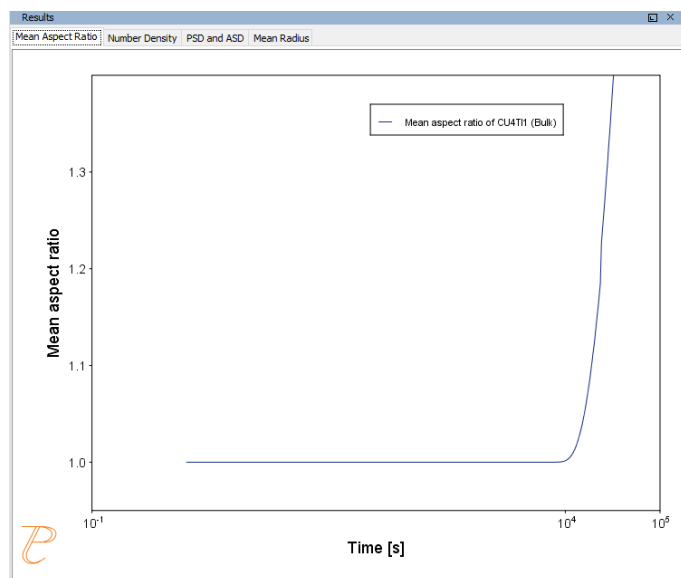
#### System (System Definer)

Database package

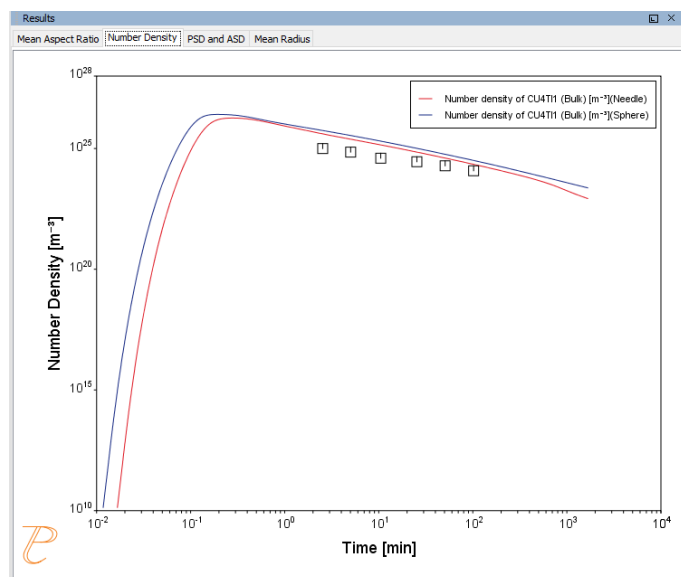
Demo: Copper-based alloys (CUDEMO and MCUDEMO)

|   |  |
|---|--|
| Elements  | Cu, Ti   |
| <b>Sphere and Needle Conditions (Precipitation Calculator)</b>                        |  |
| Composition   | Cu-1.9Ti Mole percent  |
| Matrix phase  | FCC_L12  |
| Precipitate phase   | CU4TI1   |
| <b>Matrix Phase Data Parameters (Precipitation Calculator)</b>                        |  |
| Mobility enhancement prefactor<br>(click <b>Show details</b> to display this setting) | 100  |
| <b>Precipitate Phase Data Parameters (Precipitation Calculator)</b>                   |  |
| Nucleation sites  | Bulk   |
| Interfacial energy  | The default  |
| Morphology (click <b>Show details</b> to display this setting)                        | For the <b>Sphere</b> node (renamed from Precipitation Calculator), keep the default.<br>For the <b>Needle</b> node (renamed from Precipitation Calculator), <b>Needle</b> is selected.  |
| Transformation strain (click <b>Show details</b> to display this setting)             | For the <b>Sphere</b> node (renamed from Precipitation Calculator), keep the default.<br>For the <b>Needle</b> node (renamed from Precipitation Calculator), <b>User defined</b> is selected. In this example, the following settings are defined: <ul style="list-style-type: none"><li>• <math>\epsilon_{11}</math> and <math>\epsilon_{22}</math> are set to <b>0.022</b></li><li>• <math>\epsilon_{33}</math> is set to <b>0.003</b></li></ul> |
| <b>Calculation Type (Precipitation Calculator)</b>                                    |  |
| Calculation type  | Isothermal   |
| Temperature   | 350° C   |
| Simulation time   | 10,000 seconds   |
| <b>Datasets (Experimental File Reader)</b>  |  |
| Borchers Mean radius vs Time and Borchers Number density vs Time                      | Data sets included with this example and imported to two Experimental File Readers. These data sets are used for the Mean Radius and Number Density plots, respectively.   |

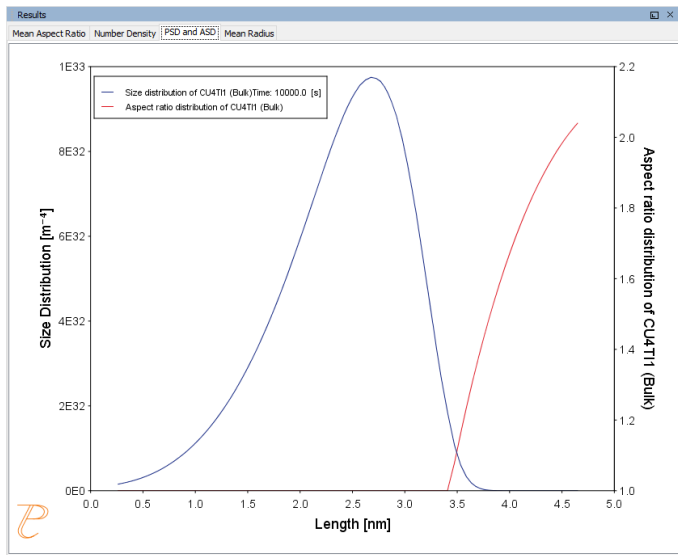
## Plot Results



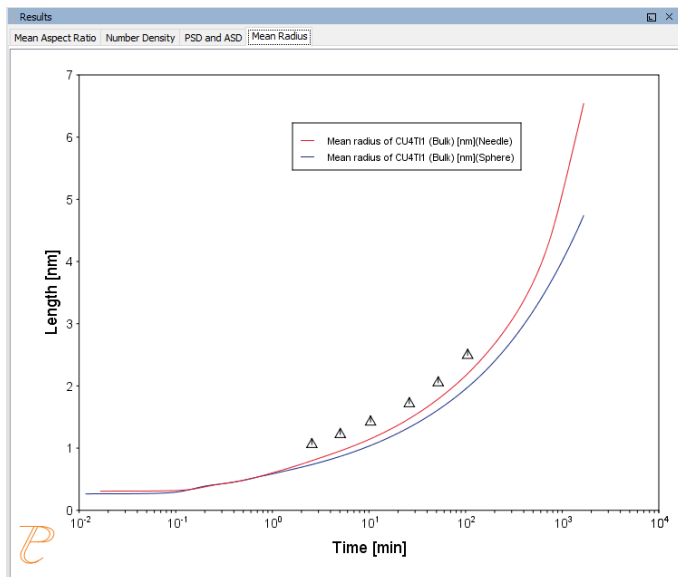
### Mean Aspect Ratio



## Number Density



## PSD and ASD



## Mean Radius

## References

[1987, Kampmann] R. Kampmann, H. Eckerlebe, R. Wagner, 1987. "Precipitation Kinetics in Metastable 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<sub>3</sub>Sc 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.

### 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

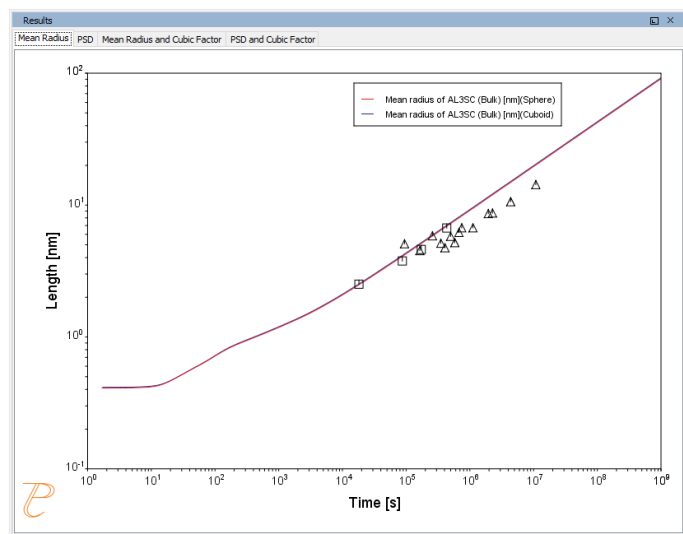


To ensure that the settings are done on the correct Precipitation Calculators, the **Sphere** and **Cuboid** nodes are renamed from **Precipitation Calculator** to match their morphology. The morphology is set in the **Precipitate Phase** section when you click **Show details**. See P\_08 for an example of this.

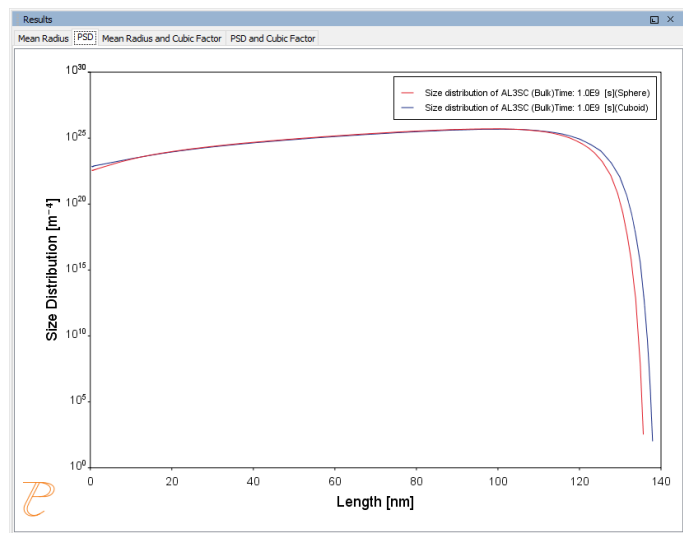
| System (System Definer)                                 |   |
|---|---|
| Database package  | Demo: Aluminum-based alloys (ALDEMO, MALDEMO) |
| Elements  | Al, Sc  |
| Sphere and Cuboid Conditions (Precipitation Calculator) |   |
| Composition   | Al-0.18Sc Mole percent                        |
| Matrix phase  | FCC_A1  |

|   |   |
|---|---|
| Precipitate phase   | AL3SC   |
| <b>Matrix Phase Data Parameters (Precipitation Calculator)</b>            |   |
| Elastic properties (click <b>Show details</b> to display this setting)    | <p>For the <b>Sphere</b> node (renamed from Precipitation Calculator), the default, <b>Disregard</b> is kept.</p> <p>For the <b>Cuboid</b> node (renamed from Precipitation Calculator), choose <b>Cubic</b>. 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</p> <ul style="list-style-type: none"><li>• c11 is <b>108.2</b> GPa</li><li>• c12 is <b>61.3</b> GPa</li><li>• c44 is <b>28.5</b> GPa</li></ul> |
| <b>Precipitate Phase Data Parameters (Precipitation Calculator)</b>       |   |
| Nucleation sites  | Bulk  |
| Interfacial energy  | The default   |
| Morphology (click <b>Show details</b> to display this setting)            | <p>For the <b>Sphere</b> node (renamed from Precipitation Calculator), keep the default.</p> <p>For the <b>Cuboid</b> node (renamed from Precipitation Calculator), <b>Cuboid</b> is selected.</p>  |
| Transformation strain (click <b>Show details</b> to display this setting) | <p>For the <b>Sphere</b> node (renamed from Precipitation Calculator), keep the default.</p> <p>For the <b>Cuboid</b> node (renamed from Precipitation Calculator), <b>Calculate from molar volume</b> is selected to obtain a purely dilatational strain.</p>  |
| <b>Calculation Type (Precipitation Calculator)</b>                        |   |
| Calculation type  | Isothermal  |
| Temperature   | 350° C  |
| Simulation time   | 1.0E9 seconds   |
| <b>Datasets (Experimental File Reader)</b>                                |   |
| Dataset 1 and Dataset 2   | Data sets included with this example and imported to one Experimental File Reader. It is used for the Mean Radius plot.   |

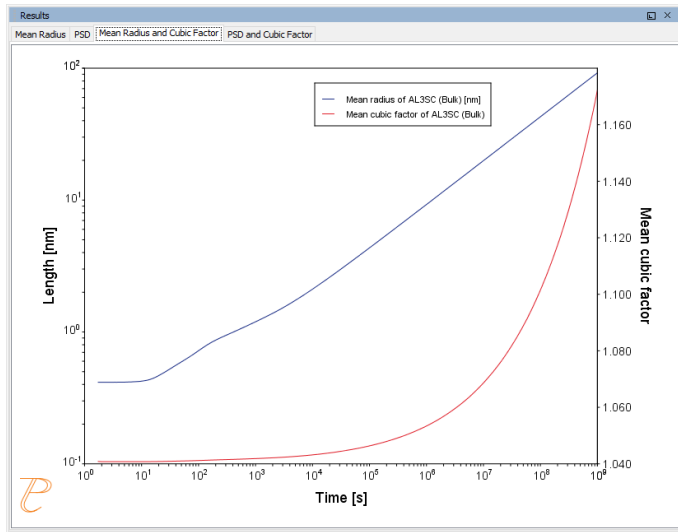
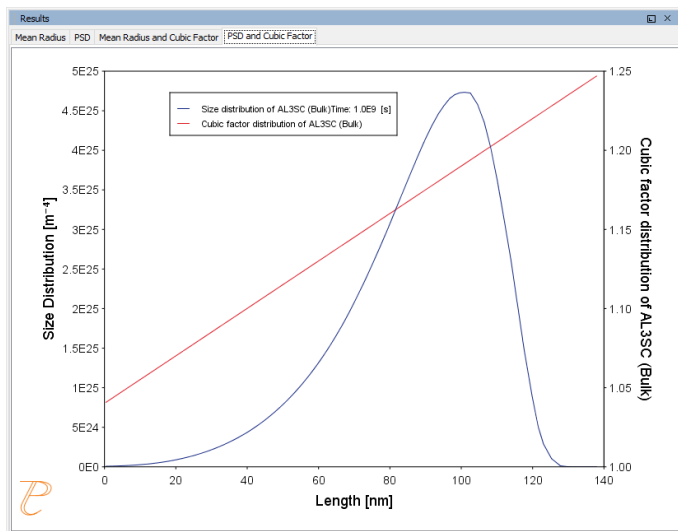
## Plot Results



### Mean Radius





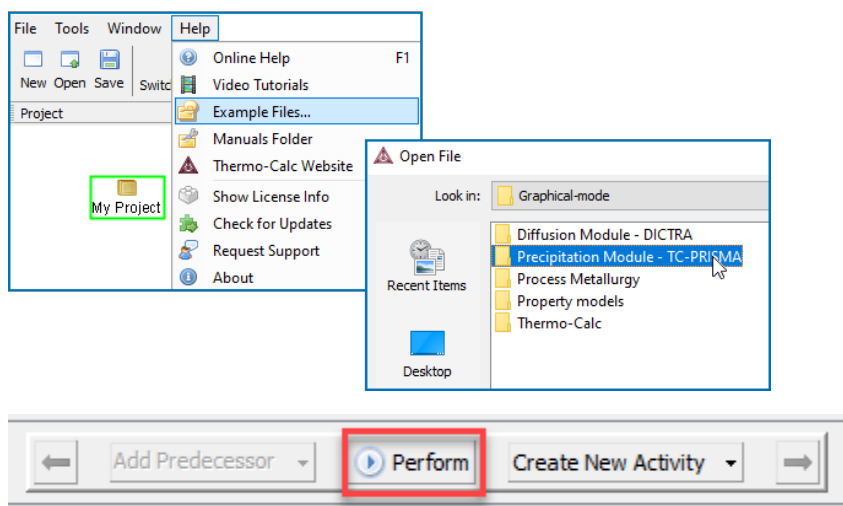
*Particle size distribution (PSD).**Mean Radius and Cubic Factor**Particle size distribution (PSD) and cubic factor.***References**

- [2001, Marquis] E. A. Marquis, D. N. Seidman, Nanoscale structural evolution of Al<sub>3</sub>Sc precipitates in Al (Sc) alloys. *Acta Mater.* 49, 1909–1919 (2001).
- [2001, Novotny] G. M. Novotny, A. J. Ardell, Precipitation of Al<sub>3</sub>Sc 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=PLfv6McToaTGSpgvuLoY3b\\_UV-8xpgLUKj](https://www.youtube.com/playlist?list=PLfv6McToaTGSpgvuLoY3b_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<sub>3</sub>Sc phase from FCC\_A1 matrix phase in an Al-Sc binary alloy using the Precipitation Module (TC-PRISMA).

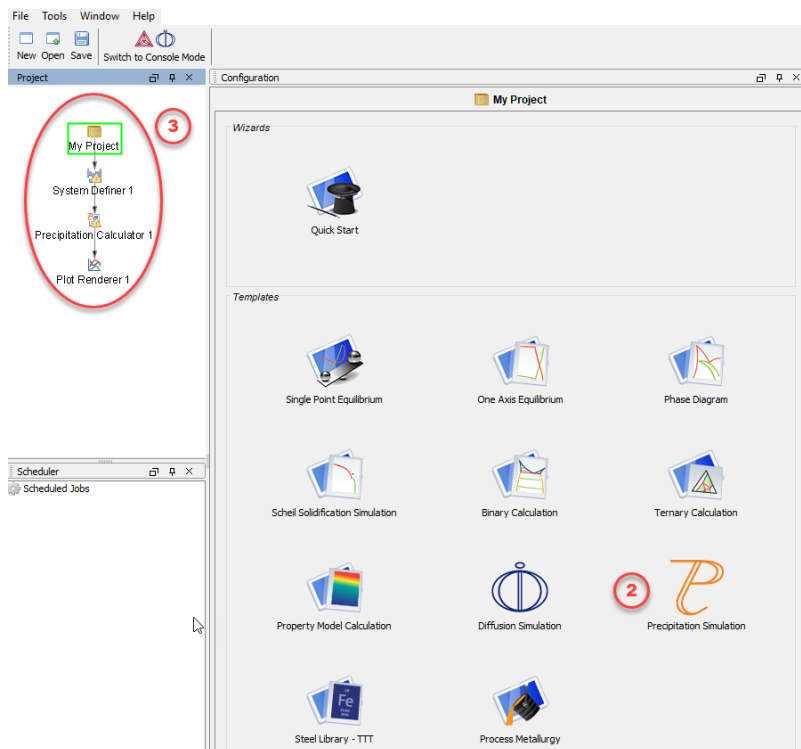
Two separate calculations are performed so you can make a comparison of the results, one assuming spherical morphology without elastic strain energy, and the other assuming cuboid morphology whose shape is determined by competition between interfacial energy and elastic strain energy.

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

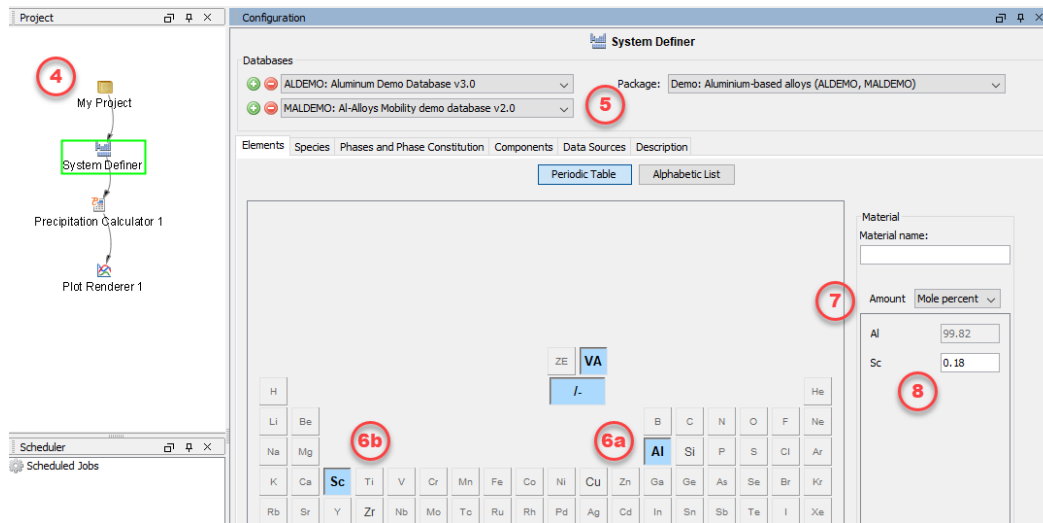
If you run the example file included in your software, the simulation results are compared with experimental data collected from Marquis and Seidman (2001) and Novotny and Ardell (2001).

## 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.



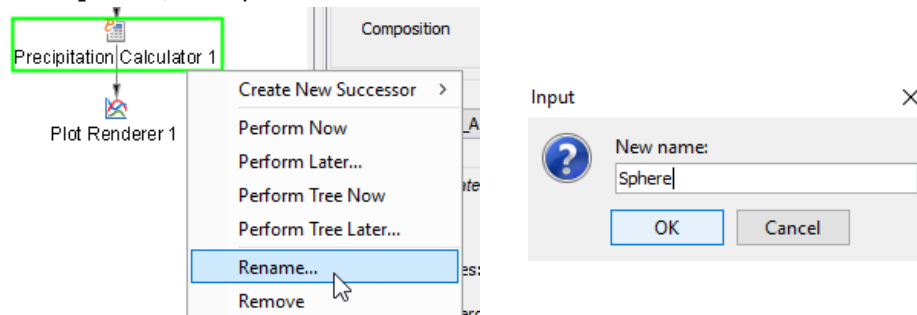
Our system is now defined. Now set up the precipitation calculations.

## SETTING UP THE PRECIPITATION CALCULATIONS

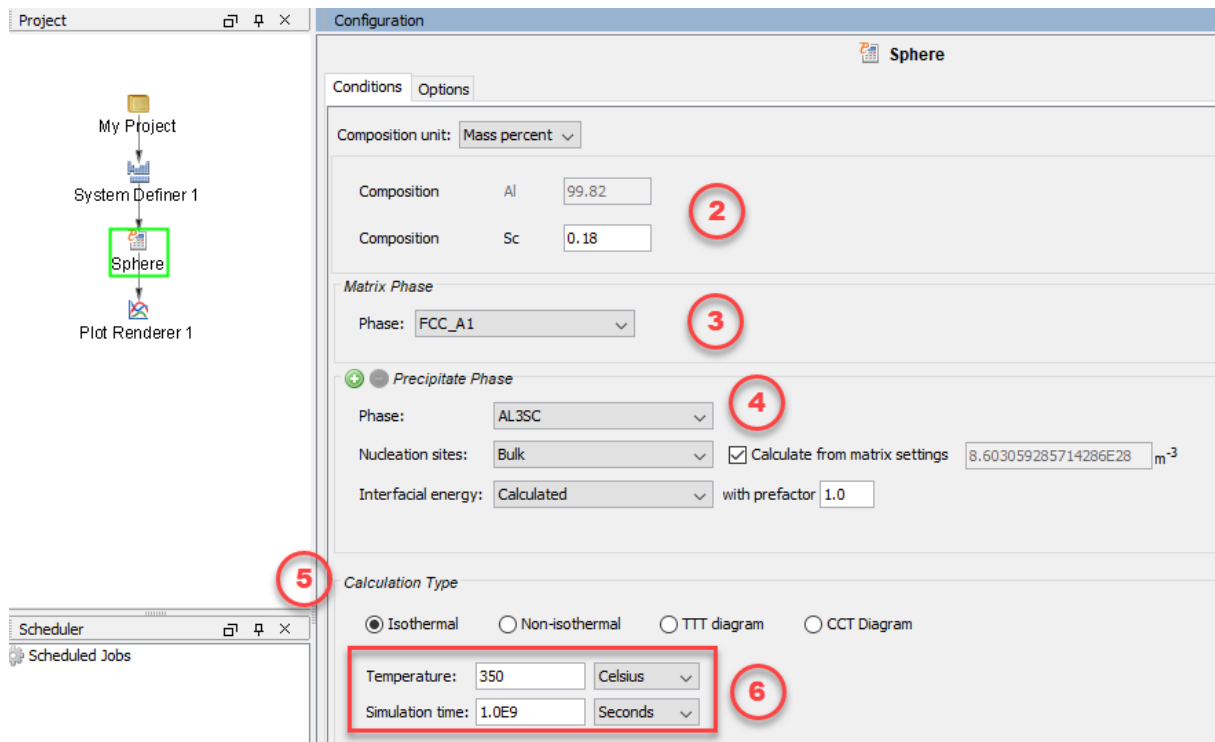
There are two precipitation calculations in this example, one assuming spherical morphology without elastic strain energy, and the other assuming cuboid morphology whose shape is determined by competition between interfacial energy and elastic strain energy. The results are then compared for both calculations.

### *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**.



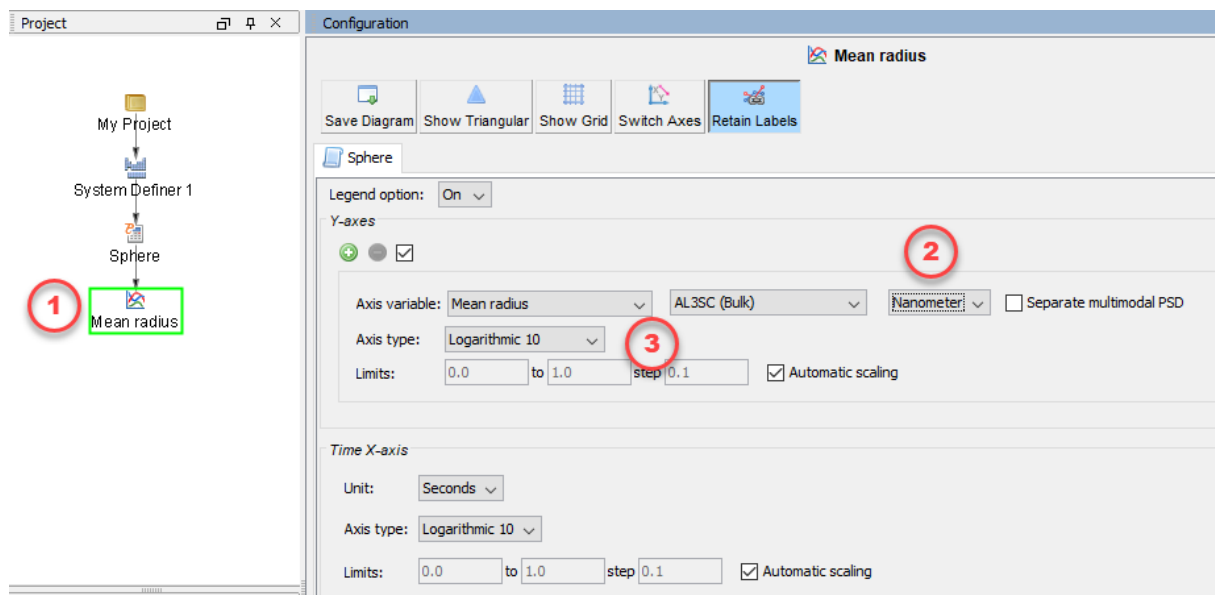
2. Notice that the composition set in the *System Definer* auto-populated on the Precipitation Calculator.
3. Under *Matrix Phase* from the *Phase* list it defaults to **FCC\_A1**.
4. Under *Precipitate Phase* from the *Phase* list select **AL3SC**.
5. Under *Calculation Type*, make sure **Isothermal** is selected, which means that the same temperature is maintained throughout the calculation.
6. Enter
  - a. 350 as the *Temperature* and select **Celsius**.
  - b.  $1.0 \times 10^9$  as the *Simulation time* and select **Seconds**.



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

### Configuring the Plot

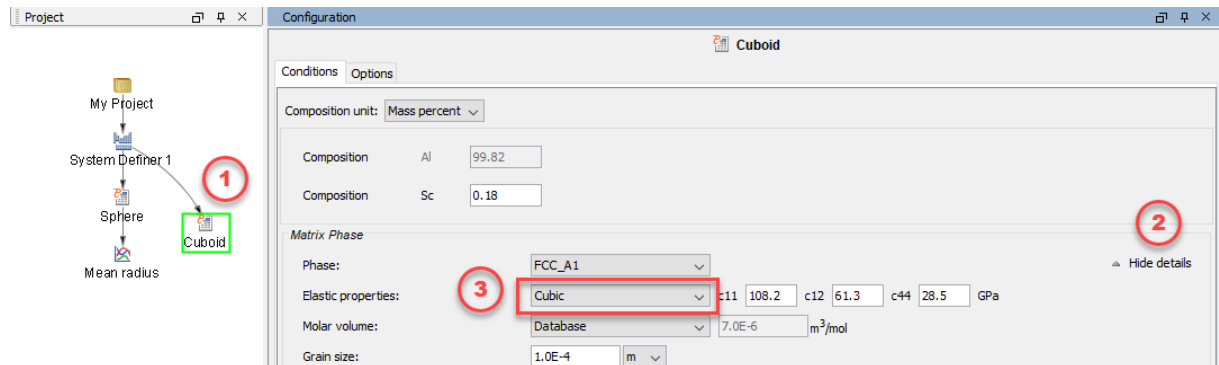
1. In the **Project** window, right-click **Plot Renderer 1** and select **Rename**. Name the plot **Mean radius** then press Enter or click **OK**.
2. Under **Y-axes** change the units to **Nanometer (nm)**.
3. From the **Axis type** list select **Logarithmic 10**.



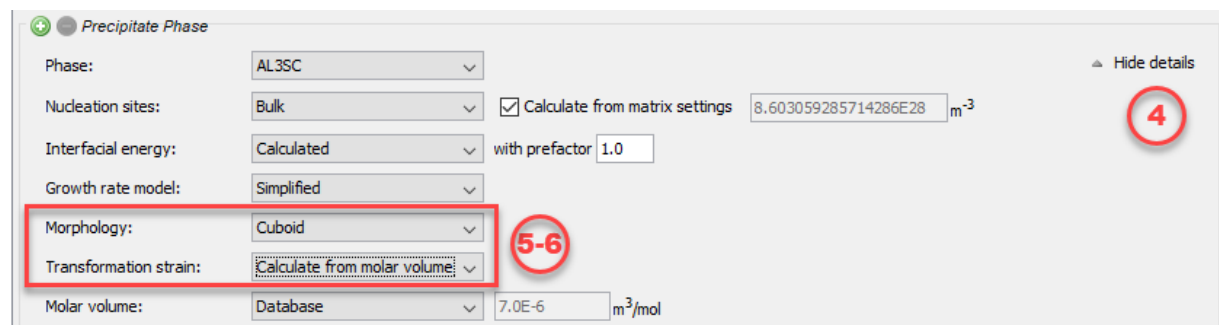
The plot is now set, but before running the simulation you set up another calculation and link it to the same Plot Renderer.

### Setting up the Precipitation Calculation with Cuboid Morphology

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



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

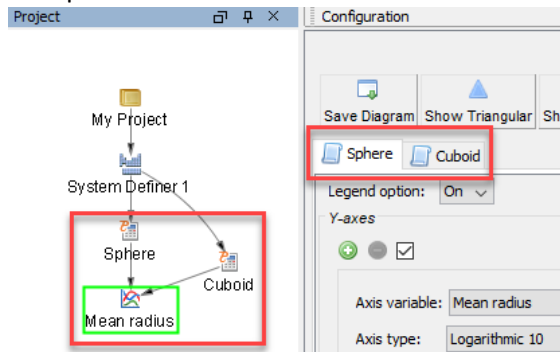


The second calculation is now set up, so now link it to the Plot Renderer node.

### Linking the Plot to the Calculation with Cuboid Morphology

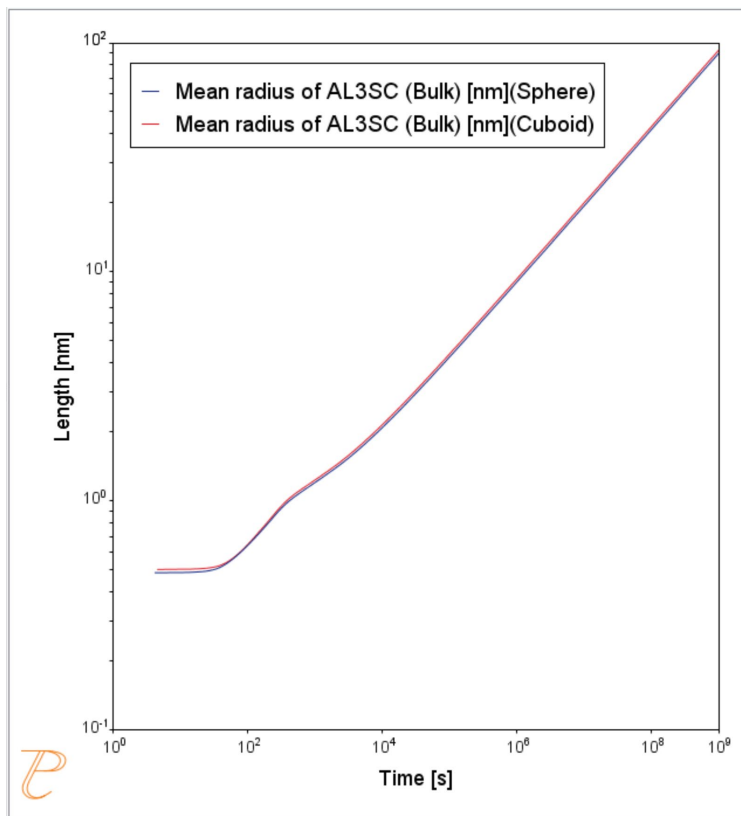
- In the **Project** window, right-click the **Mean radius** node and select **Add Predecessor** >**Cuboid**.
- Notice that in the **Configuration** window there are two tabs associated with this plot, one for **Sphere** and one for **Cuboid**. The Sphere settings are already configured, so you just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

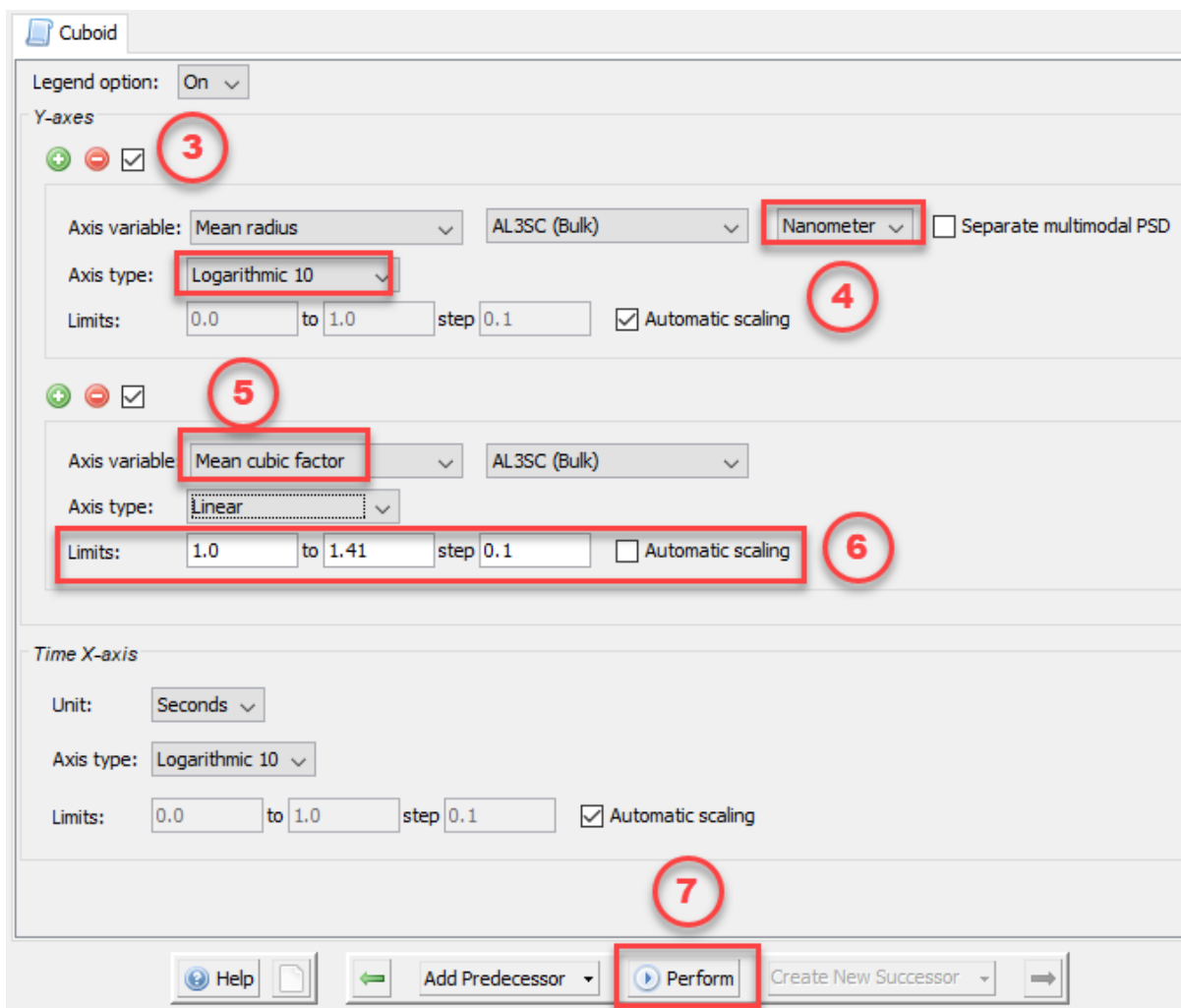
## PLOTTING ADDITIONAL VARIABLES

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*.

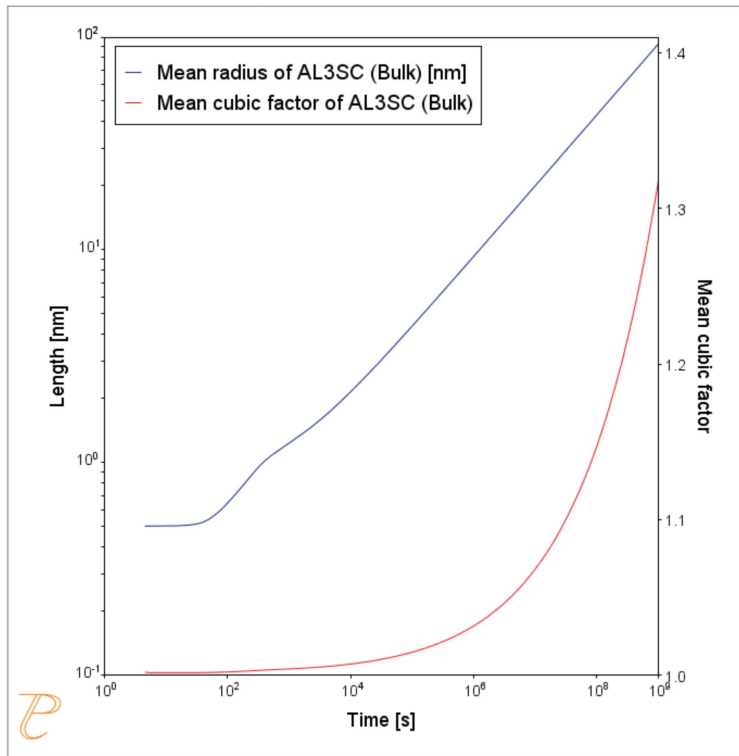
1. Right-click the **Cuboid** node and add a **Plot Renderer**.
2. Right-click the new node and rename it *Mean radius and Cuboid factor*.
3. Under *Y-axes* click the green plus sign to add another axis.
4. Keep *Mean radius* as the first axis variable but change the units to **Nanometers (nm)** and 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**.



The screenshot shows the 'Cuboid' plot configuration window. The 'Legend option' is set to 'On'. The 'Y-axes' section contains two axes. The first axis is 'Mean radius' with units 'Nanometer' and 'Logarithmic 10' axis type. The second axis is 'Mean cubic factor' with 'Linear' axis type. The 'Time X-axis' is set to 'Seconds' with 'Logarithmic 10' axis type. The 'Perform' button is highlighted.



### ***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.

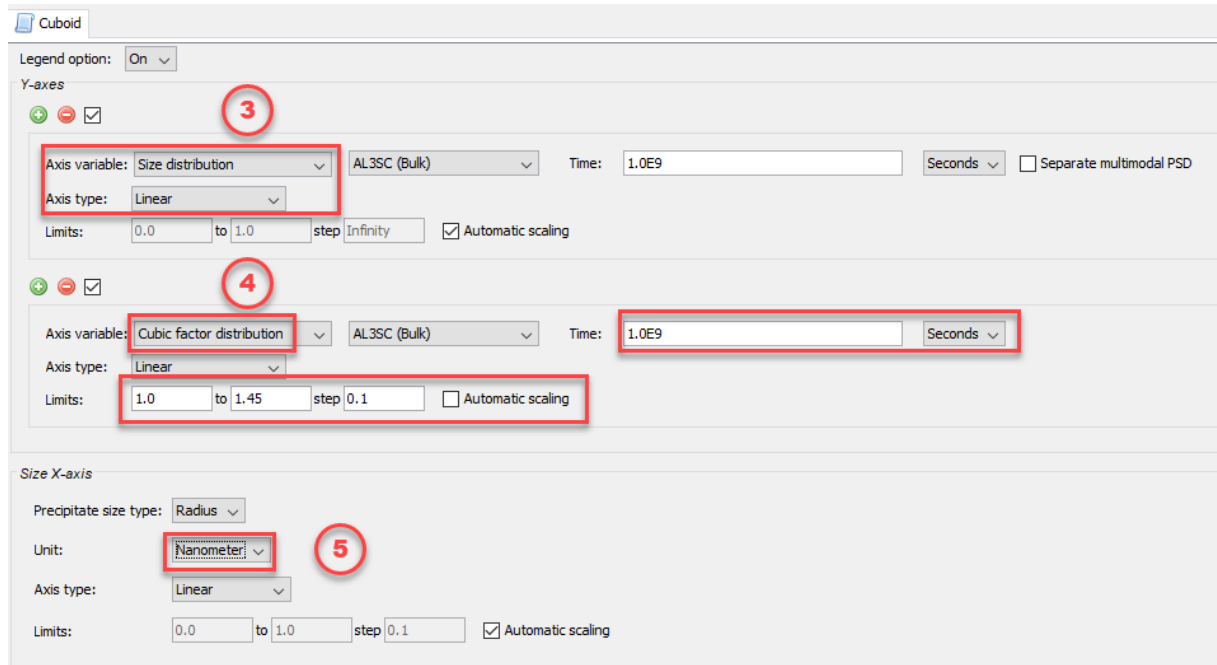
### ***Plotting Particle Size and Cubic Factor Distribution***

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.



**Y-axis 1 (Size distribution):**

- Axis variable: Size distribution
- Axis type: Linear
- Limits: 0.0 to 1.0 step Infinity
- Automatic scaling: ☒

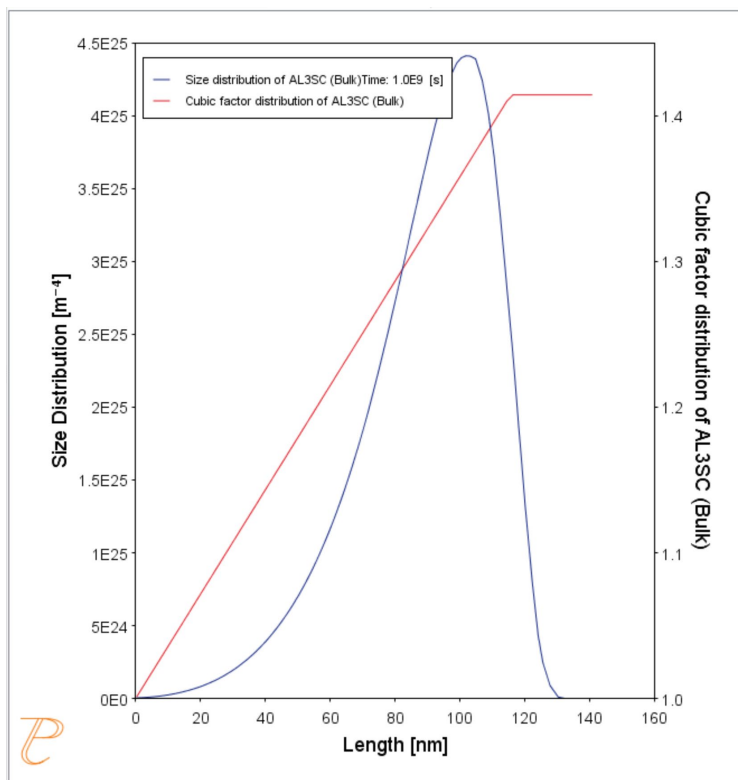
**Y-axis 2 (Cubic factor distribution):**

- Axis variable: Cubic factor distribution
- Axis type: Linear
- Limits: 1.0 to 1.45 step 0.1
- Automatic scaling: ☐

**Size X-axis:**

- Precipitate size type: Radius
- Unit: Nanometer
- Axis type: Linear
- Limits: 0.0 to 1.0 step 0.1
- Automatic scaling: ☒

### 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.

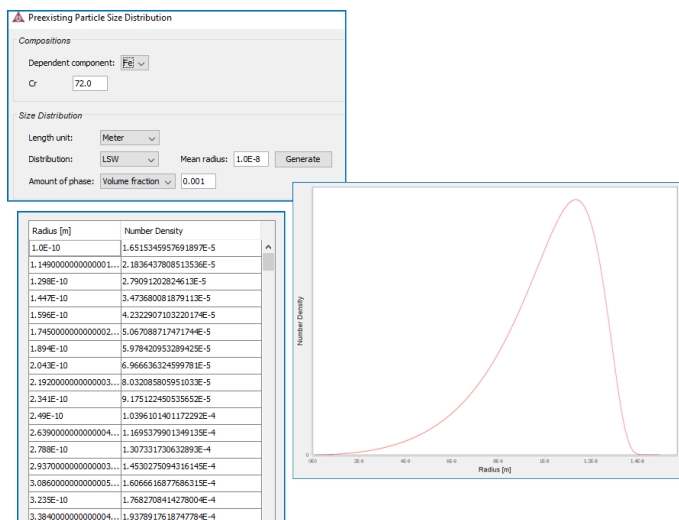
### ***References***

1. Marquis, E.A, and D.N Seidman. 2001. "Nanoscale Structural Evolution of Al<sub>3</sub>Sc Precipitates in Al(Sc) Alloys." *Acta Materialia* 49 (11): 1909–19.
2. Novotny, Gabriel M., and Alan J. Ardell. 2001. "Precipitation of Al<sub>3</sub>Sc 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.



The Preexisting Particle Size Distribution (PSD) settings window for example P\_10.

### 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

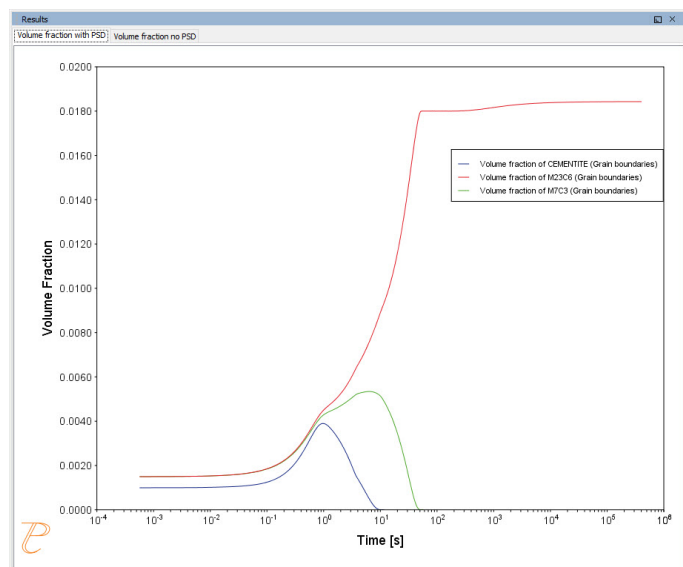
#### System (System Definer)

Database package

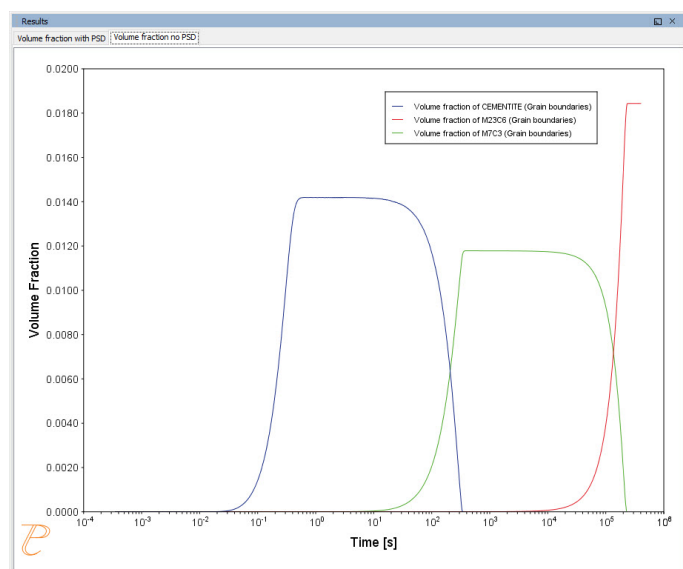
Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO)

|  |   |
|--|---|
| Elements   | Fe, C, Cr   |
| <b>Conditions (Precipitation Calculator)</b>   |   |
| Composition  | Fe-0.1C-12Cr Mass percent   |
| Matrix phase   | BCC_A2<br>All other defaults are kept.  |
| Precipitate phases   | CEMENTITE, M23C6 and M7C3   |
| <b>Precipitate Phase Data Parameters (Precipitation Calculator)</b>                  |   |
| 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): <ul style="list-style-type: none"><li>• CEMENTITE: 0.167 J/m<sup>2</sup></li><li>• M23C6 0.252 J/m<sup>2</sup></li><li>• M7C3 0.282 J/m<sup>2</sup></li></ul>  |
| Preexisting size distribution<br>(click <b>Show details</b> to display this setting) | For the Precipitation Calculator including particle size distribution, and for all precipitate phases, this check box is selected.<br><br>For each precipitate phase (CEMENTITE, M23C6 and M7C3), click <b>Edit particle size distribution</b> to make changes to the parameters. A window opens with a graphical representation of the radius vs number density. |
| <b>Calculation Type (Precipitation Calculator)</b>                                   |   |
| Calculation type   | Isothermal  |
| Temperature  | 1053 K  |
| Simulation time  | 400 000 seconds   |

## Plot Results



Volume fraction with initial particle size distribution (PSD).



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

## P\_11: Interfacial Energy Function

In some cases, interfacial energy may be a function of temperature and/or particle radius. This example uses four Precipitation Calculators at four temperature points in 30 K increments: 673 K, 703 K, 733 K, and 763 K. It is an isothermal calculation to examine the mean radius of an Al-0.12Sc system. It uses an FCC\_A1 matrix phase and Al3Sc precipitate phase with bulk nucleation sites and user-defined interfacial energy function. The user defined interfacial energy function uses an error function to set a smooth transition of the interfacial energy from 0.065 J/m<sup>2</sup> to 0.085 J/m<sup>2</sup> for particle radii below and above 1e-8m and 5e-8m, respectively.

A dataset based on Iwamura and Miura (<sup>1</sup>) data is compared with the calculated results.

### 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<br>All other defaults are kept.        |

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

Precipitate phase

AL3SC

Nucleation sites (all calculations): Bulk ( $6.025 \times 10^{28} \text{ m}^{-3}$ )Interfacial energy (all calculations): User-defined function  $f(r,T)$ :  $0.075 + 0.011 \cdot \text{erf}((r - 3 \times 10^{-8}) / 1 \times 10^{-8} \text{ J/m}^2)$ **Calculation Type (Precipitation Calculator)**

Calculation type

Isothermal (all calculations)

Temperature

Four temperature points in 30 K increments: 673 K, 703 K, 733 K, and 763 K.

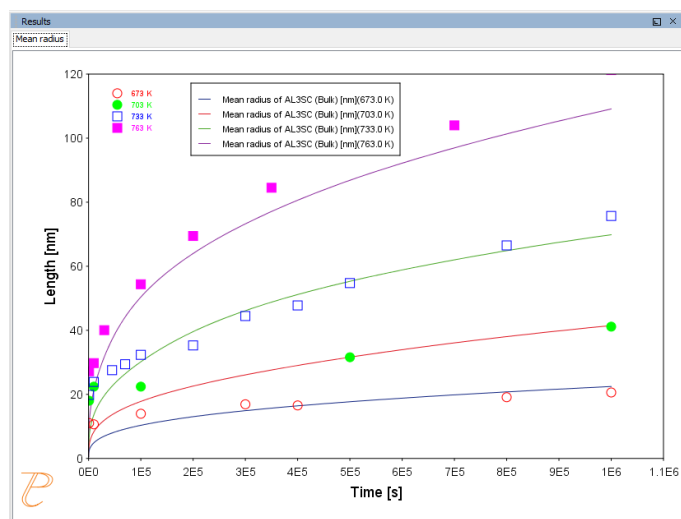
Simulation time

1 000 000 seconds (all calculations)

**Datasets (Experimental File Reader)**

Wamura 2004 (Dataset 1)

Data set included with this example and imported to one Experimental File Reader.

**Plot Results**

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



## 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 Knippling et al. [2008] data is compared with the calculated results.

### 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.

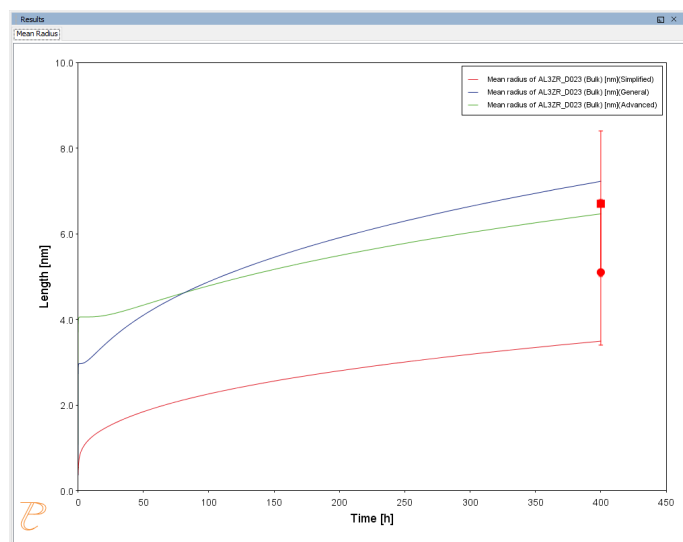
### Example Settings

#### System (System Definer)

|                  |   |
|------------------|---|
| Database package | Demo: Aluminum-based Alloys (ALDEMO, MALDEMO) |
|------------------|---|

|  |  |
|--|--|
| Elements   | Al, Zr   |
| <b>Conditions (Precipitation Calculator)</b>       |  |
| Composition  | Al-0.2Zr Mole percent  |
| Matrix phase                                       | FCC_A1<br>All other defaults are kept.   |
| Precipitate phase                                  | AL3ZR_D023<br>Click <b>Show details</b> to select the <b>Growth rate model (Simplified, Advanced and General)</b> . All other defaults are kept. |
| <b>Calculation Type (Precipitation Calculator)</b> |  |
| Calculation type                                   | Isothermal   |
| Temperature  | 425 Celsius  |
| Simulation time                                    | 400 hours  |
| <b>Datasets (Experimental File Reader)</b>         |  |
| 2008 Knipling                                      | Data set included with this example and imported to one Experimental File Reader.  |

## Plot Results



Result comparing the mean radius of the spheres for each AL3ZR\_D023 precipitate phase calculated for each type of growth rate model.

## 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.

### Project File and Video Tutorial Information

- Folder: Precipitation Module - TC-PRISMA
- File name: *P\_13\_Precipitation\_Fe-C-Cr\_Paraequilibrium\_Precipitation\_of\_Cementite.tcu*



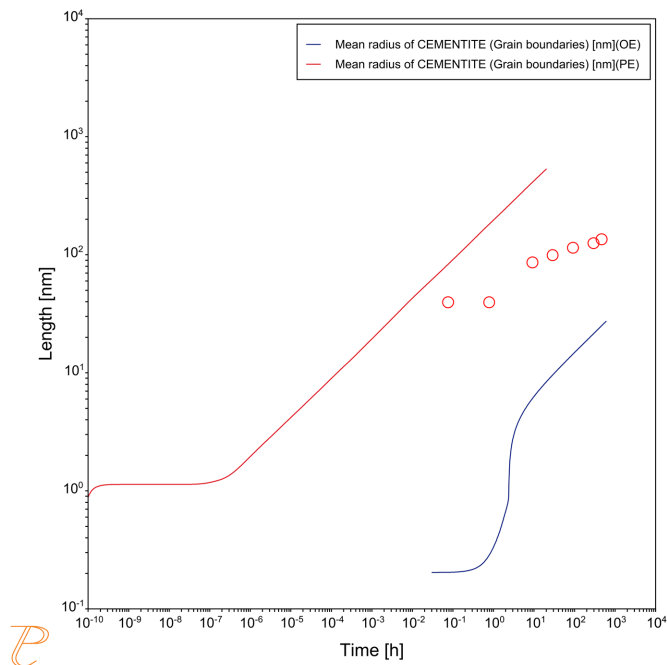
Also see [our website](#) and [YouTube channel](#) for other examples of the Precipitation Module.

### 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<br>All other defaults are kept.       |

|  |   |
|--|---|
| Precipitate phase                                  | CEMENTITE<br>Click <b>Show details</b> to select the <b>Growth rate model (Simplified and Para-eq)</b> . All other defaults are kept. |
| <b>Calculation Type (Precipitation Calculator)</b> |   |
| Calculation type                                   | Isothermal  |
| Temperature  | 773 Kelvin  |
| Simulation time                                    | 20 hours for the paraequilibrium model and 600 hours for the simplified model.  |
| <b>Datasets (Experimental File Reader)</b>         |   |
| 1980 Sakuma  | Data set included with this example and imported to one Experimental File Reader.   |

## Plot Results



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

## 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).