Precipitation Module (TC-PRISMA) User Guide

Thermo-Calc Version 2026a

Thermo-Calc Software AB

Råsundavägen 18, SE-169 67 Solna, Sweden

+46 8 545 959 30

https://thermocalc.com/

Contents

Introduction to the Precipitation Module (TC-PRISMA) 5

About the Precipitation Module (TC-PRISMA) 6

Available Options 9

Network License Restrictions 12

Help Resources: Installed and Web Versions 13

Typographical Conventions 15

Using the Precipitation Calculator 19

Precipitation Calculator 20

Define the Precipitation Calculator 22

Matrix Phase Settings 23

Selecting the Disordered Phase as a Matrix Phase 29

Precipitate Phase Settings 30

Particle Size Distribution (PSD) 37

Calculation Type Settings 43

Precipitation Calculator Thermal Profile 45

Guidelines for Importing Data Files to Thermal Profiles 49

Options Tab 51

Precipitation Calculator Plot Renderer 57

Quantities Groups Available for Plots and Tables 65

Pause, Resume, and Cancel Precipitation Calculations 73

Theoretical Models and Numerical Methods 76

Theory Overview 77

Nucleation Theory 79

Homogeneous Nucleation 80

Heterogeneous Nucleation 87

Nucleation During a Non-isothermal Process 93

Growth 94

Coarsening 104

Continuity Equation 105

Mass Conservation 106

Numerical Method 107

Estimation of Coherent Interfacial Energy 112

Precipitation Morphology 113

Normal Grain Growth 116

Stereology 121

Microstructure Descriptions 128

Precipitation Module (TC-PRISMA) References 129

Precipitation Module (TC-PRISMA) Examples Collection 132

P_01: Isothermal Precipitation of Al3Sc 134

P_02: Stable and Metastable Carbides - Isothermal 139

P_03: Stable and Metastable Carbides - TTT Diagram 143

P_04: Precipitation of Iron Carbon Cementite 147

P_05: Precipitation of γ’ in Ni Superalloys - Isothermal 150

P_06: Precipitation of γ’ in Ni Superalloys - Non-isothermal 155

P_07: Continuous Cooling Transformation (CCT) Diagram of Ni-Al-Cr γ-γ’ 162

P_08: Precipitation of Cu-Ti CU4TI with Assumptions of Sphere and Needle Morphologies 165

P_09: Precipitation of Al-Sc AL3SC with Assumption of Sphere and Cuboid Morphologies 172

P_10: Initial Particle Size Distribution of Fe-Cr-C 178

P_11: Interfacial Energy Function 185

P_12: Comparing Growth Rate Models for an Al-Zr System 189

P_13: Paraequilibrium Precipitation of Cementite Fe-C-Cr 193

P_14: Grain Growth and the Zener Pinning Effect 197

P_15: Smooth Transition from Paraequilibrium to Ortho-equilibrium 202

P_16 Isothermal Coarsening and a 3D to 2D Stereological Conversion 207

Introduction to the Precipitation Module (TC-PRISMA)

In this section:

About the Precipitation Module (TC-PRISMA) 6
Available Options 9
Network License Restrictions 12
Help Resources: Installed and Web Versions 13
Typographical Conventions 15

About the Precipitation Module (TC-PRISMA)

The Precipitation Module, or TC-PRISMA, is an Add-on Module to Thermo-Calc and it is available in Graphical Mode as the *Precipitation Calculator*.

The Module treats concurrent nucleation, growth/dissolution and coarsening under arbitrary heat treatment conditions in multi-component and multi-phase systems using Langer-Schwartz theory and the Kampmann-Wagner numerical approach. It is a general computational tool for simulating kinetics of diffusion controlled multi-particle precipitation processes in multicomponent and multiphase alloy systems.

You can use the Precipitation Module for:

- Concurrent nucleation, growth/dissolution and coarsening of precipitates
- Normal grain growth and Zener pinning
- Temporal evolution of particle size distribution
- Average particle radius and number density
- Volume fraction and composition of precipitate
- Nucleation rate and coarsening rate
- Time-Temperature-Precipitation (TTP) diagrams
- Continuous-Cooling-Transformation (CCT) diagrams
- Estimation of multi-component interfacial energy
- Estimation of yield stress using the Yield Strength Property Model

The configuration of the Yield Strength Property Model is completed on the Property Model Calculator and then accessed as a variable with the Plot Renderer or Table Renderer.

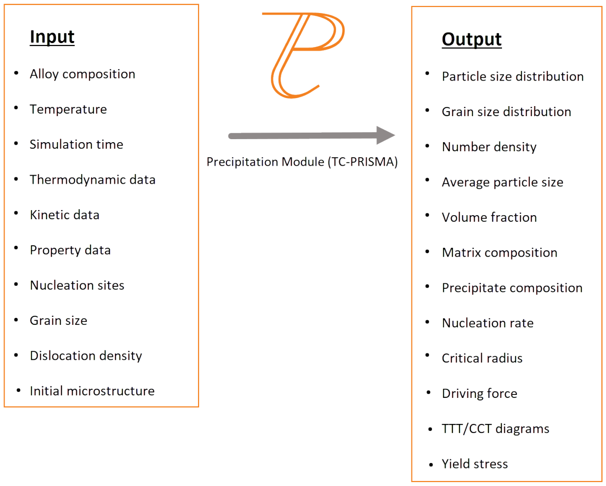
In order to perform a simulation in the Precipitation Module, both a thermodynamic database and a kinetic database is needed. The thermodynamic database is a normal Thermo-Calc database, whereas the kinetic database contains information about the atomic mobility of individual elements in various phases.

Precipitation, formation of particles of a second phase, or second phases from a supersaturated solid solution matrix phase, is a solid state phase transformation process that has been exploited to improve the strength and toughness of various structural alloys for many years. This process is thermochemically driven and fully governed by system (bulk and interface) thermodynamics and kinetics.

Typically, a precipitation process has three distinctive stages: nucleation, growth, and coarsening. However, under certain conditions, these can also happen at the same time. With the Precipitation Module, the kinetics of concurrent nucleation, growth, and coarsening can be simulated by calculating the evolution of the probability distribution of the particle number densities, usually called particle size distribution (PSD). The simulation results can be used to understand and guide how to obtain desirable precipitates with certain PSD or to avoid undesirable precipitations during heat treatments of alloys such as aging and tempering.

A summary for the input and output of the Precipitation Module is shown.

Input and Output of the Precipitation Module



The Precipitation Module relies on CALPHAD-based software tools and databases to provide the necessary bulk thermodynamic and kinetic data for phases in multicomponent systems. The CALPHAD approach has been developed for more than 50 years and is routinely applied to design new alloys and optimize existing materials within various metal industries, such as steels and alloys of nickel, titanium, aluminum and magnesium.

The power of this approach is due to the adopted methodology where free energy and atomic mobility of each phase in a multicomponent system can be modeled hierarchically from lower order systems, and model parameters are evaluated in a consistent way by considering both experimental data and ab-initio calculation results. The Precipitation Module is directly integrated into Thermo-Calc, a CALPHAD-based computer program for calculating phase equilibrium. Another Add-on Module, the Diffusion Module (DICTRA) is available for diffusion controlled phase transformation in multicomponent systems.

With Thermo-Calc and the accompanying thermodynamic and mobility databases, almost all fundamental phase equilibrium and phase transformation information can be calculated without unnecessary and inaccurate approximations. For example you can calculate:

- Driving forces for nucleation and growth
- Operating tie-lines under local equilibrium conditions
- Deviations from local equilibrium at interfaces due to interface friction
- Atomic mobilities or diffusivities in the matrix phase

In addition to bulk thermodynamic and kinetic data, a few other physical properties, such as interfacial energy and volume, are needed in precipitation models. These additional physical parameters can be obtained by experiments or other estimation models or first principles calculations. Volume data are available in most of our thermodynamic databases . The Precipitation Module has an estimation model available for interfacial energy.

This guide is a supplement to the full Thermo-Calc documentation set. It is recommended that you use the Online Help, which you can access in Thermo-Calc by pressing F1 or from the main menu choose **Help** → **Online help**.

See "Help Resources: Installed and Web Versions" on page 13 to learn how to access this information if you have not already done so.

Available Options

The Precipitation Module, previously referred to as TC-PRISMA, is an Add-on Module to the core Thermo-Calc software.

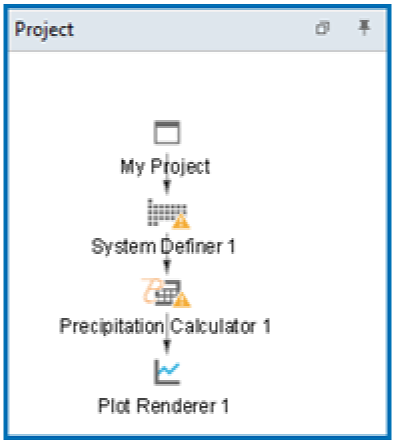
A separate license is required to perform calculations for more than three elements. Without it you are able to use the module in *Demo Mode*.

Precipitation Template

A **Precipitation** template under **Non-Equilibrium Calculations** is available to all Thermo-Calc users when in Graphical Mode. If you are in DEMO mode then this is indicated by the addition of **DEMO** text.

Using the Template

After opening Thermo-Calc in Graphical Mode, in the templates section under **Non-Equilibrium**, click the **Precipitation** button to add a *System Definer*, *Precipitation Calculator*, and *Plot Renderer* to the **Project** tree.

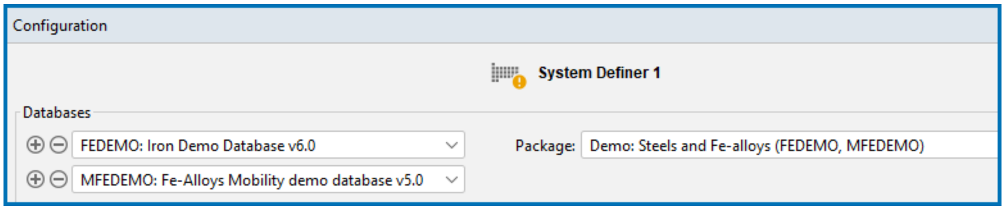


Precipitation Calculator

A Precipitation Calculator allows you to set the conditions for, and perform, a precipitation calculation.

Demo Database Packages for the Examples Collection

Both a thermodynamic and mobility database are required to run the Precipitation Module simulation. If you have a Precipitation Module (TC-PRISMA) license you can run all the examples as the demonstration database packages are included with your installation. Select the database packages from the **System Definer** → **Configuration** window to run a simulation.



Databases
FEDEMO: Iron Demo Database v6.0
MFEDEMO: Fe-Alloys Mobility demo database v5.0
Package: Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)

Demonstration (Demo) Mode

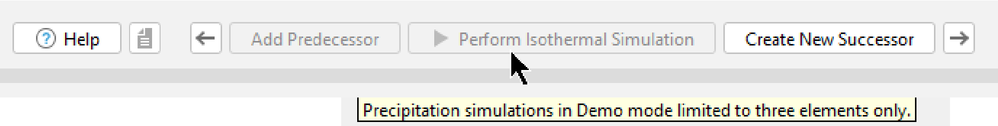
The Precipitation Module, and some examples, are available to all Thermo-Calc users but only for simulations of alloys with up to three elements. If you do not have a license for the Precipitation Module then you are in *Demonstration Mode* when using the Precipitation Calculator or Precipitation Simulation template.

A **Precipitation** template under **Non-Equilibrium Calculations** is available to all Thermo-Calc users when in Graphical Mode. If you are in DEMO mode then this is indicated by the addition of **DEMO** text.

Precipitation Calculator

If you are experimenting with the Precipitation Calculator in Demo Mode, you may have access to a variety of databases based on your license. However, you can only define up to three elements for a demo simulation.

If you define more than three elements on the System Definer, when you go to the Precipitation Calculator, the **Perform** button is unavailable and the tooltip explains why. In this case one of the chosen elements needs to be removed and then the Perform button is made available.



Precipitation simulations in Demo mode limited to three elements only.

Even if you have more than three elements, the Plot Renderer or Table Renderer **Perform** button is still available. However, if you click the button and try to run the simulation the Event Log displays an error message.

Additive Manufacturing (AM) Module

There is connectivity between the Diffusion Module (DICTRA) or the Precipitation Module (TC-PRISMA) and the Additive Manufacturing (AM) Module when you have full licenses available for all relevant Add-on Modules and databases.

You can add a Diffusion Calculator or Precipitation Calculator as a successor to the AM Calculator and then when probes are included with the AM Calculator this data can be further used with the thermal profile.

Network License Restrictions

The Precipitation Module (TC-PRISMA) requires a separate license. If you are using a network client installation of Thermo-Calc, then you may not be able to use it even if you have access to a license server with a valid network license file. The reason for this is because other clients who are part of your network installation may have checked out all instances of the network license allowed to run simultaneously.

For users with a network license, you must exit Thermo-Calc to release the license for other users. The license is checked out as soon as you add a Precipitation Calculator and remains unavailable to other users until you exit the program.

With a network license, and if as per above you temporarily do not have access to a license, you are automatically put into *Demo Mode*. Then the Precipitation Calculator is available with three elements.

Search the online help or see the *Thermo-Calc Installation Guide* for more about network licenses.

Help Resources: Installed and Web Versions

The technical content is available in HTML format as an Online Help system that you can access from two locations. Both versions are viewed in your browser.

Go to these locations to access the same content:

- **Locally Installed Help**: When in Thermo-Calc, press F1 to open the current version of the help in a local browser. You can also click **Online Help** from the **My Project** page to open the file. Then search or navigate to the applicable folder to browse the contents. This does not not require an Internet connection.
- **Web Help**: Go to the Documentation page to link to the most recent version of the web help. Then search or navigate to a relevant folder to browse the contents.

> Between releases there may be minor updates to the web version compared to the installed version. All updates made to the web version are included in the next installed release version.

> There are several resources available on our website to help you learn how to use Thermo-Calc and other Add-on Modules. Go to the Getting Started Guides page and choose one of the guides that provides new users an introduction to setting up simple calculations in Graphical Mode. The information there is also in this help documentation.

Opening the Web Version of the Help

A web version **specific to only the most recent release version** is available at https://help.thermocalc.com/2026a/content/intro/help-home.htm

Opening the Installed Help: No Internet Required

There are several ways to access online help in a browser. The content opens in a browser but uses local content so you do not need an Internet connection except for links to external websites.

First open Thermo-Calc, then choose one of these options to go to the local browser version of the help:

- Press <F1> on the keyboard.
- Select **Help →** **Online Help**.
- On the **My Project Configuration** window, click **Online Help**.
- At the bottom of any **Configuration** window, click **Help**.

Typographical Conventions

The following typographical conventions are used throughout the documentation, both online and in the PDF documents.

Text

Convention	Definition
Forward arrow symbol →	The forward arrow symbol → instructs you to select a series of menu items in a specific order. For example, **Tools → Options** is equivalent to: From the **Tools** menu, select **Options**.
Boldface font	A **boldface** font indicates that the given word(s) are shown that way on a toolbar button or as a menu selection. For example, if you are told to select a menu item in a particular order, such as **File → Save Project**, or to click **Save**.
Italic font	An *italic* font in the body of the text indicates the introduction of important terminology. Expect to find an explanation in the same paragraph or elsewhere in the guide.
COMMAND	For features in Thermo-Calc that use Console Mode (i.e. the command line), this font and all capital letters indicates that this is a Console Mode COMMAND. Examples of how you can use a command are written with code font. For example: Use DEFINE_ELEMENTS followed by a list of the elements that you want in your system. (To list the elements that are available in your current database, use LIST_DATABASE and choose `Elements`).
HELP	Text in blue and underline and a page number is a link to another topic in the current or referenced guide. Command names are often also topics. Clicking the link takes you to more detail about a particular command or subject in the PDF or documentation set.
<Enter>	Text with <angle brackets> indicates a keyboard entry. Usually to press <Enter> (or Return) or to use a series of keys such as <Ctrl + S>.
`code` and **`code bold`**	A `code` font shows a programming code or code example. The **`code bold`** font highlights the entry. It is also used for file names or paths to help distinguish it from other text. e.g. • For Windows users, the documents, materials, examples and other folders that sometimes require additional licenses are installed in C:\Users\Public\Public Documents\Thermo-Calc\<*version*>."
click vs press	In general, you *click* with the mouse to perform an action on the screen (e.g. click **Save**) and you *press* keys on a keyboard to enter a set of commands (e.g. press Ctrl+S).

Convention	*Definition*
	>_ When working in Console Mode, you can use keyboard shortcuts. Sometimes a window opens where you have the option to **Save**, **Cancel** or **Open** a file, for example. In these cases the instructions might say *click* Save, whereas you would need to *press* the applicable keys to perform the action.

Icons

Convention	*Definition*
Important	! Provides important information. It is recommended that you read the text or follow the link.
License Required	🔑 This indicates that additional licenses are required for the feature, database, or example.
Note	📄 The information can be of use to you. It is recommended that you read the text or follow the link to more information.
Time	⌛ Indicates that something you are going to do will take some time, usually related to running an example.
Tip	💡 This is general information that can be of use but is not required knowledge.

Convention	*Definition*
Read More	Read more at the link, which may be to our website or another source of general information.
See More	Go to the link or guide to see more general information about the topic being discussed.
Training	Indicates there may be training opportunities available, usually related to a specific feature.
Link to more information	Click the link to more information in the content.
Examples	Go to the example collection to learn more.
Console Mode	This note relates specifically to something in Console Mode.
Video	Indicates there is a video tutorial on our website, usually in relation to an example.
Graphical Mode	This note relates specifically to something in Graphical Mode.
Diffusion Module (DICTRA)	This indicates that the information relates to the Add-on Diffusion Module (DICTRA).
Precipitation Module (TC-PRISMA)	This indicates that the information relates to the Add-on Precipitation Module (TC-PRISMA).
Process Metallurgy Module	This indicates that the information relates to the Add-on Process Metallurgy Module.

Convention	***Definition***
Property Models	This indicates that the information relates to the Property Models. This includes all material specific libraries, i.e. Steel Model Library, Nickel Model Library, etc. as well as the general Models included with all installations.
Additive Manufacturing (AM) Module	This indicates that the information relates to the Add-on Additive Manufacturing (AM) Module.

Using the Precipitation Calculator

In this section:

Precipitation Calculator 20

Define the Precipitation Calculator 22

Matrix Phase Settings 23

Selecting the Disordered Phase as a Matrix Phase 29

Precipitate Phase Settings 30

Particle Size Distribution (PSD) 37

Calculation Type Settings 43

Precipitation Calculator Thermal Profile 45

Guidelines for Importing Data Files to Thermal Profiles 49

Options Tab 51

Precipitation Calculator Plot Renderer 57

Quantities Groups Available for Plots and Tables 65

Pause, Resume, and Cancel Precipitation Calculations 73

Precipitation Calculator

The Precipitation Calculator is available with three elements if you do not have the additional Precipitation Module (TC-PRISMA) license. With the Add-on Module you can use all available elements. See "Available Options" on page 9 for details about this and other options available with additional licenses.

A **Precipitation Calculator** allows you to set the conditions for, and perform, a precipitation calculation. You can add the calculator to the System Definer directly (right-click and select it from the **Create New Successor** menu)

There is also a **Precipitation** template available under **Non-Equilibrium** that you can use to quickly set up a simulation.

Once you have added a Precipitation Calculator, the **Configuration** window has **Conditions** and **Options** settings tabs where there are many available conditions to set and then continue the settings with the specialized **Plot Renderer**.

Conditions

Set the conditions for your calculation that define the *Matrix phase* and *Precipitate phase*. Choose the *Calculation Type*.

"Matrix Phase Settings" on page 23

"Precipitate Phase Settings" on page 30

"Calculation Type Settings" on page 43

Options

Modify *Numerical Parameters* that determine how the conditions are calculated.

"Options Tab" on page 51

Plot Renderer

There are also unique settings available for this calculator once you add a "Precipitation Calculator Plot Renderer" on page 57.

Working with these simulations is an advanced topic. It is recommended you review the documentation and videos available or search for a specific topic.

"Precipitation Module (TC-PRISMA) Examples Collection" on page 132

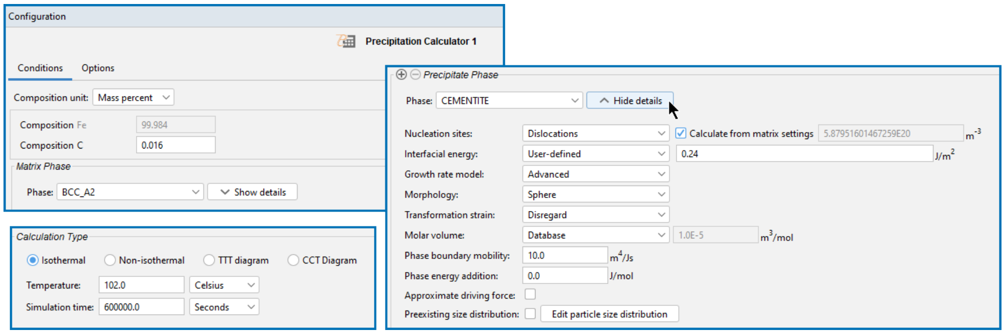
Define the Precipitation Calculator

1. Add a **Precipitation Calculator** node to the System Definer. If you used the **Precipitation** template (on the 🗀 **My Projects Configuration** window under **Non-Equilibrium**), click the node to display the **Configuration** settings window.
2. In the Precipitation Calculator **Configuration** window, enter the settings on the **Conditions** and **Options** tabs. These are described separately:
   - Matrix Phase
   - Precipitate Phase
   - Calculation Type and "Precipitation Calculator Thermal Profile" on page 45
   - Options Tab Advanced Settings
3. Once you have finished defining the Precipitation Calculator, you also choose settings on the **Plot Renderer**. Some additional settings are specific to the "Precipitation Calculator Plot Renderer" on page 57.

Matrix Phase Settings

Below are details about the settings available for the *Composition* and *Matrix Phase*, which is selected from the **Conditions** tab on the calculator **Configuration** window.

There are additional **Conditions** tab settings described for the Precipitate Phase and Calculation Type.



Composition unit: Mass percent
Composition Fe: 99.984
Composition C: 0.016

Matrix Phase
Phase: BCC_A2

Calculation Type
● Isothermal ○ Non-isothermal ○ TTT diagram ○ CCT Diagram
Temperature: 102.0 Celsius
Simulation time: 600000.0 Seconds

Precipitate Phase
Phase: CEMENTITE
Nucleation sites: Dislocations ☑ Calculate from matrix settings 5.87951601467259E20 m^{-3}
Interfacial energy: User-defined 0.24 J/m^2
Growth rate model: Advanced
Morphology: Sphere
Transformation strain: Disregard
Molar volume: Database 1.0E-5 m^3/mol
Phase boundary mobility: 10.0 m^4/Js
Phase energy addition: 0.0 J/mol
Approximate driving force: ☐
Preexisting size distribution: ☐

There are three distinct settings areas for the Configuration window for example P_04_Precipitation_Fe-C_Cemetite. In this case, Show Details is expanded to show the Precipitate Phase settings.

You can change these settings locally for a specific Calculator or globally for some defaults in the **Options** *window* (a different location than the tab).

To open the **Options** window:

- Windows: Select **Tools** → **Options**.
- Mac: Select **Thermo-Calc** <*version*> → **Preferences** or **Settings** or press <⌘> on the keyboard.

then click the **Graphical Mode** tab and the **Precipitation** node in the tree.

SHOW OR HIDE DETAILS

Click **Show Details** to view some of the additional settings listed below. You can also set the default to display in **Phase view mode** on the **Options** window then click the **Graphical Mode** tab and the **Precipitation** node in the tree. Click **Hide Details** to hide the information.

Composition Settings

COMPOSITION UNIT

Select the **Composition unit**: **Mass percent**, **Mole percent**, **Mass fraction**, or **Mole fraction**.

Matrix Phase Settings

"Selecting the Disordered Phase as a Matrix Phase " on page 29

PHASE

> Only phases with kinetic data can be selected as the matrix phase. If the list is empty, go to the System Definer to confirm that both thermodynamic and kinetic databases are selected and defined.

Choose a **Phase** from the list. The list is based on the settings for the System Definer. When setting up a system, choose a matrix phase with kinetic data available in the database.

ELASTIC PROPERTIES

See "Homogeneous Nucleation" on page 80 for theory.

Choose **Disregard** to ignore the elastic properties.

Default elastic constants for **Isotropic** or **Cubic** are based on the major element of the alloy system. The elastic properties can affect nucleation rate, nuclei size, and particle shape.

- For **Isotropic**, enter values for **Shear modulus** (in GPa) and **Poisson's ratio** as required.
- For **Cubic**, enter values for **c11**, **c12**, and **c44** as required. c_{11}, c_{12}, c_{44} are the elastic constants.

MOLAR VOLUME

Use the **Database** value (if the molar volume for the phase is defined in the thermodynamic database) or select **User-defined** to enter another value in m^3/mol.

If you select the **Grain growth** checkbox, see the separate Grain Growth Settings section for details.

GRAIN SIZE

If the **Grain growth** checkbox is NOT selected then this version of the **Grain size** section is available in order for the **Average diameter** of the grain size to be entered.

Grain size is the "diameter" of a grain. The **Grain size** value changes the available nucleation sites when **Grain boundaries**, **Grain edges**, or **Grain corners** is selected along with **Calculate from matrix settings** in the *Precipitate Phase*. Enter a numerical value and choose a unit from the list. The default is `1.0E-4` m.

See "Precipitation Morphology" on page 113 and "The Number of Available Heterogeneous Nucleation Sites" on page 91 for theory.

GRAIN ASPECT RATIO

For an elongated grain with a minor axis and a major axis, one may use the minor axis as grain size and the major/minor ratio as the grain aspect ratio to characterize the grain. The **Grain aspect ratio** value also changes the available nucleation sites when **Grain boundaries**, **Grain edges**, or **Grain corners** is selected along with **Calculate from matrix settings** in the *Precipitate Phase*. Enter a numerical value. The default is 1.0.

If the **Grain growth** checkbox is selected, the aspect ratio is fixed at 1.0 and can not be changed. See Grain Growth Settings.

See "Precipitation Morphology" on page 113 and "The Number of Available Heterogeneous Nucleation Sites" on page 91 for theory.

DISLOCATION DENSITY

The **Dislocation density** value changes the available nucleation sites when **Dislocations** is selected along with **Calculate from matrix settings** in the *Precipitate Phase*. Enter a numerical value. The default is 5.0E12 m^{-2}.

See "Precipitation Morphology" on page 113 and "The Number of Available Heterogeneous Nucleation Sites" on page 91 for theory.

MOBILITY ADJUSTMENT

The **Mobility adjustment** parameters modify the atomic mobility data from a database.

Choose **Same for all elements**, which applies the adjustment to all elements, or **Per element** to adjust to each individual element. Then for the following settings, enter one set of values for **Same for all elements**, or individually for **Per element**.

- **Prefactor** (unitless) is a parameter that multiplies to the mobility data from a database. This value scales the mobility by a constant amount.

  For the Precipitation Calculator, this can be useful, for example, when the material has a higher than normal vacancy concentration at the start of the precipitation simulation. (e.g. from a prior solutionizing and quenching treatment).

- The **Activation energy** (J/mol) is a value that adds to the activation energy of mobility data from a database. This value scales the mobility by a temperature-dependent amount. Similar usage as the **Mobility adjustment >Prefactor** setting.

Grain Growth Settings

GRAIN GROWTH

Select the **Grain growth** checkbox to use this to calculate the temporal evolution of grain size distribution (GSD). The grains are assumed of spherical morphology when modeling the growth rates. Nucleation is not considered, thus an initial GSD is necessary to start the simulation.

After selecting the checkbox, there are additional settings made available as described in this section.

This checkbox is not available when a **TTT diagram** or **CCT diagram** *Calculation Type* is selected.

See "Normal Grain Growth" on page 116 and "Zener Pinning" on page 118 for theory.

GRAIN SIZE >> GRAIN SIZE DISTRIBUTION

When the **Grain growth** checkbox is selected, then this version of the **Grain size** settings section is available. This is where you access the grain *Size distribution* settings.

Click **Edit grain size distribution** to open the *Size distribution* settings window. In this window, you can edit the parameters and generate a graph comparing the radius and number density for initial grains.

Select a **Length unit**: **Meter**, **Micrometer**, **Nanometer**, or **Ångström**.

Select a **Distribution**: **Normal**, **Log normal**, or **From file**.

- If **Normal** or **Log normal** is selected, enter values for **Mean radius** and **Std** (standard deviation). The default Std is different for each choice.
- If **Hillert** is selected, enter a value for the **Mean radius**.
- If **From file** is selected, click **Import** and navigate to the file containing the required information and click **Open**. This file can be in .xls, .xlsx, .csv or .txt formats. The file should consist of two columns with values where the first column contains **radius** data and the second contains **number density** data.

A similar setup can also be found in the "Particle Size Distribution (PSD)" on page 37.

Once the size distribution is defined, click **Generate** to view or update the graph comparing the radius and number density for initial grains.

GRAIN BOUNDARY ENERGY

This setting is available when the **Grain growth** checkbox is selected.

Enter a value for the **Grain boundary energy**. The default is 0.5 J/m^2.

See "Normal Grain Growth" on page 116 for theory.

GRAIN BOUNDARY MOBILITY

This setting is available when the **Grain growth** checkbox is selected.

The **Prefactor** (m^4/Js) is a parameter that represents the magnitude of the grain boundary motion.

The **Activation energy** (J/mol) is a parameter that describes the temperature dependence of the grain boundary mobility.

See Grain Boundary Mobility Values for theory and recommended values.

ZENER PINNING

This setting is available when the **Grain growth** checkbox is selected.

Select the **Zenner pinning** checkbox to consider the effect of precipitates on inhibiting normal grain growth. When this checkbox is selected, there are additional settings available in the **Precipitate Phase** section.

See "Zener Pinning" on page 118 for theory.

"P_14: Grain Growth and the Zener Pinning Effect" on page 197

Selecting the Disordered Phase as a Matrix Phase

The following information is about using disordered FCC as a matrix phase with the following thermodynamic and mobility database packages:

- TCCU and MOBCU (Cu-based alloys)
- TCNI and MOBNI (Ni-based alloys)

In the TCNI/MOBNI and TCCU/MOBCU packages, the well-known order/disorder two-sublattice model is used to describe the Gibbs energy of both FCC_A1 and FCC_L12. With this treatment, FCC_L12 is becoming FCC_A1 if the site fractions of each element on both sublattices are identical, which means that FCC_A1 is only a special case of FCC_L12. Therefore, FCC_A1 is not shown in the phase list on the *Phases and Phase Constitution* tab on the System Definer activity and in subsequent equilibrium calculation results. Instead it is shown only as FCC_L12. The real ordered FCC_L12 is shown as FCC_L12#2.

In precipitation simulations, the matrix phase is quite often the disordered FCC phase. You can directly select FCC_L12 as the matrix phase and run a simulation. However, the speed is not optimal due to the sophisticated model used for both Gibbs energy and atomic mobilities. A better and more convenient way is to deselect FCC_L12 and FCC_L12#2 from the phase list on the *Phases and Phase Constitution* tab on the **System Definer** if the ordered phase is irrelevant in the alloy under investigation, such as in most Cu alloys. Once these are unchecked (i.e. not selected), the FCC_A1 phase is available and can later be selected as the matrix phase.

For Ni-based superalloys using the TCNI/MOBNI package, the ordered FCC_L12#2 (gamma prime) has to be included as the precipitate phase in most of calculations. In this case, you can select DIS_FCC_A1 from the phase list on the *Phases and Phase Constitution* tab and then select it as the matrix phase in the **Precipitation Calculator**.

Precipitate Phase Settings

Below are details about the settings for the *Precipitate Phase*, which is selected from the **Conditions** tab on the Precipitation Calculator **Configuration** window.

There are additional **Conditions** tab settings described for the Matrix Phase and Calculation Type.

To open the **Options** window:

- Windows: Select **Tools** → **Options**.
- Mac: Select **Thermo-Calc** *<version>* → **Preferences** or **Settings** or press <⌘> on the keyboard.

then click the **Graphical Mode** tab and the **Precipitation** node in the tree.

SHOW OR HIDE DETAILS

Click **Show Details** to view some of the additional settings listed below. You can also set the default to display in **Phase view mode** on the **Options** window then click the **Graphical Mode** tab and the **Precipitation** node in the tree. Click **Hide Details** to hide the information.

PHASE

The phases available to choose have both thermodynamic and kinetic data. If the list is empty, go to the System Definer to confirm that both types of databases are selected and defined.

Choose a **Phase** from the list. The list is based on the System Definer settings.

NUCLEATION SITES

See "Homogeneous Nucleation" on page 80 and "Heterogeneous Nucleation" on page 87 for theory.

The number of different nucleation sites is dependent on the shape and size of grains in the matrix. Grain size is the "diameter" of a grain. Choose one of the following from the list.

- **Bulk**, **Grain boundaries**, **Grain edges**, **Grain corners**, or **Dislocations**.
- For **Grain boundaries**, **Grain edges**, and **Grain corners**, enter the **Wetting angle (0-90)** in addition to the matrix settings. **Wetting angle** defines the deviation from spherical shape (or dihedral angle).

Click to select the **Calculate from matrix settings** checkbox to calculate the initial number density of sites from the matrix grain size or dislocation density.

To enter a specific value for the number of **Nucleation sites**, click to clear the checkbox.

INTERFACIAL ENERGY

See "Estimation of Coherent Interfacial Energy" on page 112 and "Interfacial Energy Anisotropy" on page 101 for theory.

Choose **Calculated** to use the estimated value. To adjust the estimate, enter a different **prefactor** or choose **User-defined** to enter a value in J/m^2. For the User-defined option, you can also enter it as a function of radius (r) and temperature (T).

GROWTH RATE MODEL

Select **Simplified**, **General**, **Advanced**, **Para-eq**, **NPLE**, or **PE Automatic** (where Para-eq and PE are both abbreviations for *paraequilibrium*).

> All models treat a particle (precipitate) of stoichiometric composition or with negligible atomic diffusivity. Except for the **PE Automatic** model, local equilibrium or paraequilibrium at the precipitate-matrix interface is assumed. The **PE Automatic** model enables smooth transition from paraequilibrium to local equilibrium.

In the documentation and on the GUI, the abbreviations *Para-eq* and *PE* are both used for paraequilibrium. There is also the use of OE as an abbreviation for *ortho-equilibrium* and LE for *local equilibrium*.

See "Growth" on page 94.

MORPHOLOGY

See "Precipitation Morphology" on page 113 for theory.

Choose the particle shape: **Sphere** (default), **Cuboid**, **Plate**, or **Needle**. Options are based on the **Elastic properties** selected for the **Matrix** phase:

- For a **Cubic** elastic property, **Sphere**, **Plate**, **Needle**, and **Cuboid** are available.
- For an **Isotropic** elastic property, **Sphere**, **Plate** and **Needle** are available.

If **Sphere** is selected, there is an option to use a **3D → 2D** conversion on the Plot or Table Renderer for certain variables. See "Stereology" on page 121 for theory details.

For **Plate** or **Needle**, select the **Calculate aspect ratio from elastic energy** checkbox or enter a numerical value in the **Aspect ratio** field to provide a constant aspect ratio.

See "Particle Shape Determination" on page 100 for theory.

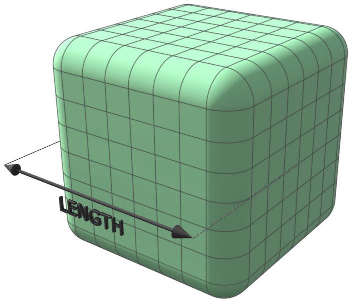


Figure 1: The cuboid shape is described by a supersphere. Cuboids have six faces, which form a convex polyhedron.

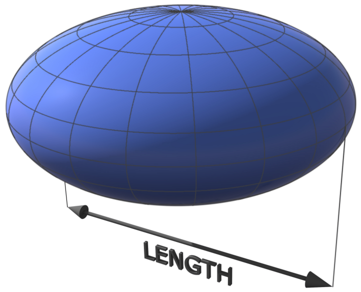


Figure 2: The plate is described as oblate spheroid. Oblate spheroids have rotational symmetry around an axis from pole to pole.

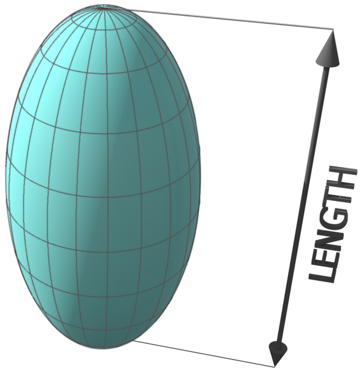


Figure 3: The needle shape is described as prolate spheroid. A prolate spheroid is a surface of revolution obtained by rotating an ellipse about its major axis.

TRANSFORMATION STRAIN

Choose **Disregard** to ignore the transformation strain. When **Isotropic** or **Cubic** is chosen in **Elastic properties** in Matrix Phase, you can also choose **Calculated from molar volume** to obtain a purely dilatational strain. If **Plate** or **Needle** is selected as the **Morphology**, you can alternatively choose **User-defined** and enter the properties for **ε11**, **ε12**, **ε13**, **ε22**, **ε23**, and **ε33**.

? See "Particle Shape Determination" on page 100 for theory.

MOLAR VOLUME

Use the **Database** value (if the phase molar volume is defined in the thermodynamic database) or select **User-defined** to enter another value.

ZENER PINNING PARAMETERS

These parameters are available when the **Zener pinning** checkbox is selected under the **Matrix Phase** settings. These settings are to consider the effect of precipitates on inhibiting normal grain growth.

- **Cutoff size**: Precipitates with radius smaller than this value are neglected in pinning force calculation. Default value : 7 x 10^{-7} m.
- **Kinetic prefactor**: Dimensionless kinetic coefficient in Zener equation. Default value: 0.5.
- **Exponent**: Exponent of precipitate volume fraction in Zener equation. Default value: 0.93.

See "Zener Pinning" on page 118 for theory.

"P_14: Grain Growth and the Zener Pinning Effect" on page 197

PHASE BOUNDARY MOBILITY

A parameter that accounts for interface-controlled growth. Only effective if a very small, positive value is used. Use with caution due to a tentative treatment.

See "Simplified Growth Rate Model" on page 95 for theory.

TRANS-INTERFACE MOBILITY ADJUSTMENT

This setting is available when **PE Automatic Growth rate model** is selected.

The **Trans-Interface mobility adjustment** parameters modify the atomic mobility data from a database.

Choose **Same for all elements**, which applies the adjustment to all elements, or **Per element** to adjust to each individual element.

The transition kinetics from Para-Equilibrium (PE) to Ortho-Equilibrium (OE) is controlled by the ratio of atomic mobility of substitutional elements to that of interstitial elements. This implies that the option of **Same for all elements**—while useful to the case that the atomic mobility data for all elements are needed to be scaled with the same factor to match experimental trans-interface mobility data—does not change the PE-OE transition kinetics. Therefore, the change of transition kinetics separately requires adjustment of individual elements, which is when the **Per element** setting is useful.

Then for the following settings, enter one set of values for **Same for all elements**, or individually for **Per element**:

- **Prefactor** (unitless) is a parameter that multiplies to the mobility data from a database. This value scales the mobility by a constant amount. This results in the trans-interface mobility that controls the kinetics of Para-Equilibrium (PE) to Ortho-Equilibrium (OE) transition.
- The **Activation energy** (J/mol) is a value that adds to the activation energy of mobility data from a database. This value scales the mobility by a temperature-dependent amount. Similar usage as the **Trans-Interface mobility adjustment >Prefactor** setting.

PHASE ENERGY ADDITION

An energy value that adds to the Gibbs free energy of the precipitate phase from a database. Enter a value in the field and choose a unit **J/mol formula unit** or **J/mol substitutional atom**.

See "Simplified Growth Rate Model" on page 95 for theory.

APPROXIMATE DRIVING FORCE

Select the checkbox to include this if simulations with several compositions sets of the same phase create problems.

See "Nucleation Theory" on page 79.

PREEXISTING SIZE DISTRIBUTION

Select the checkbox to include this. Click **Edit particle size distribution** to open the **Preexisting Particle Size Distribution** window where you can edit the parameters and view a graph comparing the radius and number density for the selected component.

? Press F1 and search for "Particle Size Distribution (PSD)" for detailed instructions.

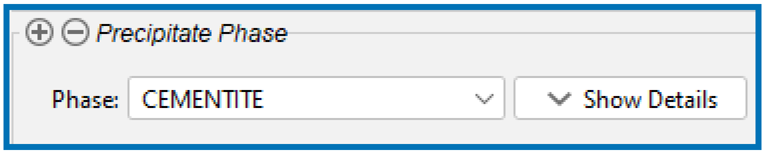
Particle Size Distribution (PSD)

📈 "P_10: Initial Particle Size Distribution of Fe-Cr-C" on page 178

On the Precipitation Calculator you can set the pre-exisiting particle size distribution (PSD) parameters in the **Show Details** section. The size distribution can be generated from a probability distribution function, by importing a file, calibrating a probability distribution function to experimental data, or by manually entering information into a table. Uni-modal distributions can be created within the Graphical Mode interface. Pre-existing multimodal distributions can be loaded from a file.

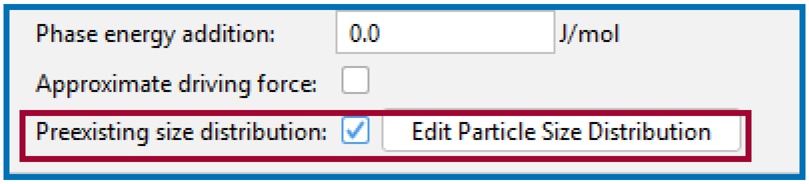
Accessing the 'Preexisting Size Distribution' Settings

1. To the right of the *Precipitate Phase* settings fields, click **Show Details**.



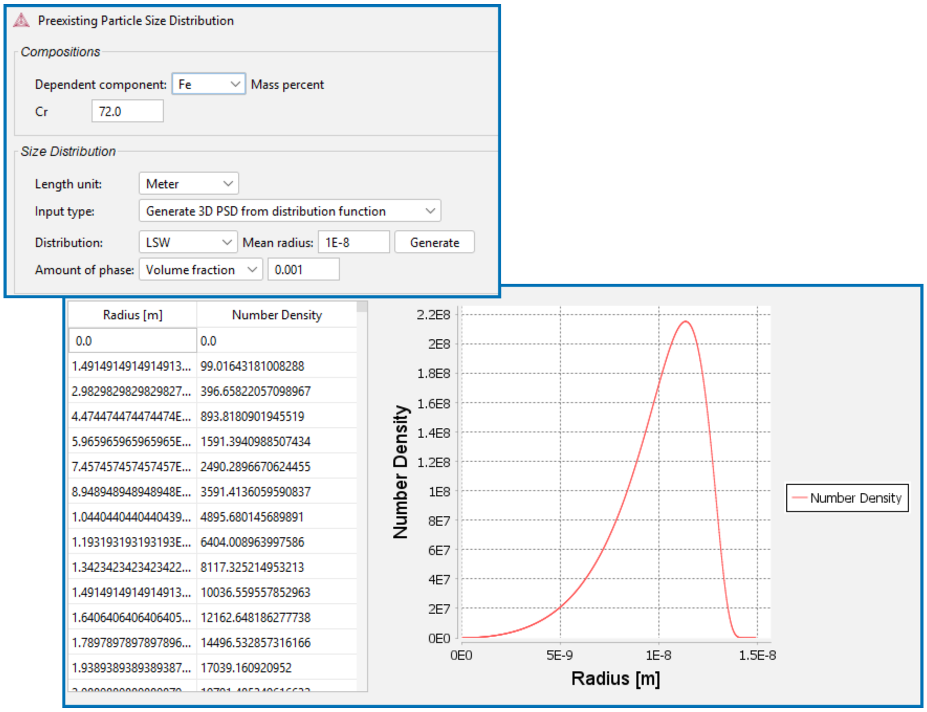
Phase: CEMENTITE

2. At the bottom of the *Precipitate Phase* section, click to select the **Preexisting size distribution** checkbox. Then click **Edit Particle Size Distribution**.



Phase energy addition: 0.0 J/mol
Approximate driving force: ☐
Preexisting size distribution: ☑

3. The **Preexisting Particle Size Distribution** window opens as shown for example P_10 CEMENTITE phase.



Dependent component: Fe Mass percent

Cr 72.0

Length unit: Meter

Input type: Generate 3D PSD from distribution function

Distribution: LSW Mean radius: 1E-8

Amount of phase: Volume fraction 0.001

Radius [m]	Number Density
0.0	0.0
1.4914914914914913...	99.01643181008288
2.9829829829829827...	396.65822057098967
4.474474474474474E...	893.8180901945519
5.965965965965965E...	1591.3940988507434
7.457457457457457E...	2490.2896670624455
8.948948948948948E...	3591.4136059590837
1.0440440440440439...	4895.680145689891
1.193193193193193E...	6404.008963997586
1.3423423423423422...	8117.325214953213
1.4914914914914913...	10036.559557852963
1.6406406406406405...	12162.648186277738
1.7897897897897896...	14496.532857316166
1.9389389389389387...	17039.160920952

Defining the Preexisting Size Distribution

Compositions

Choose a **Dependent component** from the list and enter the composition for the other component.

Length Unit

Choose a **Length unit**: **Meter**, **Micrometer**, **Nanometer**, or **Ångström**.

Amount of Phase

For all options, choose an **Amount of phase**: **Volume percent** or **Volume fraction** and then enter a number in the field.

Input Type

Choose an **Input type**: **Generate 3D PSD from distribution function**, **From File**, or **Approximate the 3D PSD from experimental data**. See the following sections for the details about each setting.

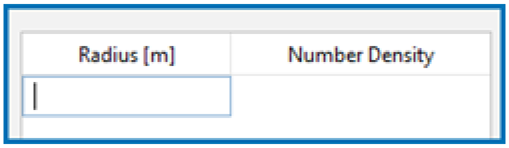
Generate 3D PSD from Distribution Function

This option allows the generation of the size distribution from a list of probability distribution functions. The **Distribution** types include **LSW**, **Normal**, **Log normal**, and **Weibull**.

- **Mean radius** The mean particle radius.
- **Sigma** The standard deviation for the chosen length unit.
- **Alpha** A dimensionless shape factor that should vary between 1.5 and 10.
- **Fraction offset** The fraction offset applied to the mean radius to shift the start of the distribution. This must be greater than or equal to zero, and less than 0.95.

Once the **Distribution** is defined, click **Generate** to create the size distribution.

You can also click in the table to manually enter numbers into the cells rather than use one of the provided probability distribution functions. The radius values must monotonically increase in size.



Radius [m]	Number Density

From File

This option lets you load the initial size distribution from a file. Click **Import** and navigate to the file containing the required information and click **Open**. This file can be in .xls, .xlsx, .csv, or .txt formats. The file should consist of two columns with values where the first column contains **radius** data and the second contains **number density** data.

The example `P_10` (available from the **Example files** → **Precipitation Module - TC-PRISMA** folder) shows this for the precipitate phase M23C6. There is also a file in this folder called `P_10_Precipitation_Initial_PSD_FeCrC_psd_3D_M23C6.csv` that is an example of a correctly formatted text file.

The imported size distribution is normalized into a probability distribution function by ensuring that the zeroth moment is unity. If you wish to import a histogram that has un-even bin spacing, it is necessary to convert the Y-axis counts of the histogram to a count density first to avoid changes to the shape of the distribution. The count density is obtained simply by dividing the count of a bin by the bin's width.

Approximate the 3D PSD from Experimental Data

The **Approximate the 3D PSD from experimental dataInput type** allows you to calibrate a continuous probability distribution function to an experimentally measured size distribution, and account for stereological considerations. There are additional settings related to this.

DIMENSIONALITY OF EXP. DATA AND IMPORT EXP. DATA

The **Dimensionality of exp. data** setting must be defined.

- For precipitate radius measurements that are a good approximation of the 3D size of the particles, select **3D**. Measurements from quantitative image analysis of Transmission Electron Micrographs (TEM) provide **3D** size data, however the precipitates can still be truncated within the TEM sample foil thickness.
- **2D** data is obtained from a cross section taken through the microstructure. Examples include micrographs taken from Scanning Electron Microscopy (SEM), and Optical Microscopy (OM). The radius measurements are obtained from calculating the equivalent radius of a circle from the areas of identified objects from quantitative image analysis of the micrographs. It is possible that the samples of interest are over-etched, revealing the full size of the precipitates. In this case the data may be more descriptive of the **3D** size, however smaller particles are removed by the etching, distorting the obtained size distribution.

- **1D** data is obtained from applying the linear intercept method to micrographs descriptive of a cross section through the dispersion. A half-linear intercept is used in this calculation, which is analogous to the radius of the particle, opposed to the diameter.

Click **Import exp. data** to import the experimental data. Navigate to the file containing the required information and click **Open**. This file can be in .xls, .xlsx, .csv, or .txt formats. The file should consist of two columns with values where the first column contains **radius** data and the second contains **number density** data.

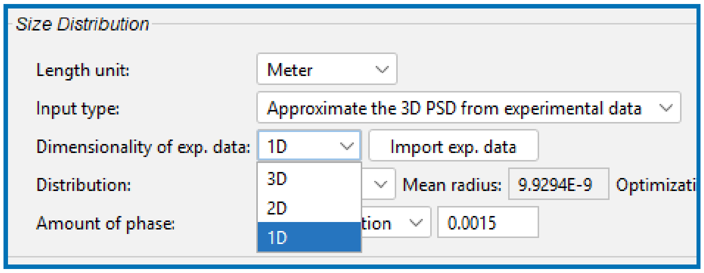
The example `P_10` (available from the **Example files** → **Precipitation Module - TC-PRISMA** folder) shows this for the precipitate phase M7C3. There is also a file in this folder called `P_10_Precipitation_Initial_PSD_FeCrC_psd_1D_M7C3.csv` that is an example of a correctly formatted text file.

DISTRIBUTION

Choose a **Distribution**: **LSW** (Lifshitz-Slyozov-Wagner), **Normal**, **Log normal**, or **Weibull**.

Click **Generate** to calibrate the chosen **Distribution** to capture the **Import exp. data** accounting for the chosen stereological **Dimensionality of exp. data**.

For 3D data, there are two datasets shown in the preview; the experimental data and the 3D model data. For 2D and 1D data, the sectioned model data is also shown and compared with the experimental data



Size Distribution

Length unit: Meter

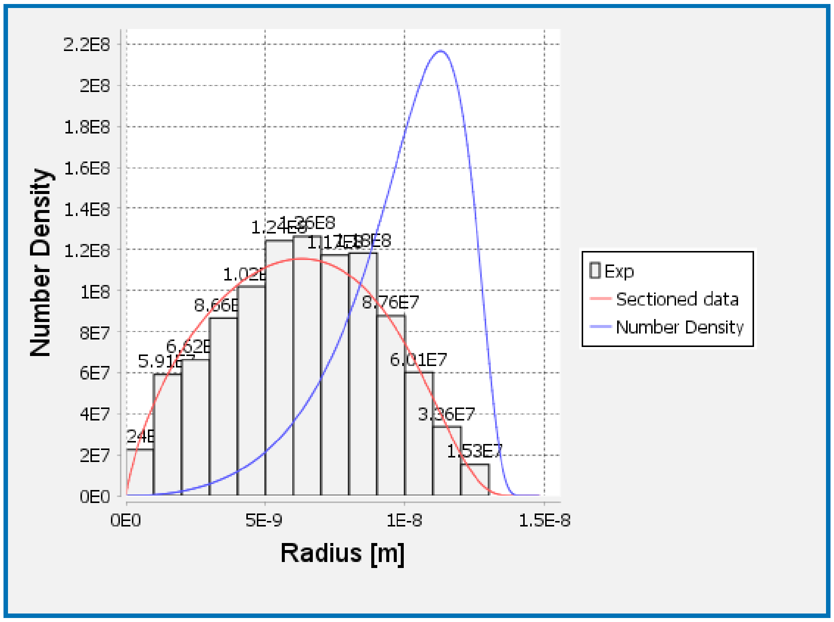
Input type: Approximate the 3D PSD from experimental data

Dimensionality of exp. data: 1D

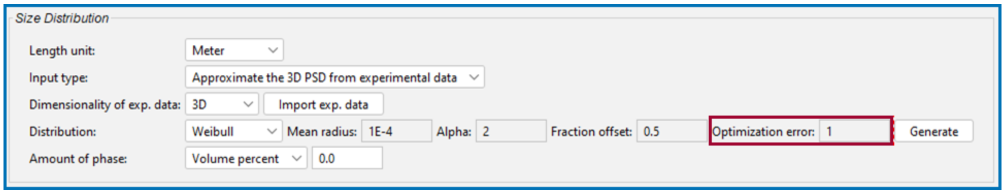
Distribution:

Mean radius: 9.9294E-9

Amount of phase: 0.0015



The Optimization error is output into the text-field highlighted below. This can be used to determine the best distribution type to use for a given dataset.



Size Distribution

Length unit: Meter

Input type: Approximate the 3D PSD from experimental data

Dimensionality of exp. data: 3D

Distribution: Weibull

Mean radius: 1E-4

Alpha: 2

Fraction offset: 0.5

Optimization error: 1

Amount of phase: Volume percent 0.0

Calculation Type Settings

Below are details about the settings for the *Calculation Type*, which is selected from the **Conditions** tab on the Precipitation Calculator **Configuration** window.

There are additional **Conditions** tab settings described for the Matrix Phase and Precipitate Phase.

ISOTHERMAL

Use an **Isothermal** calculation type to do a simulation at constant temperature.

These settings are described in the section for the "Precipitation Calculator Thermal Profile" on page 45.

NON-ISOTHERMAL

"Nucleation During a Non-isothermal Process" on page 93

Use a **Non-isothermal** calculation type to do a simulation with a user-defined temperature profile. You can enter information directly or import a data file.

These settings are described for the "Precipitation Calculator Thermal Profile" on page 45 including information about importing data files.

When you also have a license for the Additive Manufacturing (AM) Module you can include probe data from the AM Calculator in the set up of the thermal profile.

TTT DIAGRAM

Use a **TTT-diagram** to calculate the time-temperature-transformation (TTT) curve for the formation of the precipitate phase.

- **Temperature**: Enter **Min**, **Max**, and **Step** numerical values and choose a temperature **Unit**.
- **Max annealing time**: Enter a numerical value and choose a time **Unit**.
- **Stop criteria**: Choose **Volume fraction of phase** or **% of equilibrium fraction** and then enter a numerical value. For each temperature, the simulation stops when the stop criteria is fulfilled or if the maximum annealing time is reached, whichever happens first.

See example "P_03: Stable and Metastable Carbides - TTT Diagram" on page 143

CCT DIAGRAM

Use a **CCT-diagram** to calculate the continuous-cooling-transformation (CCT) curve for precipitation.

- **Temperature**: Enter **Min** and **Max** numerical values and choose a temperature **Unit**.
- **Cooling rate(s)**: Enter a range of values in the field, e.g.`.01 .1 1 10 100`. These values are equal to **K/s**, **°C/s** or **°F/s** per second based on the temperature **Unit** selected.
- **Stop criteria**: Enter a numerical value for the **Volume fraction of phase**. For each temperature, the simulation stops when the stop criteria is fulfilled.

See example "P_07: Continuous Cooling Transformation (CCT) Diagram of Ni-Al-Cr γ-γ’" on page 162.

Precipitation Calculator Thermal Profile

The **Thermal Profile** is set up on the **Configuration** window for a **Precipitation Calculator**. The isothermal or non-isothermal profile is viewed in the **Visualizations** window. Choose **Isothermal** to do a simulation at constant temperature. Choose **Non-isothermal** to enter or import data for a user-defined temperature profile.

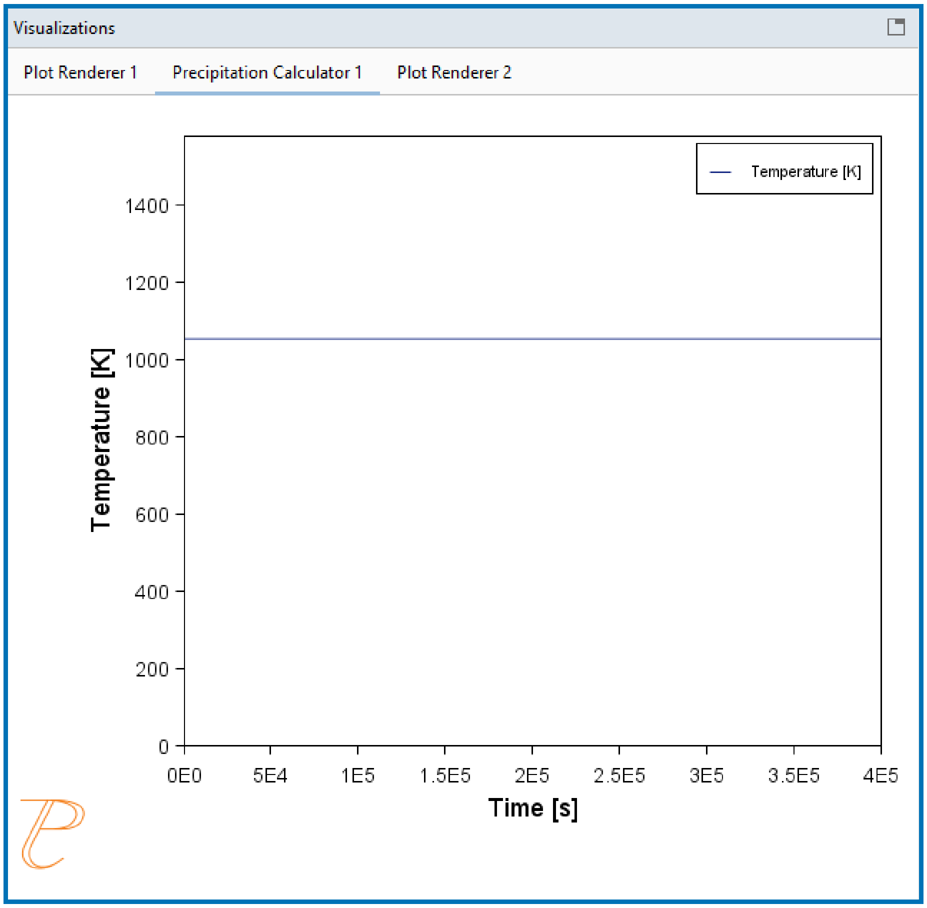
When connected to an AM Calculator (see Including Probe Data from an AM Calculator) the **Isothermal** and **Non-isothermal** options are not visible as it is not relevant to that view.

Isothermal Calculations

Many of the Graphical Mode examples for this Add-on Module are isothermal calculations, e.g. *P_02_Precipitation_Fe-C-Cr_Cementite-M7C3-M23C6*.

1. On the Precipitation Calculator **Configuration** window, first enter the required *Matrix Phase* and *Precipitate Phase* settings.
2. Under **Calculation Type**, click to choose **Isothermal** to do a simulation at constant temperature.
3. Enter a **Temperature** and choose a unit (**Kelvin**, **Celsius**, or **Fahrenheit**).
4. Enter an **End time** and choose a unit: **Seconds**, **Minutes**, **Hours**, or **Days**. The *Simulation time* is displayed as text.

   The profile is displayed on the **Precipitation Calculator** tab in the **Visualizations** window showing the constant temperature entered.



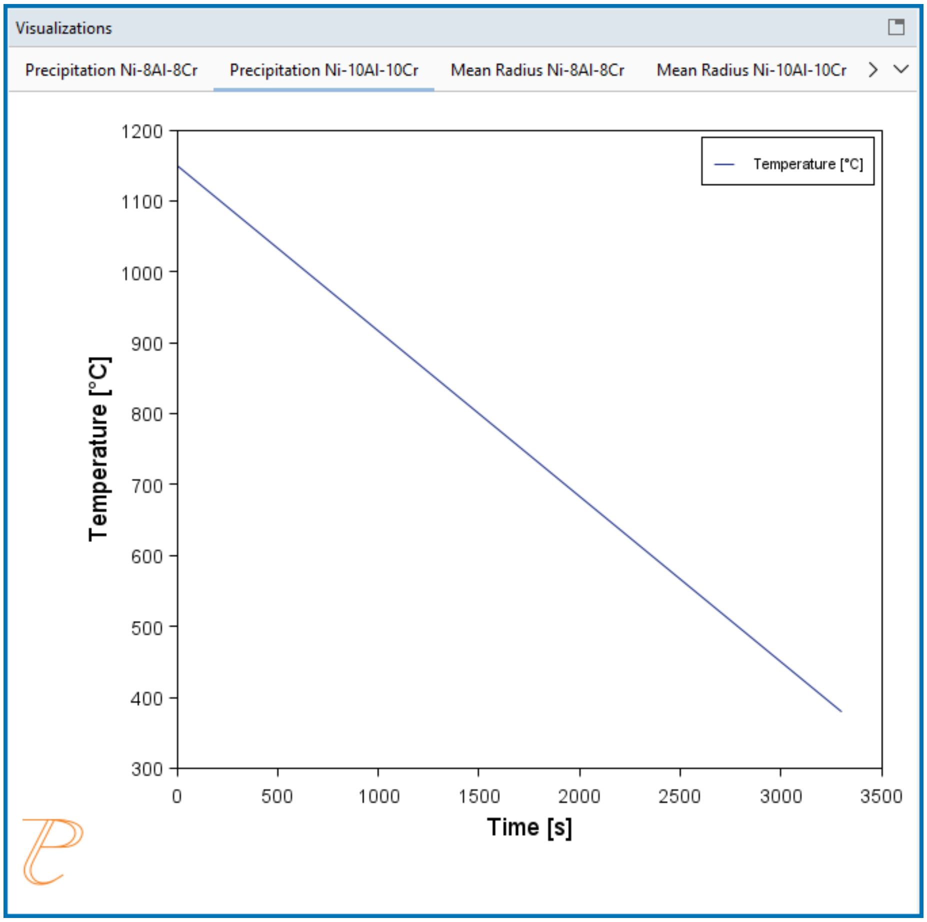
5. For this calculation type this completes the settings you need to enter for the Thermal Profile.

Non-isothermal Calculations

1. On the Precipitation Calculator **Configuration** window, first enter the required *Matrix Phase* and *Precipitate Phase* settings.
2. Under **Calculation Type**, click to choose **Non-isothermal** to enter or import data for a user-defined temperature profile.
3. Select a **Temperature unit**: **Kelvin**, **Celsius**, or **Fahrenheit**.
4. Enter an **End time** and choose a unit: **Seconds**, **Minutes**, **Hours**, or **Days**. The *Simulation time* is displayed as text.

   You can next either directly enter **Time** and **Temperature** coordinates into the table or import the information from a file. A minimum of two points is required.

5. To enter directly into the table:
    1. Click in each cell under the applicable columns, **Time** and **Temperature** then directly enter the values in the table.
    2. Press `<Enter>` to add rows and use the scroll bars to navigate the table.
6. To import a data file:
    1. Although it is a simple set of data, prepare the data file as in "Guidelines for Importing Data Files to Thermal Profiles" on page 49.
    2. When the data file is ready, to the right of the **Import from file** field, click the file 📁 button.
    3. Navigate to a data file such as an MS Excel spreadsheet (with ***.xls** or ***.xlsx** extensions) or a ***.csv** file. You can also use other programs (e.g. Google Sheets) to enter data and export to a CSV format that can be read by the software. Click **Open** to import the data to the **Configuration** window table.
    4. If there are issues with the above import, experiment with choosing the delimiter type that corresponds to the data in the file: **Comma** (,), **Colon** (:), **Equals sign** (=), **Semicolon** (;), or **Tab**. Click the **Reload** button 🔄. The data is imported to the **Configuration** window table.
7. For this calculation type this completes the settings you need to enter for the profile, which is displayed on the **Precipitation Calculator** tab in the **Visualizations** window. Make adjustments to the settings as needed and watch it dynamically change in the window.



This is from the non-isothermal calculation example, *P_06_Precipitation_Ni-Al-Cr_Non-isothermal_Gamma-Gamma_prime*.

Including Probe Data from an AM Calculator

When you also have a license for the Additive Manufacturing (AM) Module you can include probe data from the AM Calculator in the set up of the thermal profile.

There is connectivity between the Diffusion Module (DICTRA) or the Precipitation Module (TC-PRISMA) and the Additive Manufacturing (AM) Module when you have full licenses available for all relevant Add-on Modules and databases.

You can add a Diffusion Calculator or Precipitation Calculator as a successor to the AM Calculator and then when probes are included with the AM Calculator this data can be further used with the thermal profile.

Guidelines for Importing Data Files to Thermal Profiles

The **Thermal Profile** settings are done on the **Configuration** window for a Precipitation Calculator. The profile is then previewed in the **Visualizations** window.

You can import data from a file. There are specific guidelines needed to correctly prepare the data in this file to ensure it imports without errors.

Data File Requirements

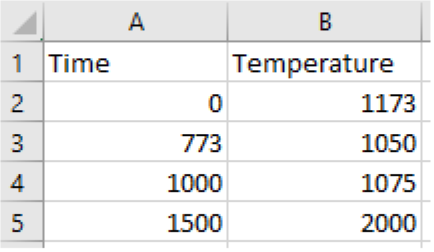
For a Thermal Profile you can either directly enter **Time** and **Temperature** coordinates into the table on the **Configuration** window, or import the data from a file. A minimum of two points is required.

Although there are only two columns to define, it is still important to ensure the file is set up correctly. In order for the data to be included in the calculation, the column and row definitions in the file must adhere to certain rules of entry.

General Rules

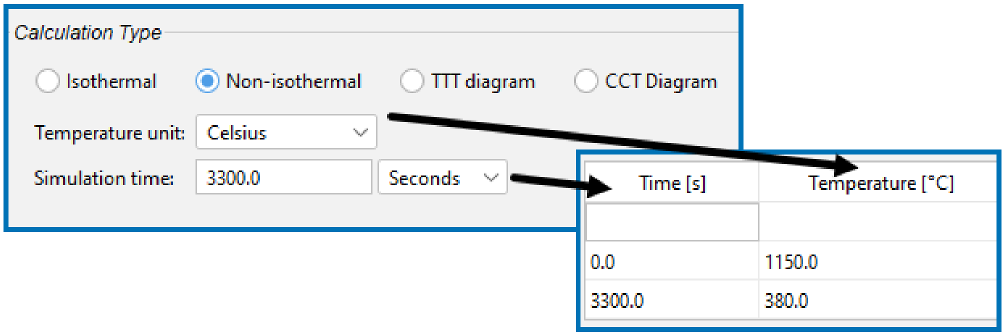
- No abbreviations are allowed in the header.
- A header is not actually required in this file but in order to know which column is which, it is recommended to include it.
- All header text must be in English, i.e. no translations into other languages will be read correctly by the data file.

> Only the columns described here are read / used in the calculation. It is important to enter the information exactly as described. It is recommended that the data file is cleaned up before importing / loading it and performing calculations.



	A	B
1	Time	Temperature
2	0	1173
3	773	1050
4	1000	1075
5	1500	2000

Figure 4: This is an example of data entered into an Excel spreadsheet (which is then converted to csv format). Columns A and B show the data entered to create the Thermal Profile.



Calculation Type

○ Isothermal ● Non-isothermal ○ TTT diagram ○ CCT Diagram

Temperature unit: Celsius

Simulation time: 3300.0 Seconds

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

Figure 5: The units shown on the Configuration window for the Time and Temperature correspond to settings that can ONLY be selected on the Configuration window. The data file does not contain any information about the units.

Column Heading Requirements and Options	***Row Cell Requirements and Options***
Time This is column A as in Figure 4 Enter the text `Time`. No abbreviations allowed but it is not case sensitive. It is also not required but recommended to include so you know which column of data it applies to.	Valid format and entries for each row in this column: • Any numerical input for the time that corresponds to the unit selected on the Configuration window e.g. `0.0`, `773`, `1000`, `1500`, are times in seconds, which is the unit chosen in the example shown in Figure 5.
Temperature This is column B as in Figure 4 Enter the text `Temperature`. No abbreviations allowed but it is not case sensitive. It is also not required but recommended to include so you know which column of data it applies to.	Valid format and entries for each row in these columns: • Any numerical input for the temperature that corresponds to the unit selected on the Configuration window e.g. `1173`, `1050`, `1075`, are temperatures in Celsius, which is the unit chosen in the example shown in Figure 5

Options Tab

The Precipitation Calculator settings including the sections *Numerical Parameters*, *Save Options*, *Preprocessing Operations*, and *Interpolation Scheme* are located on the **Configuration** window → **Options** tab.

For equations and details about these settings, see "Numerical Method" on page 107.

You can change these settings locally for a specific Precipitation Calculator or globally for some defaults in the **Options** window settings.

Numerical Parameters

MAX TIME STEP FRACTION

The **Max time step fraction** is the maximum time step allowed for time integration as fraction of the simulation time. The default is 0.1.

NO. OF GRID POINTS OVER ONE ORDER OF MAGNITUDE IN RADIUS

The default number of grid points for every order of magnitude in size space. The default is 150.0.

MAX NO. OF GRID POINTS OVER ONE ORDER OF MAGNITUDE IN RADIUS

The maximum allowed number of grid points in size space. The default is 200.0.

MIN NO. OF GRID POINTS OVER ONE ORDER OF MAGNITUDE IN RADIUS

The minimum allowed number of grid points in size space. The default is 100.0.

MAX RELATIVE VOLUME FRACTION OF SUBCRITICAL PARTICLES ALLOWED TO DISSOLVE IN ONE TIME STEP

The portion of the volume fraction that can be ignored when determining the time step. The default is 0.01.

MAX RELATIVE RADIUS CHANGE

The maximum value allowed for relative radius change in one time step. The default is 0.01.

RELATIVE RADIUS CHANGE FOR AVOIDING CLASS COLLISION

Set a limit on the time step. The default is 0.5.

MAX OVERALL VOLUME CHANGE

This defines the maximum absolute (not ratio) change of the volume fraction allowed during one time step. The default is 0.001.

MAX RELATIVE CHANGE OF NUCLEATION RATE IN LOGARITHMIC SCALE

This parameter ensures accuracy for the evolution of effective nucleation rate. The default is 0.5.

MAX RELATIVE CHANGE OF CRITICAL RADIUS

Used to place a constraint on how fast the critical radium can vary, and thus put a limit on time step. The default is 0.1.

MIN RADIUS FOR A NUCLEUS TO BE CONSIDERED AS A PARTICLE

The cut-off lower limit of precipitate radius. The default is 5.0E-10 m.

MAX TIME STEP DURING HEATING STAGES

The upper limit of the time step that has been enforced in the heating stages. The default is 1.0 s.

MAXIMUM RELATIVE SOLUTE COMPOSITION CHANGE AT EACH TIME STEP

Set a limit on the time step by controlling solute depletion or saturation, especially at the isothermal stage. The default is 0.01.

Save Options

Save Options

From the **Save frequency** list, select an option that can reduce file size and speed up post-processing: **Medium** (the default), **High**, **Low**, or **Last result**. There is also an option to use **Original** settings and in some cases this is automatically selected.

When using the **High**, **Medium**, or **Low** save frequency settings, the particle size distribution (PSD) information is interpolated from the closest saved results. This is the most accurate when using the **High** setting as it reduces the error from the interpolation.

- **High** aims to capture all behavior, but may save more data than needed, with larger file sizes. This is a good option for scenarios where multimodal precipitate dispersions form, or you are interested in the change in the particle size distribution during the simulation.
- **Low** aims to only save when a dispersion changes. It may miss behavior but keeps the file size small.
- A **Medium** setting is a compromise between the High and Low settings, and is the default.
- The **Last result** option only saves information about the precipitates for the last time-step. This can be of interest to keep a small file size during high throughput calculations.

If you are modeling grain growth or doing CCT or TTT simulations, then **High**, **Medium**, **Low**, and **Last result** are not available. In these cases, **Original** is automatically selected by the software and then the same save logic as used as in Thermo-Calc versions 2025b and older.

Preprocessing Operations

Preprocess Equilibrium Data

Select the **Preprocess equilibrium data** checkbox to calculate the required phase equilibrium properties as a function of temperature for stable and metastable conditions. This speeds up the computation time of non-isothermal simulations or isothermal simulations where there is difficulty with losing precipitate phases during the calculation.

When the checkbox is selected, the stable and meta-stable property diagram data for all simulated precipitate phases is preprocessed. This preprocessing avoids repeating global equilibrium calculations, and speeds up computational time. It also allows for an improved description of precipitate kinetics under severe dissolution conditions. This can occur when temperatures are too high, where the phase is no longer detected in equilibrium calculations, or if the matrix is depleted of precipitate forming species, and the precipitate phase is lost when calculating the driving force.

This feature is used primarily for non-isothermal simulations. For isothermal simulations it can be used when there is difficulty losing precipitate phases during the calculation. In this case, it alters the predicted dissolution kinetics in certain conditions where the precipitation phase is lost and then it also speeds up these calculations.

Include Incipient Melting

To use the **Include incipient melting** checkbox requires that the thermodynamic database (i.e. TCFE, TCNI, and so on) includes the liquid phase. If the liquid phase is not included, then the **Perform** button is not available (it is grayed out with a message explaining why) until either a liquid phase is included or this checkbox is deselected.

This is available when the **Preprocess equilibrium data** checkbox is selected.

Select the **Include incipient melting** checkbox to approximate the melting temperature of precipitate phases. The precipitates are removed upon exceeding this temperature.

Incipient melting is a phenomenon where, due to rapid heating rates, a solid-state precipitate is in solution at temperatures where it would normally dissolve. It liquidates rather than dissolves into the matrix. Being able to include (or exclude) the incipient melting is relevant to simulations involving welding and AM. Including incipient melting in AM calculations is useful to avoid excessive computation time modeling the dissolution of precipitates which would melt. The precipitates are assumed to melt instantaneously upon reaching their incipient melting temperature.

Interpolation Scheme

Use Interpolation Scheme

Select the **Use interpolation scheme** checkbox to turn on an interpolation scheme for thermodynamic and mobility calculations. This can accelerate the computation time.

The advantage of using interpolation is mainly with CCT calculations, where the same matrix compositions are revisited repeatedly as several precipitation simulations are executed in sequence under different cooling rates.

Many precipitate simulations, however, do not reduce simulation times when using interpolation. For example, in isothermal precipitation, the matrix composition gradually changes from the initial oversaturated to the equilibrium composition during the simulation. By default, interpolation is therefore turned off.

The interpolation scheme is not compatible with the advanced growth-rate and is turned off automatically if this option is used in a simulation. It is also not recommended for use with the para growth-rate.

Largest improvements to computation time are seen with the simplified growth rate. In some cases, decent performance improvements have been obtained with the general and NPLE descriptions. Minor improvements are obtained for PE Automatic. Simulation times with the interpolation scheme are slower with the para-equilibrium growth-rate.

The interpolation scheme does not take advantage of pre-processed data, making it liable to issues where the precipitate phase is lost in equilibrium calculations, incurring error. This can happen at high super-solvus temperatures, or when the matrix is highly depleted from precipitate forming elements.

Discretization Method

The **discretization** can be either **Linear** or **Logarithmic** (the default). Logarithmic discretization is best when modeling interstitial elements where the composition can vary by orders of magnitude. Linear discretization works well when modeling only substitutional elements.

Number of Steps

Enter what is essentially the number of **steps in each dimension** in composition-temperature space for each equilibrium condition. In the limit where an infinite number of steps are used, exactly the same solution is obtained as without the interpolation scheme. However, excellent results can be obtained with a reasonable discretization.

Memory to Use

You can define the upper limit to how much **Memory to use** to store previous results for interpolation. The limit can be set in either **Megabyte** or a **Fraction of free** physical memory available at the start of the simulation.

Precipitation Calculator Plot Renderer

The following is information about the settings available for a **Plot Renderer** when it is a successor to a **Precipitation Calculator**.

"Quantities Groups Available for Plots and Tables" on page 65 for a general list of quantities. However, for the Precipitation Calculator Plot Renderer there are no defined groups to choose from.

Plot Settings

LEGEND OPTION

Select whether the diagram’s legend displays **On** or **Off**.

Y- AND X-AXES VARIABLES

Set the state variable you want plotted along the X-axis and the Y-axis. The available variables in the list are based on how your system is set up.

Below are additional details related to the axis variable chosen.

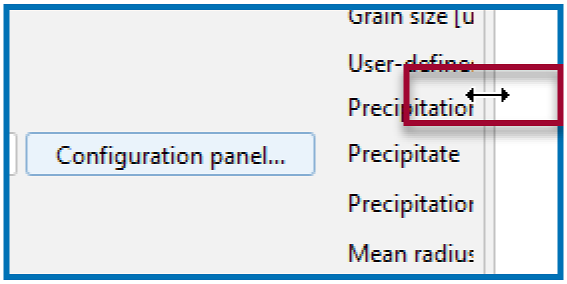
- **Separate Multimodal PSD:** If you select **Mean radius**, **Number density**, **Volume fraction**, **Size distribution**, **Number density distribution**, or **Normalized number density distribution** then the **Separate multimodal PSD** checkbox is available. For variables with time for the X-axis, the number of **Points** used to sample the results can be modified. The **Inflection neighbors** and **Smoothing iterations** are used to identify individual particle populations. See Separate Multimodal PSD below for more detail.
- **3D → 2D:** For a spherical morphology, and if you select **Mean radius**, **Number density**, **Volume fraction**, **Size distribution**, **Number density distribution**, or **Normalized number density distribution** as an axis variable, you can also select the **3D → 2D** checkbox to convert the 3D property to the corresponding 2D property considering the resulting 2D size distribution obtained from sectioning a 3D spherical dispersion. See 3D to 2D Conversion below for more detail.
- **Yield Strength**: If you select this as an axis variable there are additional settings. See Yield Strength below for more detail.

Yield Strength

If you choose **Yield strength** as an *Axis variable*, you can further define the model. Click to expand the drop down list to the right of the *Axis variable*, then select any or all of the checkboxes listed below to plot the respective contributing elements to the yield strength.

Click **Configuration Panel** toggle between the settings options and to further fine-tune the model. The greyed out sections (e.g. the **Matrix**, **Precipitate** phases, and **Grain size**) are defined on the **Precipitation Calculator** and cannot be changed.

> To see these settings after clicking **Configuration Panel**, you need to expand the **Plot Renderer Configuration** window to the right. Either detach the window to resize, or hover with the mouse until you see the double arrow, then click and drag to expand the window.



- Total yield strength
- Intrinsic strength
- Solid solution strengthening
- Solid solution strengthening FCC
- Solid solution strengthening BCC
- Solid solution strengthening HCP
- Grain boundary strengthening
- Total precipitation strengthening
- Precipitation strengthening per phase
- Constant strength addition

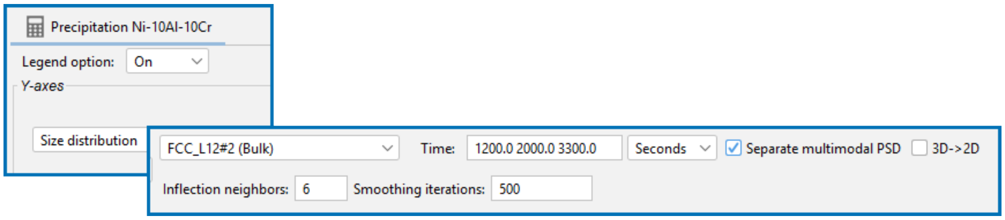
The **P_01: Isothermal Precipitation of Al3Sc** example demonstrates the use of this Yield Strength Model.

Separate Multimodal PSD

This setting is available if you select **Mean radius**, **Number density**, **Volume fraction**, or **Size distribution** as the *Axis Variable*.

When the **Separate multimodal PSD** checkbox is selected on a **Plot Renderer** activity for the **Precipitation Calculator**, the size distribution is evaluated at the given time steps and results for individual particle populations are identified and presented. These are separated and used to calculate the specified property.

"P_06: Precipitation of γ′ in Ni Superalloys - Non-isothermal" on page 155



Precipitation Ni-10Al-10Cr

Legend option: On

Y-axes

Size distribution

FCC_L12#2 (Bulk)

Time: 1200.0 2000.0 3300.0 Seconds

☑ Separate multimodal PSD ☐ 3D->2D

Inflection neighbors: 6

Smoothing iterations: 500

POINTS

This field is available when the **Separate multimodal PSD** checkbox is selected. It is not available with the **Size distribution** variable.

Since the evaluation of multimodality at each time step is costly, you can specify how many evaluation **Points** to use. The points are geometrically distributed over the time scale where nucleated particles are found. The default is 40 points.

INFLECTION NEIGHBORS

This field is available when the **Separate multimodal PSD** checkbox is selected.

Enter the **Inflection neighbors**, which are the number of neighboring points with consistent gradient direction to identify inflection points. The default is 6. As a guide, too low a number is sensitive to noise and too high a number can fail to detect particle populations.

SMOOTHING ITERATIONS

This field is available when the **Separate multimodal PSD** checkbox is selected.

Enter the number of **Smoothing iterations** performed to reveal significant particle populations. The default is 500. As a guide, too small a number can fail to remove noise, and too high a number can remove the particle populations of interest.

3D to 2D Conversion

When the *Precipitate Phase* **Morphology** is set to **Sphere** on the Precipitation Calculator, the following options are available when certain axis variables are also selected.

Select the **3D → 2D** checkbox if you want to make a direct comparison between the predicted three-dimensional (3D) radius of the precipitates and the two-dimensional (2D) data obtained from a cross-section taken through the dispersion.

> The stereological conversion is described in the theory for spherical particles. See "Stereology" on page 121.

These variables can be converted to 2D:

- **Mean radius**: The average circular radius of cross sections of particles obtained by taking a section through the dispersion, assuming spherical precipitates.
- **Number density** The number concentration of precipitates found on a 1 m^2 cross-section through the microstructure.
- **Volume fraction** The area fraction of precipitates found on a cross-section taken through the microstructure.
- **Size distribution**: The number density of particle cross sections that have a radius varying within a given size class in a unit area.
- **Number density distribution**: The number of particle cross sections that have a radius varying within a given size class in a unit area.
- **Normalized number density distribution**: The probability of finding particle cross sections with a cross sectional radius varying within the size class. The radius is normalized by the volumetric mean of the dispersion.

AXIS TYPE

Select the type of axis scale: **Linear**, **Logarithmic**, **Logarithmic 10**, or **Inverse**.

LIMITS

Specify the range along the axis to show in the plot. In the fields, enter the minimum and maximum values of the axis variable. You can also determine the **step** size between the tick marks along each axis.

Select the **Automatic scaling** checkbox to allow the program to set the limits.

UNIT (TIME X-AXIS)

Choose a **Unit**: **Seconds**, **Hours**, or **Days**.

ADD AN AXIS AND REMOVE THIS AXIS BUTTON

Use the ⊕ **Add an axis** and ⊖ **Remove this axis** buttons to add additional *X*- and/or *Y*-axes to a plot or to merge plots (to overlay one plot with another in the same diagram). When merging plots, you define this variable as the *Z*-axis.

AVAILABLE AXIS VARIABLES

? "Quantities Groups Available for Plots and Tables" on page 65 for a general list of quantities. However, for the Precipitation Calculator Plot Renderer there are no defined groups to choose from.

- **Mean radius**: Spherical radius of average volume of all particles for a specific phase and nucleation type, regardless of their actual shapes. If the matrix phase is selected, it outputs the average grain radius.
- **Conventional mean radius**: Is available for precipitates and grains. The result can be split into individual populations, and sectioned to approximate the 2D size distribution. See "Microstructure Descriptions" on page 128.
- **Critical radius**: Spherical radius of critical nuclei for a specific phase and nucleation type. If the matrix phase is selected, it outputs critical grain radius.
- **Yield strength**: To use the Yield Strength Property Model to calculate yield stress.
- **Matrix composition**: Instantaneous compositions of the matrix phase.

- **Precipitate composition**: To track the instantaneous composition of precipitate particles. In particular, it is useful to distinguish different composition sets of the same phase (for example, FCC_A1#2 and FCC_A1#3). Further choose **Solutes** or **All**.
- **Number density**: Instantaneous number of particles per unit volume for a specific phase and nucleation type. If the matrix phase is selected, it outputs instantaneous number of grains per unit volume.
- **Size distribution**: Number of particles, or grains if the matrix phase is selected, varying with their sizes per unit volume per unit length, for a specific phase and nucleation type, at a specific time.
- **Number density distribution**: Retrieve the number density (number of particles per unit volume) of precipitates, or grains if the matrix phase is selected, distributed in different particle sizes.
- **Normalized Number density distribution**: Retrieve the number density (number of particles per unit volume) of precipitates, or grains if the matrix phase is selected, normalized by total number of particles or grains per unit volume, distributed in different particle sizes normalized by average size.
- **Volume fraction**: Instantaneous volume fraction for a specific phase and nucleation type.
- **Nucleation rate**: Instantaneous number of nuclei per unit volume per unit time for a specific phase and nucleation type.
- **Normalized driving force**: Instantaneous nucleation driving force per unit mole of elements for a specific phase and nucleation type. It is normalized with RT and therefore, dimensionless.
- **Temperature**
- **Mean cubic factor**: Average cubic factor of cuboid particles. Available only when cuboid is selected as the **Morphology**.

The following settings area available as indicated when **Needle**, **Plate**, or **Cuboid** are selected as the **Morphology** in the *Precipitate Phase* section on the Precipitation Calculator.

- **Cubic factor distribution**: Variation of cubic factor with particle size at a specific time. Available with a cuboid morphology.
- **Mean aspect ratio**: Average aspect ratio of non-spherical particles. Available with a needle or plate morphology. Note that this is always larger than 1, where 1 = a sphere.
- **Mean particle length**: Diameter of non-spherical particles along the longer axis.

Available with a needle or plate morphology.

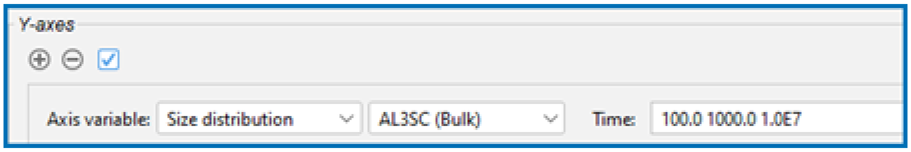
- **Aspect ratio distribution**: Variation of aspect ratio with particle size at a specific time. Available with a needle or plate morphology.

TIME (Y-AXES)

This field is available when **Size distribution** or **Number density distribution** is selected as the Y-axes variable. Enter one or a series of numbers in the field, separated by a space.

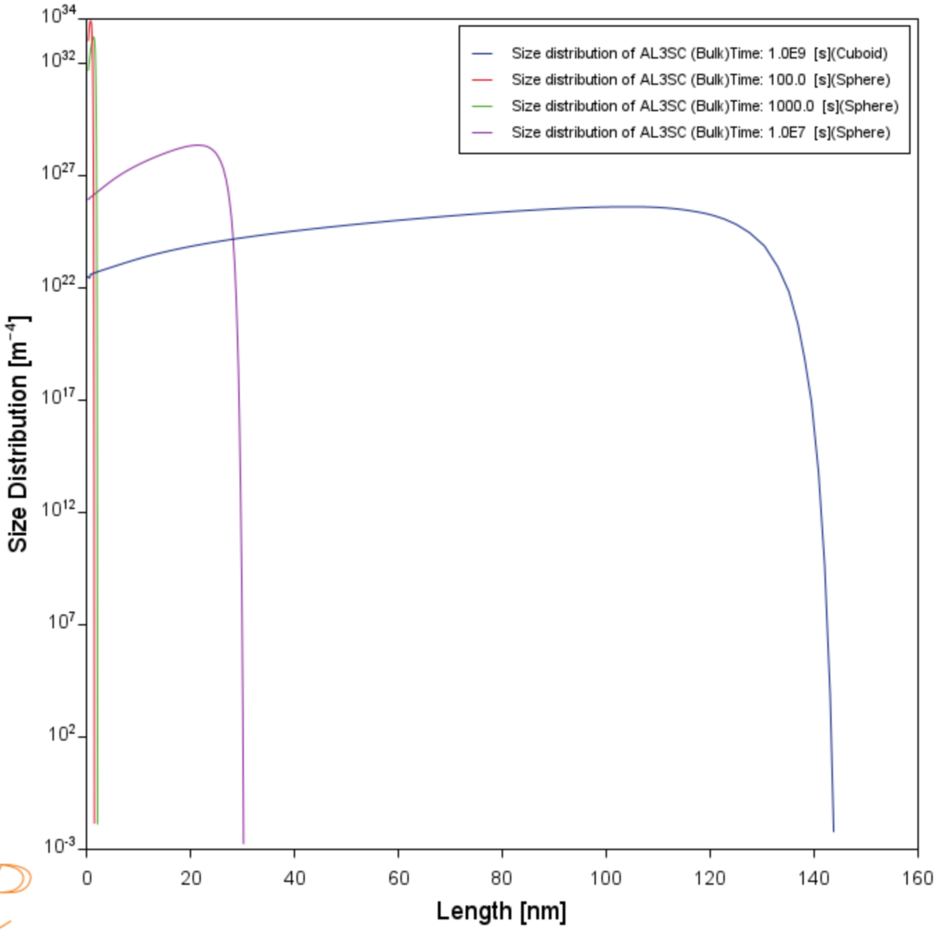
"P_09: Precipitation of Al-Sc AL3SC with Assumption of Sphere and Cuboid Morphologies" on page 172

If you open the example P_09, then change the **Time** settings on the **PSD** Plot Renderer to be `100.0 1000.0 1.0E7`:



Axis variable: Size distribution | AL3SC (Bulk) | Time: 100.0 1000.0 1.0E7

When you click **Perform** the series of times are plotted:


Size distribution of AL3SC (Bulk)Time: 1.0E9 [s](Cuboid)
Size distribution of AL3SC (Bulk)Time: 100.0 [s](Sphere)
Size distribution of AL3SC (Bulk)Time: 1000.0 [s](Sphere)
Size distribution of AL3SC (Bulk)Time: 1.0E7 [s](Sphere)
Size Distribution [m^-4]
10^{34}
10^{32}
10^{27}
10^{22}
10^{17}
10^{12}
10^{7}
10^{2}
10^{-3}
0
20
40
60
80
100
120
140
160
Length [nm]

Quantities Groups Available for Plots and Tables

The following table lists the common quantities available as axis variables (plots) or columns (tables) when working in Graphical Mode. All the quantities are listed alphabetically in conditions, quantity function definitions, and table and plot results.

About Quantity Groups

The quantities are sometimes grouped into categories on the Plot Renderer or Table Renderer. Availability of the list and the variables themselves, is based on several factors, including the database selected, the Calculator used, and the type of calculation being performed. Other differences are based on the *Plot type* selected, e.g. what you see on the **Configuration** window changes if you use **Flexible Mode** or **Grouped Mode**. Other plot types do not group the quantities and each Calculator handles the information differently.

When working on a Plot Renderer (e.g. associated to the *Axes* X, Y, and Z) or Table Renderer (associated to *Columns*), there is sometimes the option to choose a quantity group from a list. When applicable, these are the categories:

- All variables
- System variables
- Phase equilibria
- Physical properties
- Aqueous properties
- Kinetic properties
- Elastic properties

After selecting the group, you next choose from the available variables and continue to define each based on the additional settings specifically available, i.e. select a unit or a phase, and many other options that are only displayed when relevant.

These quantities are also available in Console Mode but are entered manually.

Each quantity is selected on the **Configuration** window as required either as **Axis variables** for the Plot Renderer or when choosing the **Columns** for a Table Renderer.

Quantity	*Group (when available)*	*Units*	*Additional Settings or Link to More Information*
Activity of component	Phase equilibria	dimensionless	Click to deselect the SER checkbox to use the reference state you have selected. Choose an element from the list or choose All.
Activity of water in aqueous phase	Aqueous properties	dimensionless	
Activity referred to a phase	Phase equilibria	dimensionless	Choose a phase and an element.
Affinity per electron	Aqueous properties	Joule, Calorie, Electron volt, Gigajoule, Watt hour, Kilowatt hour	
Amount of component	Phase equilibria	Mole, Gram, Kilogram, Tonne, Pound	Select the Normalization variable or No normalization if you do not want to normalize the quantity. Choose a specific element or All and a unit.
Amount of component in phase	Phase equilibria	Mole, Gram, Kilogram, Tonne, Pound	Select the Normalization variable or No normalization if you do not want to normalize the quantity. Choose a specific element or All, then a specific phase or All phases, and a unit.
Amount of phase	Phase equilibria	Mole, Gram, Kilogram, Tonne, Pound	Select the Normalization variable or No normalization if you do not want to normalize the quantity. Choose a specific phase or All phases and a unit.
Bohr magneton number	Phase equilibria	dimensionless	Choose a specific phase or All phases
Bulk modulus	Elastic properties	Pascal, Gigapascal, Atmospheres, Bar	Choose All phases or a specific phase. Select a unit.
Chemical diffusion coefficient	Kinetic properties	$m^2/$	Choose the diffusing element, Gradient element, and Reference element.
Chemical potential of component	Phase equilibria	Joule, Calorie, Electron volt, Gigajoule, Watt hour, Kilowatt hour	Click to deselect the SER checkbox to use the reference state you have selected.

Quantity	***Group (when available)***	***Units***	***Additional Settings or Link to More Information***
Chemical potential referred to a phase	Phase equilibria	Joule, Calorie, Electron volt, Gigajoule, Watt hour, Kilowatt hour	Choose a phase, an element, and a unit.
Composition	System variables	Mass percent, Mole percent, Mass fraction, Mole fraction	Choose All or a specific element and a unit.
Composition of a phase	Phase equilibria	Mass percent, Mole percent, Mass fraction, Mole fraction	Choose a specific element or All, then a specific phase or All phases, and a unit.
Curie temperature	Phase equilibria	Kelvin, Celsius, Fahrenheit	Choose a specific phase or All phases, and a unit.
Density	Physical properties	Gram per cubic meter, Kilogram per cubic meter, Gram per cubic centimeter, Pound per cubic inch	Choose All phases, an individual phase, or System. Choose a unit.
Dynamic viscosity	Physical properties	Pascal-second, milliPascal-second, Poise, centiPoise	This defaults to the LIQUID phase. Choose a unit. About Thermophysical Properties Data Parameters
Electric conductivity	Physical properties	S/m	Choose All phases, an individual phase, or System. About Thermophysical Properties Data Parameters
Elastic constant	Elastic properties	Pascal, Gigapascal, Atmospheres, Bar	Choose the elastic constant C11, C12, C13, C33, or C44. Choose All phases or an individual phase. Select a unit. Elastic Properties Variables
Electric potential (Eh)	Aqueous properties	Volt, Millivolt	

Quantity	***Group (when available)***	***Units***	***Additional Settings or Link to More Information***
Electric resistivity	Physical properties	Ωm	Choose All phases, an individual phase, or System. ? About Thermophysical Properties Data Parameters
Enthalpy	Physical properties	Joule, Calorie, Electron volt, Gigajoule, Watt hour, Kilowatt hour	Select the Normalization variable or No normalization if you do not want to normalize the quantity. Click to deselect the SER checkbox to use the reference state you have selected. Choose All phases, an individual phase, or System. Select a unit.
Entropy	Physical properties	Joule per Kelvin, Calorie per Kelvin, Electron volt per Kelvin	Select the Normalization variable or No normalization if you do not want to normalize the quantity. Click to deselect the SER checkbox to use the reference state you have selected. Choose All phases, an individual phase, or System. Select a unit.
Function	All variables	No units.	This option is only available when you choose the group **All variables**. Select **Function** when you want to choose a user-defined function. For example, if `fraction_solid` is predefined defined on the **Functions** tab for an Equilibrium Calculator and you want to plot this, choose **Function**.
Gibbs energy	Physical properties	Joule, Calorie, Electron volt, Gigajoule, Watt hour, Kilowatt hour	Select the Normalization variable or No normalization if you do not want to normalize the quantity. Click to deselect the SER checkbox to use the reference state you have selected. Choose All phases, an individual phase, or System. Select a unit.
Heat capacity	Physical properties	Joule per mole Kelvin, Calorie per mole Kelvin, Joule per kilogram Kelvin, BTU per pound Fahrenheit	Choose All phases, an individual phase, or System. Select a unit.
Helmholtz energy	Physical properties	Joule, Calorie, Electron volt, Gigajoule, Watt	Select the Normalization variable or No normalization if you do not want to normalize the quantity.

Quantity	*Group (when available)*	*Units*	*Additional Settings or Link to More Information*
		hour, Kilowatt hour	Click to deselect the SER checkbox to use the reference state you have selected. Choose All phases, an individual phase, or System. Select a unit.
ln(activity of component)	Phase equilibria	dimensionless	Click to deselect the SER checkbox to use the reference state you have selected. Choose an element from the list or choose All.
ln(activity referred to a phase)	Phase equilibria	dimensionless	Choose a phase and an element.
Internal energy	Physical properties	Joule, Calorie, Electron volt, Gigajoule, Watt hour, Kilowatt hour	Select the Normalization variable or No normalization if you do not want to normalize the quantity. Click to deselect the SER checkbox to use the reference state you have selected. Choose All phases, an individual phase, or System. Select a unit.
Intrinsic diffusion coefficient	Kinetic properties	m^2/s	Choose the diffusing element, Gradient element, and Reference element.
Ionic strength	Aqueous properties	dimensionless	
Isothermal compression	Physical properties	1/Pa	Choose All phases, an individual phase, or System.
Kinematic viscosity	Physical properties	Square meter per second, Stokes, Centistokes	This defaults to the LIQUID phase. Choose a unit. ? About Thermophysical Properties Data Parameters
L''	Kinetic properties	m^2/Js	Choose the diffusing element, Gradient element, and Reference element.
log10(Chemical diffusion coefficient)	Kinetic properties	m^2/s	Choose the diffusing element, Gradient element, and Reference element.
log10(Intrinsic diffusion coefficient)	Kinetic properties	m^2/s	Choose the diffusing element, Gradient element, and Reference element.
log10(Mobility)	Kinetic	m^2/s	

Quantity	*Group (when available)*	*Units*	*Additional Settings or Link to More Information*
	properties		
log10(Tracer diffusion coefficient)	Kinetic properties	m^2/s	
Logarithm of electron activity	Aqueous properties	dimensionless	
Mobility	Kinetic properties	m^2/s	
Molality	Aqueous properties	mol/kg H_2O	Choose **All** or select specific solute species from the list.
Mole fraction solvent	Aqueous properties	dimensionless	
Mole number	Aqueous properties	Mole	Choose **All** or select specific solute species from the list.
Normalized driving force	Phase equilibria	dimensionless	Select the Normalization variable - Per mole, Per mass in gram, Per volume in cubic meter, or Per mole formula unit. Then choose All phases or a specific phase.
Osmotic coefficient	Aqueous properties	dimensionless	
Phase stability function	Phase equilibria	dimensionless	Choose All phases or a specific phase.
pH of aqueous solution	Aqueous properties	dimensionless	
Pressure	System variables	Pascal, Atmospheres, Bar	Choose a unit.
Shear modulus	Elastic properties	Pascal, Gigapascal, Atmospheres, Bar	Choose All phases or an individual phase. Select a unit. ? Elastic Properties Variables
Site fraction	Phase equilibria	dimensionless	Choose All phases or a specific phase. Where

Quantity	***Group (when available)***	***Units***	***Additional Settings or Link to More Information***
			applicable for individual phases also select a sublattice and then a specific element for the sublattice.
Surface tension	Physical properties	Joule per m^2, Millijoule per m^2	This defaults to the LIQUID phase. Choose a unit. ? About Thermophysical Properties Data Parameters
System size	System variables	Mole, Gram, Kilogram, Tonne, Pound	Choose a unit.
Temperature	System variables	Kelvin, Celsius, Fahrenheit	Choose a unit.
Thermal conductivity	Physical properties	W/mK	Choose All phases, an individual phase, or System. ? About Thermophysical Properties Data Parameters
Thermal diffusivity	Physical properties	m^2/s	Choose All phases, an individual phase, or System. ? About Thermophysical Properties Data Parameters
Thermal expansivity	Physical properties	per Kelvin, per Fahrenheit	Choose Linear or Volumetric. Choose All phases, an individual phase, or System. Select a unit.
Thermal resistivity	Physical properties	mK/W	Choose All phases, an individual phase, or System. ? About Thermophysical Properties Data Parameters
Thermodynamic factor	Kinetic properties	m^2/s	Choose the diffusing element, Gradient element, and Reference element.
Total molality	Aqueous properties	moles per kg	
Tracer diffusion coefficient	Kinetic properties	m^2/s	

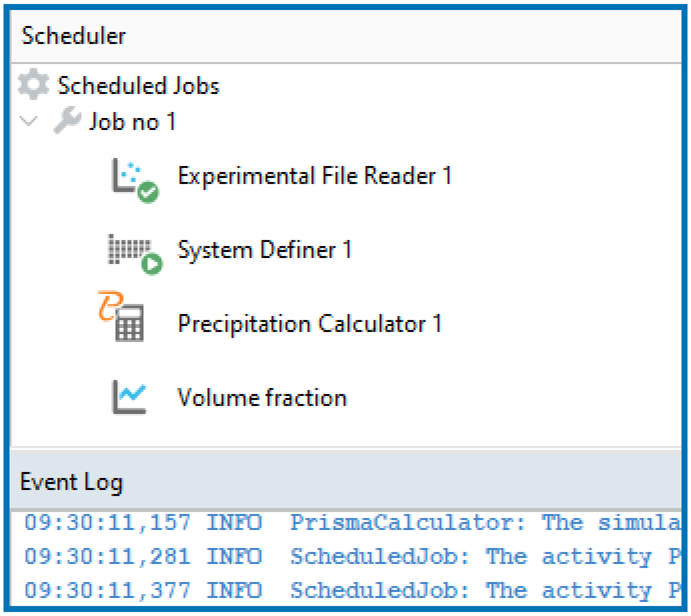
Quantity	***Group (when available)***	***Units***	***Additional Settings or Link to More Information***
u-fraction	Phase equilibria	dimensionless	Choose an element and then from the Components in denominator list, you can select or deselect specific elements using the checkboxes. ? The u-Fraction Variable
User-defined	System variables	No units.	Enter another axis variable.
Volume	Phase equilibria	Cubic meter, Cubic decimeter, Cubic centimeter, Normal cubic meter	Select the Normalization variable or No normalization if you do not want to normalize the quantity. Click to deselect the SER checkbox to use the reference state you have selected. Choose All phases, an individual phase, or System. Choose a unit.
Volume fraction of phase	Phase equilibria	dimensionless	Choose All phases or an individual phase.
Young's modulus	Elastic properties	Pascal, Gigapascal, Atmospheres, Bar	Choose All phases or an individual phase. Select a unit. ? Elastic Properties Variables

Pause, Resume, and Cancel Precipitation Calculations

Precipitation calculations are often complex simulations that take some time to complete. Sometimes you may want or need to pause or resume a calculation, or make adjustments to your compositions and start again. You pause and resume from the Precipitation Calculator **Configuration** window.

To Pause and Resume a Job

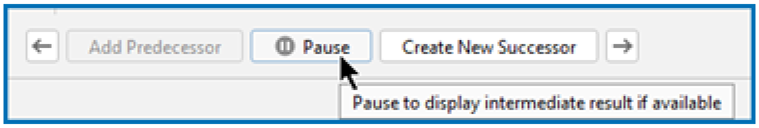
1. Run the job (i.e. click **Perform Tree**). In the **Scheduler**, you can see the job listed and in the **Event Log** you can follow the progress of the calculation.



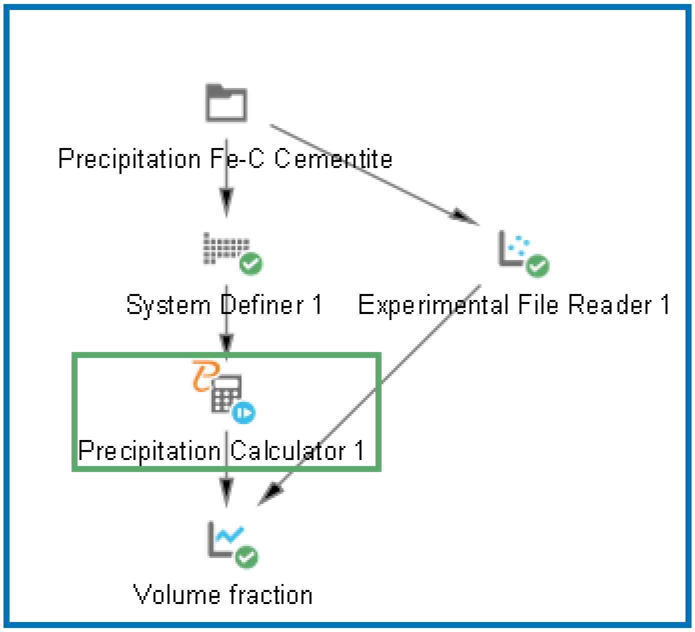
```
09:30:11,157 INFO  PrismaCalculator: The simula
09:30:11,281 INFO  ScheduledJob: The activity P
09:30:11,377 INFO  ScheduledJob: The activity P
```

2. In the **Project** window, click the **Precipitation Calculator** node.

3. In the **Configuration** window at the bottom, click **Pause**. Observe that the **Precipitation Calculator** in the **Project** window has a pause indicator. If there are intermediate results available these will be listed in the **Event Log**.

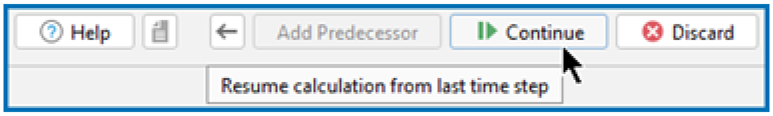


Pause to display intermediate result if available



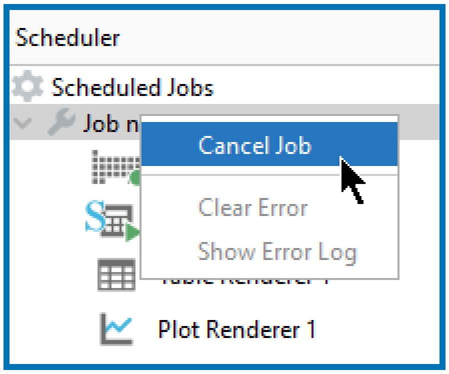
4. When pausing the calculation, you can make changes to a variety of settings under the *Matrix Phase* or *Precipitate Phase* sections (click **Show Details**), plus the **Interfacial energy**, **Temperature** (for non-isothermal calculations), and **Simulation time**. The rest of the **Configuration** window settings are grayed out and no other editing can be done while paused.

5. When ready, click ▶ **Continue** to resume your calculations from the last time step or click ⊗ **Discard** to discard the calculation (then click **Yes** or **No** on the window that opens).



To Cancel a Job

- In the **Scheduler** window, right-click the job you want to cancel and select **Cancel Job**.



Theoretical Models and Numerical Methods

In this section:

Theory Overview 77

Nucleation Theory 79

Homogeneous Nucleation 80

Heterogeneous Nucleation 87

Nucleation During a Non-isothermal Process 93

Growth 94

Coarsening 104

Continuity Equation 105

Mass Conservation 106

Numerical Method 107

Estimation of Coherent Interfacial Energy 112

Precipitation Morphology 113

Normal Grain Growth 116

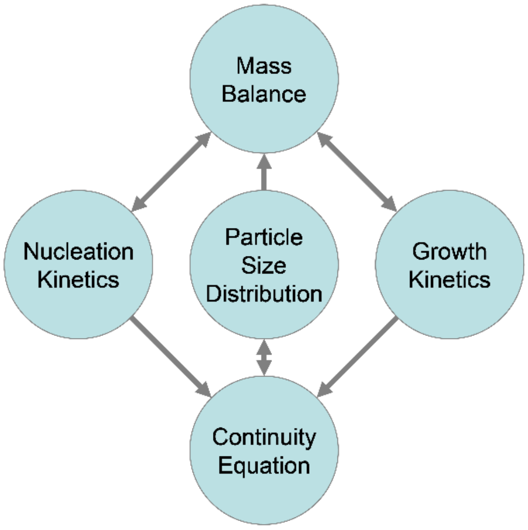
Stereology 121

Microstructure Descriptions 128

Theory Overview

Based on the theory from Langer-Schwartz [1980Lan] the Precipitation Module (TC-PRISMA) adopts Kampmann-Wagner numerical (KWN) [2013Wag] method to simulate the concomitant nucleation, growth, and coarsening of precipitates in multicomponent and multiphase alloy systems. The KWN method is an extension of the original Langer-Schwartz (LS) approach and its modified (MLS) form, where the temporal evolution of the mean radius and particle density over the whole course of precipitation are predicted by solving a set of rate equations derived with certain assumptions for the rates of nucleation and growth, as well as the function of particle size distribution (PSD). The MLS approach differs from the LS with respect to the Gibbs-Thomson equations used for calculating equilibrium solubilities of small particles. The former applies the exact exponential form, whereas the latter takes the convenient linearized version. Instead of assuming a PSD function *a priori* and working with rate equations for determining only mean radius and particle density, the KWN method extends the LS and MLS approaches by discretizing the PSD and solving the continuity equation of the PSD directly. Therefore, the time evolution of the PSD and its n^{th} moment (*0*: number density; 1^{st}: mean radius; 3^{rd}: volume fraction) can be obtained altogether during the simulation. The key elements of the KWN method are the models for nucleation and growth under the mean field mass balance condition and the numerical algorithm for solving the continuity equation of the PSD. Coarsening comes out naturally without any *ad hoc* treatment.

The key elements of the KWN method and their relationship as implemented in the Precipitation Module (TC-PRISMA).



Integration of the Precipitation Module into Thermo-Calc

Precipitation Module (TC-PRISMA) is integrated with Thermo-Calc in order to directly get all necessary thermodynamic and kinetic information required in the KWN method. For industry relevant multicomponent alloys, thermodynamic and kinetic databases and calculation tools have to be used in order to obtain various quantities in the multicomponent models for nucleation and growth, such as the driving forces for the formation of embryos and their compositions, the atomic mobilities or diffusivities in the matrix, the operating interface compositions under local equilibrium conditions, the Gibbs-Thomson effect, and the deviation from local equilibrium due to interface friction etc. With Thermo-Calc and the Diffusion Module (DICTRA) as well as the accompanying databases, all these properties and effects can be calculated without unnecessary and inaccurate approximations.

In the following topics, various models and numerical methods implemented in Precipitation Module (TC-PRISMA) are introduced. Unless specified, spherical particles are assumed in the discussion.

References

[1980Lan] J. S. Langer, A. J. Schwartz, Kinetics of nucleation in near-critical fluids. Phys. Rev. A. 21, 948–958 (1980).

[2013Wag] R. Wagner, R. Kampmann, P. W. Voorhees, 'Homogeneous second phase precipitation', in Materials Science and Technology, R. W. Cahn, P. Haasen, E. J. Kramer, Eds. (Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany, 2013), pp. 213–304.

Nucleation Theory

Precipitation starts from the nucleation of clusters that can be considered as embryos of new phases with distinctive structures or compositions. In a perfect single crystal, nucleation happens homogeneously. In an imperfect crystal or polycrystalline materials, nucleation tends to occur heterogeneously due to the presence of dislocations, grain boundaries, grain edges, and grain corners. These imperfections or defects reduce the nucleation barrier and facilitate nucleation. However, if supersaturation or driving force is very large homogeneous nucleation is also possible since all sites including those inside a grain can be activated.

The following sections further elaborate on this theory.

- "Homogeneous Nucleation" on the next page
- "Heterogeneous Nucleation" on page 87
- "Nucleation During a Non-isothermal Process" on page 93

Homogeneous Nucleation

The classic nucleation theory (CNT) [2000, Kashchiev; 1980, Russell] has been extended for the purpose of modeling nucleation in multicomponent alloy systems. The time-dependent nucleation rate $J(t)$ is given by

[*Eq. 1*] $$J(t) = J_s exp\left(\frac{-\tau}{t}\right)$$

where

- J_s is the steady state nucleation rate,
- τ is the incubation time for establishing steady state nucleation conditions, and
- t is the time.

The steady state nucleation rate J_s is expressed by

[*Eq. 2*] $$J_s = Z\beta^* N exp\left(\frac{-\Delta G^*}{kT}\right)$$

where

- Z is the Zeldovich factor,
- β^* is the rate at which atoms or molecules are attached to the critical nucleus,
- N is the number of available nucleation sites (of a particular type) per unit volume. In the case of homogeneous nucleation, initially, each atom in the whole volume of the mother phase is a potential nucleation site. As precipitation proceeds, the number of available nucleation sites decreases due to the occupancy of part of the matrix volume by formed secondary phase particles. In the case of heterogeneous nucleation, the initial number can also be estimated, given the grain size or dislocation density in the matrix phase. It decreases also with time but at different rates.
- ΔG^* is the Gibbs energy of formation of a critical nucleus,
- k is Boltzmann's constant,
- T is absolute temperature.

The Gibbs energy of formation of a critical nucleus is expressed as

[*Eq. 3*] $$\Delta G^* = \frac{16\pi\sigma^3}{3\left(\Delta G_m^{\alpha\to\beta}/V_m^\beta\right)^2}$$

where

- σ is the interfacial energy,
- $\Delta G_m^{\alpha\rightarrow\beta}$ is the molar Gibbs energy change for the formation of the β precipitate of the critical composition X_i^β from the α matrix, i.e. the maximum driving force for the $\alpha \rightarrow \beta$ phase transformation
- V_m^β is the molar volume of the β precipitate phase.

If elastic strain energy is excluded, $\Delta G_m^{\alpha\rightarrow\beta}$ is the chemical driving force for nucleation. There are two ways to calculate the nucleation driving force $\Delta G_m^{\alpha\rightarrow\beta}$ and the critical composition X_i^β, as shown in Figure 6 for a prototype binary system. The standard calculation in Figure 6 is to obtain the maximum driving force by finding the parallel tangent lines or surfaces passing through the alloy composition of the matrix, which is a routine calculation in the Thermo-Calc software. The approximate calculation in Figure 6 is performed by using the Gibbs energy difference corresponding to the equilibrium composition in the precipitate phase. It can be used when the standard calculation fails, mostly within a miscibility gap. Additionally, the standard calculation is also used for driving force under paraequilibrium conditions, while the approximate calculation is used for driving force under NPLE (Non-Partitioning Local Equilibrium) conditions.

? "Growth" on page 94

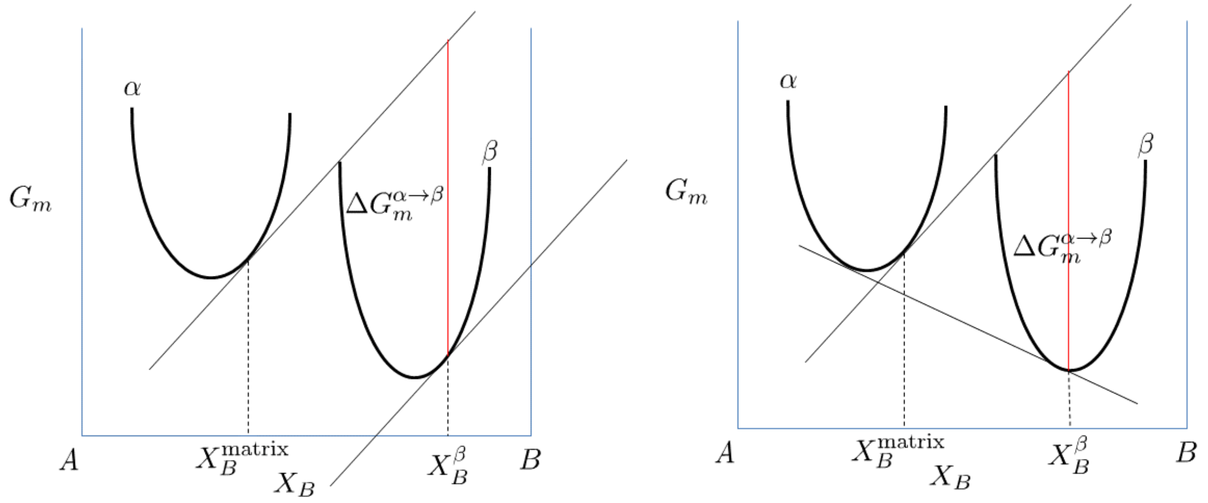


Figure 6: Methods to calculate the nucleation driving force $\Delta G_m^{\alpha\rightarrow\beta}$ and the critical composition X_i^{β}. The standard calculation (left) and an approximate calculation (right).

Nucleation is a stochastic process and can be considered formally as a diffusion process or Brownian movement in the particle size space. Supercritical nuclei with radius slightly larger than the critical radius have a probability of passing back across the free energy barrier and dissolve in the matrix. The Zeldovich factor (Z) is a measure of such probability and is related solely to the thermodynamics of the nucleation process in

[*Eq. 4*]

$$Z = \frac{V_m^{\beta}}{2\pi N_A r^{*2}}\sqrt{\frac{\sigma}{kT}}$$

where N_A is the Avogadro number and r^*, the critical radius, is given by

[*Eq. 5*]

$$r^* = -\frac{2\sigma V_m^{\beta}}{\Delta G_m^{\alpha\rightarrow\beta}}$$

The atomic or molecular attachment rate β^* reflects the kinetics of mass transport in the nucleation process and is given by Svoboda et al. [2004Svo].

[*Eq. 6*]

$$\beta^* = \frac{4\pi r^{*2}}{a^4}\left[\sum_{i=1}^{k}\frac{\left(X_i^{\beta/\alpha} - X_i^{\alpha/\beta}\right)^2}{X_i^{\alpha/\beta} D_i}\right]^{-1}$$

where

- a is the lattice parameter,
- $X_i^{\beta/\alpha}$ and $X_i^{\alpha/\beta}$ are the mole fractions of element *i* at the interface in the precipitate and matrix, respectively.
- D_i is the corresponding diffusion coefficient in the matrix.

The incubation time τ for an isothermal reaction is

[*Eq. 7*] $$\tau = \frac{1}{\theta Z^2 \beta^*}$$

where θ differs from one derivation to another. The value 2 from Feder et al. [1966Fed] is adopted.

Elastic Strain Energy

Elastic strain energy, E_{el}, reduces the nucleation driving force, $\Delta G_m^{\alpha\to\beta}$ in Eq. 3, hence affecting nucleation rate and nuclei size. It also changes the shape of the particle by competing with interfacial energy.

Cuboid Particle

"Precipitation Morphology" on page 113

The numerical simulations by Onaka et al. [2003Ona] indicate that the elastic strain energy is reduced almost linearly with increasing cubic factor η. Since the numerical simulations are computationally expensive, we assume that the elastic strain energy follows the linear relationship with η, and the elastic strain energy for spherical ($\eta = 1$) and cubic ($\eta = \sqrt{2}$) are calculated based on Khachaturyan’s approximation [1983/2008Kha].

[*Eq. 8*] $$E_{\mathrm{el}} = \tfrac{1}{2}(c_{11} + 2c_{12})\epsilon_0^2 V[A_1 + A_2]$$

where

- ϵ_0 is the lattice misfit strain,
- c_{11}, c_{12}, c_{44} are elastic constants in a cubic system,
- V is particle volume,
- A_1 and A_2 are expressed as

$$A_1 = 2\tfrac{c_{11}-c_{12}}{c_{11}} - 12\tfrac{c_{11}+2c_{12}}{c_{11}}\tfrac{c_{11}-c_{12}-2c_{44}}{c_{11}+c_{12}+2c_{44}}I_1$$

$$A_2 = -54\tfrac{c_{11}+2c_{12}}{c_{11}}\tfrac{(c_{11}-c_{12}-2c_{44})^2}{(c_{11}+c_{12}+2c_{44})(c_{11}+2c_{12}+4c_{44})}I_2$$

with

Sphere

$$I_1 = \frac{1}{15} \qquad I_2 = \frac{1}{105}$$

Cubic

$$I_1 = 0.006931 \qquad I_2 = 0.000959$$

Ellipsoidal Particle (Plate and Needle)

"Precipitation Morphology" on page 113

Since they are ellipsoidal shape, it is convenient to use Eshelby's theory [1957/1959Esh] with a reasonable computational cost. The Eshelby's tensor can be calculated by simply performing a surface integral over a unit sphere

[*Eq. 9*]
$$D_{ijkl} = -\frac{abc}{4\pi}\int_0^{\pi}\int_0^{2\pi}\Omega_{ij}n_kn_l\frac{\sin\theta}{\beta^3}d\phi d\theta$$

where

- a, b, c are ellipsoid axes,
- $n_i(i = 1, 2, 3)$ are unit directional vector normal to the spherical surface and

$$\beta = \sqrt{(a^2\cos^2\phi + b^2\sin^2\phi)\sin^2\theta + c^2\cos^2\theta}$$

For matrix phase with cubic crystal symmetry, we have for $\Omega_{ij}(i, j = 1, 2, 3)$. See [1983Kha].

$$\Omega_{ii}(\vec{n}) = \frac{c_{44}+(c_{11}-c_{44})(n_j^2+n_k^2)+\xi(c_{11}+c_{12})n_j^2n_k^2}{c_{44}D(\vec{n})}$$

$$\Omega_{ij}(\vec{n}) = -\frac{(c_{12}+c_{44})(1+\xi n_k^2)}{c_{44}D(\vec{n})}n_in_j$$

where

$$\xi = \frac{c_{11}-c_{12}-2c_{44}}{c_{44}}$$

$$D(\vec{n}) = c_{11} + \xi(c_{11} + c_{12})(n_1^2n_2^2 + n_1^2n_3^2 + n_2^2n_3^2) + \xi^2(c_{11} + 2c_{12} + c_{44})n_1^2n_2^2n_3^2$$

The Eshelby S tensor can then be calculated as

[*Eq. 10*]
$$S_{ijmn} = -\frac{1}{2}C_{lkmn}\left(D_{iklj} + D_{jkli}\right)$$

The total strain ϵ_{ij} at each location inside the particle is related to its transformation strain (eigenstrain) ϵ^*_{ij} as

[*Eq. 11*] $$\epsilon_{ij} = S_{ijkl}\epsilon^*_{kl}$$

Combined with elastic stress calculated as

$$\sigma_{ij} = C_{ijkl}\left(\epsilon_{kl} - \epsilon^*_{kl}\right)$$

The elastic strain energy can be then obtained

[*Eq. 12*] $$E^{el} = -\frac{1}{2}\sigma_{ij}\epsilon^*_{ij}V$$

with V the particle volume.

Spherical Approximation for Nuclei

In the Precipitation Module, the user-input or calculated interfacial energy is assumed to be the coherent interfacial energy that applies to the habit plane, $\sigma^{\mathrm{sph}}_{\mathrm{coh}}$, consistent with the approximation made by the embedded interfacial energy model. When calculating the critical nuclei, the interfacial energy in Eq. 3 is assumed to be that of a spherical particle with constant specific interfacial energy $\sigma^{\mathrm{sph}}_{\mathrm{coh}}$. This is consistent with the fact that the nuclei tend to be spherical due to dominant interfacial energy. Interfacial energy penalty assuming a nucleus with pre-defined, and most likely large, aspect ratio is thus over-estimated, and has been found to shut down nucleation event abnormally.

Under spherical approximation, the elastic strain energy is calculated using spherical expression in Eq. 8 for spherical and cuboidal particles, or by setting $a = b = c$ in Eq. 9 for ellipsoidal particles.

References

[1957Esh] J. D. Eshelby, The Determination of the Elastic Field of an Ellipsoidal Inclusion, and Related Problems. Proc. R. Soc. A Math. Phys. Eng. Sci. 241, 376–396 (1957).

[1959Esh] J. D. Eshelby, The Elastic Field Outside an Ellipsoidal Inclusion. Proc. R. Soc. A Math. Phys. Eng. Sci. 252, 561–569 (1959).

[1966Fed] J. Feder, K. C. Russell, J. Lothe, G. M. Pound, Homogeneous nucleation and growth of droplets in vapours. Adv. Phys. 15, 111–178 (1966).

[1980Rus] K. C. Russell, Nucleation in solids: The induction and steady state effects. Adv. Colloid Interface Sci. 13, 205–318 (1980).

[2000Kas] D. Kashchiev. Nucleation. Butterworth-Heinemann, 2000.

[2003Ona] S. Onaka, N. Kobayashi, T. Fujii, M. Kato, Energy analysis with a superspherical shape approximation on the spherical to cubical shape transitions of coherent precipitates in cubic materials. Mater. Sci. Eng. A. 347, 42–49 (2003).

[2004Svo] J. Svoboda, F. D. Fischer, P. Fratzl, E. Kozeschnik, Modelling of kinetics in multi-component multi-phase systems with spherical precipitates. Mater. Sci. Eng. A. 385, 166–174 (2004).

[2013Kha] A. G. Khachaturyan, “Habit Plane and Orientation Relations in Precipitates: Comparison with Experimental Data.” in Theory of Structural Transformations in Solids (Dover Publications, Inc., New York, 2013.

Heterogeneous Nucleation

All equations remain the same for the calculation of heterogeneous nucleation rate within the framework of classic nucleation theory (CNT), but the nucleation energy and available nucleation site are different.

To a first approximation, the nucleation energy may be calculated by assuming an effective interfacial energy for each heterogeneous nucleation site.

For a rigorous treatment of heterogeneous nucleation the effect of wetting angles need to be considered.

Non-Spherical Particles and the Effect of Wetting Angle

"Precipitation Module (TC-PRISMA) References" on page 129

Non-spherical particles have been considered for grain boundary (GB) precipitation. Three morphologies are implemented for grain boundary, grain edge and grain corner precipitation, respectively, as shown in Figure 7. The parameter that defines the deviation from spherical shape is wetting angle (or dihedral angle), θ, as described in Figure 8 and taken from Clemm and Fisher [1955Cle].

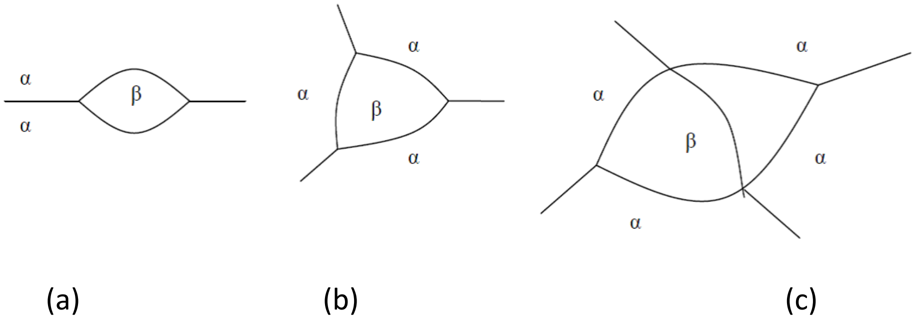


Figure 7: Non-spherical particles (β) that precipitate at grain boundaries of matrix phase(α) (a) grain boundary (two-grain junction) (b) grain edge (three-grain junction) (c) grain corners (four-grain junction). Images from [2004Zan].

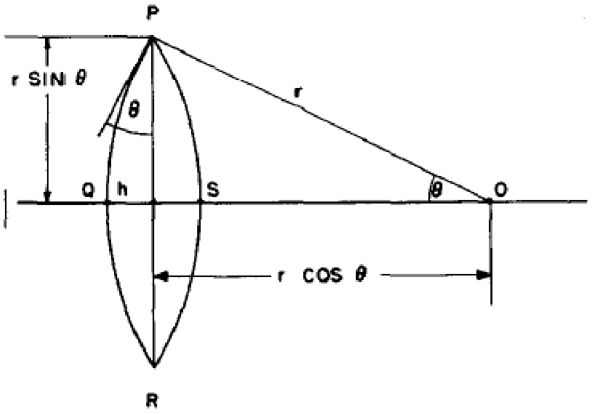


Figure 8: The nucleus at the grain boundary. Image from [1955Clem].

Some physical parameters, mainly in nucleation models, have to be modified for the effect of the wetting angle. The following discussions contribute to this effect.

Shape Factors

Following Clemm and Fisher, the eliminated grain boundary area between $\alpha - \alpha$ grains due to the formation of nucleus of a new phase β is:

[*Eq. 1*] $$A_{\alpha\alpha} = ar^2$$

Where r is the radius of curvature of the nucleus. The surface area of the nucleus is:

[*Eq. 2*] $$A_{\alpha\beta} = br^2$$

and the volume of the nucleus is

[*Eq. 3*] $$V = cr^3$$

The expression of a, b, c in Eq. 1 and Eq. 3 for grain boundary (two-grain junction), grain edge (three-grain junction) and grain corner (four-grain junction) can be found in the paper by Clemm and Fisher [1955Cle].

Critical Radius and Activation Energy

The energy change due to the formation of the new particle is thus

[*Eq. 4*] $$\Delta F = \frac{\Delta G_m^{\alpha \to \beta}}{V_m} \cdot cr^3 + br^2 \sigma_{\alpha\beta} - ar^2 \sigma_{\alpha\alpha}$$

where $\sigma_{\alpha\beta}$ and $\sigma_{\alpha\alpha}$ are the interfacial energy and grain boundary energy, respectively.

Then the critical radius should be

[*Eq. 5*]
$$r^* = -\frac{2\left(b\sigma_{\alpha\beta} - a\sigma_{\alpha\alpha}\right)V_m}{3c\Delta G_m^{\alpha\rightarrow\beta}}$$

And the activation energy barrier for nucleation is

[*Eq. 6*]
$$W = \frac{4}{27}\frac{\left(b\sigma_{\alpha\beta} - a\sigma_{\alpha\alpha}\right)^3 V_m^2}{c^2\left(\Delta G_m^{\alpha\rightarrow\beta}\right)^2}$$

The interfacial energy, grain boundary energy and wetting angle can be related as

[*Eq. 7*]
$$k = \cos\theta = \frac{\sigma_{\alpha\alpha}}{2\sigma_{\alpha\beta}}$$

i.e.

[*Eq. 8*]
$$\sigma_{\alpha\alpha} = 2k\sigma_{\alpha\beta}$$

which can be replaced into Eq. 5 and Eq. 6.

[*Eq. 9*]
$$r^* = -\frac{2\left(b - 2ak\right)\sigma_{\alpha\beta}V_m}{3c\Delta G_m^{\alpha\rightarrow\beta}}$$

[*Eq. 10*]
$$W = \frac{4}{27}\frac{\sigma_{\alpha\beta}^3 V_m^2}{\left(\Delta G_m^{\alpha\rightarrow\beta}\right)^2}\frac{\left(b - 2ak\right)^3}{c^2}$$

The bulk, spherical precipitation equation is recovered by:

[*Eq. 11*]
$$a = 0, \quad b = 4\pi, \quad c = \frac{4\pi}{3}$$

so that

[*Eq. 12*]
$$r^* = -\frac{2\sigma_{\alpha\beta}V_m}{\Delta G_m^{\alpha\rightarrow\beta}}$$

[*Eq. 13*]
$$W = \frac{16\pi}{3}\frac{\sigma_{\alpha\beta}^3 V_m^2}{\left(\Delta G_m^{\alpha\rightarrow\beta}\right)^2}$$

And also the grain boundary precipitation with spherical shape (with weighting angle 90°) follows Eq. 12 and Eq. 13 by $k = \cos\theta = 0$.

Zeldovich Factor

The Zeldovich factor is modified as

[*Eq. 14*] $$Z = Z_b\sqrt{f}$$

with Z_b the original value, and f the volume factor that is the ratio of the c in Eq. 3 to the spherical shape factor $4\pi/3$.

[*Eq. 15*] $$f = \frac{3c}{4\pi}$$

Impingement Rate

The surface area factor in impingement rate calculation is changed from $4\pi(r^*)^2$ to $b(r^*)^2$.

Nucleation Site Density

In each time step, the occupied grain boundary area

[*Eq. 16*] $$A_{\text{red}} = a \cdot nr^2$$

is deducted when calculating available nucleation site density.

Growth Rate

The radius r defined in previous equations is the curvature of the precipitate surface (the Big radius) as shown in Figure 8. It is exactly the definition in the growth rate whose coarsening consideration relates to the curvature effect. Therefore, the growth rate equation can be directly used with r being defined here. Again, for bulk, spherical precipitation it automatically corresponds to the particle radius.

Output

The volume of the precipitate should be calculated appropriately as cr^3 with r being the curvature of the particle surface as defined above. For output of the particle size (mean radius, critical radius and particle size distribution) in the user interface, it seems better to use the radius of the eliminated grain boundary area, i.e.

[*Eq. 17*] $$r' = \sqrt{\frac{a}{\pi}} \cdot r$$

With a defined in Eq. 1.

For example, the size of the precipitate at grain boundary (two-grain junction) is the radius of the lens shown in Figure 8.

$$r' = r\sin\theta = r\sqrt{1-k^2}$$

The Number of Available Heterogeneous Nucleation Sites

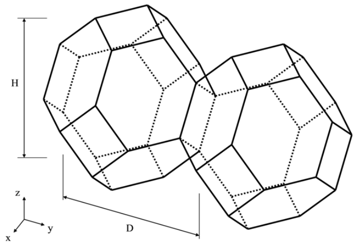


Figure 9: An example of tetrakaidecahedron approximation of grains.

The number of different nucleation sites is dependent on the shape and size of grains in the matrix. Assuming all grains are equally large tetrakaidecahedra with the distance between one pair of square faces as H, and that between the other two pairs as D we obtain the densities ρ_2, ρ_1, and ρ_0 for the grain boundary area, edge length, and grain corner number, respectively in

[*Eq. 18*]

$$\rho_2 = \frac{6\sqrt{1+2A^2}+1+2A}{4A}D^{-1}$$

[*Eq. 19*]

$$\rho_1 = 2\frac{\sqrt{2}+2\sqrt{1+A^2}}{A}D^{-2}$$

[*Eq. 20*]

$$\rho_0 = \frac{12}{A}D^{-3}$$

where $A = H/D$ is the aspect ratio, defining the degree of elongation of the grains.

By default, the aspect ratio is set to 1 and the densities are then the same as obtained by Cahn [1956Cah]. Once the densities are known, if taking boundary thickness as one atomic layer, the available nucleation sites can be calculated by

[*Eq. 21*]

$$N_i = \rho_i \left(\frac{N_A}{V_m^\alpha}\right)^{i/3} \quad i = 2, 1, 0$$

where V_m^α is the molar volume of the matrix phase and N_A is the Avogadro number.

For a crystalline material, given a dislocation density ρ_d, the number of nucleation sites at the dislocations N_d can be calculated with the same form as in

[*Eq. 22*]

$$N_d = \rho_d \left(\frac{N_A}{V_m^\alpha}\right)^{1/3}$$

References

[1955Cle] P. J. Clemm, J. C. Fisher, The influence of grain boundaries on the nucleation of secondary phases. Acta Metall. 3, 70–73 (1955).

[1956Cah] J. W. Cahn, Transformation kinetics during continuous cooling. Acta Metall. 4, 572–575 (1956).

[2004Zan] L. Zang, Lecture 13: Heterogeneous Nucleation: Effects of Grain Boundaries and Surface Defects, The University of Utah, (2004), (available at http://www.eng.utah.edu/%7B$~$%7Dlzang/images/lecture-13.pdf).

Nucleation During a Non-isothermal Process

Under non-isothermal conditions, temperature dependency of key parameters such as nucleation driving force, solute diffusivities and solute concentrations, etc., have been taken into account, and are updated automatically during a simulation.

Another important parameter that depends on thermal history is the incubation time, defined by

[Eq. 1]

$$\tau = \frac{1}{\theta Z^2 \beta^*}$$

for an isothermal condition. In a non-isothermal process, the exact calculation of the incubation time requires a solution to the Fokker-Planck equation. In the Precipitation Module, an approximation approach has been employed to deal with the transient nucleation, which gives the incubation time as an integral form of past thermal history [2004Jou] as in

[Eq. 2]

$$\int_o^\tau \beta^*(t')dt' = \frac{1}{\theta Z^2(\tau)}$$

where

τ is the incubation time, β^* is the impingement rate for solute atoms to the critical cluster as defined in

[Eq. 3]

$$\beta^* = \frac{4\pi r^{*2}}{a^4}\left[\sum_{i=1}^{k}\frac{\left(X_i^{\beta/\alpha} - X_i^{\alpha/\beta}\right)^2}{X_i^{\alpha/\beta} D_i}\right]^{-1}$$

and Z is the Zeldovich factor, previously defined in

[Eq. 4]

$$Z = \frac{V_m^\beta}{2\pi N_A r^{*2}}\sqrt{\frac{\sigma}{kT}}$$

but now as a function of τ derived from temperature change.

The starting point of the integral $t' = 0$ is either the starting time if there is an initial nucleation driving force, or the latest time when the nucleation driving force is vanished.

Reference

[2004Jou] H.-J. Jou, P. Voorhees, G. B. Olson, Computer simulations for the prediction of microstructure/property variation in aeroturbine disks. Superalloys, 877–886 (2004).

Growth

Spherical Particles

The growth rate models implemented in the Precipitation Module are called **Advanced**, **Simplified**, **General**, **Para-eq**, **NPLE**, and **PE Automatic**. All models treat a spherical particle (precipitate) of stoichiometric composition or with negligible atomic diffusivity.

All models treat a particle (precipitate) of stoichiometric composition or with negligible atomic diffusivity. Except for the **PE Automatic** model, local equilibrium or paraequilibrium at the precipitate-matrix interface is assumed. The **PE Automatic** model enables smooth transition from paraequilibrium to local equilibrium.

In the documentation and on the GUI, the abbreviations *Para-eq* and *PE* are both used for paraequilibrium. There is also the use of OE as an abbreviation for *ortho-equilibrium* and LE for *local equilibrium*.

Advanced Growth Rate Model

The *Advanced* model is proposed by Chen, Jeppsson, and Ågren (CJA) [2008Che]. In this 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.

According to the CJA model, the interface velocity v can be obtained together with interface concentrations by numerically solving $2n-1$ equations, comprising of the flux balance equations for $n-1$ independent components and the local equilibrium conditions for all n components as in

[*Eq. 1*] $$v(c_i^{\beta/\alpha} - c_i^{\alpha/\beta}) = c_i^{\alpha/\beta} M_i \frac{\mu_i^{\alpha} - \mu_i^{\alpha/\beta}}{\xi_i r}$$

[*Eq. 2*] $$\mu_i^{\alpha/\beta} = \mu_i^{\beta/\alpha} + \frac{2\sigma V_m^{\beta}}{r}$$

where

- $c_i^{\beta/\alpha}$ and $c_i^{\alpha/\beta}$ are the volume concentrations of component i at the interface in the precipitate and matrix, respectively,
- M_i is the corresponding atomic mobility in the matrix,
- μ_i^{α} and $\mu_i^{\alpha/\beta}$ are the chemical potentials in the matrix of the mean-field concentration and at the interface, respectively.
- $\mu_i^{\beta/\alpha}$ is the chemical potential at the interface in the precipitate.

In the above local equilibrium condition, the multicomponent Gibbs-Thomson effect has been taken into account by adding a curvature induced pressure term to the Gibbs energy of the precipitate phase.

The introduced effective diffusion distance factor, ξ_i, for each independent component is given by

[Eq. 3]
$$\xi_i = \frac{\Omega_i}{2\lambda_i^2}$$

where

$$\Omega_i = \frac{c_i^{\alpha} - c_i^{\alpha/\beta}}{c_i^{\beta/\alpha} - c_i^{\alpha/\beta}}$$

is the so-called dimensionless supersaturation for an individual component, and λ_i is obtained via

[Eq. 4]
$$2\lambda_i^2 - 2\lambda_i^3\sqrt{\pi}\exp\left(\lambda_i^2\right)\mathrm{erfc}(\lambda_i) = \Omega_i$$

Simplified Growth Rate Model

In some cases, the **Advanced** model fails to find the solution to flux-balance equations. Even when it does, the calculation can be time consuming. Therefore, a simple and efficient, albeit less rigorous, model is preferred in many applications. The **Simplified** model [2022Ågr], in a pseudo-steady state approximation, is developed by solving Laplace equation along radial direction, and is expressed as

[Eq. 5]
$$v = \frac{K}{r}\left[\Delta G_m - \frac{2\sigma V_m^{\beta}}{r}\right] = \frac{2\sigma V_m^{\beta} K}{r}\left[\frac{1}{r^*} - \frac{1}{r}\right]$$

where ΔG_m is the nucleation driving force and r^* is the radius of critical nuclei. K is the kinetic parameter that is related to solute composition and mobility. Neglecting cross diffusion, it is expressed as

[*Eq. 6*]

$$K = K^{\text{simplified}}_{\text{sphere}} = \left[\sum_i \frac{\left(X_i^{\beta/\alpha}(r) - X_i^{\alpha/\beta}(r)\right)^2 \xi_i}{X_i^{\alpha/\beta}(r) M_i}\right]^{-1}$$

The interface compositions (mole fractions) $X_i^{\beta/\alpha}(r)$ and $X_i^{\alpha/\beta}(r)$ for precipitate and matrix phase, respectively, are tie-line compositions across the matrix composition. To avoid time-consuming equilibrium calculations and also realizing that precipitate composition $X_i^{\beta/\alpha}(r)$ only appears in the difference term

$$\left(X_i^{\beta/\alpha}(r) - X_i^{\alpha/\beta}(r)\right)$$

Equation 6 is further simplified by replacing $X_i^{\beta/\alpha}(r)$ with nuclei composition from nucleation driving force calculation, and $X_i^{\alpha/\beta}(r)$ with matrix composition.

The K constant defined here relates growth rate to driving force in $v = \frac{K}{r}\left[\Delta G_m - \frac{2\sigma V_m^\beta}{r}\right]$, which is not to be confused with coarsening rate constant relating mean particle radius cubed to time.

For the *Precipitation Calculator* → *Precipitate Phase* settings, **Phase energy addition** G_m^a and **Phase boundary mobility** M^B shifts the Gibbs energy of the precipitate β phase by $G_m^a + vV_m^\beta / M^B$. As a result, the driving force ΔG_m is reduced by $G_m^a + vV_m^\beta / M^B$, and the equilibrium compositions $c_i^{\beta e}$ and $c_i^{\alpha e}$ are shifted.

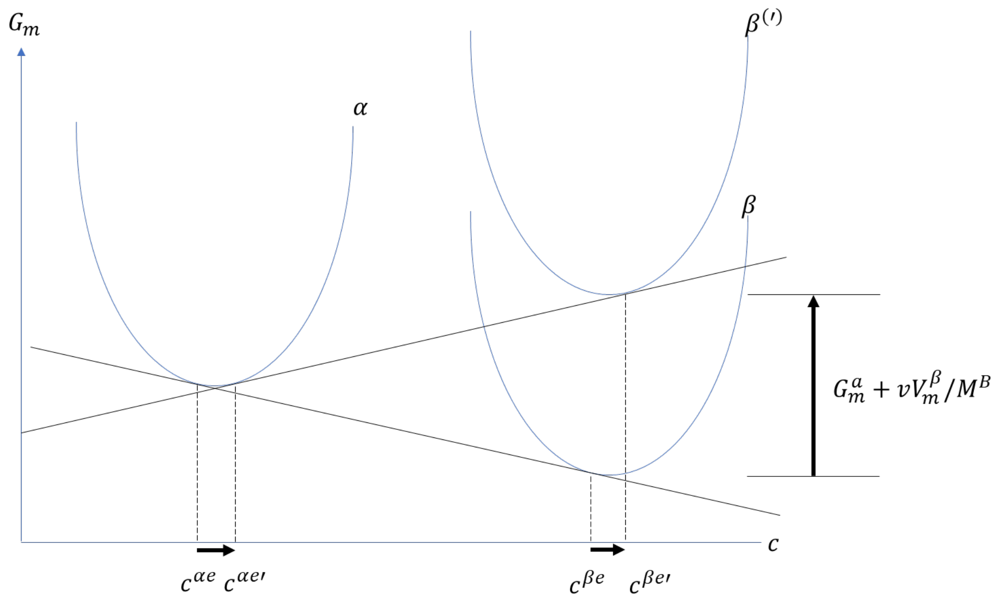


Figure 10: Effects of “Phase energy addition” G_m^a *and “Phase boundary mobility”* M^B*.*

General Growth Rate Model

The **General** model is based on the existing coarsening models [1993Uma; 1994Mor; 1995Mor], which follows the same quasi-steady state approximation as the **Simplified** model, but improves by taking into account the cross diffusion. The growth rate equation has thus the same format as that in the Simplified model, i.e., Eq. 5, with the kinetic parameter K defined as

[*Eq. 7*] $$K = K_{\text{sphere}}^{\text{general}} = \frac{1}{(\Delta X^{\alpha\beta}][\ddot{G}][D]^{-1}[\Delta X^{\alpha\beta})}$$

where $(\Delta X^{\alpha\beta}]$ and $[\Delta X^{\alpha\beta})$ are $n-1$ row and column vector, respectively, whose *i*th element is the composition difference $\left(X_i^{\beta/\alpha}(r) - X_i^{\alpha/\beta}(r)\right)$ as described in Eq. 6. $[\ddot{G}]$, a $(n-1)\times(n-1)$ matrix, is based on thermodynamic factor matrix $[G^\alpha]$ with a correction factor

[*Eq. 8*] $$[\ddot{G}] = f[G^\alpha]$$

where thermodynamic factor matrix is defined as the secondary derivative of free energy with respect to composition in the matrix phase

$$[G^\alpha]_{ij} = \frac{\partial^2 G_m^\alpha}{\partial X_i^\alpha \partial X_j^\alpha}$$

$[G^\alpha]$ is evaluated at the far-field matrix composition to consider the multicomponent Gibbs-Thomson effect [1995Mor]. For a particle with critical nuclei size r^*, the Gibbs-Thomson equation is

[*Eq. 9*] $$(\Delta X^{\alpha\beta}]\,[G^\alpha]\,[\Delta X^\alpha) \approx \frac{2\sigma V_m}{r^*} = \Delta G_m$$

where $[\Delta X^\alpha)$ is a $n-1$ column vector representing the difference between the far-field matrix composition $[X^\alpha)$ and the equilibrium (tie-line) composition of the matrix phase $[X^{\alpha/\beta})$. It has been found that Eq. 9 is not numerically accurate and sometimes the deviation can be quite significant. Therefore, a correction factor is introduced as

$$f = \frac{\Delta G_m}{(\Delta X^{\alpha\beta}][G^\alpha][\Delta X^\alpha)}$$

which then appears in Eq. 8.

$[D]^{-1}$ in Eq. 7 is the inverse of the chemical diffusivity matrix $[D]$. In some alloy systems, diffusivity is strongly composition dependent, so that an effective diffusivity is necessary. A series of numerical simulations in comparison with DICTRA calculations indicates that a good approximation can be achieved if $[D]$ is the arithmetic mean of the diffusivity with far-field matrix composition and diffusivity with equilibrium (tie-line) composition

$$[D] = \frac{1}{2}\left\{[D]_{(X^\alpha)} + [D]_{(X^{\alpha/\beta})}\right\}$$

Paraequilibrium Growth Rate Model

The paraequilibrium (**Para-eq**) growth rate model is only available for alloy systems where Fe is the major element and C is the only interstitial element, which also partitions into the precipitate phase.

The intersitial elements, e.g. C, N, etc., usually have remarkably faster diffusion rate than the substitutional elements. Meanwhile, they are assumed to have negligible volume contribution, and as a result the composition variables in Eq. 6 to Eq. 9 are replaced by *u*-fractions when interstitial elements are included in the system. The paraequilbrium growth rate model is designed specifically to address the fast diffusion of C in Fe alloys. Based on the *Simplified* growth rate model, it holds a paraequilbrium condition [1953Hil] at the migrating interface, in that, instead of assuming that all alloying elements are in equilibrium at the interface as the regular ortho-equilibrium condition states, only C assumes equilibrium state, while the substitutional elements are immobile and thus have the same compositions (*u*-fractions) across the interface. Therefore, only composition of C and its mobility appear in Eq. 6.

PE Automatic Growth Rate Model

The tempering of martensite in steels induces the precipitation of cementite particles. The growth kinetics initially follows the paraequilbrium (abbreviated here as PE) condition due to the fast diffusion of interstitial C, and gradually transforms to regular Local Equilibrium (LE), i.e. Ortho-equilibrium (OE), condition so that substitutional elements can reach equilibrium partitioning at the migrating interface. The **PE Automatic** model enables the smooth transition from *Paraequilibrium growth rate model* to *Simplified growth rate model*. The rate of transition process is dependent on the relative differences in diffusion between C and substitutional elements, as well as the differences in driving force between PE and OE.

NPLE Growth Rate Model

The Non-Partitioning Local Equilibrium (NPLE) growth rate model is only available for alloy systems where Fe is the major element and at least one interstitial element partitions into the precipitate phase.

The **NPLE** growth model is designed specially to deal with the fast diffusion of interstitial element (C, N, etc.) in Fe alloys. Based on the *Simplified* growth model, it still holds a local equilibrium condition at the migrating interface, but chooses a tie-line under NPLE condition [1958Kir] that the *u*-fractions of all substitutional elements and minor interstitial elements in the precipitate phase are the same as those in the far-field matrix phase (i.e. the overall instantaneous matrix composition).

Model Selections

The most efficient model is the **Simplified** model, which is the default and applicable to most alloy systems under conditions that either the supersaturation is small, or the alloying elements have comparable diffusivity. If all alloying elements are substitutional but they have remarkable diffusivity difference, e.g. in Al-Zr system, or the diffusivity is strongly composition dependent, the **General** model is preferred. If the supersaturation is high, and meanwhile there are fast-diffusing interstitial elements such as C, the **Advanced** model is more appropriate to capture the NPLE mechanism.

In some cases with the **General** model, you may need to switch to another model if the matrix composition passes through a spinodal composition space where the thermodynamic factor becomes negative, thus leading to an abnormal growth rate. When this happens, Thermo-Calc alerts you that the *Matrix Composition in Spinodal Zone*. It is then recommended to switch to other models.

Non-Zero Volume Correction

The non-zero volume correction to the velocity according to Chen and Voorhees [1993Che] is taken into account and it follows as

[*Eq. 10*] $$v' = v\left(1 + r\sqrt{4\pi N_V \langle r \rangle}\right)$$

where

- v' is the corrected velocity
- $\langle r \rangle$ is the mean radius
- N_V is the number density

Non-Spherical Particles

A reference for this section can be found in [2018Wu].

Particle Shape Determination

The shape of the cuboid particles, the cubic factor, is determined by the minimization of combined interfacial energy and elastic strain energy. If you choose **Calculated from molar volume** for the **Transformation strain** as the *Precipitation Calculator → Precipitate Phase* settings, the lattice misfit is then calculated from difference in molar volume between matrix and precipitate phase, and the elastic strain energy is calculated accordingly. If you disregard the transformation strain, the elastic strain energy is neglected and hence the particles remain spherical in shape.

If you select the **Calculated aspect ratio from elastic energy** checkbox for either a plate or needle **Morphology** on the *Precipitation Calculator → Precipitate Phase* settings, the particle shape is determined by the minimization of combined interfacial energy and elastic strain energy. Otherwise, if you enter a value for aspect ratio, the particle shape is fixed except for nucleation calculation in which a spherical particle is always assumed.

"Homogeneous Nucleation" on page 80

Interfacial Energy Anisotropy

"Precipitation Morphology" on page 113

Isotropic interfacial energy is always assumed for spherical and cuboidal particles. For plate and needle, when the aspect ratio becomes larger than 1, the interfacial energy anisotropy occurs, so that the interfacial energy at the edge is larger than that at the broad face (habit plane). This increases the overall interfacial energy which is given as follows for each morphology.

Plate

$$E_{\text{int}} = 4\pi\sqrt[3]{\alpha^2}\sigma_0^{\text{sph}}r^2$$

Needle

$$E_{\text{int}} = 4\pi\sqrt[3]{\alpha}\sigma_0^{\text{sph}}r^2$$

Where

- α is the aspect ratio
- σ_0^{sph} is the interfacial energy of the habit plane, i.e., the plane normal to the shorter axis
- r is the radius of a sphere with equivalent volume

Growth Rate Adjustment

"Precipitation Morphology" on page 113

For non-spherical particles, the growth rate equations for spherical particles are still applicable, but adjustment parameters are introduced to take into account the shape effect. The cuboid particles arise from "symmetry preserving" transformation, e.g., FCC_A1 to $L1_2$, and are thus highly isotropic and assumed growth rate equal to that of spherical particles. The plate and needle particles, on the other hand, arise from "symmetry breaking" transformations, e.g., cubic to tetragonal transformation, and are thus anisotropic leading to a significant increase of growth rate.

We define r as the radius of a sphere with equivalent volume of the non-spherical particle, so that the format of Eq. 5 keeps unchanged. In our current model, two effects are considered contributing to the growth rate for plate and needle particles, from interfacial energy anisotropy and particle shape effect. The kinetic parameter K defined in Eq. 5 is thus given as

[Eq. 11] $$K = K_\sigma \cdot K_{\text{shp}} \cdot K_{\text{sphere}}$$

with K_{sphere} defined in Eq. 6 and Eq. 7. The interfacial energy σ in Eq. 5 is that of habit plane, i.e., the plane that is normal to the shorter axis of the particle. K_σ is the parameter that takes into account the Gibbs-Thomson effect due to interfacial energy anisotropy, based on Johnson [1965Joh].

Plate

$$K_\sigma = \sqrt[3]{\alpha^2}$$

Needle

$$K_\sigma = \sqrt[3]{\alpha}$$

where α is the aspect ratio of the ellipsoidal particle. K_{shp} is the parameter that takes into account the non-spherical concentration field around the particle. Assuming a shape-conserving concentration field and thus following the derivation by Ham [1958 and 1959], it is given as

Plate

$$K_{\text{shp}} = \frac{e\sqrt[3]{\alpha}}{\arccos(0) - \arccos(e)}$$

Needle

$$K_{\text{shp}} = \frac{2\sqrt[3]{\alpha^2}e}{\ln(1+e) - \ln(1-e)}$$

where e is the eccentricity of the ellipsoidal particle.

$$e = \sqrt{1 - \frac{1}{\alpha^2}}$$

References

[1953Hil] M. Hillert, 1953. "Paraequilibrium." Internal Report, Swedish Institute for Metals Research.

[1958Ham] F. S. Ham, Theory of diffusion-limited precipitation. J. Phys. Chem. Solids. 6, 335–351 (1958).

[1958Kir] J. S. Kirkaldy, Diffusion in Multicomponent Metallic Systems: I. Phenomenological Theory for Substitutional Solid Solution Alloys. Can. J. Phys. 36, 899–906 (1958).

[1959Ham] F. S. Ham, Shape-preserving solutions of the time-dependent diffusion equation. Q. Appl. Math. 17, 137–145 (1959).

[1965Joh] C. A. Johnson, Generalization of the Gibbs-Thomson equation. Surf. Sci. 3, 429–444 (1965).

[1993, Chen] M. K. Chen, P. W. Voorhees, The dynamics of transient Ostwald ripening. Model. Simul. Mater. Sci. Eng. 1, 591–612 (1993).

[1993Uma] A. Umantsev, G. B. Olson, Ostwald ripening in multicomponent alloys. Scr. Metall. Mater. 29, 1135–1140 (1993).

[1994Mor] J. E. Morral, G. R. Purdy, Particle coarsening in binary and multicomponent alloys. Scr. Metall. Mater. 30, 905–908 (1994).

[1995Mor] J. E. Morral, G. R. Purdy, Thermodynamics of particle coarsening. J. Alloys Compd. 220, 132–135 (1995).

[2008Che] Q. Chen, J. Jeppsson, J. Ågren, Analytical treatment of diffusion during precipitate growth in multicomponent systems. Acta Mater. 56, 1890–1896 (2008).

[2018Wu] K. Wu, Q. Chen, P. Mason, Simulation of Precipitation Kinetics with Non-Spherical Particles. J. Phase Equilibria Diffus. 39, 571–583 (2018).

[2022Ågr] J. Ågren, Q. Chen, Simplified Growth Model for Multicomponent Systems - Inclusion of PARA and NPLE Conditions. J. Phase Equilibria Diffus., in press (2022).

Coarsening

Physically speaking, coarsening or Ostwald ripening where big particles grow and small particles shrink is a process driven by lowering the total surface energy of the system. From a thermodynamic point of view, the Gibbs-Thomson effect leads to inhomogeneous chemical potentials in the system if the particle sizes are not uniform. Solutes at the interface in the matrix near a particle of a radius smaller than critical radius have a higher chemical potential than that corresponding to the mean concentration of the matrix. As a result, the solutes diffuse from the precipitate/matrix interface to the inside of the matrix and cause dissolution of the particle. Conversely, particles with a radius larger than the critical size have lower interface potentials, and the solutes diffuse to the interface and cause growth of the particles.

Since it is not possible to find a closed form analytic solution for the problem of diffusion-controlled spherical particle dissolution [1970Aar], we simply apply the Growth equations 1 to 5 with the absolute value of Ω_i to calculate the interface velocity for particles of all sizes.

As can be easily seen, if $r < r^*$, then the Gibbs-Thomson Equation 1 gives $\mu_i^{\alpha/\beta} > \mu_i^{\alpha}$, and a negative velocity results from Equation 2 for particles having $r < r^*$, which means that they shrink.

Results for particles having $r > r^*$ are obtained vice versa. In all situations, when the absolute values of Ω_i are very small, the steady-state solution for either growth or dissolution are recovered. In conclusion, the dissolution is treated as the reverse of growth (1970Aar, Ibid.), and the coarsening comes out naturally either together with nucleation and growth or as a dominant process finally in the course of the evolution of the PSD.

Reference

[1970Aar] H. B. Aaron, Diffusion-Limited Phase Transformations: A Comparison and Critical Evaluation of the Mathematical Approximations. J. Appl. Phys. 41, 4404 (1970).

Continuity Equation

Let $f(r)$ be the PSD of a precipitate phase, N the number of particles per unit volume, $\langle r \rangle$ the mean radius and ϕ the particle volume fraction, is expressed as

[Eq. 1] $N = \int_0^\infty f(x)dr$

[Eq. 2] $\langle r \rangle = \int_0^\infty rf(r)dr$

[Eq. 3] $\phi = \int_0^\infty (\frac{4\pi}{3})r^3 f(r)dr$

The time evolution of $f(r)$ follows the continuity as in Langer and Schwartz [1980Lan].

[Eq. 4] $\frac{\partial f}{\partial t} = -\frac{\partial}{\partial r}[v(r)f(r)] + j(r)$

Where $v(r)$ is the growth rate of a particle of size r, and $j(r)$ is the distributed nucleation rate, which is defined by

[Eq. 5] $J = \int_{r*}^\infty j(r)dr$

where J is the nucleation rate.

Reference

[1980Lan] J. S. Langer, A. J. Schwartz, Kinetics of nucleation in near-critical fluids. Phys. Rev. A. 21, 948–958 (1980).

Mass Conservation

The matrix concentration is updated at each time step according to the law of mass conservation. If the alloy concentration, i.e. initial mole fraction of component i in the matrix phase is X_i^0, the new concentration X_i can be obtained from the following mass balance shown in

$$X_i^0 = \left(1 - \sum_p \int_0^\infty \frac{4\pi r_p^3 f(r_p)}{3V_m^p} dr_p\right) X_i + \sum_p \int_0^\infty \int_0^{t_j} \frac{4\pi r_p^2 f(r_p,t) v(r_p,t)}{V_m^p} X_i^p(r_p,t) dt dr_p$$

where

- $X_i^p(r_p,t)$ is the mole fraction of element i at the interface in the precipitate phase p of particle size r_p at time t. $f(r_p,t)$, $v(r_p,t)$ and V_m^p are the PSD function, growth rate, and molar volume of the precipitate phase p, respectively.
- t_j is the time at time step j.

Apparently, the new matrix concentration, and thus the updated supersaturation, nucleation rate, and interface velocity are all functions of the PSD function. This inevitably leads to the complex non-linear behavior of and great difficulty in solving the continuity equation.

Numerical Method

Since it is impossible to have a general close form solution, the complex non-linear continuity equation (see "Continuity Equation" on page 105) of the particle size distribution (PSD) function has to be solved numerically. Different numerical methods can be found in the literature to solve this equation, such as finite difference and method of characteristics. In all approaches, the continuous PSD is discretized into a sufficiently large number of size classes, and then integrated discretely in the time space. The Precipitation Module utilizes the method of characteristics, where the number of particles in each size class is kept constant unless particles of the same size have been nucleated.

An adaptive geometric grid allocation method has been used for particle size discretization since from nucleation to coarsening the particle size can span several orders of magnitude. In this approach, the new size grids are allocated evenly in a logarithmic scale and the number of grid points over one order of magnitude is kept almost constant during the whole process by class merging and splitting. The time step is controlled by several adjustable numerical parameters based on mechanistic quantities.

Summarized below are all numerical parameters used in this approach to control either the size grid distribution or time steps.

Maximum Time Step Fraction

$$P_{dt}^{max}$$

Maximum time step allowed for time integration as fraction of the simulation time.

Number of Grid Points Over One Order of Magnitude in *r*

$$P_{Nr}$$

Default number of grid points for every order of magnitude in size space. The number determines a default ratio between two adjacent grid points. When there is a need to create new grid points, such as nucleating at a new radius not covered by the current range of PSD, this default ratio is used to add these new radius grid points. A larger value of this parameter enforces a finer grid to allow better numerical accuracy. However, this also comes with performance penalty, since finer grid in the size space often requires smaller time step to resolve the calculations.

Maximum Number of Grid Points Over One Order of Magnitude in r

P_{Nr}^{max}

The maximum allowed number of grid points in size space. This parameter determines a lower bound limitation for the ratio of every two next nearest grid points in order to maintain adequate computational efficiency. When a ratio of two next nearest grid points is less than this limit, the middle grid point is removed and the corresponding size class merged with the two neighboring ones.

Minimum Number of Grid Points Over One Order of Magnitude in r

P_{Nr}^{min}

The minimum allowed number of grid points in size space. This parameter determines an upper bound limitation for the ratio of every two adjacent grid points in order to maintain proper numerical accuracy. When a ratio of two adjacent grid points exceeds this limit, a new grid point is then inserted between the two adjacent grids to keep the required resolution.

Maximum Relative Radius Change

P_r

The maximum value allowed for relative radius change in one time step. This parameter limits the time step according to the following relation, which is controlled by the particle growth:

$\Delta t \leq P_r \times r/(|dr/dt|)$ for $r > r_{dt}$

where r_{dt} is a cut-off subcritical size defined by the next parameter. The growth rates of supercritical particles (with $r > r_c$) are always bounded, and there is a size class and the corresponding growth rate that controls the time step. The subcritical particles (with $r < r_c$), however, has a mathematical singularity (negative infinity) in growth rate as rr approaches 0. This means that the time step can become extremely small if applying the above criterion to very small subcritical particles. In open literature, several researchers have tried mathematical transformation to avoid this singularity. Unfortunately, the transformation also complicates the formulation of the models. The Precipitation Module implementation uses a simple approach to deal with this issue by defining a cut-off size r_{dt}. All the particles with $r < r_{dt}$ may disappear within one time step. is determined by the next input parameter.

Maximum Relative Volume Fraction of Subcritical Particles Allowed to Dissolve in One Time Step

$$P_{rdt}$$

This parameter represents the portion of the volume fraction that can be ignored when determining the time step. It is used to calculate the cut-off subcritical size, r_{dt}, for the above time step control that allows a maximum relative radius changes for all particles:

$$(\int_0^{rdt} fr^3 dr)/(\int_0^\infty fr^3 dr) = P_{rdt}$$

Relative Radius Change for Avoiding Class Collision

$$P_{cc}$$

For the supercritical particles, the growth rate is non-linear – usually, it first increases with r and then decreases after a certain size. In the region(s) with growth rate decreasing with r, it is possible that the smaller size grid point can catch up with the larger size grid, if the time step is not controlled. To prevent this from happening, an additional parameter, P_{cc}, can be used to set a limit on time step according to the following relation:

$$\Delta t \le P_{cc} \times (r_{i+1} - r_i)/(dr_i/dt - dr_{i+1}/dt)$$

for

$$r_{i+1} > r_{i+1}$$

and

$$dr_{i+1}/dt < dr_i/dt$$

Maximum Overall Volume Change

$$P_\nu$$

This parameter defines the maximum absolute (not ratio) change of the volume fraction allowed during one time step. This parameter is also used in controlling allowable variation in volume fraction due to the newly created particles within one time step. That is

$$\Delta t \le P_V/10/(4\pi r_{eff}^3 J/3)$$

where r_{eff} and J are effective radius and nucleation rate, respectively.

Maximum Relative Change of Nucleation Rate in Logarithmic Scale

$$P_{logJ}$$

This parameter ensures accuracy for the evolution of effective nucleation rate. It sets a limit on time step so that the relative change of nucleation rate does not exceed the specified value, based on the information of previous step. That is

$$\Delta t \le P_{logJ} \times \Delta t_{previous} / (|log(J_1 / J_2)|)$$

where nucleation rate J_1 and J_2 occurs at the beginning and end of $\Delta t_{previous}$.

Maximum Relative Change of Critical Radius

$$P_{rc}$$

During the nucleation under high supersaturation, the critical radius can vary dramatically. Hence, this parameter can be used to place a constraint on how fast the critical radium can vary, and thus put a limit on time step:

$$\Delta t \le P_{rc} \times \Delta t_{previous} / (|r_{c1} - r_{c2} / r_{rc1}|)$$

Minimum Radius for a Nucleus to be Considered as a Particle

$$P_{rmin}$$

The cut-off lower limit of precipitate radius. Particles with radius smaller than the value specified for this parameter are discarded. In reality, the particle cannot be smaller than an atom; hence, there is no reason to keep track of particles of unphysical sizes.

Maximum Time Step During Heating Stages

$$P_{htmax}$$

The upper limit of the time step that has been enforced in the heating stages. The current algorithm may over-estimate the subsequent time increment when temperature is increased. It is thus required to reduce this value when the calculation terminates unexpectedly during or after a heating stage.

Numerical Control Parameters Default Values

Default value for numerical parameters that controls the size grid distribution and time step.

Parameter	Default value
P_{dt}^{max}	0.1
P_{Nr}	200
P_{Nr}^{max}	300
P_{Nr}^{min}	100
P_r	0.01
P_{rdt}	0.01
P_{cc}	0.5
P_{ν}	0.001
P_{logJ}	0.5
P_{rc}	0.1
P_{rmin}	5e-10m
P_{htmax}	1.0s

Estimation of Coherent Interfacial Energy

Interfacial energy is an important parameter used in precipitation simulations to calculate the rates of nucleation, growth/dissolution, and coarsening. The value of interfacial energy can vary dramatically (usually between 0.01 to 2.0 J/m^2).

The extended Becker's model functions to estimate coherent interfacial energy by using thermodynamic data from existing CALPHAD thermodynamic databases:

$$\sigma_c = \frac{n_s z_s}{N_A z_l} \Delta E_s$$

where σ_c is the coherent interfacial energy, n_s is the number of atoms per unit area at the interface, z_s is the number of cross bonds per atom at the interface, z_l is the coordination number of an atom within the bulk crystal lattice, and ΔE_s is the energy of solution in a multicomponent system involving the two phases being considered [1938Bec].

Reference

[1938Bec] R. Becker, Die Keimbildung bei der Ausscheidung in metallischen Mischkristallen. Ann. Phys. 424, 128–140 (1938).

"Interfacial Energy Anisotropy" on page 101

Precipitation Morphology

As the spherical particle is the default morphology, for precipitations within the grain, three non-spherical shapes are considered: *cuboid*, *plate* and *needle*.

- "Growth" on page 94
- "Homogeneous Nucleation" on page 80
- "Precipitate Phase Settings" on page 30

Cuboid

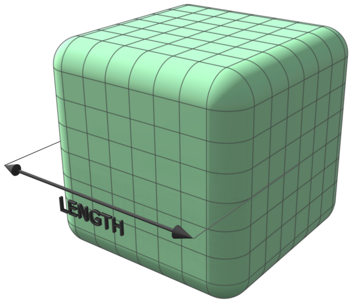


Figure 11: Cuboids have six faces, which form a convex polyhedron.

The cuboid shape is described by a supersphere

$$x_1^p + x_2^p + x_3^p = R^p \qquad (p \geq 2)$$

with p=2 being spherical shape. The larger the *p*, the more cubic the shape. Sometimes it is useful to define the cubical character as

$$\eta = \sqrt{2} \cdot 2^{-1/p}$$

Which gives a spherical shape when $\eta = 1$, and a cubic shape when $\eta = \sqrt{2}$.

Plate

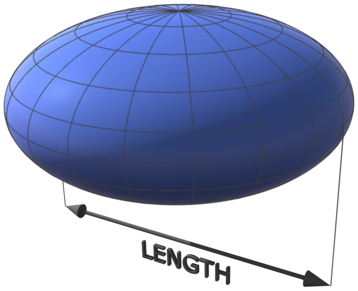


Figure 12: Oblate spheroids have rotational symmetry around an axis from pole to pole.

The plate is described as oblate spheroid

$$\frac{x_1^2}{l^2}+\frac{x_2^2}{l^2}+\frac{x_3^2}{r^2}\le 1 \qquad l>r$$

with aspect ratio

$$\alpha=\frac{l}{r}>1$$

Needle

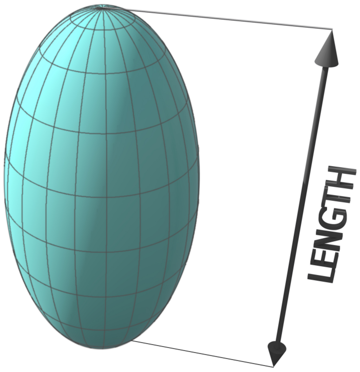


Figure 13: A prolate spheroid is a surface of revolution obtained by rotating an ellipse about its major axis.

The needle shape is described as prolate spheroid

$$\frac{x_1^2}{r^2}+\frac{x_2^2}{r^2}+\frac{x_3^2}{l^2}\le 1 \qquad l>r$$

with aspect ratio

$$\alpha=\frac{l}{r}>1$$

Precipitations at a Grain Boundary, Edge or Corner

For precipitations at a grain boundary, grain edge, or grain corner, non-spherical particles are considered based on wetting angle.

"Heterogeneous Nucleation" on page 87

"Matrix Phase Settings" on page 23

Normal Grain Growth

The normal grain growth model in the Precipitation Module (TC-PRISMA) uses a similar approach to its precipitation counterpart (see "Theory Overview" on page 77) in that it calculates the temporal evolution of grain size distribution (GSD). The grains are assumed of spherical morphology when modeling the growth rates. Nucleation is not considered, thus an initial GSD is necessary to start the simulation.

The boundary motion of a grain with radius R_i without considering pinning forces from precipitate particles, is driven by curvature and can be modeled as [1957Fel; 1965Hil]

[*Eq. 1*] $$\frac{dR_i}{dt} = \alpha M \gamma \left(\frac{1}{R_{cr}} - \frac{1}{R_i} \right)$$

where

- M is grain boundary mobility (m^4/Js)
- γ is the grain boundary energy (J/m^2)
- α is a dimensionless constant

If it should be satisfied that $k = M\gamma$, which is the parabolic growth rate of average grain size at steady-state

[*Eq. 2*] $$\bar{R}^2 - \bar{R_0}^2 = kt$$

It was found that $\alpha \approx 2$ [1965Hil].

R_{cr} in Eq. 1 is the critical grain size, which, not necessarily the average grain size, is determined by volume conservation [2008Jep]

[*Eq. 3*] $$\frac{dV}{dt} = 4\pi \sum_i \frac{R_i^2 dR_i}{dt} = 0$$

where the index i covers all the grains at each time step. Substituting Eq. 1 into Eq. 3, R_{cr} is obtained at each time step.

Grain Boundary Mobility Values

The grain boundary mobility M can be calculated as:

[*Eq. 4*] $$M = M_0 exp(-\frac{Q}{RT})$$

where

- M_0 is the prefactor (m^4/Js)
- Q is the activation energy (J/mol)

The recommended values of M_0 and Q in high purity metals such as ferritic iron, austenitic iron, nickel, and aluminum are shown in the table below.

Since grain growth is significantly affected by grain boundary segregation, precipitation, and grain boundary complexion, the accuracy of the mobility data used for the recommended values is not guaranteed.

If the grain size is in nanoscale, these parameters may not be applicable since the effects of grain boundary junction and complexion cannot be ignored in nanocrystals. For some alloys, such as Al, the parameters can also be sensitive to temperature. The temperature range in the table is the suggested best fit.

Recommended grain growth parameters for mobility prefactor M_0 and activation energy Q.

	Matrix Phase	***Temperature Range (K)***	***Prefactor M_0 (m^4/Js)***	***Activation Energy Q (J/mol)***	***Reference***
High purity iron	BCC_A2	625 ~ 875	4E-3	242000	[1997Mal]
Low alloying steel (Cr-Mo)	FCC_A1	1173 ~ 1473	3.6E-3	228302	[2008Lee]
Pure Ni	DIS_FCC_A1/FCC_L12	1098 ~ 1323	4.12E-8	123050	[2008Ran]
High purity aluminum	FCC_A1	300 ~ 548	1.02E-14	27430	[2004Yu]
		573 ~ 773	1.25E-8	73080	

References

[1957Fel] P. Feltham, Grain growth in metals. Acta Metall. 5, 97–105 (1957).

[1965Hil] M. Hillert, On the theory of normal and abnormal grain growth. Acta Metall. 13, 227–238 (1965).

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

[2004Yu] C. Y. Yu, P. L. Sun, P. W. Kao, C. P. Chang, Evolution of microstructure during annealing of a severely deformed aluminum. Mater. Sci. Eng. A. 366, 310–317 (2004).

[2008Jep] J. Jeppsson, J. Ågren, M. Hillert, Modified mean field models of normal grain growth. Acta Mater. 56, 5188–5201 (2008).

[2008Lee] S.-J. Lee, Y.-K. Lee, Prediction of austenite grain growth during austenitization of low alloy steels. Mater. Des. 29, 1840–1844 (2008).

[2008Ran] V. Randle, P. R. Rios, Y. Hu, Grain growth and twinning in nickel. Scr. Mater. 58, 130–133 (2008).

Zener Pinning

Zener [1948Smi] proposed a pinning force due to second-phase particles, so that the normal grain growth would be completely inhibited when the grain size reached a critical maximum grain size R_z. In general form, it can be expressed as [1998Man]

[*Eq. 1*] $$R_z = K\frac{r}{f^m}$$

Where

- r is the radius of the pinning particles
- f the volume fraction of the particles
- K is a dimensionless constant
- m an exponential index for f

The original Zener pinning theory gives

$$K = 4/3, m = 1$$

which has been found to be inconsistent with the experimental information and thus needs refinement.

For simplicity, the average particle radius $\bar{r}_j$ of a precipitate phase j has been used to calculate the pinning force arising from all the particles of this phase. The pinning force, z_j, can be evaluated as the inverse of $R_{z,j}$

$$z_j = \frac{1}{R_{z,j}} = \frac{1}{K_j}\frac{f_j^{m_j}}{\bar{r}_j}$$

When there are multiple precipitate phases, the overall pinning effect is the sum of that from all precipitate particles,

$$z_j = \sum_j z_j = \sum_j \frac{1}{K_j} \frac{f_j^{m_j}}{\bar{r}_j}$$

The retarding force due to Zener pinning, RF_z, is therefore [1965Hil]

$$RF_z = \sigma \cdot z = \frac{\sigma}{R_z}$$

where σ is the grain boundary energy.

Realizing that the drag force resists the grain boundary motion, no matter in the growing (positive velocity) or shrinking (negative velocity) direction, the overall growth rate is expressed as [1965Hil]

$$\frac{dR_i}{dt} = \alpha M \sigma \left[\left(\frac{1}{R_{cr}} - \frac{1}{R_i} \right) \pm \frac{1}{R_z} \right]$$

The negative sign holds when

$$\left(\frac{1}{R_{cr}} - \frac{1}{R_i} \right) - \frac{1}{R_z} > 0$$

while positive sign holds when

$$\left(\frac{1}{R_{cr}} - \frac{1}{R_i} \right) + \frac{1}{R_z} < 0$$

And $\frac{dR_i}{dt} = 0$ when R_i lies between these two limits.

In the Precipitation Module (TC-PRISMA), you can input parameters K_j and m_j for each precipitate phase. An additional parameter, *cutoff radius* (unit= m), can be used so that precipitates with a smaller size than this value are excluded from the calculation of pinning force. This adjustment avoids an unreasonably large pinning force calculated from very small precipitates (e.g. nuclei).

"P_14: Grain Growth and the Zener Pinning Effect" on page 197

References

[1948Smi] C. S. Smith, Grains, Phases, and Interfaces - an Interpretation of Microstructure. Trans. AIME. 175, 15–51 (1948).

[1965Hil] M. Hillert, On the theory of normal and abnormal grain growth. Acta Metall. 13, 227–238 (1965).

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

Stereology

Stereology is the science of assessing the three-dimensional (3D) geometry and morphology of objects utilizing data descriptive of a cross-section of the material. It is common to characterize a precipitate dispersion utilizing quantitative image analysis of micrographs obtained from light or scanning electron microscopy. In these cases, the data describes the precipitates found in a cross-section taken through the sample.

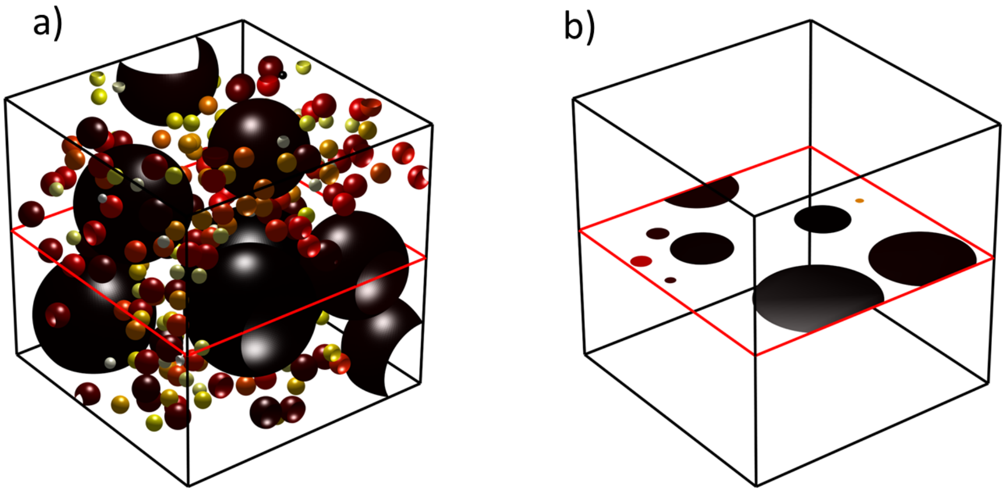


Figure 14: a) A 3D dispersion of non-penetrating polydisperse particles. b) A cross-section taken through the dispersion.

Stereological considerations are important when seeking greater quantitative accuracy comparing model calculations and experimental data. The two-dimensional (2D) size distribution is of interest for the calculation of mechanical properties as it represents the size distribution of obstacles encountered by a dislocation on a slip system.

The size of the precipitates can be expressed as the equivalent radius of a circle with the same cross-sectional area as measured from the micrograph. Figure 15, Figure 16, and Figure 17 compare the 3D and 2D size distributions of a spherical dispersion considering a left skewed, a normal, and a right-skewed distribution. Observe the changes in shape of the distribution in addition to the smaller 2D mean radius compared to the true 3D size.

The 3D to 2D conversion implementation considers spherical particles. Although the precipitates may be approximated as spherical for the approximation of the 2D size distribution, there may be a large error for geometries that differ largely from spheres.

The **3D → 2D** checkbox that is available to use this feature requires (1) that the *Precipitate Phase* **Morphology** is set to **Sphere** on the Precipitation Calculator, and then (2) one of these axis variables is selected on either the Plot or Table Renderer: **Mean radius**, **Size distribution**, **Number density distribution**, or **Normalized number density distribution**.

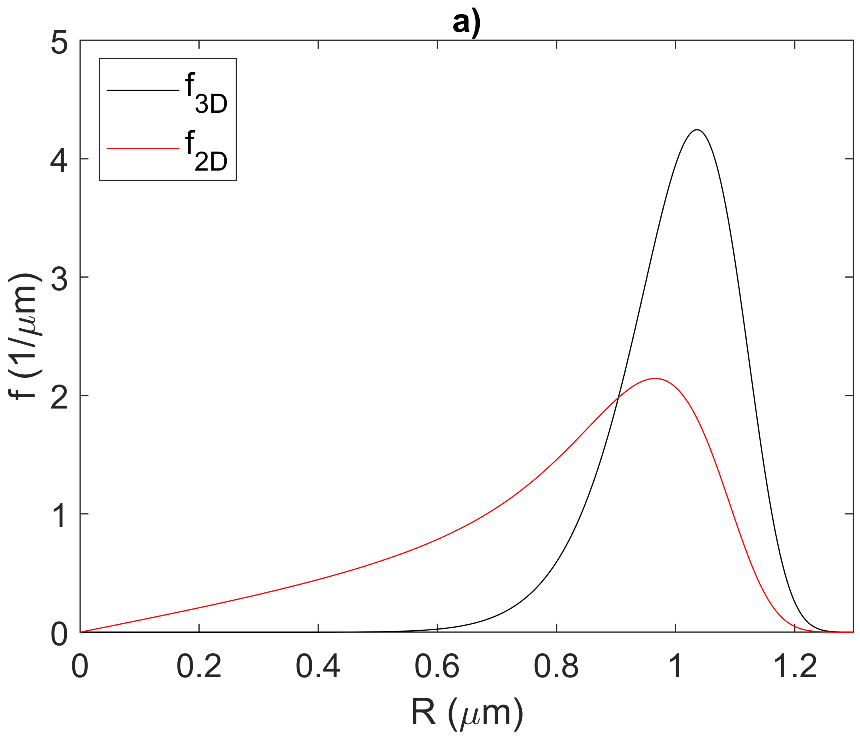


Figure 15: A comparison of the 3D and 2D particle size distributions considering a left-hand skewed Weibull distribution.

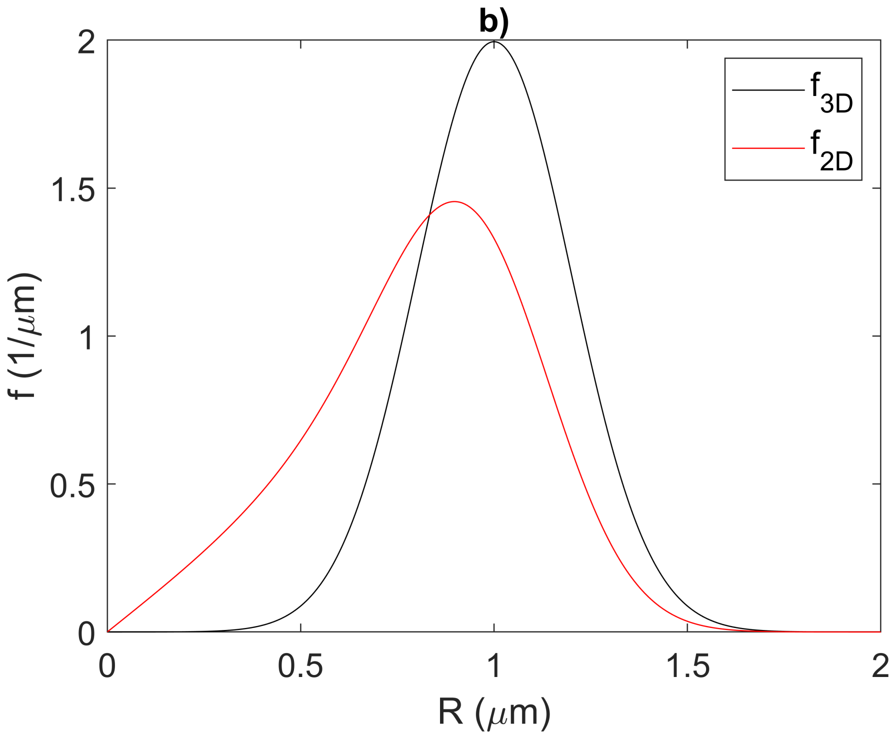


Figure 16: A comparison of the 3D and 2D particle size distributions considering a normal distribution

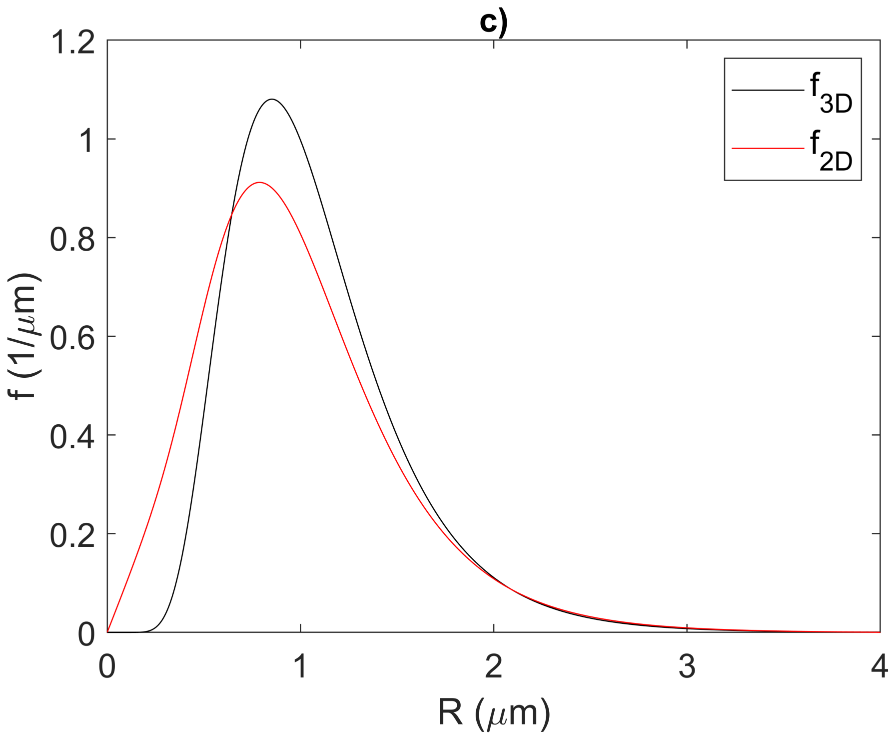


Figure 17: A comparison of the 3D and 2D particle size distributions considering a right-hand skewed log-normal distribution.

Analytical solutions exist for the determination of the 2D size distribution of impenetrable polydisperse spheres [1958Sal; 1925Wic]. Thermo-Calc has implemented the Jeppsson-Mannesson-Borgenstam-Agren (JMBA) [2011Jep] Saltykov conversion method to calculate the 2D size distribution.

Let $F_{3D}(r)dr$ describe the number of particles with radius varying between r and $r+dr$ within a unit volume. The corresponding 2D size distribution is given by $F_{2D}(r)dr$, describing the number of particle cross-sections with a radius varying between r and $r+dr$ within a unit area. Following the Saltykov method, the 2D size distribution is obtained from the following matrix calculation:

$$\underline{F_{2D}} = \underline{\underline{\alpha}}\,\underline{F_{3D}}$$

where $\underline{\underline{\alpha}}$ is a matrix of probabilities for the conversion and $\alpha_{i,j}$ describe the likelihood of obtaining a 2D cross-section of radius r_i from 3D grains of radius r_j . The JMBA model derived these probabilities as:

$$\alpha_{i,j} = \begin{cases} 2r_i \frac{\Delta \mathrm{rb_i}}{\Delta r b_j} \frac{\sqrt{r_i^2 - b_{j-1}^2} - \sqrt{r_j^2 - b_j^2}}{r_i} & i < j \\ \frac{\Delta b_j 4\pi r_j^3/3 - \sum_{i=1}^{j-1}\left(\pi r_j^2 b_i \Delta b_{i-1} \alpha_{i,j}\right)}{\Delta b_j \pi r_j^2} & i = j \\ 0 & i > j \end{cases}$$

Where b_i and b_{i+1} describe the lower and upper boundaries to the particle radii class r_i. Δr_i and Δb_i are the spacing between radii midpoints and class boundaries, respectively. For a linear discretization, $\Delta b_i = \Delta r_i$.

It is assumed that the 2D cross-section is a perfect cut through the material however there may be some error in this approximation. Figure 18 presents the idealized case with a 3D and 2D size distribution with a mean radius of 1.5 µm. In Figure 19, it is assumed that the minimum size of particles that can be quantified in the micrograph is 0.25 µm. This crops off the left-hand tail of the 2D distribution. Etching away the matrix reveals sub-surface particles. Figure 20 shows the impact of etching a depth of 30 nm, further exposing particles that have a center below the cross-section of the cut.

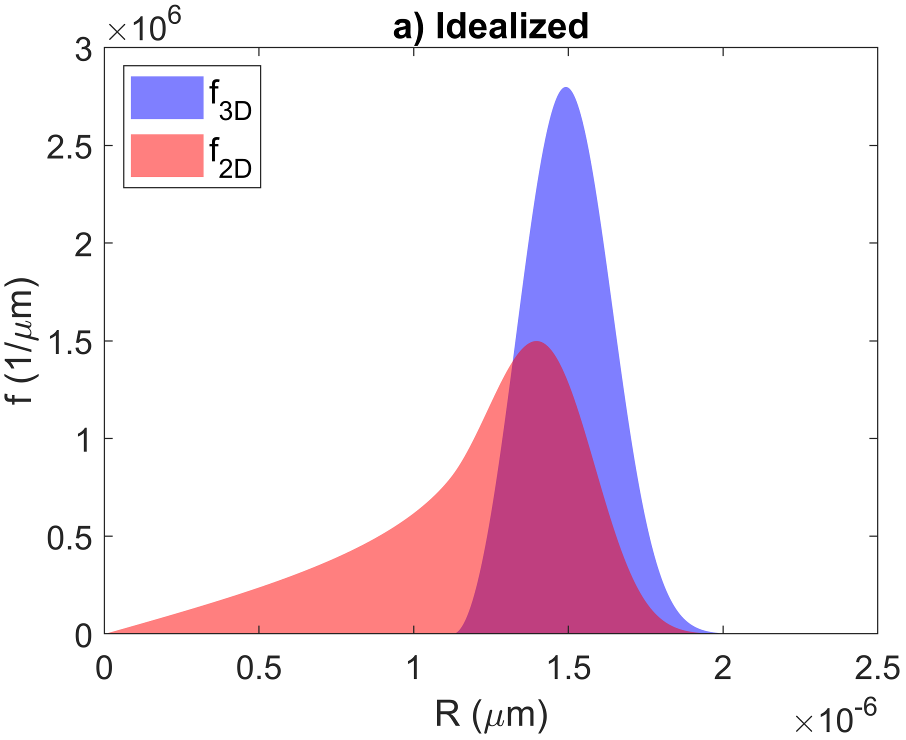


Figure 18: Potential causes of error in micrographs showing the idealized 2D size distribution.

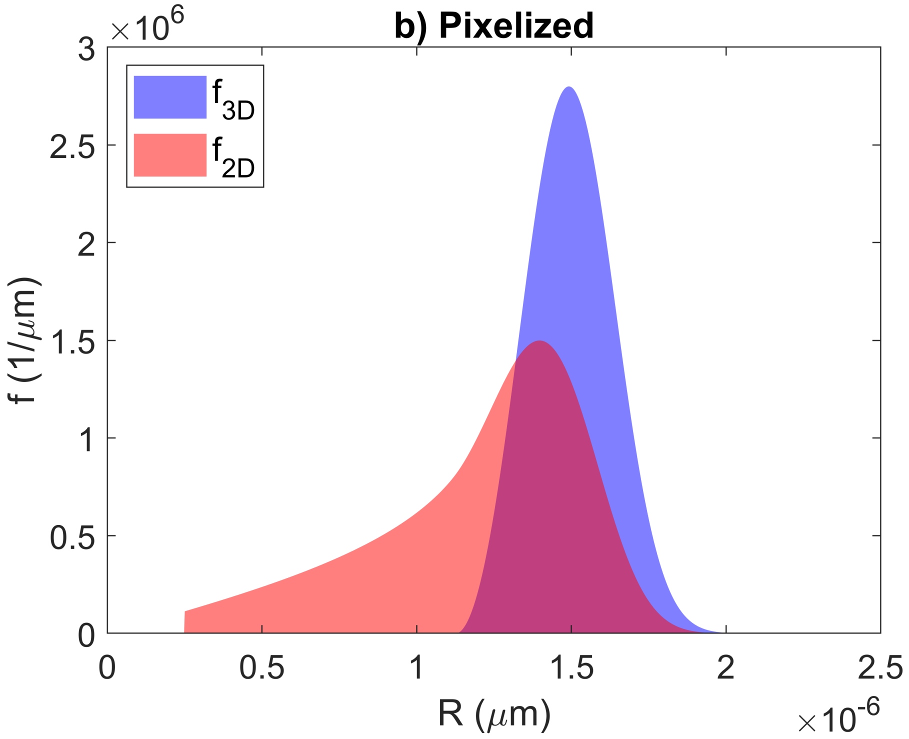


Figure 19: Potential causes of error in micrographs showing the cropped left-hand tail caused by a limiting size that can be measured from the micrograph.

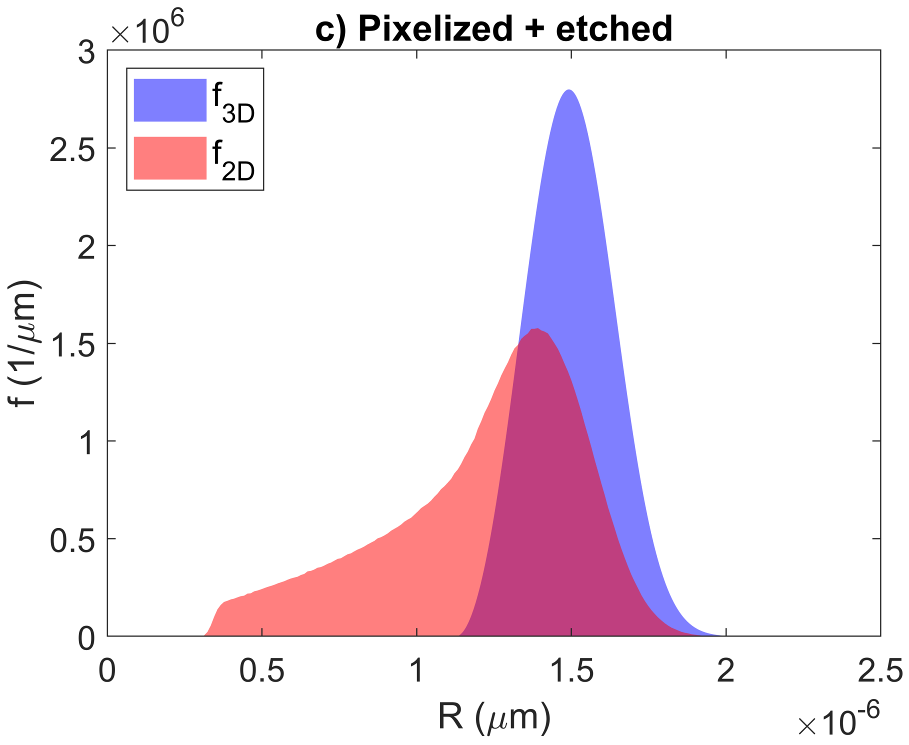


Figure 20: Potential causes of error in micrographs showing how the left-hand tail can be blurred due to etching.

References

[1925Wic] S. D. Wicksell, The Corpuscle Problem. A Mathematical Study of a Biometric Problem. Biometrika. 17, 84–99 (1925).

[1958Sal] S. A. Saltykov, Stereometric metallography (Metallurgizdat, Moscow, ed. 2nd, 1958).

[2011Jep] J. Jeppsson, K. Mannesson, A. Borgenstam, J. Ågren, Inverse Saltykov analysis for particle-size distributions and their time evolution. Acta Mater. 59, 874–882 (2011).

Microstructure Descriptions

Precipitation kinetics and grain coarsening is modeled by the evolution of size distributions. Distribution functions describe the matrix grain size, and a size distribution for each precipitate phase specific to an individual nucleation site. Let the number concentration of precipitates or grains within the size interval of r and $r + dr$ be defined by fdr. The mean radius (r), number concentration N, and volume fraction ϕ of the precipitates or matrix grains are obtained from moments taken from the distribution function. The key statistics are obtained from the first set of equations (Eq. 1), where η is the volumetric shape factor. For spherical particles, $\eta = 4\pi/3$.

[Eq. 1]

$$\langle r \rangle = \frac{\int_0^\infty fr\,dr}{\int_0^\infty f\,dr}$$

$$N_v = \int_0^\infty f\,dr$$

$$\phi = \eta \int_0^\infty fr^3\,dr$$

The default output mean radius in the Precipitation Module (TC-PRISMA) uses a cubic mean radius. This value is less sensitive to numerical noise in the solution, and provide a better approximation of the three-dimensional size of the precipitates.

The cubic mean radius are given as follows:

[Eq. 2]

$$\langle r \rangle = \left(\frac{\int_0^\infty fr^3\,dr}{\int_0^\infty f\,dr} \right)^{1/3}$$

For sectioned spherical particles, a quadratic mean radius is used.

[Eq. 3]

$$\langle r \rangle = \left(\frac{\int_0^\infty fr^2\,dr}{\int_0^\infty f\,dr} \right)^{1/2}$$

The conventional mean radius as defined in the first set of equations (Eq. 1) is available as an output from calculations for precipitates and grains. The result can be split into individual populations, and sectioned to approximate the 2D size distribution.

Precipitation Module (TC-PRISMA) References

[1938Bec] R. Becker, Die Keimbildung bei der Ausscheidung in metallischen Mischkristallen. Ann. Phys. 424, 128–140 (1938).

[1948Smi] C. S. Smith, Grains, Phases, and Interfaces - an Interpretation of Microstructure. Trans. AIME. 175, 15–51 (1948).

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

[1953Hil] Hillert, M. Paraequilibrium. Internal Report, Swedish Institute for Metals Research (1953).

[1955Cle] P. J. Clemm, J. C. Fisher, The influence of grain boundaries on the nucleation of secondary phases. Acta Metall. 3, 70–73 (1955).

[1957Esh] J. D. Eshelby, The Determination of the Elastic Field of an Ellipsoidal Inclusion, and Related Problems. Proc. R. Soc. A Math. Phys. Eng. Sci. 241, 376–396 (1957).

[1956Cah] J. W. Cahn, Transformation kinetics during continuous cooling. Acta Metall. 4, 572–575 (1956).

[1957Fel] P. Feltham, Grain growth in metals. Acta Metall. 5, 97–105 (1957).

[1958Ham] F. S. Ham, Theory of diffusion-limited precipitation. J. Phys. Chem. Solids. 6, 335–351 (1958).

[1958Kir] J. S. Kirkaldy, Diffusion in Multicomponent Metallic Systems: I. Phenomenological Theory for Substitutional Solid Solution Alloys. Can. J. Phys. 36, 899–906 (1958).

[1959Esh] J. D. Eshelby, The Elastic Field Outside an Ellipsoidal Inclusion. Proc. R. Soc. A Math. Phys. Eng. Sci. 252, 561–569 (1959).

[1959Ham] F. S. Ham, Shape-preserving solutions of the time-dependent diffusion equation. Q. Appl. Math. 17, 137–145 (1959).

[1965Hil] M. Hillert, On the theory of normal and abnormal grain growth. Acta Metall. 13, 227–238 (1965).

[1965Joh] C. A. Johnson, Generalization of the Gibbs-Thomson equation. Surf. Sci. 3, 429–444 (1965).

[1966Fed] J. Feder, K. C. Russell, J. Lothe, G. M. Pound, Homogeneous nucleation and growth of droplets in vapours. Adv. Phys. 15, 111–178 (1966).

[1970Aar] H. B. Aaron, Diffusion-Limited Phase Transformations: A Comparison and Critical Evaluation of the Mathematical Approximations. J. Appl. Phys. 41, 4404 (1970).

[1975Hel] P. Hellman, M. Hillert, On the Effect of Second-Phase Particles on Grain Growth. Scand. J. Metall. 4, 211–219 (1975).

[1980Lan] J. S. Langer, A. J. Schwartz, Kinetics of nucleation in near-critical fluids. Phys. Rev. A. 21, 948–958 (1980).

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

[1983/2013Kha] A. G. Khachaturyan, Habit Plane and Orientation Relations in Precipitates: Comparison with Experimental Data. In Theory of Structural Transformations in Solids, 299–305. Mineola, New York: Dover Publications, Inc.

[1988Hil] M. Hillert, Inhibition of grain growth by second-phase particles. Acta Metall. 36, 3177–3181 (1988).

[1991Kam] R. Kampmann, R. Wagner. "Homogeneous second phase precipitation". In R. W. Cahn, P. Haasen, & E. J. Kramer (Eds.), Materials Science and Technology (pp. 213–304). Weinheim, Germany: Wiley-VCH Verlag GmbH & Co. KGaA (1991).

[1993Che] M. K. Chen, P. W. Voorhees, The dynamics of transient Ostwald ripening. Model. Simul. Mater. Sci. Eng. 1, 591–612 (1993).

[1993Uma] A. Umantsev, G. B. Olson, Ostwald ripening in multicomponent alloys. Scr. Metall. Mater. 29, 1135–1140 (1993).

[1994Mor] J. E. Morral, G. R. Purdy, Particle coarsening in binary and multicomponent alloys. Scr. Metall. Mater. 30, 905–908 (1994).

[1995Mor] J. E. Morral, G. R. Purdy, Thermodynamics of particle coarsening. J. Alloys Compd. 220, 132–135 (1995).

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

[2000Kas] D. Kashchiev. Nucleation, (Butterworth-Heinemann, 2000).

[2003Ona] S. Onaka, N. Kobayashi, T. Fujii, M. Kato, Energy analysis with a superspherical shape approximation on the spherical to cubical shape transitions of coherent precipitates in cubic materials. Mater. Sci. Eng. A. 347, 42–49 (2003).

[2004Iwa] S. Iwamura, Y. Miura, Loss in coherency and coarsening behavior of Al3Sc precipitates. Acta Mater. 52, 591–600 (2004).

[2004Jou] H.-J. Jou, P. Voorhees, G. B. Olson, Computer simulations for the prediction of microstructure/property variation in aeroturbine disks. Superalloys, 877–886 (2004).

[2004Svo] J. Svoboda, F. D. Fischer, P. Fratzl, E. Kozeschnik, Modelling of kinetics in multi-component multi-phase systems with spherical precipitates. Mater. Sci. Eng. A. 385, 166–174 (2004).

[2004Yu] C. Y. Yu, P. L. Sun, P. W. Kao, C. P. Chang, Evolution of microstructure during annealing of a severely deformed aluminum. Mater. Sci. Eng. A. 366, 310–317 (2004).

[2004Zan] L. Zang, "Lecture 13: Heterogeneous Nucleation: Effects of Grain Boundaries and Surface Defects". Lecture slides, Salt Lake City, Utah: The Zang Research Group, The University of Utah. Retrieved from http://www.eng.utah.edu/~lzang/images/lecture-13.pdf

[2008Che] Q. Chen, J. Jeppsson, J. Ågren, Analytical treatment of diffusion during precipitate growth in multicomponent systems. Acta Mater. 56, 1890–1896 (2008).

[2008Jep] J. Jeppsson, J. Ågren, M. Hillert, Modified mean field models of normal grain growth. Acta Mater. 56, 5188–5201 (2008).

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

[2008Lee] S.-J. Lee, Y.-K. Lee, Prediction of austenite grain growth during austenitization of low alloy steels. Mater. Des. 29, 1840–1844 (2008).

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

[2008Ran] V. Randle, P. R. Rios, Y. Hu, Grain growth and twinning in nickel. Scr. Mater. 58, 130–133 (2008).

[2014Che] Q. Chen, K. Wu, G. Sterner, P. K. Mason, Modeling Precipitation Kinetics During Heat Treatment with Calphad-Based Tools. J. Mater. Eng. Perform. 23, 4193–4196 (2014).

[2016Hou] Z. Hou, P. Hedström, Q. Chen, Y. Xu, D. Wu, J. Odqvist, Quantitative modeling and experimental verification of carbide precipitation in a martensitic Fe–0.16wt%C–4.0wt%Cr alloy. Calphad. 53, 39–48 (2016).

[2018Wu] K. Wu, Q. Chen, P. Mason, Simulation of Precipitation Kinetics with Non-Spherical Particles. J. Phase Equilibria Diffus. 39, 571–583 (2018).

Precipitation Module (TC-PRISMA) Examples Collection

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

When an example uses a demonstration (demo) database package, this is included with your installation.

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

In this section:

P_01: Isothermal Precipitation of Al3Sc 134
P_02: Stable and Metastable Carbides - Isothermal 139
P_03: Stable and Metastable Carbides - TTT Diagram 143
P_04: Precipitation of Iron Carbon Cementite 147
P_05: Precipitation of γ’ in Ni Superalloys - Isothermal 150
P_06: Precipitation of γ’ in Ni Superalloys - Non-isothermal 155
P_07: Continuous Cooling Transformation (CCT) Diagram of Ni-Al-Cr γ-γ’ 162
P_08: Precipitation of Cu-Ti CU4TI with Assumptions of Sphere and Needle Morphologies 165
P_09: Precipitation of Al-Sc AL3SC with Assumption of Sphere and Cuboid Morphologies 172
P_10: Initial Particle Size Distribution of Fe-Cr-C 178
P_11: Interfacial Energy Function 185
P_12: Comparing Growth Rate Models for an Al-Zr System 189

P_13: Paraequilibrium Precipitation of Cementite Fe-C-Cr 193

P_14: Grain Growth and the Zener Pinning Effect 197

P_15: Smooth Transition from Paraequilibrium to Ortho-equilibrium 202

P_16 Isothermal Coarsening and a 3D to 2D Stereological Conversion 207

P_01: Isothermal Precipitation of Al_3Sc

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

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

Project File and Step-By Step Instructions

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

Example Settings

System (System Definer)	
Database package	Demo: Aluminum-based alloys (ALDEMO, MALDEMO)
Elements	Al, Sc
Conditions (Precipitation Calculator)	
Composition	Al-0.18Sc Mole percent
Matrix phase	FCC_A1
Precipitate phase	AL3SC
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk

Interfacial energy	Calculated
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	350° C
Simulation time	1.0E7 seconds
Experimental File Reader 1 and 2	
There are two Experimental File Reader nodes used. One for the mean radius plot and one to demonstrate the *Yield Strength Property Model*.	

Visualizations

This example is included as a Precipitation Module (TC-PRISMA) tutorial on our website and as part of the playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

> For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

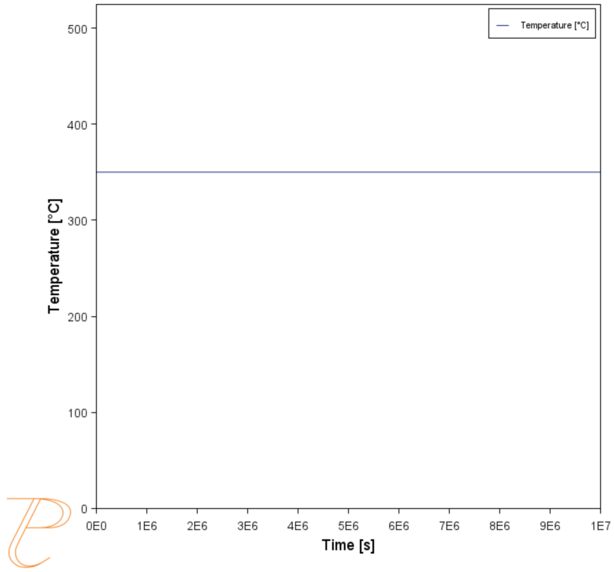


Figure 21: During set up of the calculation, preview the Thermal Profile. Click the tab in the Visualizations window to preview it. For an Isothermal Thermal Profile this shows the constant temperature as entered.

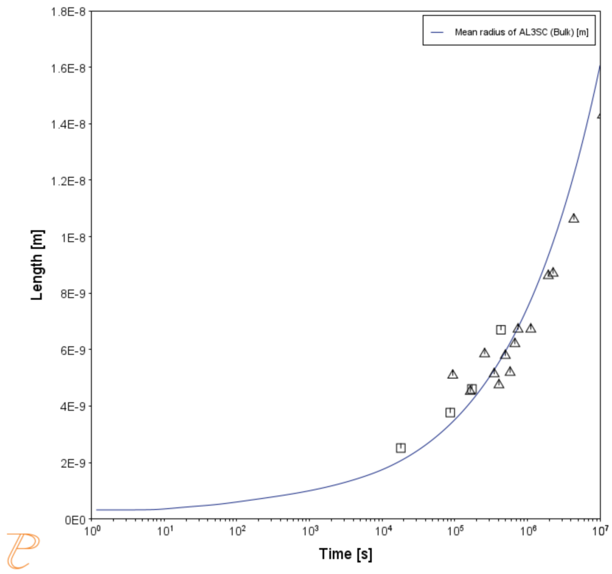


Figure 22: After performing the calculation, you can view the result on the applicable tab. This plot shows the mean radius of the AL3SC precipitate as a function of time.

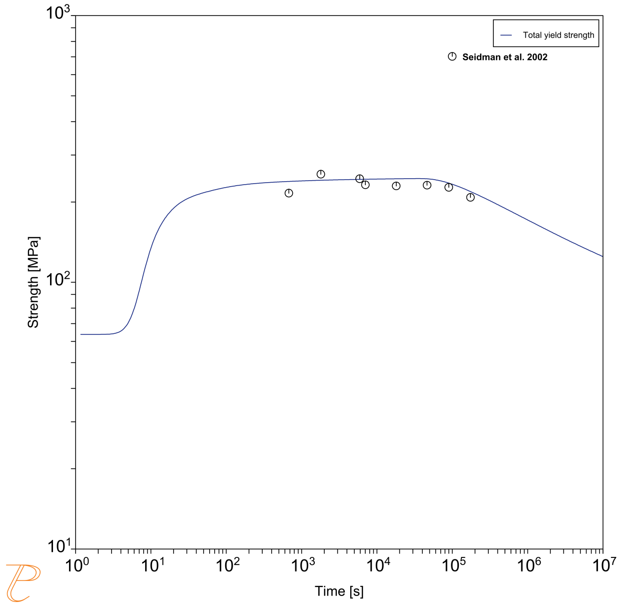


Figure 23: After performing the calculation, you can view the result on the applicable tab. This plot shows the total yield strength of the AL3SC precipitate as a function of time compared to experimental data from Siedmen et al. [2002Sei]. The model captures the over-tempering behavior from excessive coarsening of the strengthening precipitates.

References

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

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

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

P_02: Stable and Metastable Carbides - Isothermal

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

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

Project File Information

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

Example Settings

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

Interfacial energy	Cementite 0.167 J/m^2, M23C6 0.252 J/m^2, M7C3 0.282 J/m^2
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	1053 K
Simulation time	400 000 seconds

Visualizations

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 from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

> For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

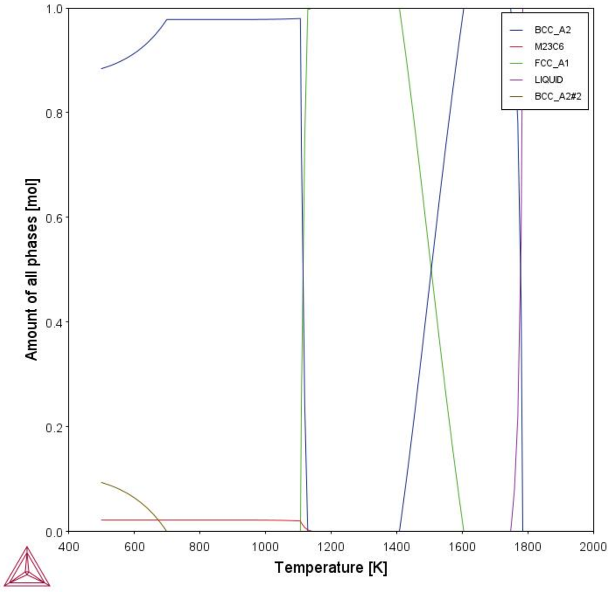


Figure 24: After performing the calculation, you can view the result on the applicable tab. This shows the equilibrium property diagram for the Fe-C-Cr alloy, highlighting what phases are predicted to be at equilibrium for a range of temperatures. The calculation shows that at 1053 K, M23C6 is the stable carbide.

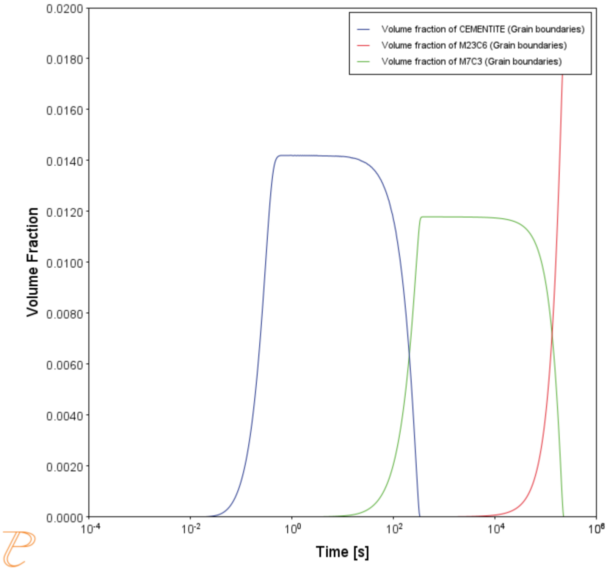


Figure 25: After performing the calculation, you can view the result on the applicable tab. This shows the evolution of the volume fraction of cementite, M7C3, and M23C6 during an isothermal heat treatment of an Fe-C-Cr alloy at 1073 K. The cementite and M7C3 are metastable at this temperature, however their nucleation kinetics are faster than the stable phase, allowing them to form and then dissolve when the next more thermodynamically stable phase nucleates.

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 Information

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

Example Settings

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

Precipitate phases	Cementite, M23C6 and M7C3
Matrix Phase Data Parameters (Precipitation Calculator)	
Grain size (click **Show Details** to display this setting)	1.0E-4 m
Precipitate Phase Data Parameters	
Nucleation sites	Grain boundaries
Interfacial energy	Cementite 0.167 J/m^2, M23C6 0.252 J/m^2, M7C3 0.282 J/m^2
Calculation Type (Precipitation Calculator)	
Calculation type	TTT diagram
Temperature	500° to 800° C with 25° C steps
Max. annealing time	1.0E8 seconds
Stop criteria	Volume fraction of phase is set to 0.0001
Options > Numerical Parameters	
No. of grid points over one order of magnitude in radius	150
Max no. of grid points over one order of magnitude in radius	200
Min no. of grid points over one order of magnitude in radius	100

Visualizations

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 from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

  For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

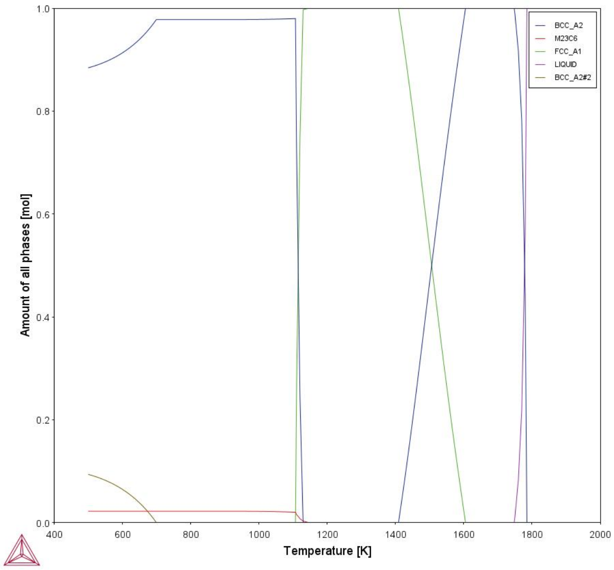


Figure 26: After performing the calculation, you can view the result on the applicable tab. Here the results from the equilibrium calculator are shown, which assesses the stability of phases across the temperature range of interest.

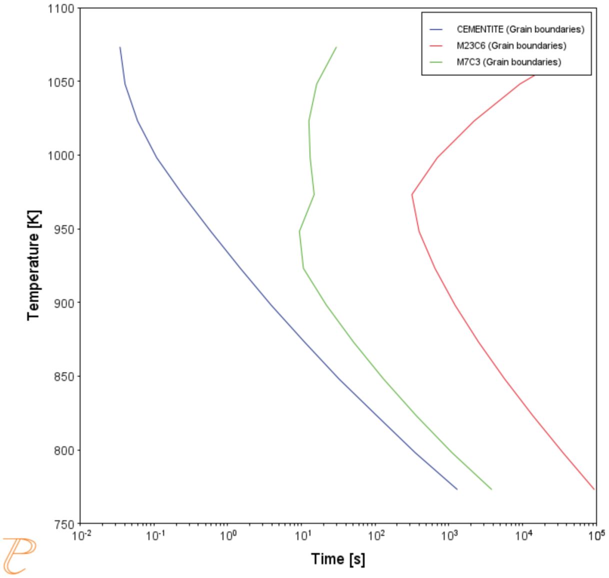


Figure 27: After performing the calculation, you can view the result on the applicable tab.This shows results from a TTT (Temperature-Transformation) simulation using the Precipitation Calculator to examine the sequence of phase transitions considering the formation of cementite, M7C3, and M23C6 carbide phases. The previous Equilibrium Calculator reveals the temperatures where the cementite and M7C3 are metastable.

P_04: Precipitation of Iron Carbon Cementite

This example is based on [1949Wer] and simulates the kinetics of precipitation of carbides from a BCC Fe solution phase. This isothermal calculation example uses the Precipitation Calculator plus two Experimental File Reader activities to plot the volume fraction of the cementite phase.

Project File Information

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

Example Settings

System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO)
Elements	Fe, C
Conditions (Precipitation Calculator)	
Composition	Fe-0.016C mass percent
Matrix phase	BCC_A2
Precipitate phase	Cementite
Matrix Phase Data Parameters (Precipitation Calculator)	
Grain aspect ratio (click **Show Details** to display this setting)	1.0
Dislocation density (click **Show Details** to display this setting)	1.5e11m^{-3}
Precipitate Phase Parameters (Precipitation Calculator)	
Nucleation sites	Dislocations
Interfacial energy	0.24 J/m^{2}

Growth rate model (click **Show Details**)	Advanced
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	102° C
Simulation time	600 000 seconds

Visualizations

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 from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

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

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

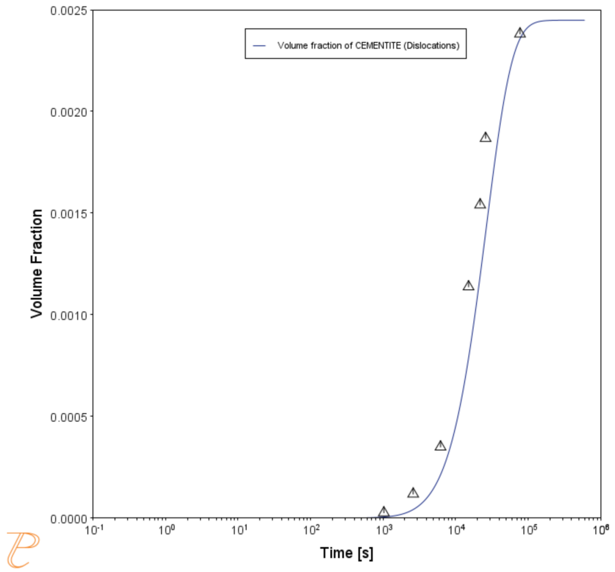


Figure 28: After performing the calculation, you can view the result on the applicable tab. The result compares the predicted evolution of the volume fraction of cementite with the measurements of [1949Wer].

Reference

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

P_05: Precipitation of γ' in Ni Superalloys - Isothermal

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

This example uses three Experimental File Reader activities with the Precipitation Calculator. It does an isothermal calculation to plot the volume fraction, mean radius, and number density of the cementite phase.

DIS_FCC_A1 needs to be selected on the System Definer. See "Selecting the Disordered Phase as a Matrix Phase " on page 29 for details.

Project File Information

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

Example Settings

System (System Definer)	
Database package	Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO)
Elements	Ni, Al Cr
Conditions (Precipitation Calculator)	
Composition	Ni-9.8Al-8.3Cr Mole percent
Matrix phase	DIS-FCC_A1 See "Selecting the Disordered Phase as a Matrix Phase " on page 29

Precipitate phase	FCC_L12#2
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk
Interfacial energy	0.012 J/m^2
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	800° C
Simulation time	1 000 000 seconds

Visualizations

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 from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

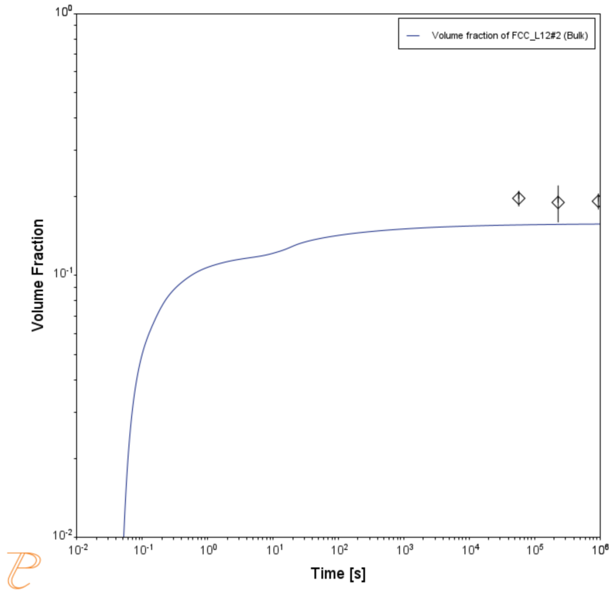


Figure 29: After performing the calculation, you can view the result on the applicable tab. This plot compares the predicted evolution of the volume fraction of gamma prime with the measurements of [2008Sud].

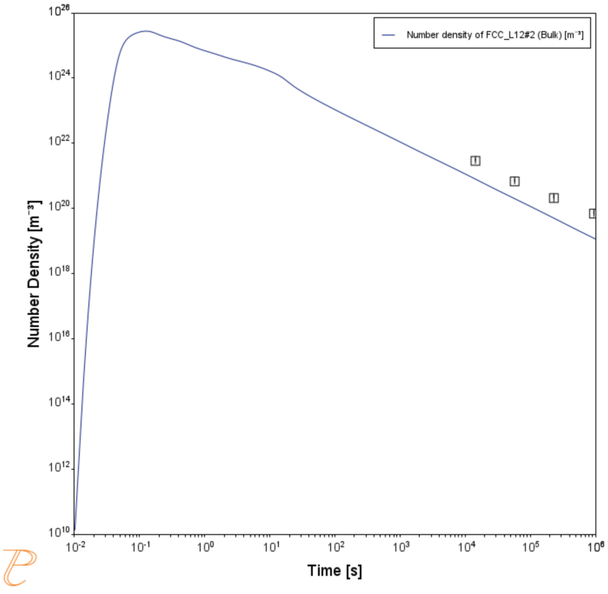


Figure 30: After performing the calculation, you can view the result on the applicable tab. This plot compares the predicted evolution of the number density of gamma prime with the measurements of [2008Sud].

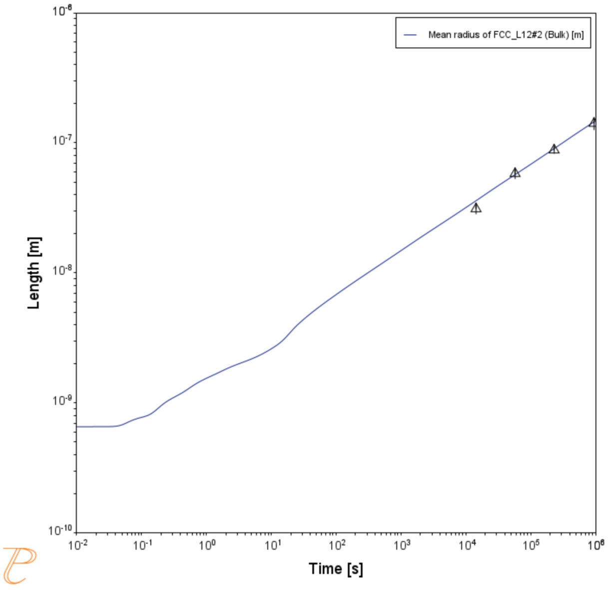


Figure 31: After performing the calculation, you can view the result on the applicable tab. This plot compares the predicted evolution of the mean particle radius of gamma prime with the measurements of [2008Sud].

Reference

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

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

This example simulates the kinetics of precipitation of gamma prime (γ') phase from gamma (γ) phase in Ni-8Al-8Cr and Ni-10Al-10Cr at.% alloys during continuous cooling from a super-solvus temperature. The simulation results can be compared with experimental results from Rojhirunsakool et al. [2013Roj].

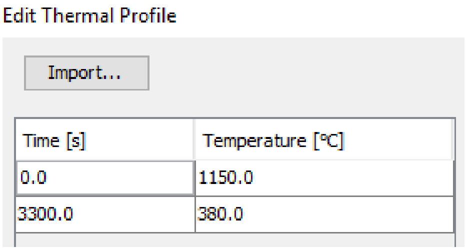
DIS_FCC_A1 needs to be selected on the **System Definer** for both the thermodynamic and mobility databases. See "Selecting the Disordered Phase as a Matrix Phase " on page 29 for details.

Project File Information

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

Example Settings

System (System Definer)	
Database package	Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO)
Elements	Ni, Al, Cr
Conditions (Precipitation Calculator)	
Composition (Ni-8Al-8Cr)	Ni-8Al-8Cr Mole percent
Composition (Ni-10Al-10Cr)	Ni-10Al-10Cr Mole percent
Matrix phase	DIS_FCC_A1 See "Selecting the Disordered Phase as a Matrix Phase " on page 29

<table>
<tr><td>Precipitate phase</td><td>FCC_L12#2</td></tr>
<tr><td colspan="2">Matrix Phase Data Parameters (Precipitation Calculator)</td></tr>
<tr><td>Mobility adjustment > Prefactor (click Show Details to display this setting)</td><td>Keep the default, Same for all elements, then enter 5.0 for the Prefactor.</td></tr>
<tr><td colspan="2">Precipitate Phase Data Parameters (Precipitation Calculator)</td></tr>
<tr><td>Nucleation sites</td><td>Bulk</td></tr>
<tr><td>Interfacial energy</td><td>0.023 J/m^2</td></tr>
<tr><td colspan="2">Calculation Type (Precipitation Calculator)</td></tr>
<tr><td>Calculation type</td><td>Non-isothermal</td></tr>
<tr><td>Temperature unit</td><td>Celsius</td></tr>
<tr><td>Time unit</td><td>Seconds</td></tr>
<tr><td>Temperature</td><td>1150 - 380 °C

Edit Thermal Profile
<table>
<tr><th>Time [s]</th><th>Temperature [°C]</th></tr>
<tr><td>0.0</td><td>1150.0</td></tr>
<tr><td>3300.0</td><td>380.0</td></tr>
</table></td></tr>
<tr><td>Simulation time (Ni-8Al-8Cr)</td><td>3300 s</td></tr>
<tr><td>Simulation time (Ni-10Al-10Cr)</td><td>3300 s</td></tr>
<tr><td colspan="2">Multimodal PSD (Plot Renderer)</td></tr>
<tr><td>Separate multimodal PSD checkbox is selected for 8Al-8Cr for both the Mean radius and PSD plots.</td><td>Mean Radius and PSD plots: The Inflection neighbors and Smoothing interactions defaults are kept.
Mean Radius plot: The Points are set to <code>15</code>.</td></tr>
<tr><td>Separate multimodal PSD checkbox is selected for 10Al-10Cr for both the Mean radius and PSD plots.</td><td>Mean Radius and PSD plots: The Inflection neighbors and Smoothing interactions defaults are kept.</td></tr>
</table>

- Mean Radius plot: The **Points** are set to `50`.

Visualizations

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 from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

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

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

  For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

In this example, all nodes are renamed in the **Project** window, and this matches each of the tab names in the **Visualizations** window.

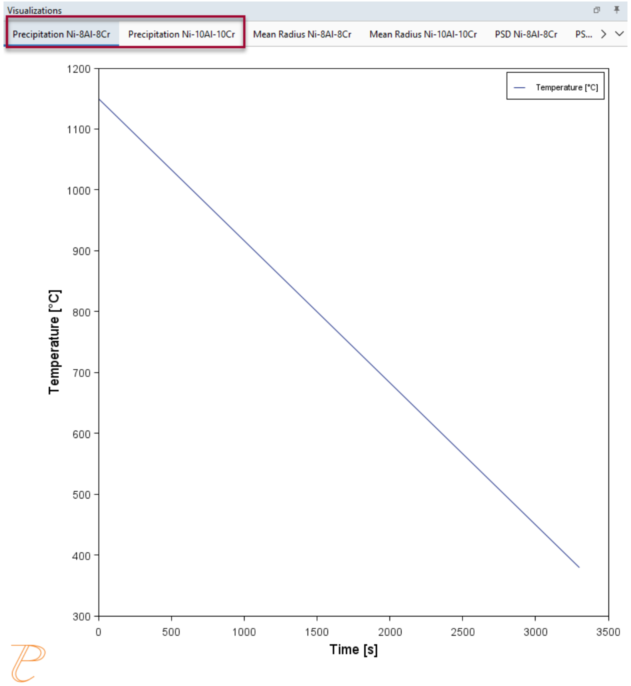


Figure 32: During set up of the calculation, you can preview the non-isothermal Thermal Profile(s). Click the tab in the Visualizations window to adjust settings on the Precipitation Calculator Configuration window. In this case the heat treatment is a continuous cooling curve, however any thermal profile can be modeled using the Non-isothermal Calculation Type.

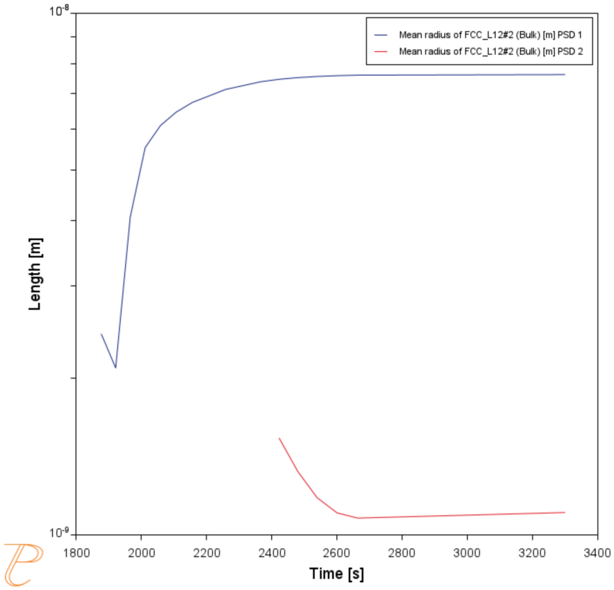


Figure 33: These results show the predicted evolution of the mean radius of gamma prime populations nucleating during the quench for the Ni-8Al-8Cr alloy. Note that the tertiary particles (second particle population) are very small, and this dispersion would appear monomodal without TEM characterization.

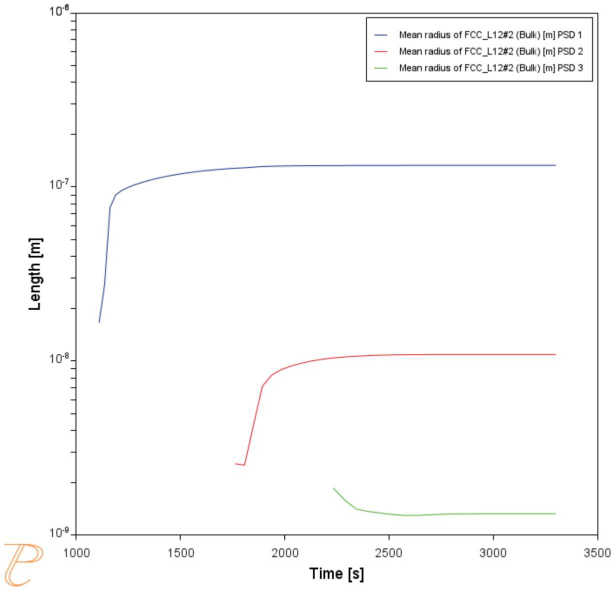


Figure 34: These results show the predicted evolution of the mean radius of gamma prime populations nucleating during the quench for the Ni-10Al-10Cr alloy. In this case three distinct particle populations are simulated to form, agreeing with [2013Roj].

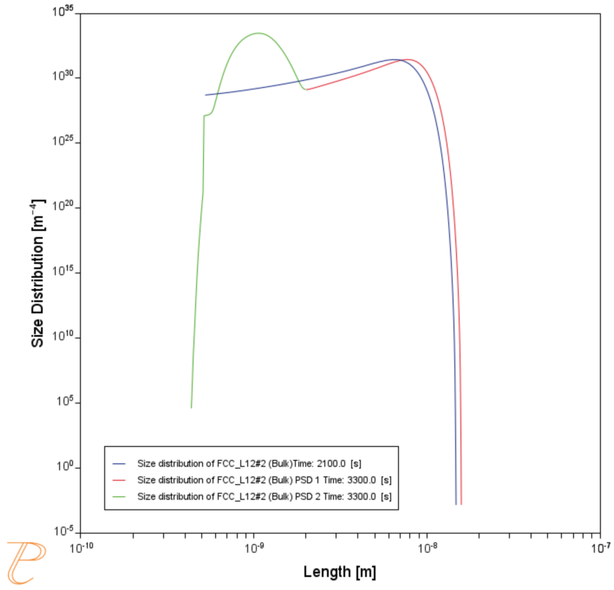


Figure 35: These results show the predicted size distributions of precipitates at different times during the quench of the for the Ni-8Al-8Cr alloy. The individual particle populations are distinguished using the "Separate multimodal PSD" option showing a bimodal distribution with very small nano-meter sized tertiary particles.

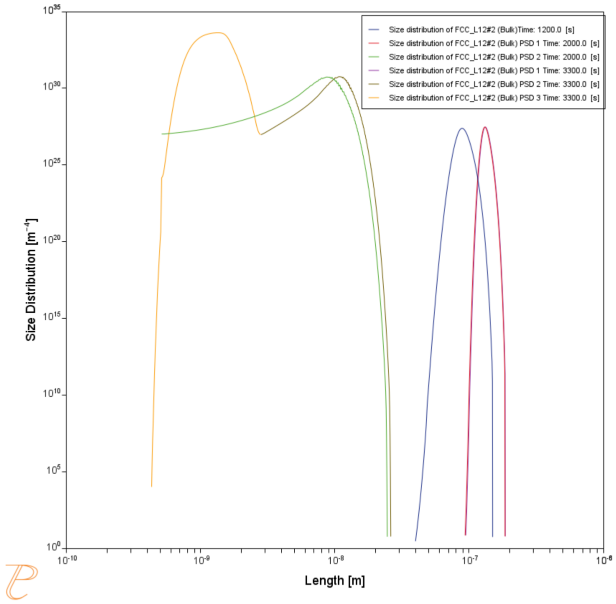


Figure 36: These results show the predicted size distributions of precipitates at different times during the quench for the Ni-10Al-10Cr alloy. The individual particle populations are distinguished using the "Separate multimodal PSD" option showing the formation of a tri-modal dispersion.

Reference

[2013Roj] T. Rojhirunsakool, S. Meher, J. Y. Hwang, S. Nag, J. Tiley, R. Banerjee, Influence of composition on monomodal versus multimodal γ′ precipitation in Ni–Al–Cr alloys. J. Mater. Sci. 48, 825–831 (2013).

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

This example shows you how to simulate a CCT (Continuous Cooling Transformation) diagram for gamma prime (γ’) precipitation in a Ni-Cr-Al alloy using the Precipitation Calculator. A CCT calculation maintains the same cooling rate the entire time.

The system is a Ni-10Al-10Cr γ - γ’ alloy and it is calculated and plotted with superimposition of the cooling rate values.

Project File and Step-By Step Instructions

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

Example Settings

System (System Definer)	
Database package	Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO)
Elements	Ni, Al, Cr
Conditions (Precipitation Calculator)	
Composition	Ni-10Al-10Cr Mole percent
Matrix phase	DIS_FCC_A1
Precipitate phase	FCC_L12#2
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk
Interfacial energy	0.023 J/m^2
Calculation Type (Precipitation Calculator)	
Calculation type	CCT Diagram
Temperature Min to Max	500 to 1200 Kelvin

Cooling rate(s)	.01 .1 1 10 100 K/s
Stop criteria	Volume fraction of phase 1.0E-4

Visualizations

This example is included as a Precipitation Module (TC-PRISMA) tutorial on our website and as part of the playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

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

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

  For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

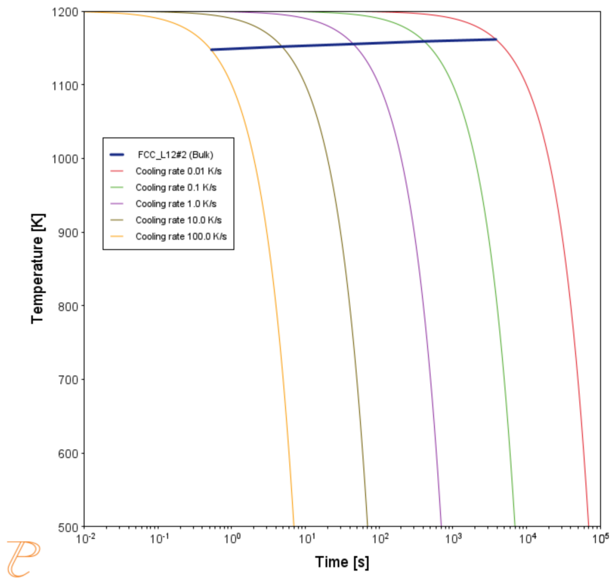
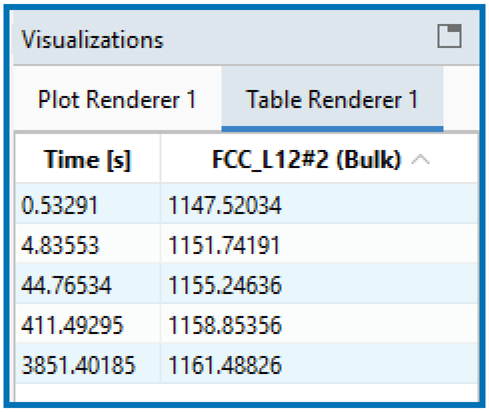


Figure 37: In this plot, the blue horizontal line shows the time it takes for γ' to transform at each of the cooling rates according to the stop criteria, which is set as 1e-4 volume fraction. The cooling rates are represented by the multicoloured curved lines.

If you hover your mouse over the intersection of the blue line and any of the vertical lines, a yellow box shows the approximate time it takes for γ' to transform according to the stop criteria, which is a volume fraction of 1e-4, followed by the approximate temperature.



Time [s]	FCC_L12#2 (Bulk)
0.53291	1147.52034
4.83553	1151.74191
44.76534	1155.24636
411.49295	1158.85356
3851.40185	1161.48826

Figure 38: An example of the table shown in the Visualizations window, which shows the same information as in the plot - for each cooling rate the temperature and the time it takes for γ' to transform according to the stop criteria, which is a volume fraction of 1e-4.

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

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

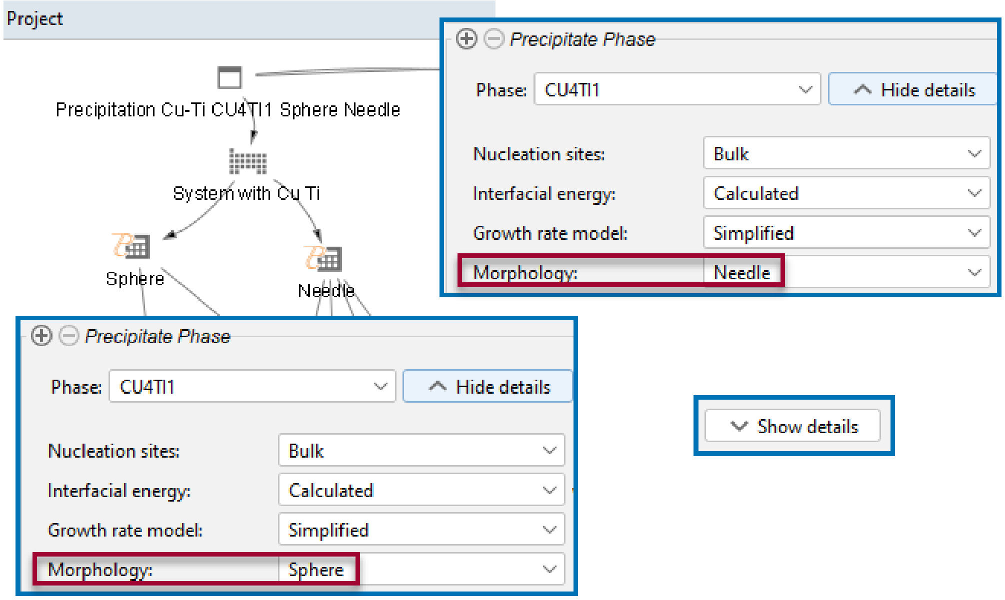
> For more details about the background theory, see "Precipitation Morphology" on page 113.

Project File Information

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

Example Settings

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



Phase: CU4TI1

Nucleation sites: Bulk

Interfacial energy: Calculated

Growth rate model: Simplified

Morphology: Needle

Phase: CU4TI1

Nucleation sites: Bulk

Interfacial energy: Calculated

Growth rate model: Simplified

Morphology: Sphere

System (System Definer)

Database package	Demo: Copper-based alloys (CUDEMO and MCUDEMO)
Elements	Cu, Ti

Sphere and Needle Conditions (Precipitation Calculator)

Composition	Cu-1.9Ti Mole percent
Matrix phase	FCC_L12
Precipitate phase	CU4TI1

Matrix Phase Data Parameters (Precipitation Calculator)

Mobility adjustment > Prefactor (click **Show Details** to display this setting)	Keep the default, Same for all elements, then enter 100 for the Prefactor.

Precipitate Phase Data Parameters (Precipitation Calculator)

Nucleation sites	Bulk
Interfacial energy	The default
Morphology (click **Show Details** to display this setting)	For the **Sphere** node (renamed from Precipitation Calculator), keep the default.

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

Visualizations

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 from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

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

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

  For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

In this example, all nodes are renamed in the **Project** window, and this matches each of the tab names in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

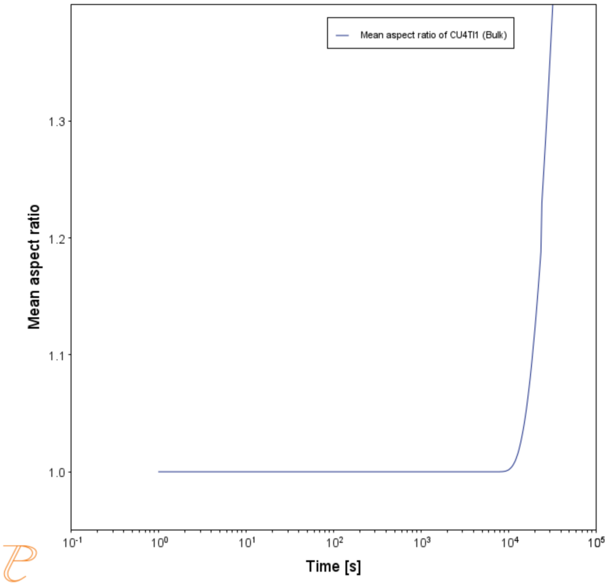


Figure 39: The predicted evolution of the morphology of needle shaped precipitates, showing how the mean aspect ratio changes during the isothermal heat treatment.

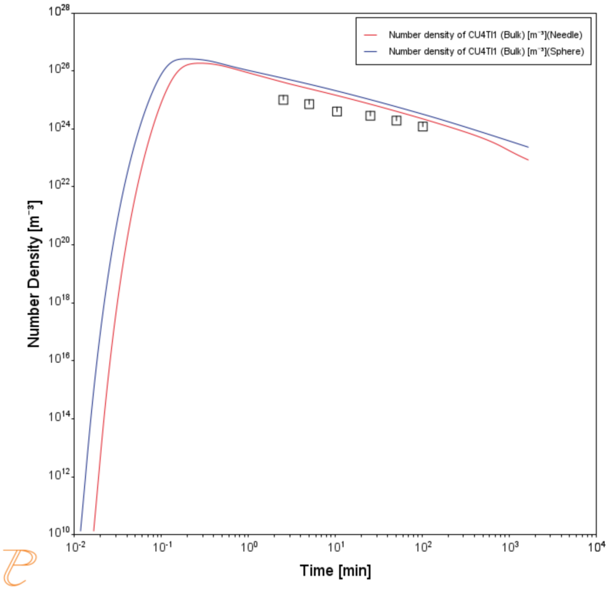


Figure 40: The results compare the predicted evolution of the mean size of precipitates with the experimental data from [1987Kam], comparing the spherical and needle shaped approximations of the precipitate morphology. Note how the needle shape approximation is closer to the experimental data.

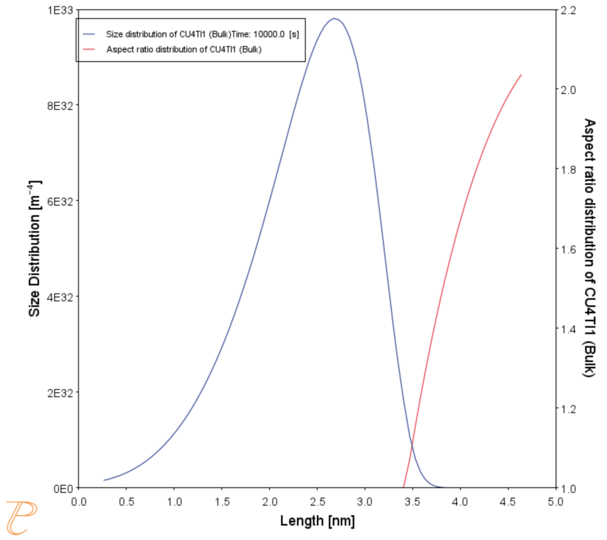


Figure 41: These results show both the predicted final particle size distribution from the needle shape simulation and the predicted relationship between the length of the precipitate and the needle aspect ratio.

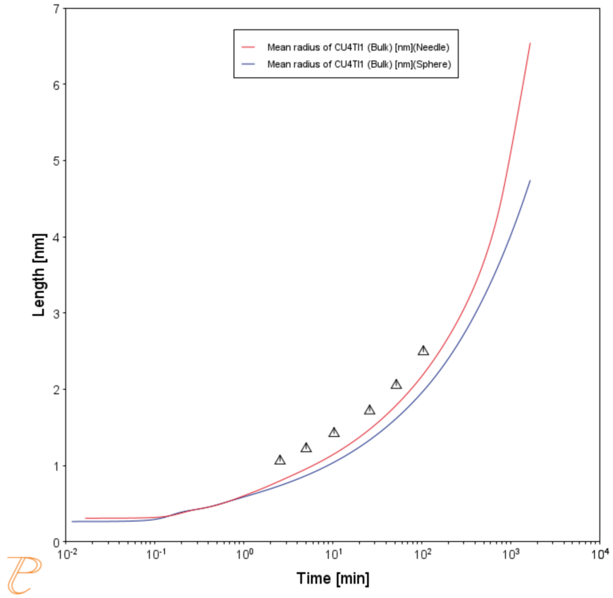


Figure 42: This shows the approximates the size of the needle shaped precipitates as a sphere of equivalent volume, and compares the experimental results of [1987Kam] with those obtained from a spherical and needle shaped approximation.

References

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

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

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

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

For more details about the background theory, see "Precipitation Morphology" on page 113.

Project File and Step-By Step Instructions

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

Example Settings

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

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

Elements	Al, Sc
Sphere and Cuboid Conditions (Precipitation Calculator)	
Composition	Al-0.18Sc Mole percent
Matrix phase	FCC_A1
Precipitate phase	AL3SC
Matrix Phase Data Parameters (Precipitation Calculator)	
Elastic properties (click **Show Details** to display this setting)	For the **Sphere** node (renamed from Precipitation Calculator), the default, **Disregard** is kept. For the **Cuboid** node (renamed from Precipitation Calculator), choose **Cubic**. Then enter the elastic constants accordingly. Default elastic constants are given based on the major element of the alloy system. In this example that is • c11 is **108.2** GPa • c12 is **61.3** GPa • c44 is **28.5** GPa
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Bulk
Interfacial energy	The default
Morphology (click **Show Details** to display this setting)	For the **Sphere** node (renamed from Precipitation Calculator), keep the default. For the **Cuboid** node (renamed from Precipitation Calculator), **Cuboid** is selected.
Transformation strain (click **Show Details** to display this setting)	For the **Sphere** node (renamed from Precipitation Calculator), keep the default. For the **Cuboid** node (renamed from Precipitation Calculator), **Calculate from molar volume** is selected to obtain a purely dilatational strain.
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	350° C

Simulation time	1.0E9 seconds
Datasets (Experimental File Reader)	
Dataset 1 and Dataset 2	Data sets included with this example and imported to one Experimental File Reader. It is used for the Mean Radius plot.

Visualizations

This example is included as a Precipitation Module (TC-PRISMA) tutorial on our website and as part of the playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

  > For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

In this example, all nodes are renamed in the **Project** window, and this matches each of the tab names in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

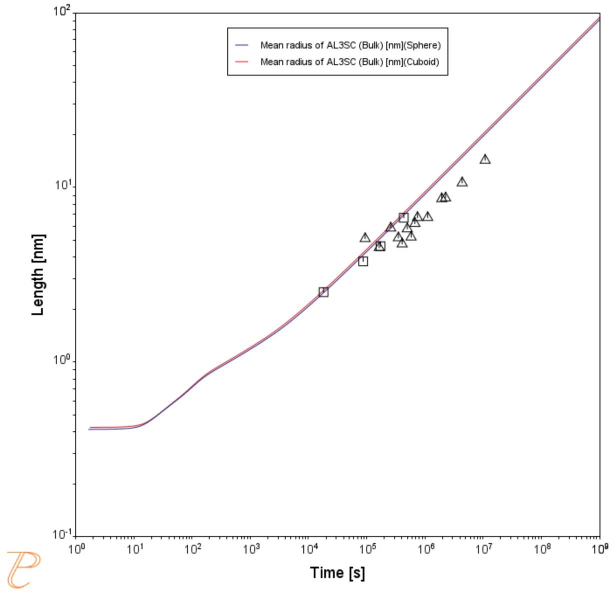


Figure 43: This shows the predicted evolution of the mean size of precipitates with the experimental data from [2001Mar, 2001Nov], comparing the spherical and cuboidal shaped approximations of the precipitate morphology. Although there is not significant difference in the results, capturing the correct geometry of the precipitate is important in subsequent calculations of precipitate spacing used in property calculations.

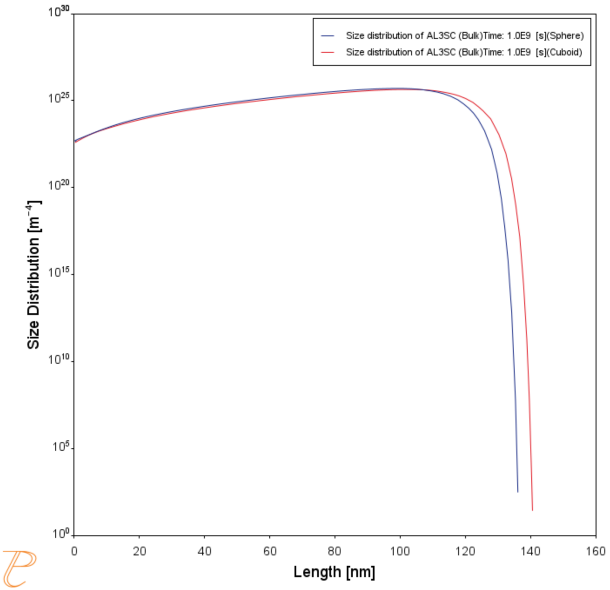


Figure 44: These results compare the predicted size distributions after heat treatment considering the spherical and cuboidal approximations of the precipitate morphology.

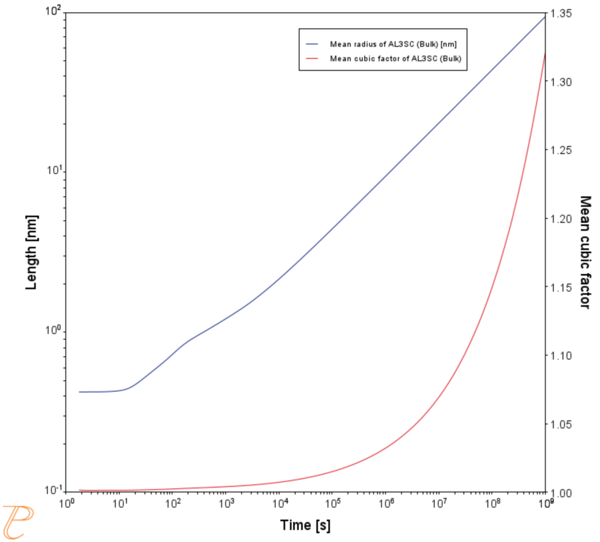


Figure 45: These results compare the predicted evolution of the mean particle radius and mean aspect ratio from using the cuboidal approximation of the precipitate morphology. In this case, the radius of a sphere of equivalent volume to the cuboidal precipitate is shown.

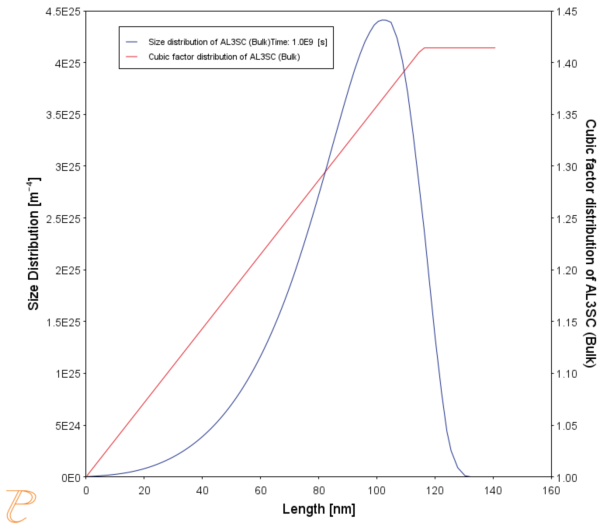


Figure 46: These results show the predicted size distribution of the precipitates obtained from the cuboidal approximation of the precipitate morphology. Also shown is the calculated size dependent cubic factor of the cuboids associated with this dispersion.

References

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

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

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

This example demonstrates the effect of initial particle size distribution (PSD) of the precipitate phases on the overall precipitation kinetics. It uses two Precipitation Calculators to simulate and compare carbide precipitations from a ferritic BCC_A2 matrix in a Fe-0.1C-12Cr alloy. Three carbides, CEMENTITE, M23C7, and M7C3 are included in the calculations simulating a complex precipitation sequence with stable and meta-stable precipitate phases. The results show a large difference in predicted behaviour, with meta-stable precipitates dissolving earlier as a result of the stable precipitates existing in the initial condition.

This example also shows the different ways to create the initial size distribution.

- **Generate 3D PSD from distribution function**: CEMENTITE's PSD is approximated from an LSW distribution.
- **From File**: M23C6's PSD is loaded from a file.
- **Approximate the 3D PSD from experimental data**: M7C3's PSD is approximated from 1D experimental data descriptive of halved linear intercepts.

Project File Information

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

There are also two *.csv files available for you to use as a template for when you are importing data from a file.

- Input data for M23C6: `P_10_Precipitation_Initial_PSD_FeCrC_psd_3D_M23C6.csv`
- Input data for M7C3: `P_10_Precipitation_Initial_PSD_FeCrC_psd_1D_M7C3.csv`

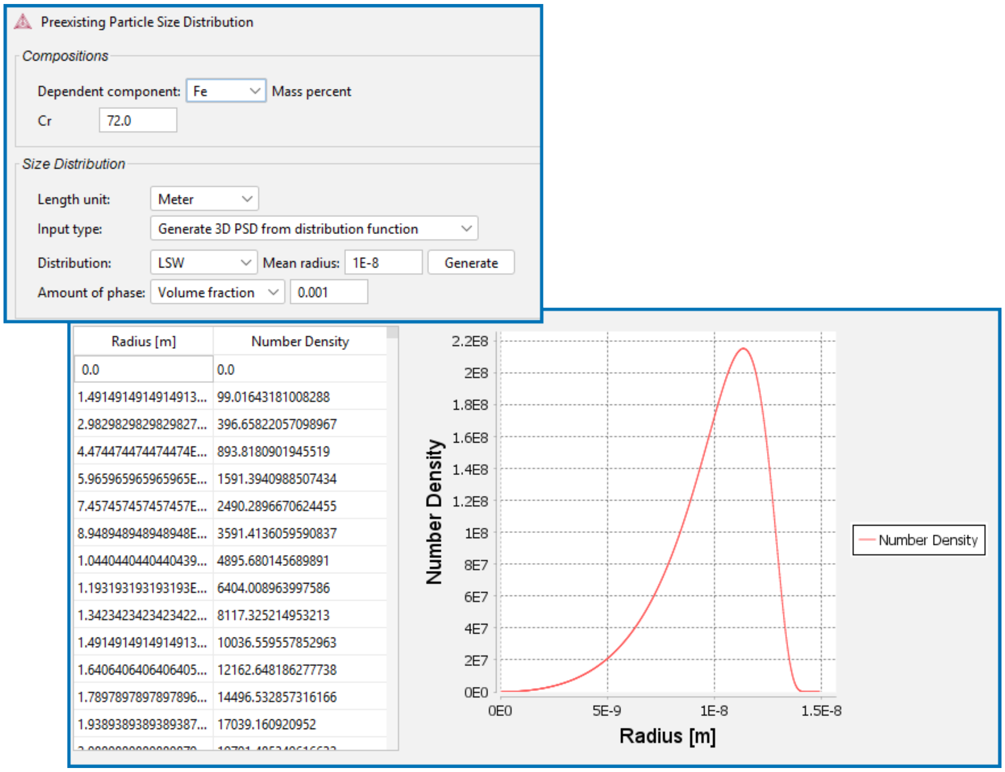
Preexisting Particle Size Distribution

The **Preexisting Particle Size Distribution** window shown in Figure 47 is a graphical representation of the radius versus corresponding number densities, with fields available to enter the initial precipitate composition and volume fraction. An editable table is also provided for the particle size distribution.

"Particle Size Distribution (PSD)" on page 37

Cementite

The amount of Fe and Cr must be defined for Cementite for this alloy. Fe is set to the dependent component, and 72 mass percent of Cr is set. The option **Generate 3D PSD from distribution function** is chosen to create the PSD for Cementite. The initial volume fraction of 0.001 % is assumed. An LSW distribution is selected with a mean radius of 1E-8m.



Dependent component: Fe Mass percent

Cr 72.0

Length unit: Meter

Input type: Generate 3D PSD from distribution function

Distribution: LSW Mean radius: 1E-8

Amount of phase: Volume fraction 0.001

Radius [m]	Number Density
0.0	0.0
1.4914914914914913...	99.01643181008288
2.9829829829829827...	396.65822057098967
4.474474474474474E...	893.8180901945519
5.965965965965965E...	1591.3940988507434
7.457457457457457E...	2490.2896670624455
8.948948948948948E...	3591.4136059590837
1.0440440440440439...	4895.680145689891
1.193193193193193E...	6404.008963997586
1.3423423423423422...	8117.325214953213
1.4914914914914913...	10036.559557852963
1.6406406406406405...	12162.648186277738
1.7897897897897896...	14496.532857316166
1.9389389389389387...	17039.160920952

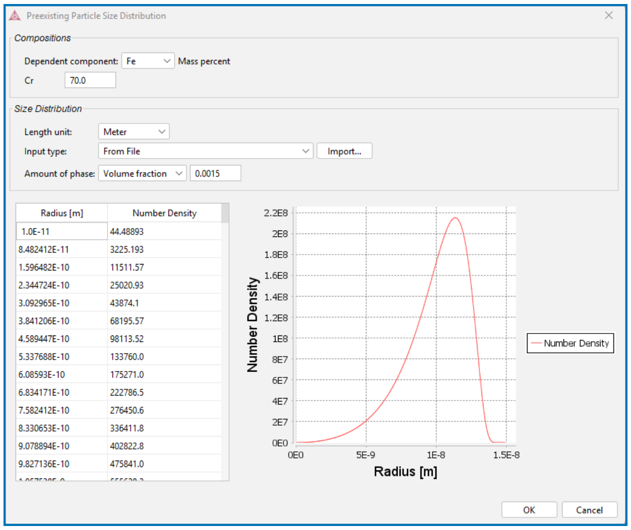
Figure 47: An LSW distribution with a mean radius of 1E-8m is used.

M23C6

The amount of Fe and Cr must be defined for M23C6 for this alloy. Fe is set to the dependent component, and 70 mass percent of Cr is set. The **From File** option is used to create the PSD.

> The file loaded for M23C6 is available from the **Example files** → **Precipitation Module - TC-PRISMA** folder and is named `P_10_Precipitation_Initial_PSD_FeCrC_psd_3D_M23C6.csv`.

You can import data from a spreadsheet or text file (.xls, .xlsx, .csv, or .txt formats are acceptable). The initial volume fraction of 0.15 % is assumed.



Compositions

Dependent component: Fe Mass percent

Cr 70.0

Size Distribution

Length unit: Meter

Input type: From File

Amount of phase: Volume fraction 0.0015

Radius [m]	Number Density
1.0E-11	44.48893
8.482412E-11	3225.193
1.596482E-10	11511.57
2.344724E-10	25020.93
3.092965E-10	43874.1
3.841206E-10	68195.57
4.589447E-10	98113.52
5.337688E-10	133760.0
6.08593E-10	175271.0
6.834171E-10	222786.5
7.582412E-10	276450.6
8.330653E-10	336411.8
9.078894E-10	402822.8
9.827136E-10	475841.0

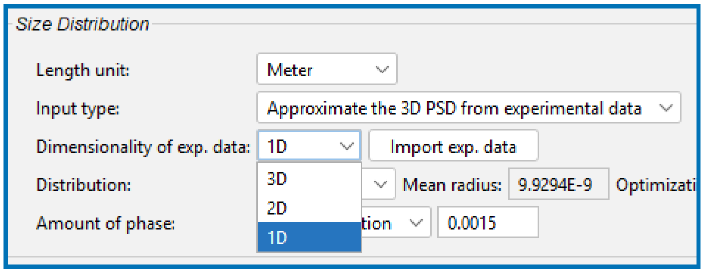
M7C3

The amount of Fe and Cr must be defined for M7C3 for this alloy. Fe is set to the dependent component, and 83 mass percent of Cr is set. The Approximate the 3D PSD from experimental data option is used to create the PSD.

In this example, the linear intercept method is used to measure the size distribution of M7C3 from micrographs descriptive of sectioning the dispersion. A size distribution of halved linear intercepts is created and is available as a file you can use as a template.

The file loaded for M7C3 is available from the **Example files** → **Precipitation Module - TC-PRISMA** folder and is named `P_10_Precipitation_Initial_PSD_FeCrC_psd_1D_M7C3.csv`.

The **Dimensionality of the exp. data** is set to 1D. The experimental data is loaded by importing the above named *.csv file. An **LSW Distribution** is used. When you click **Generate**, it calibrates the chosen distribution and stereology description to the experimental data. The initial volume fraction of 0.15 % is assumed.



Size Distribution

Length unit: Meter

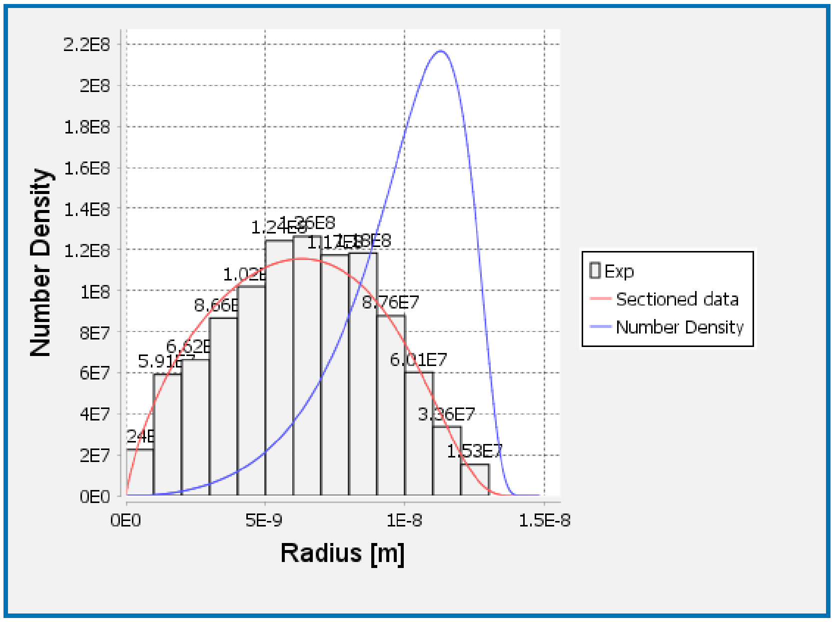
Input type: Approximate the 3D PSD from experimental data

Dimensionality of exp. data: 1D

Distribution:

Mean radius: 9.9294E-9

Amount of phase: 0.0015



Example Settings

System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO)
Elements	Fe, C, Cr
Conditions (Precipitation Calculator)	
Composition	Fe-0.1C-12Cr Mass percent
Matrix phase	BCC_A2 All other defaults are kept.
Precipitate phases	CEMENTITE, M23C6 and M7C3
Precipitate Phase Data Parameters (Precipitation Calculator)	
Nucleation sites	Grain boundaries (all calculations): Calculated from the matrix settings with a

	wetting angle of 90°
Interfacial energy	User-defined function f(r,T) (all calculations): - CEMENTITE: 0.167 J/m^2 - M23C6 0.252 J/m^2 - M7C3 0.282 J/m^2
Preexisting size distribution (click **Show Details** to display this setting)	For the Precipitation Calculator including particle size distribution (PSD), and for all precipitate phases, this checkbox is selected. For each precipitate phase (CEMENTITE, M23C6 and M7C3), click **Edit Particle Size Distribution** to make changes to the parameters. A window opens with a graphical representation of the radius vs number density. **Input type** - Generate 3D PSD from distribution function - CEMENTITE uses this option in the example - From File - M23C6 uses this option in the example - Approximate the 3D PSD from experimental data - M7C3 uses this option in the example.
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	1053 K
Simulation time	400 000 seconds

Visualizations

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 from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

  For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

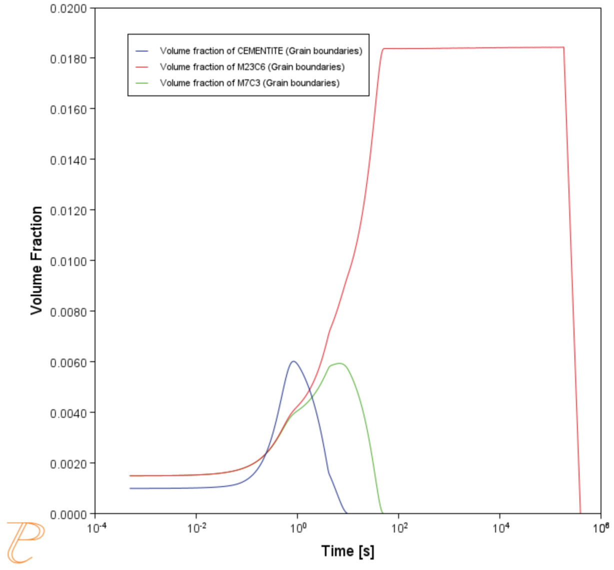


Figure 48: These results show the predicted volume fraction of cementite, M23C6, and M7C3 during an isothermal aging with an initial particle size distribution of each precipitate phase. The predicted kinetics are sensitive to the initial size, volume fraction, and composition of these precipitates.

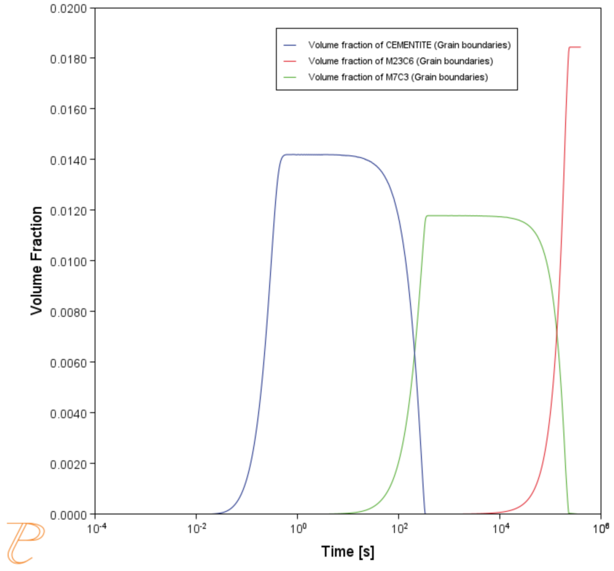


Figure 49: The predicted volume fraction of cementite, M23C6, and M7C3 during an isothermal aging with no precipitates in solution in the initial condition.

P_11: Interfacial Energy Function

In some cases, interfacial energy may be a function of temperature and/or particle radius. This example uses four Precipitation Calculators at four temperature points in 30 K increments: 673 K, 703 K, 733 K, and 763 K. It is an isothermal calculation to examine the mean radius of an Al-0.12Sc system. It uses an FCC_A1 matrix phase and AL3SC precipitate phase with bulk nucleation sites and user-defined interfacial energy function. The user defined interfacial energy function uses an error function to set a smooth transition of the interfacial energy from 0.065 J/m^2 to 0.085 J/m^2 for particle radii below and above 1e^{-8}m and 5e^{-8}m, respectively.

A dataset based on Iwamura and Miura [2004Iwa] data is compared with the calculated results.

"Interfacial Energy Anisotropy" on page 101

Project File Information

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

Example Settings

System (System Definer)	
Database package	Demo: Aluminum-based Alloys (ALDEMO, MALDEMO)
Elements	Al, Sc
Conditions (Precipitation Calculator)	
Composition	Al-0.12Sc Mole percent
Matrix phase	FCC_A1 All other defaults are kept.

Precipitate phase	AL3SC Nucleation sites (all calculations): Bulk (6.025E28 m^{-3}) Interfacial energy (all calculations): User-defined function f(r,T): 0.075+0.011*erf((r-3e-8)/1e-8 J/m^2)
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal (all calculations)
Temperature	Four temperature points in 30 K increments: 673 K, 703 K, 733 K, and 763 K.
Simulation time	1 000 000 seconds (all calculations)
Datasets (Experimental File Reader)	
Wamura 2004 (Dataset 1)	Data set included with this example and imported to one Experimental File Reader.

Visualizations

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 from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

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

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

> For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

> For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

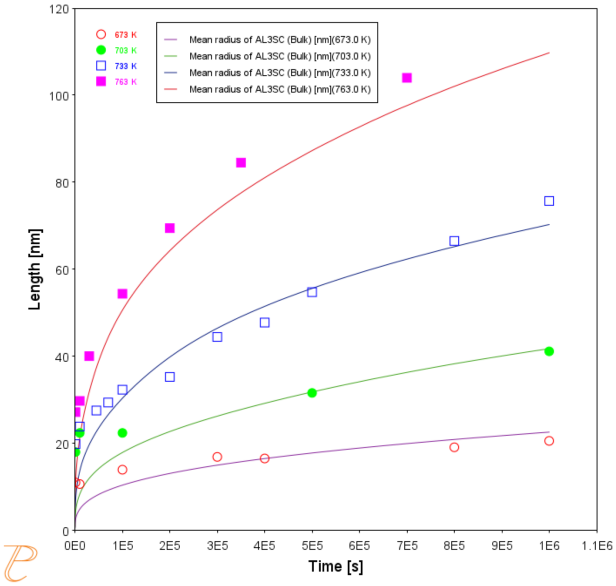


Figure 50: The results of an isothermal calculation to examine the mean radius of an Al-0.12Sc system with experimental data from [2004Iwa].

Reference

[2004Iwa] S. Iwamura, Y. Miura, Loss in coherency and coarsening behavior of Al3Sc precipitates. Acta Mater. 52, 591–600 (2004).

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

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

All models treat a spherical particle (precipitate) of stoichiometric composition or with negligible atomic diffusivity. Local equilibrium at the precipitate-matrix interface is assumed.

When you use the *Advanced* model, the velocity of a moving phase interface and the operating tie-line are solved together from flux-balance equations. This model can treat both high supersaturation and cross diffusion rigorously. It can also capture the transition between NPLE (non-partitioning local equilibrium) and PLE (partitioning local equilibrium) without any *ad hoc* treatment.

The *Simplified* model is based on the quasi-steady state diffusion approximation, and estimates solute partitioning with matrix composition and nuclei composition instead of time-consuming stepwise tie-line calculations. It also neglects cross diffusion for simplicity.

The *General* model can be considered the same theoretical approximation as, but an improvement over, the *Simplified* model, with cross-diffusion terms taken into account, as well as adjustment of Gibbs-Thomson effect and effective diffusivity implemented. A dataset based on Knipling et al. [2008Kni] data is compared with the calculated results.

For more background information, see the theory described in "Growth" on page 94.

Project File Information

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

Example Settings

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

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

Visualizations

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 from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

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

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

  > For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

> For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

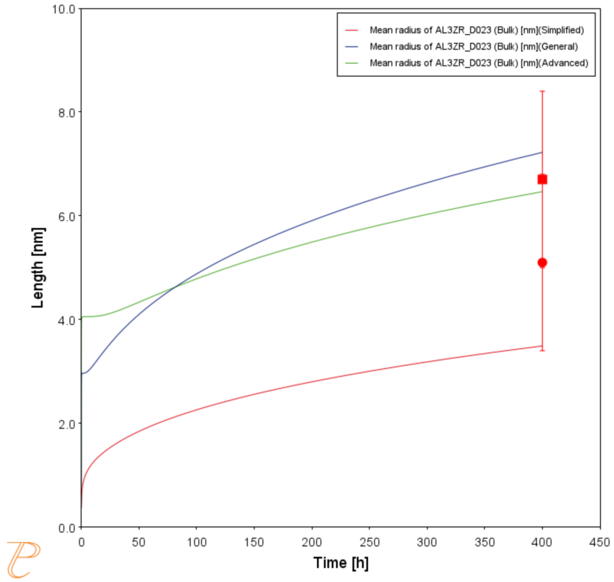


Figure 51: This shows the impact of the available growth rate settings options and compares the mean radius measurements of [2008Kni] with results obtained from the simplified, general, and advanced growth rate models. The experimental data includes measurements taken from different dendrites.

Reference

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

P_13: Paraequilibrium Precipitation of Cementite Fe-C-Cr

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

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

For more background information, see the theory described in "Growth" on page 94.

Project File Information

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

Example Settings

System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)
Elements	Fe, Cr, C
Conditions (Precipitation Calculator)	
Composition	Fe-0.95Cr-1.065C Mass percent
Matrix phase	BCC_A2

	All other defaults are kept.
Precipitate phase	CEMENTITE_D011 Click **Show Details** to select the **Growth rate model** (**Simplified** (OE) and **Para-eq**) (PE). All other defaults are kept.
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	773 Kelvin
Simulation time	20 hours for the paraequilibrium model and 600 hours for the simplified model.
Datasets (Experimental File Reader)	
1980 Sakuma	Data set included with this example and imported to one Experimental File Reader.

Visualizations

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 from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

When you run (Perform) this example, it can take over two hours to complete the calculations.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

  For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

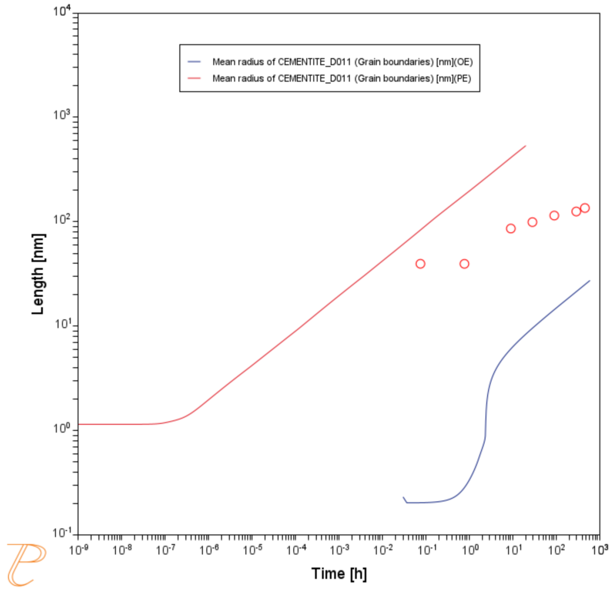


Figure 52: These results compare the predicted and measured evolution of the mean radius of cementite with the experimental data from [1980Sak] to simulation predictions obtained from the ortho-equilibrium (OE), and para-equilibrium (PE) approximations of the precipitate composition. The precipitate growth kinetics exhibited by cementite can be rationalized by the transition from PE to OE.

Reference

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

P_14: Grain Growth and the Zener Pinning Effect

This example demonstrates the simulation of normal grain growth and the pinning effect [1948Smi; 1998Man] of precipitated second-phase particles on the grain boundary motion.

To investigate the grain growth and Zener pinning effect, an Fe-0.2C (wt.%) binary alloy, with a BCC_A2 matrix phase and CEMENTITE precipitate phase, is simulated and uses the demonstration steel databases, FEDEMO and MFEDEMO. These databases are available to all users (i.e. you do not need a license for the Precipitation Module (TC-PRISMA)) and contain the necessary thermodynamic and kinetic data needed for the calculation.

> For more details, see the theory described in "Normal Grain Growth" on page 116 and "Zener Pinning" on page 118.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: `P_14_Precipitation_Fe-C-Ferrite-Grain_Growth_with_Zener_Pinning.tcu`

Example Settings

System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO)
Elements	Fe, C
Conditions (Precipitation Calculator)	
Composition	Fe-0.2C Mass percent
Matrix phase	BCC_A2 • Grain boundary energy (J/m^2): 0.5 • Grain boundary mobility: Prefactor(m^4/Js): 2 x 10^{-15} • Click to **Edit grain size distribution**. Then Initial grain size distribution: Hillert distribution with average radius of 3.2 x 10^{-6} m

	• Mobility adjustment: Same for all elements. Prefactor 0.08.
Precipitate phase	CEMENTITE • Zener pinning parameters: Cutoff size (m): 8.0 x 10^{-7}
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	722 °C
Simulation time	35 hours
Datasets (Experimental File Reader)	
[1975Hel]	Data sets included with this example and imported to two Experimental File Readers.

Visualizations

This example is included as a Precipitation Module (TC-PRISMA) tutorial on our website and as part of the playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

The calculated equilibrium volume fraction of CEMENTITE at 722 °C (0.02786), using FEDEMO, matches that (0.02787) of a Fe-0.2C-0.004S-0.0004O-0.001N-0.001Al (wt.%) multicomponent commercial alloy, calculated using the latest version of the TCS Steel and Fe-alloys Database (TCFE), an alloy that was studied by Hellman and Hillert [1975Hel]. The mobility adjustment assures the precipitation kinetics of CEMENTITE phase in Fe-C system matches that of experimental data [1975Hel] of the commercial counterpart (and shown in Figure 53)

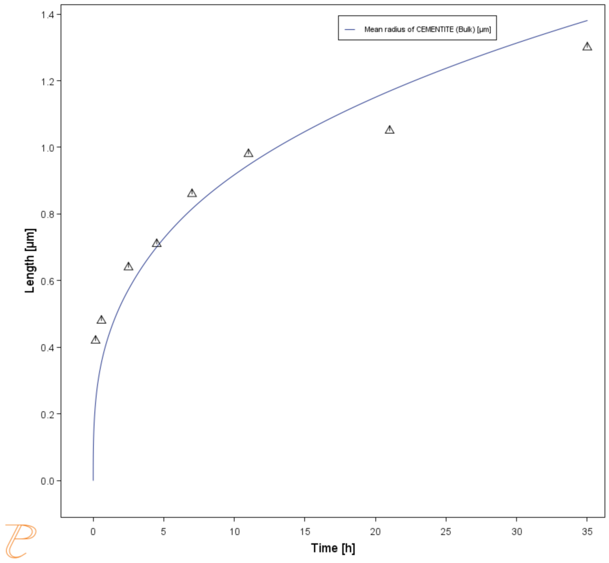


Figure 53: The evolution of the mean radius of cementite comparing the experimental data from [1975Hel] with the Precipitation Calculator results.

The grain boundary energy was chosen to be a reasonable value of 0.5 J/m^2. There is a large discrepancy, in several orders of magnitude, among experimental data regarding the grain boundary mobility. In the present calculation, a value of 2x10^{-15} m^4/Js was chosen.

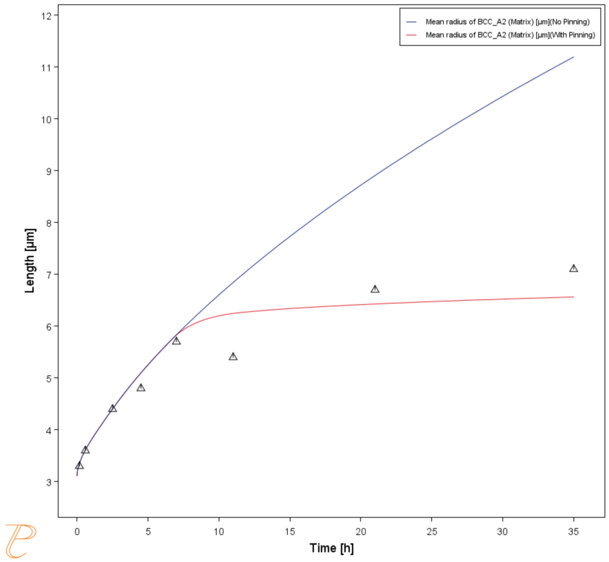


Figure 54: The evolution of the mean grain radius of ferrite comparing the experimental data from [1975Hel] with predictions made with and without Zener pinning from an evolving dispersion of cementite precipitates.

References

[1948Smi] C. S. Smith, Grains, Phases, and Interfaces - an Interpretation of Microstructure. Trans. AIME. 175, 15–51 (1948).

[1975Hel] P. Hellman, M. Hillert, On the Effect of Second-Phase Particles on Grain Growth. Scand. J. Metall. 4, 211–219 (1975).

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

P_15: Smooth Transition from Paraequilibrium to Ortho-equilibrium

In this example, the precipitation of cementite during tempering of an Fe-Mn-C steel is simulated considering three interface conditions: the usual ortho-equilibrium (OE) condition; paraequilibrium (PE) condition; and a smooth transition from paraequilibrium to ortho-equilibrium condition (PE-OE). The simulation results are compared with the experimental data from Miyamoto et al. [2007Miy].

> The Precipitation Calculator nodes are renamed in the example to match the abbreviations for the three interface conditions considered: OE, PE, and PE-OE. Also see the video to learn how to create this example.

This example demonstrates that the early stage of the cementite precipitation follows a PE condition, under which the precipitation kinetics is controlled by the diffusion of C. At a later stage, gradual transition from PE condition to OE condition occurs, and if the tempering time is long enough the diffusion of Mn has a dominating effect on the coarsening of cementite. While a *Simplified* model follows the OE condition and a *Para-eq* model follows PE condition, the *PE Automatic* model enables the smooth transition from PE condition at early stage to OE condition at a late stage.

The example uses the demonstration steel databases, FEDEMO and MFEDEMO. These databases are available to all users (i.e. you do not need a license for the Precipitation Module (TC-PRISMA)) and contain the necessary thermodynamic and kinetic data needed for the calculation.

> For more details, see PE Automatic Growth Rate Model described in the "Growth" on page 94 theory section.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: `P_15_Precipitation_Fe-C-Mn_PE-OE_Precipitation_of_Cementite.tcu`

Example Settings

System (System Definer)	
Database package	Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO)
Elements	Fe, Mn, C
Conditions (Precipitation Calculator)	
Composition	Fe-1.96Mn-0.61C mass percent
Matrix phase	BCC_A2 Click **Show Details**: • Grain size: Average radius 1.0E-7m • Grain aspect ratio: 100.0 • Mobility adjustment: Keep the default, Same for all elements, then enter 0.008 for the Prefactor, and -7e4 J/mol for the Activation energy. All other defaults are kept.
Precipitate phase	CEMENTITE_D011 Click **Show Details** to select the Growth rate model (**Simplified**, **Para-eq**, and **PE Automatic**). All other defaults are kept.
Calculation Type (Precipitation Calculator)	
Calculation type	Isothermal
Temperature	923.15 Kelvin
Simulation time	1E6 seconds for Simplified and PE Automatic models, and 5 seconds for Para-eq model
Datasets (Experimental File Reader)	
Mean Radius Exp	Data set including experimental mean radius of cementite
Mn Concentration	Data set including experimental Mn composition in cementite

Visualizations

This example is included as a Precipitation Module (TC-PRISMA) tutorial on our website and as part of the playlist on our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

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

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

  For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

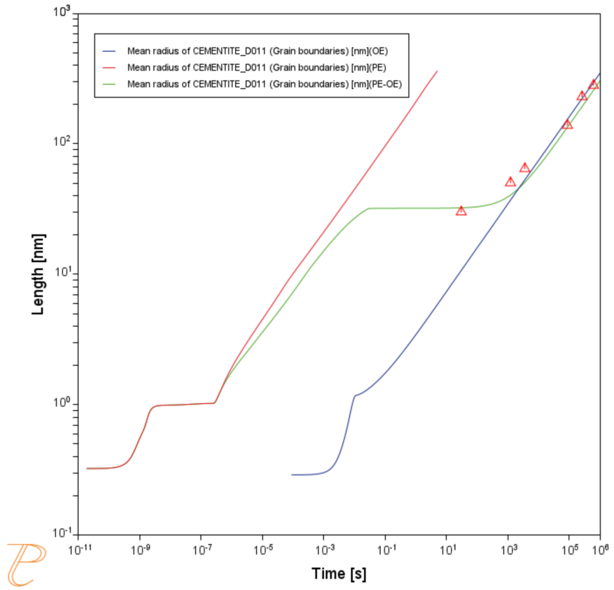


Figure 55: A comparison between the measurements of mean cementite radius from [2007Miy] with the simplified (OE), para-eq (PE), and PE Automatic (PE-OE) growth models. The PE-OE model is needed to capture the nucleation, growth, and coarsening behavior of cementite.

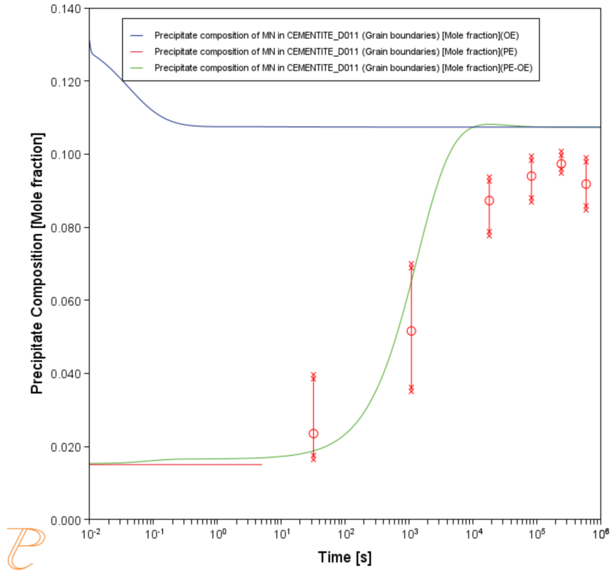


Figure 56: A comparison of the evolution of the cementite Mn composition during isothermal aging at 923.15 K between the experimental data from [2007Miy] with model predictions obtained from the simplified (OE) growth model, the para-eq (PE) growth model, and the PE Automatic (PE-OE) growth model. The PE-OE model captures the behavior shown in the experimental data, where the Mn composition transitions from the initial ferrite composition towards the equilibrium cementite composition.

Reference

[2007Miy] G. Miyamoto, J. Oh, K. Hono, T. Furuhara, T. Maki, Effect of partitioning of Mn and Si on the growth kinetics of cementite in tempered Fe–0.6 mass% C martensite. Acta Mater. 55, 5027–5038 (2007).

P_16 Isothermal Coarsening and a 3D to 2D Stereological Conversion

This example demonstrates the use of the **3D → 2D** stereological conversion functionality to compare Precipitation Module (TC-PRISMA) predictions with experimental data obtained from Scanning Electron Micrographs (SEM).

The **3D → 2D** setting is available on a **Plot** or **Table Rendere**r that is a successor to the **Precipitation Calculator**, and when certain axis variables are selected for a spherical morphology.

For more background information, see the theory described in "Stereology" on page 121.

The isothermal coarsening kinetics of γ' precipitates in a Ni-Al-Cr alloy is modeled. The experimental data is from [2008Sud], which investigates isothermal coarsening kinetics at a temperature of 873 K for up to 264 h.

It is assumed that there are no precipitates in solution at the beginning of the isothermal heat treatment.

Project File Information

- Folder: **Precipitation Module - TC-PRISMA**
- File name: `P_16_Precipitation_Ni-Al-Cr_Stereology.tcu`

Example Settings

The example also includes an Equilibrium Calculator and Table Renderer to first confirm the stability of the precipitate phase for this system (FCC_L12#2), then determine particle composition at 1073 K, and this information is used with the Precipitation Calculator set up.

System (System Definer)	
Database package	Demo: Nickel-based superalloys (NIDEMO and MNIDEMO)
Elements	Ni, Al, Cr
Conditions (Precipitation Calculator)	
Composition	Ni-10l-8.5Cr Mole percent
Matrix Phase	DIS_FCC_A1 - Click **Show Details** and for the **Mobility adjustment** enter `0.5` for the **Prefactor**. - All other defaults are kept.
Precipitate Phase	FCC_L12#2 Click **Show Details** and adjust the default settings as indicated: - **Interfacial energy**: Select **User-defined** and enter `0.01` J/m^2.
Calculation Type (Precipitation Calculator)	
Calculation Type	Isothermal
Temperature	1073 Kelvin
Simulation time	300 h
Datasets (Experimental File Reader)	
2008 Sudbrack et al	Data sets are included with this example and are imported using the Experimental File Reader activity. There are 2D size distributions comparing results after a total of 16 h aging, 64 h aging, and 264 h of aging, and a comparison of the experimental and predicted 2D mean radius versus time.

Visualizations

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 from the main My Project window, click **Video Tutorials**. Alternately, you can go to the website or our YouTube channel.

Open the example project file to review the node setup on the **Project** window and the associated settings on the **Configuration** window for each node. For some types of projects, you can also adjust settings on the **Plot Renderer Configuration** window to preview results before performing the simulation. Click **Perform Tree** to generate plots and tables to see the results on the **Visualizations** window.

There is a variety of information shown in the **Visualizations** window that can be viewed during configuration and after performing the calculation.

- **Thermal Profile**: When setting up a calculator on a **Configuration** window for **Isothermal** or **Non-isothermal** *Calculation Types*, you can preview the profile and adjust settings as needed. When you click a calculator node in the **Project** window, the matching name of the node is on the tab(s) displayed in the **Visualizations** window.

  For **TTT Diagram** and **CCT Diagram** calculations there is nothing shown for the Precipitation Calculator tab in the **Visualizations** window as there is no Thermal Profile to be defined.

- **Plot** or **Table** results: After completing the set up and performing the calculation, to view the matching name of the node on tab(s) in the **Visualizations** window, either click a **Plot Renderer** or **Table Renderer** node in the **Project** window or click the tabs individually in the **Visualizations** window.

For this **Isothermal** example, its **Thermal Profile** is also displayed in the **Visualizations** window showing the constant temperature entered for this calculation type. The tab names match the node names in the **Project** window.

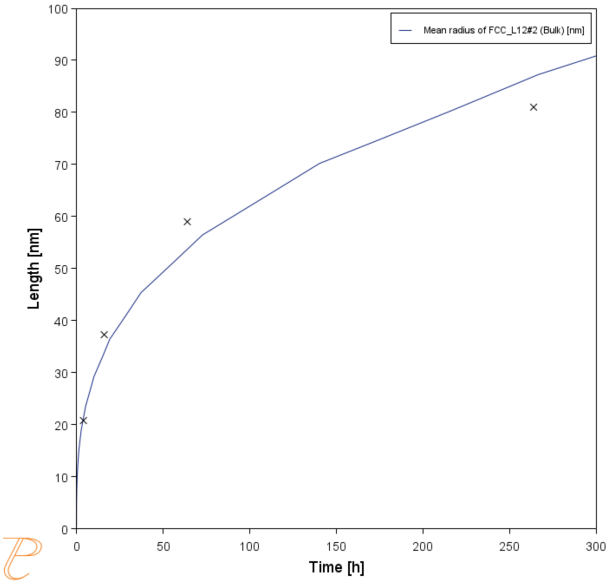


Figure 57: A comparison of the evolution of the mean 2D precipitate radius measurements of [2008Sud] with model predictions.

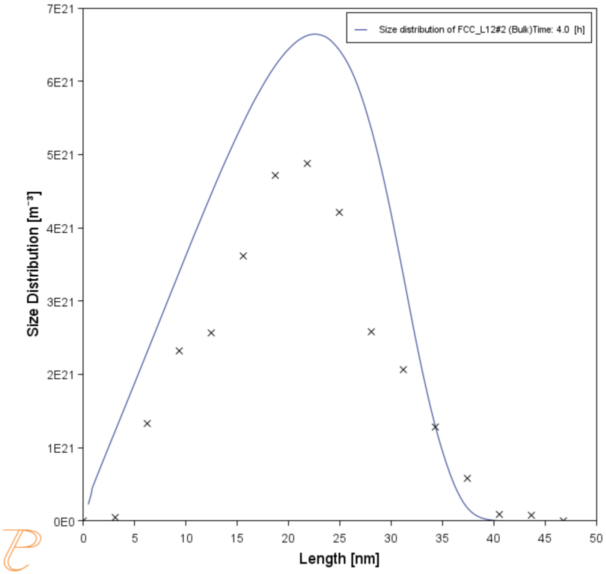


Figure 58: A comparison of the predicted and measured 2D size distribution after 4 h of aging.

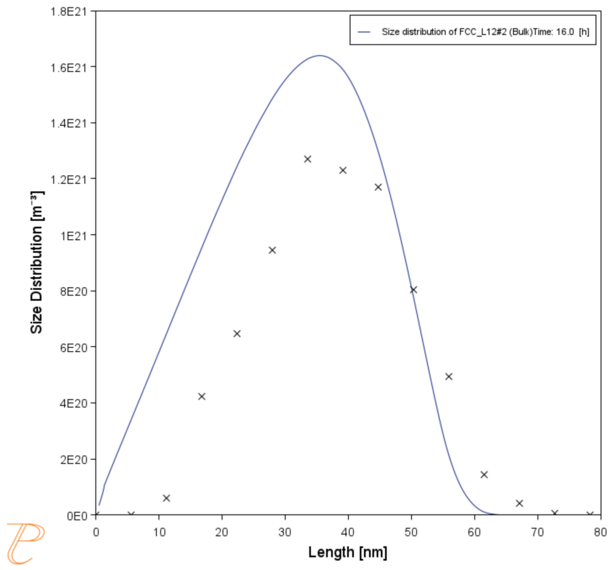


Figure 59: A comparison of the predicted and measured 2D size distribution after 16 h of aging.

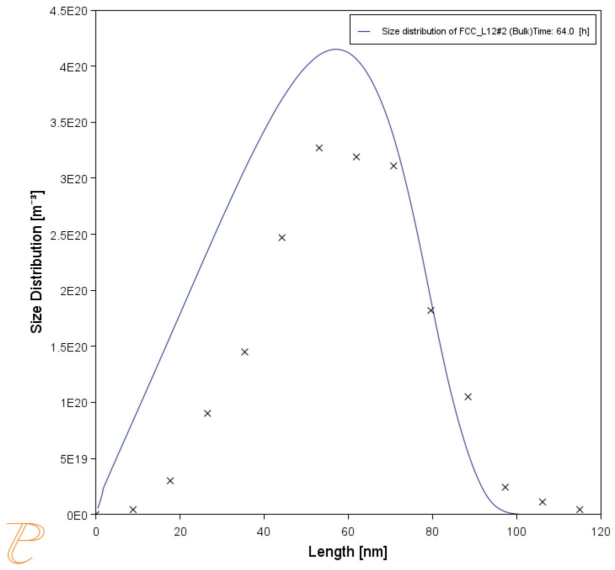


Figure 60: A comparison of the predicted and measured 2D size distribution after 64 h of aging.

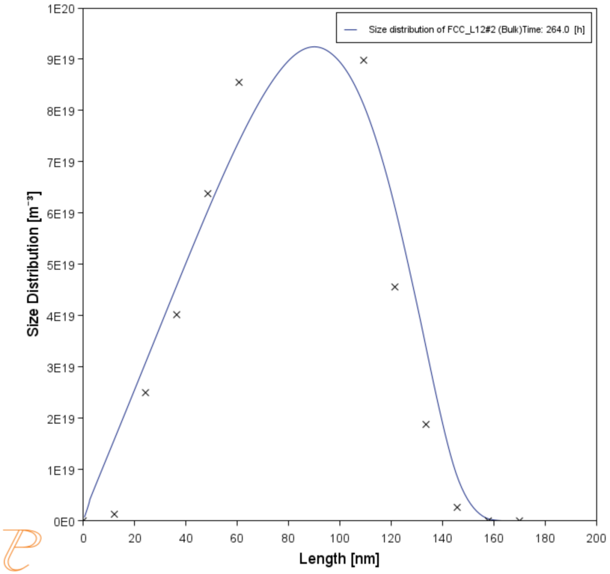


Figure 61: A comparison of the predicted and measured 2D size distribution after 264 h of aging.

Reference

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