Release Notes:

Thermo-Calc Software Package and Databases

Version 2023a

Contents

Thermo-Calc Version 2023a Highlights

Highlights

★ Thermo-Calc:

- New dark mode
- Full gas description added to many major databases for use with calculations
- New evaluation method for many Scheil properties

★ Property Models and Model Libraries:

- Energy addition for T-Zero Temperature Property Model
- New homogenization functions for Freeze-in Temperature Models
- Updates to the Steel Model Library CCT and TTT Property Models to include new quantities and to automatically detect the most-probable type of carbide in pearlite and bainite

★ Precipitation Module (TC-PRISMA):

- New para-equilibrium automatic growth rate model available to handle the smooth transition for para-equilibrium and local equilibrium

★ Databases:

- New thermodynamic databases for oxides (TCOX12) and titanium (TCTI5)
- New kinetic databases for zirconium (MOBZR1) and high entropy alloys (MOBHEA3)
- Updated high entropy (TCHEA6.1), aluminum (TCAL8.2), and copper (TCCU5.1) thermodynamic databases
- Updated kinetic titanium (MOBTI4.1) database

★ Additive Manufacturing Module (Beta Release):

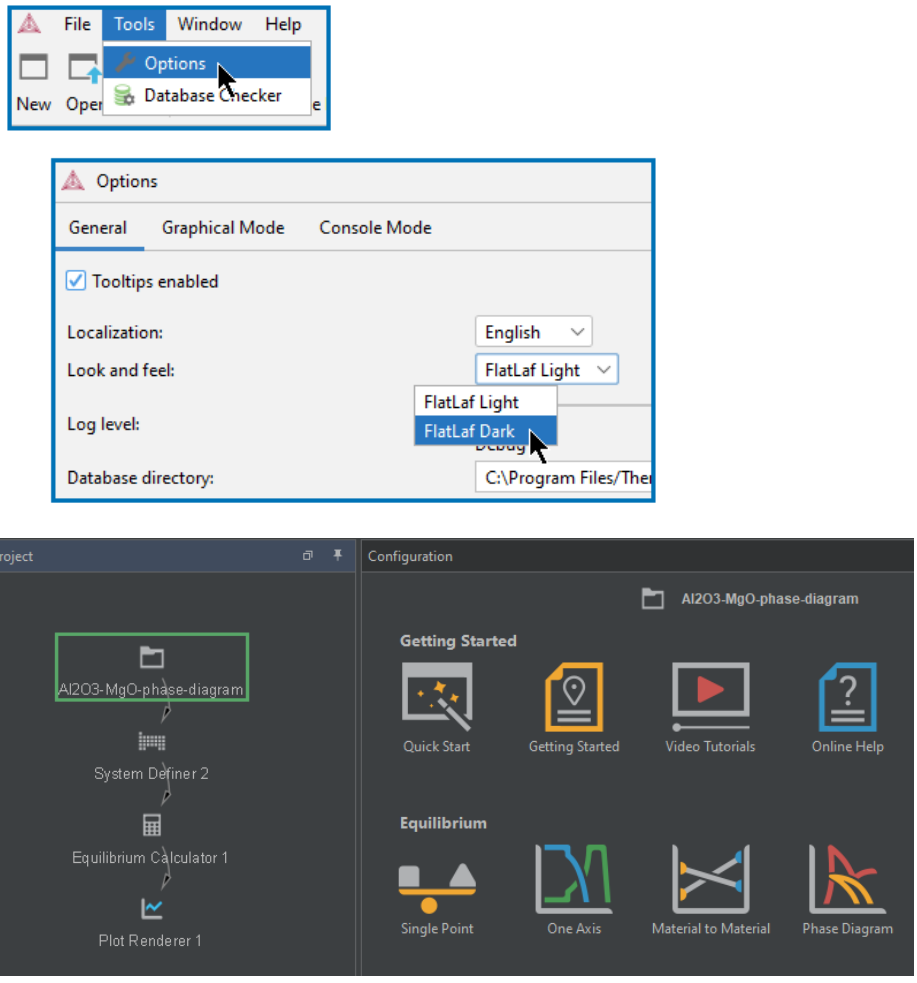
- The Additive Manufacturing Module is currently in closed-beta testing. It will be available for purchase as an Add-on Module in Thermo-Calc and is scheduled for release in June 2023 (version 2023b). A beta version is included with the 2023a installation. You are able to add the new AM Calculator node and template, as well as apply settings, but you cannot calculate any results.

Thermo-Calc

New Dark Mode

A new dark mode is available for the Graphical User Interface (GUI). This much requested feature is available as a new *Look and feel* called FLATLAF Dark. For many users, this interface can make it easier on the eyes and offer better visibility. Change the interface to the new dark mode from the **Tools > Options** menu, then on the **General** tab, select **FlatLAF Dark** from the list.

Also as of this release, there are only two *Look and feel* options available: The default **FlatLAF Light** and the new **FlatLAF Dark**. The options Metal, Nimbus, CDE/Motif, Windows, and Windows Classic are now deprecated.



Switch to the new dark mode from the Options window. An example of what dark mode looks like on the Project and Configuration windows.

Full Gas Descriptions in Most Major Databases

Over the past several years, we have been working to add full gas descriptions to all major databases. With the full gas description incorporated in each database, you can do several simulations without needing to append the gas description from other databases such as the STGE SSUB Substances Database, and thus reduce or eliminate complication and incompatibility issues.

The benefits include:

- Simulating the gassing and degassing processes.
- Calculating the temperature and enthalpy of evaporation.
- Calculating the evaporation properties in a Scheil simulation.

Starting with the 2023a release, full gas descriptions are available with:

- TCOX12: Metal Oxides Solutions Database
- TCTI5: Ti/TiAl-based Alloys Database
- Demo database OXDEMO (from this release v 4.0)

The following databases already have the full gas descriptions available starting with the indicated version in brackets:

- TCNI12: Nickel-based Superalloys Database (from v 12.0)
- TCCU5: Copper-based Alloys Database (from v 5.0)
- TCSLD4: Solder Alloy Solutions Database (from v 1.0)
- TCUHTM1: Ultra-high Temperature Materials Database (from v 1.0)
- TCZR1: Zr-based Alloys Database (from v 1.0)
- TCHEA6: High Entropy Alloys Database (from v 6.0)
- TCMG6: Mg-based Alloys Database (from v 6.3)
- Demo database NIDEMO (from v 1.0)

New and Improved Scheil Features

In preparation for the upcoming full release of the new Additive Manufacturing Module in 2023b, some Scheil features are implemented in this release. In addition, a new evaluation method is implemented for many Scheil properties. These changes also have applications to users working with multiphysics solidification simulations in general, where as-cast material properties are needed in the temperature range from room temperature up to evaporation temperature.

New Evaluation Method for Many Scheil Properties

The way properties are evaluated in the Scheil Calculator is improved for several properties. The new evaluation method uses an average of the “frozen-in” profile that considers all previous calculation steps for each step of the simulation.

In previous versions, the solid properties at each step in a Scheil calculation only evaluated the part that was solidified at that step. The portion of the material that had already been solidified was not considered. This method works well for thermodynamic calculations and some properties calculations. However, several of the new properties recently added to the software require this new method.
The properties using the new method are:

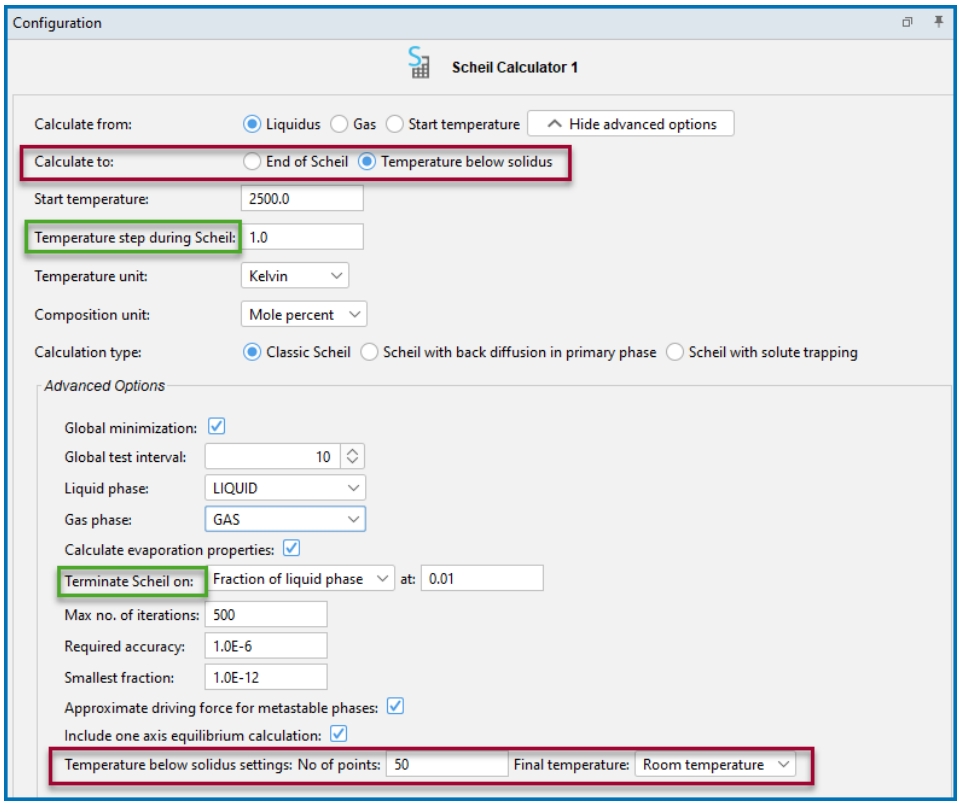
- Thermal conductivity, resistivity, and diffusivity
- Electrical conductivity and resistivity
- Heat per mole/gram,
- Apparent heat capacity per mole/gram
- Density
- Molar volume
- Apparent volumetric thermal expansion coefficient

Temperature Below Solidus

There are new settings available to calculate solid state properties at temperatures below the solidus temperature, using the phase compositions and fractions from Scheil calculations. The calculation is performed at a set number of temperatures between the solidus temperature and a lower temperature, which is by default set to room temperature. The end temperature and the number of points can be changed.

- In Graphical Mode, the settings are added to the main Configuration window (*Calculate to*) as well as additional settings under Advanced Options (*Temperature below solidus settings*). Two other settings have adjusted wording—Temperature step *during Scheil* and Terminate *Scheil* on.
- In Console Mode a new command is added called `CALCULATE_BELOW_SOLIDUS`.
- In TC-Python and TC-Toolbox for MATLAB® this feature can be turned on with `calculate_to_temperature_below_solidus` under `ScheilOptions`.

Temperature below solidus additions and changes to the Graphical Mode Scheil Calculator Configuration window. Red areas are new settings, green is text that is updated to be clearer about the use. Note that some settings are under Advanced Options.



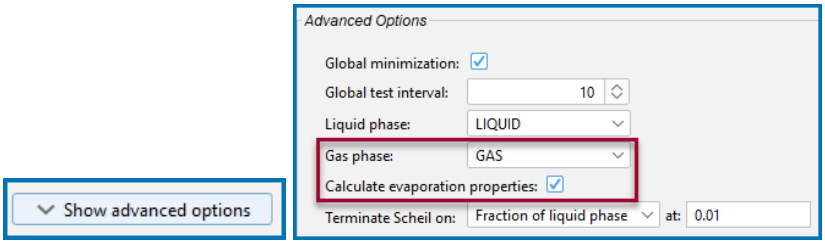
Evaporation Properties Above Liquidus

In Graphical Mode, an option is added to the Scheil Calculator under the *Advanced Options* section to calculate three new evaporation properties: Molar mass of gas, driving force for evaporation, and evaporation enthalpy.

In the Console Mode Scheil module, the command is called `CALCULATE_EVAPORATION_PROPERTIES`.

In TC-Python and TC-Toolbox for MATLAB® this option can be turned on with `enable_evaporation_property_calculation` under `ScheilOptions`.

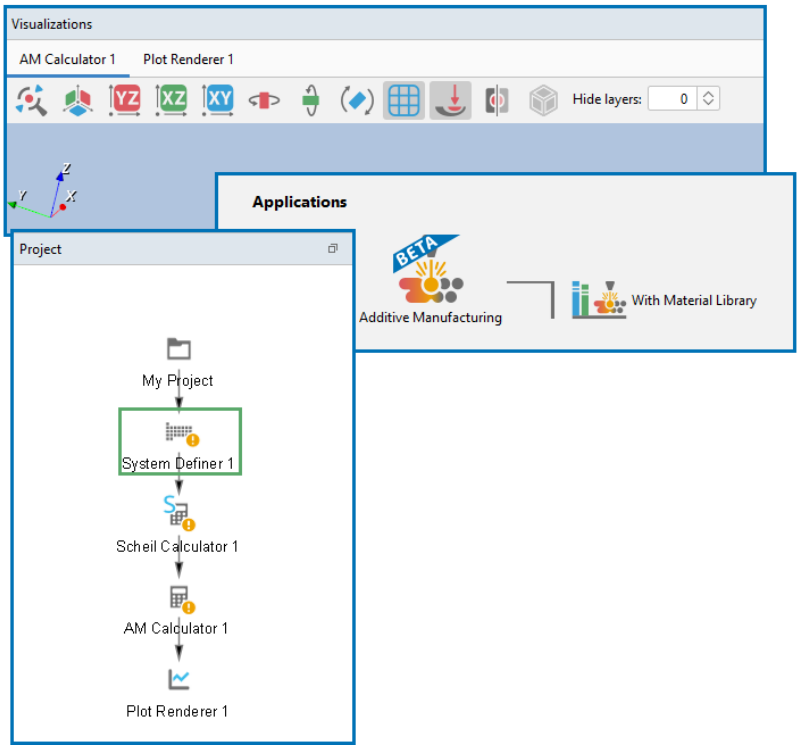
A gas phase is required to calculate these properties.



*For Graphical Mode, on the Scheil Calculator Configuration window, click **Show advanced options** to locate the settings.*

Graphical Mode Results Window Renamed to Visualizations

In connection to the upcoming release of the Additive Manufacturing Module in 2023b, the **Results** window in Graphical Mode is renamed to **Visualizations**. This will accommodate the new ability to visualize and work with the design configuration and set up before *and* after a calculation is performed. Nothing has changed with respect to how plots are displayed for the existing features and calculators after a calculation is performed.



*The **Results** window is now called **Visualizations**. You can take a sneak peek at the upcoming set up for the new Additive Manufacturing Module by adding an **Additive Manufacturing** template under Applications.*

Additive Manufacturing Module - Closed Beta Release

The Additive Manufacturing Module is currently in closed-beta testing. It will be available for purchase as an Add-on Module in Thermo-Calc and is scheduled for release in June 2023 (version 2023b)

The Module is primarily designed for modeling the powder bed fusion process in Additive Manufacturing. Special focus has been to have a unified treatment of alloy dependent material properties and process parameters when solving the multiphysics problem of a moving heat source that melts and solidifies metal powder. The multiphysics simulation involves thermal conduction, fluid flow, evaporation-, radiation- and convective-heat loss.

A beta version is included with your installation. You are able to add the new AM Calculator node and template, as well as apply settings, but you will not be able to calculate any results.

You can learn more about the upcoming Additive Manufacturing Module on our website. Or sign up to our newsletter to be one of the first to learn more about this exciting new addition to our product line.

Features Already Available in 2023a

In preparation for the upcoming full release of the new Module, some Scheil features are implemented in 2023a. This includes Scheil with temperature below solidus and calculation of three new evaporation properties: Molar mass of gas, driving force for evaporation, and evaporation enthalpy. In addition, there is the update to include full gas descriptions in most major databases and the Results window is renamed to Visualizations.

Note that except for periphery features (such as the new Scheil features and renamed Results window) there is no documentation specifically about the Additive Manufacturing Module included in the help at this time.

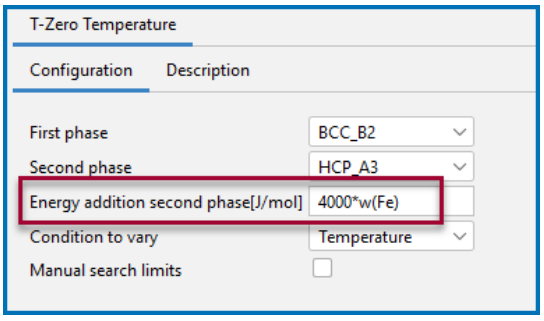
Thermo-Calc Property Models and the Property Model Calculator

Below are improvements and bug fixes for the Property Models included with Thermo-Calc and available with the Property Model Calculator. Some items are also included in the Thermo-Calc Improvements and Bug Fixes section.

T-Zero Temperature Property Model

New Energy Addition for T-Zero Temperature Martensite Calculations

For the Graphical Mode Property Model, *T-Zero Temperature*, you can now include an energy barrier for martensitic phase transformations. There is a new field **Energy addition second phase** where the Gibbs energy addition to the second phase of the T-Zero calculation is entered.



New Example for T-Zero Martensite Energy Addition

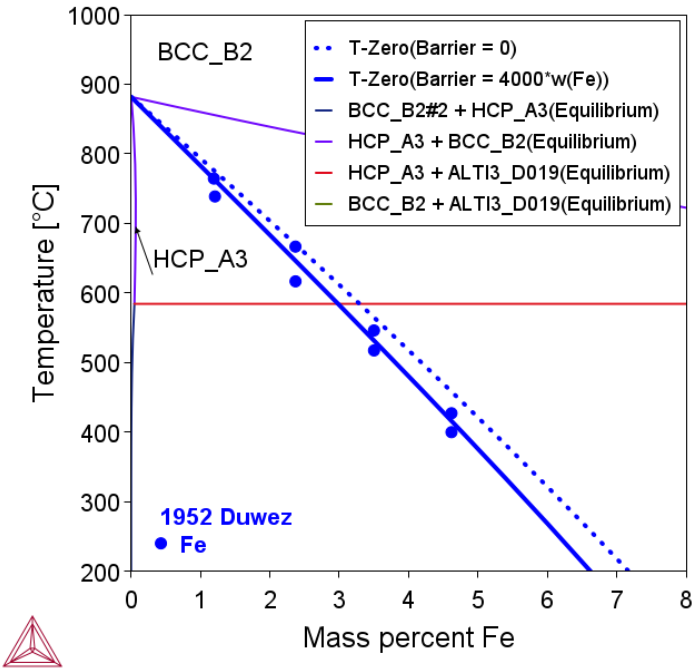
There is a new General Property Model example that uses the new energy addition setting for the martensitic BCC → HCP transformation for a binary Ti-Fe system.

There are different ways to open the examples folder:

- From the menu in Thermo-Calc choose **Help > Example Files**
- Click the top level **My Project** node then on the **Configuration** window click the **Example Files** button.

Then from the **> Property Models > General** folder select **PM_G_14_Ti_Fe_T-Zero_Martensite.tcu**

Note that a license for the TCS Ti/TiAl-based Alloys Database (TCTI) is needed to run the example.



*Dotted blue line is the T-Zero temperature without energy addition, the solid blue line is the T-Zero temperature with an energy addition of 4000*w(Fe) [J/mol], that well reproduces the experimental data.*

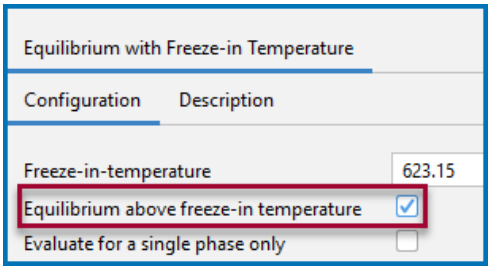
Equilibrium with Freeze-in Temperature Property Models (General and Nickel)

The feature settings described in this section are for the Property Models *Equilibrium with Freeze-in Temperature* (under the **General** models), available to all users, and *Equilibrium with Freeze-in Temperature - Ni* (under **Nickel Models**), which requires a licence to the Nickel Model Library.

New Equilibrium Above Freeze-in Temperature Setting

A new default setting is available on the Configuration windows for both the General and Nickel Property Models. Typically, freeze-in of the microstructure occurs during cooling of a material where equilibrium can be assumed above the freeze-in temperature. The new setting is the **Equilibrium above Freeze-in-temperature** checkbox, which is selected by default. In cases where the frozen structure should be evaluated at a higher temperature than the freeze-in temperature, you can click to clear the checkbox.

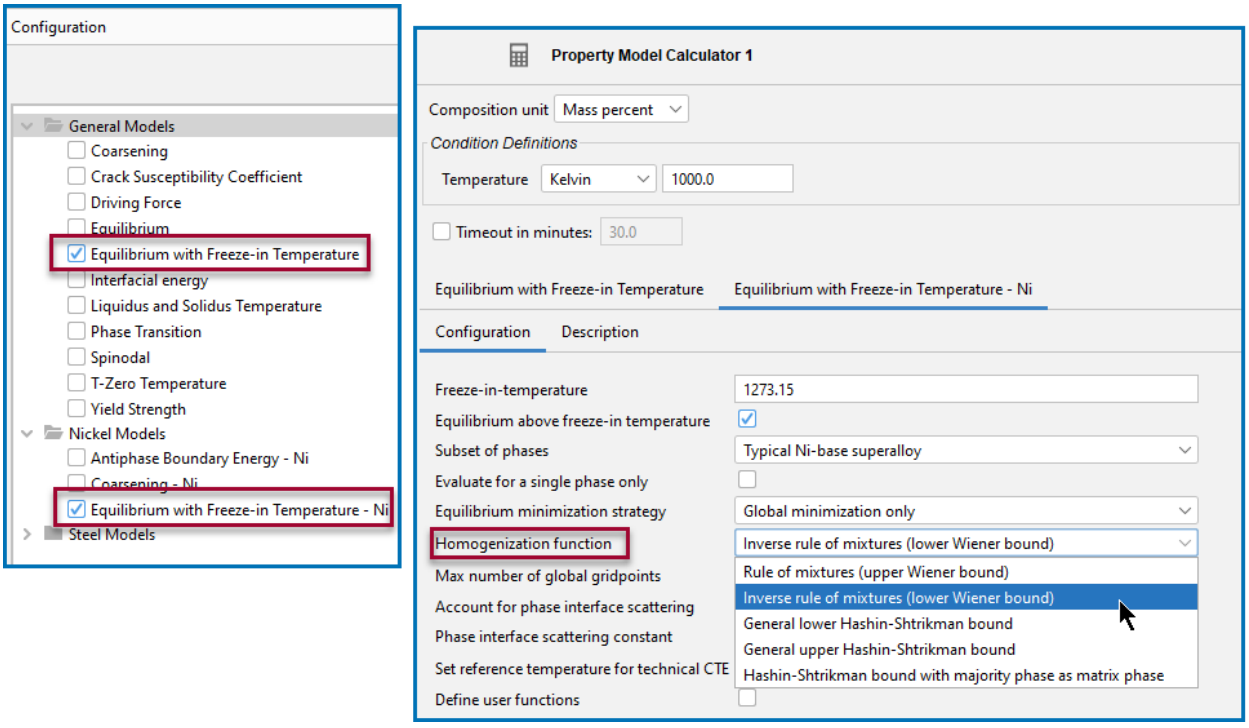
The previous versions of these models used the freeze-in-temperature equilibrium to evaluate the properties for temperatures both below and above the freeze-in-temperature.



New Homogenization Functions

For the *Equilibrium with Freeze-in Temperature* Property Models a selection of homogenization functions is available for the evaluation of thermal- and electric-properties. Thermal and electric properties depend on the microstructure and the geometrical representation of phases in the microstructure can be linked to different homogenization functions. The homogenization function is applied on thermal- and electrical-resistivity. The electric conductivity, thermal conductivity, and thermal diffusivity are evaluated from the resistivities.

The homogenization function settings are for the Property Models *Equilibrium with Freeze-in Temperature* (under the **General Models**), available to all users, and *Equilibrium with Freeze-in Temperature - Ni* (under **Nickel Models**), which requires a licence to the Nickel Model Library.



Yield Strength Property Model

These improvements and bug fixes are completed for the *Yield Strength* Property Model available with the Property Model Calculator.

- The Precipitate Size Distribution (PSD) as calculated by the Precipitation Module (TC-PRISMA) is now used for Yield Strength calculations after the simulation.
- Yield Strength after a Precipitation Calculator simulation is calculated only for a selected number of timesteps. The time steps for which Yield Strength is calculated is determined by the rate of change in precipitate volume fraction and/or precipitate radius.

Phase Transition Property Model

The *Phase Transition* Property Model has a bug fix. Previously, the model returned *Temperature* or *Composition* in Mass%, Mass fraction, Mole% or Mole fraction, depending on which condition was relaxed. The return quantity was sometimes converted to a unit corresponding to what was set in the Property Model Calculator. Now it always returns *Temperature* in Kelvin or Mass%, which now makes it possible to convert the result to other units in plots and tables.

Thermo-Calc Improvements and Bug Fixes

Below are various improvements and bug fixes related mostly to the main Thermo-Calc features unless otherwise indicated. Also see some items listed for the Yield Strength Property Model and Phase Transition Property Model.

Reduce Loading Times when Creating Templates and Opening Projects

- Fixed an issue where the Property Models sometimes did not load correctly, causing errors in logs.
- Fixed an issue for macOS where some calculations caused an error: `se.thermocalc.core.CalculationEngineException: java.nio.file.NoSuchFileException`.
- In some cases, calculations on disc were not cleaned from temporary files and/or left hanging processes. This behaviour is now improved where possible.
- Fixed a bug which could cause a Scheil calculation to hang at start when running from TC-Python or Graphical Mode.

Graphical Mode Only

Calculation Related

- Scheil Calculator is refactored to have caching enabled.
- Fixed an issue for the Property Model Calculator, Process Metallurgy Calculator, and Material to Material Calculator where the caching mechanism picked up the wrong result and the plot reflected the second result instead of the first when multiple changes were made to the calculation. i.e. the problem sometimes happened with a particular sequence of events. For example, a first set of calculations is performed and plotted, then the calculation settings are adjusted. Then the second set of calculations is performed and plotted, but if you revert to the original settings, the results would not update correctly.
- Fixed an issue related to re-performing an uncertainty calculation in the Property Model Calculator or Process Metallurgy Calculator, where previously no new randomized dataset was created.

Plotting Related

- Fixed a memory leak in the 3D plotting. Creating a 3D plot could cause excessive memory usage in Thermo-Calc 2022b. 2023a instead uses a CPU-based rendering backend instead of the GPU-based that introduced the problem in 2022b.
- Improved performance in regard to user interactions in the Property Model Calculator, Process Metallurgy Calculator and these plot types.
- Composition sets created during a material to material calculator not selectable for plotting.

Both Graphical and Console Mode

Plotting Related

- When in plot properties *Plot Area Size* section, and the "Fit plot area to a square…" button is selected AND the "Scale plot attributes using the system scaling factor" checkbox is NOT selected, the saved image now has the same dimension as the fixed plot area size has with a height and width of 600.
- Improved performance when plotting surface tensions.
- In batch/probability calculations in the Property Model Calculator, the lines are not added to the plot when line width changes, and the data points are always shown even if no data points marker is selected.

Calculation Related

- Increased a limit which allows more than 1000 phase regions in a phase diagram mapping.

General or Other

- The 3rd party dependency Apache commons-text is now updated to the latest (1.10.0) version, which has no known security problems.
- Fixed an issue with opening files with UNC paths.
- Support IPv6 only network environments.

Console Mode

Plotting Related

- Revision of conditions to show axis values in scientific format automatically so that the positive and negative numbers show the same behaviour.
- Fixed an issue that caused repeated tabulation of the variables NS, BS, and NN to change values.

Database Related

- `List-Data` command with GES6 now ignores V-parameters from the PARROT module.

General or Other

- Fixed a bug where starting a stand-alone console with a file argument works again.

Property Model Libraries

Visit the Steel Model Library and Nickel Model Library on the website to learn more about these sets of Property Models designed to help experts working with steel and nickel, respectively.

Nickel Model Library

Below are details about the **Nickel** Property Models included with Thermo-Calc with the addition of a licence for the Nickel Model Library.

Equilibrium with Freeze-in Temperature Property Model

See Equilibrium with Freeze-in Temperature Property Model (General and Nickel) for two new settings available to both the General and Nickel Property Models.

Coarsening-Ni Property Model

Fixed a calculation error that occurred for some Ni alloys in the *Coarsening-Ni* Property Model.

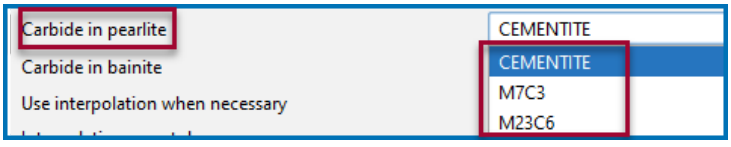
Steel Library

Below are details about the **Steel** Property Models included with Thermo-Calc with the addition of a licence for the Steel Model Library.

CCT and TTT Diagram Property Models

Custom Carbide Calculation Settings

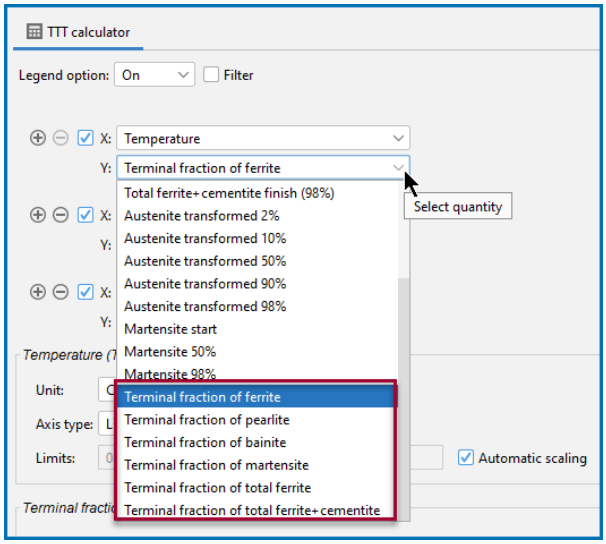
The software now automatically detects the most-probable type of carbide in pearlite and bainite. This selection option is for the *CCT Diagram* and *TTT Diagram* Property Models where two new sections are available as **Custom** calculation settings: **Carbide in pearlite** and **Carbide in bainite**. This allows for the choice of carbide to be present in the pearlite and bainite, respectively. These new selections are particularly useful for steels with higher Cr contents, where now one can select M7C3 and M23C6 to be the carbide in pearlite, and M7C3 for bainite.

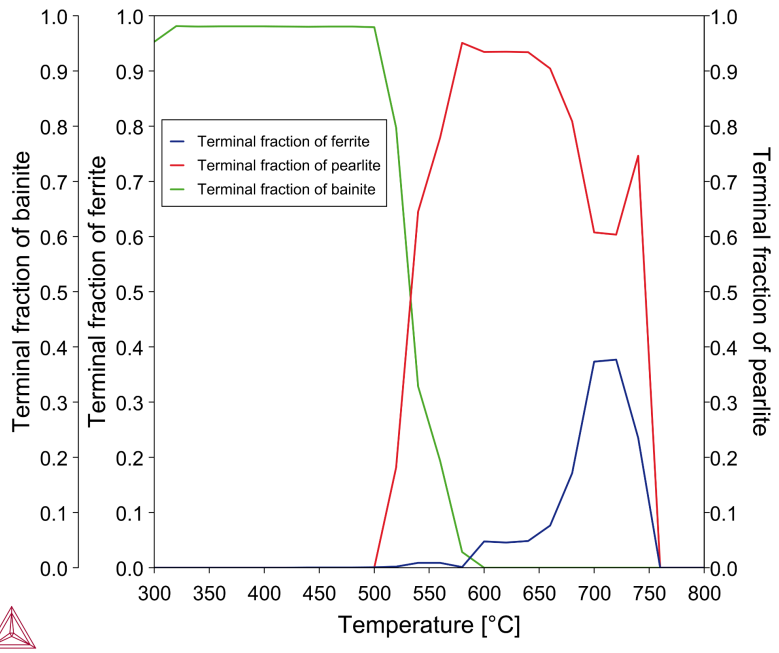


New Result Quantities and Updated Examples

Nine new result quantities are added to the *CCT Diagram* and *TTT Diagram* Property Models:

- *Austenite transformed 10%*, *Austenite transformed 90%*, and *Total ferrite+cementite finish (98%)*. For CCT these are both defined in time (t) and temperature (T), and for TTT as time (t) quantity only.
- *Terminal fraction of ferrite*, *Terminal fraction of pearlite*, *Terminal fraction of bainite*, *Terminal fraction of martensite*, *Terminal fraction of total ferrite*, and *Terminal fraction of total ferrite+cementite*. Terminal fractions are unit-free quantities.
- Examples *PM_Fe_06_Fe-C-Mn-Si-Cr-V_TTT.tcu* and *PM_Fe_08_Fe-C-Mn-Si-Cr-V_CCT.tcu* are updated to include these new quantities. These examples are available in the **> Example Files > Property Models > Steels** folder.





The plot from example PM_Fe_06 now also includes the terminal fractions quantities for bainite, ferrite, and pearlite, which are plotted against the cooling rate for the Fe-C-Mn-Si-Cr-V alloy. Example PM_Fe_08 is also updated.

Precipitation Module (TC-PRISMA)

Visit the Precipitation Module (TC-PRISMA) on the website to access resources such as training videos, publications, application examples, and much more.

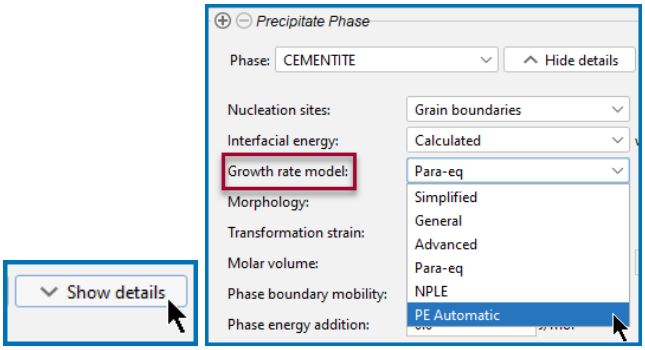
Handle Smooth Transition Para-equilibrium and Local Equilibrium

New Para-equilibrium (PE) Automatic Growth Rate Model

A new growth rate model is available—the *Para-equilibrium (PE) Automatic Growth Rate Model*, or *PE Automatic* for short. It is available with the Precipitation Calculator and a new example and companion video is included with the installation.

The tempering of martensite in steels induces the precipitation of cementite particles. The growth kinetics initially follows the Para-Equilibrium (PE) condition due to the fast diffusion of interstitial C, and gradually transforms to regular Local Equilibrium (LE), known in Thermo-Calc as 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 (*Para-eq*) 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 paraequilibrium and ortho-equilibrium.

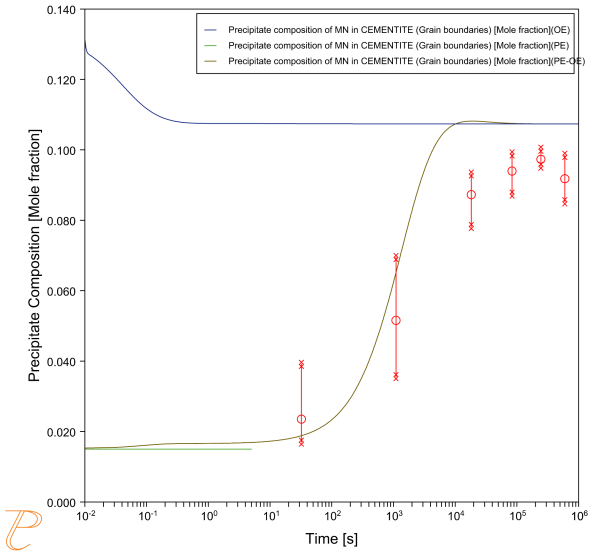


*Click **Show details** to toggle and view the **Growth rate model** list. Then the **PE Automatic** model is available under the Precipitate Phase settings on the Precipitation Calculator.*

New Example and Video: Smooth Transition from Paraequilibrium to Ortho-equilibrium

In this new 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; the paraequilibrium (PE) condition; and a smooth transition from the paraequilibrium (PE) to the ortho-equilibrium (OE) condition. The example *P_15_Precipitation_Fe-C-Mn_PE-OE_Precipitation_of_Cementite.tcu* is available in the **> Example Files > Precipitation Module (TC-PRISMA)** folder.

There is also a companion video showing the step-by-step setup of this example. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or you can go to the website or our YouTube channel.



Comparing calculated Mn composition in cementite from Simplified (OE), Para-eq (PE), and PE Automatic (PE-OE) growth models.

Improvements and Bug Fixes

See Yield Strength Property Model.

Diffusion Module (DICTRA)

Visit the DIffusion Module (DICTRA) on the website to access resources such as a tutorial, training videos, publications, application examples, and much more.

Improvements and Bug Fixes

Some items are also included in the Thermo-Calc Improvements and Bug Fixes section.

Both Console and Graphical Mode

- Resolved an issue causing incorrect values for QI and FI if diffusing and gradient elements differ.
- Fixed an issue in POLY-3 which crashed after calculating intrinsic diffusivities for phases without vacancies.
- Resolved an issue that could cause the application to crash or consume too much memory. That could happen when switching boundary conditions, and/or the simulation switched back and forth to the homogenization model.

Console Mode Only

- Fixed the Console Mode command, INPUT_SCHEIL_PROFILE, which now sets the majority element as dependent, instead of the last read.
- Fixed a bug in the auto-generated column in tables in the POST module.
- Fixed several issues related to DICTRA cell calculations.

Process Metallurgy Module

Visit the Process Metallurgy Module on the website to access resources such as training videos, publications, application examples, and much more.

Improvements and Bug Fixes

- The configured “transfer of phase group” rate is now exactly maintained even if the mass transfer coefficient is large.

Also see the TCS Metal Oxide Solutions Database (TCOX12) section. The following is updated in the Process Metallurgy Module to match the changes made to the new version of the database.

- Introduced support for TCOX12, which now includes new gas constituents.
- Handle BO3-3 added to TCOX12.

TC-Python API and TC-Toolbox for MATLAB®

Improvements and Bug Fixes

Some items are also included in the Thermo-Calc Improvements and Bug Fixes section.

- Added a method `get_name` to the enum ProcessDatabase - this is especially useful to determine the actually used database if using the “latest” one.
- Improve error handling of additions with invalid composition.
- *TC-Toolbox only*: Fixed the functions `GrainGrowthModel.fixed_grain_size()` and `GrainGrowthModel.grain_growth()` in the Precipitation package that were failing with an error.

Legacy TC-Toolbox for MATLAB®: Deprecation with Version 2023a

The legacy version of TC-Toolbox for MATLAB® is no longer supported as of Thermo-Calc version 2023a (December 2022) and users are encouraged to migrate scripts to the new TC-Toolbox.

Legacy TC-Toolbox for MATLAB® documentation is no longer available in the Thermo-Calc help. Legacy documentation as a PDF is available from the website Documentation archive. It is also available with any previously installed version of Thermo-Calc (2022b and earlier).

Removed Functions in TC-Python and TC-Toolbox - Deprecation with 2023a

The following functions are renamed, and the old versions are removed in this release 2023a. Users are required to update any scripts to the latest.

Old Name	New Name
`set_grain_radius`	`with_grain_growth_model(GrainGrowthModel.fixed_grain_size)`
`set_grain_aspect_ratio`	`with_grain_growth_model(GrainGrowthModel.set_grain_aspect_ratio)`
`density_of_solid_phase`	`density_of_phase`

New Thermodynamic and Kinetic Databases

All the thermodynamic and kinetic databases have dedicated web pages where new and updated Technical Information and Example Collections are available in addition to links to examples, publications, webinars, and many other resources can be found.

TCS Zr-alloys Mobility Database (MOBZR1)

The TCS Zr-alloys Mobility Database (MOBZR) is a kinetic database containing mobility data for Zr-based alloys. Data is present in a format suitable for simulation of diffusion controlled phenomena using the add-on Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA). It can also be used together with any Thermo-Calc programming interface such as TC-Python.

TCS Zr-alloys Mobility Database (MOBZR) is intended for use in combination with the TCS Zr-based Alloys thermodynamic database, which is currently at version 1 (TCZR1).

Together with the Diffusion Module and TCZR1, you can use the database to study diffusion-controlled phenomena in zirconium alloys, e.g. microsegregation during solidification, homogenization kinetics, growth/dissolution kinetics of precipitates, interdiffusion, and so forth. You can also use it with the Precipitation Module to simulate concurrent nucleation, growth, and coarsening of precipitates in Zr-based alloys.

- Included elements (8): Cr, Fe, Nb, Ni, Sn, O, H, Zr (the same as with TCZR1)
- Included phases: BCC_A2, HCP_A3 and LIQUID

- Assessed systems (BCC_A2 and HCP_A3): The unary systems and some of the binaries (Cr-Fe, Cr-Ni, Cr-H, Fe-H, Fe-Ni, Fe-O, Nb-H) already exist in the other mobility databases. The mobility parameters were tested for compatibility and combined with the assessments. Mobility parameters for the Zr-Cr, Zr-Fe, Zr-H, Zr-Nb, Zr-Ni, Zr-O, and Zr-Sn systems have been assessed.

TCS Metal Oxide Solutions Database (TCOX12)

New Elements and Related Binary, Ternary, and Higher Order Systems

- Added three new elements: B, Hf, and Yb. Now it is a 32 element framework.
- Added Hf: Assessed or added from literature 24 binary, 11 ternary, and 8 higher order systems.
- Added Yb: Assessed or added from literature 24 binary, 10 ternary, and 8 higher order systems.
- Added B: Assessed or added from literature 20 binary, 21 ternary, and 12 higher order systems.

New Assessed Systems

Cu-F-O	Cu-K-O	F-Na-O-Si	F-K-O-Si
Ca-F-Fe-O-Si	Ca-F-K-O-Si	Ca-F-Na-O-Si	$NaF-SiF_4$
Na-Si-F-O	$CaCO_3$-$MgCO_3$	$CaCO_3$-$FeCO_3$	$FeCO_3$-$MgCO_3$
Nb_2O_5-ZrO_2	Al_2O_3-TiO_2-ZrO_2	Gd_2O_3-La_2O_3-ZrO_2	Cr_2O_3-MgO-SiO_2
MnO-SiO_2-TiO_2	TiO_2-Y_2O_3-ZrO_2	CaO-Gd_2O_3-ZrO_2	Al_2O_3-CaO-Gd_2O_3
Al_2O_3-Fe-O-Y_2O_3	Al_2O_3-CaO-SiO_2-Y_2O_3		

Reassessed Systems

Al_2O_3-CaO	Al_2O_3-CaO-SiO_2	Al_2O_3-CaO-FeO_x	Al_2O_3-CaO-MgO
Al_2O_3-CaO-Y_2O_3	Al_2O_3-Na_2O-SiO_2	Al_2O_3-CaO-FeO_x-SiO_2	Al_2O_3-CaO-MgO-SiO_2
Al_2O_3-CaO-Na_2O-SiO_2	Cu-F	Ca-F-Mn	Al-O-V
Fe-Na-O	Al_2O_3-SiO_2-TiO_2	Reassessed ZrO_2-mono/tetra T0 for • ZrO_2-Al_2O_3 • ZrO_2-Gd_2O_3 • ZrO_2-Y_2O_3.	

Other Changes

- Extended the GARNET phase description.
- Included complete gas description.

TCS Ti/TiAl-based Alloys Database (TCTI5)

- Updates to Ti-Al-B, Ti-Al-C, Ti-Al-Cr, Ti-Al-Mo, Ti-Al-Nb, Ti-Al-O, Ti-Al-Si, Ti-Al-Sn, Ti-Al-W, and Ti-Al-Zr.
- Modeled the Ti-Si-Zr ternary system.
- Full gas descriptions are added.
- There is a change to default settings. From this release, the GAS phase is restored by default when retrieving the data from the database. In order to reject it when it is not required for a calculation, you have to now manually reject it.

The following volume parameters are updated for:

- Liquid in Ti-V and Ti-Al-V
- AlTi3_D019 in Ti-Al-O
- BCC_A2 in Ti-H
- HCP_A3 in Ti-O and Ti-N

TCS High Entropy Alloy Mobility Database (MOBHEA3)

- Atomic mobility parameters for all BCC_A2 binary systems have been assessed or estimated and then updated.
- The database was validated in the Fe-Ti, Zr-Nb-Ta-Ti, Zr-Nb-Hf-Ti and Al-Fe-Cr-Mn-V systems.

Updated Thermodynamic and Kinetic Databases

TCS High Entropy Alloys Database (TCHEA6 Updated to v 6.1)

Reassessed Binary, Ternary, and Quinary Systems

- Binary: Two reassessments, Cr-Mn and Ir-Nb.
- Ternary: Seventeen (re-)assessments: Al-Cr-V, Co-Cr-Fe, Co-Cr-Mn, Co-Cr-Ni, Co-Fe-Mn, Co-Fe-Ni, Co-Mn-Ni, Cr-Fe-Mn, Cr-Mn-Ni, Cr-Mo-Nb, Cr-Mo-Ti, Cr-Nb-V, Fe-Mn-Ni, Fe-Ni-W, Mo-Nb-V, Re-Nb-V, and Re-V-W.
- Quinary: Validation of the Co-Cr-Fe-Mn-Ni system in full temperature and composition space (7 isopleths).

TCS Al-based Alloy Database (TCAL8 Updated to v 8.2)

- Corrected an error in the molar volume of the B2 phase in the Al-Fe-Ni system.

TCS Cu-based Alloys Database (TCCU5 Updated to v 5.1)

- Corrected an error in the molar volume of the B2 phase in the Al-Fe-Ni system.

TCS Ti-alloys Mobility Database (MOBTI4 Updated to v 4.1)

- Modified the impurity diffusivity parameter of nitrogen in HCP_A3 titanium.

OXDEMO (Version 4)

OXDEMO version 4 is identical to TCOX12 for the elements included. These are all changes that affect the OXDEMO database:

- Reassessed CaO-Al_2O_3 and CaO-Al_2O_3-SiO_2 systems. Updated CaO-Al_2O_3-Fe-O, CaO-Al_2O_3-Fe-O-SiO_2 due to changes in CaO-Al_2O_3, CaO-Al_2O_3-SiO_2 systems.
- Added full gas description instead of the reduced one.
- Added surface tension.
- Updated viscosity and molar volume descriptions.
- Updated all metallic systems to be the same as in the TCFE database.
- Fixed an error in molar volume of FCC_A1 and BCC_A2 phases.
- Assessed $CaCO_3$-$FeCO_3$.
- Renamed the following phases: C1A1F2 -> A1C1F2, CF -> CAV2O4, CA2SIO4_ALPHA -> CA2SIO4_ALPHA_A.

Installation

Reminder for TDB Editor Installations to Update the Plugin

For anyone who installed the new TDB Editor (released with 2021a), you will need to update the plugin for this after installing a new version of Thermo-Calc. When Thermo-Calc is updated to a new version, VSCode should be updated too with the VSIX extension of the new release. This then includes the latest bug fixes and any other changes or improvements.

If VSCode is not updated with a new VSIX extension, it will continue to work as before with the language server of a previous release, as long as this release is not uninstalled. If the release is uninstalled, the VSIX extension (and thus the TDB Editor) will cease to work.

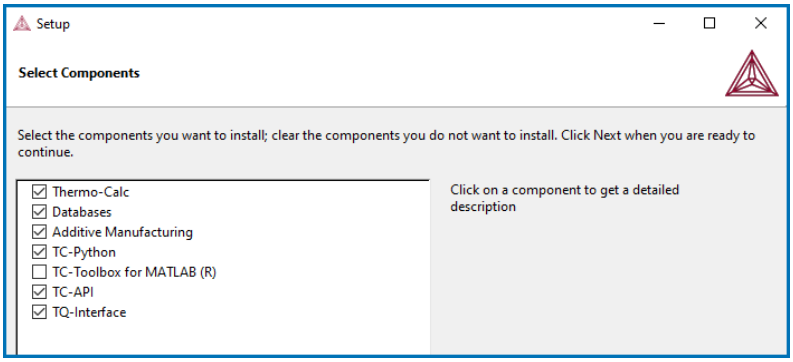
This installation is done after Thermo-Calc is installed. Search the help (press F1 in Thermo-Calc) for *Installing VSCode and the TDB Editor*.

Installation Changes

If you are doing a custom installation, there are changes to the Select Components window during installation. The Legacy TC-Toolbox is removed and Additive Manufacturing is included with the installation although it is currently in Beta mode only. See the *Thermo-Calc Installation Guide*, available from various places including our website.

See also

- Legacy TC-Toolbox for MATLAB®: Deprecation with Version 2023a
- Additive Manufacturing Module - Closed Beta Release



Documentation and Videos

In Thermo-Calc, press F1 to search the online help.

New Examples

These are the new examples:

- From the **> Example Files > Property Models >General** folder: *PM_G_14_Ti_Fe_T-Zero_Martensite.tcu.* The example uses the Property Model Calculator and the T-Zero Temperature Property Model to demonstrate the martensitic BCC ⟶ HCP transformation for a binary Ti-Fe system.
- From the **> Example Files > Thermo-Calc** folder: *T_17_Al2O3-MgO_phase_diagram.tcu.* This example uses an Equilibrium Calculator to calculate a phase diagram of the pseudo-binary system Al2O3-MgO. It also demonstrates how to change components in the System Definer.
- From the **> Example Files > Precipitation Module (TC-PRISMA)** folder: *P_15_Precipitation_Fe-C-Mn_PE-OE_Precipitation_of_Cementite.tcu.* In this example, precipitation of cementite during tempering of an Fe-Mn-C steel is simulated considering three interface conditions: the usual ortho-equilibrium (OE) condition; the paraequilibrium (PE) condition; and a smooth transition from the paraequilibrium (PE) to the ortho-equilibrium (OE) condition.

Updated Examples

- The TCSLD Examples Collection (figure 15, switched location of plot labels for Ag_3Sn and Cu_6Sn_5_HT). This was updated on the website in August 2022 and is included in the help as of 2023a.
- Steel Model Library, Property Model examples from the **Help > Example Files > Property Models > Steels** folder, PM_Fe_06_Fe-C-Mn-Si-Cr-V_TTT and PM_Fe_08_Fe-C-Mn-Si-Cr-V_CCT are both updated to include the new properties described in New Result Quantities.
- Most of the installed or application Process Metallurgy examples that use TCS Metal Oxide Solutions Database (TCOX) are updated to use the latest version of this database (TCOX12).

Videos

When in Thermo-Calc, from the menu select **Help** → **Video Tutorials**, or you can go to the Video Tutorials page on the website or our YouTube channel.

- Companion Video for P_15, see New Para-equilibrium (PE) Automatic Growth Rate Model
- The 2023a Release Overview video and blog are available on the website.

Platform Roadmap and System Requirements

For information about platforms being phased out visit our Roadmap for Platform Support.

For information about disk space requirements for installation and calculations, review the System Requirements page on our website.