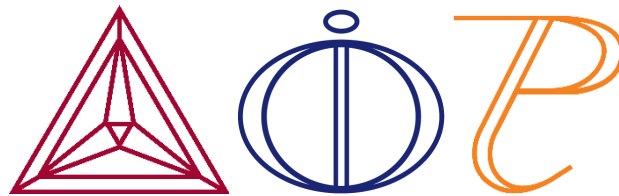




Release Notes:

Thermo-Calc Software Package and Databases

Version 2022b



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Thermo-Calc Version 2022b Highlights

Highlights

★ **Thermo-Calc**

- Improved look and feel throughout the graphical user interface
- New plot themes and several related plot improvements
- New calculation examples for thermophysical properties and a new additive manufacturing application example
- For Scheil simulations you can now calculate from the gas/liquid transition temperature
- Plus many additional bug fixes and improvements for all products

★ **Property Models and Model Libraries**

- In the Steel Model Library there is a new Ferrite Property Model and improved CCT and TTT
- Several improvements to the Yield Strength Property Model

★ **TC-Python and TC-Toolbox for MATLAB®**

- Process Metallurgy Module now available
- New timeout available for calculations

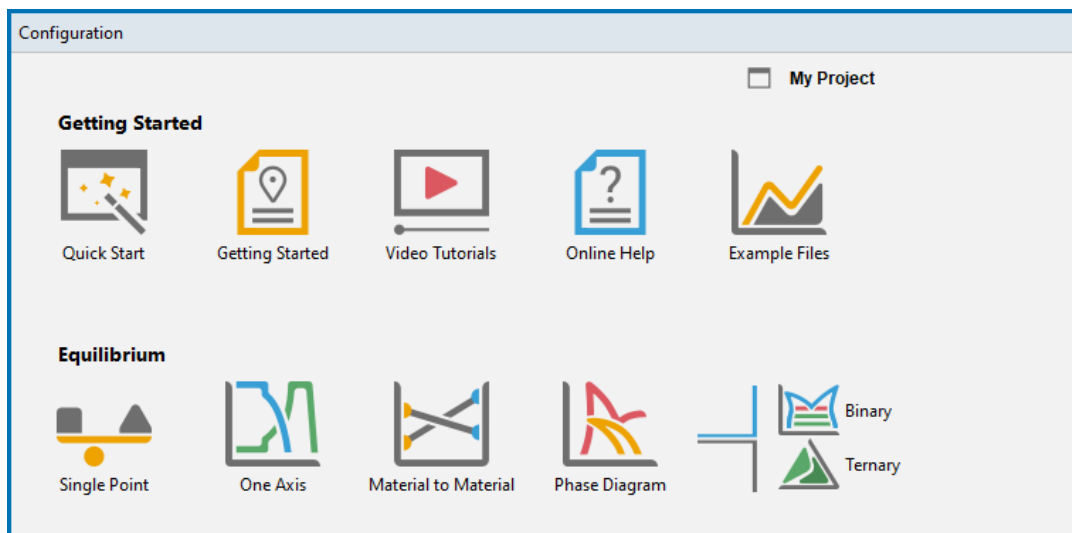
★ **Databases**

- New database for ultra-high temperature materials (TCUHTM1)
- New versions of databases for nickel (TCNI12 and MOBNI6), copper (TCCU5 and MOBCU5), high entropy alloys (TCHEA6), and nuclear materials (MEPH20 and NUCL20)
- Updated databases for solders (TCSLD4.2) and magnesium (TCMG6.3)

Thermo-Calc

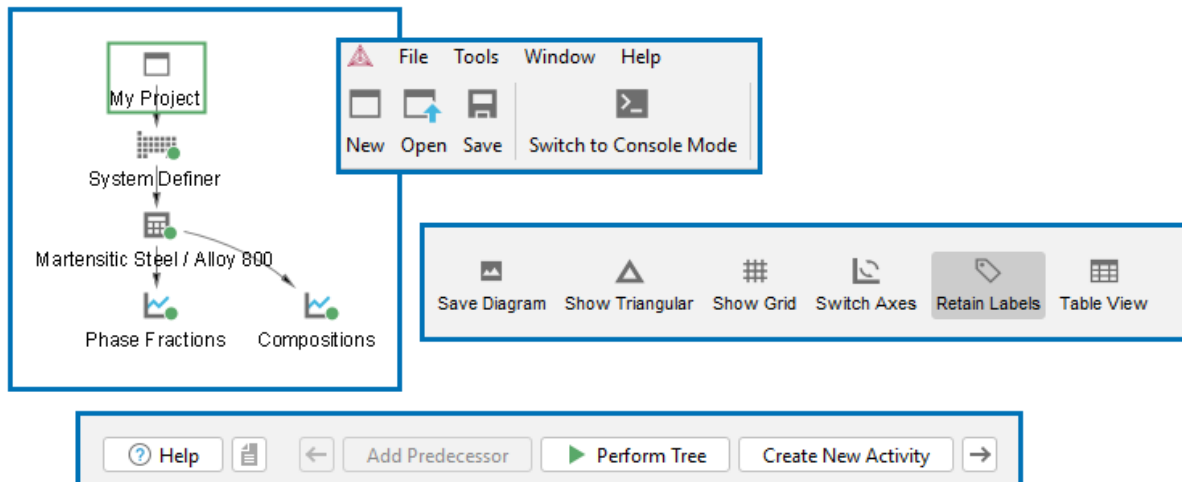
Improved Look and Feel

Thermo-Calc has a new look and feel with the 2022b release. The primary purpose is to have a more modern graphical user interface (GUI) and improve the user experience. As the Thermo-Calc Software product line has expanded in recent years with additional modules and property libraries, the software has become increasingly complex. For those working in Graphical Mode, the main **My Projects Configuration** window is reorganized into categories to help you more easily locate templates and additional resources. A *Getting Started* section is added to help new users learn about or gain a deeper understanding of the software.

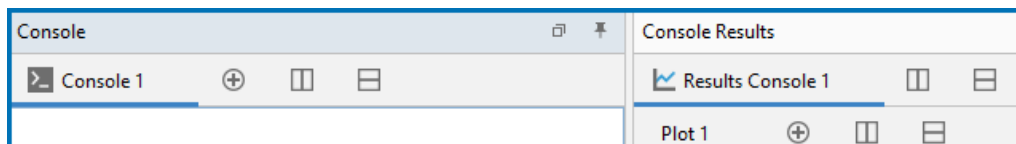


Some of the new categories on the My Projects Configuration window, which include links to the website (the Getting Started guide and video tutorials) as well as local resources (the help and example files). All the templates are still accessed from this window but are reorganized into categories and have new icons.

Additionally, all of the icons in the software are updated with a simpler, more modern feel so that they are easy to identify on the range of screen sizes and resolutions in use today. The overall appearance of the software, such as the buttons and form fields, has also been simplified to make it easier to navigate through the program.



An example of the new icons you will see when working in Graphical Mode. There are also some changes to the icons in the Console and Console Results windows when working in Console Mode as shown below.



New Plot Themes and Related Plot Improvements

The 2022b release introduces predefined themes to provide more flexibility when designing and setting up your plot outputs. A useful change for some users compared to previous software versions is that you can have different global settings applied for Graphical Mode or Console Mode plots at the same time. There are also several other plotting improvements related to the implementation of the new themes as well as various bug fixes described in these release notes.



There is additional information related to the new themes described in the Help. In Thermo-Calc press F1 and search for “plot theme”.

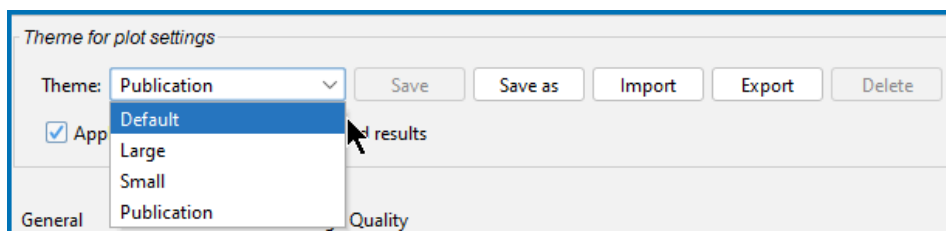
Predefined or Custom Plot Themes

A new section - **Theme for plot settings** - is available with predefined themes for both Graphical and Console Mode. You can also work with themes from both the global or local settings windows, which are accessed slightly differently for the two modes although the options are mostly the same.

- Global settings are accessed on the **Tools > Options** window.
- Local plot settings are accessed from the **Results** window when you right-click an individual plot and choose **Properties**.

Apply Predefined Themes

There are four predefined themes: **Default**, **Large**, **Small**, and **Publication**. The four predefined themes have most of the same settings where key differences include attribute changes to font sizes, plot area size and type, scaling, data point marker radius, tick mark length, line width, and image quality. Predefined themes cannot be renamed or deleted, but can be exported and used as a template for custom themes.



Create and Apply Custom Themes

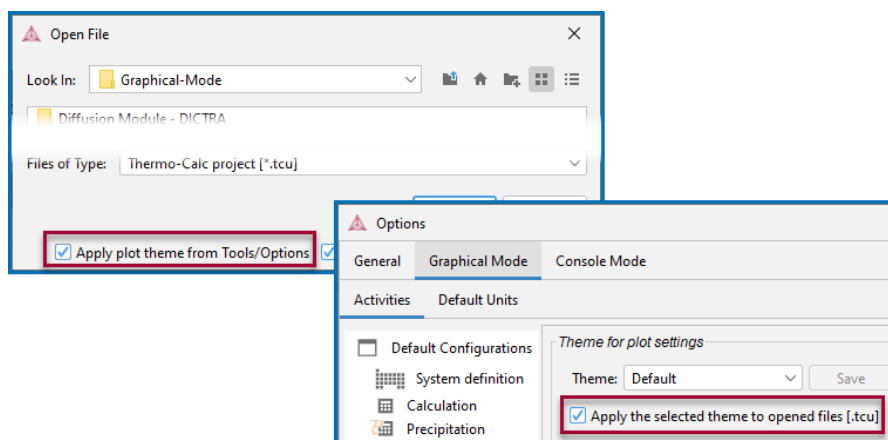
In the **Theme for plot settings** section, and if you make a change based on a predefined theme, it can be saved as a new custom theme (**Save as**), and these custom themes can be reused to create additional themes. Themes (including the predefined ones) can be exported and you can import your own custom themes using *.json files. Once a custom theme is available in the list, it can also be updated (by clicking **Save**) and deleted as needed from the list.

There are many options to work with the settings, either to create a custom theme used and assigned globally from the **Options** section, or when working in the **Results** window for a specific plot.

Apply Themes Locally or Globally to Project Files

For Graphical Mode only, and when opening project files, a predefined or custom plot theme can be automatically applied to all plots (global setting), or just for a specific file (local). There are two check boxes that control this:

- Locally on the **Open File** window, it is called *Apply plot theme from Tools/Options*
- Globally in the **Theme for plot settings** section for Graphical Mode, it is called *Apply the selected theme to opened file [.tcu]*
- NOTE: If you double-click or drag and drop to open a project file it automatically uses the global settings in Thermo-Calc (which may or may not be to apply a theme, i.e. the *Apply the selected theme to opened file [.tcu]* check box may be selected).

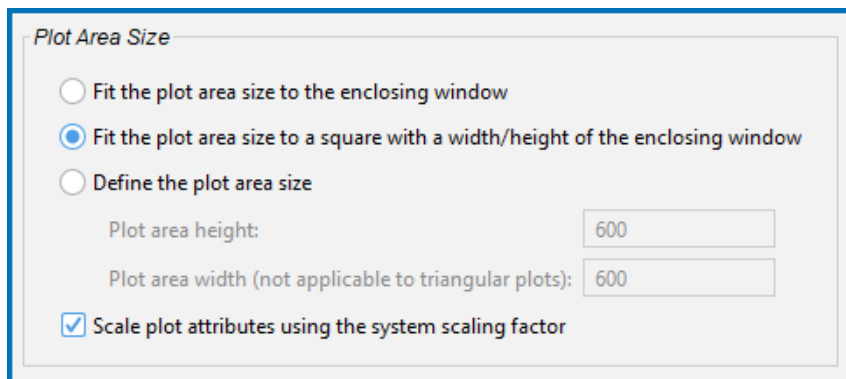


Plot Area Size Improvements

Additional functionality is also added to the **Plot Area Size** section to support and expand on the new theme settings.

The two new sections are used by default for the **Publication** theme. The **Fit the plot area size to a square with a width/height of the enclosing window** option means that the minimum value of the width and height of the **Results** window is used as the dimension of the fixed plot area and in a square.

The new **Scale plot attributes using the system scaling factor** checkbox is selected by default for all themes. This maintains consistent attribute sizing between different plots. Click to deselect it to scale all plot attributes (i.e. labels, font size, axes, tick marks, etc.) independently of the screen size and resolution.



The default settings for the Publication theme under the Plot Area Size section.

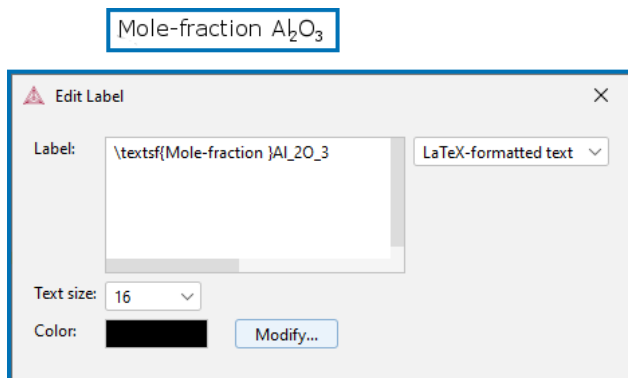
Note that there are also additional improvements and bug fixes for plots listed below in the applicable sections, i.e. [Thermo-Calc Improvements and Bug Fixes](#).

LaTeX Label Improvements

Several improvements have been made to LaTeX formatted text, which can be used in plot labels, plot axis labels, and plot titles. The most significant improvement is that LaTeX output is now made in vector format instead of using an overlaid image, which often was rendered too blurry. The LaTeX output is now as crisp as anything else on the plots. This improves the quality of images saved to file.

Some other important updates to LaTeX labels are:

- The default text style has been changed to non-italic sans serif, to better match the default plain text font.
- The color of LaTeX labels can be changed.



An example of a label created using the LaTeX formatted text option in either Graphical or Console Mode. Details about how to enter this information is found in the help (press F1 and search for LaTeX). You can also now choose a color to apply to the label text.

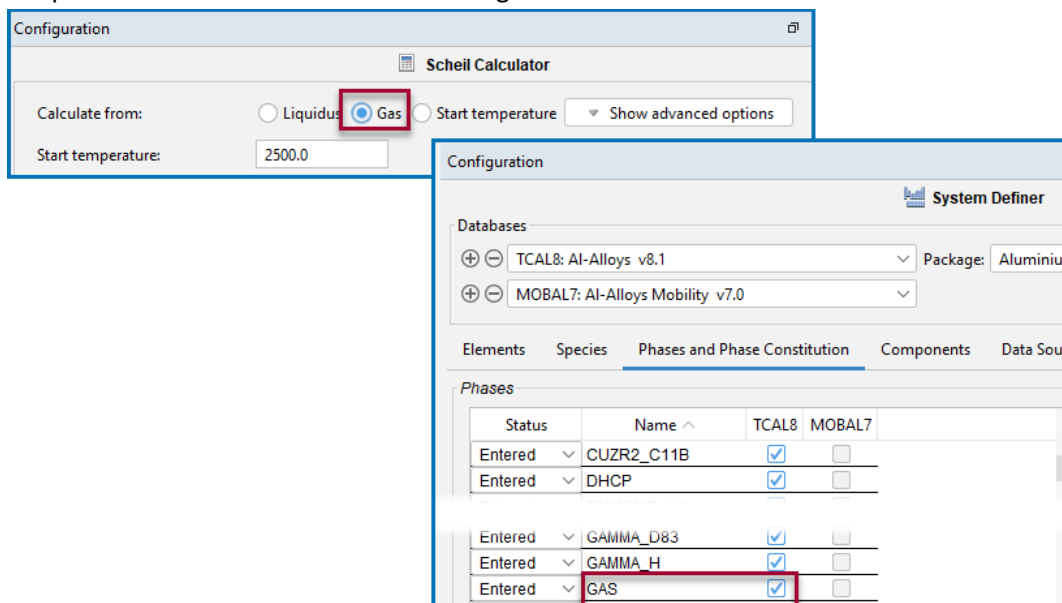
Scheil: Calculate from the Gas/Liquid Transition Temperature

The option to calculate from the gas/liquid temperature, i.e. from the temperature above which the liquid phase is no longer stable, is added to the Scheil calculation options in Graphical Mode, Console Mode, TC-Python, and TC-Toolbox for MATLAB®.

- In Graphical Mode the new option is added as an option on the Scheil Calculator Configuration window.
- In TC-Python and TC-Toolbox for MATLAB® a new method `calculate_from_gas` is added to the `ScheilOptions`.
- In Console Mode there is a new command `CALCULATE_FROM_GAS`.

When choosing the option, equilibrium calculations are performed at set temperature intervals above the liquidus temperature. These equilibrium calculations are performed at 5 K intervals in the two-phase region between the gas/liquid temperature and the liquid/gas temperature, which is the temperature below which the gas phase is no longer stable. When nearing the phase change at liquid/gas temperature the equilibria are calculated at decreasing intervals. Between the liquid/gas temperature and the liquidus temperature the equilibrium calculations are performed at 50 K intervals, and from the liquidus temperature the Scheil solidification simulation is performed as usual.

When running in Graphical Mode, the gas/liquid temperature, liquid/gas temperature and liquidus temperature are collected in the Event Log at the end of the simulation.



An example of where in Graphical Mode to find the new option **Calculate from: Gas** on the Scheil Calculator. This **Calculate from** section has also been moved from the **Advanced Options** section compared to previous versions. The option on the **Phases and Phase Constitution** tab is available when a gas phase is selected for the database on the System Definer.

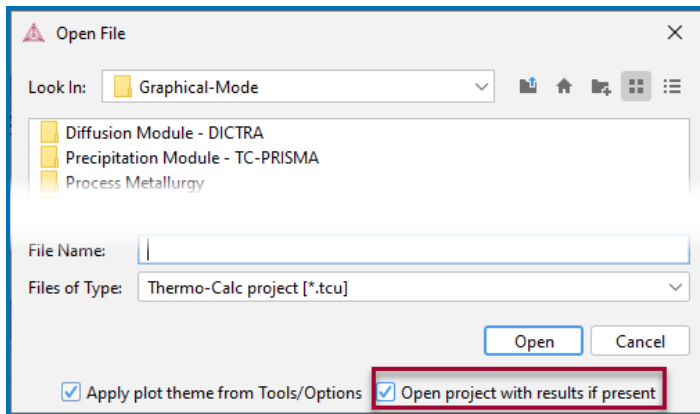
Changes to Graphical Mode Project File Handling

A project file has the extension *.tcu and is specific to working in Graphical Mode. A variety of important changes are introduced in this release to address the ongoing challenges of backward compatibility and the continued improvements and additions to the design and settings within Thermo-Calc. As the result of several recent bug reports of extremely slow opening of project files, where once opened there were still many errors, it is now NOT possible to open project files with results in a different version of the software in which the results were originally saved, i.e. a 2022b project file including results is best opened in version 2022b. Now a project file is converted and maintains the structure and design of the simulation, but no results are included.

The primary changes are related to project files with or without results (for new versions of Thermo-Calc), a new option to open recent files, and that old project files containing results will be converted without results. There is also a related and new check box described for the [New Plot Themes and Related Plot Improvements](#).

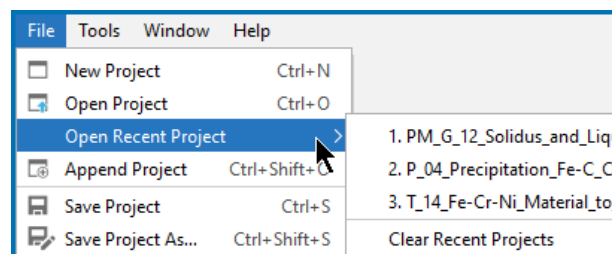
Opening Projects without Results

Starting with 2022b project files, It is now possible to open projects without results, even if the project has saved results. The **Open project with results if present** check box on the **Open File** window controls this. Note that for older project files between 2015a and 2022a, these are now always opened without results even if this check box is selected. In this case an additional window prompts the user for what to do next. See [Converting Old Projects with Results](#).



Opening Recent Project Files

A new menu option is available. Select **File** → **Open Recent Project** and choose from the list of projects or click **Clear Recent Projects** to reset the list. Up to the last 10 projects are listed and numbered in the order in which they were last opened.



Converting (Opening) Old Projects with Results

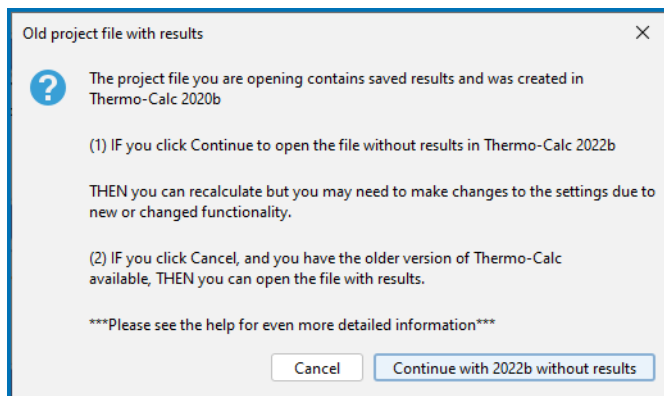
Starting with Thermo-Calc version 2022b, you can continue to open and thus convert an older project file created between versions 2015a to 2022a but if it also includes saved results from a previous version, these are now not immediately available. You can still convert the file and regenerate the results. Whenever a file is converted, a backup file is created, which you can rename and reuse in the original version of the software where it was created. The backup file is saved in the same folder as the original file.

These changes are introduced due to the challenges of backward compatibility and the continued improvements and additions to the design and settings within Thermo-Calc.

The new way that Thermo-Calc handles opening project files that include results is that you are prompted with information to either open the file without results or cancel the action. The version in which the results were calculated is identified in the **Old project file with results** window as well as the version (in this case, 2022b) of the software in which you are opening it in.



There are extensive instructions included in the help detailing all the options related to saving and opening project files, both with and without results. In Thermo-Calc press F1 and search for “converting a project file”.



The prompt window that gives you the option to open an old project file with or without results in 2022b. If you click Cancel, you can open the project file in the original software version, in this case 2020b. If you click Continue, the project file is converted and the results are overwritten. There is a backup file saved in this case, which you can rename and reuse as needed.

Other Bug Fixes Related to Project Files

Also see bug fixes in the section [Project File Related](#), which generally are improved or eliminated with the new way of handling project files.

New Thermo-Calc Examples

There are also several new examples described elsewhere in this document:

- TC-Python and TC-Toolbox for MATLAB® see [Five New Examples](#).
- Ferrite Property Model see [New and Updated Examples](#).

Thermophysical Properties General Examples

Five new examples in both Console Mode and Graphical Mode are available to demonstrate the use of these thermophysical properties: Molar volume, electrical resistivity and thermal conductivity.

Molar Volume and Thermal Expansion

The molar volume examples calculate volumetric thermal expansion coefficients of the L12-type Al3Sc and the L12-type Al3Zr, respectively. Both Al3Zr and Al3Sc are modeled as the same phase (named as AL3SC, since Al3Sc is stable while Al3Zr is metastable).

In Graphical Mode there is one project file and in Console Mode there are two macro files to demonstrate this. When in GM or CM, from the menu choose **Help > Example Files > Thermo-Calc**

- Graphical Mode: **T_15_Molar_Volume_and_Thermal_Expansion_Coefficient.tcu**
- Console Mode: open the **tcex58** and **tcex59** folder for the examples

Electrical Resistivity and Thermal Conductivity

The electrical resistivity and thermal conductivity examples calculate the electrical resistivity (ELRS) and thermal conductivity (THCD) of pure Cu. The example makes a one axis (Graphical Mode) / step (Console Mode) calculation over a wide temperature range, covering both the FCC_A1 state and the liquid state. It plots thermal conductivity of the system (both FCC_A1 and liquid) and that of a single phase (taking FCC_A1 as an example), respectively. Also it plots electrical resistivity of the system and that of FCC_A1.

The same example is also provided in Console Mode as tcex60.

- Graphical Mode: **T_16_Electrical_Resistivity_Thermal_Conductivity_Cu.tcu**
- Console Mode: open the **tcex60** folder for the example



There is a companion video available for the Graphical Mode version of this example (T_16). Go to the [Video Tutorials](#) page on the website or our [YouTube channel](#) to access various playlists.

Additive Manufacturing Applications

This is a new in-depth application example included with your installation. It uses the Property Model Calculator and batch calculations to find the optimal composition for a titanium-based alloy to be used for additive manufacturing applications. This application example, including detailed descriptions and step-by-step instructions, is [showcased on our website](#).

From the menu in Thermo-Calc choose **Help > Example Files > Property Models > General**

- File name: **PM_G_13_Ti_Alloy_Design_for_AM.tcu**

Thermo-Calc Improvements and Bug Fixes

Below is grouped into related categories and whether it is fixed in Graphical Mode, Console Mode, or both Modes. There are also sometimes related items listed in other sections and grouped by Add-on Module as there are often multiple related items.

Graphical Mode

Project File Related

- When projects with calculated results created with a different GES version than selected from the **Tools > Options** window, the results are discarded, since they are not 100% compatible.
- Fixed an issue when opening project files with results and calculations that were then still run even if there was an incorrect GES version or other things stored in the cache for certain calculators such as Property Model, Material to Material, and Process Metallurgy. This is also fixed based on the new functionality where old project files with results cannot be opened in 2022b.

Table Related

- Improved readability of the list of constituents in the Table Renderer output. Now these are shown in several rows in the equilibrium table instead of extending in one row across.
- Fixed a bug for the Table Renderer where previously tabulating activity referred to a phase did not work for partitioned ordered phases.
- Diffusion quantities (tracer/intrinsic/chemical diffusion coefficient, and mobility quantities) are now shown in the Table Renderer when the composition is used as a stepping quantity.
- Fixed a bug where the volume fraction of a phase was not listed in the Table Renderer if the phase name was not written in all capital letters in the database.
- Fixed a bug where the creation of new composition sets during a step calculation could sometimes prevent tabulating quantities with the *All Phases* option selected.

Plotting Related

- Previously when the unit of temperature was saved in Celsius for a TTT plot it always loaded as Kelvin when a project (*.tcu) file was opened, i.e. it ignored the Celsius unit when originally saving the file.
- 3D plot charts now support hardware rendering (GPU rendering) for all operating systems.
- Fixed an issue during plotting where the software could hang after clicking the Perform button a few times.
- Fixed a bug where tracer diffusion coefficients for different components did not plot correctly.

Calculation Related

- Fixed a bug related to using uncertainty calculations in the Property Model Calculator. Previously, after selecting elements in the System Definer, the settings for the randomized quantities were sometimes mixed up when opening a project file or when cloning or creating a calculator.
- The formula for density of phase is corrected.
- Previously, for the Equilibrium Calculator, the temperature, pressure, and system size were reset in condition input fields to the average stepping value when used as the stepping quantity and the condition value is lower/higher than the min/max stepping value. These are now only reset in calculation.

- Fixed an issue on Windows where spaces in the path to the temporary directory caused calculations using the Diffusion Calculator and Scheil Calculator to fail. Also see [File Names and File Paths](#).

General

- Fixed a bug on the System Definer where the reference temperature and pressure did not change with the unit.
- Improved several dialog box prompts where there was inconsistent behaviour for the *Close (X)*, *OK*, and *Cancel* buttons.

General Property Models

Below are improvements and bug fixes for the **General** Property Models included with Thermo-Calc. Also see [Yield Strength Model](#), [Steel Model Library](#), and [Nickel Model Library](#).

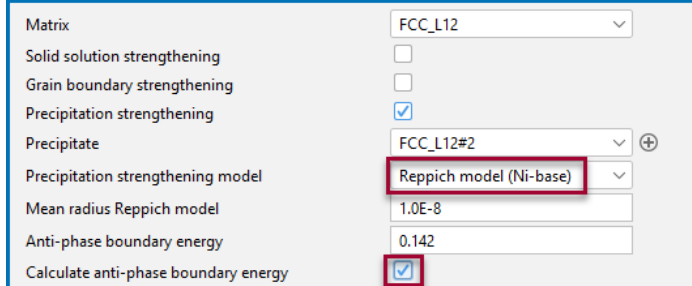
- For the **Equilibrium** Model, added some missing quantities to the Quantity Definitions list: *Thermal conductivity*, *Thermal resistivity*, *Thermal diffusivity*, *Electric conductivity*, *Electrical resistivity*, *Dynamic viscosity*, *Kinematic viscosity*, and *Surface tension*.
- The temperature is shown once for the grid option in the Z-axis quantity list in a Plot Renderer. The composition and temperature are shown for the one-axis option in the quantity list in Plot Renderer when they are not selected as stepping quantities.
- The Property Model configuration panel now expands for readability as expected when parameters are added.

Yield Strength Property Model

The Yield Strength Model is a **General** Property Model included with Thermo-Calc. It is further specialized and also available with the Precipitation Module (TC-PRISMA). Also see [General Property Models](#), [Steel Model Library](#), and [Nickel Model Library](#).

- The following is implemented for the **Simplified model (general)** and **Seidman model (Al-base)**. The mean precipitate radius given by the user is transformed to a Lifshitz-Slyozov-Wagner particle size distribution (LSW PSD). The distribution is stepwise integrated and the mean radius for all sections are used to calculate a partial precipitate strengthening contribution. The use of a PSD smoothes the transition between the cutting and Orowan regions.
- A change is made to the standalone Yield Strength Property Model to make it consistent with the Precipitation Module (TC-PRISMA) version. Previously the standalone model used mole fraction of precipitate and yield strength, now both use volume fraction precipitate.
- Specifically for the Precipitation Module (TC-PRISMA) version of the Yield Strength Model:
 - Implemented the use of precipitate size distribution (PSD), which uses the calculated mean radius from a precipitation simulation instead.
 - Fixed where it sometimes had the wrong precipitate phase selected.
- Fixed a calculation failure when only one element is selected for the **Single Calculation type**.

- When using the Yield Strength Property Model with the **Reppich model (Ni-base)** as the **Precipitation strengthening model** in a calculation, you can select a new checkbox to calculate the antiphase boundary energy. The software uses the stand alone APBE model in the Ni-library from within the Yield Strength Model for the calculation. *Note:* The APBE can only be calculated for gamma prime. If the selected precipitate phase is not gamma prime, the user defined value in the configuration panel is used.



Matrix	FCC_L12
Solid solution strengthening	<input type="checkbox"/>
Grain boundary strengthening	<input type="checkbox"/>
Precipitation strengthening	<input checked="" type="checkbox"/>
Precipitate	FCC_L12#2
Precipitation strengthening model	Reppich model (Ni-base)
Mean radius Reppich model	1.0E-8
Anti-phase boundary energy	0.142
Calculate anti-phase boundary energy	<input checked="" type="checkbox"/>

- A temperature dependence of the form $A \cdot \exp(-B/T)$ is implemented for pure elements in the Yield Strength Property Model. The relevant elements are: Ag, Al, Au, Be, Ce, Co, Cr, Cu, Dy, Er, Fe, Gd, Hf, Ho, Ir, La, Mg, Mo, Nb, Nd, Ni, Pd, Pt, Rh, Sm, Ta, Ti, U, V, W, Y, Zn, and Zr. Further to this improvement all solid solution strength model parameters have been re-optimized to maintain accuracy stated in the original model.
- Result quantity *Fraction of precipitate* was not set. The result quantity for volume fraction of precipitate phases existed in earlier versions and is now replaced.
- One of the general Property Model examples has an adjustment to the plot variable used. **PM_G_04_Yield_Strength.tcu** is now changed to plot *Total precipitation strengthening* instead of *Total yield strength*.

Both Graphical and Console Mode

Plotting Related

- When a plot is reopened having a max limit for temperature lower than the default minimum value (500), the default maximum value (3000) was shown as the max limit.
- A single point data is shown as a star (symbol 208) even if the *None* data points marker is selected.
- From the **Tools > Options** window (Plotting), fixed a bug related to when you clicked **Reset to original settings** (at the bottom of all of the Options settings windows). Now when you click the button on the applicable window, the **Border width**, **Data points marker size**, **Header font**, and **Line width** defaults are correctly reset.
- Fixed a bug that caused extremely slow tabulation when tabulating composition of all phases.
- For Scheil with back diffusion or with fast diffusers, the variable *Distribution of component in phase* is temporarily unavailable. The reason for this is a so far unresolved issue with the amounts not summing up correctly.
- Fixed a bug that prevented images from being saved when you right-clicked in the **Results** window or clicked the button on the **Configuration** window.
- The automatically selected line colors in plots had a random behavior regarding which color was selected for a given quantity. This is fixed.

File Names and File Paths

- Saving POLY3 files no longer defaults to the `/tmp` directory. See below.
- Double clicking PAR and TDB files now works if the paths contain white space. See below.

- From the **Tools > Options** window (**General** tab) you can now change the path to the **Temporary Directory** folder, where files are stored during calculation, such as Console Mode state files (e.g. `State_4064824901731140183.POLY3`), log files, and so forth.
- In the `tc_initd.tdb` file it is now possible to add databases with absolute file names with white space, if the path is surrounded by quotation marks, e.g.:

```
TEST "G:\My Drive\My Folder\Test.TDB" My test database v0.1!
```

IMPORTANT. The use of absolute paths should be used with caution as these are not portable.

General

- Ionic liquid model with only VA in the second sublattice, failed when using global minimization.
- Improvements in Scheil with solute trapping calculations when the primary solid phase is first formed.

Console Mode

Plotting Related

- Addressed issues with some Console Mode plot settings not being honored. Improves the behavior of: `SET_RASTER_STATUS`, `SET_TIC_TYPE`, `PLOT_SYMBOLS_AT_NODE_POINTS`, and `SYMBOL_SIZE`.
- Bug fixes related to Console Mode plots using the inverse axis include correcting the size of symbols for experimental data, adding tooltips on the diagram to show both the linear and inverse values, showing the inverse axis label as 1 over the quantity name, and including tick marks and header fonts when the axis type changes to inverse.
- The `SET_PREFIX_SCALING` command, which enables scientific notation, works now. The exponent part is placed under the X-axis and on the left side of the Y-axis.

Gibbs Energy System (GES5 and GES6)

Below relates to improvements and bug fixes for the core calculation engine used throughout the product range.



For further information about the changes to GES, see the [2019b](#), [2020b](#), [2021a](#), [2021b](#), and [2022a](#) release notes on the website.

Database Related

- POLY3 and DIC files using user database(s) with GES6 are now portable.
- `LIST_DATA` command (GIBBS module) GES6 fixes:
 - Fixed an issue where the command would sometimes fail.
 - It now lists only the species that are actually used by the selected phases.
 - Fixed so the command includes the V parameters that are used by PARROT.
 - Previously it sometimes printed the phase in parameter definitions using upper case when the phase definitions used lower case.
- The order in the database of constituents on the second sublattice no longer matters.

General

- Improved the user experience when changing the system interactively in Console Mode.
- Neutral reference in ionic liquids now gives the correct results.
- Fixed wrong magnetic contributions for so-called partitioned never disorder phases in GES5 and GES6.

Steel Model Library

Below are details about the **Steel** Property Models included with Thermo-Calc with the addition of a licence for the Steel Model Library. Also see [General Property Models](#), [Yield Strength Model](#), and [Nickel Model Library](#).

New Ferrite Model and Improved CCT and TTT

A Ferrite Property Model is added to the Steel Model Library. This new model calculates the transformation product from austenite that happens when you have low carbon and hold it at a high temperature for a long time.

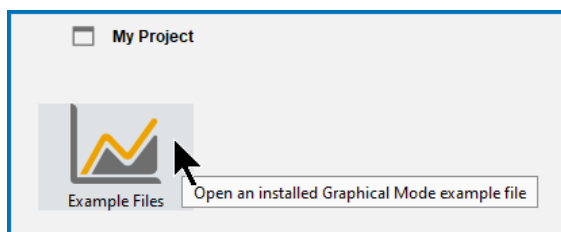
The new Ferrite model has also been incorporated into the TTT Diagram and CCT Diagram Models, which combine the Pearlite, Bainite, Martensite, and Ferrite Property Models and calculate the kinetics of concurrent transformation of austenite into pearlite, bainite, martensite, and ferrite.

This new Ferrite model is available to users who have a licence for the Steel Model Library and a valid Maintenance and Support Subscription. Learn more about the [Steel Model Library on our website](#) where there are links to additional resources.

New and Updated Examples

A new example is added to help users learn about this **Ferrite** Property Model. Three existing examples are updated for the **TTT Diagram** Property Model and **CCT Diagram** Property Model. For these examples, from the menu in Thermo-Calc choose **Help > Example Files > Property Models > Steel**, then select files demonstrating the use as follows.

- TTT Diagram = **PM_Fe_06_Fe-C-Mn-Si-Cr-V_TTT.tcu**
- TTT Diagram, CCT Diagram, and other Steel Models = **PM_Fe_07_Hardenability_Design_of_Steel.tcu**
- CCT Diagram = **PM_Fe_08_Fe-C-Mn-Si-Cr-V_CCT.tcu**
- Ferrite = **PM_Fe_09_Fe-C-Ni_Ferrite.tcu**



Tip: As of this release, you can also click the Example Files icon on the My Project Configuration window to directly access the file location.

Improvements and Bug Fixes

Improved algorithm for time integration for **Pearlite** and **Bainite** Property Models, which fixes some previous problems including:

- In some cases, calculation gives incomplete austenite-to-pearlite transformation when the transformation should be complete;
- In some cases, when cooling rate is lowered in a CCT Diagram calculation, *Pearlite-start* can be unphysically overtaken by *Bainite-start*.

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. Also see [General Property Models](#), [Yield Strength Model](#), and [Steel Model Library](#).

Bug Fix

A correction to spelling for a phase name for the **Coarsening** Property Model. Previously M23C6 was incorrectly named M6C3 when selecting it from the precipitates list.

TC-Python and TC-Toolbox for MATLAB®

Process Metallurgy in TC-Python and TC-Toolbox for MATLAB®

The Process Metallurgy Module is now available in both TC-Python and TC-Toolbox for MATLAB®, our two most powerful APIs. All functionality that is currently available in the Graphical Mode version of the Process Metallurgy Module is now available in both of these APIs, including equilibrium calculations and kinetic process simulations.

The integration into the APIs now gives the full power of a programming language to the Process Metallurgy Module. But it also makes it easier to use for integrating calculations and process simulations directly with the data available in steel plants, for example, from a data warehouse. However, such integrations currently need to be developed by the user.

The strength of the Process Metallurgy Module is that thermodynamic calculations and even full simulations of a liquid steelmaking process, such as a ladle furnace, can be set up easily, and the results can be easily interpreted. For example, slag composition is directly available per component (CaO, Al₂O₃, FeO, Fe₂O₃, etc...), not only per element.

This new integration is available to users who have a licence for the Process Metallurgy Module and either TC-Python or TC-Toolbox for MATLAB®. Contact your local representative to learn how to obtain a licence for these powerful new tools.

Five New Examples

Five new examples are available in TC-Python and TC-Toolbox for MATLAB® to demonstrate how the Process Metallurgy Module can be used in these APIs. Brief descriptions of the examples are also included in the help.

TC-Python

- `pyex_PMET_01_Single_adiabatic_equilibrium.py`
- `pyex_PMET_02_Stepping_adiabatic_equilibrium.py`
- `pyex_PMET_03_Mapping_isothermal_equilibrium.py`
- `pyex_PMET_04_Simple_process_simulation.py`
- `pyex_PMET_05_VOD_process_simulation.py`

TC-Toolbox for MATLAB®

- `matex_PMET_01_Single_adiabatic_equilibrium.m`
- `matex_PMET_02_Stepping_adiabatic_equilibrium.m`
- `matex_PMET_03_Mapping_isothermal_equilibrium.m`
- `matex_PMET_04_Simple_process_simulation.m`
- `matex_PMET_05_VOD_process_simulation.m`

Timeout to Stop a Calculation

TC-Python and TC-Toolbox for MATLAB® now allow users to set timeouts for each calculation in a project in order to prevent the program from hanging on incorrectly formatted calculations. If a calculation cannot be completed in the set time, the program moves on to the next calculation, rather than aborting the entire project. The timeout parameter is set in the **Calculate** method and is available with all calculation types except for Single equilibrium stateless calculations.

Almost all calculation methods now have this optional parameter:

```
result = calc.calculate(timeout_in_minutes=2.0)
```

When used, the calculation runs at maximum for the time specified, and if not finished by then it throws an `UnrecoverableCalculationException`.

Scheil: New Method

Also see [Scheil: Calculate from the Gas/Liquid Transition Temperature](#) where In TC-Python and TC-Toolbox for MATLAB® a new method `calculate_from_gas` is added to the `ScheilOptions`,

Improvements and Bug Fixes in TC-Python and TC-Toolbox

- User database paths with white space now work. Also see [File Names and File Paths](#).
- Fixed a bug with the method `get_system_function` where it would not always return a value for zero-valued database functions.
- Fixed a bug that caused the method `get_phase_parameter` to return at most 256 characters of a database parameter description.

Installation Related

Also see [Installation](#) for other changes related to general Thermo-Calc installations.

- A Python installation version 3.9 is included in the Windows installation to make it possible to run TC-Toolbox on MATLAB® version R2022a and later. It's installed in a folder, with the name python39, next to the old python 3.7 installation.
- Fixed the installer to correctly find the location of MATLAB® 2022a.
- Fixed a bug that prevented TC-Toolbox for MATLAB® from being selected as an option on the installation window if the first attempt failed because MATLAB® was not found.



Details about the TC-Python and TC-Toolbox for MATLAB® installations are available in the *Thermo-Calc Installation Guide*, which among other places, can be [found on our website](#).

Deprecation and Removed Function Reminders

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

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

Removed Functions: No Longer Supported as of Version 2022b

The following functions were deprecated starting with 2021b and as of this release are no longer supported.

Old Name	New Name
<code>set_fast_diffusing_elements</code> in class <i>ScheilCalculation</i>	<code>set_fast_diffusing_elements</code> in <i>ScheilCalculationType</i> Use it with the method <code>with_calculation_type</code>
<code>with_back_diffusion</code>	<code>with_calculation_type</code>
<code>set_homogenization_function</code>	<code>with_function</code>

Removed Functions: Stop Supporting as of Version 2023b

The following functions are renamed, and the old versions will be removed in 2023b (June 2023). Users are recommended to update any scripts as soon as possible.

Old Name	New Name
<code>get_system_for_scheil_calculations</code>	use the regular <code>get_system</code> instead

Process Metallurgy Module



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

Included with TC-Python and TC-Toolbox for MATLAB®

The Process Metallurgy Module is now available with TC-Python and TC-Toolbox for MATLAB®. See [Process Metallurgy Included with TC-Python and TC-Toolbox for MATLAB®](#)

Improvements and Bug Fixes

- Fixed a bug related to when the unit of transfer of phase group was potentially wrong in the table for a process simulation. This happened when heat was added to the process model and then Transfer of Phase Group was added by reopening the Edit Process Model dialog.
- For Process Simulations, the setting option **Absolute Amount** is no longer selectable as an **Input Type** because the option was not useful in this context.
- Fixed that the unit of a gas addition was not set in certain situations if the configuration had been loaded from a file.
- There is a significant improvement to the performance of process simulations using extensively continuous additions. For example, tests using this feature for industrial ladle furnace simulations to model slow dissolution of additions have confirmed a performance improvement of around 35%.

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.

Improvements and Bug Fixes

- See the [Yield Strength Model](#) for details of bug fixes applicable to the Property Model, which is also available in an advanced form in the Precipitation Module (TC-PRISMA).
- On the Precipitation Calculator, the *Preexisting size distribution* checkbox is no longer wrongly deselected after a calculation has finished.

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

Graphical Mode

- Several issues in plotting with diffusion calculations having regions created during the simulation are fixed.
- Previously after opening project files (or cloning calculators) with a Diffusion Calculator, simulations failed when calculating stoichiometric phases.
- Fixed a rare case that made plotting diffusion simulation results impossible after resaving the project file.

Both Console and Graphical Mode

- Fixed an inconsistent equation shown in both Console Mode help and the online help. Now the equations as part of the text for the two boundary condition commands, Activity Flux Function and Potential Flux Function (as part of `SET_CONDITION` command) include molar volume expression.
- Fixed an issue with diffusion coefficients calculated wrongly if the interpolation scheme was turned on, DICTRA classic with complex phases was used, and temperature depended on time.

Console Mode Only

- Resolved an issue that made the following variables unavailable: DT, QT, QC, QI, FC, FT and FI.

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 Ultra-high Temperature Materials Database (TCUHTM1)

The TCS Ultra-high Temperature Materials Database (TCUHTM1) is a thermodynamic database for ultra-high temperature materials that can be used for hypersonic aircraft and space vehicles. These are typically non-oxides with melting/decomposition temperatures in excess of 3000 °C. Examples include borides, nitrides, and carbides of Group IV-V metals in the periodic table, such as ZrB₂, HfB₂, ZrC, HfC, TaC, and HfN. SiC was used to improve oxidation resistance. The database can be used to calculate phase diagrams and thermodynamic properties of assessed systems, but also for predicting phase equilibria, melting temperatures, and simulating operation processes for a wide range of compositions.

TCUHTM1 enables predictions (such as multicomponent phase equilibria calculations, equilibrium solidification simulations, and Scheil solidification simulations) to be made for multicomponent systems and alloys of industrial importance. This means that the database can be used to extrapolate to higher-order systems by combining several critically assessed systems.

There are seven included elements B, C, Hf, N, Si, Ta, and Zr.

A hybrid approach of experiments, first-principles calculations and CALPHAD modeling have been used to obtain thermodynamic descriptions of the constituent binary and ternary systems over the whole composition and temperature ranges. All the stable solution phases and intermetallic compounds that exist in each assessed system are included. In most cases phases having the same crystal structure are merged as the same phase.

The database contains:

- 21 assessed binary systems
- 26 assessed ternary systems
- 35 phases



There is a new [Ultra-high Temperature Materials](#) page on our website where you can access an example collection and the technical information.

TCS Ni-based Superalloys Database (TCNI12)

New Element

- Phosphorus (P) is added to make it a 31 element framework.

20 New Binary Systems

- The following systems are at least partially assessed. Al-P, B-P, C-P, Ca-P, Co-P, Cu-P, Cr-P, Fe-P, Mn-P, Mo-P, Nb-P, Ni-P, P-Pd, Pt-P, Ru-P, S-P, Si-P, Ti-P, V-P, and W-P.

29 New Ternary Systems

Al-Fe-P	B-Ni-P	C-Fe-P	Co-Fe-P	Co-Ni-P	Co-P-V
Co-P-W	Cr-Fe-P	Cr-Nb-P	Cr-Ni-P	Cr-P-Ti	Cu-Fe-P
Cu-Ni-P	Fe-Mn-P	Fe-Mo-P	Fe-Nb-P	Fe-Nb-Si	Fe-Ni-P
Fe-P-Si	Fe-P-Ti	Fe-P-V	Fe-P-W	Nb-Ni-P	Nb-P-Ti
Ni-P-Ti	Ni-P-V	Ni-P-W	Ni-Si-P	P-V-W	

Binary and Ternary System Updates

- Fe-Nb updated, improved MU and C14_LAVES boundaries.
- Nb-Ni, Fe-Si, Nb-Si updated metastable C14_LAVES description.
- Co-W updated so that Co3W D019 is stable to low temperature.
- Fe-Nb-Si added.
- Fe-Nb-Ni updated, improved Laves boundaries.
- Co-Ni-Ti updated to correspond better with available phase diagram data.
- Al-Co-Ni updated to better fit thermodynamic and phase diagram data.
- Al-Co-W updated to destabilize FCC_L12#2 (gamma-prime)
- Co-Ni-W updated metastable FCC_L12 towards an improved description of Al-Co-Ni-W
- Nb-Ni-Ti fixed a bug relating to a slightly destabilized ternary phase.

Thermophysical Properties

- Viscosity and Surface tension updated:
 - Viscosity is now described for the ionic liquid phase (IONIC_LIQ)
- Electrical and thermal properties improved:
 - High-temperature trends of THCD are now better for commercial alloys.
 - ELRS of Cr-Fe rich Ni-base alloys were before quite over-estimated, now improved.

Phase Names/Phase Information

- AL-FE-SI ternary phases renamed to use their modern Greek letters, e.g. ALFESI_ALPHA > ALFESI_ALPHA_TAU5.
- D01_MO2B5 renamed to MO2B5_D8I, correct strukturbericht.
- All phase descriptions updated to our new standardized crystallographic information format.

Bug Fix

- Corrected minor typo in the Gibbs energy of the MUFEMO function, used in the MU_PHASE.

TCS Ni-alloys Mobility Database (MOBNI6)

This database is compatible with TCS Ni-based Superalloys Database (TCNI12).

New Element

- Phosphorus (P) is added to make it a 29 element framework.

FCC_A1 Phase

Mobility parameters for 29 binary or ternary systems are added or reassessed:

- Four (4) binaries: Co-Mn, Co-Re, Cr-Pt and Ni-P
- Twenty-five (25) ternaries: Co-Cr-Mo, Co-Cr-W, Co-Mo-W, Co-Ti-V, Co-V-W, Ni-Al-Co, Ni-Al-Nb, Ni-Al-Ta, Ni-Al-W, Ni-Co-Cr, Ni-Co-Mo, Ni-Co-Re, Ni-Co-Ru, Ni-Co-W, Ni-Cr-Mo, Ni-Cr-Nb, Ni-Cr-Ti, Ni-Cr-V, Ni-Cu-Cr, Ni-Cu-Mo, Ni-Cu-Ti, Ni-Fe-Ti, Ni-Fe-V, Ni-Mo-Ta, and Ni-Mo-W

FCC_L12 Phase

- Mobility parameters for three (3) ternary system are added or reassessed: Ni-Al-Ta, Ni-Al-Re, and Ni-Al-W

BCC_B2 Phase

- Mobility parameters for one ternary system are assessed: Ni-Al-Co

LIQUID Phase

- Mobility parameters for one binary system are added: Ni-P

TCS Cu-based Alloys Database (TCCU5)

New Elements

- Two new elements, Ce and La.

New Binary and Ternary Systems

- 13 new binary systems: Cr-O, Cu-La, Cu-Ce, Cr-La, La-Zr, La-Ni, Ce-La, Al-Ce, Ni-Ce, Nb-Ni, Nb-Ti, Ni-Ti, and Zr-O
- 11 new ternary systems: Ag-Cu-Si, Ag-Cr-Cu, Al-Ce-Cu, Ce-Cu-La, Ce-Cu-Ni, Cr-Cu-La, Cu-La-Ni, Cu-La-Zr, Cu-Nb-Ni, Cu-Nb-Ti, and Cu-Ni-Ti

New Volume Data

- Volume data for the newly added phases are assessed or estimated.

TCS Cu-alloys Mobility Database (MOBCU5)

This database is compatible with TCS Cu-based Alloys Database (TCCU5).

New Elements

- Two new elements: Ce and La.

New Diffusion Data for FCC_A1 and LIQUID Phases

- The self-diffusion and related impurity diffusion data for Ce and La were included in both FCC_A1 and LIQUID phases.

New System Assessments

- The complete and critical assessments for the following systems are implemented:
 - FCC Cu-Ti, Co-Mn, Ni-Mo, Cu-Ni-Mo, Cu-Ni-Ti, Cu-Co-Mn, Cu-Mn-Si, Cu-Ni-Al-Zn and Cu-Ni-Al-Sn.
 - Liquid: Al-Ce and Cu-Ce.

Updated Description

- The description for FCC Ni-Ti is updated.

TCS High Entropy Alloys Database (TCHEA6)

In this release of the database, there is one new ternary system assessment plus major changes to 18 critically assessed systems. In addition, 19 ternary systems also had some minor changes and a complete description of the gas phase is added.

Ternary Systems: New and Reassessed

- One new ternary assessment added: Al-V-Zr
- Reassessed 18 ternary systems: Al-Co-Ti, Al-Cr-Ti, Al-Mn-Ti, Al-Mo-Ti, Al-Ni-Ti, Al-Sn-Ti, Al-Ta-Ti, Al-V-Zr, Co-Mo-Ti, Cr-Mn-Ti, Cr-Ti-Zr, Fe-Ti-V, Mo-Ti-V, Mo-Ti-Zr, Nb-Ti-W, Ta-Ti-V, Ti-V-W, and Ti-V-Zr

Ternary Systems: Minor Modifications

- Adjustments for 19 ternary systems: Al-B-Ti, Al-C-Ti, Al-Fe-Ti, Al-N-Ti, Al-Si-Ti, Co-Sn-Ti, Cr-Si-Ti, Cu-Ti-Zr, Mo-Nb-Ti, Mo-Ta-Ti, Mo-Ti-W, Nb-Sn-Ti, Nb-Ta-Ti, Nb-Ti-V, Nb-Ti-Zr, Si-Ti-W, Ta-Ti-W, Ta-Ti-Zr, and Ti-W-Zr

Gas Phase Description

- Added a complete description of the gas phase in the 26 element framework.

IRSN Mephista-20 Nuclear Fuels Database (MEPH20)

New Element

- Added element Cr

New Binary Systems

- Added 14 binary systems related to the addition of Cr. All X-Cr (with X=Ba, C, Ce, Cs, Fe, La, Mo, O, Pu, Ru, U, Si, Sr, Zr) are modeled.

New Ternary Systems

- Added 6 fully modeled ternary systems related to the addition of Cr. Cr-Fe-O, Cr-Fe-Zr, C-Cr-Fe, Ce-Cr-O, Cr-Mo-O, and Cr-O-Zr.

New Pseudo-binary Sections

For the following ternary systems where there is not enough experimental data, only pseudo-binary sections are modeled:

- Ba-Cr-O modeled as BaO – Cr₂O₃
- Cr-La-O modeled as Cr₂O₃ – La₂O₃,
- Cr-O-Si modeled as CrO – SiO₂ and Cr₂O₃-SiO₂
- Cr-O-Sr modeled as Cr₂O₃ – SrO
- Cr-O-U modeled as Cr₂O₃ – UO₂

IRSN NUCLEA-20 Nuclear Alloys-Oxides Database (NUCL20)

Binary Systems

- Updated binary system: Ag-In as taken from E. Fischer et al., Calphad, 64:292–305, 2019
- Change to B-Ni: The name of the compound B0414NI0586 is changed to B7NI10.

Pseudo-binary Systems

- A bug fix for the pseudo binary system, Ba-Ca-O BaO-CaO

Ternary Systems

Change of name for three ternary stoichiometric phases:

- Fe-U-Zr: The name of the ternary stoichiometric phases, FE333U250ZR417(e), FE6U71ZR23(l), and FE503U18ZR32(k) are changed to FE4U3ZR5, FE6U71ZR23, and FE253U9ZR16, respectively.

Pseudo-ternary Systems

Two new systems and one reassessment:

- Al-Ca-O-Zr: Modeling of the CaO-Al₂O₃-ZrO₂ pseudo-ternary system
- Al-O-Si-Zr: Reassessment of the Al₂O₃-SiO₂-ZrO₂ pseudo-ternary system
- Ca-Mg-O-Zr: Modeling of the CaO-MgO-ZrO₂ pseudo-ternary system

Updated Thermodynamic and Kinetic Databases

TCS Solder Alloy Solutions Database (TCSLD4.2)

- Bi-Sn is re-assessed.
- Au-Co is updated.

TCS Mg-based Alloys Database (TCMG6.3)

- Remodeled Ag-Mg over the entire composition range, with a focus on the Mg-rich corner.
- The Al-Mg-Y description was refined via stabilizing the Al₂Y phase.
- The GAS phase now has a complete thermodynamic description within the framework of the database.

Aluminium Demo Database (ALDEMO 4.1)

- Synchronization with TCAL8.1: updated thermal expansion of L1₂-type Al₃Zr and Al₃Sc (both named as AL3SC); updated thermal conductivity of liquid Cu and electrical resistivity of solid Si.
- Added the list of ASSESSED_SYSTEMS, so that the assessed binaries and ternaries could be calculated with the BINARY and TERNARY modules, respectively, in the Console Mode.

Installation

Thermo-Calc Changes

- Thermo-Calc communicates internally with its own subprocesses using network sockets. On Windows, firewall rules are now added that prevents outside traffic from reaching those processes. Before, the users sometimes were queried for this and that could result in unnecessarily permissive settings. The details are described in the *Thermo-Calc Installation Guide*, available from various places including [our website](#).
- The Thermo-Calc update now checks if the calculation-engine dll is locked and kills all processes that may be locking it when the user confirms to update.
- There are some installation fixes related to TC-Python and TC-Toolbox for MATLAB®. See [Installation Related](#).

Option to Save Backup User Created Files During Thermo-Calc Software Updates

Occasionally after a full release (such as 2022b), an interim release version, an update, is required to fix a serious bug or to address an external issue that occurred after the full release. During the installation process, several default folders are added to your system that include Documentation, Materials, and Example files. Starting with 2022b, and **only for an updated version of an installation**, Thermo-Calc runs a check of these default folders to determine if there are changed or new user files also saved to these folders. For example, you might have saved a completely new project *.tcu file into the Examples folder, or after running one of the included examples such as **T_06_Serial_Equilibrium_Calculators.tcu**, the default file is changed and now includes results.

There are operating system differences regarding what backup files are saved if you are installing an update on Windows versus macOS or Linux.

- On **Windows** operating systems, Thermo-Calc gives you the opportunity after the installation to specifically save a backup folder of these user created or modified files to your Documents folder when you open Thermo-Calc for the first time after the update. Note that the following file types are not kept, i.e. these are excluded during the backup process: dll, exe, lib, mlbtx, pdf, whl, html, and htm.
- For **macOS** and **Linux** operating systems, the behavior is different due to limitations enabling the identification of changes to some files. In this case, a backup of the full Examples folder is saved, regardless of whether there are additions or changes to any file. No backups of Materials or Documentation folders are made.



In Thermo-Calc, press F1 to search the help for *Updating the Software* for details about the location of the backup folders as well as the different behavior based on the operating system. This information is specifically in the full [Installation Guide PDF](#), a copy of which is found on our website.

Educational Package Updates of Note

The [Educational Package](#) is available after filling in a short form on our website. Most users are unlikely to perform an update between releases and instead request, download, and install the latest version. However, the following information is included for completeness.

- The Precipitation Module (TC-PRISMA) example P_01 now opens without errors. This is automatically included with any new educational download.
- The Precipitation Module (TC-PRISMA) example P_11 is now available for users. This was released with an updated version for 2022a in March i.e. automatically included with any download since then.

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 Disk Space Requirement

Due to precompiled databases added to the Thermo-Calc installation, 5 GB of disk space is recommended for the 2022b installation. However, for Process Metallurgy Module users, due to the complexity of the calculations, it is recommended that at least 50 GB of disk space is available.

Platform Roadmap



For information about platforms being phased out visit our [Roadmap for Platform Support](#).