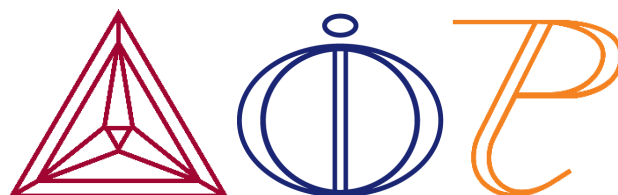Release Notes:

Thermo-Calc Software Package and Databases

Version 2021b

Contents

Thermo-Calc Version 2021b Highlights

★ **Thermo-Calc:** Scheil with solute trapping, batch calculations with the Property Model Calculator, export/save plot results as tabular data, filter quantities in plots and tables, and much more

★ **Property Models and Steel Model Library**: batch calculations, new CCT Diagram Property Model and CCT template, plus updated TTT template and a new TTT Diagram Property Model, new plotting modes to compare experimental data to calculated results, plus new examples

★ **Diffusion Module (DICTRA):** caching added, homogenization functions added to TC-Python

★ **TC-Toolbox for MATLAB®:** entirely rewritten with extensive new functionality

★ **TC-Python:** debug Property Models, all the homogenization functions for the Diffusion Module (DICTRA) now added

★ **Databases:** 7 new databases (TCNI11, TCHEA5, TCOX11, TCAL8, TCCU4, MOBCU4, and TCSLD4) and 1 updated database (TCMG6.1)

★ **Thermophysical Properties**: Properties and many new examples added -
  ○ Surface tension of liquid: TCHEA5, TCOX11 (oxide slag), TCCU4, TCSLD4
  ○ Viscosity of liquid: TCCU4 and TCSLD4
  ○ Thermal conductivity and electrical resistivity: TCHEA5 and TCNI11

Thermo-Calc

Scheil with Solute Trapping for High Solidification Speeds such as Additive Manufacturing (AM)

A new model for solute trapping considers multicomponent systems and is implemented in Thermo-Calc's Graphical Mode Scheil Calculator. It is also available in Console Mode (where you use the new command SOLUTE_TRAPPING to turn on the feature) and then new prompts are included with the Scheil module Start Wizard. The feature is also available with the SDKs, TC-Python and the new TC-Toolbox for MATLAB®.

For equilibrium- and Scheil-type solidification simulations thermodynamic equilibrium is established at the solid-liquid interface. This means that solutes are partitioned between the solid and liquid phases according to solidus and liquidus lines of the phase diagram. The assumption of thermodynamic equilibrium at the solid-liquid interface however breaks down for very fast solidification rates, that are encountered for example during additive manufacturing.

> You can read more about the model and the assumptions that are made, either in the online help (press F1 in Thermo-Calc) or read a presentation about the model's development, which is available from the Scheil page on our website.

New Examples

An example of using the new Scheil model is available in different formats, either from within Thermo-Calc for Graphical or Console Mode, or when using one of our SDKs.

For Thermo-Calc examples, select **Help > Example Files >** then navigate to the applicable folder as indicated. The default folder that opens depends on whether you are in Console Mode or Graphical Mode to begin. You can also navigate to the examples for the SDKs this way, and the examples will also be available within the SDK application (e.g. TC-Python or TC-Toolbox for MATLAB®).
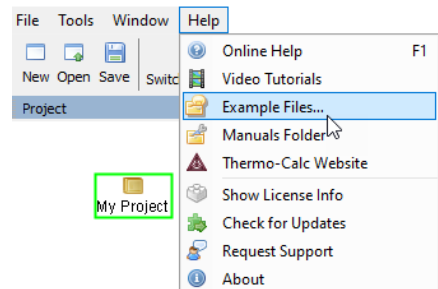
- *Graphical Mode* **Thermo-Calc > T_13_Scheil_with_Solute_Trapping.tcu**
- *Console Mode* **Thermo-Calc > tcex57 > tcex57.TCM**

When you have a license for these SDKs, locate these example file names either starting via the menu in Thermo-Calc or within the SDK itself. See the documentation for details.

- *TC-Python* **SDK > TC-Python > Examples > pyex_T_16_Scheil_Solute_Trapping_Al_Si_Cu.py**
- *TC-Toolbox for MATLAB®* **SDK > TC-Toolbox-MATLAB > matex_T_16_Scheil_Solute_Trapping_Al_Si_Cu.m**
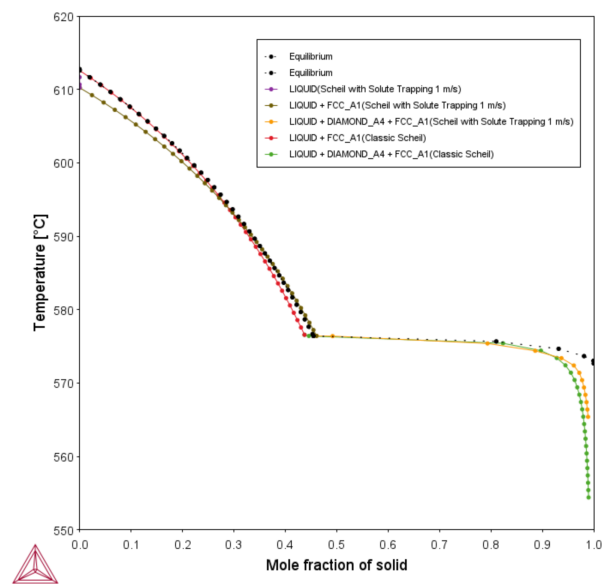
The results of the Graphical Mode example T_13 showing the effect of Scheil solidification with solute trapping of a Al-7.5Si-0.2Cu alloy compared to equilibrium and a Classic Scheil calculation.

> 💡 In Thermo-Calc, press F1 to search the help for *Scheil solute trapping* for details about this new feature and Scheil calculations in general such as classic Scheil, Scheil with back diffusion, and Scheil with fast diffusers. There is also a table comparing the different ways to access each model in Graphical Mode versus Console Mode.

Batch Calculation Type Added to the Property Model Calculator

A new calculation type called *Batch* allows for high throughput calculations. This new calculation type allows the Property Model Calculator, which is available in Graphical Mode, to read input from a file, such as a spreadsheet, rather than, for example, having a fixed grid in one or several dimensions allowing the program to read in significant amounts of input data. Results from batch calculations can then be compared to experimental values as long as these are included in your data file.

The program uses information from uploaded data to configure your calculation and offers validations to help ensure that files are formatted correctly. Additionally, users can set timeouts for each row in order to prevent the program from hanging on incorrectly formatted rows.
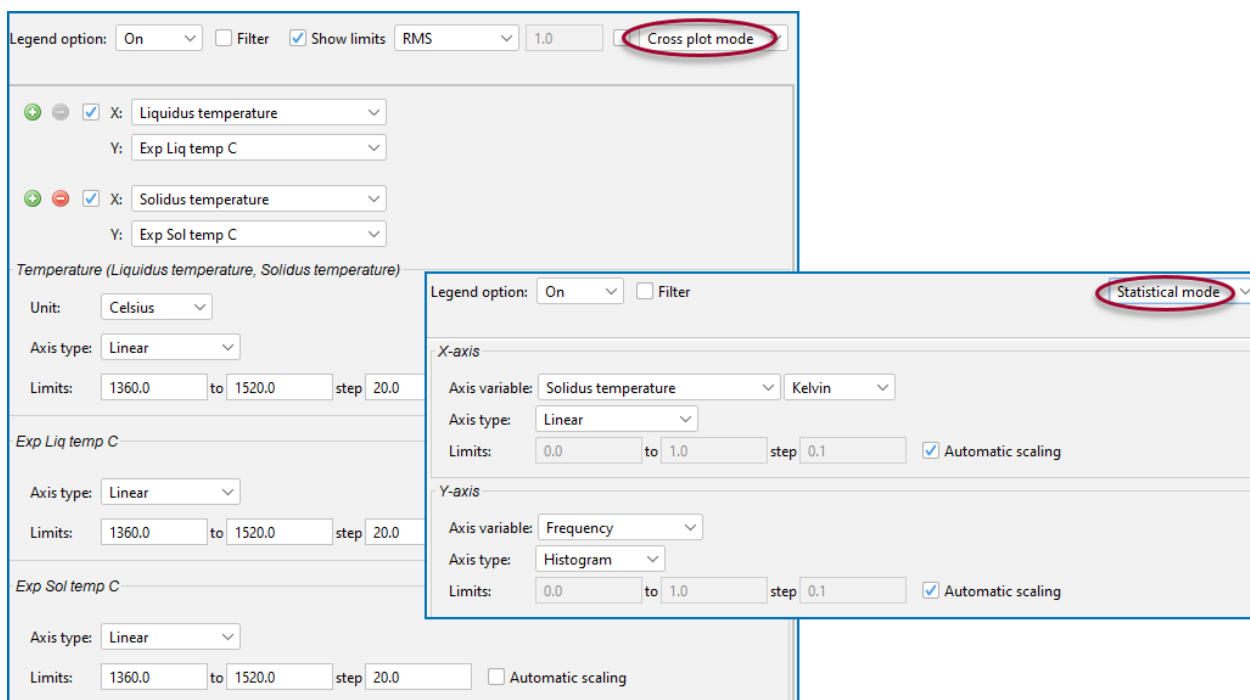
There are two new plotting modes available on the Plot Renderer that can be used with the Batch calculation - *Cross plot mode* and *Statistical mode*.

New Cross Plot and Statistical Modes on the Plot Renderer

The Property Model Calculator has both Batch and Uncertainty calculation types, and the Process Metallurgy Module also has the Uncertainty calculation type.

- **Statistical mode** is available with both **Batch** or **Uncertainty** calculation types. Use **Statistical mode** to select Frequency or Normal probability as the Axis variable and then the Axis type is set to Histogram or Probability, respectively.
- **Cross plot mode** (aka a parity plot) is available with both **Batch** or **Uncertainty** calculation types. Use Cross plot mode to plot the experimental data from a Batch calculation with the calculated result, e.g. you might be looking at liquidus temperature and now can plot both to compare the experimental data against the Thermo-Calc calculated results. You choose the experimental data value (which is read from the data file) as an X- or Y- Axis variable and then the calculated result as the other X- or Y- Axis variable.

Also see the New CCT and TTT Plot Modes for the Steel Model Library.

Switching between Cross plot mode versus Statistical mode on the Plot Renderer for the new PM_G_12 example.

New Example and Video Tutorial

Open the Thermo-Calc project file in Thermo-Calc then watch and follow the video tutorial to learn more. Search the help for "Working with Batch Calculations" to fully understand the requirements for creating a good datafile. From the menu, select **Help > Example Files > Property Models > General > PM_G_12_Solidus_and_Liquidus_Batch_Calculation.tcu**

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📹 There is a video tutorial associated with the new example available with the Property Model Calculator examples on our website.
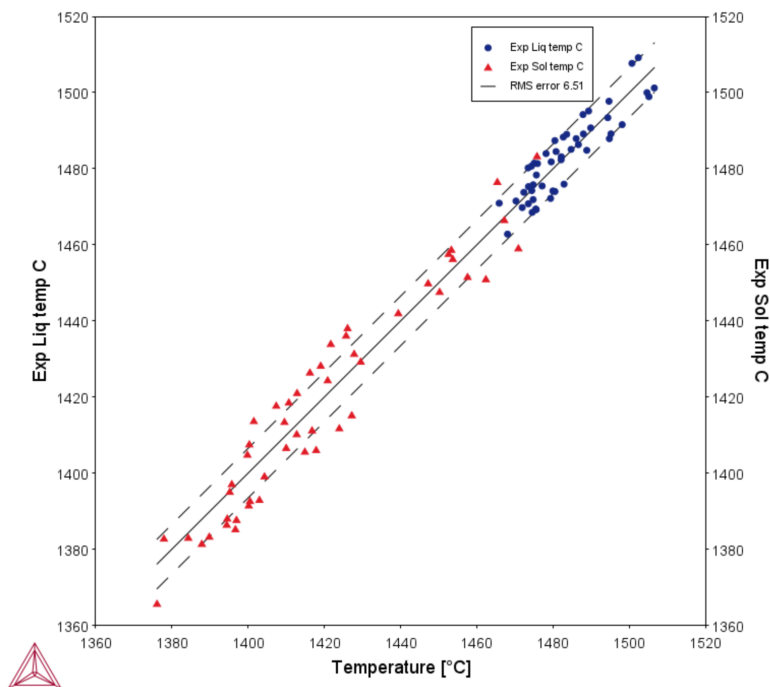
The results from example PM_G_12 showing a comparison of experimental liquidus and solidus data using the Cross plot mode with a Batch calculation. A root mean square (RMS) setting shows the distribution of the data points.

Save (Export) Tables from the Plot Renderer

For all calculation types and calculators, you can now convert a plot to table data from the Plot Renderer. A new **Table View** button allows you to toggle displaying the Plot or Table in the Results window as well as Save the table and export to file, for example to a spreadsheet.

When you click the button to toggle ON, click **Perform** to regenerate as a Table. When you click to toggle OFF, click **Perform** to regenerate the Plot. For example, set up the Plot Renderer and click **Perform** to display the Plot. Then click **Table View** and **Perform** to see the results in a table format in the Results window.
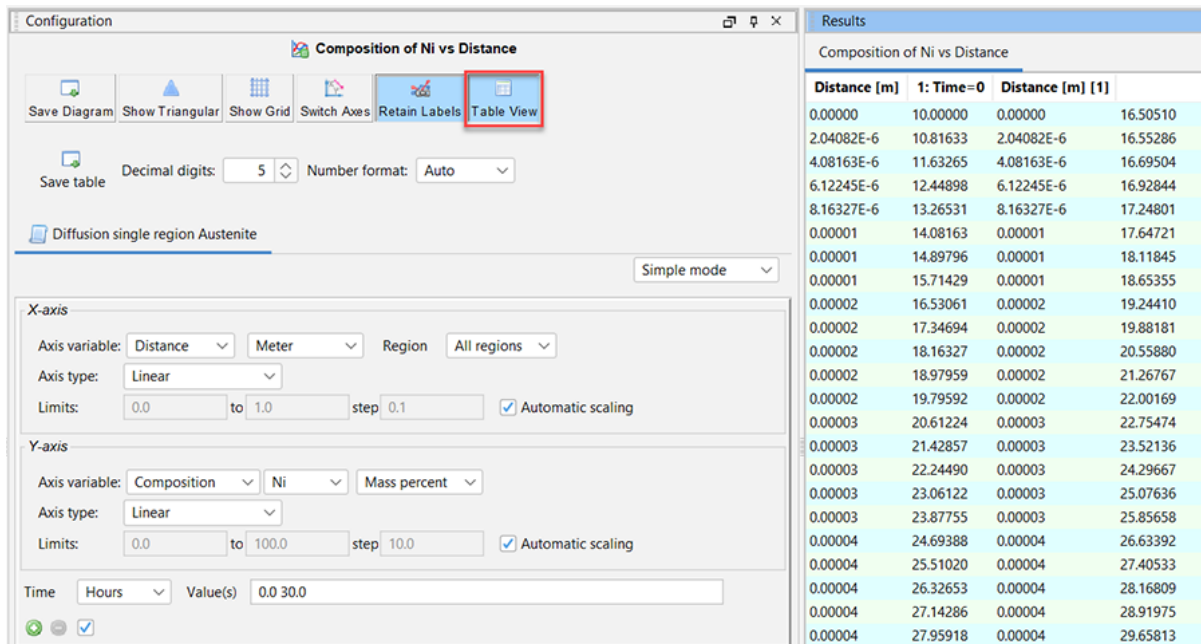
Table View button in the Graphical Mode of Thermo-Calc allows you to easily convert plot results into tabular data.

Filter Quantities in Plots and Tables

A new check box is available on the Plot Renderer and is available with the Property Model Calculator and Process Metallurgy Calculator. Use the *Filter* check box to filter the data that is visualized on the plot or table data and based on the set up of the calculation. For example, enter a *Min* and *Max* and choose an axis variable such as *Ms Temperature* and the unit *Kelvin* to adjust the output in the **Results** window. Click **Perform** each time you add or remove a filter for the results to update.
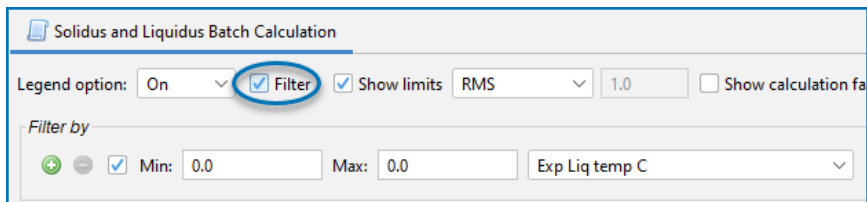
An example of the Filter check box available on the Plot Renderer that is a successor to the Property Model Calculator. This is a screenshot from the new Batch calculation example PM_G_12.

3D Plots Restored to macOS and Linux

3D plotting is available with *Grid* calculations using the Equilibrium, Property Model, and Process Metallurgy Calculators. For 2021a, this plot type did not work with macOS and Linux but this is now fixed and available again.

Other fixes and improvements for all operating systems include that ternary plots are now possible in 3D for all operating systems, 3D plots scale better on high resolution screens, and various bugs were fixed

such as where fullscreen or detached plot windows turned black, and where previously trying to open a project file after generating a 3D plot gave an error.
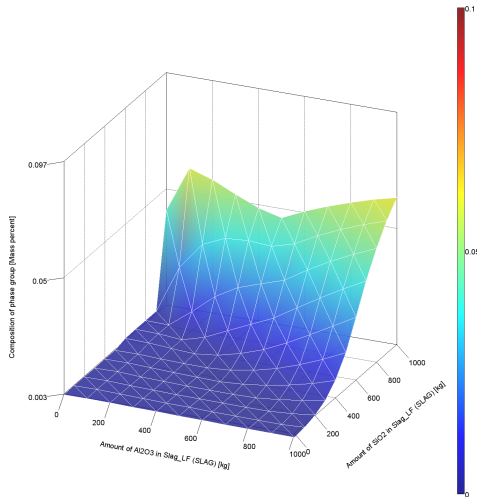
Improvements and Bug Fixes

Graphical Mode

Plotting Related

- It is now possible to edit / remove the annotations for the contour plot lines in a contour plot.
- When trying to save a plot in PNG format with a too high resolution there are two new windows that open depending on the issue that happened. One window opens to suggest saving the image at a lower resolution, or if a different error has occurred there is a message describing this.
- Fixed a bug that caused disabled plot axes in Grouped Mode plots to be saved as enabled.
- Fixed the U-fraction plot in the GUI that previously had missing lines in some cases.

Project File Related

- Fixed a bug related to the wrong reference state phase being selected when a project file was opened, even though it was correctly set in the System Definer.
- Project files with Property Model Calculators containing results were sometimes not opened with these results.
- It was not possible to perform with an Equilibrium Calculator that was added to a System Definer from a project saved with results.
- User-defined system components were sometimes lost when opening a saved project file.

Calculation Related

- In Scheil with back diffusion settings, the calculated value of secondary dendrite arm spacing is now shown.

For the Property Model Calculator:

- Fixed an exception that occurred when changing calculation type.
- Fixed a bug where Min/Max calculations with more than two quantities were not configured correctly.

- Fixed a bug found in version 2021a that the default values of model configurations were not honored as the Mean for Min/Max and Uncertainty types of calculations.
- The Property Model min/max and uncertainty calculations now update the arguments.

Both Graphical and Console Mode

Plotting Related

- In plots after a Scheil calculation, it is now possible to plot thermophysical properties such as surface tension and viscosity.

Calculation Related

- Made mapping faster for a case where there are no tie-lines in the plane.
- Scheil with back diffusion has a revision to the algorithm. With small amounts of slow diffusers back diffusion could previously have very little effect, with the revised treatment this is no longer the case.
- Fixed a crash that could happen if both an ionic liquid and an option B or F phase were used.
  - Option F: An ordered FCC or HCP solution phase with four substitutional sublattices and an optional interstitial sublattice.
  - Option B: An ordered BCC solution phase with four substitutional sublattices and an optional interstitial sublattice.
- Suspending and restoring components could result in the wrong equilibrium if it was preceded by equilibrium calculations based on other suspended components.

Database Related

- Fixed a bug where database parameters were not read into the software if the phase name is an abbreviation of another phase, and in particular when there are more than 500 phases in the system.
- The parser of TDB files that is used in the Thermo-Calc *Database Checker* and *TDB Editor* applications now gives warning messages for tab characters that are encountered in TDB files. Although tab characters are valid whitespace characters in most contexts, these have previously on occasion caused issues in the Thermo-Calc application.
- Increased internal data structures to be able to read all of the TCNI11 database.

General or Other

- Improved the GUI to have better support for high resolution screens, native Windows 10 window snapping and scaling, and more.
- Fixed a bug that occurred when moving a mouse over a plot, making the tooltips flicker and sometimes these were not displaying.
- The splash screen no longer hangs if the application cannot retrieve a valid license. Instead an error message is displayed.

Property Models and/or the Steel Model Library

Steel Library: New CCT Diagram and TTT Diagram Models

Two new Property Models are available for the Steel Model Library, which requires a valid maintenance license plus licenses for both the TCFE (version 9 and higher) and MOBFE (version 4 and higher) databases.
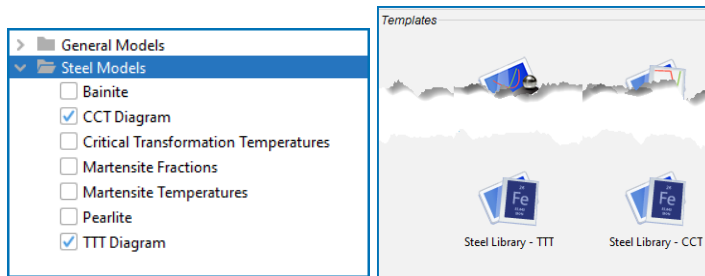
New CCT Diagram and TTT Diagram Property Models and an updated Steel Library TTT template and new CCT template.

CCT Diagram Property Model

A **CCT Diagram** Property Model, or continuous cooling transformation (CCT) diagram, is added to the Steel Model Library. This model combines the Pearlite, Bainite, and Martensite Property Models and calculates the kinetics of concurrent transformation of austenite into pearlite, bainite, and martensite under continuous cooling conditions. There is a new **Steel Library - CCT** template available where the CCT Diagram Model is automatically selected on the Property Model Calculator with all settings by default.

A new example *PM_Fe_08_Fe-C-Mn-Si-Cr-V_CCT.tcu* is available in the **Property Models > Steel** folder in Graphical Mode.

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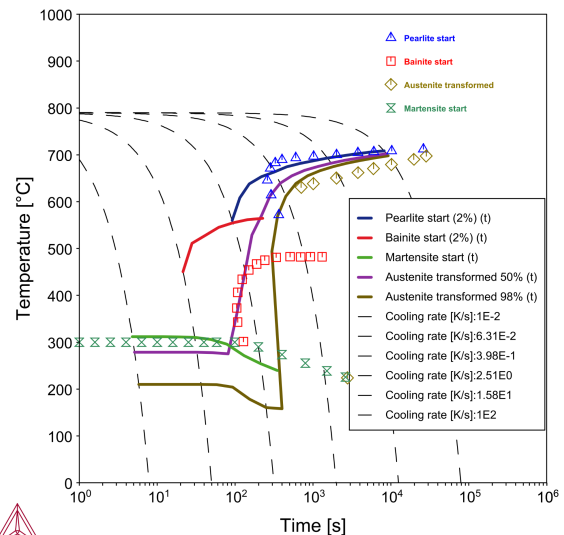
TTT Diagram Property Model

The **TTT Diagram** calculation is improved to calculate the concurrent transformation of austenite into pearlite, bainite, and martensite under isothermal conditions. In previous releases, pearlite, bainite, and martensite were calculated separately. The concurrent transformation is now handled in a new Property Model named TTT Diagram. The **Steel Library - TTT** template is updated to reflect the changes, where the TTT Diagram Model is automatically selected with all settings by default.

A new example *PM_Fe_06_Fe-C-Mn-Si-Cr-V_TTT.tcu* is available in the **Property Models > Steel** folder in Graphical Mode.
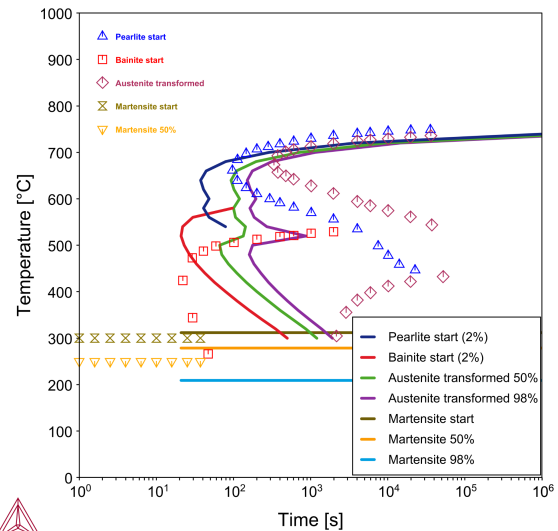
New CCT and TTT Plot Modes

These plotting modes are available with the Plot Renderer associated with a Property Model Calculator with either a CCT Diagram or TTT Diagram Property Model selected.

- Use *CCT mode* to make a CCT diagram from a One-axis calculation with log10(cooling rate) from the CCT Diagram Property Model. The x- and y-axes are time and temperature, respectively. Result quantities defined as time-temperature pairs are identified and plotted. Cooling curves are also automatically added in the plot.
- Use *TTT mode* to make a TTT diagram from a One-axis calculation with temperature. The x- and y-axes are time and temperature, respectively. Temperature axis quantities (such as Ms, M50) are independent of time and plotted as horizontal lines.

Also see New Cross Plot and Statistical Modes on the Plot Renderer.

An example of the Steel Library - CCT template showing the new CCT and TTT plotting modes available.

Certain defaults are set up on the Property Model Calculator (renamed Steel models) and the Plot Renderer (renamed CCT) and when you add either this or the Steel Library - TTT template.
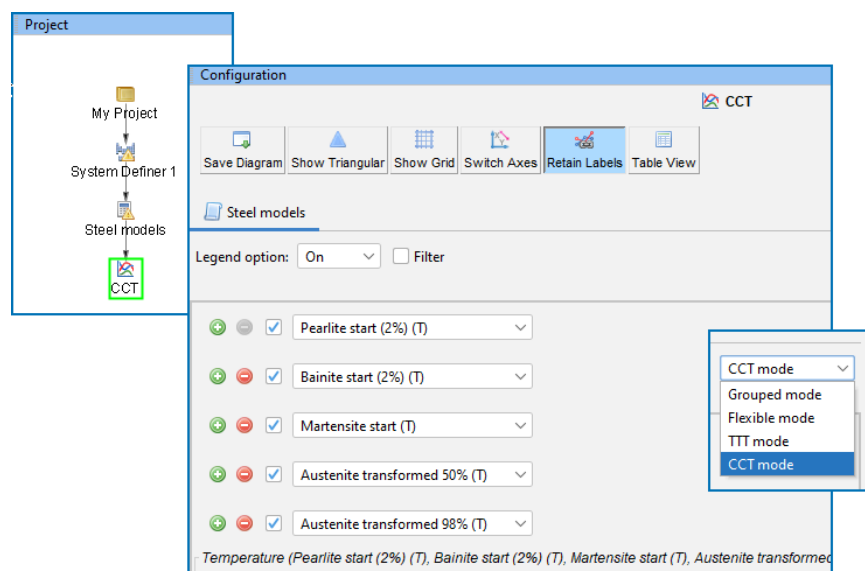
New Timeout Option to Stop a Calculation after a Set Time

On the Property Model Calculator Configuration window, there is a new check box available. Use this when you are running a complex or unknown outcome and do not want it to take computer time. The number entered in the field means that this is the maximum amount of time that each line can take for an individual calculation. This is useful in particular for a Batch or Uncertainty calculation.

☐ Timeout in minutes: 30.0

Property Models: Bug Fixes and Improvements

Also see Thermo-Calc Improvements and Bug Fixes for some general Property Model Calculator changes.

Martensite Temperatures and Martensite Fractions Property Model (TC-Python)

The **Martensite Temperature** and the **Martensite Fractions** Property Models are now converted into the new TC-Python based Property Model framework. Execution time of the models is improved. Project files from earlier releases are compatible with the new models. See TC-Python API for additional changes to that SDK.

Freeze-in Equilibrium Property Model

- Generalized the empirical handling of scattering on grain boundary phases and the selection of matrix phase, which is no longer required. The electrical resistivity due to phase interface scattering is now evaluated as the scattering constant times sum of the interaction between the volume fraction of all the phases. The contribution to thermal conductivity is assumed to be related to that to electrical resistivity, following the Wiedemann-Franz law.
- Also fixed a problem when grid calculations of the Freeze-in Equilibrium model included zero amount compositions.

Crack Susceptibility Coefficient Property Model

- Fixed an issue in cases when the Scheil simulation has endothermic reactions so it no longer gives negative result values.
- This Property Model now automatically selects a liquid phase in cases where *None* was selected for the liquid. Previously, the model only matched the phase named LIQUID before and this failed (for example with IONIQ_LIQUID) when there is no phase named LIQUID.
- The Property Model sometimes failed to find the A1 temperature when carbonitrides were stable at this temperature.

Reminder for Legacy Property Model Development Framework

The Property Model Development Framework is now integrated into TC‑Python. The Property Models that previously used the Jython API are discontinued. Existing Jython-based Property Models will continue to be supported until the June 2022 release of Thermo‑Calc (version 2022a). It is recommended that users migrate to the new TC-Python Property Model framework that is based on regular Python 3 and has full support for any Python package including NumPy, SciPy, and so forth. Also see Property Models in TC-Python.

Process Metallurgy Module

New Features

New Statistical mode is available on the Plot Renderer when using an Uncertainty calculation type. See [New Cross Plot and Statistical Modes on the Plot Renderer](). Also see [Filter Quantities in Plots and Tables]().

Improvements and Bug Fixes

- Normalizing any material composition without any threshold if "Normalize to total of 100%" is chosen (previously the scaling was actually only performed if the sum of components was below 99%), this fixes calculations failures occurring for material compositions summing to ca. 99% as well.
- In some cases there is an improvement to calculation performance. By preventing multiple license checkouts during a calculation (which previously happened approximately once per second), it will reduce the load on the license server and potentially speed up the calculation.
- In addition to the TCOX11 database updates, also fixed an issue related to the Process Metallurgy Module. In TCOX11, all carbides and nitrides available in the steel database (TCFE) were added. This prevents calculation failures during the initial enthalpy calculation of additions with high carbon and nitrogen content (such as ferroalloys) that were previously a problem.
- Support for TCOX11, which is mostly related to the addition of the new element K and all its components in slag and gas.
- Fixed that the heating efficiency specified in the Process Model was not saved to disk. It was always reset to 100% when reloading the file previously.
- Fixed a bug where no matter what activity is chosen on the Plot Renderer, the first option was plotted instead of the one selected by the user.
- Show correct component composition (Na_2O, Al_2O_3, Fe_2O_3) for $NaFeO_2$ and $NaAlO_2$.
- Fixed a bug that showed the component activities twice in the Table Renderer.
- Fixed a bug that made the liquid metal / slag determination fail for one-sublattice ionic liquids such as pure S or Fe. This prevented usage of zones consisting of pure metal with one element only, for example Fe.
- No longer throwing an exception if the mass of exhaust gas is plotted but no exhaust gas is present in the calculation.

Gibbs Energy System (GES6)

GES6 Improvements and Bug Fixes

- Fixed an issue with GES6 being unaware of fixed variables set to zero in PARROT.
- Improved the performance of ideal phases in GES6, most notably the gas phase.
- The consistency checking of disordered and ordered phases is improved. The improved consistency checking applies to the Thermo-Calc application, the Database Checker and the TDB Editor.
- Magnetic contributions to electric properties were previously not supported by GES5 in error.

- TERNARY, QUATERNARY, and QUINARY ionic liquid parameters gave wrong contributions in GES6 when there were many constituents selected in the phase.
- Some ionic liquid interaction parameters were not reaching GES6, instead they produced an error "END MEMBERS MUST HAVE DEGREE ZERO"

Also see the Thermo-Calc Improvements and Bug Fixes section for additional items.

> 💡 **Important note for custom user databases that were previously accepted by older versions of Thermo-Calc.** It is recommended and probably required that the user database needs to be checked and corrected for errors before the TDB file can be used in 2021b.

> 📖 For further information about the changes to GES, see the 2019b , 2020b, and 2021a release notes on the website.

Thermophysical Properties

Important thermophysical properties continue to be added as shown in this summary of the major additions starting with 2020a.

Viscosity of Liquid	***New! TCCU4 and TCSLD4 2021b*** ● TCHEA4 and TCFE10 as of 2020a ● TCAL7, TCNI10 and TCOX10 as of 2020b ● TCTI3 and TCMG6 as of 2021a
Surface Tension of Liquid	***New! TCHEA5, TCOX11*, TCCU4, TCSLD4 as of 2021b*** ● TCAL7 and TCNI10 as of 2020b ● TCTI3, TCMG6 and TCFE11 as of 2021a *surface tension of oxide slag
Thermal Conductivity and Electrical Resistivity	***New! TCHEA5, TCNI11 as of 2021b*** *Updates for TCAL8 and TCMG6.1 in 2021b* ● TCAL7 as of 2020b ● TCMG6 as of 2021a
Molar Volume	Molar volume has been included with many databases for some time. Below lists more recent additions: ● TCOX10 as of 2020b ● TCMG6 as of 2021a

💡 In Thermo-Calc, press F1 to search the help for *Thermophysical Properties* (or search by database name) for model details and much more. You can also find information on our website about the [properties that can be calculated with Thermo-Calc and the Add-on Modules](). Additional resources will also be made available on our website in the near future so keep checking back or [subscribe to our newsletter]().

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

- Fixed a bug with the Yield Strength Property Model (found in Graphical Mode with the Property Model Calculator), which previously could not be loaded nor could any plots with results be plotted.
- Sometimes project files containing plots using the Yield Strength model could not be opened. This has been fixed.
- Fixed a bug that gave the incorrect initial volume fraction when pre-existing PSD (particle size distribution) was input for non-spherical particles at grain boundaries with a wetting angle different from 90°.

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 Only

- Caching is added, meaning that calculations you have previously run in the Diffusion Module (DICTRA) during your current session will be read from disk rather than re-calculated, saving time if you re-run the calculation. As a side-effect, project files containing diffusion calculations with results created in previous versions will be opened without results.
- When users change the configuration of the calculation to a configuration that has already been calculated, the results of that calculation will automatically be found and used instead of re-running the calculation. Since diffusion calculations often take a long time to run, this can be a significant time-saver.

- *Mixed zero flux and activity* Boundary Conditions can be used as a function in diffusion simulations. The function is entered using the same syntax as with Console Mode functions. These are included the Help (search for "Operators and Functions")
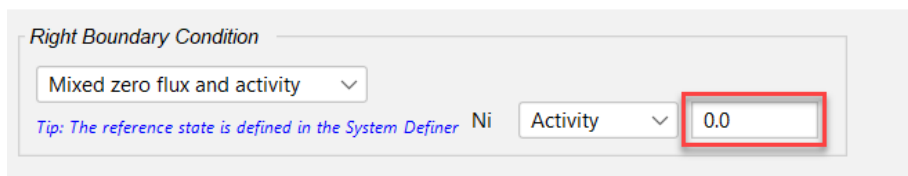
Also Applicable to TC-Python

- You can now enter the Activity boundary condition as a function. Previously it was just a numeric entry. This is also available in TC-Python.
- *Diffusion Improvements in TC-Python to Simulate Carburization Process:* several improvements to diffusion simulations in TC-Python allow users to calculate and optimize the carburization process if you work with the low pressure carburization process in furnaces. See Diffusion Model in the TC-Python section.

TC-Toolbox for MATLAB®

New TC-Toolbox for MATLAB® Entirely Re-Written

TC-Toolbox for MATLAB® (TC-Toolbox) provides an interface to the commonly used MATLAB® software for scientific and engineering computing. This software development kit (SDK) is ideal for fast realization of ideas and visualization of results during research and development activities. The API includes all calculation types available in Thermo-Calc Graphical Mode, such as single point equilibrium, property (step) and phase (map) diagrams, Scheil solidification simulations, as well as all the general Thermo-Calc Property Models (e.g. yield strength, spinodal, driving force, etc.).

With the addition of licenses for the applicable software and databases, you can further maximize your integration with MATLAB® to include the capabilities of the Steel Model Library Property Models (e.g. bainite, pearlite, etc.), as well as access the range of functionality included with the Diffusion Module (DICTRA) and the Precipitation Module (TC-PRISMA).

TC-Toolbox for MATLAB® is available on Windows platforms. Also see the product webpage for more information.

Legacy vs New Version of TC-Toolbox

As of 2021b TC-Toolbox for MATLAB® (TC-Toolbox) is completely rebuilt. The previous version, now referred to as *legacy* TC-Toolbox for MATLAB® (or legacy TC-Toolbox) can be installed along-side the new version. You can run both versions at the same time in MATLAB® although there is no communication between the two programs.

Compared to the new TC-Toolbox, the legacy version of TC-Toolbox for MATLAB® can only perform single equilibrium calculations, limiting the scope of simulations available. The rebuild includes significant upgrades compared to the legacy version and allows for easier implementation of new features in the future. If both versions are installed in parallel there is an example available (Benchmark Toolboxes) to run a comparison between the two to see that there is no significant change to the speed of calculations, even though there are many other differences making the new version more robust for most users.

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

Documentation and Examples

New Version

The new *TC-Toolbox for MATLAB® API Reference Documentation* is available either as interactive help (in HTML format or when in MATLAB® using tab completion or accessed via different menus or key combinations) or as a standalone PDF. Only information related to the new version of the software is included.

There are these ways to access the content:

- Directly in MATLAB® via the Help menu then under Supplemental Software click TC-Toolbox. Help is also available when writing code and using the tab completion feature and/or pressing different key combinations as described in the Best Practices section of the help.
- From the website: HTML Help or PDF
- Locally in a Thermo-Calc installation:
  - HTML: Help > Manuals Folder > TC-Toolbox_MATLAB, then click any HTML file.
  - PDF: Help > Manuals Folder > Software Development Kits (SDKs), then double-click to open the TC-Toolbox for MATLAB® API Programmer Guide. This is a copy of the HTML API reference documentation.

After installing Thermo-Calc, and when you first open the program, the set of folders containing the examples is copied from the source Public\Documents location into a user Documents folder: for example, *C:\Users\<user>\Documents\Thermo-Calc\<version>\SDK\TC-Toolbox-MATLAB\Examples*

Legacy Version

Legacy TC-Toolbox for MATLAB® documentation is no longer available in the Thermo-Calc help. The exception is for installation instructions, which are included as required. Legacy documentation as a PDF is available from the website documentation archive (for example, see the 2021a PDF on our website). It is also available with any previously installed versions of Thermo-Calc.

TC-Python API

Diffusion Model

Several improvements have been made to the diffusion calculations in TC-Python.

NOTE: Some of these changes also affect Graphical Mode when working with the Diffusion Module (DICTRA) and the Diffusion Calculator. These improvements are listed.

Resume Calculations

It is now possible to run a *DiffusionCalculation* and from the *DiffusionResult*, change some of the normal settings and then continue the calculation. This makes it possible to optimize, for example, carburization processes.

On *DiffusionResult* there is a new function

        with_continued_calculation

it returns a *ContinuedDiffusionCalculation*, which is a diffusion calculation with a subset of the normal functionality. On that calculation you can change settings and then call `calculate()` which returns a normal *DiffusionResult* (on which you can call `with_continued_calculation`, among other things)

Enter Activity Boundary Condition as a Function

You can now enter the Activity boundary condition as a function. Previously it was just a numeric entry. This is also applicable to Thermo-Calc Graphical Mode.

You can also specify a "time" upto which the function is used, thereby allowing you to set different functions for different time intervals.

Time Parameter Added

A "time" parameter is added to the following functions

- with_timestep_control
- with_options
- with_solver
- with_left_boundary_condition
- with_right_boundary_condition

This makes it possible to have these settings "per time interval". Before they could only be set for the entire simulation.

New Boundary Conditions with a New Example

Two new boundary conditions are added: `activity_flux_function` and   .

A new example for the `ActivityFluxFunction` boundary condition is available with the possibility to calculate and continue using *with_continued_calculation*

The example is found in the installation when you update to 2021b.

- `pyex_D_08_Diffusion_Carburization_Multiphase_Boost_And_Diffusion`

More Homogenization Functions for the Diffusion Module (DICTRA)

Several homogenization functions are added. To make this possible there is a new function to set the homogenization function. This means that the old function is deprecated and will be removed in 2022b. Users are encouraged to migrate their code before that.

Added homogenization functions:

- hashin_shtrikman_bound_prescribed(cls, phase: str):
- labyrinth_factor_f(cls, phase: str):
- labyrinth_factor_f2(cls, phase: str):

- general_lower_hashin_shtrikman_excluded_phase(cls, phase_list: List[str] = list()):
- general_upper_hashin_shtrikman_excluded_phase(cls, phase_list: List[str] = list()):
- hashin_shtrikman_bound_prescribed_excluded_phase(cls, phase: str, phase_list: List[str] = list()):
- hashin_shtrikman_bound_majority_excluded_phase(cls, phase_list: List[str] = list()):
- rule_of_mixtures_excluded_phase(cls, phase_list: List[str] = list()):
- inverse_rule_of_mixtures_excluded_phase(cls, phase_list: List[str] = list()):

Users need to migrate their code

To set these new functions (and also the once already present) use:

```
with_function
```

Migrate your code to that function from:

```
set_homogenization_function
```

These functions are present in the class `HomogenizationSolver`.

Property Models in TC-Python - Now Can Debug Models

As of 2021a, the Property Model Development Framework is now fully available via TC-Python.

When developing new Property Models you can start and debug a model from TC-Python. Previously this was only possible from Thermo-Calc Graphical Mode.

When developing Property Models, you can now have "common" source code that is shared between several Property Models.

Also see Martensite Temperatures and Martensite Fractions Property Model.

Bug Fixes

- Fixed the incorrect parameter name `constituent_name_to_deselect` to `constituent_name_to_select` in the the methods `system.SystemBuilder.select_constituent_on_sublattice` and `system.MultiDatabaseSystemBuilder.select_constituent_on_sublattice`
- Revised the doc-strings regarding spelling, grammar and method links

- Fixed not working caching of precipitation calculations if it used automatic calculation of the nucleation density (which is the default)

Removed Functions in TC-Python - Deprecation with 2021b

The following functions are renamed, and the old versions will be removed in this release, 2021b (June 2021). Users are recommended to review and update their scripts.

- The two methods *with_back_diffusion* and *set_fast_diffusing_elements* have been deprecated and the new method *with_calculation_type*, where you choose and configure one of three possible *ScheilCalculationTypes* should be used instead.
- NOTE. The parameter 'function' in the method *def get_system_function(self, function: str)* had to be renamed to 'f', without being deprecated for one year.

	Old Name	New Name
Class ElementProfile	`def function(cls, dictra_console_mode_function: str)`	`def funct(cls, dictra_console_mode_function: str):`
Diffusion options	`def enable_automatic_forced_starting _values_in_equilibrium_calculati ons()`	`def enable_automatic_forced_starting_v alues_in_eq_calculations()`
Diffusion options	`def set_default_driving_force_for_ph ases_allowed_to_form_at_interfac es()`	`def set_default_driving_force_for_phas es_allowed_to_form_at_interf()`
System	`get_ges_parameter` `set_ges_parameter,` `run_ges_command`	`get_system_data` `Moved to with_system_modifications in all calculation classes.`

New 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 Metal Oxide Solutions Database (TCOX11)

New Element

- Addition of K

Binary, Ternary and Higher Order System Updates

- K: Assessed or added from literature 24 binary, 13 ternary and 14 higher order systems.
- Added carbide and nitride phases.
- The following systems have been assessed: Al_2O_3-CaO-MgO.
- The following systems have been reassessed: Al_2O_3-CaO-MgO-SiO_2.
- Reassessed Fe-solubility in $MgSiO_3$ (ortho-pyroxene).
- Updated all metallic systems to be the same as in the TCFE database.

Thermophysical Properties

- Addition of surface tension of the ionic liquid phase.
- Addition of viscosity of the ionic liquid phase for the systems containing K.

TCS Al-based Alloy Database (TCAL8)

New Assessments

- 5 new elements: Nd, Pr, S, Se and Te
- 8 new assessed binaries: Al-Nd, Al-Pr, Al-S, Al-Se, Al-Te, Bi-Mg, Mg-Sc and Si-Y
- 9 new assessed ternaries: Al-Bi-Mg, Al-Cu-Ti, Al-Mg-Sc, Al-Mg-Sn, Al-Mg-Zr, Al-Mn-Ti, Al-Si-Y, Bi-Mg-Sn and Mg-Sc-Si
- 2 new assessed quaternaries: Al-Bi-Mg-Sn and Al-Mg-Sc-Si
- Surface tension, viscosity and volume of liquid, and electrical resistivity and thermal conductivity of some previously unassessed systems and some of the new systems have been modelled, e.g. viscosity for 175 binaries and surface tension for 70 binaries.

Other Updates

- Al-V and Al-Sc: the (Al) solvus is better described.
- Mg-Sn and H-Zn: new thermodynamic descriptions.
- Al-Li-Si: the ternary phases are refined to better account for their melting.
- Al-Ni-Si: the B2 description is refined.
- Al-Cr-Mg: Al18Mg3Cr2 (AL18MG3TM2) is refined.
- The partitioning ORD_L12 is removed. The compounds that it describes are merged into L12_FCC. This causes negligible changes in Al-Ce-Ni and Al-Mg-Ni, and triggers minor adjustments of Ag-Mg, Al-Ni, Fe-Ni, Ge-Ni, Mn-Ni, Ni-Si, Al-Cu-Ni, Al-Fe-Ni, Al-Mn-Ni, Al-Ni-Si, Al-Ni-Zn, Cu-Fe-Ni, Cu-Mn-Ni, Cu-Ni-Si, Fe-Mg-Ni, Fe-Mn-Ni, Mg-Mn-Ni, Fe-Ni-Si, Fe-Ni-Zn, Mg-Ni-Si, Mn-Ni-Si, Mn-Ni-Zn, and Ni-Si-Zn.
- ETA_PRIME, which is an important aging hardening precipitate, is refined in Al-Mg-Zn and Al-Cu-Mg-Zn.
- AL9FENI is identified as the metastable Al9Fe2 phase being stabilized by the Ni addition and thus renamed as Al9M2. The family of Al-Fe metastable phases is almost completely described.
- Thermophysical properties descriptions of many systems and for many phases are improved. These properties include viscosity and surface tension of liquid, molar volume, electrical resistivity, and thermal conductivity.

TCS Ni-based Superalloys Database (TCNI11)

Addition of the thermophysical properties Electrical Resistivity (ELRS) and Thermal Conductivity (THCD), which means that the derived properties Electrical Conductivity (ELCD), Thermal Resistivity (THRS) and Thermal Diffusivity (THDF) are readily available. In most cases, it is recommended to use the Property Model "Equilibrium with Freeze-in Temperature" to correctly predict these properties for an alloy.

TCS Cu-based Alloys Database (TCCU4)

- Two binary systems Cr-P and Ni-P are added.
- Three ternary systems Cu-Ni-P, Cu-Co-Si, and Ni-Sn-Zn are added.
- Addition of viscosity and surface tension data.

TCS Cu-alloys Mobility Database (MOBCU4)

This database is compatible with TCS Cu-based Alloys Database (TCCU4). The complete and critical assessments for FCC Cu-Al-Sn and Cu-Ni-Sn ternary systems and liquid Ni-P binary system are implemented. The description for FCC Cu-Al-Ni is updated.

TCS High Entropy Alloys Database (TCHEA5)

Addition of surface tension of liquid phase. Addition of electrical resistivity and thermal conductivity of liquid, BCC (A2, B2), FCC (A1, L12) and HCP solution phases.

TCS Solder Alloy Solutions Database (TCSLD4)

Addition of thermophysical properties: viscosity and surface tension.

Updated Database

TCS Mg-based Alloys Database (TCMG 6.1)

New Assessments

- The interaction parameters for liquid viscosity of 30 binary systems and 1 ternary system.
- The interaction parameters for surface tension of the liquid of 12 binary systems.

Other Updates

- Viscosity parameters of Al-Mg and Al-Ga systems were re-assessed.
- Surface tension parameters of the Al-Ga system were re-assessed.
- Improved thermal conductivity for systems including but not limited to:
    - hcp_A3 Mg-Al, Mg-Ce, Mg-Gd, Mg-Nd, Mg-Sm, Mg-Y, Mg-Zn, and Mg-Gd-Y.
    - fcc_A1 Al-Mg, Cu-Zn, Fe-Ni, Fe-Si, Mn-Ni, Ni-Si, and Ni-Zr
    - bcc_A2 Al-Fe, Fe-Ni, Fe-Si, and Ni-Zr
    - liquid Fe-Ni and more
- Improved electrical resistivity for systems including but not limited to:
    - hcp_A3 Mg-Sm, Mg-Nd, Mg-Gd, and Mg-Y
    - fcc_A1 Cu-Fe, Fe-Si, Mn-Ni, Ni-Si, and Ni-Zr
    - bcc_A2 Al-Fe, Cu-Fe, Fe-Mn, Fe-Ni, Fe-Si, and Ni-Zr
- Electrical resistivity and thermal conductivity were reassessed for Mg12Ce, Mg41Sm5, Mg5Gd, Mg41Nd5, Al12Mg17, MGZN and AlFe.
- Phase equilibria of Ce-La was extrapolated.

Installation

Thermo-Calc Changes

See TC-Toolbox for MATLAB® for the differences between the two versions. There are new instructions related to whether you are installing the new or legacy version or both. The details are described in the *Thermo-Calc Installation Guide*, available from various places including our website.

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, 2 GB of disk space is recommended for the 2021b 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.

Installation Folder Name Changed

If another installation folder than the default was chosen the folder name was <installationfolder>/Thermo-Calc/2021.1.82843-259. It has been changed to <installationfolder>/Thermo-Calc/2021b.

Documentation

Software Examples

There are several new examples described elsewhere in this document:

Scheil with Solute Trapping

- Thermo-Calc > Graphical Mode T_13_Scheil_with_Solute_Trapping.tcu
- Console Mode tcex57.TCM
- TC-Python pyex_T_16_Scheil_Solute_Trapping_Al_Si_Cu.py
- TC-Toolbox for MATLAB matex_T_16_Scheil_Solute_Trapping_Al_Si_Cu.m
- See New Examples.

Batch Calculations

- Property Models> General > PM_G_12_Solidus_and_Liquidus_Batch_Calculation.tcu.
- See New Example and Video Tutorial.

Steel Property Models

- Property Models> Steel > PM_Fe_06_Fe-C-Mn-Si-Cr-V_TTT.tcu
- Property Models> Steel > PM_Fe_08_Fe-C-Mn-Si-Cr-V_CCT.tcu
- See New - CCT Diagram and TTT Diagram Models

TC-Toolbox for MATLAB®

- See Documentation and Examples for information about the new and legacy versions.

Application Examples Now Included with the Installation

Several examples that were available on the website are now available with the Thermo-Calc installation. Details are included in the help or you can read more via the individual application website pages.

Database Examples of Thermophysical Properties

Surface Tension and Viscosity

There are 60 new example plots that are updated in the following Example Collections, which you can find on the website for each database and in the Thermo-Calc help when you press F1.

- Steels (TCFE), Magnesium (TCMG), Aluminum (TCAL), Nickel (TCNI), High Entropy Alloys (TCHEA), Titanium (TCTI), Copper (TCCU), and Solder (TCSLD)

Electrical Resistivity and Thermal Conductivity

The Magnesium (TCMG), Aluminum (TCAL), Nickel (TCNI), and High Entropy Alloys (TCHEA) databases all have these thermophysical properties and new examples are also included in the above Example Collections accessed via the website or in the help.

New Videos

There is a video tutorial associated with the new Batch calculation example available with the Property Model Calculator examples on our website. There is also a new release video available on the Release News section of the website.

Other Changes

Further to the Property Model Development Framework being integrated into TC-Python, the legacy PDF has been removed from the installation as of 2021b. The old PDF is available on the web and new documentation is part of TC-Python as described elsewhere. Also see Reminder for Users of the Legacy Property Model Development Framework.

Also being discontinued is the legacy version of TC-Toolbox for MATLAB®. As of 2021b, the documentation for the legacy version is only available on the website or in older installations of Thermo-Calc. See Legacy vs New Version of TC-Toolbox.

Platform Roadmap

A reminder to any users still using Windows 7 or Windows 8 to upgrade as soon as possible. Thermo-Calc stops supporting these platforms as of this release 2021b (June 2021).

Those who have used the Property Models Development Framework to develop Property Models are encouraged to migrate these to TC-Python as soon as possible based on the new integration with TC-Python.

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