Release Notes:

Thermo-Calc Software Package and Databases

Version 2022a

Contents

Thermo-Calc Version 2022a Highlights

★ **Thermo-Calc: New** Material to Material Calculator, updates to Scheil simulations, Quantities available for plotting and tables without the need for defining functions, General Einstein Model, performance improvements, and more

★ **Property Models and Model Libraries**: **New** Nickel Model Library with 3 Property Models

★ **Precipitation Module (TC-PRISMA)**: **New** grain growth and particle pinning

★ **Databases: New** and **Updated** databases

- 3 new databases TCZR1, TCPMAG1, MOBNOBL1
- 5 new versions of databases: Steel (TCFE12/MOBFE7), Aluminum (MOBAL7), Titanium (TCTI4), SGTE Solutions (SSOL8)
- 6 updated databases: Magnesium (TCMG6.2), Solders (TCSLD4.1), High Entropy Alloys (TCHEA5.1), Aluminum (TCAL8.1), Oxides (TCOX11.1), Nickel (TCNI11.0.1)

★ **Thermophysical Properties**: TCFE12 and TCTI4 have electrical resistivity (ELRS) and thermal conductivity (THCD) added. TCZR1 and TCPMAG1 are new databases where volume, surface tension, and viscosity are included.

Thermo-Calc

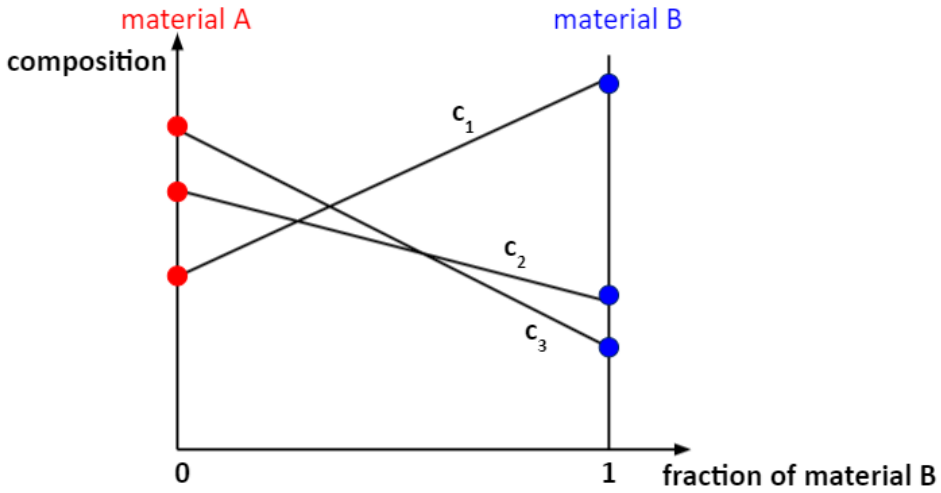
Material to Material Calculator

A Material to Material Calculator allows you to set the conditions for, and perform, a calculation to examine how materials can transition from one into the other. The calculator can be applied in any situation where different materials are in contact with each other and will react significantly, usually at high temperatures, or in instances where they will gradually transition into each other by design.

Typical applications include:

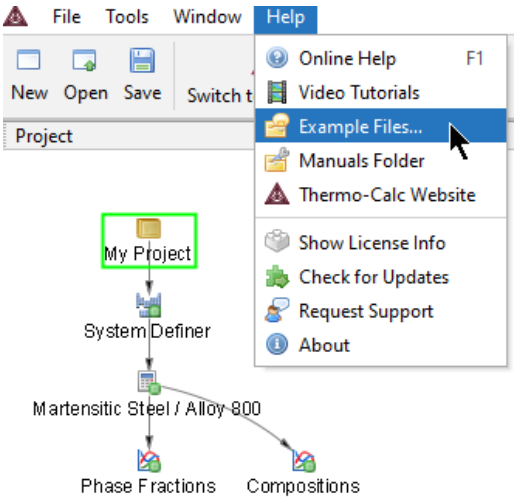
- Graded materials produced by additive manufacturing or other methods
- Non-similar material joints such as welds of titanium with nickel-based superalloys
- Reaction of two materials, for instance, the influence of volcanic ash on a turbine component in an engine
- and more

For example, you can look at the transitions of phase compositions (c_1, c_2, c_3 in the diagram) for two materials, A and B and then calculate an equilibrium, one axis (similar to a property diagram), or phase diagram to examine, for example, what phases may form at the interfaces or to see what kinds of reactions there might be at specific points in the transition. You can plot the fraction of the second material on the axis to compare to the composition or temperature, for example.

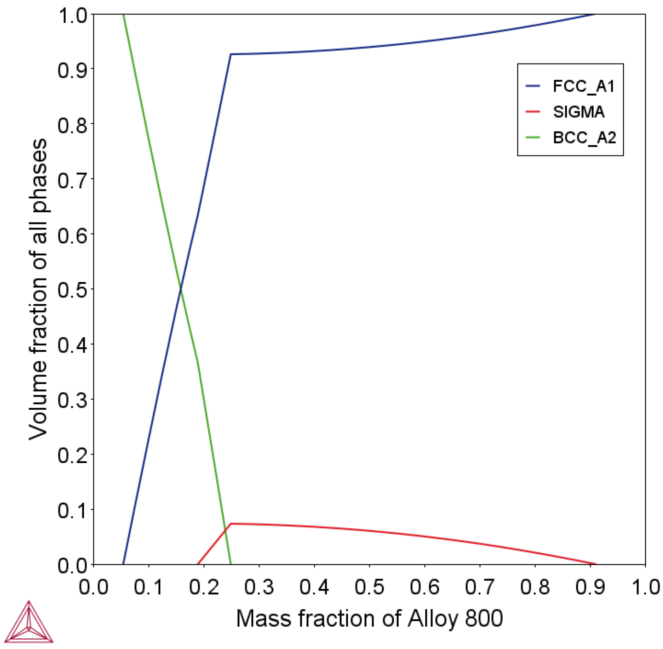


New Example, Video, and Webpage

A new example is included in the installation and an accompanying video tutorial is available. There is also a new webpage.



The example is included with the Thermo-Calc installation. From the **Help** → **Example Files** menu, navigate to the **Thermo-Calc** folder and open *T_14_Fe-Cr-Ni_Material_to_Material.tcu*. The calculations in this example search for potential deleterious phases during heat treatment of alloys joined together. See the help for more information.



This plot from the new example shows the volume fraction of phases when changing composition from the Martensitic Steel (First material) to the Alloy 800 (Second material).

The accompanying video tutorial for the *T_14* example can be found via our website or the Graphical Mode Examples playlist on our YouTube channel. There is also a new dedicated webpage about the Material to Material Calculator available.

Scheil Simulation Updates

The following changes are for all Scheil simulations. The location or way to implement a setting is based on whether you are in Thermo-Calc Graphical or Console Mode or if you are using TC-Python or TC-Toolbox for MATLAB®. Settings for Graphical Mode are found on the Scheil Calculator Configuration window, and for Console Mode there are updated or new commands. These individual commands are added in order to not break existing macros that users may have in place. Further details are included with the descriptions below or found in the help.

Global Minimization Turned On by Default and New Global Test Interval Option

The setting for global minimization is now turned on by default for all simulations. There is also a way to control the global test interval. By default this test interval is set to every 10th step, but a global test is also always performed when the set of stable phases changes. Note that in prior Thermo-Calc versions the test was made every step if global minimization was turned on.

- Graphical Mode: Scheil Calculator under Advanced settings. Settings are called **Global minimization** and **Global test interval**
- Console Mode: New command `TEST_INTERVAL_FOR_GLOBAL`
- TC-Python and TC-Toolbox for MATLAB®: For the new setting use the method `set_global_minimization_test_interval` in `ScheilOptions`

New: Equilibrium of Liquid Above Liquidus

A new setting to start the calculation from the start temperature has been added, which includes the results for the liquid phase above liquidus and up to the start temperature.

- Graphical Mode: Scheil Calculator under Advanced settings. Setting is called **Calculate from**
- Console Mode: New command `CALCULATE_FROM_START_TEMPERATURE`
- TC-Python and TC-Toolbox for MATLAB®: New `ScheilOptions` methods `calculate_from_liquidus` and `calculate_from_start_temperature`

New: Calculate Scheil without the Equilibrium Solidification Line

It is now possible to perform Scheil calculations without the one axis (step) equilibrium solidification that is done before the actual Scheil calculation. The one axis/step calculation is used to plot the equilibrium solidification curve, which is shown for comparison if the default axis variables are used. For Thermo-Calc users, this is set on by default. For TC-Python and TC-Toolbox for MATLAB® this setting is disabled by default because turning it on generally would not provide any benefits.

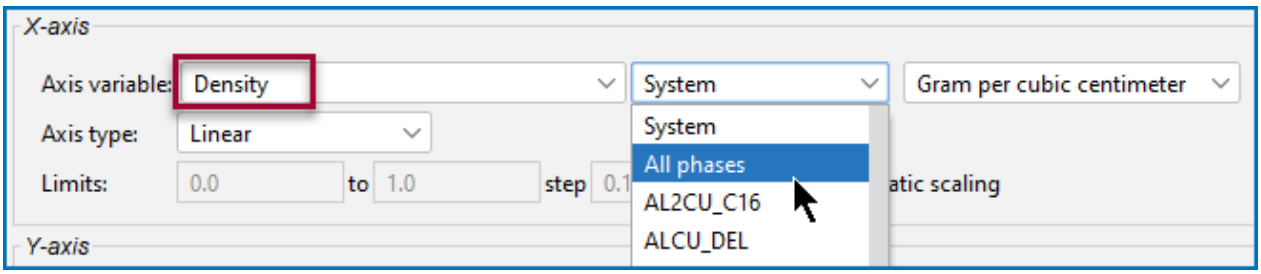
- Graphical Mode: Scheil Calculator under Advanced settings. Setting is called **Include one axis equilibrium calculation**. Enabled by default.
- Console Mode: New command `SKIP_STEP_CALCULATION`. Enabled by default.
- TC-Python and TC-Toolbox for MATLAB®: Use the new `ScheilOptions` methods `disable_equilibrium_solidification_calculation` and `enable_equilibrium_solidification_calculation`.

Scheil Plotting-related Improvements

For both Console Mode and Graphical Mode, generally, fixed several issues with plot legends after Scheil calculations. It is also now possible to plot and tabulate the density of liquid (DS(LIQUID)).

Density of Phase Quantity Deprecated and Replaced with New Setting Options

In Graphical Mode, a plot quantity, called *Density of phase*, is removed from the plot quantities lists (e.g. on the Plot Renderer when choosing an axis variable). This is because the *Density* quantity is now configurable per phase.



An example of the new settings on a Plot Renderer available for the Density quantity which has been expanded to include options for both the System and individual phases.

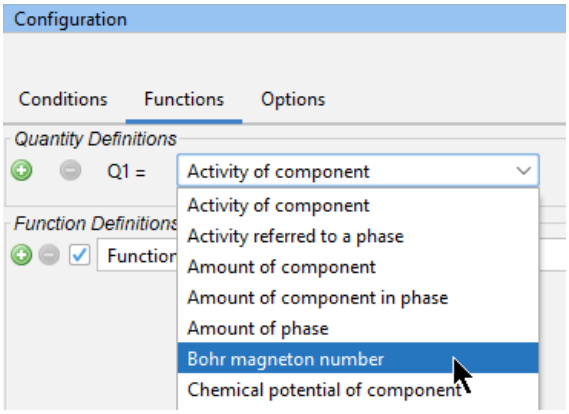
Improvements to Thermal and Electric Properties After Scheil

The evaluation for thermal conductivity, thermal resistivity, electrical conductivity, and electrical resistivity has been made more accurate in this release.

Thermo-Calc Quantities Available for Plotting and Tabulating Instead of Entering as a Function

The following quantities are now available directly for plotting and tabulating in Graphical Mode and via the Equilibrium Calculator when defining a quantity. Previously these needed to be entered/defined as specific functions.

- Bohr magneton number
- Curie temperature
- Density
- Heat capacity
- Isothermal compressibility for the system
- Phase stability function
- Thermal expansivity for the system
- Volume fraction of phase

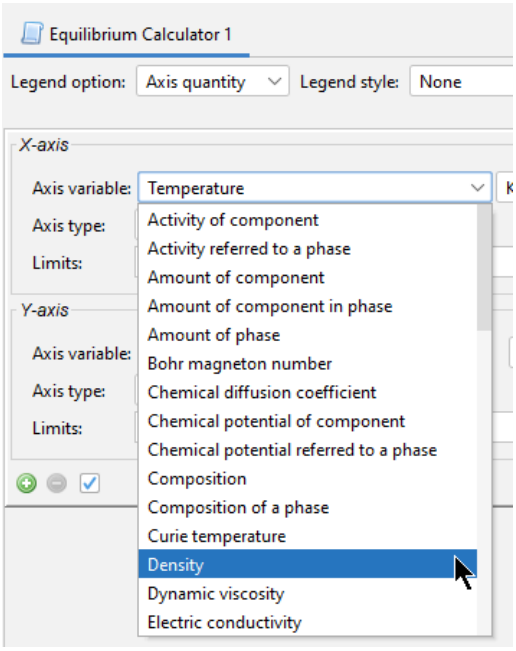


An example of where to find the new quantities on the Equilibrium Calculator Configuration window. Previously these quantities had to be defined as Function Definitions whereas now you can choose from the Quantity Definitions list.

All quantities (not just those listed) are also in alphabetical order in the drop-down menus for Equilibrium Calculator Conditions, Quantity Definitions (on the **Functions** tab), and table and plot results specifically for these types of calculations: *One axis* equilibrium, *Phase diagram*, and for binary and ternary calculations.

The change means that you can choose these quantities from the drop-down lists instead of having to go to the Functions tab and then name and define these functions as an extra step. So for example, for plots and tables, each quantity is selected on the **Configuration** window as required either as **Axis variables** for the Plot Renderer or when choosing the **Columns** for a Table Renderer.

*An example where you can find these quantities on a Plot Renderer for an Equilibrium Calculator. Here you can now choose these specific quantities from the **Plot Renderer** or **Table Renderer** drop-down lists (for example) instead of having to define it on the **Configuration** window → **Functions** tab.*



Improvements and Bug Fixes

Graphical Mode

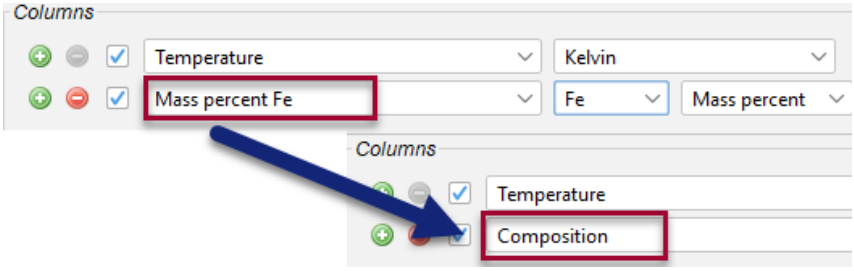
General

- Fixed a bug with some Functions that required unit conversion of quantities in the Equilibrium Calculator.
- Fixed a bug where grid equilibrium calculations did not include the max coordinates of the grid.
- Scrolling actions from the various Configuration windows is improved.
- Database cache for Graphical Mode is now installed and not created on a user's machine. This means that you do not need to wait (sometimes a long time) for the cache to be created the first time a database is opened in Graphical Mode, especially for a new release.
- Fixed an issue with the Scheil Calculator where previously in error a non-liquid phase could be selected by default instead of the liquid phase. This previously occurred with some databases when elements were selected and then deselected.
- When cloning some calculators that had calculated results, and then saving the project there was a bug that prevented saving without errors. This has now been fixed.

Plotting Related

Some plotting items included with the Property Models section instead of here

- Fixed a bug on the Plot Renderer that caused the incorrect scaling of an axis after opening a project file, i.e. After entering the scaling settings manually, it was applied to the wrong axis in the plot.
- Grid calculation results can now be visualized using Log10 and Ln scaling along the Z axis. This applies to all plot types: Contour, Heat Maps and 3D.
- The diffusion coefficients shown in single equilibrium table views were not the ones selected in the configuration.
- When all components were selected for the composition quantity, the result for only one element was shown in one axis plot.
- Change in quantity list selection option. **Composition** is now available from drop-down lists and replaces the text, ***Mass percent** X*, where *X* was a component. This is applicable in the following quantity lists:
    - Table columns
    - Equilibrium Calculator: Quantity definitions under Functions
    - Property Model Calculator (Equilibrium model): Quantity definitions under Configuration



Both Graphical and Console Mode

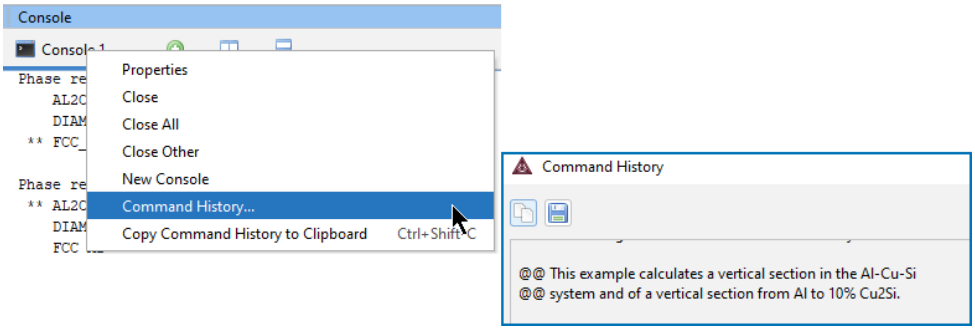
- Fixed a bug where long-running calculations used increasing amounts of memory. This bug, which affected all calculations, sometimes led to out-of-memory conditions and application crashes. Also, the application's memory management is significantly improved, which reduces the application's memory footprint in general. For large databases, the reduced memory usage may amount to several hundred megabytes per process.
- Fixed two items for Scheil calculations. Calculations now start correctly when the alloy is still liquid at room temperature. Also fixed a bug that sometimes caused calculations to finish immediately after the initial step calculation before results were actually calculated.

Console Mode

- You can now double-click a macro file to open it in an already running instance of Thermo-Calc. Previously, a new instance of the software was launched each time. When Thermo-Calc is already open, Console Mode files open in a new tab. Otherwise a new instance of Thermo-Calc is launched to open the files. This behavior now also occurs when you drag and drop a file on the executable, or start Thermo-Calc from the command line with a file argument, that is if Thermo-Calc is already open it launches the relevant file in the running instance. Note that the exception to this is when you are using the advanced pipe or redirect output data option in Console Mode where a new instance of Thermo-Calc is always started. That is, the behavior has not changed.

New Ways to Copy or Save a Command History

You can now copy a command history to the clipboard or save it to a macro (.TCM) file from any Console Mode window tab.



- To save a history, right-click any tab and select **Command History** then click the Save button to save all the commands in a .TCM file format.
- There are multiple ways to copy commands to a clipboard: Press CTRL + Shift + C in the window or tab where you want to copy the command history, right-click any tab and select **Copy Command History to Clipboard** from the menu, or right-click any tab and select **Command History** then click the **Copy** button to copy all the commands to the clipboard. In all cases, paste in a text editor as required.

Property Models and Material Specific Model Libraries

New Nickel Model Library

A new set of Property Models is available for Nickel-based alloys and systems. The Nickel Model Library is a package of pre-built Property Models that allow for easy set up of some common calculations used by those working with nickel-base alloys.

The Nickel Model Library includes these Property Models for nickel:

- **Antiphase Boundary Energy**: Calculates the antiphase boundary energy for the gamma prime (γ') phase in Ni-base alloys. The new example, PM_Ni_02, uses this Property Model.
- **Coarsening**: Calculates the coarsening rate coefficient K of one or several precipitate phases in a matrix phase, assuming spherical geometry of the precipitating phase(s).

- **Equilibrium with Freeze-in Temperature**: Calculates equilibrium at the freeze-in temperature and evaluates the properties at a different temperature. The new example, PM_Ni_01, uses this Property Model.

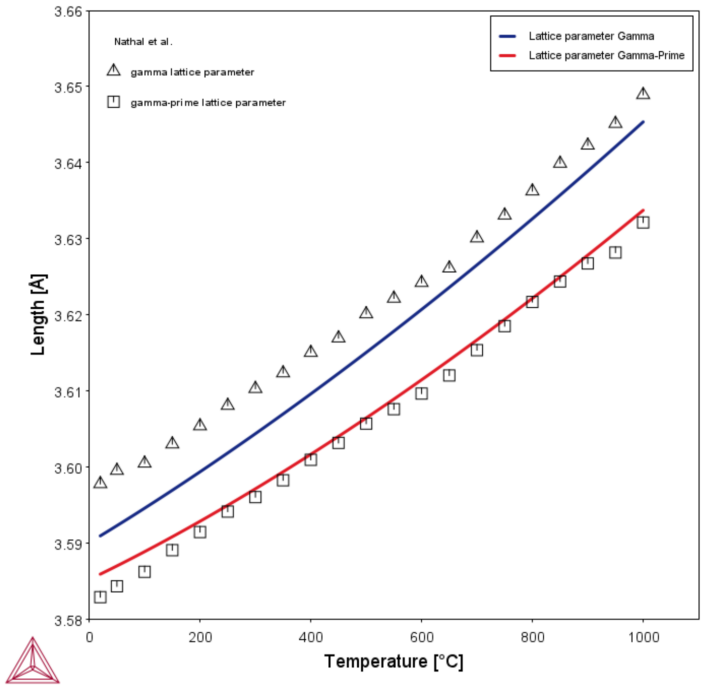
The Nickel Models require a license for the Nickel Model Library, which is available for free to all users with licenses for the databases TCNI (version 11 and newer) and MOBNI (version 5 and newer), plus a valid Maintenance & Support Subscription (M&SS).

New Examples and Webpage

Two new examples are included in the installation and there is also a new webpage—Nickel Model Library.

The examples are included with the Thermo-Calc installation. From the **Help→Example Files** menu, navigate to the **Property Models→Nickel** folder to open the examples.

- PM_Ni_01_Lattice_Parameter_of_Gamma_Gamma_Prime.tcu
- PM_Ni_02_Antiphase_Boundary_Energy_of_Gamma_Prime.tcu



A plot from the new example PM_Ni_01 showing the lattice parameters for γ and γ' plotted against experimental data. For more information see the Help.

Steel Library

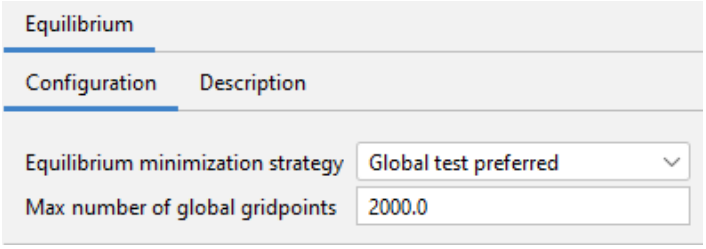
Bug Fixes and Improvements

- Improved code robustness for TTT and CCT Property Models when interpolation is used (for example, Calculation Setting "Quick")

General Property Models and the Property Model Calculator

Bug Fixes and Improvements

- The Property Model Calculator is refactored and now when running the same Property Model with the same input for a second time, the caching functionality finds the previous result and uses that instead of recalculating.
- For all Property Models, fixed inconsistent error messages when a Property Model name was suppressed.
- Fixed a bug that threw an exception on the Plot when changing calculation types in the Property Model Calculator.
- Updated a Precipitation Module (TC-PRISMA) example using the **Yield Strength** Property Model. Example *P_01_Precipitation_Al-Sc_AL3SC.tcu* now uses
    - The precipitation strengthening model now uses Seidman model (Al-base)
    - The interfacial energy prefactor changed to 0.75*calculated
    - The antiphase boundary energy changed to 0.6
- **Yield Strength**: intrinsic strength different with and without solution strengthening.
- Bug fixes YS-model - Solid solution strengthening for FCC_L12 phases are no longer evaluated if these are found to be either a carbonitride or gamma prime.
- The interfacial energy calculations used in the **Coarsening** and **Interfacial Energy** Property Models are rewritten from Jython to a TC-Python based API.
- Fixed a bug in the **Driving Force** model that could result in metastable phases not converging, thus resulting in the wrong driving force (the numerical setting *Approximate driving force for metastable phases* is now turned off).
- The **Equilibrium** Property Model is rewritten and is now TC-Python based. Also added the **Equilibrium minimization strategy** options to its settings.



- When selecting the **Equilibrium** model in the Property Model Calculator and using functions, the functions in the plot were not updated when changed on the Calculator.

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 no longer be supported as of this release of Thermo-Calc (version 2022a)**. It is recommended that users migrate to the new TC-Python Property Model framework that is based on Python 3 and has full support for any Python package including NumPy, SciPy, and so forth.

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.

Grain Growth and Particle Pinning

A new model has been added to the Precipitation Module (TC-PRISMA) that allows users to calculate normal grain growth and particle pinning, also known as Zener pinning. The new model calculates the temporal evolution of grain size distribution. The grains are assumed to be of spherical morphology and nucleation is not considered. A full description of the theory behind this new implementation is included in the help (press F1 when in Thermo-Calc).

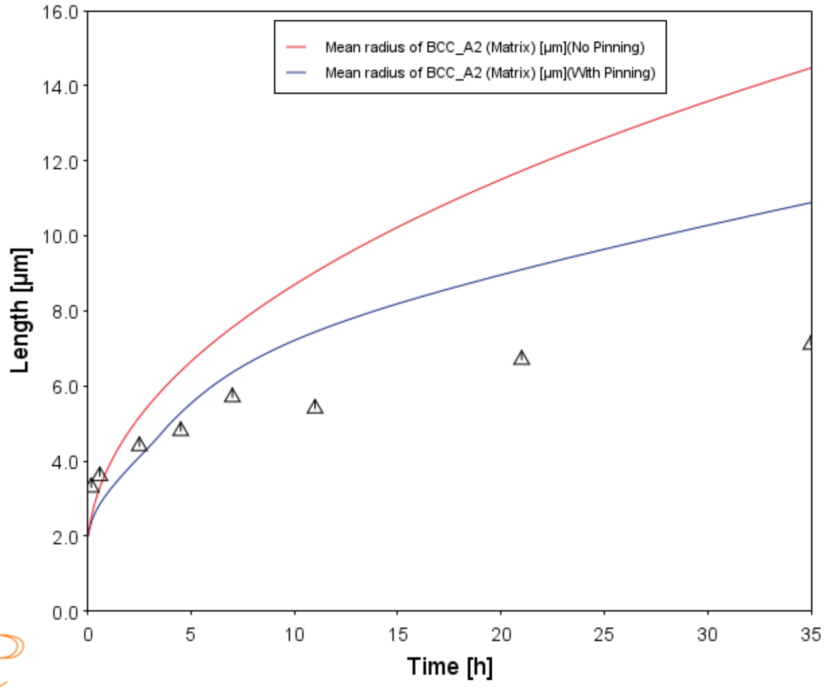
New Example and Video Tutorial

A new example is included in the installation and an accompanying video tutorial is available.

This example demonstrates the simulation of normal grain growth and the pinning effect of precipitated second-phase particles on the grain boundary motion.

The example is included with the Thermo-Calc installation. From the **Help** → **Example Files** menu, navigate to the **Precipitation Module (TC-PRISMA)** folder to open *P_14_Precipitation_Fe-C-Ferrite-Grain_Growth_with_Zener_Pinning.tcu*

The P_14 example is also available as a video tutorial on our website or via the Precipitation Module (TC-PRISMA) Examples playlist on our YouTube channel.



A plot from the new P_14 example comparing the ferrite mean grain radius with and without pinning for the BCC-A2 phase and compared to experimental data. See the help for more details.

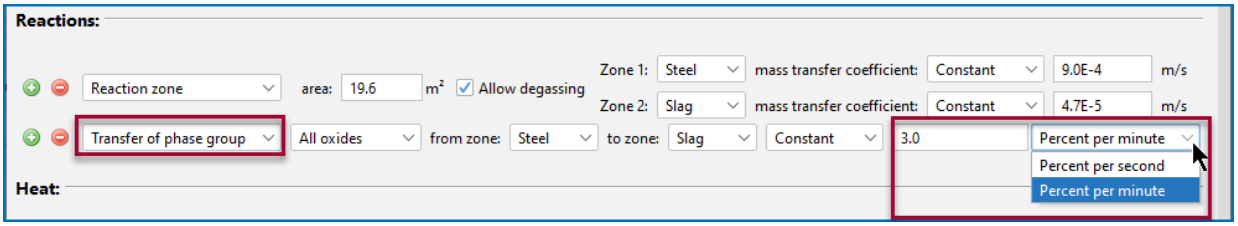
Improvements and Bug Fixes

- For some databases, deselecting phases in the System Definer could cause the Precipitation Module (TC-PRISMA) configuration to be out of sync with the System Definer and sometimes would cause the program to crash.

Process Metallurgy Module

Improvements and Bug Fixes

- When working with the *Process simulation* branch on a Process Metallurgy Calculator, the **Transfer of phase group** setting found on the **Edit Process Model** window now has the option to be defined as a function of time. This adjustment is useful, for example, for flotation of inclusions from steel to slag.



- The checkbox *Reference is liquid oxide* for the activity in the plot configuration had been ignored since 2021b due to a bug. Instead, IONIC_LIQ had always been used as a reference. This is fixed.

Gibbs Energy System (GES6)

General Einstein Model

A new general Einstein model is added to the Gibbs Energy System (GES) version 6. With this model it is possible for database developers to describe Cp at low and intermediate temperatures. Up to five Einstein temperatures (with corresponding weight functions) can be added.

The model is only available in Gibbs Energy System version 6 and it is enabled by using the new database parameters `LNTHETA1`, `LNTHETA2`, `LNTHETA3`, `LNTHETA4`, and `LNTHETA5` together with the corresponding weight functions `THETAF1`, `THETAF2`, `THETAF3`, `THETAF4`, or `THETAF5`.

 For more details about the model, in Thermo-Calc, press F1 and search for *Einstein*.

GES6 Improvements and Bug Fixes

- Fixed a memory leak that occurred when creating very many new systems, and eventually could lead to out of memory errors.
- In the GES module in Console Mode, when specifying a magnetic phase, the `AMEND_PHASE_DESCRIPTION → Magnetic ordering` command now works with GES6. Previously the magnetic contributions were ignored unless you switched to using GES5.
- In the GES module, for both Graphical Mode and Console Mode, for the `ENTER_PHASE` command, GES6 supports Option B and F, 4SL (*four Substitutional-Sublattice Ordering Model*) ordering phase models.
- Fixed a bug for ionic liquid that gave wrong contributions from some ternary and higher order database parameters.
- Activities with user defined reference states were wrong for ionic liquid

 **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 2022a.

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

Diffusion Module (DICTRA)

Improvements and Bug Fixes

Graphical Mode Only

- Updated the example *D_04_Diffusion_Fe-C_Moving_Boundary_Austenite_to_Ferrite,* which previously did not have the option to plot a position of the interface.
- Fixed a bug that stopped the simulation with the error message “NO SUCH CONDITION for inactive phase”, if a phase using the dilute diffusion model was allowed to form on the system’s left or right side.
- Fixed an issue for phases with complex constituents, causing the simulation to fail with the error message “The dependent element must be unique”.

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

TC-Python API and TC-Toolbox for MATLAB®

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

Improvements and Bug Fixes

- TC-Python auto-complete broken in PyCharm of versions later than 2020.3.5 due to a bug in PyCharm. This has now been fixed.
- The possibility to get interfacial_energy from a SingleEquilibriumCalculation has been added. This is used internally in several property models, but can also be used in any “normal” python scripts using TC-Python.
- Bookmarked single equilibrium calculation states now also contain the component status (for example “entered”, “suspended”), which will now be correctly set when loading a bookmarked state using *set_state_to_bookmark()*.
- Before Property Models that returned several values did not return anything in case of errors but raised an exception. Now the errors are instead logged, and the corresponding value is set to NaN. That means that the values that are correct in case of errors now are returned.
- Retrieving result values could fail in TC-Python: In the rare case of having result data with multiple identical values on the x-axis, the `get_values_of` method (and similar) of Scheil, Property Diagram and Phase Diagram result objects could fail with an exception.
- The functions for adding and removing dynamic arguments to Property Models is improved. Now you can specify the index of newly created arguments, and as input to the functions you get the index of all previously created arguments.

- The single equilibrium calculator is now ignoring special elements (i.e., vacancies, positrons, or electrons) defined in the system, when checking if the system elements and defined components are matching.
- The Property Model SDK is improved regarding how models control visibility of graphical input fields.
- The method `add_initial_equilibrium` if fixed for phase diagram calculations. Previously there was a problem if it was called before creating the axes.

Removed Function in TC-Python and TC-Toolbox

The following function is renamed, and the old version will be removed in 2023a. Users are recommended to review and update their scripts.

	Old Name	**New Name**
Class ScheilQuantity	density_of_solid_phase	density_of_phase

TQ-Interface

Bug Fix

Retrieving activities or chemical potentials relative to a user specified partitioned phase no longer breaks subsequent calls using the partitioned phase's index.

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.

TCS Permanent Magnetic Materials Database (TCPMAG1)

A thermodynamic and properties database for rare-earth permanent magnetic materials. It can be used for a wide range of compositions from pure $Nd_2Fe_{14}B$ to very complex NdFeB-based commercial permanent magnetic materials.

Included in this first version:

- 6 elements: B, Ce, Fe, La, Nd, and Pr
- All 15 binary systems
- 11 ternary systems that are assessed based on the published experimental data B-Ce-Fe, B-Ce-Nd, B-Fe-La, B-Fe-Nd, B-Fe-Pr, Ce-Fe-La, Ce-Fe-Nd, Ce-Fe-Pr, Ce-La-Pr, Fe-La-Nd, Fe-Nd-Pr
- 19 phases

In addition to thermodynamic data, it contains the following thermophysical properties data:

- Molar volume of all solid phases and liquid
- Viscosity of liquid
- Surface tension of liquid

TCS Zr-based Alloys Database (TCZR1)

A thermodynamic and properties database for zirconium-based alloys. It can be used for a wide range of compositions from pure zirconium to complex zirconium-based commercial zirconium alloys. It can be used for calculating phase diagrams and thermodynamic properties of assessed systems, but also for predicting phase equilibria and simulating solidification processes for a wide range of zirconium alloys of industrial relevance, including but not limited to:

- Nuclear-grade zirconium alloys
- Experimental zirconium alloys under development

In addition to thermodynamic data, it contains the following thermophysical properties data:

- Molar volume of all solid phases and liquid
- Viscosity of liquid
- Surface tension of liquid

Included in this first version:

- 8 elements (Cr, Fe, H, Nb, Ni, O, Sn, Zr)
- All 28 assessed binary systems
- 19 assessed ternary systems
- 69 phases

TCS Noble Metal Alloys Mobility Database (MOBNOBL1)

This new database is the kinetic database for being used together with TCNOBL1. It contains the atomic mobility descriptions of Ag-Au-Cu-Pd-Pt based alloys for the FCC and liquid phases.

- 21 elements are included: Ag, Au, Cu, Pd, Pt, Al, Co, Cr, Fe, Ga, Ge, In, Ir, Mn, Ni, Re, Rh, Ru, Sn, Ti, and Zn
- 90 binary systems are included for FCC phase: 27 systems were assessed in their full composition range based on experimental information and the rest have parameters for self- and impurity-diffusivities.
- 90 binary systems are included for liquid phase: 6 systems were assessed in their full composition range based on experimental information and the rest have parameters for self- and impurity-diffusivities.
- 3 ternary systems were assessed for the FCC phase.

New Versions of Databases

TCS Steel and Fe-alloys Database (TCFE12)

New Thermophysical Properties

- Electrical resistivity is modeled for crystalline phases and liquid. The descriptions can be used for deriving electrical conductivity.
- Thermal conductivity is modeled for crystalline phases and liquid. The descriptions can be used for deriving thermal resistivity as well as thermal diffusivity (by combining with our density and heat capacity data).

Added Tin (Sn)

- 26 Binaries Sn-X (X=Al, B, C, Ca, Ce, Co, Cr, Cu, Fe, Mg, Mn, Mo, Nb, Ni, O, P, Ru, S, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr)
- 13 Ternaries: Fe-Sn-X (X=C, Cr, Cu, Mn, Nb, Ni, O, S, Si, W, Zn, Zr), and Al-C-Sn

Updated Zinc Corner

As well as updated systems related for the galvanization process:

- Remodeled and unified all gamma-brass D82 phases stable in Fe-Zn, Cu-Zn, Ni-Zn, Mn-Zn, Co-Zn with a 4SL FE3ZN7_D82.
- Added Al-Fe-Mg, Cu-Fe-Zn, Fe-Ni-Zn, Fe-Si-Zn, Fe-Mg-Si, Fe-Mg-Ni, Fe-Mn-Zn, Mg-Si-Zn

Other Updates

- Unified several phases with the same crystallography
- Corrected the low melting pseudobinary in Fe-O-Si
- Extended a ternary phosphide: FEMP_C37 (CO,CR,FE,NB,NI,TI,V,W)1(CO,CR,FE,NB,NI,TI,V,W)1P1
- Revised C-Ca and estimated C-Ca-Fe

TCS Steels/Fe-Alloys Mobility Database (MOBFE7)

- Addition of Sn in BCC, FCC, and liquid phases.

TCS Ti/TiAl-based Alloys Database (TCTI4)

- Added data for electrical resistivity and thermal conductivity
- 2 new assessed ternary systems: Ti-Al-Ni and Ti-Cu-Ni.
- Updated volume descriptions for α2 and γ phases.
- Updated description of BCC_A2 in Mo-V and Mo-Ti-V.

TCS Al-alloys Mobility Database (MOBAL7)

- Addition of five elements Nd, Pr, S, Se, and Te in the FCC and liquid phases.
- The atomic mobility data of Hf in the fcc phase was updated.
- A typo error that leads to wrong interaction between Si and Sn in the fcc phase was corrected.

SGTE Solutions Database (SSOL8)

New Binary and Ternary Systems

102 new systems added

- In total, SSOL8 contains 783 binaries and 144 ternaries.
- 1 new ternary: B-Mo-Ti.
- 101 new binary systems as listed in the table below:

Ag-Co	Am-Fe	B-Ce	Be-V	Bi-Rb	Ca-Ti	Ce-Nd	Cu-Na	Ga-Li	Ge-Hf	Si-Te
Ag-La	Am-Ga	B-Ga	Bi-Cs	Bi-Sr	Ca-V	Ce-Sn	Cu-Se	Ga-Na	Ge-K	
Ag-Na	Am-Np	Ba-Bi	Bi-Dy	Bi-Te	Cd-Fe	Ce-Ti	Er-Ge	Ga-Sr	Ge-Mn	
Al-Ba	Am-Pu	Ba-Ni	Bi-Er	Bi-Ti	Cd-Mg	Ce-Zn	Er-Ti	Ga-Tb	Ge-Nb	
Al-Pu	Am-U	Ba-Pb	Bi-Fe	Bi-U	Cd-Mn	Ce-Zr	Er-Zr	Ga-Tl	Ge-Sc	
Al-Re	Am-Zr	Ba-Ti	Bi-La	Bi-V	Cd-Pu	Co-Re	Eu-Pb	Ga-V	Ge-Yb	
Al-S	Au-Ce	Ba-V	Bi-Li	Bi-Yb	Cd-Se	Co-Sr	Eu-Te	Ga-Zr	Ge-Zr	
Al-Te	Au-Nd	Be-Mo	Bi-Mg	C-Ge	Cd-Sr	Co-U	Fe-In	Gd-Pb	Hf-Mn	
Al-U	Au-Sc	Be-Pu	Bi-Mn	Ca-In	Cd-Ti	Cr-Na	Fe-Np	Gd-Y	Li-Sb	
Al-Yb	B-Cd	Be-Si	Bi-Na	Ca-Sn	Cd-V	Cu-Hg	Ga-La	Gd-Zn	Mg-Pb	

New Phases Added

645 new phases are added to SSOL8. All 2023 phases are listed in the technical information document found on the website and included in the Help and installation. Boron (B) has been added to the gas phase.

Updated Databases

TCS Mg-based Alloys Database (TCMG6.2)

- Electrical resistivity (ELRS) and thermal conductivity (THCD) descriptions for hcp_A3 Mg-Ca/Mn/Sn/Zr are derived based on experimental data.
- The Mg-Y hcp_A3 THCD description is refined.
- Mg-Cu hcp_A3 ELRS and THCD are re-estimated. ELRS and thermal conductivity (THCD) of $CuMg_2$ are tentatively estimated with experimental data from (Mg)+$CuMg_2$ two-phase alloys.
- Mg-Dy and Mg-La ELRS and THCD are re-estimated.
- Molar volume and thermal expansion coefficient of DHCP and liquid Pr are updated.

TCS Solder Alloy Solutions Database (TCSLD4.1)

- Sn-Bi binary system is updated.
- More viscosity and surface tension parameters were added. All thermodynamically assessed systems now have VISC/SURF parameters.
- Viscosity of Ag-Au is re-assessed and added for Ag-Au-Cu.
- The description of the molar volume of BCT_A5 Sn is corrected.

TCS High Entropy Alloys Database (TCHEA5.1)

- Improved the BCC (A2/B2) phase descriptions in the framework of the Al-Cr-Nb-Ti-V-Zr system. Updated assessments of the Al-V, Mo-V and Ti-V binaries. Updated assessments of the Al-Nb-Ti, Al-Ti-V and Al-Ti-Zr ternaries.
- Improved the MC carbide description in the framework of the (Hf, Nb, Ta, Ti, V, Zr)C system. Added assessments of the C-Hf-Nb, C-Hf-V, C-Nb-Ta, C-Ta-V, C-Ta-Zr, C-Ti-V and C-V-Zr ternaries. Updated assessment of the C-Hf-Ta, C-Hf-Ti, C-Nb-Ti, C-Nb-V, C-Nb-Zr and C-Ti-Zr ternaries.
- Minor bug fixed for ternary-related calculation of the Al-Fe-W, Al-Hf-Nb, Al-Mo-Nb and Al-Mo-Ni systems.

TCS Al-based Alloys Database (TCAL8.1)

- Updates to the surface tension, viscosity, and volume data for liquid.
- All assessed binary systems now have the SURF/VISC parameters.
- Updates to electrical resistivity and thermal conductivity of several solid phases (Al_2Cu, Al_6Mn, $Al_9Fe_2Si_2$ and Si) and liquid in several binaries (Ag-Al, Ag-Cu, Al-Cu, Al-Si and Al-Zn), as well as molar volume and thermal expansivity of Pr.
- Modeling of the Y solubility in (Al).

TCS Metal Oxide Solutions Database (TCOX10.2 and 11.1)

- Fixed an error in molar volume of FCC_A1 and BCC_A2 phases.

TCS Ni-based Superalloys Database (TCNI11.0.1)

- A typographical correction was made to the molar volume of the M6C phase

Other

TCS Fe-containing Slag Database (SLAG3.2.1)

This database is discontinued as of 2020b. However, for any users still using version 3 (SLAG3) of this database, a bug was fixed in the gas phase where the wrong function was assigned to N_2O_3. Note that it is recommended to upgrade to the latest version of TCOX for full functionality.

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! TCZR1 and TCPMAG1*** ● TCHEA4 and TCFE10 as of 2020a ● TCAL7, TCNI10 and TCOX10 as of 2020b ● TCTI3 and TCMG6 as of 2021a ● TCCU4 and TCSLD4 as of 2021b
Surface Tension of Liquid	***New! TCZR1 and TCPMAG1*** ● TCAL7 and TCNI10 as of 2020b ● TCTI3, TCMG6 and TCFE11 as of 2021a ● TCHEA5, TCOX11*, TCCU4, TCSLD4 as of 2021b *surface tension of oxide slag
Thermal Conductivity and Electrical Resistivity	***New! TCFE12, TCTI4*** ● TCAL7 as of 2020b ● TCMG6 as of 2021a ● TCHEA5, TCNI11 and updates for TCAL8 and TCMG6.1 as of 2021b
Molar Volume	***New! TCZR1 and TCPMAG1*** Molar volume has been included with many databases for some time. Below lists more recent additions: ● TCOX10 as of 2020b ● TCMG6 as of 2021a ● TCTI2 as of 2019a

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.

Installation

Bug Fix

Fixed a bug, which made the installer abort if there was an error while checking for multiple users. This check is only used for installation of the TC-Toolbox for MATLAB® and the error should not affect the entire installation.

Thermo-Calc Changes

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 2022a 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.

Documentation

New and Updated Software Examples

There are several new examples described elsewhere in this document:

Material to Material Calculator

- T_14_Fe-Cr-Ni_Material_to_Material.tcu

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

- Calculates the phases occurring for a material mixture, in this case for a mixture of a martensitic stainless steel with Alloy 800.
    - TC-Python: pyex_T_17_Material_to_Material_single_fraction_of_B.py

    - TC-Toolbox: matex_T_17_Material_to_Material_single_fraction_of_B.m
- Calculates the phases occurring during a gradual transition between two materials, in this case from a martensitic stainless steel to Alloy 800.
    - TC-Python: pyex_T_18_Material_to_Material_step_along_fraction_of_B.py
    - TC-Toolbox: matex_T_18_Material_to_Material_step_along_fraction_of_B.m
- Calculates the phases occurring for a material mixture with varying temperature, in this case for a mixture of a martensitic stainless steel with Alloy 800.
    - TC-Python: pyex_T_19_Material_to_Material_step_along_temperature.py
    - TC-Toolbox: matex_T_19_Material_to_Material_step_along_temperature.m
- Calculates a "phase diagram" for a material mixture, in this case for a mixture of a martensitic stainless steel with Alloy 800.
    - TC-Python: pyex_T_20_Material_to_Material_phase_diagram.py
    - TC-Toolbox: matex_T_20_Material_to_Material_phase_diagram.m

Precipitation Module (TC-PRISMA)

- P_14_Precipitation_Fe-C-Ferrite-Grain_Growth_with_Zener_Pinning.tcu

Nickel Model Library

- PM_Ni_01_Lattice_Parameter_of_Gamma_Gamma_Prime.tcu
- PM_Ni_02_Antiphase_Boundary_Energy_of_Gamma_Prime.tcu

Graphical Mode Example Changes and Updates

- The application example *PMET_04_Basic_Oxygen_Furnace_Kinetics.tcu* (without any suffix) is removed from the installation. This example was replaced in 2021b by the examples with the same name and an “a, b, or c” suffix. In other words, this example is now available as three different versions and the original is obsolete.
- Updated the example *D_04_Diffusion_Fe-C_Moving_Boundary_Austenite_to_Ferrite,* which previously did not have the option to plot a position of the interface.
- Updated a Precipitation Module (TC-PRISMA) example using the **Yield Strength** Property Model. Example *P_01_Precipitation_Al-Sc_AL3SC.tcu* now uses
    - The precipitation strengthening model now uses Seidman model (Al-base)
    - The interfacial energy prefactor changed to 0.75*calculated
    - The antiphase boundary energy changed to 0.6

Console Mode Example Changes and Updates

Several updates were made to the Console Mode examples for both Thermo-Calc and the Diffusion Module (DICTRA). Two examples were removed from the collections. Other changes addressed some minor bugs with the macros or adjusted the use of databases to either use demo versions or to upgrade to newer versions. Some of the key changes are noted below.

- tcex25 and tcex40d are deleted.
- tcex10 - now uses TCOX11 instead of the discontinued SLAG database.
- tcex15 and tcex51 - now use the FEDEMO database instead of TCFE.
- tcex32 - Uses TCOX11 now instead of both TCFE and SSUB.
- tcex41, 42, and 43 all use TCFE11 now instead of TCFE9 (that is, if you have the latest version of the database, otherwise the example will run with earlier versions of TCFE).

TC-Toolbox Legacy Notes

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.

Other Changes

The Graphical Mode Context Help (which had minimal content) is disabled. When you click the Help button in the Thermo-Calc program, the online help is opened instead. Press F1 at any time to open the Help or from the menu, select **Help** → **Online Help**.

New Webpages and Videos

Webpages

- **Permanent Magnetic Materials** (TCPMAG1 database): https://thermocalc.com/products/databases/permanent-magnetic-materials/
- **Zirconium-based Alloys** (TCZR1 database): https://thermocalc.com/products/databases/zirconium-based-alloys/
- **Nickel Model Library**: https://thermocalc.com/products/add-on-modules/nickel-model-library/
- **Material to Material Calculator**: https://thermocalc.com/products/thermo-calc/material-to-material-calculator

Videos

- **Material to Material Calculator**: The accompanying video tutorial for the T_14 example can be found via the Graphical Mode Examples playlist on our YouTube channel or our website.
- **Grain growth / Zener pinning model:** The accompanying video tutorial for the P_14 example is on our website or via the Precipitation Module (TC-PRISMA) Examples playlist on our YouTube channel.
- **2022a Release News**: Visit our website for all the release videos or go to the homepage of our YouTube channel.

Platform Roadmap

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.