Release Notes:

Thermo-Calc Software Package and Databases

Version 2021a

Contents

Thermo-Calc Version 2021a Highlights

★ **Thermo-Calc:** A new website was launched with new application examples and resources. To improve your experience on high resolution monitors, a new look and feel for the GUI is implemented. Thermophysical properties are added to the steel (TCFE11), magnesium (TCMG6), and titanium (TCTI3) databases, which are also available in Thermo-Calc as model parameters and variables.

★ **Property Models and Steel Model Library:** Six new Property Models are available -- four general models (Crack Susceptibility Coefficient, T_0 Temperature, Spinodal, and Equilibrium with Freeze-in Temperature) and two steel-specific models (Bainite and Critical Transformation Temperature).

★ **Process Metallurgy Module:** You can now change the pressure and reaction kinetics in the process schedule, valuable features for vacuum degassing processes. A new example shows these new features and how to set up a Vacuum Oxygen Decarburization (VOD) process.

★ **TC-Python:** Thermo-Calc Property Model Development Framework is now integrated into TC-Python so you can create your own property models. This allows the Property Models to perform any calculation type that is available in Thermo-Calc. There is also a new bundled version of a TC-Python installation or you can choose your own IDE.

★ **Diffusion Module (DICTRA):** For the Diffusion Calculator you can now edit the left and right boundary conditions. This is in addition to already being able to edit the simulation time while a calculation is paused. This change is useful, for example, when you want to simulate carburization.

★ **Databases:** There are nine new and seven updated databases. New are both the thermodynamic and kinetic ones for steel and Fe-alloys (TCFE11 and MOBFE6), magnesium (TCMG6 and MOBMG2), and titanium (TCTI3 and MOBTI4), plus the aluminum kinetic database (MOBAL6). The two IRSN nuclear databases (Mephista-19 and NUCLEA-19) have new versions and for those who develop their own databases, the new TDB Editor is available with all installations.

New Thermo-Calc Website

We are excited to announce the launch of our new website, which was completely redesigned to highlight the many applications of our software to materials research and engineering. The new site includes many resources to show you how others are using our tools and a new Support Center to better serve user needs.

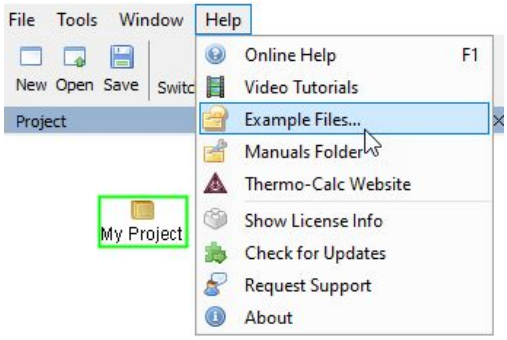
There are dozens of application examples demonstrating how our tools can be used to predict a wide range of materials property data and gain insights into materials processing and behavior through the materials life cycle. The examples are included in the new Solutions section, and the pages are divided by materials and applications, so no matter your area of focus, you can easily find your solutions.

Things that you will find on the new website that are also described in these release notes include:

- All the thermodynamic and kinetic databases have dedicated pages where new and updated Technical Information and Example Collections are available in addition to links to examples, publications, webinars, and much more.
- A useful reference document, Properties that Can Be Calculated with Thermo-Calc and the Add-on Modules includes updated information based on this 2021a release.
- The release notes and more are available on the Release News page.
- The new Process Metallurgy Module example about Vacuum Oxygen Decarburization (VOD) demonstrates the new product features and a companion PDF is available discussing the example in detail.
- Applicable links are included throughout this document.

General Property Models and Steel Model Library

Thermo-Calc 2021a has six new property models - four general models available to all users (Crack Susceptibility Coefficient, T_0 Temperature, Spinodal, and Equilibrium with Freeze-in Temperature) and two steel-specific models (Bainite and Critical Transformation Temperature), which are available to users with the applicable licenses. Each includes an example demonstrating how the model works.



General Models

Crack Susceptibility Coefficient

The **Crack Susceptibility Coefficient** Property Model is used to calculate the hot tearing tendency during solidification. Hot tearing is one of the most common and serious defects encountered during the casting of aluminum and magnesium alloys, and this model can help users choose the right alloy composition to reduce the occurrence of this issue.

Example PM_G_07_Hot Crack Susceptibility demonstrates how to set up the model. An accompanying video of the same name walks users step-by-step through setting up the calculation, offers an analysis of the results, and gives a basic description of the model.

For this and other Video Tutorials, visit the new website.

T-Zero Temperature

T_0 Temperature is a Property Model that calculates the so-called T_0 line. The T_0 temperature is defined as the temperature where two phases of identical chemical compositions have the same molar Gibbs free energy. This temperature is an important quantity in the field of diffusionless phase transformations, such as martensitic transformation, since it is the upper limit where diffusionless phase transformations can occur. It is also important for processes such as CVD and PVD (chemical and physical vapour deposition), where partitioning typically does not occur and the phase with the lowest Gibbs energy is deposited.

Example PM_G_09_T-Zero Temperature demonstrates this new model.

Spinodal Model

The **Spinodal** Property Model calculates the spinodal line. The spinodal is defined by the condition where the second derivative of Gibbs free energy is zero (d2G/dx2 = 0). The locus of these points is known as the spinodal curve. Inside the spinodal phase separation is spontaneous (i.e. does not require nucleation and growth) as any fluctuation in composition results in a lowering of the Gibbs free energy. Phase separation proceeds by amplification of these fluctuations.

One new example includes demonstrating this new model, *PM_G_08_Spinodal*.

Equilibrium with Freeze-in Temperature

The **Equilibrium with Freeze-in Temperature** Property Model calculates equilibrium at the freeze-in temperature and evaluates the properties at a different temperature. The model can evaluate several properties such as electrical and thermal resistivity / conductivity, density, coefficient of thermal expansion, and others.

Two examples are included in this release demonstrating the new model: *PM_G_10_Freeze in Thermal Conductivity* and *PM_G_11: Freeze in Electric Conductivity*.

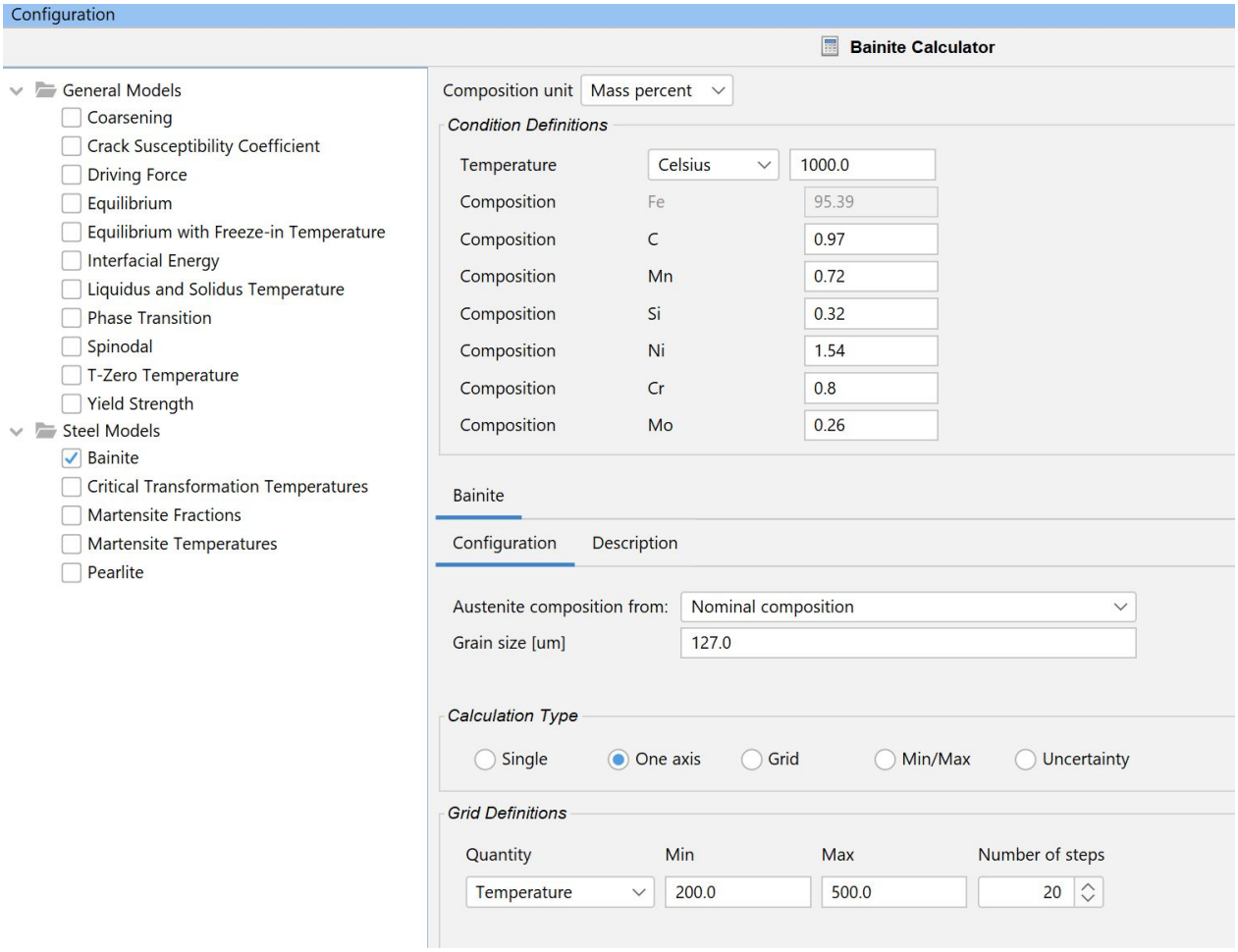
Steel Model Library Models

The **Bainite** and **Critical Transformation Temperature** Models require a license for the Steel Model Library, which is currently available for free to all users who have the databases TCFE9 or newer and MOBFE4 or newer and a valid maintenance and support subscription.

Bainite

The **Bainite** Model describes the thermodynamics and isothermal kinetics of bainite transformation from austenite. It can calculate bainite start temperature, transformation times, bainite plate lengthening rate, and phase constitution at the final state. Bainite is also available to be used with the TTT

(Time-Temperature-Transformation) template and TTT-mode plotting options. The new example, *PM_Fe_05_Fe-C-Mn-Si-Ni-Cr-Mo_Bainite*, demonstrates the model and the use of the TTT diagram.



The Bainite Property Model (and all the Property Models) available with the Property Model Calculator when you have the Steel Model Library.

Critical Transformation Temperature

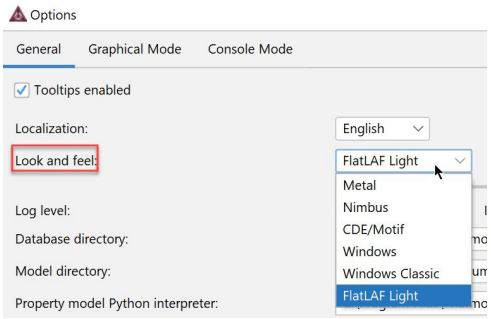
Critical Transformation Temperature is used to calculate critical transformation temperatures for steels. It can output the common transformation temperature for steels including liquidus, solidus, A0, A1, and more. The new example, *PM_FE_04_Critical Temperature*, demonstrates this new model.

In Thermo-Calc, press F1 to search the help to learn more about any of these Property Models.

Thermo-Calc New Features, Improvements, and Bug Fixes

New Look and Feel for the GUI

A new Look and Feel called **FlatLAF Light** is the default for the graphical user interface (GUI) for all Thermo-Calc installations. The change is implemented because it is better for working with higher resolution screens.



Note that if you have very different resolutions between a laptop and monitor, for example, it can require that you manually resize windows you are working with.

If you prefer to change the setting to the previous default (**Windows**), it is under the **Tools > Options** menu.

Gibbs Energy System (GES6)

Starting with Thermo-Calc 2019b, the part of the calculation engine known as the Gibbs Energy System module (GES) was updated from version 5 (GES5) to version 6 (GES6). GES6 is now enabled by default.

LIST_DATA Command Improved in Console Mode

The behavior of the LIST_DATA command in Console Mode is improved. The LIST_DATA command is used to retrieve and list the data included with a database in the DATA module or directly entered in the GIBBS module. All data for the current system that is defined within the current GIBBS workspace is written in a readable manner in the output file.

The improvements to the command are listed below. The output as a result of this command differs slightly based on whether you are using GES6 (the default) or GES5. For details of these differences search the online help for the *LIST_DATA* command.

In GES6 after entering the command and when option **N** is selected, the output data consists of:

- A list of all elements and the data followed by a list of all phase definitions.
- The data associated with the phases, sorted by system.
- For an unencrypted database using option N, there is a further subcommand that allows filtering of phase parameters with respect to the property type e.g., to include only volume parameters and/or viscosity parameters in the output.

Additional information for GES6 included in the list:

- Automatically suspended phases
- Maintains the original reference citation that is used in the database making it clearer if you need to clarify the source of the information.

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

Thermophysical Properties Added to TCFE11, TCMG6, and TCTI3 Databases

There are 16 new and updated databases detailed in these release notes. Important thermophysical properties continue to be added as shown in this summary of the major additions starting with 2020a.

Viscosity of Liquid	• TCHEA4 and TCFE10 as of 2020a • TCAL7, TCNI10 and TCOX10 as of 2020b • TCTI3 and TCMG6 as of 2021a
Surface Tension of Liquid	• TCAL7 and TCNI10 as of 2020b • TCTI3, TCMG6 and TCFE11 as of 2021a
Thermal Conductivity and Electrical Resistivity	• 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 thermophysical 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.

Improvements and Bug Fixes

Graphical Mode

- EXP file renderer now accepts PROLOGs called PROLOGUE.
- Appending (i.e. loading) a user database on top of a regular database is working again. For 2020b it was not.
- Fixed a bug for the Scheil Calculator with a Table Renderer as a successor. Sometimes when a saved project file was opened there would be incorrect column data included.
- Fixed a bug for the Ternary Calculator on the Plot Renderer settings window where the list of phases were not available in the drop-down list when certain quantities were selected.

Both Graphical and Console Mode

- User-defined functions can now use the trigonometric functions tan, asin, and acos, and the hyperbolic trigonometric functions sinh, asinh, cosh, acosh, tanh, and atanh.
- A license issue related only to Thermo-Calc version 2020b was fixed. When there were old license features available, the program sometimes was unable to obtain a license, which caused the program to occasionally freeze or crash.
- Fixed a crash or wrong value when computing equilibria with AC & ACR(Species,Phase) constraint and no Pressure constraint.

Console Mode

- When entering the POST module, unnecessary composition sets are no longer occasionally created.
- Fixed a bug related to the Scheil with back diffusion option in the Start Wizard. Previously any user selected primary phase was ignored in error.
- The advanced option command `KEEP_COMP_SET_NUMBERS` no longer tries to re-assign composition sets that have the status set as FIXED. This change also affects any SDKs that have the corresponding option available (e.g. TC-Python).

Important: 3D Plots for Linux and macOS Temporarily Not Supported

3d plots in Graphical Mode on Linux and OSX are not supported in 2021a, however the development work required to fix this bug is planned for implementation in 2021b.

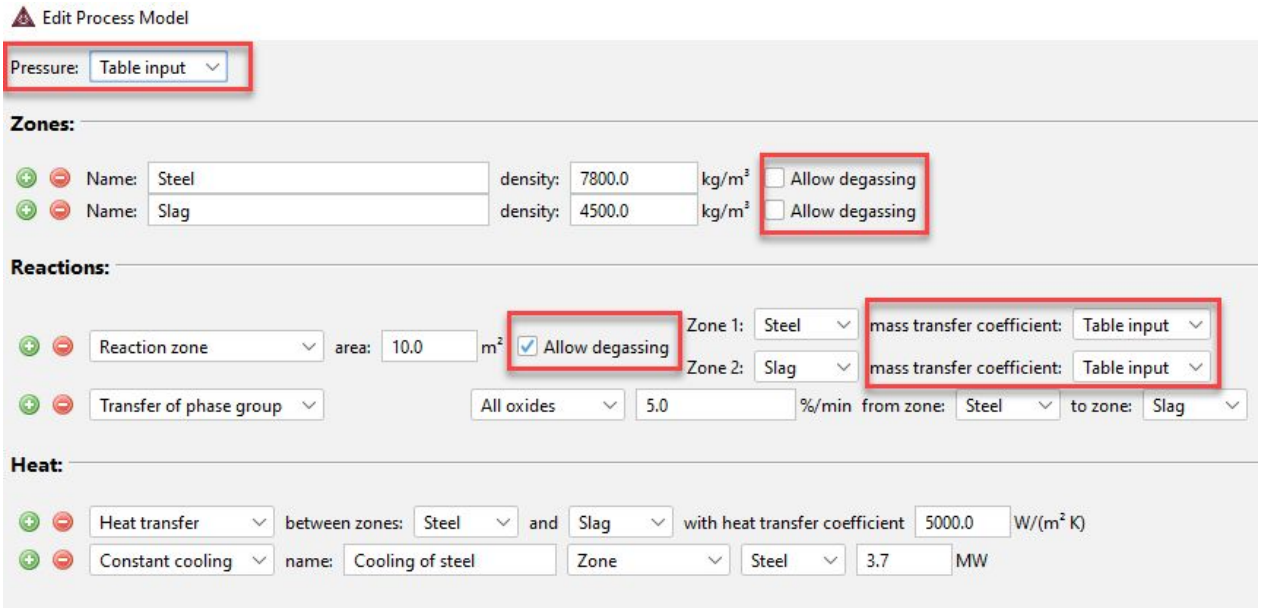
Process Metallurgy Module

New Features and a VOD Example

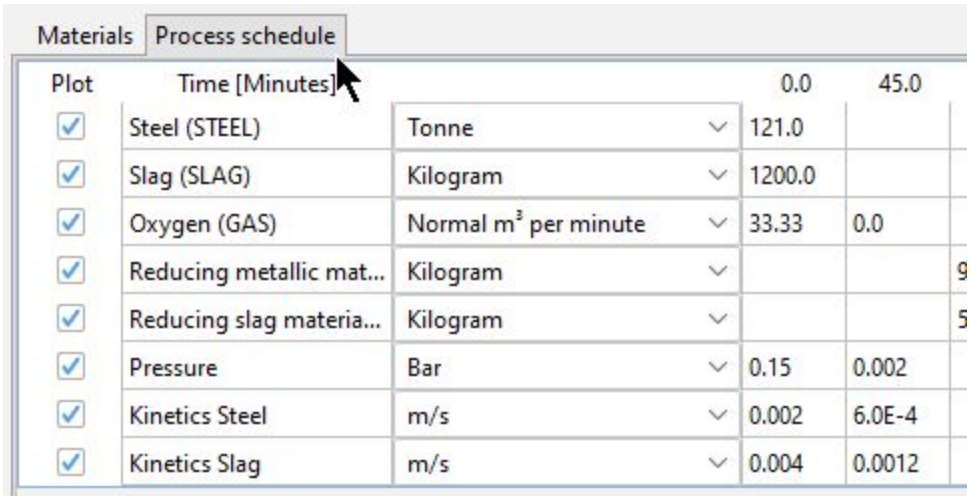
The Process Metallurgy Module for steel and slag now allows users to change the pressure and reaction kinetics in the process schedule, valuable features for vacuum degassing processes. The new example (*PMET_07_Vacuum_Oxygen_Decarburization_Kinetics)* shows how to set up the VOD process when using the Process Simulation (EERZ model). Use of the new features is highlighted.

Visit the website Application Examples→Process Metallurgy page for more background information as well as more in depth analyses of this and other examples. Also visit the Process Metallurgy Module page to access resources such as training videos, presentations, publications, webinars, and much more.

- You can define in both the **Zones** and the **Reactions** sections on the **Edit Process Model** window which zone the gas can escape from. If the **Allow degassing** checkbox is selected, all the gas phase formed is removed from the zone in each timestep and moved to the exhaust gas zone. This functionality gives some control over degassing kinetics. Allowing degassing in all zones results in very fast removal due to degassing, which in most cases is probably not realistic.
- Variable pressure is now available as a function of time. This is set first on the **Edit Process Model > Pressure** section where you can select it to be **Constant** or choose **Table input** to then enter the information in the **Process schedule** table.
- Change of reaction kinetics in function of time during the process i.e. the mass transfer coefficient of the reaction zone can now be input directly in the **Process schedule** table after selecting Table input on the **Edit Process Model** window.



The Edit Process Model window where the new Table input option is available so that variable pressure or mass transfer coefficients can be entered in the Process schedule as a function of time.

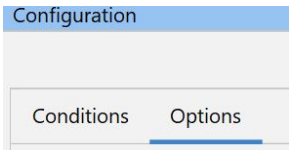


*The Process Schedule table for the new example.*Process Metallurgy Bug Fixes and Improvements

Improvements and Bug Fixes

Some changes are located on the Process Metallurgy Calculator Configuration window as indicated.

Options Tab



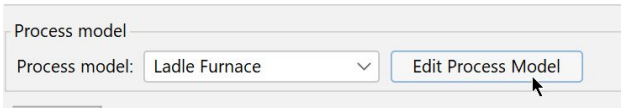
Material Manager Improvements

- To make it more easily accessible, the **Material Manager** (only available for the Process Metallurgy Module) is moved from its old location (*Tools>Options>Graphical Mode>Process Metallurgy Calculation*) to the **Options** tab on the Process Metallurgy Calculator's Configuration window.
- Material groups created in the Material Manager now appear in all of the Process Metallurgy Calculator dropdown lists, and these are also globally removed. Deleted group data directories are moved to the computer's trash/bin.
- A material saved in any of the material configuration panels is now directly accessible globally in the Process Metallurgy Calculator Configuration window. When a material is removed in the Material Manager panel it is globally removed from the Process Metallurgy Calculator.

Default Value Change

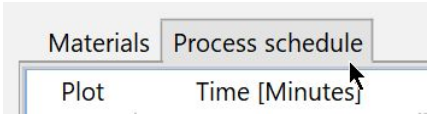
- For a more stable calculation, the default value for the setting "Maximum number of Iterations" is changed to 2000.

Edit Process Model



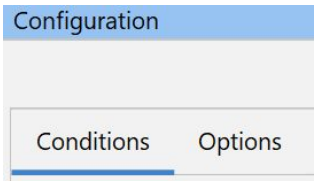
On the **Edit Process Model** window, the kinetic simulations now allow for multiple phase groups to be transferred ("Transfer of Phase Group") through each reaction zone.

Process Schedule Tab



In addition to the new functionality discussed above, there is improved ability to move around the Process Schedule table. You can now scroll vertically and horizontally. This is particularly useful when there are complex process schedules entered.

Conditions Tab



- Fixed a bug that prevented saving a material if it was obtained after opening a project file (instead of saving it directly). Now you can correctly save the material to disk from the Material section, click **Show composition** and then **Save material** as normal.
- Each branch (**Equilibrium** and **Process simulation**) now has separate setting options for **Database**, **Temperature unit**, and **Time unit** allowing for different branch settings to be used in the same project.

Event Log

For EERZ calculations that do not work, and to make debugging easier, more detailed information was added to the error messages available in the Event Log.

Calculation-Related Fixes

- The performance of adiabatic stepping and mapping equilibrium calculations is improved
- Reimplemented the algorithm to distinguish between metallic and non-metallic phase groups to be more accurate in corner-cases.
- Fixed a bug to prevent calculation failures related to adjusting the time-step control after additions. Now after any addition or other change such as pressure or mass-transfer coefficient, a time-step with minimal length is performed.
- Fixed a bug in the process simulation where the heat values sometimes were not saved in the project file.

General Improvements and Bug Fixes

- The liquid “oxide” phase group contains now (additional to CaF2) all fluorides that are present in the database: FeF3, CrF3, CuF2, NbF5, CoF3
- French locale issues fixed: Fixed errors in French translation as well as the material delete button that did not work.

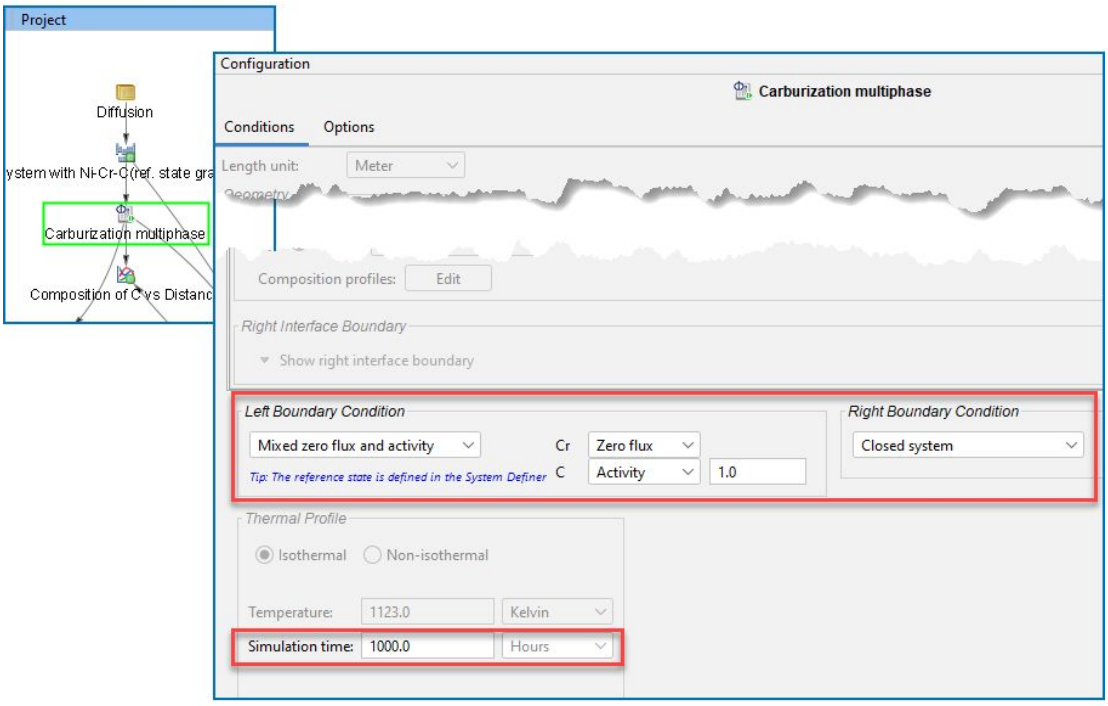
Diffusion Module (DICTRA)

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

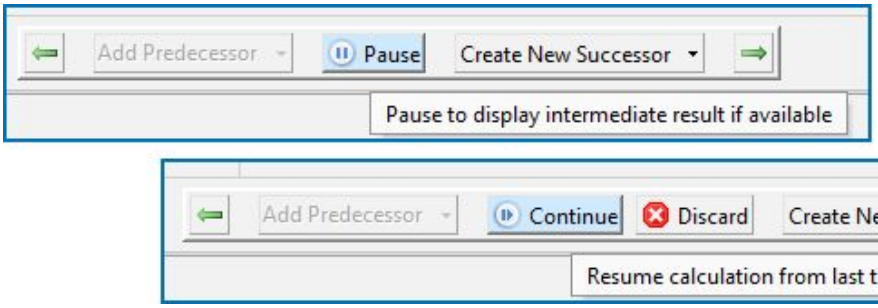
Edit Boundary Conditions and Simulation Time while Paused

When using the Diffusion Calculator in Graphical Mode, you can now edit the left and right boundary conditions. This is in addition to already being able to edit the simulation time while a calculation is paused.

This change is useful, for example, when you want to simulate carburization. In this case it is common to first have a step with high carbon activity in the furnace for the actual carburization and then lower it and allow the carbon in the specimen to diffuse without further increased carbon content. Now you can set up your Diffusion Calculator, start the simulation, then pause it to see if adjustments need to be made. If so, you can edit the fields and continue the simulation, or you can discard the calculation and start again.



The Diffusion Module example (D_07_Diffusion_Carburization_Multiphase.tcu) calculation was paused. Both the boundary settings (new this release) and simulation time can be edited as necessary.



During the diffusion simulation, you can pause it, and then when you have made the changes continue the simulation (or discard it and start again).

Bug Fix

For both Console and Graphical Mode, a bug fix was completed related to plotting of DC and DI.

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.

Bug Fixes

- Fixed an issue related to when the Yield Strength Property Model is used with the Precipitation Calculator and the plot after a calculation did not work if the system was changed.
- Corrected a bug that led to instability when some solute elements are depleted in the matrix phase.
- Corrected a bug that failed to reclaim the workspace for storage, resulting in a simulation crash with the message “TMAKE Error”.

Thermo-Calc Property Model Development Framework Now Part of TC-Python

Thermo-Calc 2021a introduces a new way for users to develop Property Models using TC-Python. Previously, users could develop Property Models using a Jython-based API called the Property Model Development Framework, but Jython is no longer being supported, so we are introducing a new framework.

This new system allows for easier development of Property Models and significantly expands what can be done with user developed models. For example, because this new API uses the Python language, users can use any Python library, such as NumPy, SciPy, or scikit-learn, within the Property Models, making model development quite powerful.

This new system also allows the Property Models to perform any calculation type that is available in Thermo-Calc. Previously, only single equilibrium calculations were supported.

Property Models created in TC-Python automatically show up in the Property Model Calculator in the Graphical Mode of Thermo-Calc. Here, they can be further configured, combined with other models, and run.

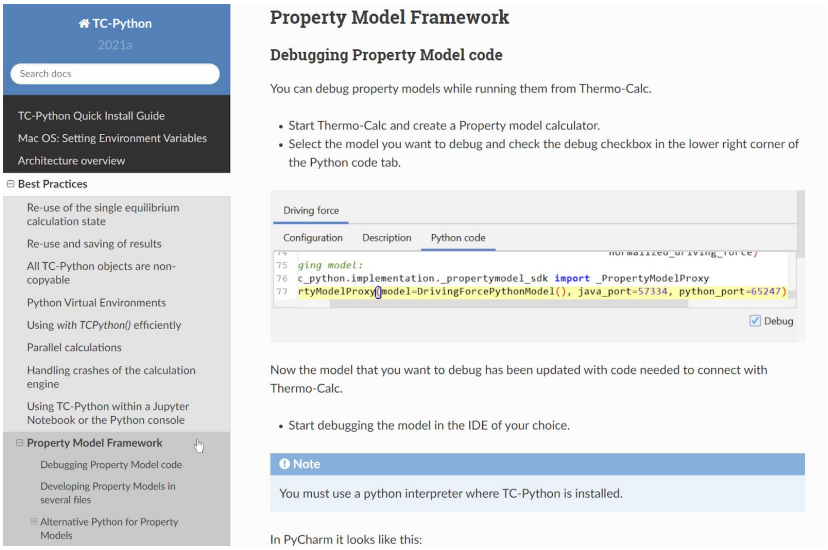
Users who previously used the Property Models Development Framework to develop Property Models can still use their models in Thermo-Calc, but they are encouraged to migrate them to TC-Python as soon as possible (supported unitl the 2022a release). This new feature requires a license for TC-Python.

New Property Model Documentation in TC-Python

The old documentation for the Jython Property Models is available on the website or temporarily in the installation. Existing Jython-based Property Models are guaranteed to function in Thermo-Calc until the 2022a release.

The new documentation is included in the TC-Python help available both on our website or as part of your installation. There is also information found in the Best Practices section.

The same information contained in the online TC-Python help is included in a PDF version, also included with your installation.



TC-Python

Also see Thermo-Calc and TC-Python: New Bundled Python Interpreter

New Features

Save and Restore State of Single Equilibrium Calculations

Added a feature to “bookmark”, i.e. save and restore the state of single equilibrium calculations. This can be used to improve convergence and performance in many advanced use cases.

Remove Composition Conditions

The function `set_component_to_suspended` on single equilibrium and batch equilibrium calculations now have the option to also remove composition conditions for the component if they are defined.

New and Updated Examples

- A new example (*pyex_PM_3_Property_model_self_developed_model.py*) that shows how to make and use a property model written in the new API `propertymodel_sdk` is added.
- The existing example *pyex_PM_2_Property_model_parameter_fitting.py* is updated to use a model created with `propertymodel_sdk`.

TC-Python Improvements and Bug Fixes

- Clearer exceptions are now thrown in case of misconfiguration of the database (no elements, phases, mixing user and regular databases)
- The method `BatchEquilibriumCalculation.get_components()` is now working.
- Fixed that the global equilibrium setting was lost if the `with_options()` method was called afterwards (affected Scheil, Property Diagram, Phase Diagram, and Batch Equilibrium calculations).

Renamed Functions in TC-Python - Deprecation with 2021b

The following functions are renamed, and the old versions will be removed in the next release, 2021b (June 2021). Users are recommended to update any scripts as soon as possible.

	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_calculations()`	`def enable_automatic_forced_starting_values_in_eq_calculations()`
Diffusion options	`def set_default_driving_force_for_phases_allowed_to_form_at_interfaces()`	`def set_default_driving_force_for_phases_allowed_to_form_at_interf()`

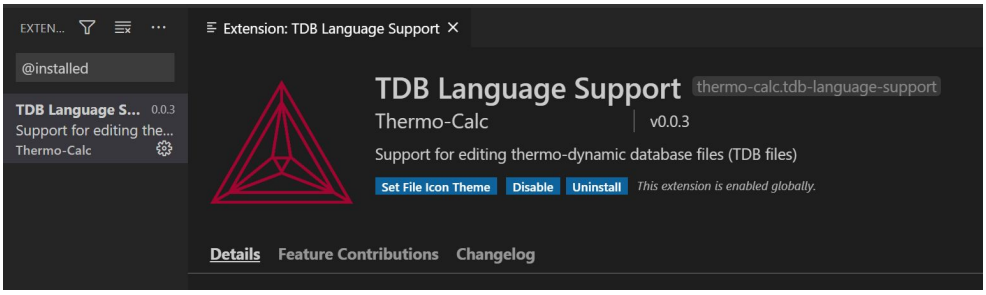
TQ-Interface

Bug Fixes

- Fixed an issue that caused a crash that happened if `tq_keep_cs_numbers` was enabled and equilibrium calculations failed
- Fixed a bug that could cause `tq_ceg` not to use the global equilibrium.

TDB Editor Extension for Custom Database Development

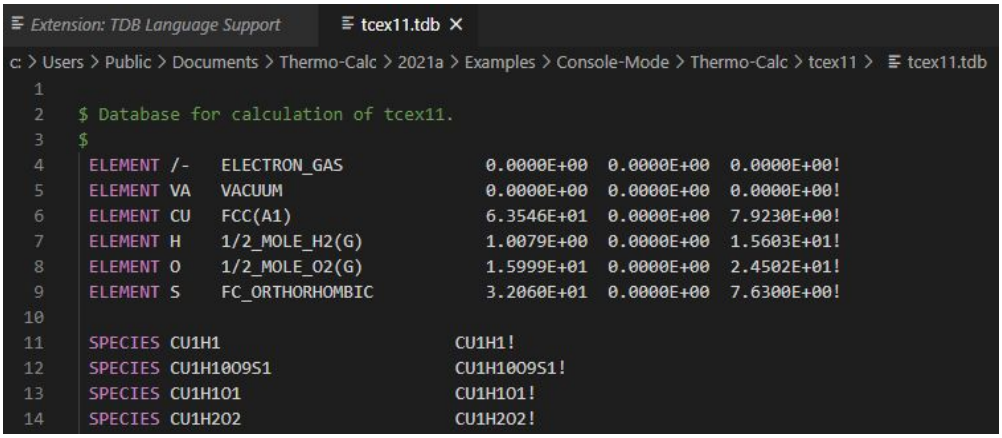
A new tool, the TDB Editor, is available for those who develop their own custom databases for use with Thermo-Calc or other applications. The advantage to using the TDB Editor compared to a basic text editor is that it generally speeds up the editing process. The TDB Editor extension provides features that give immediate feedback such as syntax coloring and checking, formatting of TDB files, and generally easier navigation to items of interest in the TDB file such as functions and references. The Thermo-Calc Database Format (TDB) is an international standard for the CALPHAD-type thermodynamic calculations and kinetic simulations.



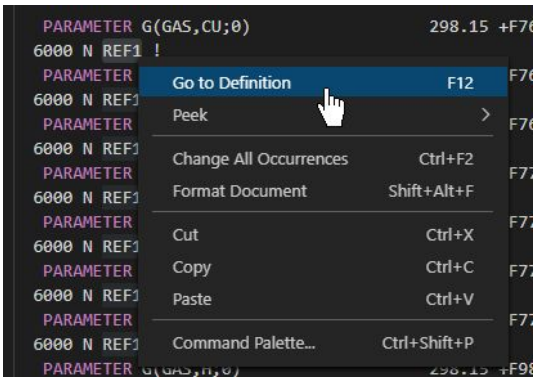
The TDB Editor has two components:

- An installed extension to the open source code editor Microsoft Visual Studio Code (VSCode), which has the user interface for the TDB Editor. VSCode is available for free.
- A server application that runs invisibly in the background and provides the VSCode extension with services specific to the TDB format.

The syntax checker uses the same text parsing engine as the Database Checker tool (already available with Thermo-Calc) and the Thermo-Calc application itself. This means that an edited TDB file with no errors shown in the TDB Editor, is also accepted by the Thermo‑Calc application.



An example of an unencrypted database TDB file open in the new TDB Editor.



The new TDB Editor makes it easier to navigate the TDB file during database development.

In Thermo-Calc, press F1 to search the help for *TDB Editor* where there are details about installing the tool and the features that are available, such as custom colors.

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.

Also see Thermophysical Properties Added to TCFE11, TCMG6 and TCTI3 Databases.

TCS Mg-based Alloys Database (TCMG6)

New Thermophysical Properties

- Electrical resistivity assessed or estimated for all the phases (except for GAS)
- Thermal conductivity assessed or estimated for all the phases (except for GAS)
- Viscosity assessed for liquid
- Surface tension assessed for liquid
- Molar volume and thermal expansivity assessed for all the phases

New Elements

- Bi and H

Newly Assessed Thermodynamic Systems

11 ternary and 12 binary systems are newly assessed.

- 4 binaries and 3 ternaries are within the scope of Mg-Bi-based alloys:
  - Bi-Ca, Bi-Mg, Bi-Mn, Bi-Zn,
  - Bi-Ca-Mg, Bi-Mg-Mn, Bi-Mg-Zn
- 8 binaries and 5 ternaries are among the core systems of hydrogen storage Mg alloys:
  - Ce-H, Cu-H, La-Zn, H-La,
  - H-Mg, H-Nd, H-Ni, H-Zn,
  - Ce-H-Mg, Cu-H-Mg, H-La-Mg,
  - H-Mg-Nd, Mg-H-Ni
- 3 more important ternary systems:
  - Al-Ce-Mn, Al-La-Mg, La-Mg-Zn

New Metastable Precipitates

The metastable precipitates Mg_7R, Mg_3R ($D0_3$), Mg_3R ($D0_{19}$) that form during aging of Mg-RE (rare earth) alloys have been modeled in the following systems:

- Mg-Gd
- Mg-Nd
- Mg-Y

Updated Phase Equilibria

- Cu-Gd: thermodynamic descriptions are improved for several compounds
- Mg-Nd-Zn: remodeled based on the recent experimental data
- Mg-Al-Ce: remodeling of the Mg-rich $Mg_{12}Ce$ phase and the ternary C15 and $Al_{13}CeMg_6$ phases
- Mg-Si-Sn: the mutual solubility of Mg_2Si and Mg_2Sn (modelled as the same phase as MG2SI) are reassessed

TCS Steel and Fe-alloys Database (TCFE11)

New Thermophysical Properties

- Added surface tension of the metallic liquid.
- Updated molar volume of the liquid.

New Elements and Systems

- Added binary M-H systems where M=Al, Ca, Ce, Co, Cr, Cu, Fe, Mg, Mn, Mo, Nb, Ni, Ru, Si, Ta, Ti, V, W, Y, Zn, Zr.
- Liquid, FCC, BCC and HCP solutions and important hydrides are included. In addition, ternary C-Fe-H, Fe-H-Si, Cr-Fe-H, Al-Fe-H, Fe-H-Mo, Fe-H-Ni, Fe-H-V, Fe-H-W, Al-H-Ti, H-Ni-Ti, H-Ti-Zr systems and quaternary C-Fe-Mn-H, Cr-Fe-H-Ni systems were verified against the experimental data.
- Al-Fe-Nb, Fe-Nb-Ni, Co-Fe-Nb, Al-Cr-Nb
- Al-Fe-Zr, Cr-Fe-Zr, Cu-Fe-Zr
- Ca-P, Ca-Ti, Ca-V, Ca-W
- Ce-Nb, Ce-Ta, Ce-Ti, Ce-W
- Ca-N, N-Y, Ce-N
- Nb-Zn, Ta-Zn, W-Zn, Fe-Nb-Zn
- P-V, Fe-P-V
- S-Ta

Updated Systems and Phases

- Fe-N and C-Fe-N are updated to a more recent modeling work including the non-stoichiometric composition of Fe_4N nitride.
- Fe-Si and C-Fe-Si are updated to avoid a high temperature miscibility gap in the liquid.
- Cr-Si, Cr-Fe-Si, and C-Cr-Si are updated to a more recent modeling work.
- FeNbP, FeTiP, NbCrP, NbNiP, CrNiP are modeled as FEMP_C23 phase.
- Co-Nb, Cr-Nb, and Cr-Nb-Ni are updated to separate C15 and C14 laves phases.
- Fe-Y is updated to a more recent modeling work.
- Fe-Zr and Fe-Si-Zr are updated to a more recent modeling work.
- Fe-Nb is updated with an updated formation energy of MU_D85 phase.
- Nb-N is updated to a more recent modeling work.
- Ni-S is updated to assess the solubility of S in Fcc nickel.

TCS Ti/TiAl-based Alloys Database (TCTI3)

- Added Copper (Cu), which is a minor-alloying element in titanium alloys.
- Ti-Cu, Cu-Fe, Cu-H, Cu-N, Cu-Nb, Cu-O, Cu-Si, Cu-Sn, Ti-Cu-C, Ti-Cu-Fe, Ti-Cu-H, Ti-Cu-N, Ti-Cu-Nb, Ti-Cu-O, Ti-Cu-Si, and Ti-Cu-Sn are modeled. Now it is possible to perform calculations for titanium alloys within the framework of Ti-Cu-Sn-Nb-Si. Moreover, the reliability can be enhanced by the availability of considering the effects from common impurities: C, Fe, H, N, and O.
- Al-Cu and Ti-Al-Cu are modeled, which is useful for both Ti- and TiAl-based alloys where alloying effects of Cu are of interest.

- Ti-Hf-Ta, Ti-B-Hf, Ti-Hf-Zr, and B-C-Si are modeled. These systems are of particular use for those involved in the development of biomedical materials because it combines cytocompatibility and improves mechanical properties.
- Viscosity and surface tension of liquid are included with the database as of this release.

TCS Ti-alloys Mobility Database (MOBTI4)

MOBTI4 is compatible with TCTI3. A new element Cu was added in the Bcc_A2, Hcp_A3, and liquid phases.

TCS Al-alloys Mobility Database (MOBAL6)

Three elements added to the database: Nb, P, and Y.

TCS Steels/Fe-Alloys Mobility Database (MOBFE6)

Addition of Hydrogen (H) to the database with the following assessed systems:

- FCC_A1: Al-H, Co-H, Cu-H, Fe-H, H-Ni, Fe-H-Ni, Cr-Fe-H, Co-H-Ni
- BCC_A2: Cr-H, Fe-H, Mo-H, Nb-H, Ti-H, Ta-H, V-H, Fe-H-Si, Cr-Fe-H, H-Mo-Ti, H-Nb-V, H-Ti-V
- HCP_A3: Al-H, Co-H, Ti-H
- LIQUID: Al-H, Cu-H, Fe-H, Mg-H, H-Ni, H-Si, Co-Fe-H, Cr-Fe-H, Cu-Fe-H, Fe-H-Mn, Fe-H-Mo, Fe-H-Ni, Fe-H-Nb, Fe-H-V, Fe-H-W

TCS Mg-alloys Mobility Database (MOBMG2)

- Nine elements added to the database: Bi, Dy, Er, Ga, H, Ho, In, Sb, and Sm
- Existing descriptions of the HCP_A3 are improved taking into account the new available experimental data and CALPHAD assessments.

IRSN Mephista-19 Nuclear Fuels Database (MEPH19)

Binary Systems

- Cr-Ru and Fe-Ru: The lattice-stability of Ru(BCC_A2) available in the Unary 5.0 SGTE database taken into account
- Fe-Si: Y. Yuan et al. Calphad, 44:54–61, 2014.
- Fe-U: The lattice-stabilities of Fe(ORT_A20) and Fe(TET) available in the Unary 5.0 SGTE database taken into account
- La-U: Improvement of liquid thermodynamic properties
- La-Zr: N. Mattern et al. Calphad, 52:8–20, 2016.
- Ru-U: The lattice-stability of Ru(BCC_A2) and U(hcp_A3) available in the Unary 5.0 SGTE database taken into account. The Ru_3U compound is now modeled as a solution phase, CxRU3U1(SS).
- Si-Sr: Li et al., Calphad, 35(4):594–600, 2011.
- Si-Zr: Revised to suppress the appearance of a miscibility gap at the liquid state.
- U-Zr: The lattice-stability of U(hcp_A3) available in the Unary 5.0 SGTE database taken into account. Improvement of the modeling of liquid and DELTA_UZr_2 thermodynamic properties

Pseudo-binary Systems

- Ba-O-Si BaO-SiO_2: Additional compound in the BaO-rich part, BA3O5SI1(S).
- La-O-U La_2O3-UO_2: Improvement of the oxygen potential above the solid solution FCC_C1.
- La-O-Si La_2O_3-SiO_2: Improvement of the thermodynamic properties of $La_2Si_2O_7$
- O-Si-Sr SiO_2-SrO: Improvement with consideration of new experimental data.
- O-Si-Zr SiO_2-ZrO_2: Improvement of the description of the $ZrSiO_4$ compound (thermodynamic properties and decomposition temperature)

Ternary Systems

- C-O-Zr: Improvement with consideration of new experimental data.
- Reassessment of the Fe-O-U, Fe-O-Zr, and O-U-Zr systems

IRSN NUCLEA-19 Nuclear Alloys-Oxides Database (NUCL19)

Binary Systems

- Ag-Mg: The lattice-stability of Mg(FCC_A1) available in the Unary 5.0 SGTE database taken into account.
- Ag-Zr: Change of the decomposition nature of AG1ZR1 and AG1ZR2, to congruent and peritectic respectively
- Al-Fe: Sundman et al., Acta Materialia, 57(10):2896–2908, 2009.
- Al-Mg: Liang et al. Z. Metallkde., 89(8):536–540, 1998.
- B-Cr: Revision of the thermodynamic properties of the stoichiometric phases.
- B-Ni: Sun et al., International Journal of Materials Research, 100:59–67, 2009.
- B-Si: The lattice-stability of metastable B(dia_A4) available in the Unary 5.0 SGTE database taken into account
- Ba-Mg: Error correction
- Ba-Si: Three additional stoichiometric phases, BA2SI1, BA5SI3, BA1SI1, BA3SI4.
- Ca-La: FCC_A1 is not more stable above 1500 K.
- Cr-Ru: The lattice-stability of Ru (BCC_A2) available in the Unary 5.0 SGTE database taken into account
- Cr-Zr: Yang et al. Journal of Nuclear Materials, 441(1-3):190–202, 2013.
- Fe-Ni: Introduction of the $FeNi_3$ phase as a stoichiometric phase.
- Fe-Ru: The lattice-stability of Ru (BCC_A2) available in the Unary 5.0 SGTE database taken into account
- Fe-Si: Y. Yuan et al. Calphad, 44:54–61, 2014.
- Fe-U: The lattice-stabilities of Fe(ORT_A20) and Fe(TET) available in the Unary 5.0 SGTE database taken into account
- In-Mg: The lattice-stabilities of Mg (FCC_A1) and In (FCC_A1) available in the Unary 5.0 SGTE database taken into account.
- In-O: Improvement of the modeling of solubility of oxygen in indium liquid
- La-Mg: F. Zhang, Journal of Alloys and Compounds, 663:279–288, 2016.
- La-U: Improvement of liquid thermodynamic properties
- La-Zr: N. Mattern et al. Calphad, 52:8–20, 2016.
- Mg-U: The lattice-stability of U(hcp_A3) available in the Unary 5.0 SGTE database taken into account.
- Mg-Zr: R. Arroyave et al., Calphad, 29(3):230–238, 2005.

- Ni-U: The lattice-stability of U(FCC_A2) available in the Unary 5.0 SGTE database taken into account.
- Ru-U: The lattice-stability of Ru(BCC_A2) and U(hcp_A3) available in the Unary 5.0 SGTE database taken into account. The Ru3U compound is now modeled as a solution phase, CxRU3U1(SS).
- Si-Sr: Li et al. System. Calphad, 35(4):594–600, 2011.

Pseudo-binary Systems

- Al-Ba-O Al_2O_3-BaO: Introducing two new stoichiometric compounds in the BaO-rich region, AL2BA4O7(S), and AL2BA7O10(S)
- Al-La-O Al_2O_3-La_2O_3: Improvement of $AlLaO_3$ thermodynamic properties.
- Al-O-Sr Al_2O_3-SrO: $Al_{12}SrO_{19}$ melts congruently whereas its decomposition was previously considered to be peritectic.
- Ba-O-Si BaO-SiO_2: Additional compound in the BaO-rich part, BA3O5SI1(S).
- Ca-O-Sr CaO-SrO: Improvement with consideration of new experimental data.
- Ca-O-Zr CaO-ZrO_2: Description of the solubility of CaO in the ZrO_2 tetragonal phase, and the solubility of ZrO_2 in the CaO FCC_B1.
- In-O-Zr In_2O_3-ZrO_2: Improvement of the modeling in the zirconia-rich region.
- La-O-U La_2O_3-UO_2: Improvement of the oxygen potential above the solid solution FCC_C1.
- La-O-Si La_2O_3-SiO_2: Improvement of the thermodynamic properties of $La_2Si_2O_7$
- O-Si-Sr SiO_2-SrO: Improvement with consideration of new experimental data.
- O-Si-Zr SiO_2-ZrO_2: Improvement of the description of the $ZrSiO_4$ compound (thermodynamic properties and decomposition temperature)

Ternary Systems

- C-O-Zr: Improvement with consideration of new experimental data.
- Cr-O-Zr: Modeling of the ternary system in the metallic-oxidic part.
- Reassessment of the Fe-O-U, Fe-O-Zr, and O-U-Zr systems

Pseudo-ternary Systems

Ca-O-Si-Zr: Modeling of the CaO-SiO_2-ZrO_2 pseudo-ternary system

Updated Databases

TCS Aluminium-based Alloys (TCAL7.1)

- Modeling of Mg-Si-Sn
- Update Al-Mo
- Update of molar volume data
- Update of electrical resistivity and thermal conductivity data

TCS High Entropy Alloys Database (TCHEA4.2)

Added the assessment of three binary systems- Ir-W, Mo-Rh, and Rh-W.

TCS Metal Oxide Solutions Database (TCOX10.1)

Thermophysical Property Updates

- Added viscosity for the liquid oxides of MoO_2, MoO_3, NbO, Nb_2O_5 and Y_2O_3.
- Replaced the molar volumes of metallic liquid with the unified molar volumes, which is now consistent with all the other databases.
- Added molar volumes for both liquid and solid phases which had missing values in the previous version.

Binary, Ternary, and Higher Order System Updates

- N: Added NO_3^{-1} to the liquid phase.
- Fixed a bug in NiO that made the function not continuous at T=1800 K. These systems are reassessed due to the change in NiO description: Ca-Ni-O, Gd-Ni-O, La-Ni-O, Nb-Ni-O, Ni-O-P, Ni-O-Si, Ni-O-Ti, Ni-O-V, Ni-O-Y, CaO-NiO-SiO_2, MgO-NiO-SiO_2, Co-La-Ni-O.
- Updated NbO_2 to the latest description.
- Decreased stability of $FeSiO_3$ ortho-pyroxene (should not be stable, but was in version 10.0).
- The following systems are assessed: AlF_3-NaF, $Ca(NO_3)_2$, Mg(NO3)2, MgF_2-NaF, $NaNO_3$, NaF-Na_2CO_3, $NaNO_3$-Na_2CO_3, Na_2CO_3-Na_2S, $Ca(NO_3)_2$-$Mg(NO_3)_2$, $Ca(NO_3)_2$-$NaNO_3$, $NaNO_3$-NaF, $Mg(NO_3)_2$-$NaNO_3$. Estimations: Al_2O_3-Na_2O-ZrO_2, Na_2O-SiO_2-ZrO_2.
- The following systems are reassessed: Updated liquid AlF_3 to [2013 Lambotte]. AlF_3-CaF_2, AlF_3-MgF_2. Reassessed solubility of Al in V3O5_HT and M4O7. Reassessed solubility of Mg in V3O5_HT.
- Assessed a separation between liquid NaF and oxides in the following NaF-MeO_x systems: MeO_x= CuO, $FeO_{3/2}$, $MnO_{3/2}$, $NbO_{5/2}$, SiO_2.

SALT1: SGTE Molten Salts Database (SALT1.3)

Corrected a bug in the description for liquid LiCl.

TCS Steel and Fe-alloys Database 8.2 and 9.3

For users who have TCFE8 and TCFE9 and also use the Steel Model Library, there was an update to correct the volume of liquid Zn.

If you use these older databases it is recommended you update to the latest software version to have this improvement available with the subversion of the databases.

TCS Ti-alloys Mobility Database (MOBTI3.1)

The diffusivity of O in Bcc_A2 Ti was corrected.

Installation

Thermo-Calc and TC-Python: New Bundled Python Interpreter

Install with the Bundled Python-interpreter

This is a straightforward installation where TC-Python is preinstalled together with some popular Python packages. You just need to also install an IDE, for example PyCharm, in order to run the examples. This is the recommended option for new users to TC-Python who may only want to run the examples. The available preinstalled packages (e.g. numpy, scipy, scikit-learn, and matplotlib) can also be sufficient for many advanced users.

Install with a Python-interpreter of Your Choice

This installation requires additional steps and is the recommended option for more advanced use and has full flexibility. For previous Thermo-Calc versions (2020b and earlier), this is how the installation has been done, using Anaconda for example to do a pip installation of TC-Python.

Updating TC-Python from 2020b to 2021a (Nonbundled Installations)

This is only applicable to the users who will continue to use a Python interpreter of their own choice. There is now a bundled installation option included with Thermo-Calc downloads (and when there is a license for TC-Python).

However, if you installed earlier versions of TC-Python with Thermo-Calc, then when updating to a newer version of Thermo-Calc, you also need to install the latest version of TC-Python. It is not sufficient to run the installer of Thermo-Calc. See the section “Updating to a newer version” in the TC-Python Quick Installation Guide. A PDF of this manual is available on our website or search the online help if you have already installed Thermo-Calc.

Details about the TC-Python installations are available in the *2021a Thermo-Calc Installation Guide*, which among other places, can be found on our website.

Sentinel RMS License Management Software: Upgraded to Version 9.7

Thermo-Calc Software was alerted to a security issue related to older versions (v9.6 or earlier) of the Sentinel RMS License Manager (Windows) and License Server (Linux) software. The issue was related to the potential for a Denial of Service [DoS] to the Sentinel RMS License Manager through a remote memory corruption vulnerability in Sentinel RMS License Manager

The latest version of **Sentinel RMS, 9.7**, has fixed this issue. For new network licenses, version 9.7 is automatically provided with the download provided by Thermo-Calc. Existing customers were directly informed about this issue but it is important that any network license users install and use the latest 9.7 version.

Details about upgrading or new installations are in the *2021a Thermo-Calc Installation Guide*, which among other places, can be found on our website.

OpenSuse (Linux) - TC-Python Installations and Lib

If this error appears when running TC-Python:

```
ImportError: libffi.so.6: cannot open shared object file: No such file or directory
```

The following third party link has instructions to install libffi6:

https://software.opensuse.org//download.html?project=home%3Afstrba&package=libffi6

Installation Disk Space Requirement

Due to precompiled databases added to the Thermo-Calc installation, 2 GB of disk space is recommended for the 2021a 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 and Videos

New Examples

There are several new examples described elsewhere in this document. The Property Models and Process Metallurgy examples are available from within Thermo-Calc (Help > Example Files). TC-Python is available either from your IDE or by navigating to its installation location.

Property Models > General

- PM_G_07_Hot_Crack_Susceptibility.tcu
- PM_G_08_Spinodal.tcu
- PM_G_09_T-Zero_Temperature.tcu
- PM_G_10_Freeze_in_Thermal_Conductivity.tcu
- PM_G_11_Freeze_in_Electric_Conductivity.tcu

Property Models > Steel

- PM_Fe_04_Critical_Temperatures.tcu
- PM_Fe_05_Fe-C-Mn-Si-Ni-Cr-Mo_Bainite.tcu

Process Metallurgy

- PMET_07_Vacuum_Oxygen_Decarburization_Kinetics.cu

TC-Python > \SDK\TC-Python\Examples\PropertyModel

- pyex_PM_3_Property_model_self_developed_model.py

Videos

A new 2021a release video, plus one about the new Hot Crack Susceptibility Property Model, are available on the website and YouTube channel.

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

Changes to Documentation PDF Names

TC-Python Installation Guide

The *TC-Python Quick Installation Guide* is now just called *TC-Python Installation Guide*. This information continues to be included in the online TC-Python help and as part of the *Thermo-Calc Installation Guide*. The change is related to the new installation details.

New and Updated Database Technical Documentation and Examples Collections

All of the following is specific to the PDFs available on the website or included with the installation. All content continues to be available in the Thermo-Calc help. Example Collection PDFs are NOT included in the installation.

- Previously called Extended Information, the new databases also have new Technical Information and Examples Collections for TCFE11, TCMG6, and TCTI3.
- Updated Technical Information and Example Collections related to new subversions or with improvements: TCAL7, TCOX10, and TCHEA4.
- Updated Technical Information and Example Collections for TCNI10 and TCSLD3 to include new website links, formatting improvements, and to make consistent with all other database documents.

Renamed to Technical Information

The following database Technical Information documents include the release history. The information continues to be available in the Thermo-Calc help.

- MOBFE6, MOBAL6, MOBMG2, and MOBTI4

The 3rd Party IRSN databases also have a PDF renamed to Technical Information and this is combined with what was a separate document called an Overview. The information continues to be available in the Thermo-Calc help.

- NUCLEA-19 (NUCL19) and Mephista-19 (MEPH19)

Platform Roadmap

A reminder to any users still using Windows 7 or Windows 8 to upgrade as soon as possible. Thermo-Calc will stop supporting these platforms as of 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.