Thermo-Calc Software

Release Notes:

Thermo-Calc Software Package

Version 2016b
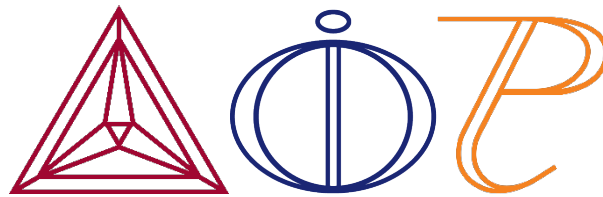
Contents

Thermo-Calc 2016b

This release focusses on fixing some outstanding issues as described in the sections below. The primary fixes relate to the Scheil Calculator in Graphical Mode and the Scheil Module in Console Mode.

👁 For more information about Thermo-Calc and the add-on module features, open Thermo-Calc, select **Help → Online Help** and enter a key word or phrase.

Thermo-Calc

Compute Transition now uses Global minimization (Console Mode, Scheil, Property Model Calculator)

- The COMPUTE_TRANSITION command now uses Global minimization for the equilibrium calculations to verify that the found transition is a global minimum. This improves:
  - o Finding correct liquidus temperature in Scheil simulations,
  - o The console command for compute transition, and
  - o Property Model calculator model *Compute Transition*

Diffusivity (Console Mode and SDK)

Fixed an issue where showing the diffusivity was wrong for complex phases when dependent component was not last in alphabetic order.

📝 This issue was not related to diffusion simulations in the Diffusion module (DICTRA). It was limited to listing diffusivities in Poly-3 and when retrieving them using the SDKs.

Property Model Calculator (Graphical Mode)

- Fixed a bug for the Property Model Calculator where changing an axis did not automatically update all the corresponding plot axes.
- Compute Transition model now uses global minimization.

Equilibrium Calculator and Table Renderer (Graphical Mode)

- For a single-equilibrium calculation, fixed an issue where phases with zero (0) amounts were displayed.

Scheil Calculator (Graphical Mode) and Scheil Module (Console Mode)

The robustness of the Scheil simulations has improved.

- Compute transition now uses global minimization and has improved in finding the correct liquidus temperature.
- Phases that were deselected in System Definer could appear in the simulations.
- Improved handling of miscibility gaps in the liquid phase.
- Numerical options for the equilibrium calculations are now included in Graphical mode and Console Mode. In rare cases these may need to be altered when the equilibrium calculations do not converge.

- o The SET_NUMERICAL_LIMITS command is now available for Scheil calculations (Console Mode).
- o Settings from the SET_NUMERICAL_LIMITS Console Mode command are now available for Scheil calculations (These are in the **Scheil Calculator > Advanced Settings** options).

Start temperature:	2500.0
Temperature step:	1.0
Temperature unit:	Kelvin
Composition unit:	Mass percent
Global minimization:	☑
Liquid phase:	LIQUID
Terminate on:	Fraction of l... at: 0.01
Max no. of iterations:	500
Required accuracy:	1.0E−6
Smallest fraction:	1.0E−12
Approximate driving force for metastable phases:	☑

The below example for an oxygen containing steel (Fe, C, Si, Mn, P,S, Al, O) is complex due to miscibility gaps in the liquid phase and can also give convergence problems in the equilibrium calculations due to small amounts of oxygen in some of the phases. The 'Smallest fraction' (the lowest allowed amount for a site-fraction on a sublattice) needs to be decreased from the default 1e-12 to 1e-14 in the numerical options to avoid these convergence problems.
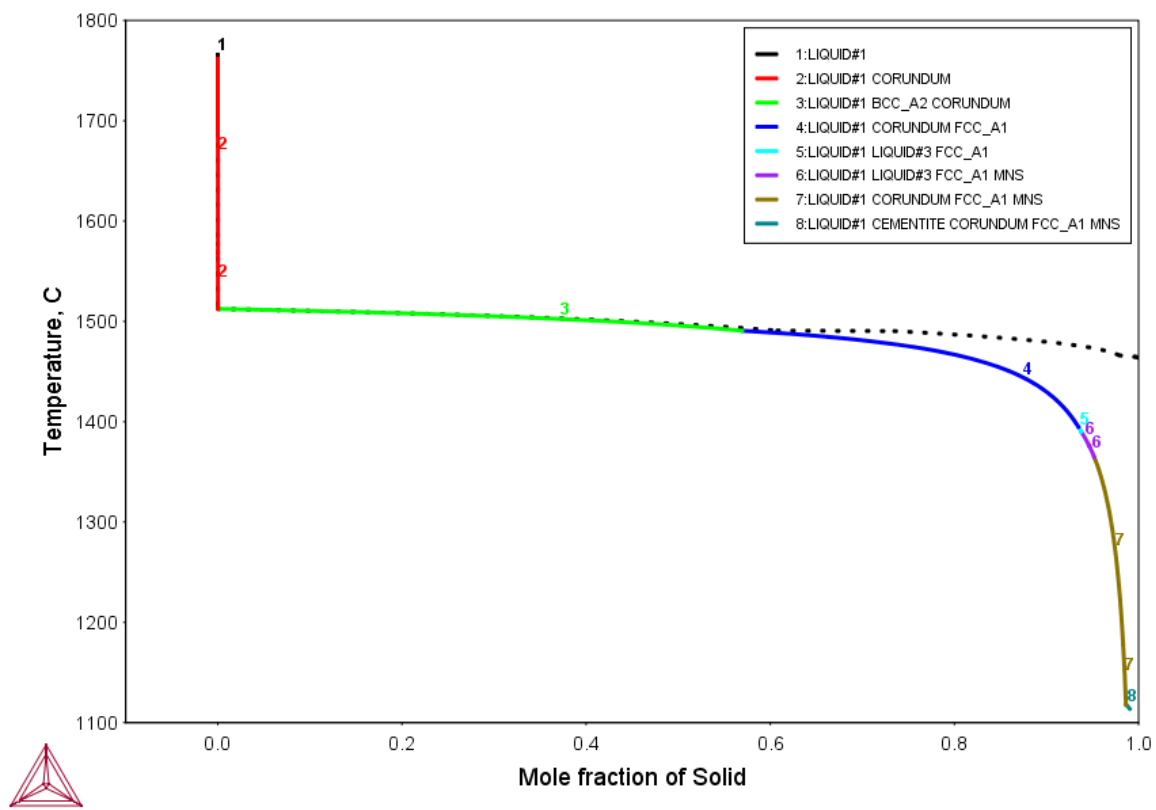
Precipitation Module (TC-PRISMA)

Fixed a problem where plots did not work as a result of languages with special characters being selected as the localization language, e.g. Chinese, Japanese or Swedish.

SDKs (Software Development Kits)

TQ-Interface

- Fixed an issue where *Show diffusivity* was wrong for complex phases when dependent component was not last in alphabetic order.
- Improved the speed of calculating the diffusion coefficient matrix in complex phases.

TC-Toolbox for MATLAB®

Fixed a bug when working with the TC-Toolbox for MATLAB and DICTRA. The dic_convert_sitefractions command now works as expected to convert from mole to weight fractions.

Databases

TCNI8

Fixed a bug in TCNI8 that caused the GUI to crash on rare occasions. It was related to carbon in combination with non-Ni/Co superalloy composition.

TCFE8

TCFE has been updated to TCFE8.1 due to the following:

- A bug fix that previously resulted in a faulty estimation of molar volume of borides, and
- The change of description of Fe-B and Fe-Ti-B systems due to incompatibility.

New version of TCAQ3

The TCAQ3 aqueous database has been updated so that all charged species (except $H+1$ and $OH-1$) are renamed with an extra prefix "A_". For example, $FE+3$ becomes A_FE+3, $CO3-2$ becomes A_CO3-2, and $FEOH+2$ becomes A_FEOH+2, and so forth. This change is to enable compatibility with other databases where phases are described by ionic CEF (e.g. the spinel phase in the TCFE or TCNI databases).

☑️It is necessary to keep the names $H+1$ and $OH-1$ for the POLY_3 module so that the LIST_EQUILIBRIUM command gives the correct pH value. Keeping these names is also required for POURBAIX Module calculations.

Installation and Licensing

- Improved the license diagnostic functions to help with support questions and issues that arise with some network license installations.
- Fixed a bug in Linux and Mac where the license diagnostic details did not display.

Documentation, Training Materials and Examples

In case you missed it, all the documentation available in PDF format is also available in the Online Help. There is also a new look and feel to the help interface. You still access it from the main menu in Thermo-Calc (**Help → Online Help**) but now it is easier to search and navigate the content by product.

👁 Send your documentation suggestions or requests to documentation@thermocalc.com.

New Examples

TC-Toolbox for MATLAB®

A new example (named *ex06_interfacial_energy.m*) is available with the TC-Toolbox for MATLAB. This example calculates the interfacial energy between BCC and M7C3 for a Fe-12Cr-0.1C alloy.

📝 Examples for the TC-Toolbox are placed under MATLAB in the same documents folder as the Thermo-Calc files (My Documents or Public Documents):

> ..\Documents\MATLAB\Thermo-Calc-Toolbox-X\Examples

Where X is the installed version number of the toolbox. For most installations the examples are available in the MATLAB window when the software is opened.

The use of the TQ-Interface with MPI

Two new examples are available with a TQ-Interface installation. These are to show how to speed up calculations with the TQ-Interface by performing calculations in parallel processes using MPI (Message Passing Interface).

- MPExample1: This is an MPI (Message Passing Interface) example that calculates the Gibbs energy for a composition grid C with a density of "npoints" at 1273K in the Mn-Ni-Fe system.
- MPExample2: This is an MPI (Message Passing Interface) example where a set of equilibrium calculations are distributed over all processes. Then the Gibbs energy of the system is retrieved and collected in a single vector in the master process.

📝 The examples are included in the SDK installation directory. For example, for a network installation on Windows, the directory is here:

> C:\Users*username*\Documents\Thermo-Calc*version*\SDK\TQ\Windows

Platform Roadmap

As per the platform roadmap, Linux 32-bit is no longer supported. For information about other platforms being phased out visit http://www.thermocalc.com/products-services/software/system-requirements/platformroadmap/.