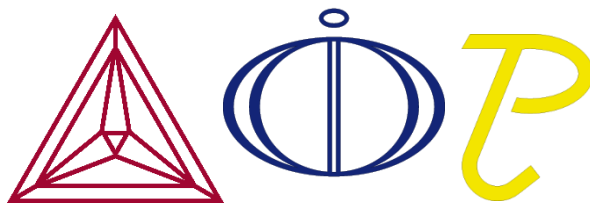


**Thermo-Calc
Software**

Release notes:

Thermo-Calc software package 4.1



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Release notes

Introduction

This document provides information on new products, features and bug fixes in version 4.1 of the Thermo-Calc software package.

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1 Delivery contents

The release includes the following:

- New version 4.1 of the Thermo-Calc program.
- New database product MOBSI1.
- New version 9.1 of the TQ-Interface Software Development Kit.
- New version 7.1 of the TC-API and the TC-Toolbox for MATLAB Software Development Kits.
- Revised releases of the databases TCNI7, MOBNI3 and TCSI1.

2 New products in Thermo-Calc software package 4.1

2.1 New mobility database MOBSI1

MOBSI1 contains self and impurity diffusivities in both solid and liquid Si. The database can be used together with TCSI1 to simulate diffusion phenomena for the production of solar cell grade Si. See section 6.1.1 for more information.

3 Thermo-Calc

3.1 New functionality

3.1.1 Graphical Mode specific

- A new “Property grid” calculation type has been added. A property grid plots a property as a surface on a plane defined by two independently varied variables. For example, the amount of a certain phase can be varied when the compositions of two components are varied. The value of the plotted property—that is, the amount of the phase—is represented either by colour-coded pixels in a heat map, or as coloured contours that trace certain values of the plotted property (akin to how height is traced by contours on a topographic map). To calculate a property grid, select the “Property grid” calculation type in the Configuration window of an Equilibrium Calculator and select which quantities that the stepping operations should be performed on. In the Plot Renderer, specify which property that should be plotted and select whether to present the diagram as a “Heat map” or a “Contour” plot.
- A new plot variable, “u-fraction”, has been added to the Graphical Mode. It was previously only available in the Console Mode. See section 6.1.1 in the *Thermo-Calc Console Mode User guide* for general information about u-fraction.
- When the results of a Scheil Calculator are plotted with the default plot axes (“Mole fraction of solid” on the X-axis and “Temperature Celsius” on the Y-axis), the results of normal equilibria calculations are automatically plotted in the same diagram as the Scheil calculations.

3.1.2 Console Mode specific

- In the “Console” window, tabs can be opened and closed in additional ways. A pop-up menu is shown when the header of a tab is selected. This menu contains options for closing all tabs (“Close All”), closing all other tabs (“Close Other”), closing the selected tab (“Close”) and opening a new tab (“New Console”).
- New Plot tabs can be opened and closed in the Results window while you are working in a tab in the Console window. To open a new Plot tab, press Ctrl+Shift+T. To close the currently shown Plot tab, press Ctrl+Shift+W or Ctrl+Shift+F4.

3.1.3 DICTRA-module specific

- Each curve in a DICTRA plot is now associated with a unique number and colour. The number is displayed in the tooltip next to the cursor when the tip is held on the curve. To display the numbers as labels beside the curves inside the plot and in a legend, use the POST command LABEL_CURVES Y. To change the colour of a curve, click it and choose a colour from the palette that is opened. To change the label shown beside a curve, click the label and enter a new one in the “Edit Label” window.

3.2 Improvements

3.2.1 Console Mode and Graphical Mode

- Graphical design improvements have been made to the tick labels on diagram axes with logarithmic scales.
- The default colour settings in Plot Properties have changed. The default background colour is now white instead of light grey and the default colour for all texts and lines is black instead of dark grey. Note that these default colour settings are applied even if the settings from an earlier version of Thermo-Calc are imported when Thermo-Calc 4.1 is installed.
- When saving plots, the default image file format is now PNG instead of SVG.

3.2.2 Graphical Mode specific

- Plot Renderer tabs are no longer automatically updated when changes are made in the Plot Renderer’s Configuration window. To update the plot, perform the activity tree. If a plot has not been updated, then a warning sign in the form of an exclamation mark enclosed in a yellow triangle is shown on the header of the Plot Renderer tab.
- Plot Renderer activities are now automatically reconfigured when changes are made to the tree to which it belongs. For example, if the quantities that a phase diagram mapping will be performed on is changed, then the Plot Renderer’s axis variables are automatically updated with the appropriate default values.
- Some single-equilibrium, property diagram and phase diagram calculations are now completed faster.

3.3 Bug fixes

3.3.1 Console Mode and Graphical Mode

- The rendering of the Thermo-Calc user interface on high-resolution displays has been improved. This means, for example, that it is now easier to read and use the periodic table, project trees and tables in Graphical Mode on a high-resolution display.
- An error in the Ionic Liquid model that sometimes led to deviances in calculations has been fixed.

3.3.2 Graphical Mode specific

- Diagram axes now plot units or are given labels that appropriately reflect normalisation. For example, if the amount of all phases per mole is plotted on an axis, then the axis label text becomes “Mole fraction of all phases” instead of “Amount of all phases [mol]”.

3.3.3 Console Mode specific

- Thermo-Calc no longer crashes when a GES5-file is read that doesn't exist, that doesn't have a valid format or for which a license is missing.
- Thermo-Calc no longer stalls or crashes when the DATA command SWITCH_DATABASE USER is called from a macro without a user database name specified. Nor does the program stall or crash if you click «Cancel» when the “Open” file window opens in response to SWITCH_DATABASE USER.
- When the cursor is held above a phase region in a liquidus projection plot, the phase is now displayed in the tooltip next to the cursor (as it is in other phase diagrams).
- It is now possible to continue to work with a console tab if the user has tried to open an encrypted database (TDC) file as a user database.

3.4 Compatibility

The 4.1 version of the Thermo-Calc program is fully backward-compatible with earlier versions of the Thermo-Calc program.

4 TC-PRISMA

TC-PRISMA does not have any new functionality and no bug-fixes have been done since Thermo-Calc 3.1. The current version of TC-PRISMA is 2.0.2.

5 Software Development Kits (SDKs)

- The SDKs TQ-Interface 9.1, TC-API 7.1 and TC-Toolbox for Matlab 7.1 are compatible with the new Thermo-Calc 4.1 version.

5.1 Bug fixes

- When TQ-Interface tries to read a GES5-file that doesn't exist or that is in the wrong format, the error message "Failed to open the data file!" is issued. If there is no license for GES5-file is trying to read, then the error message "No valid licenses" is issued instead.

6 Databases

6.1 New database

6.1.1 MOBSI1

This is a mobility database with self and impurity diffusivities in both solid and liquid Si.

- The database contains the following 28 elements: Ag, Al, As, Au, B, Bi, C, Co, Cr, Cu, Fe, Ga, Ge, In, Li, Mn, N, Ni, O, P, S, Sb, Si, Sn, Te, Ti, V, Zn.
- When used together with the thermodynamic TCSI1 database, diffusion phenomena can be simulated for the production of solar cell grade Si.

6.2 Revised database releases

What follows are the updates in the revised database releases, available for all customers who have licenses for these databases.

6.2.1 TCNI7

- Liquid without oxygen is now modelled with the ordinary substitutional solution model by default. This improves performance for alloys where oxygen does not have to be considered. If oxygen is present, then the liquid phase is modelled with the Ionic Liquid model.
- Improved description of the M6C carbide in the systems C-Cr-Ni-Mo and C-Cr-Ni-W. Previously, M23C6 was predicted as primary carbide for some commercial alloys, instead of the correct M6C. Thanks to a more accurate stability estimate for M6C, this is no longer the case.
- Improved description of the Cr-Ni-B system. Previously, the NI3B_D011 phase was too stable, which resulted in an inaccurate equilibrium with liquid.
- For ternary and quaternary systems with Y and/or Mn, constraint relations have been added for parameters describing FCC_L12 phase. This increases the stability of calculations.
- An error in volume data for systems containing Fe has been fixed.
- Various minor corrections and adjustments have been implemented.

6.2.2 MOBNI3

- The mobility of Mn has been added. This means that MOBNI3 is in complete alignment with TCNI7.

- The mobility data for the liquid phase have been adapted to the corresponding new thermodynamic descriptions in TCNI7 (see section 6.2.1).
- Various minor corrections and adjustments have been implemented.

6.2.3 TCSI1

- Description of solubility of Te in solid Si has been added.

7 Platform support

- Support has been dropped for installing and running the Thermo-Calc software package on Windows XP.
- Thermo-Calc for Windows has been tested on Windows 8 64-bit, Windows 7 SPI 32-bit and Windows 7 SPI 64-bit.
- Thermo-Calc for Linux has been tested on Ubuntu 12.04, CentOS (RedHat) 6.3 and OpenSUSE 12.2.
- Thermo-Calc for Mac OS has been tested on Mac OS X Mountain Lion (10.8) and Mac OS X Mavericks (10.9).
- TC-Toolbox for Matlab has been tested with Matlab 2013b and 2014a.

8 Installation

For more information about installation, see the Installation guides:

- *Thermo-Calc installation guide for Windows*
- *Thermo-Calc installation guide for Linux*
- *Thermo-Calc installation guide for Mac OS*

These can be found on the Thermo-Calc website under Support | Documentation.

Thermo-Calc 4.1 can be installed on a computer that already has Thermo-Calc 3, 3.1 or 4.0 installed. Thermo-Calc 4.1 will simply installed in its own home directory.

9 Roadmap

Support for installing and running the Thermo-Calc software package on all 32-bit platforms will be dropped within the next few years. Users with a 32-bit platform installation are therefore advised to migrate to a 64-bit platform in the near future.