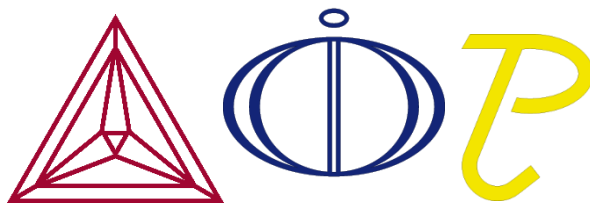


**Thermo-Calc
Software**

Release notes:

Thermo-Calc software package 3.1



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Release notes

Introduction

This document provides information on new products, features and bug fixes in version 3.1 of the Thermo-Calc software package.

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1 Delivery contents

The release includes the following:

- New database product MOBTT1 v.1.0
- New release 3.1 of the Thermo-Calc program, in both Console Mode and Graphical Mode.
- Revised release 27.0.1 of DICTRA.
- Revised release 2.0.1 of TC-PRISMA.
- Revised releases of the Software Development Kits TQ-Interface, TC-API and TC-Toolbox for MATLAB.
- New version 3.0 of database MOBAL3.
- Revised releases of the databases TCFE7, TCNI6 and TCAL2.

2 New products in Thermo-Calc software package 3.1

2.1 MOBTT1 v.1.0

MOBTT1 is a kinetic database containing mobility data for Ti-based alloys. It includes 9 elements (Al, Cr, Mo, Nb, Sn, Ta, Ti, V, Zr) and 3 phases (BCC_A2, HCP_A3 and LIQUID). Combining with the thermodynamic database TTTI, this mobility database can be used together with DICTRA, TC-PRISMA, or Thermo-Calc SDKs to simulated diffusion-controlled phase transformation or precipitation kinetics in Ti-based alloys.

3 Thermo-Calc

3.1 New functionality

3.1.1 Platform support and documentation

- Mac OS version of Thermo-Calc.
- New user manuals for Thermo-Calc. The following documents are new:
 - *Thermo-Calc installation guide for Windows*
 - *Thermo-Calc installation guide for Linux*
 - *Thermo-Calc installation guide for Mac OS*
 - *Thermo-Calc Graphical Mode User Guide*
 - *Thermo-Calc Console Mode User Guide*
 - *Thermo-Calc Console Mode Command Reference*

3.1.2 Console Mode and Graphical Mode

- The colour, stroke and line width of individual series of lines can now be changed by clicking one of the lines in the series. Whether data points should be shown for an individual series of lines can also be changed in this way. The crosshair cursor turns into a cursor resembling a pointing hand when it is placed over a line that can be clicked. However, if Ctrl is pressed down, this will not happen.

- When starting up the Thermo-Calc program for the first time after installation, the user settings from previous installed versions of Thermo-Calc 3 can be imported.
- Anchor plot labels can be set to be shown by default. To do this, select “Show anchor” on the “Plotting” tab in the Options window. This tab can be found under both the Console Mode tab and under the Graphical Mode>Activities tab.
- “Border color” and “Border width” can be changed either for a specific plot or in the default plot settings.
- “Legend background color” can be changed for specific plots or in the default plot settings.
- There are two new colour series available: “Vivid” (25 colours) and “Earth” (16 colours). The “Vivid” series is now the default colour series.
- The “Data point marker size” that is used can now be changed both for specific plots and in the default plot settings.

3.1.3 Graphical Mode specific

- Whether the tic marks on a plot’s axes should be placed inside or outside the plot surface can now be set. Select “Tick marks outside chart” on the “X Axis” or the “Y Axis” tab in the “Plot Properties” window. The tic mark size for each axis on these tabs can also be modified. Default settings for tick mark placement and size can be set in the “Options” window (to open, select “Options” from the “Tools” main menu).
- The size of the step between tic marks on each axis can be specified manually in a Plot Renderer’s “Configuration” window. For each axis, specify the size of the step in the “step” field (or select “Automatic scaling”).
- When a label is added to a plot, a “Rotation angle” can be entered to display the label at that angle.

3.1.4 Console Mode specific

- The new POST command `SELECT_PLOT <N/NEW>` can be used to select a plot in the Console Results window. “N” is the number of the plot tab to be selected. If there is no plot tab with that number or if the text “NEW” is entered instead of a number, then a new plot tab is opened.
- A new Console tab in the Console window can be opened by pressing “Ctrl-T” and a new plot tab in the Console Results window can be opened by pressing “Ctrl-Shift-T”.
- The name of a console tab can be changed by right-clicking the tab’s label and selecting “Properties” from the pop-up menu. The default name for new console tabs can be set in the “Default Appearance” tab under Console Mode in the Options window (to open, select “Options” from the “Tools” main menu).
- The POST commands `SET_CORNER_TEXT` and `SET_TIC_TYPE` are supported in Thermo-Calc 3.1.
- More types of characters can be used when adding labels to graphs with `ADD_LABEL_TEXT`. The following characters can now be used (provided that the characters in question are supported by the font used):

- Uppercase and lowercase greek letters: Enter the letters as an argument to the “^GR” code and end the string with a dollar sign (“\$”). For example, to enter “ α B γ δ ϵ Φ γ η ι φ κ ” into a label, enter “^GRa B c d e F g h i j k\$”.
- Numbers, parentheses, “+”, “-”, “i” and “n” in sub- or superscript: Enter these characters as an argument to the “^DO” code (subscript) or the “^UP” code (superscript) and end the string with a dollar sign (“\$”). For example, to enter “ 10^{2+i+n} ” into a label, enter “10^UP(2+i+n)\$”.
- Right- or left-facing arrows can be added by using the character combinations “!A” and “!B”.
- Any unicode character can be added by typing “^UC” followed by the code(s) for the character(s) that you want to include in the label. For example, to enter “ ω \hbar € X x ” into a label, enter “^UC461 452 463 46a 46b\$”.
- Labels added with ADD_LABEL_TEXT can be rotated by beginning the label text string with the command “^RO” followed by the number of degrees you want the label to be rotated. For example, to rotate the label “ 10^{2+i+n} ” forty-five degrees, enter “^RO45 10^UP(2+i+n)\$”.

3.2 Bug fixes

3.2.1 Console Mode and Graphical Mode

- When the results of a Scheil simulation is plotted in Console Mode or Graphical Mode, the composition set number is now shown in the plot.

3.2.2 Graphical Mode specific

- The number of sublattice sites is now correctly displayed in Table Renderer tabs in the Results window (when the “Constitution” or “Composition and constitution” views have been selected).
- When “Fraction of solid phases” are plotted from a Scheil simulation, curves are now correctly plotted in the Results window without displacement.
- The unit for entropy is now correctly an energy amount per temperature unit: “Joule per Kelvin”, “Calory per Kelvin” or “Electron volt per Kelvin”.

3.2.3 Console Mode specific

- The DUMP_DIAGRAM command has been fixed and now takes the parameters <FORMAT>, <FILENAME> and <Y/N>, where “y” means that if there is already a file in the working directory with the specified name, then that file will be overwritten.
- In some circumstances, labels and logotype were previous clipped when a plot was saved to an image file. This is no longer the case.
- All changes to plot properties are now immediately updated in the plot tab. There are no longer any changes that require a diagram to be plotted again for the change to take effect.
- The libraries for PDF and SVG-files have been changed and the text and symbols in a saved PDF now always gets the correct colours.
- Driving force for all phases (DGM(*)) now includes dormant phases.
- The command PATCH_WORKSPACE has been removed.

- A “Thermo-Calc\vers” folder is no longer automatically created in “My Documents” by Thermo-Calc.
- In some circumstances, Thermo-Calc 3.0.1 failed to create a socket when a proxy for internet browsing was used. This is no longer the case since Thermo-Calc no longer makes use of the Windows Java settings.
- The command SWITCH_DATABASE USER no longer changes the current directory.

3.3 Compatibility

The 3.1 version of the Thermo-Calc program is fully backward-compatible with earlier versions of the Thermo-Calc program.

4 DICTRA

4.1 New functionality in DICTRA 27.0.1

- Mac version of DICTRA.
- New user manuals for DICTRA. The following documents are new:
 - *DICTRA User Guide*
 - *DICTRA Command Reference*

4.2 Bug fixes

Some bug fixes have been implemented. This includes a bug in the evaluation of mobilities for ordered phases (interstitials are treated differently in the evaluation).

4.3 Compatibility

The 27.0.1 release of DICTRA is fully backward-compatible with earlier DICTRA releases.

5 TC-PRISMA

5.1 Bug fix in TC-PRISMA 2.0.1

An issue with retrieving mobility and diffusion data for W, Zn, and Zr in liquid systems has been fixed.

6 Software Development Kits (SDKs)

Minor bug fixes have been implemented in the SDKs TQ-Interface, TC-API and TC-Toolbox for MATLAB. The revised releases are:

- TQ-Interface 8.0.1
- TC-API 6.0.1
- TC-Toolbox for MATLAB 6.0.1

7 Databases

Besides the new database product MOBTH1 (see section 2.1), there is a new version of one database, and three new database releases.

7.1 New database versions

7.1.1 MOBTH1 v.3.0

- Mobility data for the new elements Be, Bi, Cd, Ce, Co, Ga, In and Pb in TCAL2 have been added for FCC_A1 and LIQUID phases.
- The mobility data for the interstitial elements B, C and H in the ordered phase FCC_L12 are now accessible thanks to the modified treatment of interstitials in ordered phases in DICTRA.
- The description of diffusion in the LIQUID phase has been greatly improved.

7.2 Revised database releases

7.2.1 TCAL2 v.2.1.1

- The Al-Fe-Mn-Si quaternary description had been systematically refined, including a deep revision of the Al-Fe-Si description and adjustments of the Al-Fe-Mn and Al-Mn-Si descriptions. It has been validated that this refinement improved the phase formation in a wide range of casting and wrought aluminum alloys, since Fe, Mn and Si are the most common additives and/or impurities in aluminum alloys.
- A new Al-Ni description has been adopted and adjustments were subsequently made on the Al-Ni-based ternary systems.
- The BCC_B2 description in the Ni-Zn binary system has been reassessed.
- The Al-Ni-Zn ternary has been reassessed.
- The Al-Mn-Ni description has been improved by solving some known issues.

7.2.2 TCFE7 v.7.0.1

Bug fix to prevent crash when restoring L12_FCC and Zr is in the system.

7.2.3 TCNI6 v.6.0.1

- A bug related to ternary interaction terms in the Cr-Ni-Ta system has been fixed. This bug caused a crash if DIS_FCC_A1 was restored.
- Ni17Y2 and Ni5Zr is no longer rejected by default.

8 Installation

The new versions and releases of the Thermo-Calc software package are installed in the same way in which previous versions and releases were installed.

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.

If Thermo-Calc 3.1 is installed on a computer that already has Thermo-Calc 3 or Thermo-Calc 3.0.1 installed, then the option of removing the old version of Thermo-Calc is provided as part of the installation procedure. However, the old version will only be removed if the older installation is the 3.0.1 release. To remove an installed version of Thermo-Calc 3.0, uninstall the software manually instead.