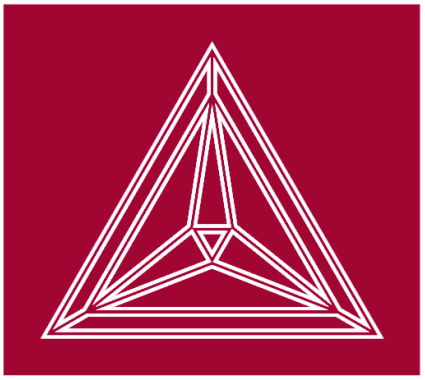
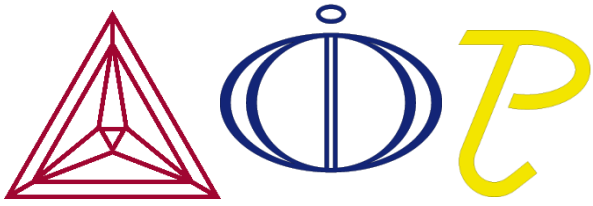


Release notes:

Thermo-Calc software package 4.0



Stockholm, Sweden

Release notes

Introduction

This document provides information on new products, features and bug fixes in version 4.0 of the Thermo-Calc software package.

Contents

1 Delivery contents

The release includes the following:

- New version 4.0 of the Thermo-Calc program, in both Console Mode and Graphical Mode, with the DICTRA program included as additional integrated module.
- New database product TCSI1.
- New version 9.0 of the TQ-Interface Software Development Kit.
- New version 7.0 of the TC-API and the TC-Toolbox for MATLAB Software Development Kits.
- New version of the databases TCNI, MOBNI, TCAL, TCMG and TCSLD.
- New installation software for all products. The Bitrock InstallBuilder now takes you through the installation process of the Thermo-Calc software package.

2 New products in Thermo-Calc software package 4.0

2.1 TCSI1

TCSI1 is a new Thermo-Calc software database for doing calculations on solar grade silicon materials.

- The database includes the following 34 elements: Ag, Al, As, Au, B, Bi, C, Ca, Co, Cr, Cu, Fe, Ga, Ge, In, Li, Mg, Mn, Mo, N, Na, Ni, O, P, S, Sb, Si, Sn, Te, Ti, V, W, Zn and Zr.
- The solubility of impurity X in diamond Si of all Si-X binaries have been assessed, except for the Si-Te binary.
- Besides the diamond phase, the liquid and the corresponding stable silicide phase with highest Si content is included in nearly all binary system that has Si as a component. The exceptions are Si-As, Si-Ga and Si-Sb.
- The binary systems Al-B and Al-P are also included.
- The ternary system Si-Al-C is included.

3 Thermo-Calc

3.1 New functionality

3.1.1 Console Mode and Graphical Mode

- On a network client installation of Thermo-Calc, it is possible to view who has checked out which license instances from the license server. This information is shown when the DISPLAY_LICENSE_INFO is used and when “Show License Info” is selected from the “Tools” main menu.

- A program that checks the syntax of database files has been added. This Database Checker can be used by database developers to check that the syntax of unencrypted Thermo-Calc or DICTRA database files is correct. The program applies the syntax rules defined in the Database Manager's Guide. Note that Thermo-Calc and DICTRA accept some deviations from these rules, so a database may work even if the Database Checker reports errors and warnings. For example, an error is reported if an abbreviated phase name is found, but phase name abbreviations are accepted by Thermo-Calc and DICTRA. The executable DatabaseChecker file is found in the Thermo-Calc home directory and can be launched by selecting "Database Checker" from the "Tools" main menu in Thermo-Calc.

3.1.2 Graphical Mode specific

- In the Configuration window, the selected activity and all activities below it in the activity tree can be performed by clicking the Perform Tree button. It is still possible to only perform the selected activity in the Project window.
- An Equilibrium Calculator activity is now easily configured by selecting "Single point", "Property diagram" or "Phase diagram" in the Configuration window.

3.1.3 Console Mode specific

- The DICTRA console is now an integrated part of the Thermo-Calc program. DICTRA exists as two Thermo-Calc modules: the DICTRA_MONITOR module and the DIC_PARROT module. Note that a separate DICTRA license is needed to use these modules.
- The POURBAIX module has been extensively revised and improved. In some circumstances, the module could previously not complete calculations of Pourbaix diagrams for systems with many elements. Significant improvements have now been implemented in the way the module handles numerical limits, hypothetical boiling temperature, acidity range, starting points and calculation of initial equilibria.

3.1.4 DICTRA-module specific

- A refined expression for the driving force for diffusion is now used in the homogenization model. The refined expression will only yield appreciably different results from the previously used expression at very high driving forces. The refined expression for the flux of component k, J_k, is the following:

$$J_k \propto \frac{-2RT}{\Delta z}\sinh\frac{\Delta\mu_k}{2RT}$$

- The mobility of a specific element in specific phases can be interactively modified with the new ENTER_ENHANCEMENT_FACTOR <PHASE> <ELEMENT> <FACTOR> command. The mobility of the specified element will be multiplied by the factor specified.
- Note that the old version numbering scheme for DICTRA has been dropped. The new version of DICTRA is referred to as DICTRA 4.0 (not DICTRA 28).

3.1.5 Documentation

- New *Data Optimisation User Guide for Thermo-Calc.*
- An appendix about "Thermodynamic variables and units" has been added to the *Thermo-Calc Console Mode User Guide*.
- New educational material document entitled *Pourbaix diagrams*.

3.2 Bug fixes

3.2.1 Console Mode and Graphical Mode

- It is now possible to select plot lines by clicking on them in ternary diagrams.
- Lines are now plotted in the correct colour also when the colour option "Legacy" is used.
- Some problems in how data from experimental data files (with filename extension "exp") were plotted previously have been fixed.
- The way that Thermo-Calc saves plots with unicode symbols and labels to PDF or SVG format has been improved.

3.2.2 Graphical Mode specific

- It is no longer possible to deselect species that represent system elements in the System Definer (on the Species tab in the "Configuration" window).

3.2.3 Console Mode specific

- Experimental data files are now saved with a lower case filename extension ("exp" instead of "EXP"). Note that both lower and upper case filename extensions are accepted when an experimental data file is read with QUICK_EXPERIMENTAL_PLOT or APPEND_EXPERIMENTAL DATA.
- When a plot is saved with DUMP_DIAGRAM in a macro file, the saved image file will now be exactly as the image depicting the plot on screen. Previously, the area around the plot were sometimes smaller in the saved image file.

3.2.4 DICTRA-module specific

- The general diffusion model has been changed. Results from calculations with this model should now be more accurate.
- It is now possible to perform DICTRA simulations involving the ionic liquid phase.
- Wildcard characters can now be used when plotting composition even if several plot conditions have been set.
- Data from several mobility databases can now be appended to a system definition.

3.3 Compatibility

The 4.0 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 9.0, TC-API 7.0 and TC-Toolbox for Matlab 7.0 are compatible with the new Thermo-Calc 4.0 version.

5.1 New functionality

- TQ-Interface has a new function TQGSE for estimating the interfacial energy between a matrix phase and a precipitate phase. The approximation model is based on Becker's bond energy approach and has been available in TC-PRISMA since version 2.0.

6 Databases

Besides the new database product TCSI1 (see section 2.1), there are new versions of the databases TCNI7, MOBNI3, TCAL3, TCMG3 and TCSLD2.

6.1 New database versions

What follows are the most important updates in the new database versions.

6.1.1 TCNI7

- The element Mn has been added. If you are going to do calculations on systems with an Mn-component, then note the following: The order-disorder model in Thermo-Calc has been used for describing the FCC_A1 and FCC_L12 phases. To reduce the time of performing calculations, Thermo-Calc uses a model with two sub-lattices rather than a more accurate (but computationally more costly) model with four sub-lattices. This means that many ternary and quaternary constraints must be added for the disordered state of FCC_A1 to be reached. However, these constraints have not yet been added in the database for systems containing Mn. The constraints will shortly be added to the database.
- The following 23 binary systems have been added: Mn-Al, Mn-B, Mn-C, Mn-Co, Mn-Cr, Mn-Fe, Mn-Hf, Mn-Mo, Mn-N, Mn-Nb, Mn-Ni, Mn-O, Mn-Pd, Mn-Pt, Mn-Re, Mn-Ru, Mn-Si, Mn-Ta, Mn-Ti, Mn-V, Mn-W, Mn-Y and Mn-Zr.
- The descriptions of the following 19 systems now includes ternary parameters: Al-Fe-Mn, Al-Mn-Ni, Al-Mn-O, Al-Mn-Si, Al-Mn-Ti, C-Fe-Mn, C-Mn-V, Co-Mn-O, Cr-Mn-N, Cr-Mn-O, Fe-Mn-N, Fe-Mn-Ni, Fe-Mn-O, Fe-Mn-Si, Mn-Ni-O, Mn-Ni-Si, Mn-O-Si, Mn-O-Y and Mn-O-Zr.
- The reappearence of phases above liquidus has been fixed for the systems C-Fe, C-Mn, C-Mo, C-Ni and Mo-Ni.
- The molar volumes in the database have been updated.

6.1.2 MOBNI3

- The descriptions for interstitial elements B, C, and N are now included.
- The description of the liquid using the ionic liquid model and MQ parameters is now available and compatible with TCNI7.
- The parameters have been updated for the following systems:
  - For the Fcc phase: Ni-Mo, Ni-O, Ni-Ru, Ni-Si, Ni-Ti, Ni-V, Ni-Y, Al-Pt, Al-Ru and Ni-Al-Pt.
  - For the L12 phase: Ni-Fe, Ni-Al-Mo, Ni-Al-Pt, Ni-Al-Ru, Ni-Al-Re and Ni-Al-V.
- The following systems have been checked against new assessments or experimental data:
  - For the Fcc phase: Ni-Hf, Ni-Nb, Ni-Pt, Ni-Re, Ni-Zr, Ni-Al-W, Ni-Al-Re, Ni-Al-Ru, Ni-Co-Re, Ni-Co-Ru, Ni-Re-Ru and Ni-Ru-W.
  - For the L12 phase: Ni-Al-Fe, Ni-Al-Si and Ni-Al-Ti
  - For the B2 phase: Ni-Al-Ru.

6.1.3 TCAL3

- The following 19 binary systems have been added: Ag-Ca, Ca-Cu, Ca-Fe, Ca-H, Ca-La, Ca-Li, Ca-Mn, Ca-Na, Ca-Ni, Ca-Sc, Ca-Si, Ca-Sr, Ca-Zn, Ag-Sc, Fe-Sc, Mn-Sc, Ni-Sc, Sc-Si and Sc-Zr.
- Metastable phases that enable the modelling of metastable precipitates have been added. More specifically, the following metastable phases and precipitates have been modelled:
  - The Al-Cu metastable precipitates GPI Zones (described as the miscibility gap of fcc_A1), θ''-Al_3Cu (that is, GPII Zones) and θ'-Al_2Cu.
  - The Al-Cu-Mg-Zn metastable phases S'-Al_2CuMg, T'-$Al_{0.3}Mg_{0.4}Zn_{0.3}$ and η'-$Al_3Mg_{2.5}Zn_{3.5}$.
  - The Al-Mg-Si metastable precipitates β''-Mg_5Si_6 (GPII zones), Al-containing β''-$Al_2Mg_5Si_4$, β'-Mg_9Si_5, U1-Al_2MgSi_2, U2-$Al_4Mg_4Si_4$ and B'-$Al_3Mg_9Si_7$.
  - The Al_mFe metastable phase (modeled as Al_4Fe). This has been observed in some as-cast aluminum alloys such as AA1xxx, AA5128 and A206.
- Volume data has been assessed for the new phases and newly introduced end-members.
- The Sn-Zn and Cu-Fe-Ni descriptions have been updated.

6.1.4 TCMG3

- The element Sc has been added.
- The following systems containing Sc have been added: Ag-Sc, Al-Sc, Mg-Sc, Mn-Sc, Cu-Sc, Fe-Sc, Sc-Si, Sc-Zr and Mg-Mn-Sc. Of them, Fe-Sc, Mg-Sc and Mn-Sc were reassessed.
- The following systems have been assessed and added: Mn-Nd, Sr-Y, La-Nd, Ce-Mg-Nd and La-Mg-Nd.
- The following systems have been thoroughly revised: La-Mg, Ce-Mg, Mg-Nd, Mg-Y-Zn and Ce-La-Mg.
- The systems La-Nd, Ca-Mn, Mg-Nd-Sr and Gd-Mg-Sr have been updated.

6.1.5 TCSLD2

Note that TCSLD2 is a complete revision of TCSLD1. The database is mainly developed for Sn-/Bi-/Au-/Zn-Al-based solder alloys and contains 133 binary and 61 ternary systems. The following elements included: Ag, Al, Au, Bi, co, Cu, Ge, In, Ni, Pb, Pd, Pt, Sb, Si, Sn, and Zn.

The important updates in TCSLD2 v. 2.0 are the following:

- The systems Ge-Pt and Pt-Sb have been added.
- The following 26 binary systems have been updated in light of new experimental data or in order to make them compatible with higher-order systems: Ag-Ge, Ag-Pd, Al-Au, Al-Bi, Al-Co, Al-Si, Au-Bi, Au-Co, Au-Ge, Au-Sb, Bi-Cu, Bi-Ni, Bi-Sn, Co-Ge, Co-Zn, Cu-Ge, Cu-Pb, Cu-Zn, Ge-Ni, Ge-Sb, In-Pb, Ni-Sn, Ni-Zn, Pb-Pt, Pb-Sb and Pb-Zn.
- The following 13 ternary systems have been added: Ag-Au-Ge, Ag-In-Pd, Al-Cu-Sn, Al-Ge-Zn, Al-Sn-Zn, Au-Cu-Sb, Au-Ge-Sn, Co-Ni-Sb, Cu-Ni-Sn, Ge-Sb-Sn, In-Pb-Sn, Pb-Sb-Sn and Pb-Sn-Zn.
- The following 21 ternary systems have been reassessed: Ag-Au-Pb, Ag-Au-Sn, Ag-Bi-Sn, Ag-Cu-In, Ag-Sb-Sn, Ag-Sb-Zn, Ag-Sn-Zn, Al-Bi-Sn, Al-Bi-Zn, Al-Cu-Zn, Au-Bi-Sn, Au-In-Sb, Au-In-Sn, Au-Ni-Sn, Au-Sb-Sn, Bi-In-Sn, Bi-Sb-Sn, Cu-In-Sn, Cu-Si-Zn, In-Ni-Sn and In-Sb-Sn.

7 Platform support

- Thermo-Calc for Windows has been tested on Windows 8 64-bit, Windows 7 SPI 32-bit, Windows 7 SPI 64-bit and Windows XP SP3 32-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 Mavericks (10.9).
- TC-Toolbox for Matlab has been tested with Matlab 2013b and 2014a.

8 Installation

The new versions and releases of the Thermo-Calc software package are installed with a new installer software, Bitrock installbuilder(www.bitrock.com).

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

9 Roadmap

After Thermo-Calc 4.0, Thermo-Calc Software will no longer develop and support the Thermo-Calc software package for the Windows XP operating system.

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.