Release Notes:

Thermo-Calc Software Package

Version 2016a

Contents

Highlights of Thermo-Calc 2016a

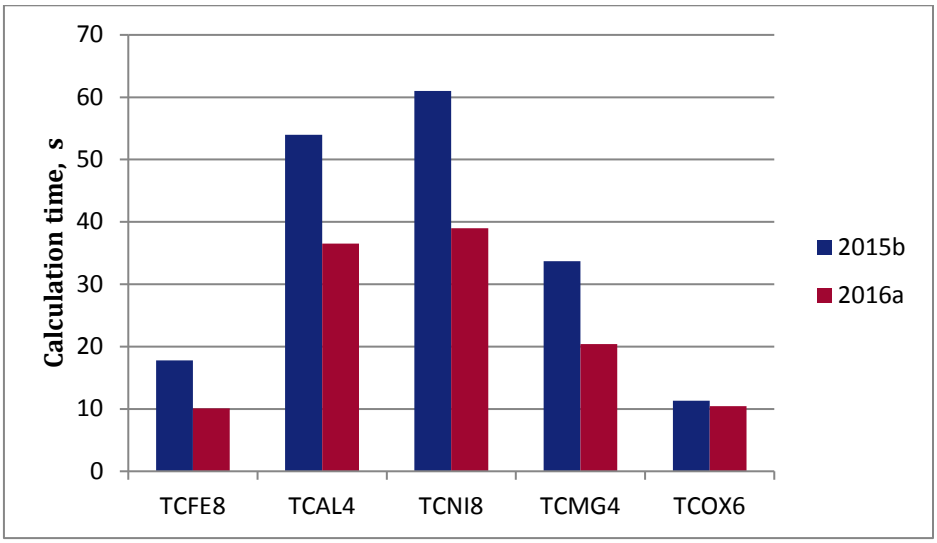
- Calculation Speed Improvements in both minimization routines and databases to decrease calculation and database loading times and make calculations faster.
- New Precipitation Module (TC-PRISMA): TC-PRISMA is integrated into Thermo-Calc Graphical Mode.
- New Copper Databases: TCCU1 (thermodynamic copper database) and MOBCU1 (Cu-alloy mobility database)
- DICTRA and TC-PRISMA Renamed as Add-on Modules: These are now referred to as the Diffusion Module (DICTRA) and Precipitation Module (TC-PRISMA).
- Online Help and PDF Documentation Improvements: a new look and feel to the Online Help, a new *Diffusion Module (DICTRA) Beginner Guide*, and much more.
- New Training Videos: Three new examples videos have been created since the last release. All three videos use DEMO databases, so all users can complete the calculations regardless of license type.

Calculation Speed Improvements

By optimizing global minimization routines and two of our large databases, the calculation speeds in Thermo-Calc are considerably faster. The following are two examples from the benchmark tests that were conducted comparing Thermo-Calc versions 2016a and 2015b.

Global Minimization Optimized

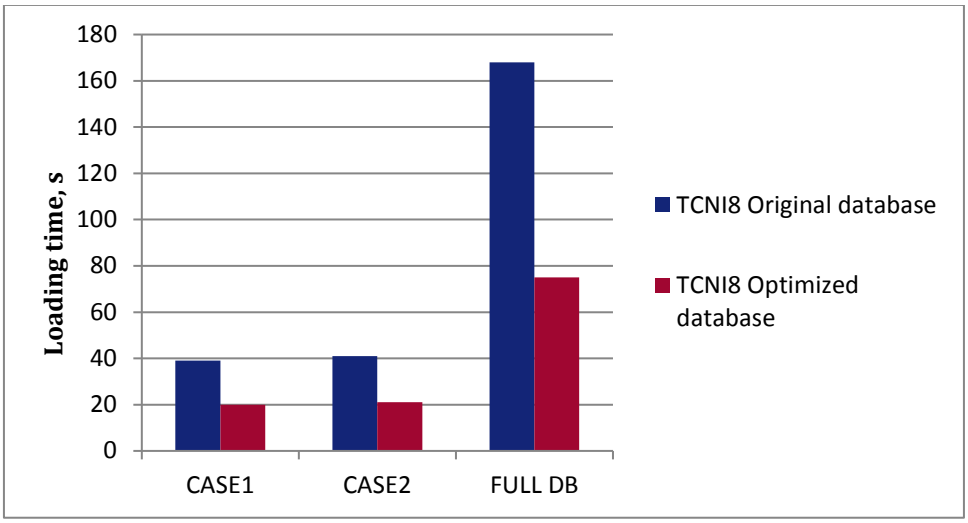
Benchmark tests quantified the calculation speed improvements seen in 2016a compared to the 2015b release. This affects most calculations such as single equilibrium, property diagrams, phase diagrams, and Scheil calculations. In tests with property diagram calculations for 5 to 8 component alloy systems, the speed improvements ranged from 9 to 38% faster, with significant improvements shown for the larger TCNI8, TCMG4 and TCFE8 databases. When the comparisons were made for phase diagram calculations at a constant temperature and with 5 to 12 component alloys, the speed improvements ranged between 5 to 17% faster.



Comparison between 2015b and 2016a showing the increased speed of Thermo-Calc calculations for different databases.

Faster TCNI8 and TCHEA1 Database Loading Times and Calculations

Benchmark tests quantified the improvements to database loading times for TCNI8 (nickel alloys) and TCHEA1 (high entropy alloys) in version 2016a compared to 2015b. The database optimization also results in faster calculation times.



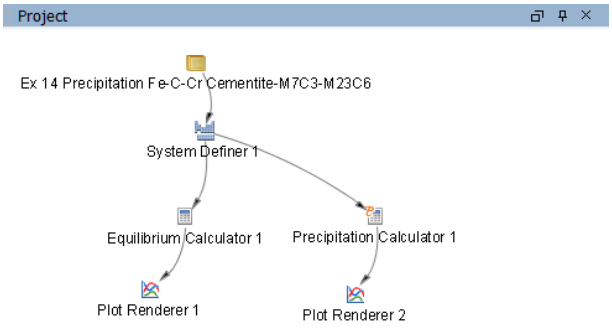
Comparison between 2015b and 2016a showing the decreased loading time for the TCNI8 database. This improved speed is also applicable to TCHEA1, TCNI6, and TCNI7.

New Precipitation Module (TC-PRISMA)

TC-PRISMA Integrated into Thermo-Calc Graphical Mode

The Precipitation Module, previously only referred to as TC-PRISMA, is an add-on module to the core Thermo-Calc software. Now it is integrated, the Precipitation Module is available for all platforms (Windows, Mac and Linux).

The benefit of this is that you can use the powerful features of the other Thermo-Calc activities, such as the System Definer and Equilibrium Calculator, to seamlessly run calculations and for the same alloy systems. For example, you can first use an Equilibrium Calculator to determine the base temperature to use in your calculations. Once that is calculated, just add the new Precipitation Calculator and a Plot Renderer, define your system and click Perform.



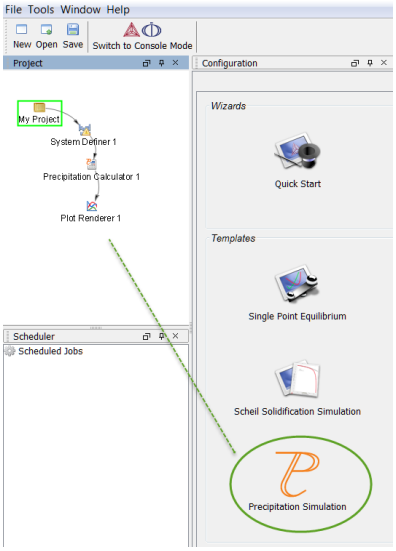
Precipitation Calculator

The Precipitation Calculator is the all-in-one precipitation activity feature. Just like the other calculators in Thermo-Calc, you can add a Plot Renderer and Table Renderer to the node.

For details and links about this feature, go to **Help → Online Help** and search for *Precipitation Calculator*.

Precipitation Simulation Template

A new **Precipitation Simulation** template is available on the dashboard. Click it to add a System Definer, Precipitation Calculator and Plot Renderer to your Project.



Test Drive the Precipitation Calculator in Demo Mode

The Precipitation Module and two examples are available to all Thermo-Calc users but only for simulations with two components. If you do not have a license for the Precipitation Module then you are in *Demonstration Mode* (Demo Mode) when using the **Precipitation Calculator** or the **Precipitation Simulation** template.

For more information go to **Help → Online Help** and search for *Demo mode*.

Key Improvements and Additions to the Precipitation Module

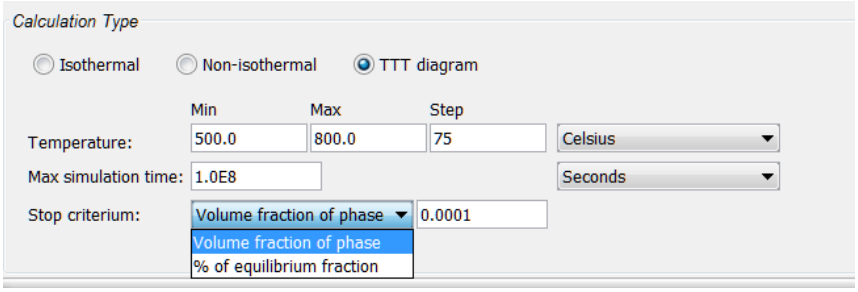
The following features are new or improved compared to previous versions of TC-PRISMA.

Non-Spherical Particles and the Effect of Wetting Angle

You can now calculate heterogeneous nucleation and consider the wetting angle and non-spherical nuclei. A new theory section has been added to the *Precipitation Module (TC-PRISMA) User Guide*, which you can find in the Online Help or included as a PDF with your installation.

TTT Simulations

- You can now run TTT simulations with multiple precipitates, something that was not available previously.
- In addition, the TTT-diagram has two stop criteria to choose from. In previous versions, only phase fraction was available (with respect to the whole system). Now you can choose either **Volume fraction of phase** or **% of equilibrium fraction**. For example, now you can calculate 50% of equilibrium fraction.



Driving Force Improvements

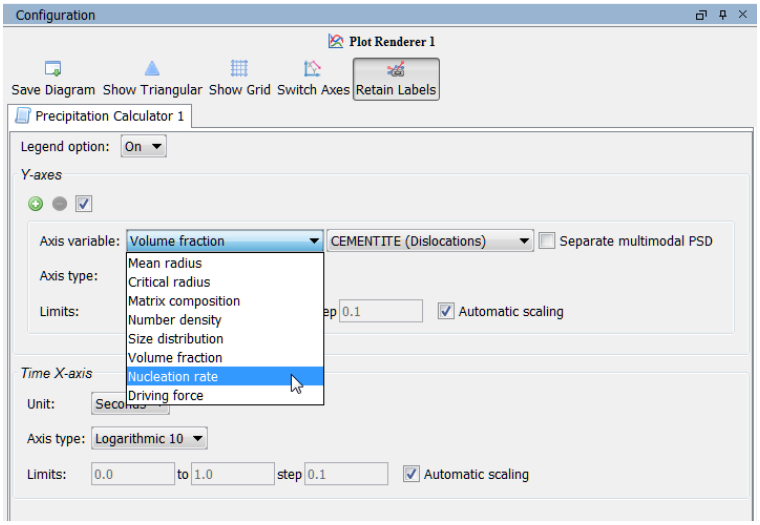
Improved the calculations to estimate driving force for phases with miscibility gaps. This is sometimes required for simulations where there is a miscibility gap between the phases that are involved in the simulation. E.g. precipitate of two FCC_A1 phases, FCC_A1#1 and FCC_A1#2.

Multiple Nucleation Sites of the Same Phase Now Possible

It is now possible to choose multiple nucleation sites for the same phase. You do this by first creating a second Precipitate phase, and then select the same phase on both, for example M23C6. Then you can select different **Nucleation sites** for the two Precipitate phases, for example you can choose **Bulk** (homogeneous) for the first and **Dislocations** for the second.

New Plot Renderer Quantities

On the Plot Renderer you can now choose **Driving force** and **Nucleation rate** to define your plot quantities.



Precipitation Module Installation

The Precipitation Module (TC-PRISMA) is no longer a separate component you need to install. You can run older versions of TC-PRISMA alongside the new version of the integrated Precipitation Module.

To learn how to uninstall older versions, see the *Thermo-Calc Installation Guide* or to **Help → Online Help** and search for *uninstalling TC-PRISMA*.

Precipitation Calculator Examples

The Precipitation Module has six examples that use the new Precipitation Calculator. Examples 13 and 16 are available to all users. The other examples require a Precipitation Module (TC-PRISMA) license to calculate and plot results. All the examples use demonstration databases, which are included with every installation.

The new set of examples are installed in the same folder as the other Graphical Mode examples. You can find these in your default directory (which is based on user-type and platform). This is a change from the older versions of TC-PRISMA where there was a separate folder and location for the examples.

On Windows, once Thermo-Calc is installed, you can locate the Manuals, Examples and Materials folders using the shortcuts located in the Start menu. Go to **Start → All Programs >Thermo-Calc** and open the applicable folder.

For other platforms, and to read detailed descriptions of the examples, go to **Help → Online Help** and search for *Default directory locations* and *Precipitation Calculator examples*, respectively.

New Copper Databases

TCCU1 TCS Thermodynamic Copper Database

TCCU1 contains most of the important Cu-based alloy phases within a 27-element framework. It can be used with Thermo-Calc and the add-on Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA) for a wide range of compositions from pure Cu to complex commercial copper alloys.

Click the image to go to the datasheet. There is also an extended information sheet available. Search for this in the Online Help or go to the Thermo-Calc website to download.

MOBCU1 TCS Cu-alloy Mobility Database

MOBCU1 is a kinetic database containing mobility data for Cu-based alloys. It is suitable for simulation of diffusion controlled phenomena using the add-on Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA). It can also be used with any Thermo-Calc programming interface (e.g. TQ-Interface or TC-API) in your own application programming needs. MOBCU1 is intended for use in combination with the TCCU thermodynamic database.

Click the image to go to the datasheet. You can also search for this in the Online Help.

DICTRA and TC-PRISMA Renamed as Add-on Modules

The integration of TC-PRISMA into Thermo-Calc has prompted a module-based approach to naming these powerful features that require Thermo-Calc as the core software.

In order to make it clearer as to how these two modules enhance the Thermo-Calc software, DICTRA has been renamed to the *Diffusion Module (DICTRA)*. Although the DICTRA name is well-known and established in the literature, this module-based approach more clearly defines how DICTRA and Thermo-Calc work together.

The same concept applies to TC-PRISMA, which is now called the *Precipitation Module (TC-PRISMA)*. It is particularly relevant to this add-on module because when you purchase a license for the Precipitation Module you get the Precipitation Calculator. The Precipitation Calculator is integrated into the Graphical Mode interface, which is part of the Thermo-Calc tree structure and calculation engines and not a standalone piece of software.

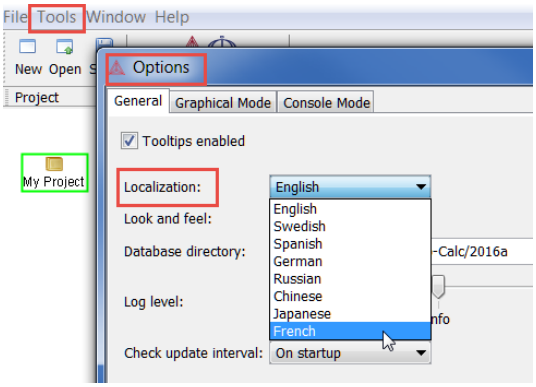
For more information about Thermo-Calc and the add-on module features, open Thermo-Calc, select **Help → Online Help** and enter a key word or phrase.

General Improvements and Bug Fixes

Thermo-Calc

French added as an interface language

You can now set the graphical user interface (GUI) in French. Go to **Tools →Options** and on the **General** tab select **French** from the **Localization** menu. You need to relaunch Thermo-Calc for the change to take effect.

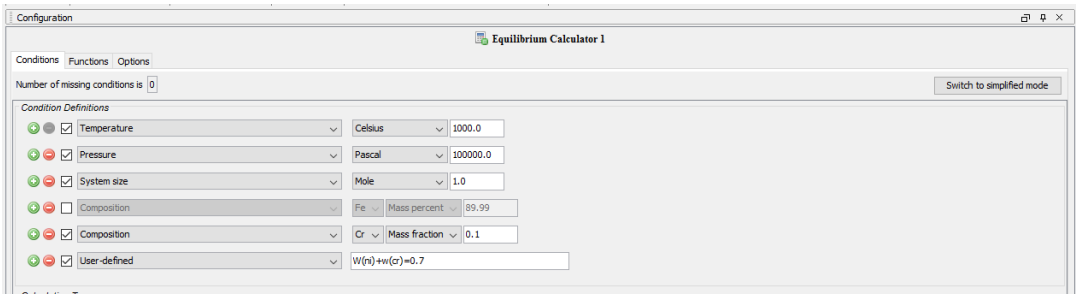


Plots and General

- Improved curve smoothness for plots: For a Grid (Property Model Calculator) or Property Grid (Equilibrium Calculator) calculation type, you can optionally use the **Interpolation**. Choose how many points of data to interpolate on a grid in order to improve curve smoothness. This is done on the Plot Renderer Configuration window.
- Fixed a bug where the incorrect legend options were made available for one axis calculations. Also fixed an issue where dotted lines displayed as solid lines.
- For a Property Diagram fixed an issue where you could select the Probability and Histogram axis types in error as these are only for Uncertainty plots (Graphical Mode).
- Fixed an issue where the transformation of the x-value was wrong for ternary diagrams (Console Mode).
- Scheil Module: A number of bugs have been fixed (Console Mode).
- For Windows users, fixed a problem where the Thermo-Calc graphical interface was too small when using a high resolution monitor.

Graphical Mode Activities

- On the Property Model Calculator, you can do a one axis calculation to plot one variable of interest on the X-axis.
- Fixed an issue with step separate in an Equilibrium Calculator.
- It is now possible on the Equilibrium Calculator to set a **User-defined** condition. This is available by clicking **Switch to advanced mode** on the Configuration window.



Customize the Default Console Directory Path

You can now add a start-up parameter to a shortcut when launching Thermo-Calc on any of the platforms. When you launch the revised shortcut, the file path is set to a user-defined default directory. The directory you want to direct Thermo-Calc to might be used for batch projects or where you have macro files used to do batch jobs. The custom directory file path can also be viewed from within Console Mode.

To learn how to set this up, go to **Help → Online Help** and search for *Default Console Directory*.

Diffusion Module (DICTRA)

Automatic Switching Between Classic and Homogenization Model

Since DICTRA version 27 there are two models available for solving moving phase boundary problems, i.e. the classic model [1,2] and the homogenization model [3,4] (the latter has evolved from a model originally intended only for single region, multiphase simulations). The classic model is computationally efficient, but can be sensitive to starting values. The homogenization model is numerically more robust, but is computationally more demanding. A feature that enables automatic switching between the two models has been available for some time and this feature has now been further refined in version 2016a. The automatic switch is enabled by default, but can be turned off with the DICTRA command SWITCH_MODEL used in Console Mode.

1. S. Crusius, G. Inden, U. Knoop, L. Höglund, and J. Ågren, *Zeitschrift Für Met*. 83, 673 (1992).
2. L Höglund, “Computer simulation of diffusion controlled transformations in multicomponent alloys”, PhD Thesis, KTH Royal Institute of Technology, Stockholm, Sweden, 1997.
3. H. Larsson and R. C. Reed, *Acta Mater.* 56, 3754 (2008).
4. 1. H. Larsson, *Calphad* 47, 1 (2014).

ENTER_MOBILITY_ESTIMATE Command Updated

The ENTER_MOBILITY_ESTIMATE command has been updated. This command is a simple way to allow you to enter mobility estimates interactively rather than setting up a user-defined database. The estimate is entered for a specific element in a specific phase. Previously only constant values were allowed, but now functions of temperature can be entered, for example Arrhenius expressions.

TQ-Interface

An optimization related to chemical diffusivities has been implemented. Chemical diffusivities are now cached, meaning that as long as the site fractions, temperature and pressure remain unchanged they are not re-evaluated when requested; they are just read from the cache.

Updated Databases

TCNI8 and TCHEA1

As described in Faster TCNI8 and TCHEA1 Database Loading Times, these databases have been optimized for this release.

SSOL6

SSOL6 contains assessed thermodynamic data from the literature and provided by SGTE members. SSOL6 includes 729 alloy systems consisting of: 575 binary systems, 133 ternary systems, 20 higher-order systems, and incorporating a total of 1331 phases.

The key changes between SSOL5 and SSOL6 are listed below.

- Hydrogen (H) is added to the database – now 79 elements.
- Many binary and ternary systems are added or updated in SSOL6 including the following systems

Ag-Te	Ce-V	Ge-Ru	Mg-Pr	Ru-Si
Al-Cr	Co-V	Ge-Si	Mg-Sr	Ru-Sn
Al-Y	Cr-Ge	Ge-Sr	Mg-Zr	Si-Sn
Bi-Tb	Cr-Y	Ge-Te	Mn-Sr	V-Y
Bi-Tm	Cr-Zn	H-Li	Mn-Zn	Cu-H-Pd
Bi-Y	Cu-Er	Ho-Mn	Mo-Y	Fe-Si-Zn
B-Mn	Cu-H	Ho-Mo	Nd-Y	Ge-Ru-Si
Ca-H	Cu-Pd	Ho-V	Ni-Sr	Ge-Ru-Sn
Ca-Sr	Eu-In	H-Pd	Pb-Pt	
Ce-Cr	Fe-Sr	In-Yb	Pb-Te	
Ce-Mo	Fe-Zn	La-V	Pd-Si	

SLAG4 Database

Based on the reassessment of phosphorus distribution between steel-making slags and liquid iron, phosphorus was re-included in the liquid slag phase in the SLAG4 database. The gas phase was simplified to accelerate the equilibrium calculation.

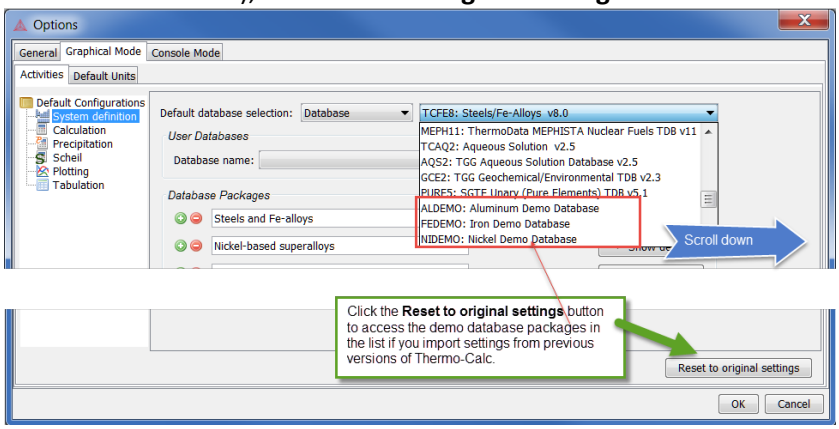
New Demo Database Packages

To accommodate the Precipitation Module examples, two database packages have been added to every installation. These database packages have both a thermodynamic and a mobility database with limited elements so you can run the examples. These are called *Demo: Aluminium-based alloys* and *Demo: Nickel-based superalloys*. The demo package called *Demo: Steels and Fe-alloys* continues to be available for these and other examples.

☑ During an upgrade installation you are prompted to import settings from the previous version of Thermo-Calc. If you do this, and want to use the demo databases you need to do the following for them to be available.

[1] In Thermo-Calc, go to **Tools → Options → Graphical Mode**.

[2] From the **System definition** section, in the lower right part of the window (you may need to scroll down), click **Reset to original settings**.



Documentation, Training Materials and Examples

Online Help and PDF Documentation Improvements

New Online Help

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 Thermo-Calc's main menu (**Help → Online Help**) but now it is easier to search and navigate the content by product.

Database Information Sheets Included

As of this release, all the database information sheets are included, both as PDFs with your installation and on the Thermo-Calc Software website http://www.thermocalc.com/products-services/databases/.

PDF Documentation

There are new user guides and PDFs available to you as part of your installation. As always these are also available in the Online Help and on the Thermo-Calc Software website.

- New *Precipitation Module (TC-PRISMA) User Guide*
- New *Diffusion Module (DICTRA) Quick Start Guide*

Based on your needs, there are PDF documentation sets available as part of your installation. The advantage to this, instead of individual PDFs, is that you can search a PDF just like you search online, and the links work between guides. These sets do not include the Database Information Sheets.

- *Thermo-Calc Documentation Set*: Includes all the manuals needed to work with Thermo-Calc including the installation guides. For the other add-on module documentation, see the separate PDFs.
- *Installation Guides*: Includes the quick install guides for Standalone Windows and Mac installations as well as the full installation guide for all platforms and installation types.
- *Diffusion Module (DICTRA) Documentation Set*: Includes Diffusion Module (DICTRA)-specific manuals plus the Thermo-Calc User Guide, Console Mode Command Reference, Data Optimization User Guide, Database Manager User Guide, and the DATAPLOT User Guide.

- *SDK (Software Development Kit) Documentation Set*: Includes TQ-Interface Programmer Guide, TC Toolbox for MATLAB® Programmer Guide, and TC-API Programmer Guide.

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

New Training Videos

Three new examples videos have been created since the last release. All three videos use DEMO databases, so all users can complete the calculations regardless of license type.

Fe-C Stable and Metastable Phase Diagrams

This video is based on the Graphical Mode example 5 and walks users through both a stable and metastable phase diagram in the Fe-C system and explains the difference between the two types of diagrams.

Scheil Solidification Simulation based on the Austenitic Stainless Steel 18/8

This video shows users how to set up a basic Scheil solidification simulation.

Precipitation Al-Sc_AL3SC

This video is based on Graphical Mode example 13. The video walks users through a precipitation calculation in the Al-Sc system and introduces uses to the newly integrated Precipitation Module, also known as TC-PRISMA.

Examples

Also see Precipitation Calculator Examples.

Diffusion Module (DICTRA) Example Updated

DICTRA example B3 (M23-carbide dissolution) has been updated to use mobility estimates for the M23-carbide.

TC-Toolbox for MATLAB Examples Moved to the Documents Folder

The MATLAB example files are now located in the documents folder. These are 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.

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/.

TCCU1: TCS Cu-based Alloys Database

Database name:	TCS Cu-based Alloys Database	*Database acronym:*	TCCU
Database owner:	Thermo-Calc Software AB	*Database version:*	1.0
Database segment:	Copper		

Brief Description

TCCU1 contains most of the important Cu-based alloy phases within a 27-element framework. It can be used with Thermo-Calc and the add-on Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA) for a wide range of compositions from pure Cu to complex commercial copper alloys.

Applications

Cu-based alloys design and processing.

Included Elements (27)

Ag Al Au As B Be Bi C Ca Cd Co Cr Cu Fe Mg

Mn Nb Ni P Pb Pt Se Si Sn Ti Zn Zr

Included Phases

TCCU1 contains 219 different solution phases and intermetallic compounds. The extended information sheet has a complete list of the phases and models and constituents. Note that compounds having the same crystal structure may have been merged into one phase. A selection of phases is shown below:

Liquid	FCC_A1	FCC_L12	BCC_A2	BCC_B2	HCP_A3
HCP_ZN	RHOMBO_A7	GAMMA_D82	GAMMA_D83	GAMMA_H	SIGMA
CU15SI4_EPSILON	CU33SI7_DELTA	CUSI_ETA	CU56SI11_GAMMA	FE5SN3_D82	NIBE7
CU3SN	CUSN_GAMMA	CU10SN3	CU6SN5_LT	CU41SN11	CU6SN5_HT
ALCU_ETA	ALCU_EPS	ALCU_ZETA	AL2CU_C16	ALCU_DEL	ALCU_PRIME
CUZR2_C11B	CO2SI_C23	AG3SN_L60	CUMG2	CU51ZR14	BE2CU
NI3SN_D019	NI2SI_HT	ZRM5_C15B	NI5SI2	MG2SI_C1	MG2NI
CU16MG6SI7	CU4MNSN	CU3MG2SI	CU5MN4SI	CUMNZN	CU2TIZR
CU3SE2	CUSE2	CU7AS3	CDCU2	CD3CU4	AG5ZN8
AL5FE2	AL5FE4	AL13FE4	CU4TI3	CU4TI1	CUTI_B11
CU3TI2	MN11SI19	MN6SI	NI11ZR9	PSI	SN3ZR5
CU3P	AL11CU5MN3	CO2SI_HT	FESI2_L	COZN_HT	ALCU3MN2

Assessed Systems

113 binary systems and 40 ternary have been assessed. These binaries and ternaries can be calculated in Thermo-Calc with the BINARY and TERNARY Modules, respectively.

Limits

As in the spirit of the CALPHAD method, predictions can be made for multicomponent systems by extrapolation into multicomponent space of data critically evaluated and assessed based on binary, ternary and in some cases higher order systems. However, critical calculations must always be verified by equilibrium experimental data; it is the user's responsibility to verify the calculations but Thermo-Calc Software AB is interested to know about any significant deviations in order to improve any future release.

Scientific Models and References

See the Thermo-Calc Software reference list and reference library at: http://www.thermocalc.com/resources/

MOBCU1: TCS Cu Alloys Mobility Database

Database name:	TCS Cu Alloys Mobility Database	*Database acronym:*	MOBCU
Database owner:	Thermo-Calc Software AB	*Database version:*	1.0
Database segment:	Copper alloys		

Brief Description

MOBCU1 is a kinetic database containing mobility data for Cu-based alloys. It is suitable for simulation of diffusion controlled phenomena using the add-on Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA). It can also be used with any Thermo-Calc programming interface (e.g. TQ-Interface or TC-API) in your own application programming needs. MOBCU1 is intended for use in combination with the TCCU thermodynamic database.

Applications

Together with the Diffusion Module (DICTRA) and a thermodynamic database for Cu-alloys (e.g. TCCU) use the MOBCU1 database to study diffusion-controlled phenomena in copper alloys, e.g. microsegregation during solidification, homogenisation kinetics, growth/dissolution kinetics of precipitates, interdiffusion, and so forth. You can also use it with the Precipitation Module (TC-PRISMA) to simulate concurrent nucleation, growth, and coarsening of precipitates in Cu-based alloys.

Included Elements (27)

Ag	Al	As	Au	B	Be	Bi	C	Ca	Cd	Co	Cr	Cu	Fe	Mg	Mn	Nb
Ni	P	Pb	Pt	Se	Si	Sn	Ti	Zn	Zr							

Included Phases

FCC_A1 LIQUID

The above phases have diffusion data included in the database. You can include other phases in a diffusion simulation. However, these phases are treated as so-called diffusion *NONE*, i.e. there is no diffusion considered in these other phases. Any phase not listed above is automatically entered as diffusion *NONE* in the DICTRA module in Thermo-Calc, as long as a thermodynamic description for the phases is retrieved prior to reading data from the mobility database.

Assessed Systems

FCC_A1

The database contains assessed impurity diffusion data in Cu for all 26 alloying elements. Complete and critical assessments for FCC_A1 in 37 binary, 26 ternary, and 1 quaternary systems have also been included.

LIQUID

Data for diffusion in liquid Cu alloys have also been assessed or estimated for all elements in the database.

Limits

The database is applicable for most commercial Cu-based alloys, care should be taken with alloys including high amounts of alloying elements. As in the spirit of the CALPHAD method, predictions can be made for multicomponent systems by extrapolation into multicomponent space of data critically evaluated and assessed based on binary, ternary and, in some cases, higher order systems. However, critical calculations must always be verified by experimental data; it is the user's responsibility to verify the calculations but Thermo-Calc Software AB is interested to know about any significant deviations to improve future releases.

Scientific Models and References

See the Thermo-Calc Software reference list and reference library at: http://www.thermocalc.com/resources/