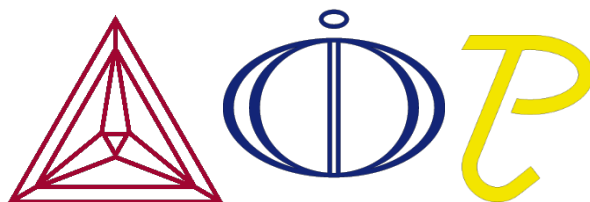




Release Notes:

Thermo-Calc Software Package

Version 2015b



These notes summarise new products and features as well as improvements and bug fixes released with version 2015b of the Thermo-Calc software package.

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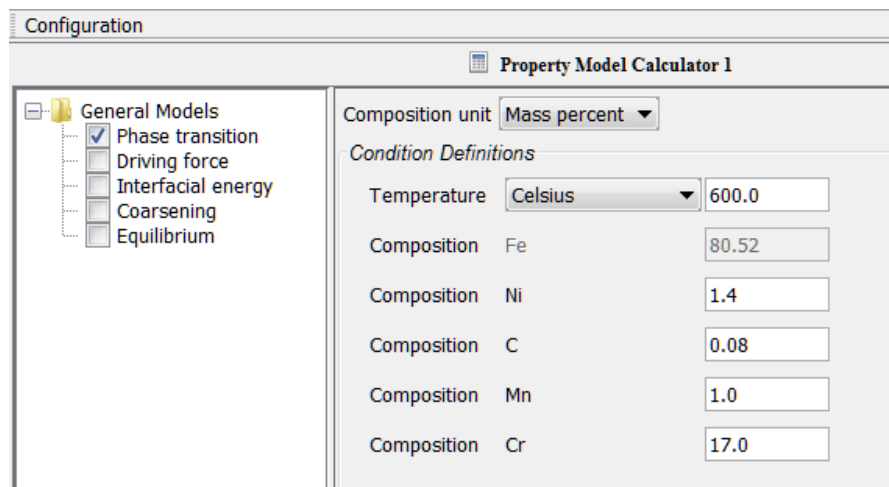
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1. New in Thermo-Calc Software Package 2015b

1.1 Property Model Calculator

A Property Model Calculator allows you to predict and optimize material properties. A set of general models is available to use: a Phase Transition, Driving Force, Interfacial Energy, Coarsening, and an Equilibrium.



- **Phase Transition:** By varying set conditions, this model calculates the point when a new phase may form. The model is useful to determine melting temperature, boiling temperature or solubility limits. It returns the phase transformation temperature, or composition, depending on the varied condition.
- **Driving Force:** Calculate the thermodynamic driving force for a phase.
- **Interfacial energy:** Estimate the interfacial energy between a matrix phase and a precipitate phase using thermodynamic data from a CALPHAD database. Note that this functionality is also available in TC-PRISMA.



Interfacial energy continues to be available in TC-PRISMA and as a subroutine with the TQ-Interface (TQGSE), TC-API, and the TC-Toolbox for MATLAB®.

- **Coarsening:** Calculate the coarsening rate coefficient of a spherical precipitate phase in a matrix phase.
- **Equilibrium:** Calculate the equilibrium for the given conditions. Optionally define additional Function Definitions. All quantities that normally can be obtained from an equilibrium calculation can also be obtained when plotting the results, as well as the defined functions.




For more information search the new [Online Help](#) for “*property model calculator*”. Include the quotation marks to limit the search results.

New Calculation Types

In addition to a **Single** calculation type, there are three new calculation types: **Grid**, **Min/Max** and **Uncertainty**.

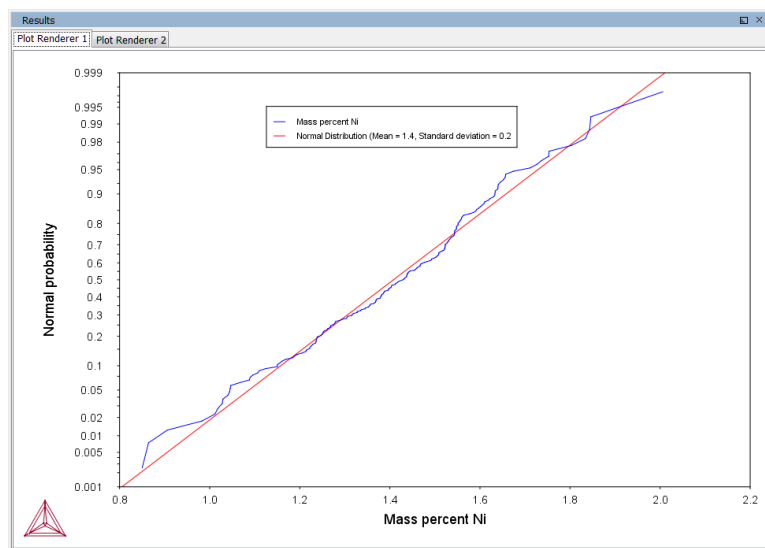
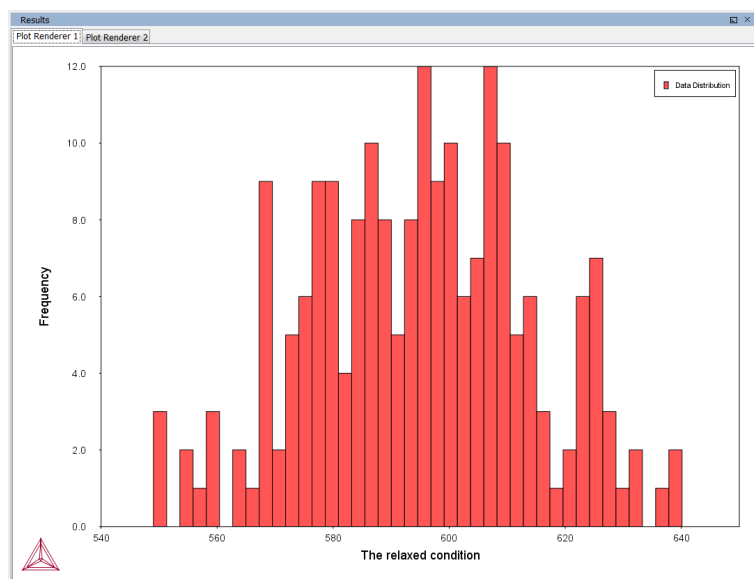
- Select a **Grid** to evaluate two axis variables of the selected quantities in the specified range and number of steps.


- The **Min/Max** calculation evaluates the property model(s) for all variations of the selected quantities at the given limits. The **Mean** field is as defined under Condition Definitions for the respective quantity. The total minimum and maximum of the model(s) results are shown in the Event log.
- The **Uncertainty** calculation evaluates the property model(s) where the values of the quantities are sampled from Gaussian distributions. The **Mean** field is as defined under Condition Definitions for the respective quantity. The result is visualized as a histogram or normal probability plot by adding a Plot Render activity.

 For more information search the new [Online Help](#) for “*property model calculator*”. Include the quotation marks to limit the search results.

New Plot Types: Histogram and Normal Probability

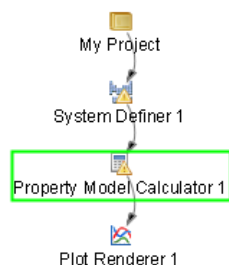
You can evaluate models simultaneously over a range of compositions and cross plot the results. You can then conduct an uncertainty analysis and plot the results as either a histogram or as a normal probability plot.



 For more information search the new [Online Help](#) for *histogram plot* or *probability plot*.

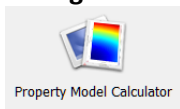
New Template

Use a Property Model Calculator Template to create all the activities for this type of calculation (System Definer, Property Model Calculator and Plot Renderer).



There are two ways to do this:

- In the **Project** window click the **My Project** node to display the templates in the **Configuration** window. Then click the **Property Model Calculator** icon.



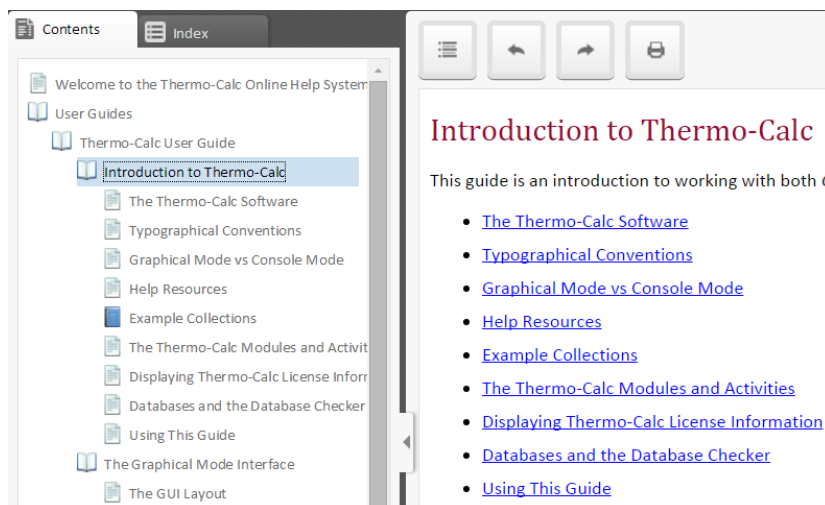
- Right-click the My Project node and from the Create New Activity → Use Template menu, select Property Model Calculator.

 For more information search [Online Help](#) for *templates*.


1.2 Online Help


A new online help includes all the documentation. It does not require an Internet connection and opens locally in your web browser. One advantage compared to using the individual PDFs is you can browse all the content and search for key words and phrases.


To learn more, open the Thermo-Calc software and select **Help → Online Help**. The **Welcome** page provides you with the basics to get started browsing and searching the software features. Or you can just browse the **Contents** tree. The topics are in the same order as in the PDF versions of the guides.




The PDF documentation continues to be located on the Thermo-Calc website (<http://www.thermocalc.com/support/documentation/>) and is always installed in a **Manuals** folder with the software. The default directories where the software and its components are installed, vary by platform and user type.

 For TC-PRISMA users, the help for TC-PRISMA is available from the Thermo-Calc software.

 You can find the details about where the folders are located by searching the online help for *installation folders*.


 For Windows users, and once Thermo-Calc is installed, you can locate the folders using the shortcuts located in the Start menu. Go to **Start → All Programs > Thermo-Calc** and click **Examples**, **Manuals**, or **Materials** as required to open the applicable folder. If you also have a license for TC_PRISMA, the **Examples** folder is currently available here **C:\Users\<user>\Documents\Thermo-Calc\2015b**.

1.3 New Databases

 For more information go to the individual database flyers located on the Thermo-Calc website <http://www.thermocalc.com/products-services/databases>.


Thermodynamic Database: TCHEA1 (High Entropy Alloys)

Thermo-Calc Software is pleased to announce the release of TCHEA1.0, a thermodynamic database for high entropy alloys (HEA) [2003Yeh, 2006Yeh], which are also known as multi-principal element alloys (MPEA) [2013Wan, 2015Sen]. TCHEA1.0 has been developed in a CALPHAD spirit based on the critical evaluation of all the binary systems and many ternary systems. A hybrid approach of experiments, first-principals calculations and CALPHAD modelling had been used to obtain reliable thermodynamic descriptions of the BCC and FCC solutions. That enables predictions to be made for multi-component alloy systems, especially for HEAs.

 See the database flyer at the end of these releases notes or on the [website](#).

Mobility Database: MOBMG1 (Magnesium Alloys)


MOBMG is a CALPHAD-type kinetic database containing atomic mobility data for Mg-based alloys. MOBMG contains all of the same elements as TCMG4 and it is compatible as well.

 See the database flyer at the end of these releases notes or on the [website](#).

Demo Databases

There are several new DEMO databases available. These were previously only available in Demo and academic versions of Thermo-Calc.

- ALDEMO: Includes Al, Cu and Si (full ternary description)
- FEDEMO: Includes Fe, Cr, Mn, Ni and C (subset of TCFE)
- SLDEMO: Includes Ag, Cu and Sn (full ternary description)
- OXDEMO: Includes Ca, Fe, Si and O (subset of TCOX) (previously called OXID4A in the Demo and Academic versions)
- SUBDEMO: Includes C, H, Fe and O (subset of SSUB) (previously called SUB4A in the Demo and Academic versions)
- PURE5: Includes critically assessed unary thermochemical data for the concerned elements
- A new DICTRA demo database MFEDEMO includes mobility data for Fe, Cr, Mn, Ni and C in BCC_A2 and FCC_A1.

 Also see the section [Databases](#) for information about updated and removed databases and bug fixes.

1.4 New Compilers Increase Processing Speeds for OS-X and Linux

In this release for OS-X and Linux operating systems now uses the Intel compilers, which can mean a large speed improvement for Thermo-Calc/DICTRA and APIs. Windows operating systems are already using the Intel compiler.

Benchmark simulations were performed on Linux (CentOS 64) on a PC with an Intel i7 processor.

- The DICTRA example b2 simulation time was reduced from 180 to 39 seconds.
- A mapping calculation with a seven component system using the TCNI8 database was reduced from 1219 to 821 seconds.

 Also see [Software Development Kits \(SDKs\)](#).

2. Improved Functionality: Thermo-Calc


For each of the following, the topic is either for Graphical Mode or Console Mode as indicated in the title.

2.1 Databases Open More Quickly in Graphical Mode

A new method of caching, or storing files for quick access, enables your databases to open more quickly.

The first time you open a database in Graphical Mode the databases will take a moment to load, especially if it is one of the large databases such as TCFE or TCNI. However, the next time the database will open quickly because of this caching.

Think of a cache as an intermediate storage area. Once a database cache is established the file is maintained even if you close the software program. It is the same concept as when you load a web page for the first time. The next time the page opens faster. This is also how it works for the databases in Thermo-Calc Graphical Mode.


 All databases that are added to the database initialization file (called *tc_initd.tdb* in Windows and *initd.tdb* in Linux and Mac) will be cached. Users who edit and use their own databases need to take note of this.

2.2 More Useful Detail Available About Licenses

The License Information window (**Help → Show License Info**) now includes the site information and user information which can be useful if trying to resolve license issues.

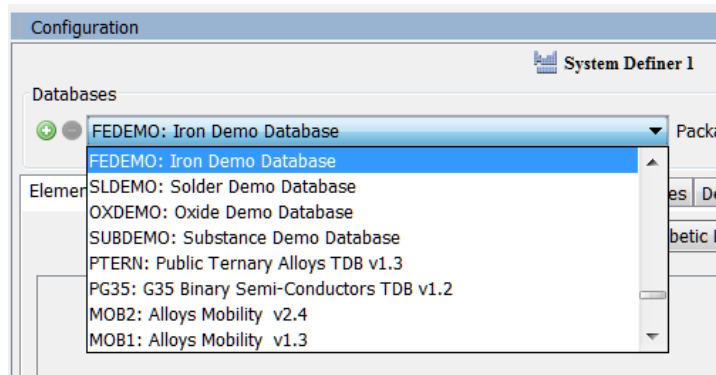
2.3 System Definer (Graphical Mode)



The System Definer has several improvements and additions to its functionality.

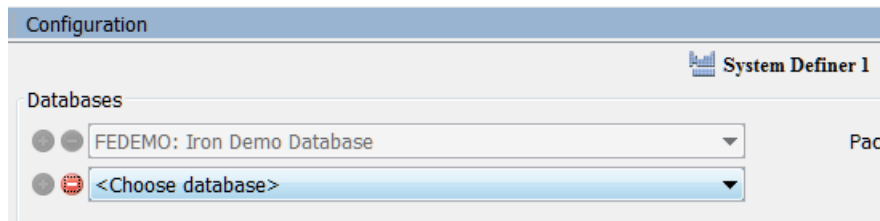
 For more information search [Online Help](#) for “*database package*” or “*system definer*”. Include the quotation marks to limit the search results.

Add More than One Database to a System Definer

You can now add more than one database at a time to the same System Definer. This functionality replaces the *Appended System* node, which was available in previous versions of Thermo-Calc.

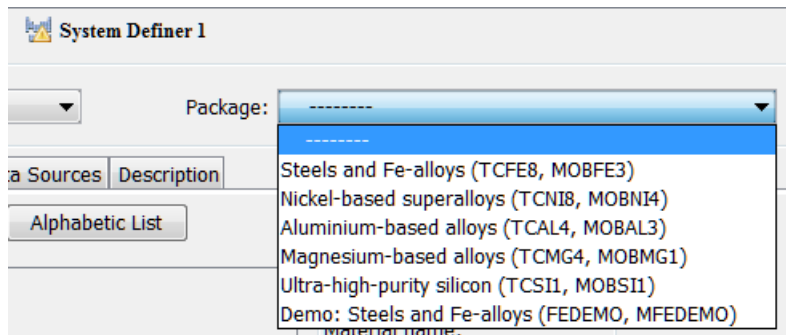


On the **System Definer Configuration** window select the first database from a list. The databases available are based on your license. To add additional databases, click the **Add a database**  button and choose another database from the list. Click **Remove this database**  button as required

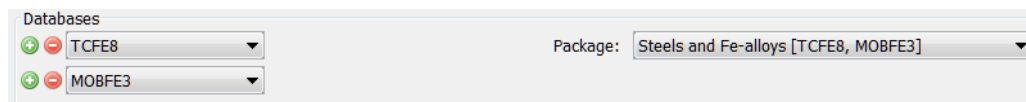


Add a Database Package to the System Definer

In addition to being able to add more than one database at a time, you can add a predefined database **Package** to the System Definer. The available predefined packages are based on your license.

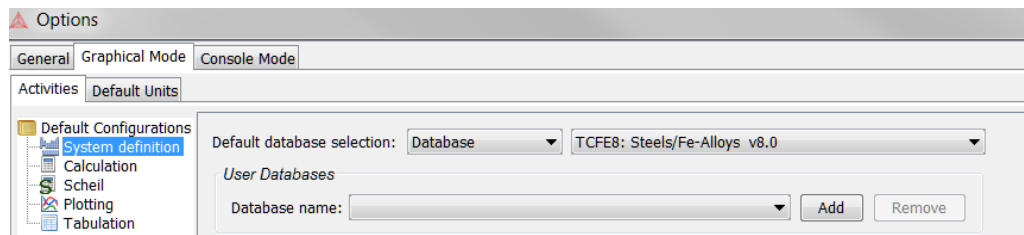


For example, if you choose **Steels and Fe-alloys**, the TCFE8 and MOBFE3 databases are added to your project (if you have a license for these databases). The package is created with the latest version of the databases that you have a license for. For example, if you have TCFE7 and MOBFE2 (instead of the most recent TCFE8 and MOBFE3) the package contains those available, in this example, TCFE7 and MOBFE2.



Set the Default Database or Database Package and Add User Databases

You can set the default database or database package to use for your projects from the **Tools → Options → Graphical Mode → System definition** window.



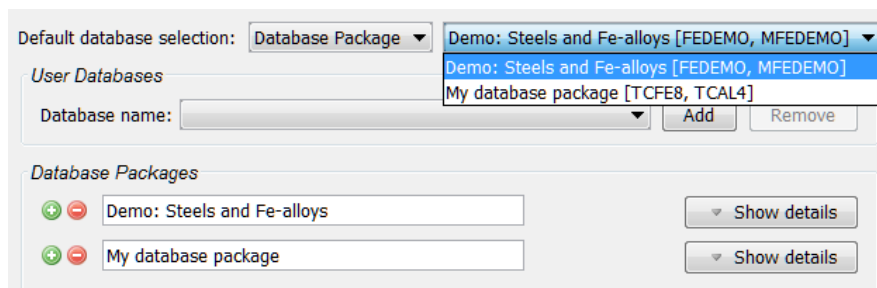
Choose a **Default database selection** - **Database** or a **Database package**.

If you choose **Database**, then select the default installed database to use globally for all System Definer nodes. For example, choose TCFE8.

If you choose **Database Package**, select an option from the list. You can choose the predefined packages or create your own. You can also Add your own user-defined database and then set this as the default.

Create Your Own User-defined Database Packages

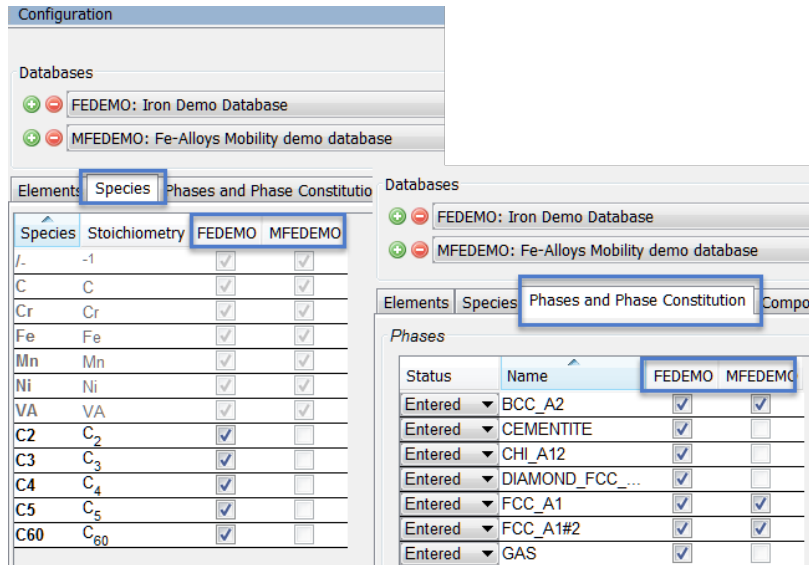
You can also create your own database packages from the **Tools → Options → Graphical Mode → System definition** window.



i The addition or removal of a database package does not take effect until a new System Definer node is defined.

Review Databases for Species and Phases in One Window

When you add more than one database to the System Definer, you can review and edit each database on the **Species** and **Phases and Phase Constitution** tabs.



Configuration

Databases

- FEDEMO: Iron Demo Database
- MFEDEMO: Fe-Alloys Mobility demo database

Elements Species Phases and Phase Constitution

Species	Stoichiometry	FEDEMO	MFEDEMO
I	-1	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
C	C	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Cr	Cr	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Fe	Fe	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Mn	Mn	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Ni	Ni	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
VA	VA	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
C2	C ₂	<input checked="" type="checkbox"/>	<input type="checkbox"/>
C3	C ₃	<input checked="" type="checkbox"/>	<input type="checkbox"/>
C4	C ₄	<input checked="" type="checkbox"/>	<input type="checkbox"/>
C5	C ₅	<input checked="" type="checkbox"/>	<input type="checkbox"/>
C60	C ₆₀	<input checked="" type="checkbox"/>	<input type="checkbox"/>

Databases

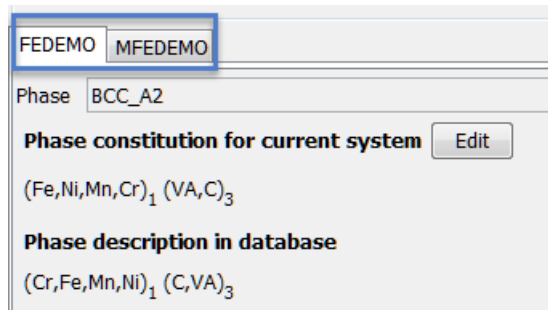
- FEDEMO: Iron Demo Database
- MFEDEMO: Fe-Alloys Mobility demo database

Elements Species Phases and Phase Constitution

Phases

Status	Name	FEDEMO	MFEDEMO
Entered	BCC_A2	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Entered	CEMENTITE	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Entered	CHI_A12	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Entered	DIAMOND_FCC_...	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Entered	FCC_A1	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Entered	FCC_A1#2	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Entered	GAS	<input checked="" type="checkbox"/>	<input type="checkbox"/>

Phase Constitution



FEDEMO MFEDEMO

Phase BCC_A2

Phase constitution for current system Edit

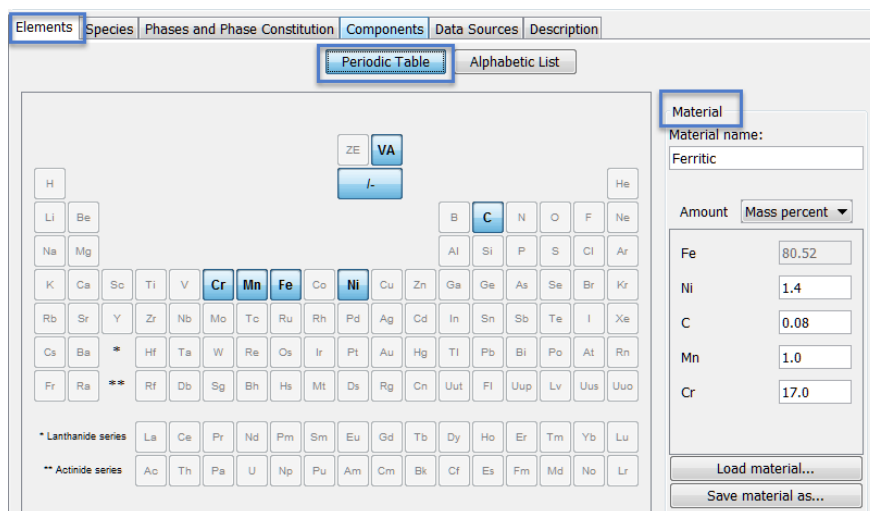
(Fe,Ni,Mn,Cr)₁ (VA,C)₃

Phase description in database

(Cr,Fe,Mn,Ni)₁ (C,VA)₃

Material Definition

The **Material** definition has been moved from its own tab to be more prominent on the **Elements** → **Periodic Table** page. This makes it easier to define your material when you are setting up the project. Another change from previous versions is that the database selection was included in the material file, whereas now you choose it from the top of the System Definer window as described above.



Elements Species Phases and Phase Constitution Components Data Sources Description

Periodic Table Alphabetic List

Material

Material name: Ferritic

Amount Mass percent

Fe	80.52
Ni	1.4
C	0.08
Mn	1.0
Cr	17.0

Load material...
Save material as...

2.4 Scheil Calculator (Graphical Mode)

The improved Scheil Calculator in Graphical Mode is now aligned with the Console Mode version. The Scheil Calculator activity is used to perform simulations of Scheil (Scheil-Gulliver) solidification processes. By default, a Scheil calculation results in an estimation of the solidification range of an alloy.


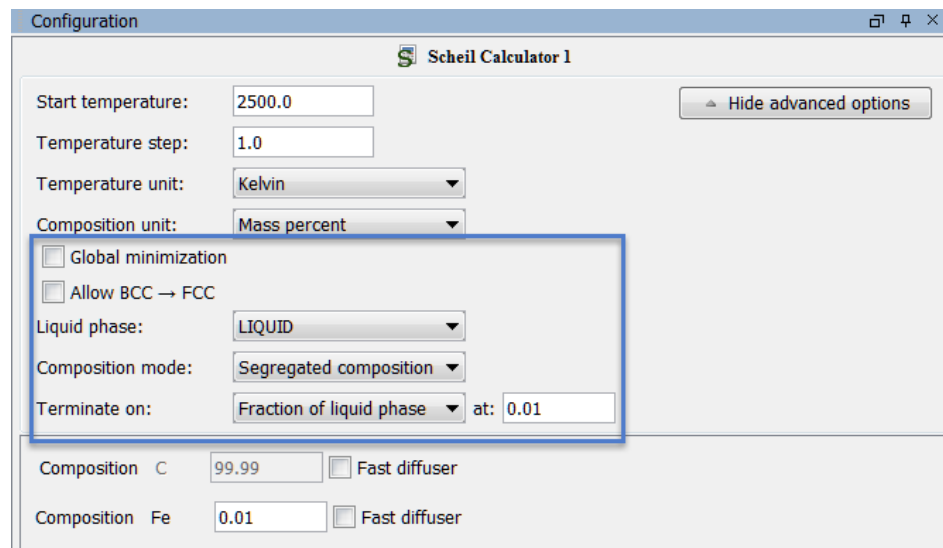
 For more information search [Online Help](#) for “*Scheil Calculator*”. Include the quotation marks to limit the search results. Also see [Scheil Module \(Console Mode\)](#), which has a new Wizard similar to using the Graphical Mode **Quick Start → Scheil solidification simulation** wizard.

Table Renderer Now Available

You can now add a **Table Renderer** to the Scheil Calculator.

New Settings in Advanced Options

The new Advanced Options settings are **Global minimization**, **Liquid phase**, **Composition mode** and **Terminate on** sections. You access these settings by clicking **Show advanced options** on the Scheil Calculator Configuration window. The **Allow BCC → FCC** check box has also been moved here.



For the Scheil Calculator, the method for calculating the segregation is the same as before but with an improvement to what and how the simulation results are stored.

In the **Advanced Options** section of the Scheil Configuration window, you can edit the Composition mode: either save as **Segregated composition** or **Average composition**. These are used when plotting composition profiles after a simulation.


2.5 Scheil Module (Console Mode)

The Console Mode Scheil module is now aligned with the [Scheil Calculator \(Graphical Mode\)](#).

A new Wizard is available (in the Scheil module type START_WIZARD) to walk you through a basic Scheil simulation. You are prompted for settings including the major element or alloy, composition input in mass (weight) percent, the alloying elements, the temperature, fast diffusing components, and whether any phase should have a miscibility gap check.

Use the other commands before running the wizard to make changes to settings that are not included in this wizard, which is intended to walk you through a basic Scheil simulation.

- BCC_TO_FCC_TRANSFORMATION
- EVALUATE_SEGREGATION_PROFILE
- GLOBAL_MINIMIZATION
- LIQUID_PHASE_NAME
- SAVE_FILE_NAME
- STORED_COMPOSITION_TYPE
- TEMPERATURE_STEP
- TERMINATION_CRITERIA

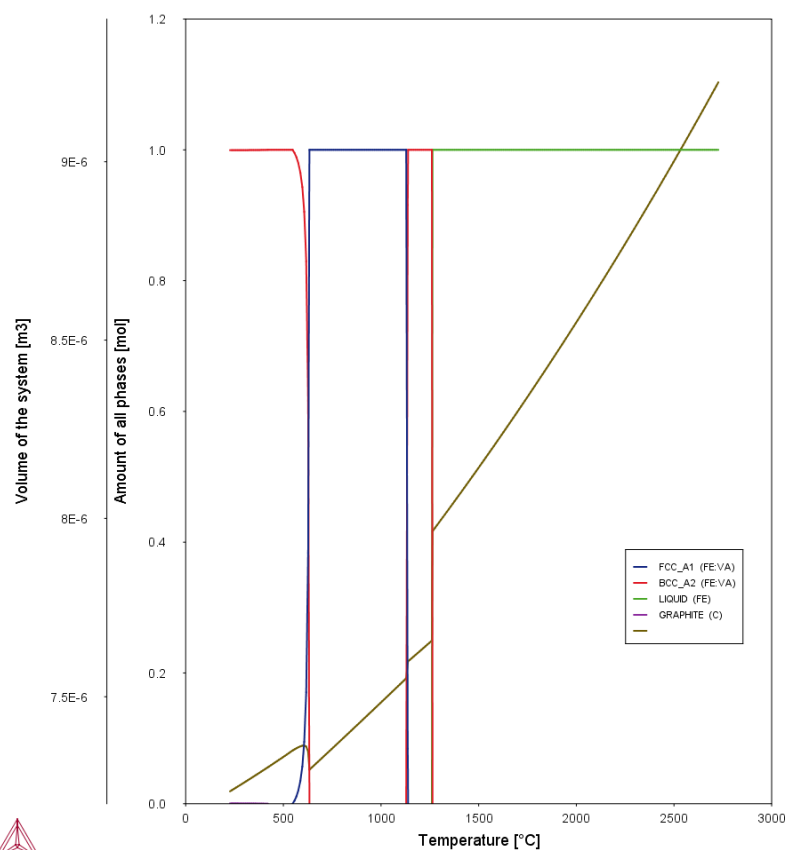
 For step-by-step instructions to use the START_WIZARD command search [Online Help](#) for “*Simulating a Scheil-Solidification*”. Include the quotation marks to limit the search results.


2.6 Plot Renderer (Graphical Mode)

The Plot Renderer displays results from the various calculator activities (Equilibrium Calculator, Property Model Calculator, Binary Calculator, Ternary Calculator, and Scheil Calculator).

Add Axes to Diagrams

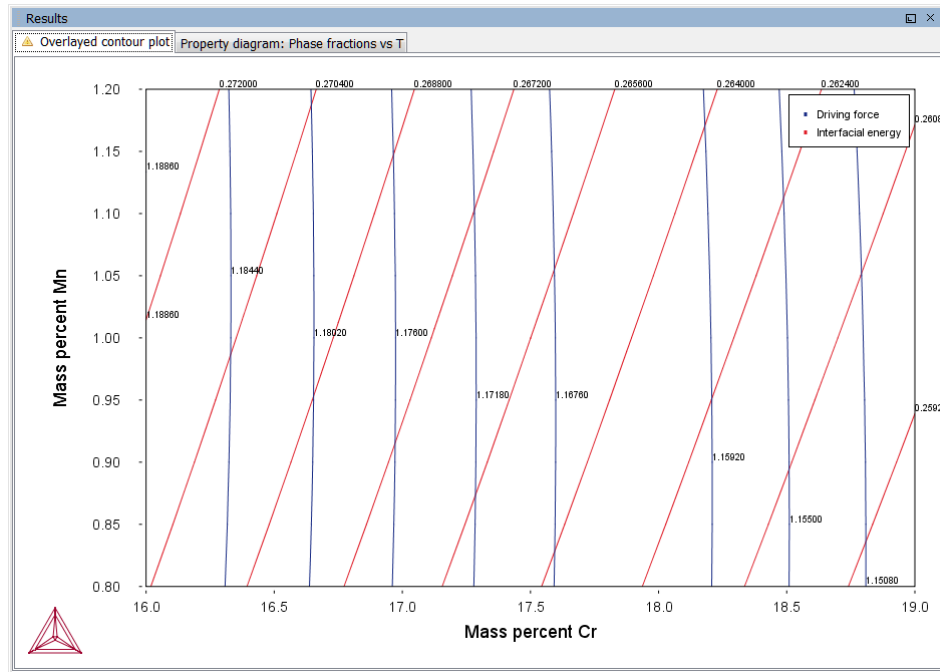
New in this release is the ability to add axes to diagrams in Graphical Mode. You can add additional X- and/or Y-axes to a plot to compare two or more variables at the same time.



 For more information search [Online Help](#) for *add axes* or *“plot renderer”*. Include the quotation marks to limit the search results.

Merge Plots into One Diagram

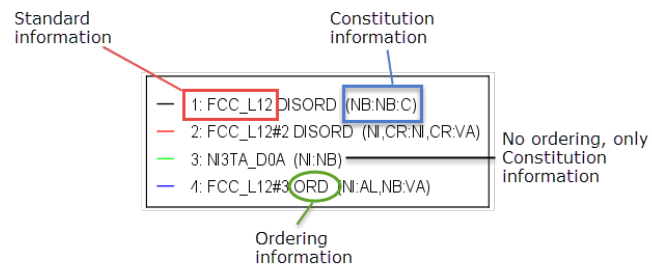
In Graphical Mode, you can also merge (or overlay) calculated results for several variables into one diagram. This is similar to adding an axis, but instead of displaying different variables along the X- and/or Y-axes, the same X and Y variables are used to compare the third variable (defined in the Plot Renderer as the Z-axis).



For more information search [Online Help](#) for *merging plots* or *“plot renderer”*. Include the quotation marks to limit the search results.

Also see

New Detailed Legend Style (Console and Graphical Modes)



There are a variety of legend styles you can use to display detail about the phases.

The same legend styles are available for both Graphical Mode and Console Mode

For Console Mode, use the command `CHANGE_LEGEND` in the POST module. In Console Mode, `LIST_EQUILIBRIUM` also displays ORD (ordered) or DISORD (disordered) (when available).

In Graphical Mode the label styles are defined when using the Plot Renderer. You can select a Legend style for the Stable phases or Axis quantity selected for Legend option.

When there is a legend in the diagram you can append constitution and/or ordering descriptions to the phase name.

If constituent description is included in the legend, then for each equilibria along a line in the diagram, the largest constituent fractions are summed until they are equal or greater than 0.6. This is done separately for each sublattice. If the equilibria along the line gets different sets of constituents these are all appended to the list for that sublattice.

The ordering description is only printed for partitioned phases (phases that have a disordered contribution) that begins with at least two identical sublattices (sublattices where the set of constituents are identical). DISORD (disordered) is shown if site fractions are identical between identical constituents on all identical sub lattices (with an error margin) otherwise ORD (ordered) is shown in the legend.

If ordering between equilibria in a line are different, then ORD + DISORD is shown in the legend.

 For more information and examples search [Online Help](#) for *legend style*.

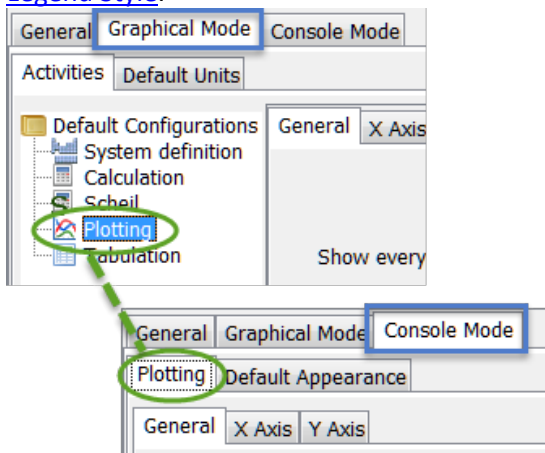
2.7 General (Graphical Mode)


Table Renderer Now Available

You can now add a **Table Renderer** to the Scheil Calculator and Binary Calculator.

Options Menu Changes

- New default configurations available for **System definition** and **Scheil** under **Options → Graphical Mode → Activities**.
 - The **System definition** section is where you create and modify database packages See [System Definer \(Graphical Mode\)](#).
 - The **Scheil** section is where you globally set global minimization, allow BCC→FCC, start temperature and temperature step. See [Scheil Calculator \(Graphical Mode\)](#).
- Under the **Options** menu **Plotting** sections, for both Console Mode and Graphical Mode, you can set the new legend phase caption style default. See [New Detailed Legend Style](#).



 For more information search [Online Help](#) for “*changing global settings*”. Include the quotation marks to limit the search results.

3. DICTRA Module

3.1 New Commands

- `STORE_HOMOGENIZATION_DATA` allows you to read/write the interpolation scheme data to file. The interpolation scheme is an option of the homogenization model that is used to speed up simulations.

The following were previously only available for the `UTILITIES_HOMOGENIZATION` command and now apply to both classic and homogenization.

- `ENTER_MOBILITY_ESTIMATE` is used to enter a constant mobility estimate for specific elements in specific phases.
- `LIST_MOBILITY_ESTIMATES` does what it says, it lists the mobility estimate entered interactively by the `ENTER_MOBILITY_ESTIMATE` command.

Also, in order to keep the size of the result file small (the ".DIC file") when the homogenization model is used, by default results are now saved at an interval corresponding to 1/1000 of the total simulation time. This default can be changed under the `UTILITIES_HOMOGENIZATION` command.

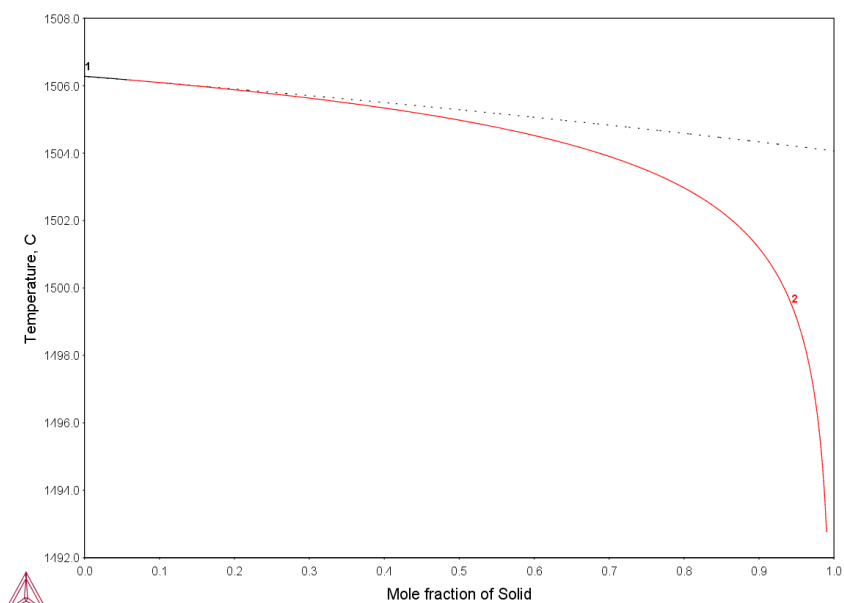
3.2 Import a Scheil Segregation Profile

In addition to all the improvements to the [Scheil Calculator \(Graphical Mode\)](#) and [Scheil Module \(Console Mode\)](#) in Thermo-Calc, a new feature in DICTRA enables you to import a previously calculated Scheil segregation profile using a new command, `INPUT_SCHEIL_PROFILE`.

A Scheil calculation is a conservative estimate of the segregation that occur during solidification and is therefore useful when estimating the necessary time/temperature for a homogenizing heat treatment. From a practical point of view it is also a simple and fast calculation compared to a more accurate, but computationally more difficult, DICTRA simulation. However, in order to limit the computational effort this feature cannot be combined with the “fast diffusers” option in the Scheil module.

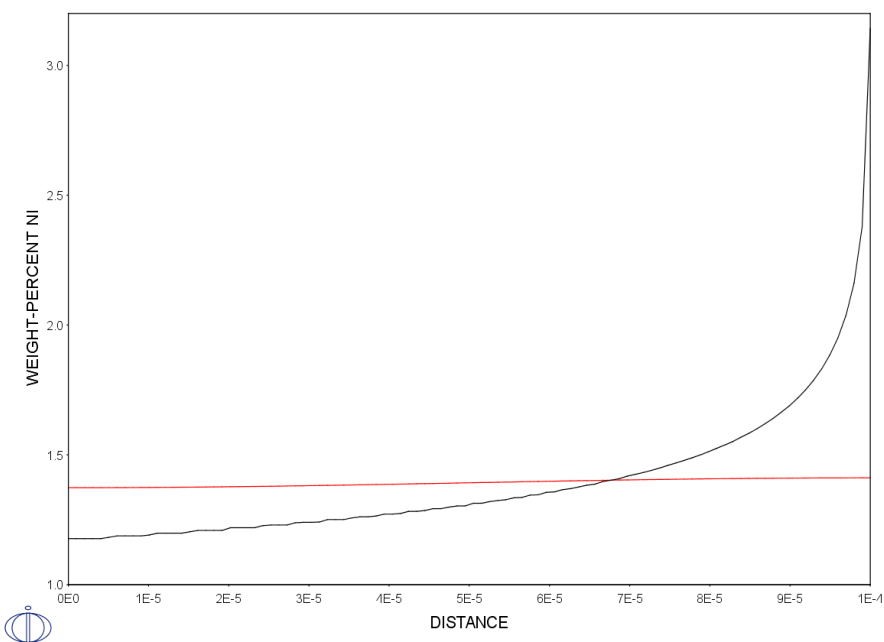
For example, the Scheil segregation profile for a ferritic stainless steel (Fe-17Cr-1.4Ni-1Mn) was calculated in the Scheil module in Thermo-Calc.

2015.11.10.11.51.39
FEDEMO: CR, FE, MN, NI
T=1779.52, W(CR)=0.17, W(NI)=1.4E-2, W(MN)=1E-2, P=1E5, N=1



The profile was then imported into DICTRA and a 1 hour homogenizing heat treatment at 1200C was simulated. For the DICTRA simulation a domain size of 100 μ m was assumed, which approximately corresponds to the secondary dendrite arm spacing. The plot below show the initial and final Ni profile.

2015.11.10.11.53.36
TIME = 0.3600
CELL #1



4. Bug Fixes

In addition to the specific fixes below, several other small fixes were completed during the development and testing process.

4.1 Thermo-Calc – Console Mode and Graphical Mode

- Fixed an issue with the automatic zoom level when plotting with Heat Map and using automatic scaling.
- Contour plots: Improved performance and speed of calculations.

4.2 DICTRA-Module



- Fixed an issue with the DICTRA Examples PDF where the setup and run section text (commands) was truncated for each example. Now it is only truncated in the plot settings section as this is repeated information during postprocessing and not required for the example setup and learning.
- Fixed an issue where the `Select_Plot /new/ option` opened the print window at the same time.

4.3 TC-PRISMA

Fixed an issue that caused TC-PRISMA to crash during TTT calculations.

5. Software Development Kits (SDKs)

New Compilers

- TQ-Interface and TC-API are available in both ifort and gfortran versions.  See [New Compilers Increase Processing Speeds for OS-X](#) and Linux for more information.
- There is a new example about using Intel-FORTRAN (ifort) in the TQ-Interface – see tqex01-ifort.  For more information search [Online Help](#) for “*TQ-Interface Examples*”. Include the quotation marks to limit the search results.

5.1 TQ Interface

New Interpolation Scheme Commands

Three new commands related to the interpolation scheme are available:

- TQIPS_WRITE_IPS_DATA_TO_FILE
- TQIPS_READ_IPS_DATA_FROM_FILE, and
- TQIPS_GET_MEMORY_USAGE

6. Databases

Two new databases are available as described in [Thermodynamic Database: TCHEA1 \(High Entropy Alloys\)](#) and [Mobility Database: MOBMG1 \(Magnesium Alloys\)](#).

There are also [Demo Databases](#) available.

 For more information go to the PDF copies of all database flyers located on the Thermo-Calc website <http://www.thermocalc.com/products-services/databases>.

6.1 Updated Databases

The following database is updated. Availability is based on having a valid license for the respective database.

TCSLD 3.1

The changes from TCSLD3.0 to TCSLD3.1 are:

- Volume data for the liquid phase are updated for some Ag/Bi/Cu/In-containing binary systems and a few Ag-containing ternary systems.
- Thermodynamic description of Au-Pb-Sn is added.

6.2 Removed Databases

With the addition of the demo databases, other databases are no longer included with the installation:

- PSUB, PBIN, PKP, PCHAT, PTERN, PION, PAQS2, PGEO and PFRIB

6.3 Bug Fixes

As part of the 2015a update in August, the following were fixed and are now included with 2015b.

TCFE8

- A revision of the liquid description in the Fe-C-Si system to improve cast iron phase equilibria
- The addition of some TYPE_DEFINITION keywords required for compatibility with DICTRA.

TCNI8

- The phase ALTI3_DO19 has been fixed in the Ni-Ti phase diagram when using the BIN module/Binary calculation in Thermo-Calc. It had been appearing incorrectly in TCNI6, TCNI7 and TCNI8.

7. Documentation, Examples and Training Materials

7.1 Documentation

In addition to the new [Online Help](#), several improvements have been made to the structure and content of all the documentation.

- The Console Mode and Graphical Mode User Guides have been merged into one guide, the *Thermo-Calc User Guide*.
- The *TQ-Interface Programmer Guide* has had a complete overhaul to make it easier to use. See section 3.2 *Using this Guide* in the PDF, or search the online help.
- The *DATAPLOT User Guide* has been updated to include LaTeX.
- There is a new *Quick Install Guide* for Mac operating systems.

7.2 New Examples

Graphical Mode

Three new examples are included with the Graphical Mode to demonstrate the Property Model Calculator. Each of these new models is shown in a new set of [Training Videos](#).

- Example 10: Uses the Property Model Calculator to predict the transition temperature to the unwanted brittle Sigma phase. The example shows how the temperature is influenced by changes to a steel alloy's composition using the uncertainty calculation type and how to create either a histogram or probability plot.
- Example 11: Uses the Property Model Calculator and both thermodynamic and kinetic demonstration steel databases. With a grid calculation type it produces three plots: a heat map, a contour plot and a cross plot with contour (where both the interfacial energy and coarsening rate is shown).
- Example 12: Uses the Property Model Calculator and a thermodynamic demonstration steel database. Using a grid calculation type it produces a contour plot comparing the driving force and interfacial energy.

DICTRA

A new DICTRA example, EXA7 is available and shown in [Import a Scheil Segregation Profile](#). This uses the new DICTRA command INPUT_SCHEIL_PROFILE.

7.3 Training Videos

Several new training videos are available:

- On the Thermo-Calc website www.thermocalc.com/training/video-tutorials/
- On our YouTube channel www.youtube.com/

Check out the new features described:

- Property Model Calculator – Phase transition, Coarsening, Interfacial energy, and the Driving force models. These use the [Graphical Mode](#).
- The new Scheil Calculator
- An overview of the new features included with this software release.

8. General

- Thermo-Calc 2015b installs in its own home directory alongside older versions of the program.
- The 2015b version of the Thermo-Calc program is fully backward-compatible with earlier versions of the Thermo-Calc program.
- Thermo-Calc supports the new operating system El Capitan for Mac OS and Windows 10.

8.1 Installation

Linux CentOS 7 Installations

If you are installing on Linux CentOS 7, it is recommended you install gtk2 before you run the installation script.

```
yum install gtk2
```

8.2 Updated EULA and General Terms and Conditions

- For the *End User License Agreement (EULA)*, a wildcard is now also accepted on the third tuple in our network licenses. See section 4.
- The General Terms and Conditions: By default you receive this via electronic download. Alternately, you can request that a paper copy is mailed to you. Section 13 also notes that a wildcard is accepted as per the details above for the EULA.
- The *General Terms and Conditions for the Software Maintenance and Support* has been updated. It is relevant to customers who add any software to an existing Thermo-Calc license and/or purchase an additional license. In both cases the free Software Maintenance and Support period for such additional license(s) is limited to the time period remaining (if any) of the Software Maintenance and Support period of the first license ordered.

For copies of these documents, visit our website

<http://www.thermocalc.com/purchase/terms-and-conditions/>

8.3 Platform Roadmap

For information about platforms being phased out visit

<http://www.thermocalc.com/products-services/software/system-requirements/platformroadmap/>.

Database name:	TCS high entropy alloy Database
Database acronym:	TCHEA
Database version:	1.0
Database owner:	Thermo-Calc Software AB
Database segment:	High entropy alloys (aka. multi-principal element alloys)

Brief description

TCHEA1.0 has been developed within a 15-element framework and contains nearly all the stable phases in the assessed systems. It can be employed to a wide range of compositions of multi-component systems.

Applications

High entropy alloys (aka. multi-principal element alloys) design and engineering

Included Elements (15)

Al Co Cr Cu Fe Hf Mn Mo Nb Ni Ta Ti V W Zr

Included Phases (163)

LIQUID:L	AL2FE	AL7V	C36_LAVES	GAMMA_H	NI2V
FCC_A1	AL2TI	AL7W3	CFC2_FENBZR	H_L21	NI3TA_D0A
FCC_L12	AL2W	AL8CR5_H	CHI_A12	HF3NI7	NI3TI_D024
BCC_A2	AL2ZR3	AL8CR5_L	CO10CU57TI33	HF8NI21	NI5ZR
BCC_B2	AL31MN6NI2	AL8MN5	CO11ZR2	HFMN	NI7ZR2
HCP_A3	AL3CO	AL8MO3	CO3VV	HFNI_ALPHA	NI8TA
DIS_FCC_A1	AL3NI1	AL8V5	CO7HF	HFNI3_ALPHA	NIT12
CBCC_A12	AL3NI2	AL9CO2	CO7M2	HFNI3_BETA	NIZR
CUB_A13	AL3NI5	AL9CR4_H	CR3MN5	HIGH_SIGMA	P_PHASE
D019_HCP	AL3ZR	AL9CR4_L	CR3SI_A15	MN3TI	R_PHASE
AL10CU10FE	AL3ZR2	ALCR2	CRNI2_OP6	MN4TI	SIGMA
AL10FEMN2	AL3ZR4	ALCU_DEL	CU10HF7	MNNI2	T1_CU2TI
AL10V	AL3ZR5	ALCU_EPS	CU10ZR7	MNTA	T1CUNITI
AL11CR2	AL4CR	ALCU_ETA	CU2TI	MNTI_HT	T2_CU3TI2
AL11CU5MN3	AL4MN_R	ALCU_PRIME	CU2TIZR	MNTI_LT	T2CUNITI
AL11MN4_HT	AL4MN_U	ALCU_ZETA	CU3TI2	MONI_DELTA	T3_CU4TI3
AL11MN4_LT	AL4W	ALCU3MN2	CU4TI1	MONI4_BETA	T4CUFETI
AL11TI5	AL4ZR5	ALMO	CU4TI3	MOSI2_C11B	T4CUNITI
AL12MN	AL5CO2_D811	ALPHA_B19	CU51HF14	MU_PHASE	T5CUFETI
AL12W	AL5FE2	ALTI_L10	CU51ZR14	MZR3_E1A	T6CUNITI
AL13CO4	AL5FE4	ALTI3_DO19	CU8HF3	NB13NI75TI12	TAAL
AL13CR2	AL5W	ALZR	CU8ZR3	NB15NI56TI29	TAAL2
AL13FE2MN2	AL62CU25FE13	ALZR2	CUTI3	NB15NI80TI5	ALMNTI_L12
AL13FE4	AL63MO37	B11	DIS_MU	NB5NI75TI20	
AL16FEMN3	AL6MN	BCT_D022	DIS_SIG	NB8NI9TI3	
AL23CUFE4	AL77W23	C14_LAVES	FCC_L10	NI10ZR7	
AL23V4	AL7CU2FE	C15_LAVES	G_PHASE	NI11ZR9	
AL28CU4MN7	AL7CU4NI	C16_THETA	GAMMA_D83	NI2TA	

In total 163 different solution phases and intermetallic compounds are included. All necessary molar volume data and thermal expansion data have been added for most of the phases.

Assessed Systems

All the binary systems and 104 ternary systems have been assessed in full range of composition and temperature. 96 more ternary systems have been tentatively assessed with extrapolations. These binaries and ternaries can be calculated in Thermo-Calc with the BINARY and TERNARY Modules, respectively.

Scientific Models & References

Scientific Models & References are available at: <http://www.thermocalc.com/resources/>

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<i>Database name:</i>	TCS Mg-alloys Mobility Database
<i>Database acronym:</i>	MOBMG
<i>Database version:</i>	1.0
<i>Database owner:</i>	Thermo-Calc Software AB
<i>Database segment:</i>	Magnesium alloys

Brief Description

MOBMG is a CALPHAD-type kinetic database containing atomic mobility data for Mg-based alloys. It is compatible with the thermodynamic database TCMG4.

Applications

Coupled with a compatible thermodynamic database, MOBMG1 can be used to calculate various diffusivities in both solid and liquid solution phases, and most importantly to simulate diffusion-controlled phenomena, such as solidification, nucleation, growth / dissolution and coarsening of precipitates, in Mg-based alloys by using DICTRA or TC-PRISMA.

Included Elements (24)

Ag	Al	Ca	Ce	Cu	Fe	Gd	K	La	Li	Mg	Mn
Na	Nd	Ni	Pr	Sc	Si	Sn	Sr	Th	Y	Zn	Zr

Included Phases

Hcp_A3 Liquid

Please note that apart from the above phases for which diffusion data are included in the database, other phases may also be included in a DICTRA simulation. However, these phases will be treated as so-called diffusion “NONE”, i.e. there will be no diffusion considered in such phases. Phases which are not listed above will automatically be entered as diffusion “NONE” in DICTRA, provided a thermodynamic description for such phases has been retrieved prior to reading data from the mobility database.

Assessed Systems

All data sets are critically assessed against experimental information whenever available. The fact that the amount of experimental diffusion data is very limited for Mg-based alloys has made it necessary to use ab-initio calculations and sound empirical rules extensively in the development of this kinetic database.

Scientific Models & References

See the Thermo-Calc Software reference list available at: <http://www.thermocalc.com/resources/>