Release Notes:
Thermo-Calc Software Package
Version 2015a

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Release notes

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

Contents

1. Contents of the Thermo-Calc software release ......................................... 3
2. New products in Thermo-Calc software package 2015a............................... 3
3. Thermo-Calc.......................................................................................................................... 3
   3.1 New release naming system ................................................................. 3
   3.2 New functionality .................................................................................. 3
      3.2.1 Graphical Mode specific ............................................................ 4
      3.2.2 Console Mode specific .............................................................. 4
      3.2.3 DICTRA-module specific ......................................................... 4
   3.3 Improvements and bug fixes ................................................................. 7
      3.3.1 Console Mode and Graphical Mode ..................................... 7
      3.3.2 Graphical Mode specific .......................................................... 8
      3.3.3 Console Mode specific ............................................................. 8
      3.3.4 DICTRA-module specific .......................................................... 8
   3.4 Compatibility .......................................................................................... 9
4. TC-PRISMA ......................................................................................................................... 9
   4.1 Improvements and Bug fixes .................................................................. 9
5. Software Development Kits (SDKs) ................................................................. 9
6. Databases ......................................................................................................................... 9
   6.1 New cemented carbide alloys database – TCCC1 ................................. 9
   6.2 Updated databases ..................................................................................... 10
      6.2.1 TCFE8 ..................................................................................... 10
      6.2.2 TCNI8 .......................................................... 10
      6.2.3 TCAL4 .................................................................................... 11
      6.2.4 TCMG4 .................................................................................... 11
      6.2.5 TCOX6 .................................................................................... 12
      6.2.6 TCSLD3 .................................................................................. 12
      6.2.7 TCSI1.2 ................................................................................... 13
      6.2.8 MOBFE3 .......................................................... 13
      6.2.9 MOBNI4 ................................................................................... 13
7. Documentation ................................................................................................................. 13
8. General installation and operation notes ......................................................... 13
9. Platform roadmap ......................................................................................................... 14
1 Contents of the Thermo-Calc software release

The release includes the following:

- New version 2015a of the Thermo-Calc program including improvements and bug fixes.
- New cemented carbide alloys database TCCC1
- New versions of several databases: TCFE8, TCNI8, TCOX6, TCAL4, TCMG4, TCSLD3, TCSI1.2, MOBFE3, and MOBNI4.
- New version 2015a of the SDKs -- TQ-Interface, TC-API and the TC-Toolbox for MATLAB®.

2 New products in Thermo-Calc software package 2015a

- A Thermo-Calc Cemented Carbide alloys database with 13 elements: C, Co, Cr, Fe, Mo, N, Nb, Ni, Ta, Ti, V, W, and Zr. See the section New cemented carbide alloys database – TCCC1 for more information.

3 Thermo-Calc

3.1 New release naming system

Previously, the versions for Thermo-Calc were in numerical order, for example 4.1, 4.0, 3.1, and so forth. In order to streamline the release naming, the new system includes the year (2015) plus a letter (a or b) to indicate whether it is the first (spring) or second (autumn) release.

The versioning system has also changed for the SDKs. In previous releases, version numbers were used for the SDK names (TQ-Interface v 9.1, TC-API v 7.1 and TC-Toolbox for MATLAB® v 7.1). These are no longer used as part of the name as the SDKs versions are synchronised with the released version of Thermo-Calc.

3.2 New functionality

- Automatically set the program to check for updates between releases. Go to Tools>Options and on the General tab from the Check update interval list, choose On startup. You can also keep the default not to check (Don’t check) for updates and do it yourself periodically by choosing Help>Check for update.

Plots

- For editing plot lines, you can see examples of the available line widths or line types. For the plot Title you can also include symbol fonts.
Label plots with LaTeX expressions in both Console and Graphical Mode. This replaces the LTEXT text formatting used in previous versions of Thermo-Calc. For users who have plots and files that use the LTEXT format, and especially when using Console Mode, the following examples show the command changes from LTEXT and its LaTeX equivalent (note that some LTEXT syntax can still be used; it is converted into LaTeX when the label or title is added). The examples below show the full command string:

<table>
<thead>
<tr>
<th>Symbol or text format</th>
<th>LTEXT</th>
<th>LaTeX</th>
</tr>
</thead>
<tbody>
<tr>
<td>Label with subscript</td>
<td>add .13 .15 n c-ZrO^DO2$</td>
<td>add .13 .15 n \latex c-ZrO_2</td>
</tr>
<tr>
<td>Greek symbol</td>
<td>ADD .05 .50 N ^GRd$</td>
<td>ADD .05 .50 N \latex \delta</td>
</tr>
</tbody>
</table>

### 3.2.1 Graphical Mode specific

- There is a new **Retain Labels** button on the Configuration window. You can toggle plot labels on or off when individual plots are updated. By default labels are retained both locally and globally. To make a global change to the plot labels, for example if you want to turn this option off, go to Tools>Options>Graphical Mode>Activities>Plotting.

### 3.2.2 Console Mode specific

- In the POLY-3 module a new command allows you to look at derivatives of Gibbs energy. The first and second derivatives of the Gibbs energy of phase are available. The derivatives are given with respect to the site-fractions and are per mole formula unit of the phase. The first derivatives are obtained through the STATE_VARIABLES command: D1G(PHASE,SPECIES#SUBLATTICE) and the second derivatives through D2G(PHASE,SPECIES#SUBLATTICE,SPECIES#SUBLATTICE). Wildcards can be applied in most cases. Enter INFO and ? at the prompt for more details about specific subjects related to this feature.

### 3.2.3 DICTRA-module specific

- For the ENTER_GRID_COORDINATES command there is a new SUB_REGION command where the grid in a specific region may also be subdivided into several parts, where the type of each part is chosen independently.
For the homogenisation model, some changes to boundary conditions make it easier to enter mobility estimates for specific elements in specific phases. See the examples below and the *DICTRA Command Reference* guide, section 2 under HOMOGENIZATION MODEL for details.

**Entering mobility estimates in DICTRA**

New subcommands for UTILITIES_HOMOGENIZATION make it easier to enter rough mobility estimates for specific elements in specific phases. The feature existed in earlier software versions but now you can enter the information directly, as explained in the example below. See Section 2 in the *DICTRA Command Reference* guide under UTILITIES_HOMOGENIZATION for details about the new commands.

In a binary Ni-Ti diffusion coupling at 1000 K the phase Ni3Ti_D024 is expected to form as a single phase layer. At the moment for this phase there is no diffusion data and simulating this diffusion coupling is not possible without mobility data. Using the new feature, a rough mobility estimate of 1e-22 is entered for both Ni and Ti in the Ni3Ti phase.

At a temperature of 1300 K a transient liquid forms if a small amount of titanium is brought into contact with nickel. As with the other example the Ni3Ti phase is expected to form. A simulation is performed where a 10 micron thick layer of Ti is put on a Ni substrate. For this simulation a mobility value for Ni and Ti in Ni3Ti of 1e-19 is entered.

![Ni-Ti phase diagram](image1)

**The Ni-Ti phase diagram**

![Ti mole fraction profile](image2)

**Ti mole fraction profile of Ni-Ti diffusion couple after 10 h at 1000 K**
Transient liquid formation in the Ni-Ti system. Ti profile after 0, 360 and 3600 s at 1300 K

**DICTRA simulation of CVD process**

The DICTRA HOMOGENIZATION MODEL [1,2] is used to simulate the deposition of NiAl β-phase by a CVD process. The resulting composition profiles were compared with experimental data by Yu et al. [3].

The experiment by Yu et al. was conducted at 1273 K for 2100 s whereby Ni and Al were co-deposited on a Ni-Al-Co-Cr substrate. The composition of the deposited coating was 51 at-% Ni and 49 at-% Al. The composition of the substrate was 29 Al, 18 Co, 16 Cr (at-%, bal. Ni). The thickness of the deposited coating was approximately 20 µm thick with a 7 µm interdiffusion zone.

The CVD process was approximated by constant fluxes of all components at the boundary such that the deposition rate and the composition of the coating corresponded to the experiment. The domain thereby grew by 20 µm during the simulation. This was not possible previously with this type of boundary condition. The figure below show the resulting composition profiles along with experimental data from Yu et al.
3.3 Improvements and bug fixes

3.3.1 Console Mode and Graphical Mode

- The four substitutional-sublattice ordering model is rebuilt and functions for all parameters, making it easier for database managers to develop a phase with four ordered substitution sub-lattices. A full explanation is in the Database Manager’s Guide (see section 3.3 Phase), which is part of your installation package or can be found on the Thermo-Calc Software website.

- The automatic scaling is improved for both linear and logarithmic axes. In addition, the logarithmic axis now only has integer exponents, rather than decimals. Decimal tick marks are also added.

- Undocked windows are hidden until you choose to display them. The window is no longer automatically placed on top of the other windows.

- One behind-the-scenes improvement is related to the format in which project files are saved. As a user, you will not notice any difference but the change provides valuable information about the project file that can be useful for troubleshooting.
Fixed an issue related to the choice of which composition set of a phase is regarded as the stable one. In this version, composition sets with the same composition as an already stable phase (composition set) are not allowed to enter the equilibrium and this retains the earlier set of phases previously calculated.

Property diagrams and plots

The plot axes settings between windows are now updated at the same time, which means you can switch from one diagram type to another without needing to do this manually. For example, say you define the calculation of a property diagram, where the x-axis is temperature and y-axis the amount of phase. When you switch to another calculation type (for example, a phase diagram), the axis definitions are updated in both the Equilibrium Calculator window and the Plot Render window (in this example, the x-axis is now mass percent and the y-axis is now temperature). In previous versions of the software you had to manually update the axes variables in the Plot Renderer.

For property diagrams, fixed an issue where sometimes the wrong default legend was added to plots.

For property diagram calculations, fixed a data filtering issue that used the (non-default) legend type "Stable phases" in error.

Fixed an issue where the x-axis for a property diagram did not default to the stepping quantity of the Equilibrium Calculator.

Fixed an issue where no default phase/constituent selection was included when any of these quantities—*Activity of constituent in a phase*, *ln(Activity of constituent in a phase)*; or *Chemical potential of constituent in a phase*—was selected as a plot axis variable.

3.3.2 Graphical Mode specific

- On the Plot Renderer, you can now use reversed axes with min>max where it is decreasing. Previously this resulted in an empty plot.
- For Scheil simulations, fixed an issue when plotting latent heat results.

3.3.3 Console Mode specific

- Fixed an issue with the TABULATE_DERIVATIVES command where previously a work around was needed to use it.
- Linux and Mac only: Fixed a command in the POST module where DUMP_DIAGRAM caused the terminal to hang.
- Fixed an issue that prevented tiled Console window properties (such as the window name) from being edited more than once.

3.3.4 DICTRA-module specific

- Obsolete command: TABULATE_MOBILITY_DATA. Use the stepping (STEP_WITH_OPTIONS) and tabulation (TABULATE) functionality in the POLY-3 module to obtain the results instead. See the Thermo-Calc Console Mode Command Reference guide for information.
- The ENTER_LABYRINTH_FUNCTION now works with the homogenization model.
3.4 Compatibility

The 2015a version of the Thermo-Calc program is fully backward-compatible with earlier versions of the Thermo-Calc program (also see New release naming system).

4 TC-PRISMA

4.1 Improvements and Bug fixes

- When using the TCNI databases for precipitation modelling in Ni-based superalloys, you can speed up simulation. Do this by selecting DIS_FCC_A1 instead of FCC_L12#1 as the matrix phase.
- Fixed an issue where TC-PRISMA stopped before reaching the end of simulation time because the results file became too large. The simulation is not interrupted now due to file size, which is always kept within an acceptable size range by saving only a reasonable number of time steps.
- Instead of diffusivity, atomic mobility is now used to calculate the atomic attachment rate and incubation time. This fixes an issue in calculating nucleation rate when a negative diagonal diffusivity occurs.

5 Software Development Kits (SDKs)

- The SDKs TQ-Interface, TC-API and TC-Toolbox for MATLAB® are compatible with the new Thermo-Calc 2015a version. Note that in previous releases, version numbers were used for the SDK names (TQ-Interface v 9.1, TC-API v 7.1 and TC-Toolbox for MATLAB® v 7.1). These are no longer used as part of the name as the SDKs versions are synchronised with the released version of Thermo-Calc. (also see New release naming system).
- For TQ-Interface fixed a bug in the header file for function TQ_GSSC.

6 Databases

6.1 New cemented carbide alloys database – TCCC1

- A Thermo-Calc Cemented Carbide alloys database with 13 elements: C, Co, Cr, Fe, Mo, N, Nb, Ni, Ta, Ti, V, W, and Zr.
- TCCC1 contains many complete and critically assessed binary and ternary systems important for cemented carbide alloy design and processing.
- TCCC1 includes data for molar volumes enabling the calculation of density and lattice parameters (for cubic structures), coefficients of thermal expansion and/or relative length change. However, the molar volume data incorporated has no pressure dependence. It can be used with satisfactory results for cemented carbides with cobalt, iron and/or nickel binder.

For more information see the TCCC1 Extended Information datasheet found on the website under Cemented carbide alloys: [http://www.thermocalc.com/products-services/databases/thermodynamic/](http://www.thermocalc.com/products-services/databases/thermodynamic/)
6.2 Updated databases

The following are the specific updates to several databases. Availability is based on having a valid license for the respective database.

6.2.1 TCFE8

The changes from TCFE7 to TCFE8 are summarised as follows.

- **Added Yttrium**, which includes these systems (either full or partial):

- **Added Zinc**, which includes these systems:
  - Al-Zn, C-Zn, Ca-Zn, Co-Zn, Cr-Zn, Cu-Zn, Fe-Zn, Mg-Zn, Mn-Zn, Mo-Zn, Nb-Zn, Ni-Zn, P-Zn, S-Zn, Si-Zn, Ti-Zn, V-Zn, Y-Zn
  - Al-Cr-Zn, Al-Fe-Zn, Al-Mg-Zn, Al-Y-Zn, C-Co-Zn, Cr-Fe-Zn, Al-Si-Zn
  - Al-Cr-Fe-Zn

- Improved Copper descriptions by adding Co-Cu, Co-Cu-Fe and Cu-Fe-Si descriptions.
- Added description of C-Co-Cr for cemented carbide applications.
- Added Fe2SiTi phase required for the Fe-Si-Ti precipitation hardening steels.
- Fixed issues in TCFE7 including:
  - Improved MnS-MnO pseudo binary description.
  - Updated Mo-Si description.
  - Improved description of liquid C-Fe-Si parameters which is common for cast irons.
  - Improved C-Fe-O description.
  - Adjusted stability of MU-Phase in Co-Nb and Co-Ta systems.
  - Adjusted stability of Sigma in Co-Cr, Al-Nb, Mn-Ta, Mo-V, Nb-V, Ta-Ti and Ta-V systems.
  - Adjusted stability of Laves_C14 in Co-Mo and Cu-Fe systems.
  - Adjusted stability of L12_FCC in Co-V system.

For more information see the TCFE8 Extended Information datasheet found on the website under **Steels and Fe-alloys**: [http://www.thermocalc.com/products-services/databases/thermodynamic/](http://www.thermocalc.com/products-services/databases/thermodynamic/)

6.2.2 TCNI8

The changes from TCNI7 to TCNI8 are summarised as follows.

- The major update to TCNI8.0 is the addition of Copper, Cu. In total 24 binary systems and 29 ternary systems were added to the database and can be calculated using the BINARY/TERNARY module in CLASSICAL MODE or by using the BINARY/TERNARY CALCULATION template in GRAPHICAL MODE using Thermo-Calc.
- These new binary systems are included in TCNI8:

- These new ternary systems are included in TCNI8:
  - Al-Cu-Fe, Al-Cu-Mn, Al-Cu-Ni, Al-Cu-Si, C-Cu-Fe, Co-Cr-Cu, Co-Cu-Fe, Co-Cu-Mn, Co-Cu-Nb, Co-Cu-Ni, Co-Cu-Ti, Cr-Cu-Fe, Cr-Cu-Nb, Cr-Cu-Ni, Cr-Cu-Si, Cu-Fe-Mn, Cu-Fe-Mo, Cu-Fe-N, Cu-Fe-Nb, Cu-Fe-Ni, Cu-Fe-Si, Cu-Fe-Ti, Cu-Fe-V, Cu-Mn-Ni, Cu-Mn-Si, Cu-Mo-Ni, Cu-Ni-Si, Cu-Ni-Ti and Cu-Ti-Zr.

For more information see the TCNI8 Extended Information datasheet found on the website under Nickel-based superalloys: [http://www.thermocalc.com/products-services/databases/thermodynamic/](http://www.thermocalc.com/products-services/databases/thermodynamic/)

### 6.2.3 TCAL4

The changes from TCAL3 to TCAL4 are summarised as follows.

- The metastable Al-Cu precipitate Ω was modelled as the Al2Cu_OMEGA phase. In the Al-Cu-Mg-Zn system, the descriptions of the metastable precipitates ETA_PRIME (η') and T_PRIME (T') were refined. In the Al-Mg-Si system, the BETA_AL_DPRIME (Al-containing β'') phase was merged into BETA_DPRIME (β'') and treated as the same phase.

- 53 Ag-, H-, Hf-, K-, La-, Li-, Na- and/or Sc-containing binary systems were added, Ag-Cu, Ag-Fe, Ag-La, Ag-Li, Ag-Mg, Ag-Mn, Ag-Na, Ag-Ni, Ag-Si, Ag-Zn, Cu-H, Cu-Hf, Cu-La, Cu-Na, Fe-H, Fe-Hf, Fe-K, Fe-La, Fe-Li, Fe-Na, H-K, H-La, H-Li, H-Mg, H-Mn, H-Na, H-Ni, H-Zn, Hf-K, Hf-Li, Hf-Mg, Hf-Mn, Hf-Na, Hf-Ni, Hf-Sc, Hf-Si, K-Li, K-Mg, K-Na, K-Zn, La-Mn, La-Ni, La-Sc, La-Si, La-Zn, Li-Mn, Li-Na, Li-Sc, Li-Zn, Na-Sc, Na-Si, Na-Zn, and Sc-Zn. The previous Ag-Al binary description was replaced.

- HCP_ZN was merged into HCP_A3. Necessary adjustments were made for the descriptions of Zn-containing systems in order to reproduce the phase equilibria.

- Zr was introduced to Al3Ti_D022 and Ti to Al3Zr_D023. Al-Ti was updated in the Al-rich region. A preliminary assessment of the Al-Ti-Zr system was conducted. The description of Al4Mn_R in the Al-Fe-Mn system was refined.

- Molar volumes and thermal expansivities were evaluated for all the newly added phases and end-members. Some existing volume data were updated as well.

For more information see the TCAL4 Extended Information datasheet found on the website under Aluminium-based alloys: [http://www.thermocalc.com/products-services/databases/thermodynamic/](http://www.thermocalc.com/products-services/databases/thermodynamic/)

### 6.2.4 TCMG4

The changes from TCMG3 to TCMG4 are summarised as follows.

- Seven Mg-containing ternary systems were assessed and added to the database: Ag-Cu-Mg, Ag-Gd-Mg, Ca-Gd-Mg, Ca-Mg-Nd, Ce-Mg-Sr, Cu-Li-Mg and Cu-Mg-Y. As a subsystem of Ce-Mg-Sr, the Ce-Sr binary system was assessed.

- Gd-Mg-Zn was completely refined and Mg-Y-Zn was updated as well.

- The binary Ca-Y and Cu-Li systems and the Mg-containing ternary Al-Ca-Mg, Ca-Mg-Y, Ce-Mg-Zn and Mg-Nd-Sr systems were reassessed.

- The ternary Ca-Sr-Zn system was extrapolated.
- HCP\_ZN was merged into HCP\_A3. Necessary adjustments were made for the descriptions of Zn-containing systems in order to reproduce the phase equilibria.

For more information see the TCMG4 Extended Information datasheet found on the website under **Magnesium-based alloys**: [http://www.thermocalc.com/products-services/databases/thermodynamic/](http://www.thermocalc.com/products-services/databases/thermodynamic/)

### 6.2.5 TCOX6

The changes from TCOX5 to TCOX6 are summarised as follows.

- The main focus in this version of the database is within the Al2O3-CaO-MgO-SiO2-Y2O3-ZrO2 system for calculations on CMAS resistant thermal barrier coatings. In addition, all systems within the Fe-Al2O3-CaO-MgO-SiO2 system are now assessed.
- The following systems are now in TCOX6
  
  
  
  - Al-Ca-Si-Y-O, C-Ca, C-Mg, Ca-Cr, Ca-Mn, Ca-Y, Ca-Mg-Mn-O, Ca-Ni-Si-O, Mg-Ni-Si-O, Mg-Ni-Si-O, Mg-Si-Zr-O (estimated)

- Modelled CaO solubility in ortho-pyroxene
- Added Ca2FeSi2O7 (Melilite) and assessed the “binaries” Ca2FeSi2O7-Ca2MgSi2O7 and Ca2FeSi2O7-Ca2AlFeSiO7
- Merged the YAM and Cuspidine phases to get complete solubility between Y4Al2O9 (YAM) and Ca2Si2Y2O9 (Cuspidine)
- Estimation of Al-Fe-Mn-O to fit a Mn/Si steel in Fe-Al-Mn-Si-O

For more information see the TCOX6 Extended Information datasheet found on the website under **Slag, molten salts, oxides and ionic solutions**: [http://www.thermocalc.com/products-services/databases/thermodynamic/](http://www.thermocalc.com/products-services/databases/thermodynamic/)

### 6.2.6 TCSLD3

The changes from TCSLD2 to TCSLD3 are summarised as follows.

- Volume data for all phases have been added.
- Element Cd has been added with focus on the Cd-Cu-Pb-Sb-Sn-Zn system.
- Element Ga has been added with focus on the Al-Ga-Mg-Zn, Cu-Ga-Sn, and Ag-Ga-Sn-Sn systems.
- Element Mg has been added with focus on the Al-Ga-Mg-Zn system.
- Element Mn has been added with focus on the Ag-Cu-Sn-Mn system.
- 15 new binary systems have been added: Ag-Ga, Al-Ga, Al-Mg, Cd-Cu, Cd-Pb, Cd-Sb, Cd-Sn, Cu-Ga, Cu-Mn, Ga-Mg, Ga-Sn, Ga-Zn, Mn-Sn, Mg-Zn.
- 6 new ternary systems have been added: Al-Ga-Zn, Al-Mg-Zn, Cd-Pb-Sn, Cd-Sb-Zn, Cu-Mn-Sn, Ga-Sn-Zn.
For more information see the TCSDL3 Extended Information datasheet found on the website under Solder alloys: [http://www.thermocalc.com/products-services/databases/thermodynamic/](http://www.thermocalc.com/products-services/databases/thermodynamic/)

6.2.7 TCSI1.2

The change from TCSI1.1 to TCSI1.2 is the improvement of the Si-C binary descriptions, specifically the solubilities of C in solid and liquid Si.

For more information see the TCSI1.2 Extended Information datasheet found on the website under Silicon-based alloys: [http://www.thermocalc.com/products-services/databases/thermodynamic/](http://www.thermocalc.com/products-services/databases/thermodynamic/)

6.2.8 MOBFE3

The change from MOBFE2 to MOBFE3 is the addition of atomic mobilities of Y and Zn in bcc, fcc and liquid Fe.

For more information see the MOBFE3 Extended Information datasheet found on the website under Steel and Fe-alloys: [http://www.thermocalc.com/products-services/databases/mobility/](http://www.thermocalc.com/products-services/databases/mobility/)

6.2.9 MOBNI4

The change from MOBNI3 to MOBNI4 is the addition of atomic mobilities of Cu in fcc, L12, B2 and liquid phases.

For more information see the MOBNI4 Extended Information datasheet found on the website under Nickel alloys: [http://www.thermocalc.com/products-services/databases/mobility/](http://www.thermocalc.com/products-services/databases/mobility/)

7 Documentation

The documentation can be found in two places. On the Thermo-Calc website (http://www.thermocalc.com/support/documentation/) and when you have Thermo-Calc installed it is available in an installation subfolder called Manuals.

- A new installation guide is available for all operating systems. This replaces the individual guides previously published.
- There is a new quick installation guide for Windows operating systems, standalone, SUNLL license. Other quick guides will follow for the next release.
- The out-of-date data plot examples guide is archived on the web.

8 General installation and operation notes

- Thermo-Calc 2015a installs in its own home directory alongside older versions of the program.
- For some users with Norton Antivirus installed, you may need to allow Thermo-Calc software to perform the automatic updates. If prompted, add the executable file called autoupdate.exe to the list of reputable companies.
Specific to a Linux CentOS 7 operating system bug, you need to launch Thermo-Calc from the terminal window instead of double-clicking the desktop icon. To launch the program, from the Thermo-Calc installation directory enter $ ./Thermo-Calc-2015a.sh.

9 Platform roadmap

For information about platforms being phased out visit http://www.thermocalc.com/products-services/software/system-requirements/platformroadmap/.