Thermo-Calc 3.0 – The new generation of Thermo-Calc

It is with great pleasure that we can now provide our maintenance and support subscribers all over the world with a completely new version of Thermo-Calc. The new release is a unified version that incorporates both a command line user interface (Console Mode) and a graphical user interface (Graphical Mode), and users may freely choose the mode of operation they find most appropriate given their experience and needs. The features of these two modes of operation are summarized on the following pages.

Our main ambitions for this new version of Thermo-Calc have been to unify the two earlier versions of Thermo-Calc (i.e. TCC and TCW) into one application, create a framework that is suitable for extension with additional modules and functionality, improve the graphics and plotting functionality, as well as to develop a modern Java based graphical user interface available for both Linux and Microsoft Windows operating systems. In addition, we have further improved the global minimization routine, introduced a new magnetic model and made numerous other small improvements. The result is Thermo-Calc 3.0 and the version number has been chosen to reflect that this is the third time in which the user-interface has been redesigned to such a large extent. Future version numbers of Thermo-Calc are expected to be 4.0, 5.0, and so forth.

Thermo-Calc 3.0 has so far been tested on both 32- and 64-bit architectures of the following operating systems; Windows (XP, 7 and 8) and Linux (Ubuntu 12.04, CentOS 6.3 and openSUSE 12.2). We plan to shortly also test Thermo-Calc 3.0 under OS X and our expectation is that soon also this operating system will be supported.

It should be noted that the installation script contains other Thermo-Calc Software products which have not been updated (such as DICTRA, TC-PRISMA and the TC-Programming Interfaces), and that we recommend you to now only install Thermo-Calc 3.0 and Databases and no other products.

We recommend you refer to the installation guide before upgrading to Thermo-Calc 3.0.

A new license file is required for running the new software version. You will be receiving the new license file from us as an e-mail attachment.

Our development efforts continue and we will within a short period release new versions for the TQ-Interface, TC-API, TC-Toolbox for MATLAB, DICTRA and TC-PRISMA.

Should you have any questions or feedback to provide, then you are always most welcome to contact us.

Enjoy using your new software!

Graphical Mode:

Thermo-Calc 3.0 features a completely new Graphical User Interface (GUI), where an activity based concept has been adopted. By this, we mean that users generate a project from specifying and configuring a sequence of separate activities. For example, there are separate activities for defining a system, defining conditions for an equilibrium calculation, and for plotting results. These activities can be performed individually or in sequence depending on choice.
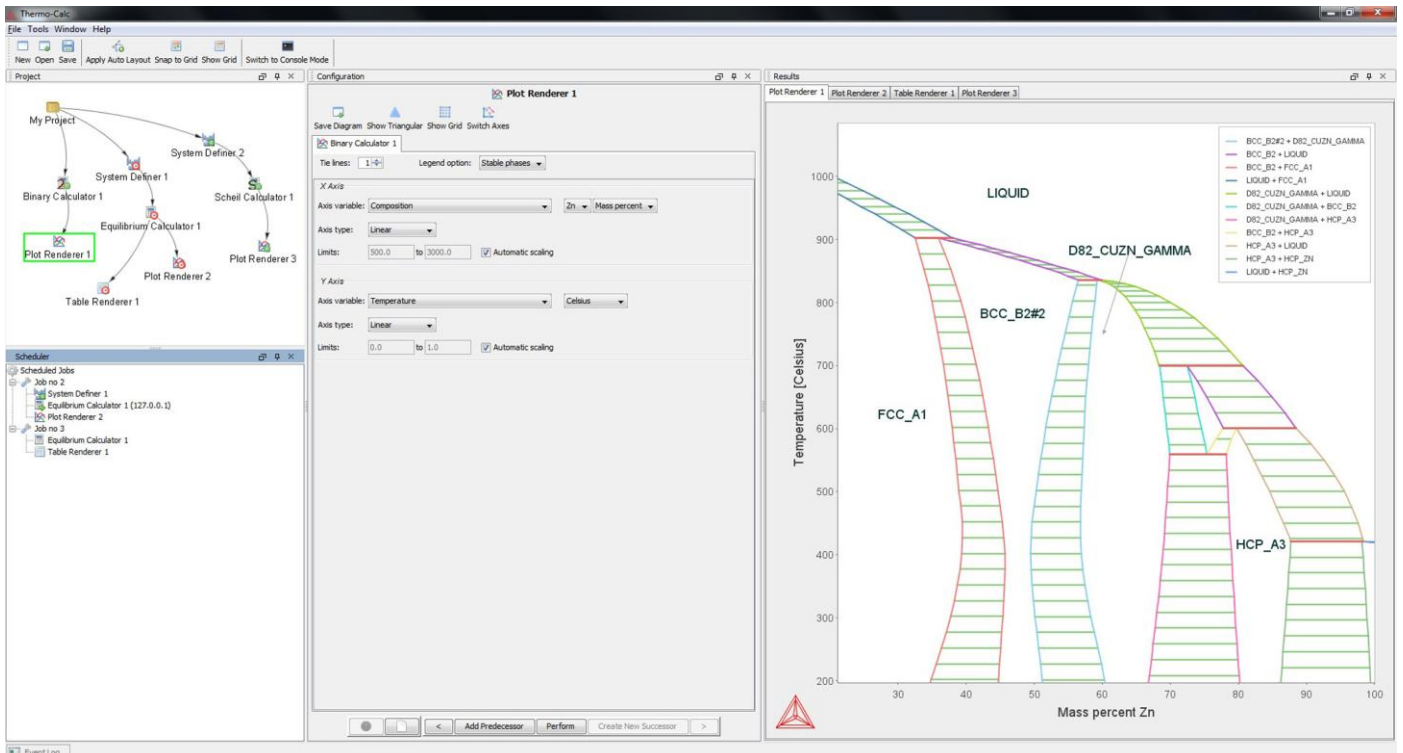
Working with projects makes it possible to save the activities and their respective configurations with or without calculation results depending on choice. This is a large advantage, since it is possible to open and modify old projects, as well as to share projects with colleagues who also have access to Thermo-Calc 3.0.

Another feature is the possibility to schedule tasks for execution (within 24 hours). In this way a user may schedule time consuming calculation tasks to start at the end of the work day.

There is also localization support available for some languages, i.e. English, Japanese, Chinese, Russian, German, Spanish and Swedish. A selection can be made in the Options present under the File menu.

To get started one may use the Quick Start wizard that will guide the user to define and perform a calculation. Alternatively, one can choose to start from one of the templates, configure the activities present in the resulting branch, followed by performing the calculation. It is also possible to define the activities one by one by either right-clicking on the icons present in the Project window (present in the upper left corner), or alternatively using the navigation bar present at the bottom of the centralized Configuration window.

We intend to shortly make videos available at www.thermocalc.com for you to watch, in order to quickly get on track and explore the new functionality.

Console Mode:

The command-line user interaction as present in Thermo-Calc Classic (TCC) has been much appreciated over the years, and is possibly the most efficient method of interaction after a user has passed the threshold of learning the relevant commands. For this reason the Console Mode in Thermo-Calc 3.0 has been designed to allow all TCC users to feel at home.
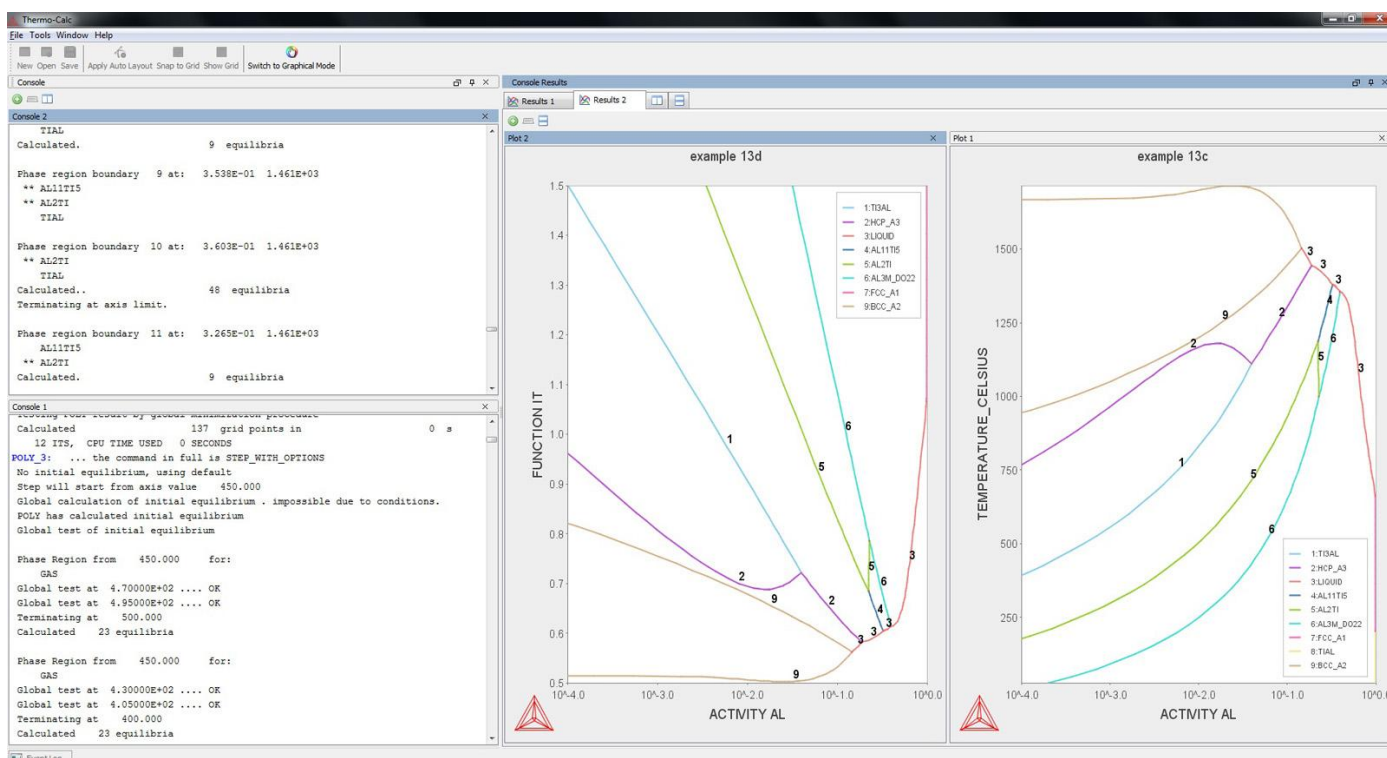
Several improvements have been made with respect to the user experience, such as the possibility to work with multiple independent console sessions (side by side or in tabs), as well as to plot and compare results in different graphs, as displayed in the above graphics.

The Console Mode, just like the Graphical Mode, features a brand new plotting facility that offers several improvements. For example, it will be possible to edit and complete diagrams for publication to a much larger extent than before. Plots will be saved with high resolution in common file formats, such as JPG, SVG, PNG, PDF, EMF, GIF and PS. To add a label or to save a plot one may optionally to command line interaction right-click in the plotted diagram and select an action form the drop down menu.

It is important to note that since the user interface is now Java-based the same user experience will be available on both Windows and Linux platforms.

It should also be emphasized that "under the hood" many improvements and corrections have also been made since the previous version. One may here specifically note in addition to the introduction of a new magnetic model, corrections to the model implementation for ionic liquid with regards to neutral liquids, molar volumes and extrapolations in higher order systems. Furthermore, all phases with a net charge are now correctly suspended in the database module, the Gibbs Energy System will only accept neutral reference states and the error "TOO LARGE WORKSPACE" that frequently could show up while saving in EDIT_EXPERIMENTS has been taken care of.