

CompuTherm Newsletter

Issue 1, 2007

Announcement of Pandat™ 7 New Release

Special points of interest:

- Enhanced Speed
- PanOptimizer
- Stability diagram
- Ru, Ir, Pt addition to PanNi
- Sn addition to PanMg

After one year's hard work, CompuTherm is pleased to make the formal announcement of the new release of Pandat 7. In addition to all the features of Pandat 6, Pandat 7 offers many new enhancements with regard to the calculation performance and functionalities. As always, Pandat 7 keeps its well-known features for being Intelligent, Reliable and User-friendly. First-time users will find it easy to calculate phase diagrams and other properties by a few mouse-clickings, while advanced users will experience the enhanced power of Pandat 7.

New features of Pandat 7

A number of important new features and upgrades are available in Pandat 7. **First of all, the overall calculation speed is improved by five times on average.** Other important highlights are:

PanOptimizer – A new module, PanOptimizer, is added into Pandat 7. It is used for optimization of thermodynamic and other property model parameters based on experimental data.

Database – Pandat 7 allows users to append new phase or parameters of the existing phase into the currently active database. It also allows users to load a materials system that is predefined in a “.PBF” script file. In addition, several free databases (*.TDB) such as SGTE pure elements and more than one hundred binaries are available with Pandat 7.

Calculation Functions – Overall calculation speed is improved by five times on average and memory usage is reduced. Other improvements and additions are (a) calculations of stability diagrams, liquidus projection with associate model in liquid phase, and Curie temperature (T_c) curves; (b) implementation of thermodynamic models for phases with ionic species and phases described by ionic liquid model. In addition, all the calculations in the current workspace can be exported into one batch file.

Table and Graph – Table of tie-line, invariant reaction, isothermal lines, and T_c curve are now automatically created in Pandat 7. An editable “worksheet” table is added. Graph “Plot Setup” has been merged with Graph “Configure”. Graph can be saved as different types of files such as “BMP”, “EPS”, “JPG” and “WMF”. “Expand/Collapse Tree Nodes” function is added for easy access of the calculation results through the left panel tree nodes in user interface.

Other improvements include miscibility gap calculation, graphic interface, bug fixing, etc.

Inside this issue:

New features of Pandat 7	1
PanOptimizer	2
Stability Diagram	3
New upgrade of PanNi	4
New upgrade of PanMg	4
Events	4

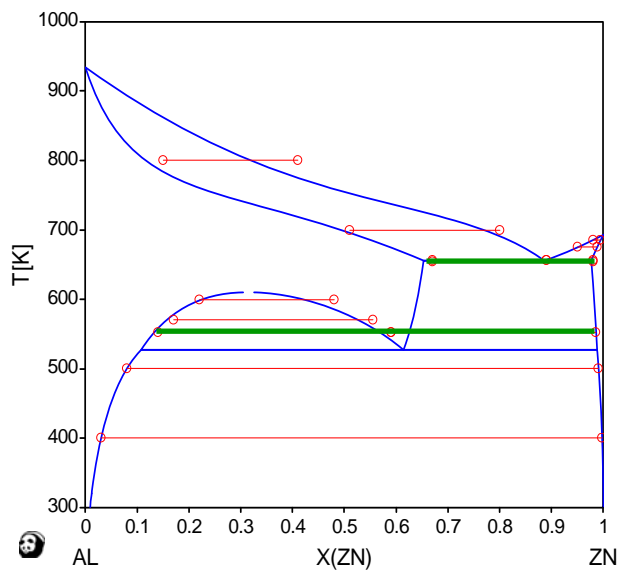
PanOptimizer

PanOptimizer is a C/C++ software package for evaluating thermodynamic, kinetic and thermo-physical model parameters based on experimental measurements. It is seamlessly integrated into Pandat as a specific module, which allows user to do real time calculation based on the instantly-obtained optimized parameters and make comparisons between the calculated values and the experimental data. A set of windows-based graphical user interfaces are deliberately designed for convenient input of the experimental data and automatic tracking of the optimization progress.

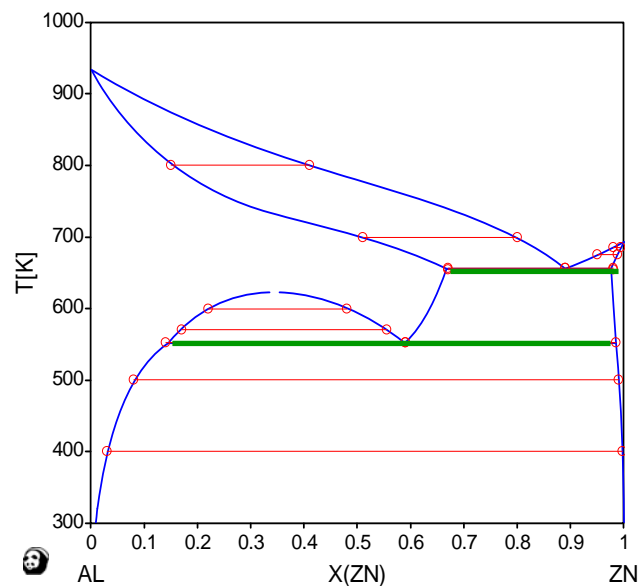
PanOptimizer is not only powerful for advanced users but also convenient for beginners. Two types of optimization process were implemented in PanOptimizer: **rough search** and **normal optimization**.

Rough search is used to obtain a rough topology of a phase diagram based on the given experimental data. It is useful for quickly estimation of the initial values of the model parameters at the beginning stage of the optimization procedure.

Normal optimization is used to obtain the best set of model parameters that can produce the best fit of experimental data.



Al-Zn phase diagram after rough search



Al-Zn phase diagram after normal optimization

Red denotes tie lines and green denotes the invariant reactions for experimental data

Free download!

Demo version of Pandat 7 with major functionalities for any binary system and the built-in Al-Cu-Mg-Si system is available for free download at

www.computherm.com

This demo version will be an excellent tool for teaching. It is also a good try-out version before you make the decision to license the full version.

Free upgrade!

The newly purchased license of Pandat 6 will be upgraded to Pandat 7 without charge. Please send your dongle information to info@computherm.com to get your free upgrade.

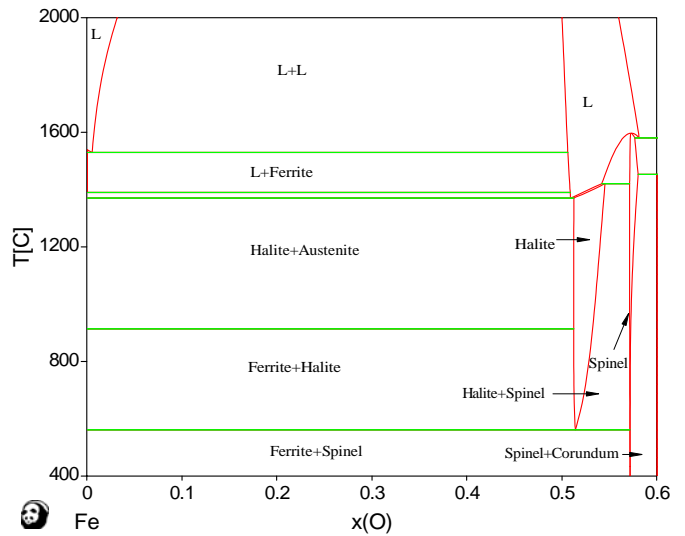
Calculation of Metal-Gas systems

Customized Training

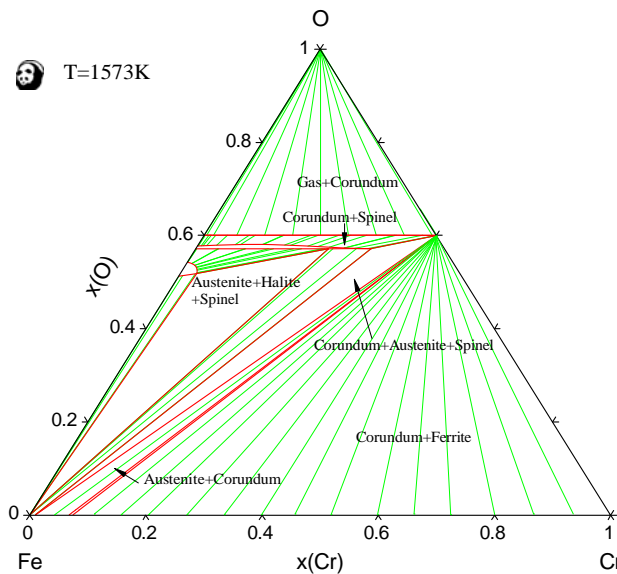
CompuTherm also provides customized training program of your interest. if you have such a demand please contact us at www.compuTherm.com

Pandat 7 has implemented the Gibbs energy functions described by ionic liquid model, compound energy model with ionic species, and associate models. Not just be able to calculate the phase diagrams of the Metal-Gas system, Pandat can work with the complex systems such as Fe-Cr-Ni-O, in which the spinal phase is described by 4 sublattices and 50 end members .

Fe-O Binary Phase Diagram



Fe-Cr-O isothermal section at 1573K



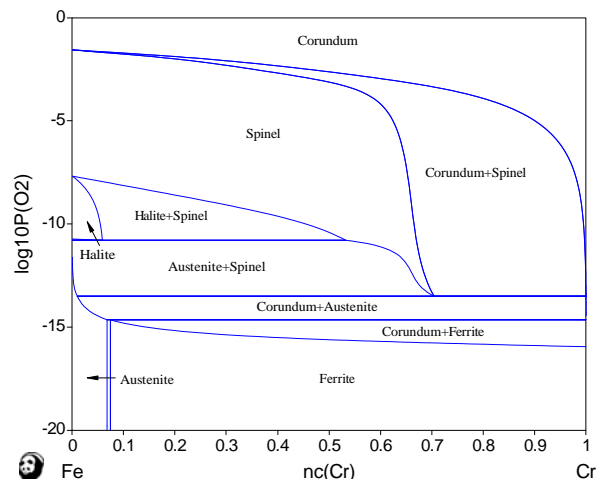
Calculation does not ask for initial values for ionic species either. Pandat automatically finds the most stable phase equilibria.

Make your Suggestions

CompuTherm honors the suggestions from customers on how to improve products. Please send your suggestions to info@compuTherm.com

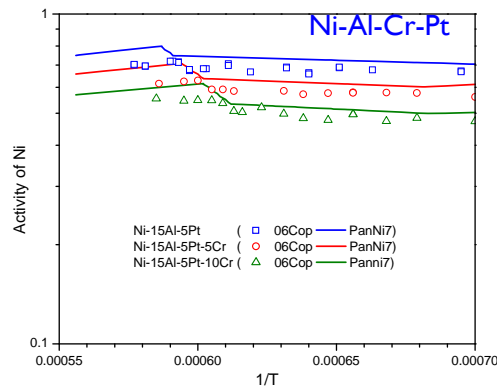
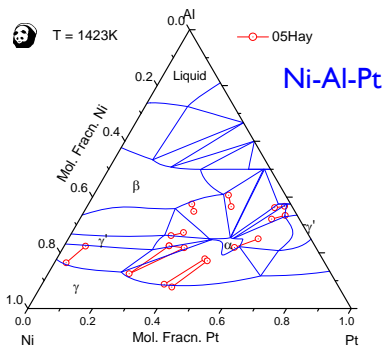
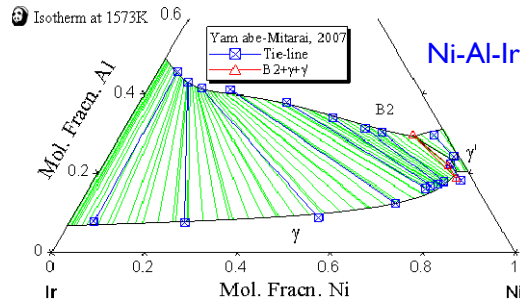
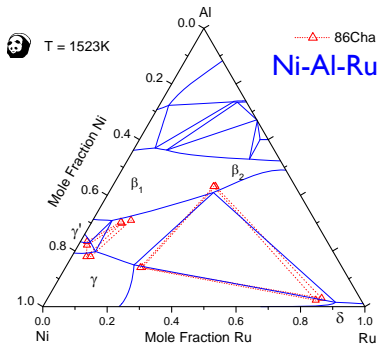
Pandat 7 can calculate the stability diagram of multicomponent systems.

Fe-Cr-O stability diagram at 1573K



New updates of PanNi

Three new elements, **Pt**, **Ru** and **Ir**, were added to PanNi, with thermodynamic descriptions developed for the following key binaries and ternaries: Ni-Pt, Al-Pt, Cr-Pt, Ni-Al-Pt, Ni-Ru, Al-Ru, Cr-Ru, Ni-Al-Ru, Ni-Cr-Ru, Ni-Ir, Al-Ir, and Ni-Al-Ir.



New updates of PanMg

A new element, **Sn**, was added to the database. The following 23 binaries and 13 ternaries were either newly developed or improved.

Ag-Ce, Ag-Sn, Al-Mn, Al-Sn, Al-Sr, Ca-Ce, Ca-Mg, Ca-Sn, Ca-Zr, Ce-Sr, Cu-Sn, Fe-Sn, Li-Sn, Mg-Mn, Mg-Sn, Mg-Sr, Mn-Sn, Mn-Sr, Si-Sn, Sn-Zn, Sn-Zr, Y-Zn, Zn-Zr

Al-Ca-Li, Al-Ca-Mg, Al-Mg-Mn, Al-Mg-Sn, Al-Mg-Sr, Al-Sn-Zn, Ca-Ce-Mg, Ca-Mg-Sn, Ca-Mg-Sr, Ca-Mg-Zn, Cu-Sn-Zn, Mg-Si-Sn, Mg-Y-Zn

EVENTS

Exhibits

MS&T 2007, September 16~20, 2007, Detroit, Michigan, USA

TMS Annual Meeting 2008, March 9~13, 2008, New Orleans, Louisiana, USA

Training Classes

Pandat and Thermodynamic databases, November 15~16, 2007, Shanghai, CHINA

Pandat and Thermodynamic databases, March 8, 2008, New Orleans, Louisiana, USA

Please contact us for more information.



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