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CompuTherm Newsletter

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New Release of Pandat™ Software and Databases Version 2025

CompuTherm is pleased to announce the release of Pandat software and databases version 2025, featuring new capabilities to enhance the user experience. The Material-to-Material calculation feature offers a novel approach to understanding phase transformations between different materials. Solute-trapping model has been implemented in the PanSolidification module to predict solute trapping during high-speed solidification. Additionally, the newly developed PandatX command-line interface enables advanced batch calculations, and its integration with the PanPython SDK significantly facilitates large-scale, high-throughput computations on both Windows and Linux. This newsletter provides a quick overview of the highlights. For further details, please refer to the Pandat Software User's Guide and Database Manuals version 2025, available on our website: www.computherm.com.

New Features and Enhancements of Pandat™ 2025

Material to Material Calculation – This new functionality in **PanPhaseDiagram** module provides users with a new perspective to understand phase transformation from one material to another material.

- **1D Line**: Calculate the phase equilibria from one material to another in terms of their relative amounts.
- **2D Isopleth**: Calculate the phase equilibria from one material to another within a temperature range.
- **2D Isotherm**: Calculate the phase equilibria among three materials at a given temperature.

Figure 1 presents three example calculations. Figure 1(a) illustrates a line calculation at 620°C, depicting the phase fraction change from SS316L to IN718. Figure 1(b) shows phase relationships between SS316L and IN718, clearly demonstrating the phase transformations that occur when these two materials are mixed. Figure 1(c) shows the isothermal section of three materials SS316L, IN718 and HEA(CoCrFeMnNi) at 900°C.

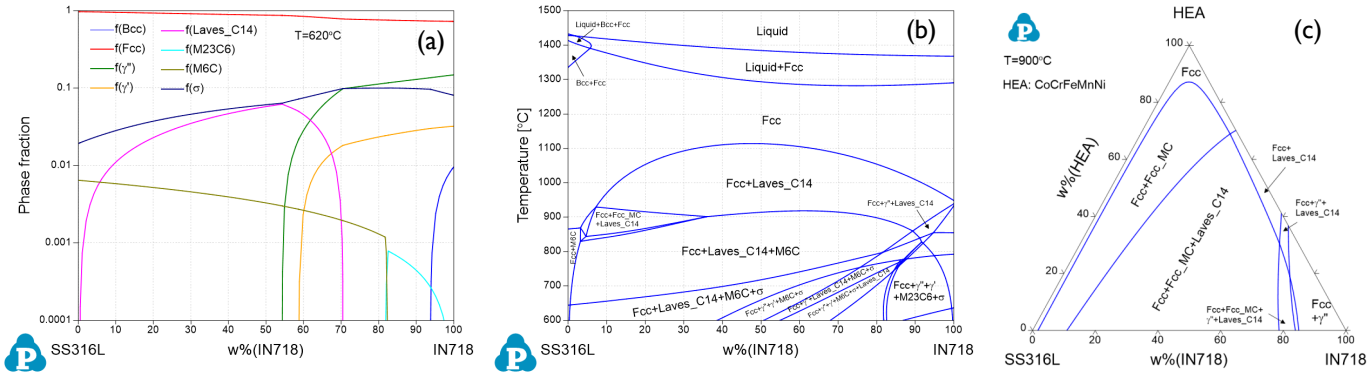

Figure 1: Three example calculations of Material to Material
(a) Line calculation; (b) Isopleth section calculation; (c) Isothermal section calculation.

Solute Trapping – The **PanSolidification** module now incorporates solute trapping effects in the "BackDiffusion" model. Solute trapping occurs during rapid solidification, i.e. when the solid/liquid interface is moving at very high velocity (0.1-1m/s), which is typical in additive manufacturing processes. The Ludwig model [1998Lud], suitable for multicomponent alloys, was implemented to account for this phenomenon. Figure 2 illustrates the Al-1.5Cu-(x)Zn isopleth, highlighting calculated liquidus and solidus lines under rapid solidification (v = 1 m/s), which reveals a reduced solidification range due to solute trapping.

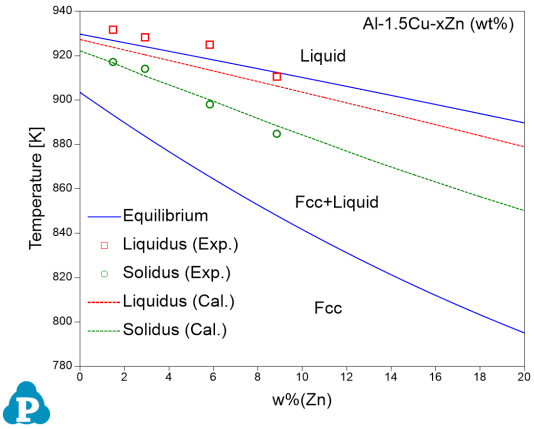

Figure 2: Isopleth diagram of Al-1.5Cu-(x)Zn with dynamic liquidus and solidus lines. Exp. Data from [2003Che].

PandatX: Command-Line Interface

PandatX is a new command-line interface that provides full access to all Pandat calculation modules.
Key features of PandatX include:

- PandatX is a cross-platform (Windows and Linux) console application that can run all batch files from any module in Pandat software.
- Compared to Pandat console mode, PandatX significantly improves efficiency, increasing performance by an order of magnitude for Point calculations.
- Performance can be further optimized by integrating PandatX with PanPython, leveraging its multithreading capabilities. The results of large-scale calculations can be stored in data files for advanced analysis and data mining.

New Databases

- Molten salt database is now available, which includes 14 chlorides, 57 binary and 4 ternary systems.
- Thermal conductivity databases were developed for multi-component Al-alloys and Mg-alloys. Three models – Scheil (as-cast), Equilibrium, and Quench (heat-treated) – enable calculations for different processing conditions.

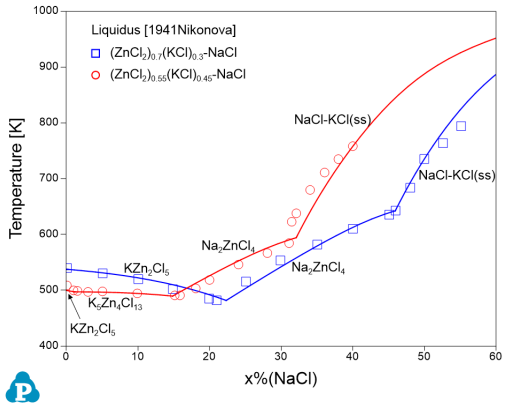

Figure 3: Calculated liquidus curves for two different vertical sections of the KCl-NaCl-$ZnCl_2$ ternary system, compared with experimental data from [1941Nik]

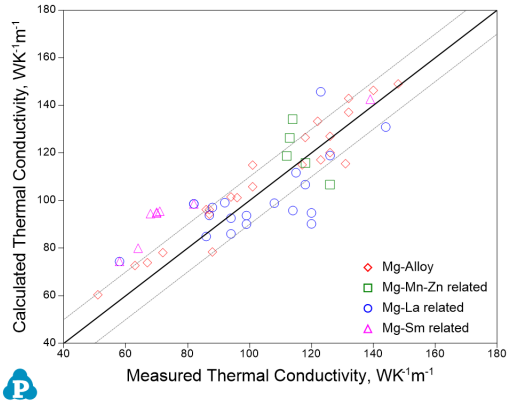

Figure 4: Comparison of calculated and measured thermal conductivity of Mg-alloys in the as-cast condition

References

[1941Nik] I.N. Nikonova, S.P. Pavlenko, A.G. Bergman, *Izv. Akad. Nauk SSSR Ser. Khim.* (1941), 391–400.
[1998Lud] A. Ludwig (1998). *Physica D: Nonlinear Phenomena*, 124(1998), 271-284.
[2003Che] F.Y. Chen, W.Q. Jie, *Acta Metallurgica Sinica*, 39 (2003), 943-947.