

# CompuTherm Newsletter

Issue 2, 2008

## Special points of interest:

### New features

- PanPrecipitation
- PanNb
- Molar Volume Database of PanFe
- Mobility Database for PanNi and PanFe

### Upgrades

- Para-Equilibrium
- 2D-Sectional Liquidus Projection
- Spinodal Decomposition Line
- Reaction Equations
- Driving Force
- Zero-Phase-Fraction Lines
- B addition to PanFe

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## Announcement of Pandat™ 8 New Release

CompuTherm is pleased to make the formal announcement of the eighth release of Pandat™ software and databases. The Pandat™ 8 release contains many improvements, some visible from the first click, and others hidden beneath the hood. This newsletter provides you with a quick glance on these new improvements. While the complete list of improvements is too lengthy to list here, we have included just a few of the reasons we're so excited about Pandat™ 8.

### New features and upgrades of Pandat™ 8

A number of important new features and upgrades are available in Pandat™ 8. Important highlights are:

**PanPrecipitation** – A new module, PanPrecipitation, is seamlessly integrated into Pandat™ 8. It is used for simulation of precipitation process. Two models, Fast Acting and Kampman Wagner Numerical models were implemented in PanPrecipitation.

**PanEngine** – Many properties can be calculated in Pandat™ 8. Examples are para-equilibrium, driving force, spinodal decomposition line, reaction equations, 2D sectional liquidus projection for  $n$ -component ( $n \geq 4$ ) system, zero-phase-fraction line, and many more.

**PanOptimizer** – The Standard Derivation and Relative Standard Derivation (RSD) for each parameter over the past 100 optimization iterations now can be calculated and traced in PanOptimizer. In addition, this version enables the optimization of model parameters for physical properties such as molar volume, density, molecular weight, surface tension and viscosity.

**Databases** – Thermodynamic database of Nb-Silicide based composites containing 10 components, molar volume database of PanFe, mobility databases for PanFe and PanNi are released in this version. B is added into PanFe.

**Miscellaneous** – More functions were implemented in Batch calculation such as defining customized tables and graphs, loop calculation for a matrix of alloys or a series of phase diagrams.

Other improvements include invariant reaction equations, graphic interface, bug fixing, etc.

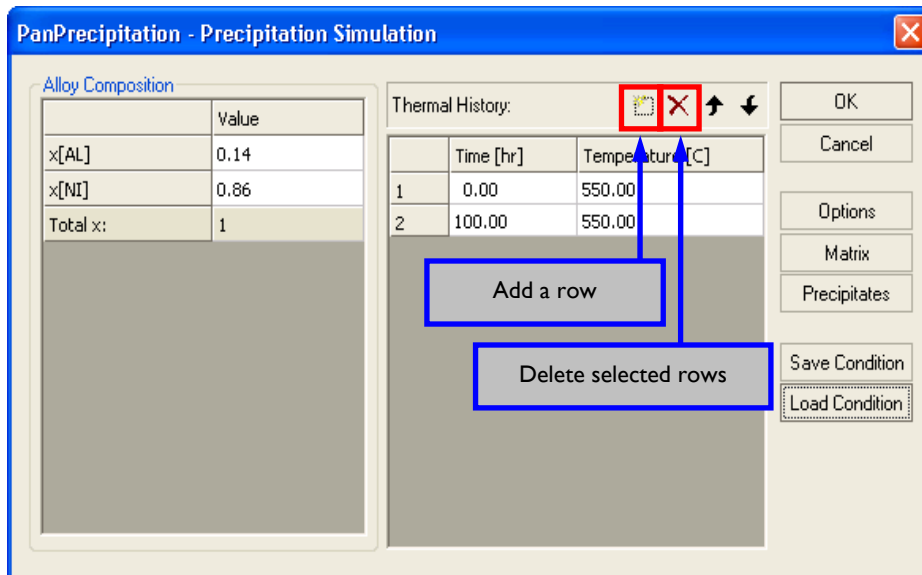
## PanPrecipitation

PanPrecipitation is designed for simulating precipitation kinetics during heat treatment processes. It is built as a shared library and integrated into Pandat as a specific module that extends the capability of Pandat for kinetic simulations, while taking full advantage of the automatic thermodynamic calculation engine (PanEngine) and the user-friendly Pandat graphical user interface (PanGUI).

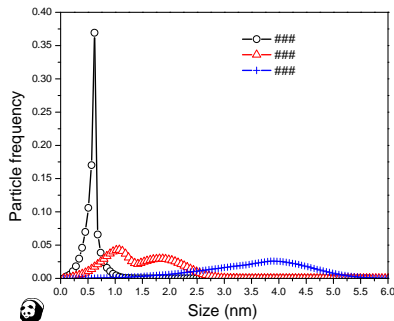
Kampman Wagner Numerical (KWN) and Fast-Acting models are built in PanPrecipitation. The input for precipitation simulation includes thermodynamic, mobility, and kinetic property databases, and alloy chemistry and thermal history. PanPrecipitation can simulate many materials properties, for example:

- Temporal evolution of average particle size
- Temporal evolution of particle size distribution
- Phase fractions
- Supersaturation in matrix phase
- Instant average composition of matrix and precipitate phases
- Growth rate of each particle size

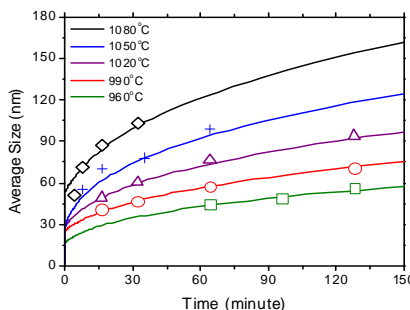
In addition to the two built-in models, Panprecipitation enables its integration with user-defined kinetic models.



Simple dialog window for precipitation simulation



KWN-predicted particle size distributions for the  $\gamma'$  particles at  $t = 21, 217$  and  $3720$  min for Ni-14 at% Al



Predicted evolution of average  $\gamma'$  particle size with time compared with the experimental data for Rene88DT

**Free download!**

Demo version of Pandat 8 with major functionalities is available for free download at

[www.computherm.com](http://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.

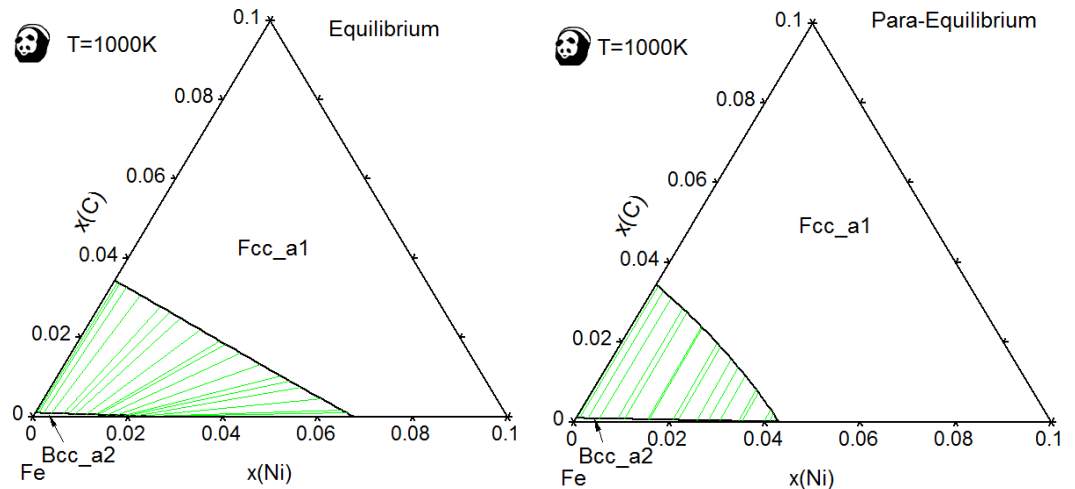
**Free upgrade!**

The newly purchased license of Pandat 7 will be upgraded to Pandat 8 without charge. Please contact

[info@computherm.com](mailto:info@computherm.com) to get your free upgrade.

# PanEngine

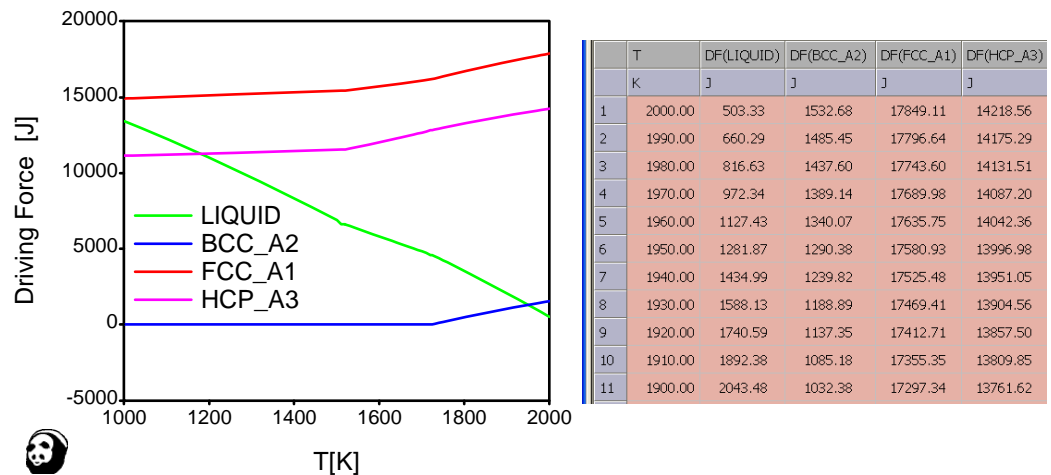
Fe-Ni-C isothermal sections (1000K) under full (left) and Para- (right) equilibrium



## Para-Equilibrium

Para-Equilibrium is often considered in a system that contains mobile and immobile elements such as Fe-Ni-C and Fe-Mn-C systems.

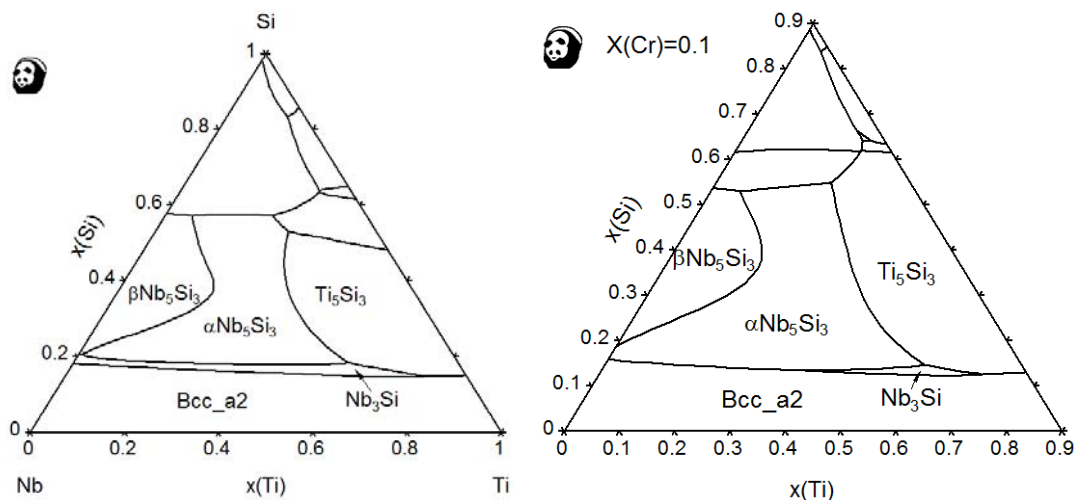
TPDF of Nb-20Ti-30Si (at%) as a function of temperature(K)



## Driving Force

Driving forces of phases are available for point and line calculations. The results are displayed in two formats: graph and table.

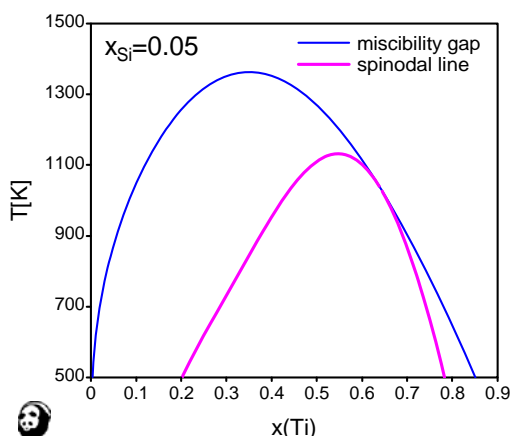
Liquidus projection of Nb-Ti-Si (left) and Nb-Cr-Ti-Si ( $x_{Cr}=0.1$ ) (right)



## 2D Sectional liquidus projection

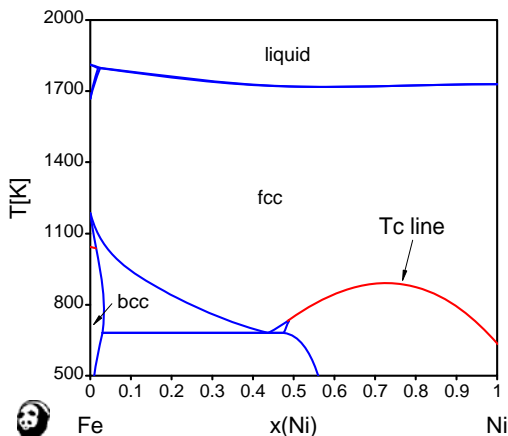
2D sectional liquidus projection makes it easy to visualize the liquidus projection of multicomponent systems ( $n \geq 4$ ).

### Spinodal Decomposition Line



Bcc\_A2 phase in Nb-Ti-Si with  $x_{Si}=0.05$

### Curie Temperature



Fe-Ni T-x phase diagram

### Training program

CompuTherm also provides customized training program of your interest. if you have such a request please contact us at [www.compuTherm.com](http://www.compuTherm.com)

## PanOptimizer

The **Standard Derivation** and **Relative Standard Derivation (RSD)** for each parameter over the past 100 optimization iterations have been calculated and traced through the “Model Parameter” dialog.

Model Parameters								
Number of parameters to be optimized is 11								
Name	Include ...	Lower Bound	Upper Bound	Value	Default Value	Std. Deviation	Relative Std. ...	
LIQUID_AA...	Active	0.0000	60000.0000	10295.9416	0.0000	5.2741	0.05%	
LIQUID_AAT...	Active	-20.0000	20.0000	-3.0334	0.0000	0.0123	0.41%	
LIQUID_BB...	Active	-60000.0000	60000.0000	-849.6646	0.0000	25.4028	3.02%	
LIQUID_BBT...	Active	-20.0000	20.0000	0.5002	0.0000	0.0095	1.89%	
HCP_A3_AA...	Active	-60000.0000	60000.0000	14713.4415	0.0000	52.9814	0.36%	
FCC_A1_AA...	Active	0.0000	60000.0000	6707.2540	0.0000	18.7172	0.28%	
FCC_A1_AA...	Active	-20.0000	20.0000	1.5538	0.0000	0.0360	2.29%	
FCC_A1_BB...	Active	-60000.0000	60000.0000	6744.2139	0.0000	27.9910	0.41%	
FCC_A1_BBT...	Active	-20.0000	20.0000	-4.9028	0.0000	0.0075	0.15%	
FCC_A1_CC...	Active	-60000.0000	60000.0000	-5160.9351	0.0000	29.0683	0.57%	
FCC_A1_CC...	Active	-20.0000	20.0000	7.0385	0.0000	0.0303	0.43%	

### Make your suggestions

CompuTherm honors suggestions from customers on how to improve products or bug report. Please send your suggestions and comments to [info@compuTherm.com](mailto:info@compuTherm.com)

Model parameters for physical properties such as molar volume, density, molecular weight, surface tension and viscosity now can be optimized in PanOptimizer

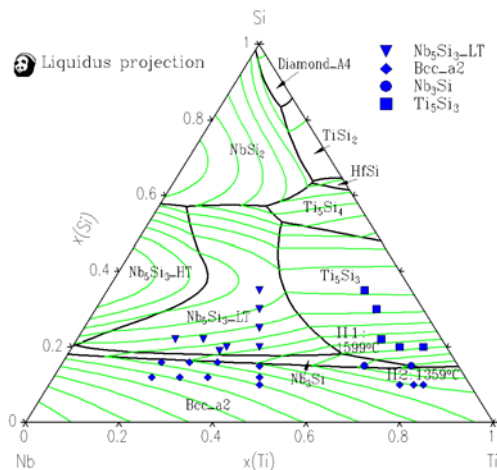
Experimental Data								
Number of experimental data is 7								
ID	Include ...	Name	Measured	Calculated	(Wtd. Residual)^2	Residual	Uncertainty	Weight
#0 (More...)	Active	log10(VM("BCC_A2"))	-5.092809	-5.089897	847.837946	0.002912	0.0001	1.0000
#1 (More...)	Active	log10(VM("BCC_A2"))	-5.104437	-5.101128	1094.786833	0.003309	0.0001	1.0000
#2 (More...)	Active	log10(VM("BCC_A2"))	-5.114531	-5.110412	1696.934515	0.004119	0.0001	1.0000
#3 (More...)	Active	log10(VM("BCC_A2"))	-5.135678	-5.138836	997.130777	-0.003158	0.0001	1.0000
#4 (More...)	Active	log10(VM("BCC_A2"))	-5.140454	-5.143543	954.479734	-0.003089	0.0001	1.0000
#5 (More...)	Active	log10(VM("BCC_A2"))	-5.144026	-5.146280	508.028015	-0.002254	0.0001	1.0000
#6 (More...)	Active	log10(VM("BCC_A2"))	-5.145293	-5.147184	357.474834	-0.001891	0.0001	1.0000

## Databases

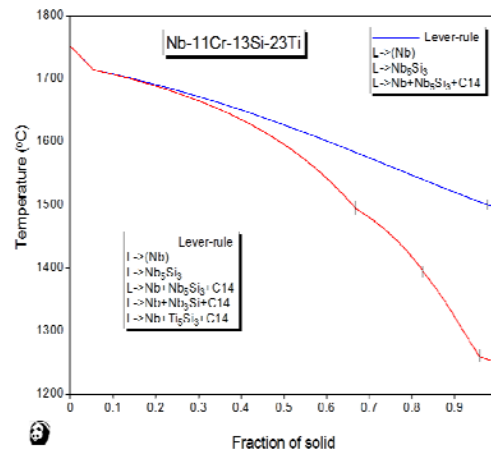
### PanNb

Thermodynamic database of PanNb contains 10 components: **Nb**, Al, Cr, Fe, Hf, Mo, Si, Ti, W, Zr. This database may be used for the alloy design of Nb silicides based Refractory Metal Intermetallic Composites (RMICs).

Nb-Ti-Si Liquidus Projection



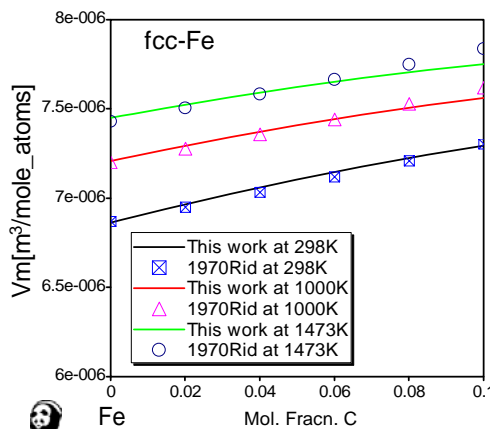
Solidification Path of Nb-11Cr-13Si-23Ti Alloy (at%)



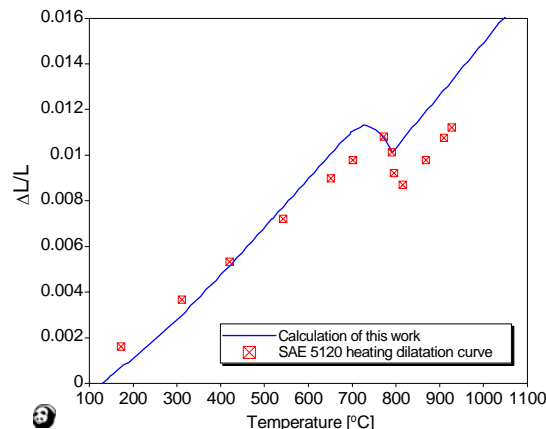
Molar Volume of Fcc in Fe-C Binary

### PanFe-Molar volume

This database contains molar volume data of the ferrite and austenite phases, involving components Fe, Al, C, Co, Cr, Cu, Mg, Mn, Mo, Nb, Ni, Si, Ti, V and W. Molar volume data of the cementite phase (Fe<sub>3</sub>C, Mn<sub>3</sub>C and Cr<sub>3</sub>C) are also included.



Dilatometric Analysis of SAE 5120\*

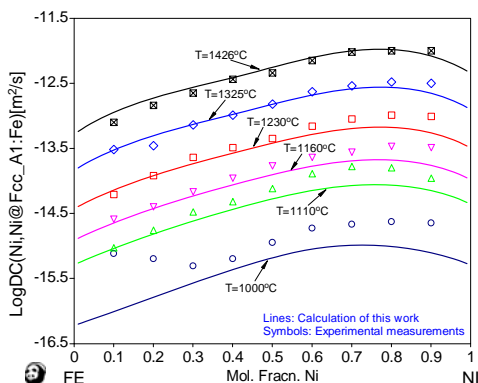


w%(Al)	w%(C)	w%(Cr)	w%(Cu)	w%(Fe)	w%(Mn)	w%(Mo)	w%(Ni)	w%(Si)
0.027	0.21	1.08	0.1	96.883	1.36	0.04	0.13	0.17

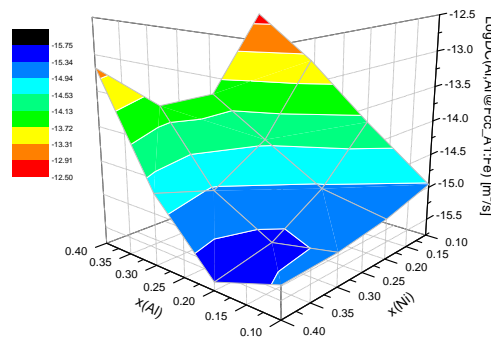
### PanMobility

This database contains mobility data of the Fcc\_A1, Bcc\_A2, and Liquid phases, involving components Al, C, Co, Cr, Cu, Fe, Hf, Mg, Mn, Mo, Nb, Ni, Pt, Re, Si, Ta, Ti, V, W, and Zn. This database is applicable to Ni-based and Fe-based alloys.

Fe-Ni Interdiffusion Coefficients



Fe-Ni-Al Interdiffusion Coefficients



## Upgrades of PanFe

**B** was newly added to the database. Thermodynamic descriptions of the following binaries ternaries were either newly developed or improved.

- Fe-B, Ni-B, Cr-B, Co-B, Mo-B, Nb-B, V-B, W-B, C-B, Si-B, Ti-B, Al-B, B-N
- Fe-B-C, Fe-B-N, Fe-C-N, Fe-Ni-B, Fe-Mn-B, Fe-Co-B, Fe-Mo-B
- Fe-Cr-B, Fe-Ti-B, Mo-Cr-B (B<33.3 at%)
- Fe-S and Mn-S have been modified.

## Upgrades of PanMg

Ni and C were newly added to the database. Thermodynamic descriptions of the following binaries and ternaries were either newly developed or improved.

- Ag-Ca, Al-Ni, Cu-Ni, Fe-Ni, Mg-Ni, Mn-Ni, Nd-Ni, Ni-Si, Ni-Sn, Ni-Y, Ni-Zn, Al-C, C-Si, Si-Zr, Al-Mn
- Al-Si-C, Cu-Mg-Ni, Cu-Ni-Si, Mg-Ni-Si, Ca-Mg-Sr, Gd-Mg-Y, Al-Ca-Mg, Al-Ca-Sr, Al-Mg-Mn

## Miscellaneous

### Batch Calculation

- Customized tables and graphs can be defined in batch calculation, which facilitates the comparison between calculated and experimental results, and the merge of different plots.
- A matrix of alloys or a series of phase diagrams can be defined as a “Loop” in batch file, which facilitates automatic execution of a large batch of calculations.

### Table and Graph

- Zero-Phase-Fraction (ZPF) lines now can be retrieved and plotted through Table and Graph functions.
- Reaction equations on phase boundaries are available from Table.

### Miedema-model calculated enthalpy of formation

- Miedema-model calculated enthalpy of formation now is available in PanOptimizer, which can be used as initial values of model parameters if experimental and First-Principles calculated data are not available.

## Events

### Exhibits

TMS Annual Meeting 2009, February 15~19, 2009, San Francisco, CA, USA

### Training Classes

Pandat and Thermodynamic databases, February 15, 2009, San Francisco, CA, USA

*Please contact us for more information.*



**CompuTherm LLC**

### Global Head Office

437 S. Yellowstone Dr.,  
Suite 217  
Madison, WI 53719  
USA

Phone: (1)608-274-1414

Fax: (1)608-274-6045

E-mail: [info@computherm.com](mailto:info@computherm.com)

Web: [www.computherm.com](http://www.computherm.com)

### Japan Agent

Materials Design Technology  
Co., LTD  
2-5 Odenmacho, Nihonbashi,  
Chuo-Ku, Tokyo 103-0011

Phone: (81)3-3660-5080

Fax: (81)3-3660-5330

E-mail: [info@materials-  
design.co.jp](mailto:info@materials-design.co.jp)

Web: [www.materials-  
design.co.jp](http://www.materials-<br/>design.co.jp)

### Korea Agent

ExpressLab Co., Ltd.  
1006 Pantheon Regency Bldg. 27  
Jeongja-dong,  
Bundang-gu, Seongnam-si,  
Gyeonggi-do 463-957

Phone : +82-31-785-7095

Fax : +82-31-785-7091

E-mail: [info@expresslab.co.kr](mailto:info@expresslab.co.kr)

Web: [www.expresslab.co.kr](http://www.expresslab.co.kr)