PANDAT™ 2020

User's Guide

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1 Pandat Basics

Pandat™ software is an integrated computational tool developed on the basis of the CALPHAD (CALculation of PHAse Diagram) approach for multi-component phase diagram calculation and materials property simulation. It has a robust thermodynamic calculation engine, a friendly graphical user interface, and a flexible post-calculation table editing function which allows user to plot variety types of diagrams. The software is designed to create a working environment that allows variety of calculation modules be integrated in the same workspace. It currently includes five modules: **PanPhaseDiagram** (phase diagram and thermodynamic property calculation), **PanPrecipitation** (precipitation simulation), **PanOptimizer** (property optimization) **PanDiffusion** (diffusion simulation) and **PanSolidification** (solidification simulation). Other modules can be easily integrated into the workspace for extended applications. The architecture of Pandat™ software is schematically shown in the Figure 1.1.

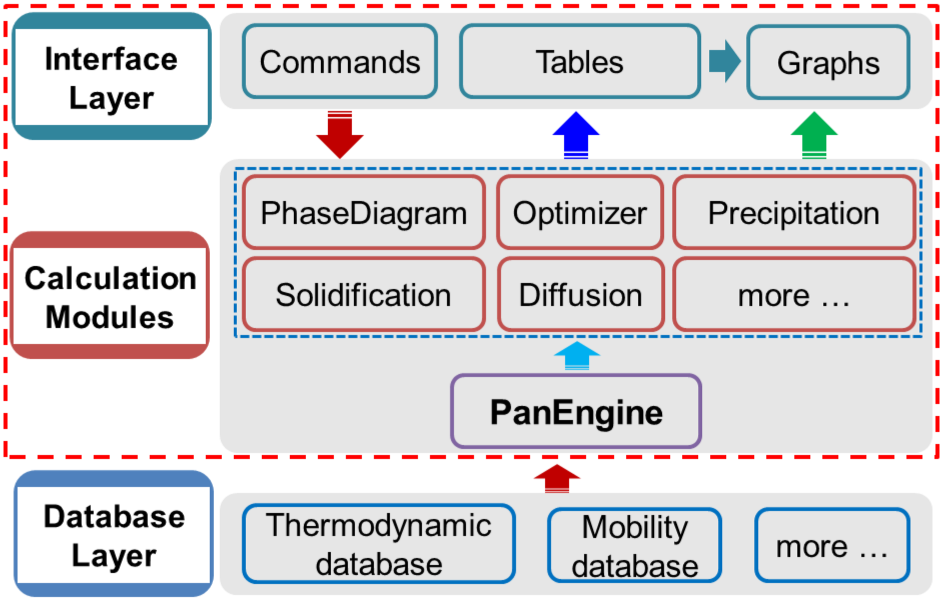
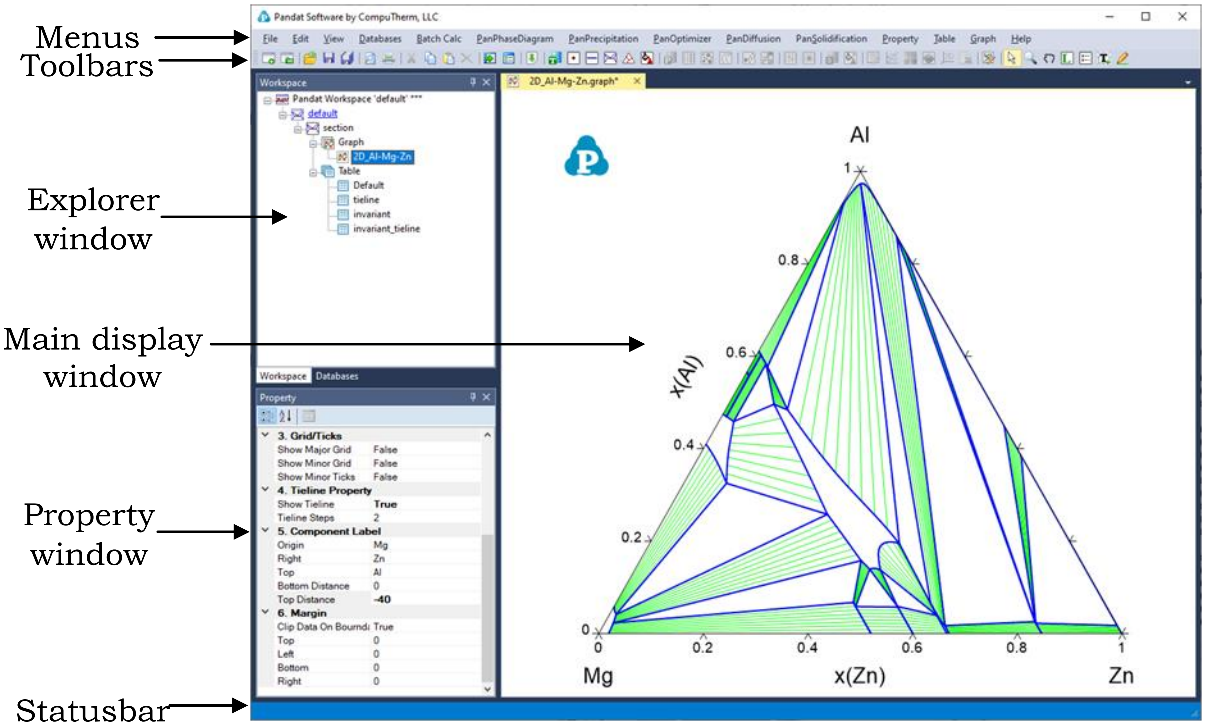


Figure 1.1 The architecture of Pandat™ software

In addition to the functionalities provided by Pandat™ as a stand-alone program being demonstrated in this manual, its calculation/optimization engine (**PanPhaseDiagram**, **PanOptimizer** and **PanPrecipitation**) are built as shared libraries and enable their integration with broader applications in the field of Materials Science and Engineering. More detailed information about Pandat software can be found in the published papers [2002Che, 2003Che, 2009Cao].

The **PanGUI** (user interface of the Pandat™ workspace) consists of six components: **Menus**, **Toolbars**, **Statusbar**, **Explorer window**, **Property window** and **Main display window** as shown in Figure 1.2.



3. Grid/Ticks	
Show Major Grid	False
Show Minor Grid	False
Show Minor Ticks	False
4. Tieline Property	
Show Tieline	True
Tieline Steps	2
5. Component Label	
Origin	Mg
Right	Zn
Top	Al
Bottom Distance	0
Top Distance	-40
6. Margin	
Clip Data On Boundi	True
Top	0
Left	0
Bottom	0
Right	0

Figure 1.2 The components of the PanGUI

1.1 Menus

Pandat menus provide commands for performing operations on the active window and other general operations such as opening and saving a workspace file (`*.pndx`) or turning on the display of a toolbar. The menus are context sensitive; that is, they change as the context in Pandat™ Main display window changes. This ensures that only Context-relevant menus and menu commands are displayed.

1.2 Toolbar

Pandat™ provides toolbar buttons for the frequently used menu commands. Like the menu commands, toolbar buttons are also context-sensitive.

When a toolbar button is pointed at with the mouse, a "tool-tip" displays the button name.

1.3 Statusbar

The Pandat™ Status bar is located at the bottom of the workspace. If the cursor is on a graph, the coordinates are displayed in the status bar.

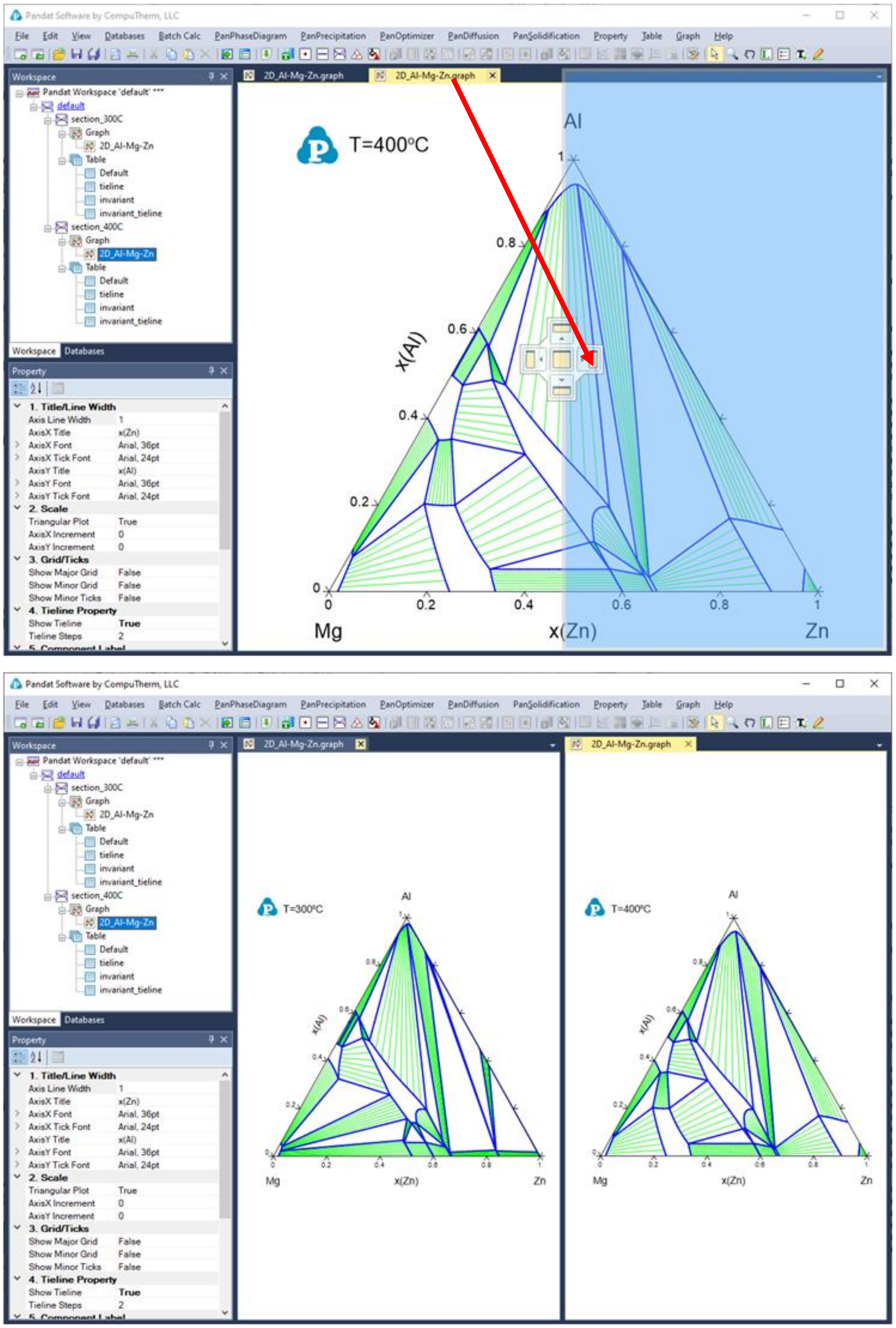
1.4 Explorer window

The Explorer window lists the contents in the current workspace. The contents are displayed in a tree structure. By clicking each node, the text, graph or table will be displayed in the Main display window of Pandat™. A node of a calculation result could be deleted.

1.5 Main display window

The Main display window displays the text, graph or table which corresponds to each node in the Explorer window.

More than one graph or table can be opened and their titles are displayed on the top bar of the Main display window. User can display several plots together in the Main display window by moving them to different positions. The following Figure 1.3 and Figure 1.4 show how to move these windows. Select the window on the top bar, hold the left button and move the mouse toward the Main display window. A dialog showing relative positions will be displayed. Move the mouse to the selected position and release the left button of the mouse. Figure 1.3 shows moving the selected window to the right side and Figure 1.4 shows moving the selected window (the Property Window) to the center position.



1. Title/Line Width
Axis Line Width 1
AxisX Title x(Zn)
AxisX Font Arial, 36pt
AxisX Tick Font Arial, 24pt
AxisY Title x(Al)
AxisY Font Arial, 36pt
AxisY Tick Font Arial, 24pt

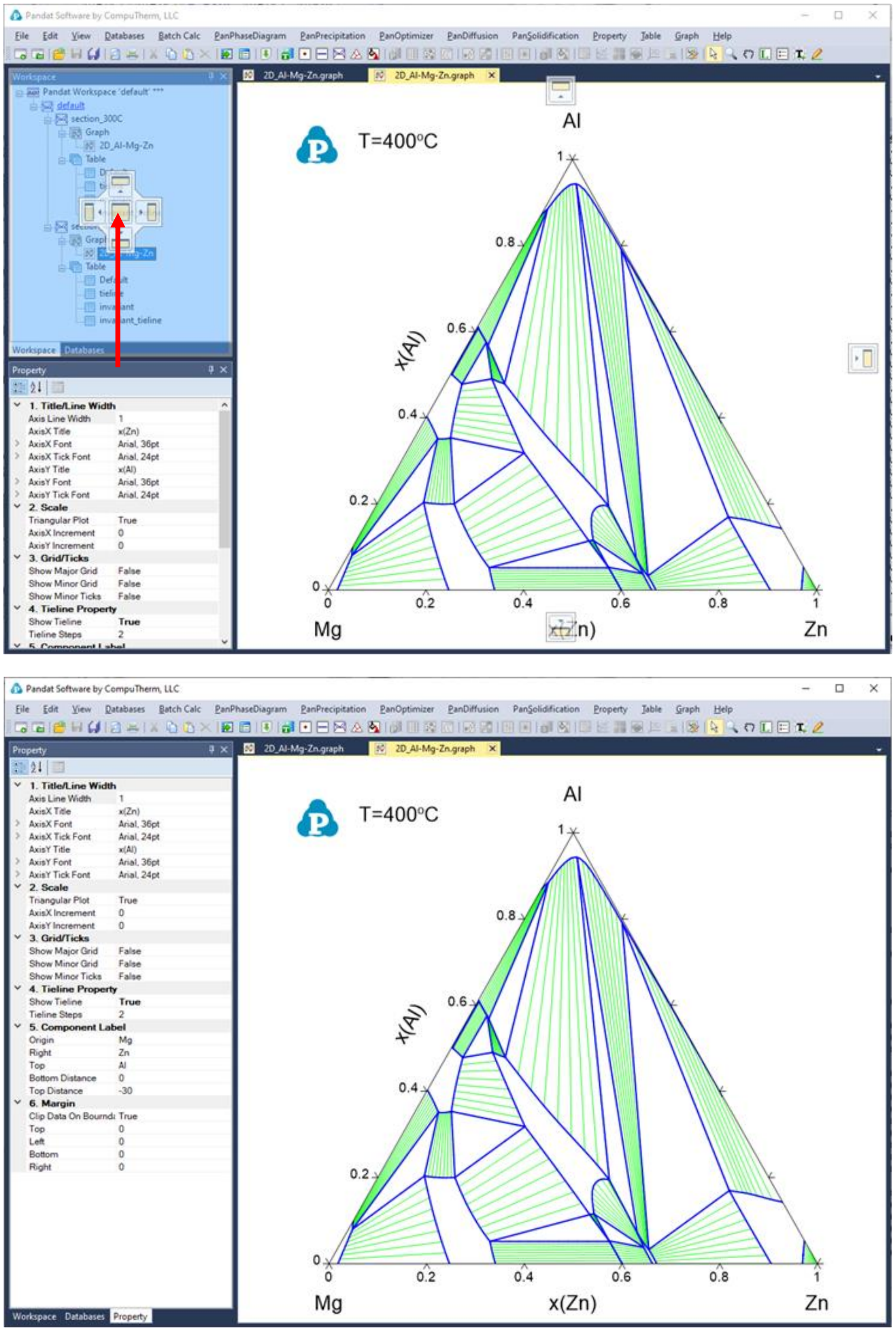
2. Scale
Triangular Plot True
AxisX Increment 0
AxisY Increment 0

3. Grid/Ticks
Show Major Grid False
Show Minor Grid False
Show Minor Ticks False

4. Tieline Property
Show Tieline True
Tieline Steps 2

5. Component Label

Figure 1.3 Rearrange the display window of Pandat™, before and after



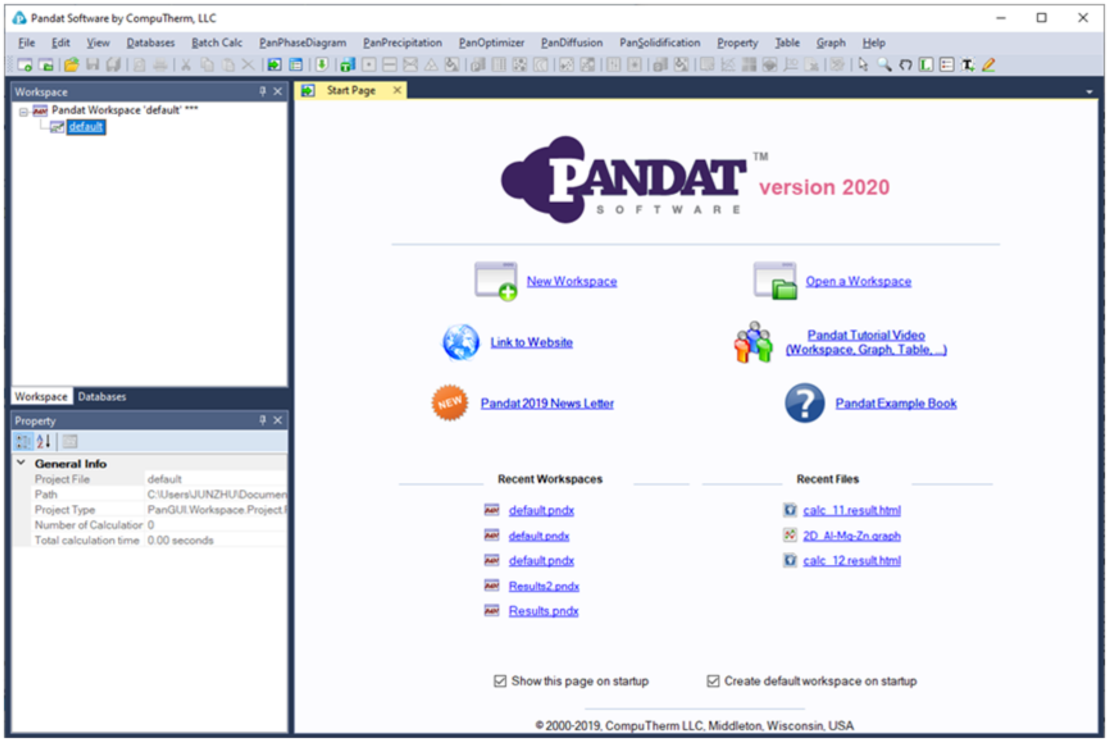
Property	
1. Title/Line Width	
Axis Line Width	1
AxisX Title	x(Zn)
AxisX Font	Arial, 36pt
AxisX Tick Font	Arial, 24pt
AxisY Title	x(Al)
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
2. Scale	
Triangular Plot	True
AxisX Increment	0
AxisY Increment	0
3. Grid/Ticks	
Show Major Grid	False
Show Minor Grid	False
Show Minor Ticks	False
4. Tieline Property	
Show Tieline	True
Tieline Steps	2
5. Component Label	

Property	
1. Title/Line Width	
Axis Line Width	1
AxisX Title	x(Zn)
AxisX Font	Arial, 36pt
AxisX Tick Font	Arial, 24pt
AxisY Title	x(Al)
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
2. Scale	
Triangular Plot	True
AxisX Increment	0
AxisY Increment	0
3. Grid/Ticks	
Show Major Grid	False
Show Minor Grid	False
Show Minor Ticks	False
4. Tieline Property	
Show Tieline	True
Tieline Steps	2
5. Component Label	
Origin	Mg
Right	Zn
Top	Al
Bottom Distance	0
Top Distance	-30
6. Margin	
Clip Data On Bounda	True
Top	0
Left	0
Bottom	0
Right	0

Figure 1.4 Rearrange the explore and property windows of Pandat™, before and after

2 Get Started

Pandat™ starts with the following start page as shown in Figure 2.1. The user can open the start page at any time by clicking the icon on the toolbar. On the start page, there are shortcuts which allow users to create a new workspace and open an existing workspace, link to CompuTherm's webpage (www.computherm.com) for recent updates and for comments and discussions from Pandat™ users. It also lists the most recent workspaces and files the user has created, so that user can reopen them easily.



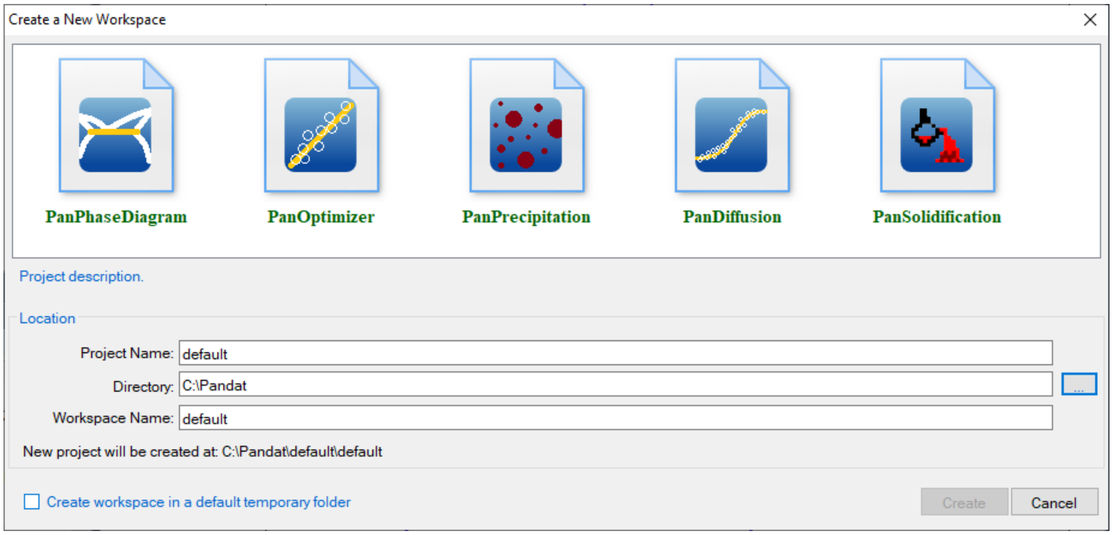
Project File	default
Path	C:\Users\JUNZHU\Documen
Project Type	PanGUI.Workspace.Project.I
Number of Calculatior	0
Total calculation time	0.00 seconds

Figure 2.1 The start page of Pandat™ software

2.1 Workspace

The workspace provides a space for user to perform Pandat™ calculations and organize the calculated results. It must be created before any Pandat™ calculation is carried out.

User can create a new workspace by clicking on the "New a Workspace" link on the start page, or the icon on the toolbar, or go through the menus (**File → Create a New Workspace**). A new window will pop out as is shown in Figure 2.2. User can define the name of the workspace and select a working directory to put the workspace. User can then select the module from the five icons: Phase diagram calculation ( ), Optimization ( ), Precipitation simulation ( ), Diffusion simulation ( ) or Solidification simulation ( ). User can also give a "Project Name" for the calculations to be performed. User may choose to create a default workspace with default project name simply by clicking the "**Create**" button or double click the selected module.



Project Name: default

Directory: C:\Pandat

Workspace Name: default

New project will be created at: C:\Pandat\default\default

☐ Create workspace in a default temporary folder

Figure 2.2 Create a new workspace dialog

After using Pandat™, user will be given an opportunity to save the workspace that the user has created. The user can open a saved workspace next time by clicking on the "**Open a Workspace**" link on the start page, or the icon on the toolbar, or going through the menus (**File → Open → Workspace**). For some most recent workspaces and files, the shortcuts listed on the start page allow the user to open them directly.

In Pandat™, only one workspace is allowed. When creating a new workspace, the user will be asked if the current workspace needs to be saved. Think twice before clicking the “**Create**” button. The old workspace will be lost if it is not saved when a new workspace is created.

2.2 Project

In the Pandat™, a workspace may contain many projects of different types. For example, a user creates a project for **PanPhaseDiagram** module which contains all calculations for phase diagrams. User can then create a new project of precipitation simulation in the same workspace using menus (**File → Add a New Project**). In this case, the workspace name and the working directory cannot be changed, but the user needs to give a new project name. The database file, table, graph and other data associated with one project can be viewed in individual tabs in the **Display** window.

When more than one project are created in one workspace, only one project will be activated at one time, and only those functions and toolbar icons associated with the activated project are available to the user at the time.

The name of the activated project will be highlighted as blue and be underlined. To select a project as the activated project, right click the mouse on the project name in the explore window and choose “**Set as Active Project**” in the popup dialog as shown in Figure 2.3.

When switching between projects, the user may also need to swtich between different databases so that the right database is used for the calculation. In the Databases view dialog in explore window, all the loaded databses are listed and the name of currently activated database is also highlighted with blue and be underlined. To activate another database, right click the mouse on the database name and choose “**Set as Activate TDB**” as also shown in Figure 2.4. Inside one project, the user may also load several databases and carry out different calculations of the same type. The user need to make sure that the correct database is activated when performing a calculation.

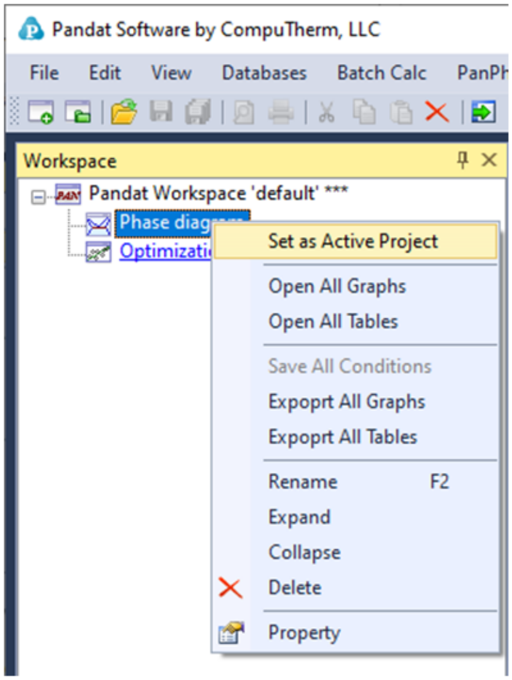


Figure 2.3 Set an active project

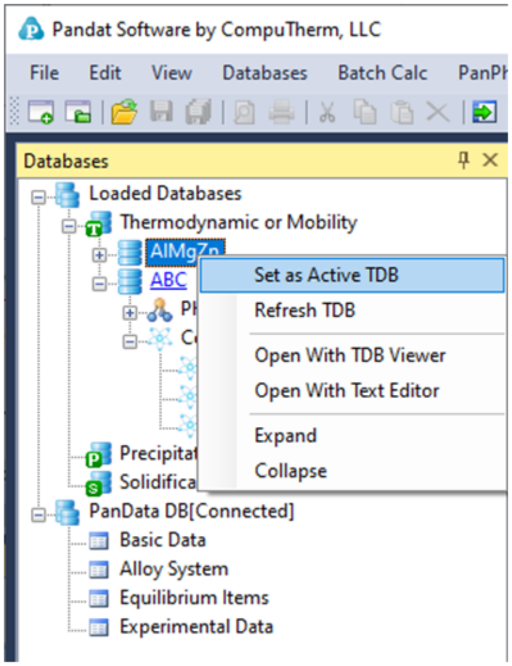


Figure 2.4 Set an active database

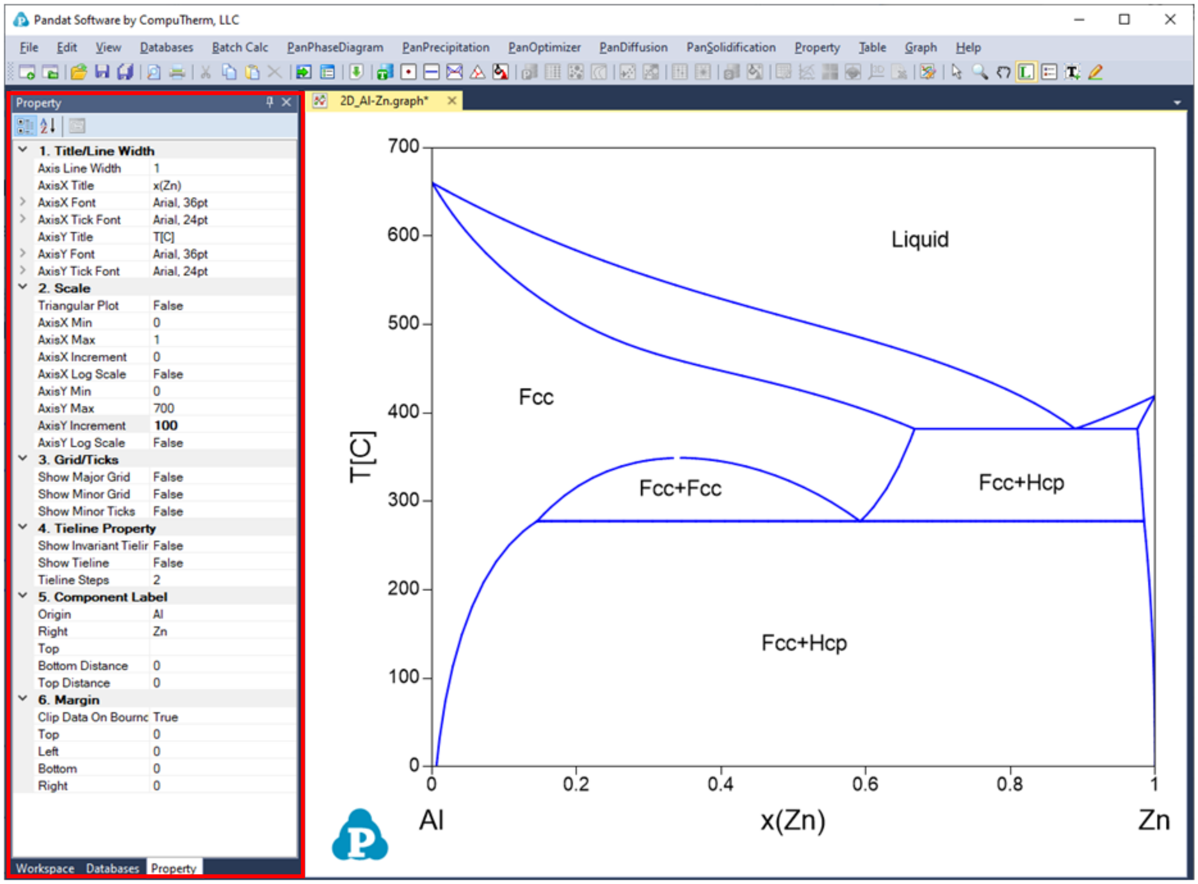
2.3 Graph

In each project, the calculated results are presented in two different formats: Graph and Table. Graph is one of the most important parts in Pandat™ interface. A typical Pandat™ graph includes at least three elements: a set of X and Y coordinate axes, one or more data plots and associated text and drawing objects. Each graph can have one or more data plots and these data plots can be configured individually. Each data plot corresponds to a data set which can be either calculated results or experiment data.

The graph is plotted in the main display window with Pandat™ logo. The Property window defines the properties for all the elements in the graph in detail. When a typical element is selected, the property of this element will be displayed in the Property window and the user may modify the graph through the Property window.

2.3.1 Property

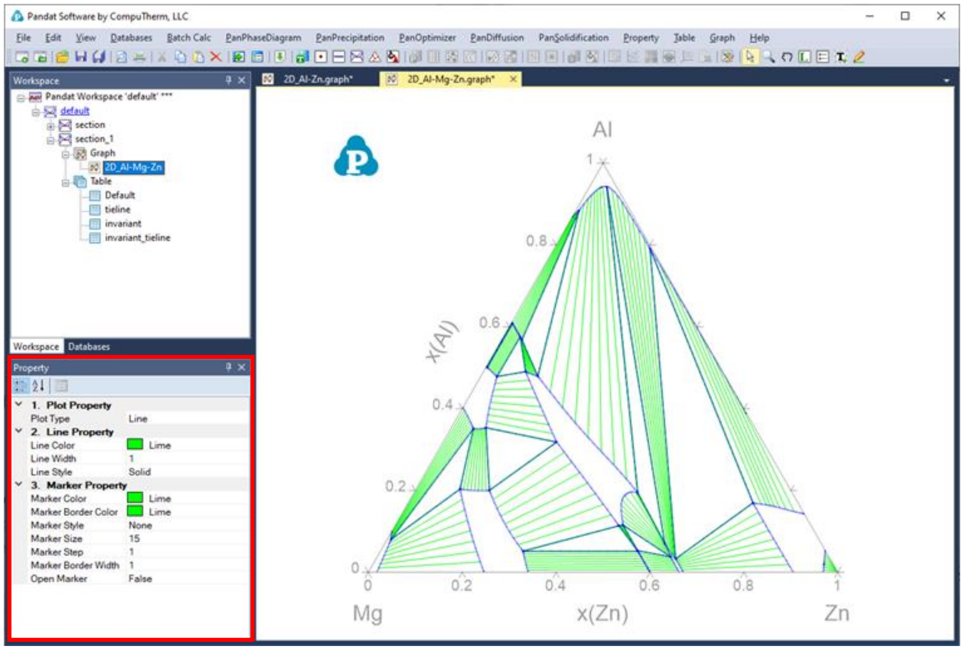
The overall property of a graph consists of six categories: **Title/Line Width**, **Scale**, **Grid/Ticks**, **Tieline Property**, **Component Label** and **Margin**, as shown in the red box area in Figure 2.5. All six categories will be shown in Property window when the whole graph is selected. The Title property defines the axis line width, the title, title font size and tick font size for both X axis and Y axis. The Scale property defines the minimum and maximum values, increment and Log scale status for both X and Y axises and a flag of Ternary Plot. If this flag is set as “True”, the figure is plotted as Gibbs triangle for a normal isothermal section and only the increments are also shown in the Scale property. If the flag is set as “False”, a Cartesian coordinate figure will be plotted. The Grid/Ticks property defines whether to show grids on the graph or ticks on the axis. The Tieline Property defines whether to show the tie-lines and the density of the tie-lines. The Component label defines the labels on the origin, right corner and Top corner of the graph. The Margin property defines the position of the plot in the Main display window.



1. Title/Line Width	
Axis Line Width	1
AxisX Title	x(Zn)
AxisX Font	Arial, 36pt
AxisX Tick Font	Arial, 24pt
AxisY Title	T[C]
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
2. Scale	
Triangular Plot	False
AxisX Min	0
AxisX Max	1
AxisX Increment	0
AxisX Log Scale	False
AxisY Min	0
AxisY Max	700
AxisY Increment	**100**
AxisY Log Scale	False
3. Grid/Ticks	
Show Major Grid	False
Show Minor Grid	False
Show Minor Ticks	False
4. Tieline Property	
Show Invariant Tielir	False
Show Tieline	False
Tieline Steps	2
5. Component Label	
Origin	Al
Right	Zn
Top	
Bottom Distance	0
Top Distance	0
6. Margin	
Clip Data On Bourn	True
Top	0
Left	0
Bottom	0
Right	0

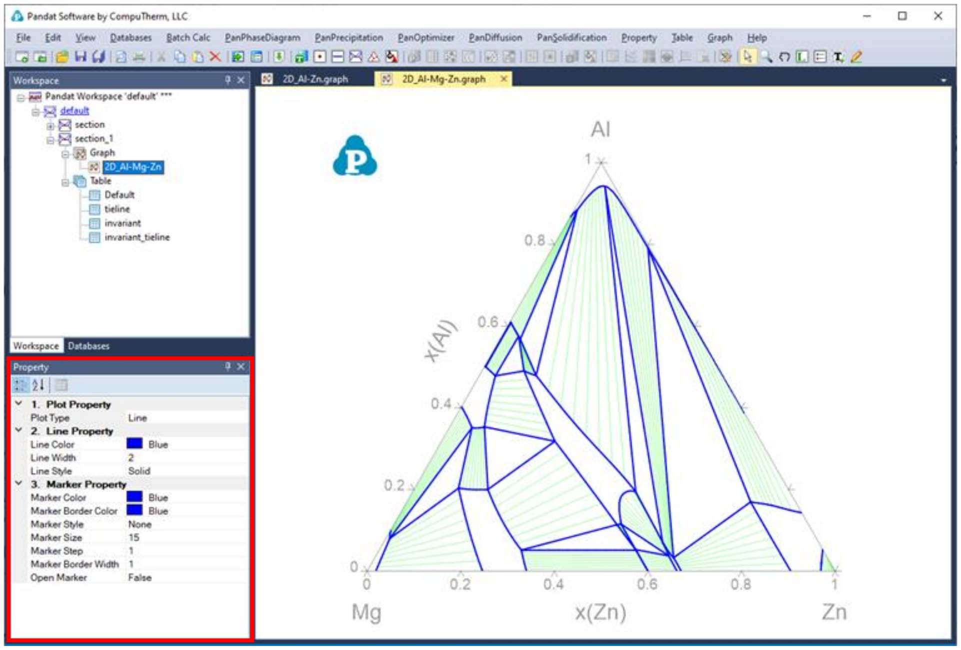
Figure 2.5 Graph property window

The other properties of the tie-lines, such as the color, the style, are defined by individual property window associated with these tie-lines. These properties can be modified when only the tie-lines on the Main Display window are selected and highlighted as shown in Figure 2.6. User can change the appearance of a set of lines belonging to the same group by selecting this line (or a group lines) only. The properties for such data plots, such as the line color, thickness, marker type, will show up in the Property window for user to modify. The data points and lines selected will be highlighted in the graph while the others will be grey. As shown in Figure 2.7, the phase boundary lines are selected as a group of lines to be modified in this case. The properties of this group lines are defined in the **Plot Property** window as “Blue, Solid, None marker” lines. All these properties can be modified in the Property Window as framed by the red line in Figure 2.7. The **Line Property** defines the property of the line and the **Marker Property** defines the property of the point on the graph.



1. Plot Property	
Plot Type	Line
2. Line Property	
Line Color	🟩 Lime
Line Width	1
Line Style	Solid
3. Marker Property	
Marker Color	🟩 Lime
Marker Border Color	🟩 Lime
Marker Style	None
Marker Size	15
Marker Step	1
Marker Border Width	1
Open Marker	False

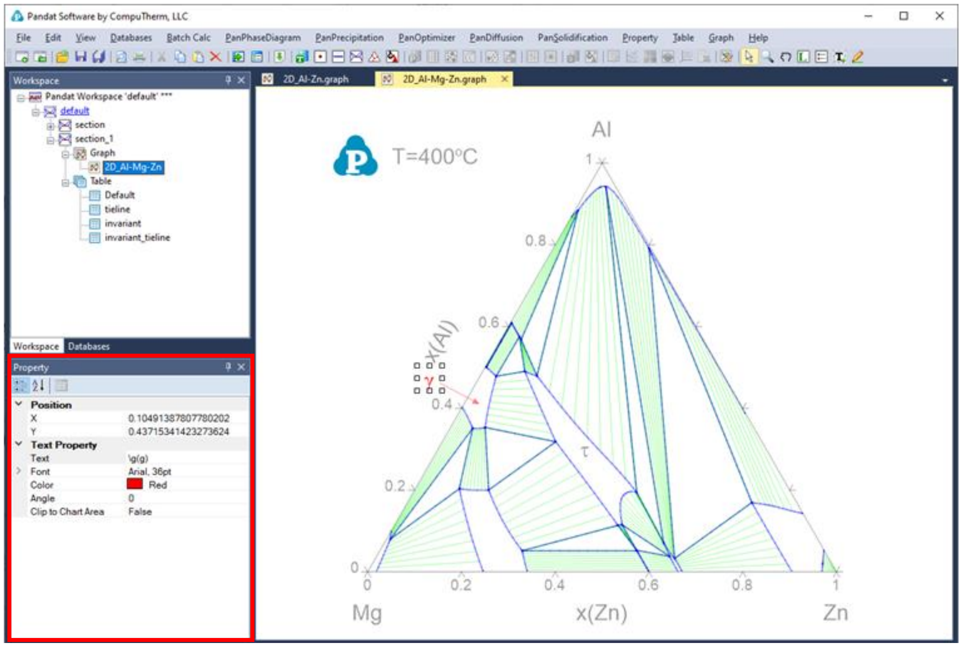
Figure 2.6 Tie-line property window



1. Plot Property	
Plot Type	Line
2. Line Property	
Line Color	🟦 Blue
Line Width	2
Line Style	Solid
3. Marker Property	
Marker Color	🟦 Blue
Marker Border Color	🟦 Blue
Marker Style	None
Marker Size	15
Marker Step	1
Marker Border Width	1
Open Marker	False

Figure 2.7 Plot property window

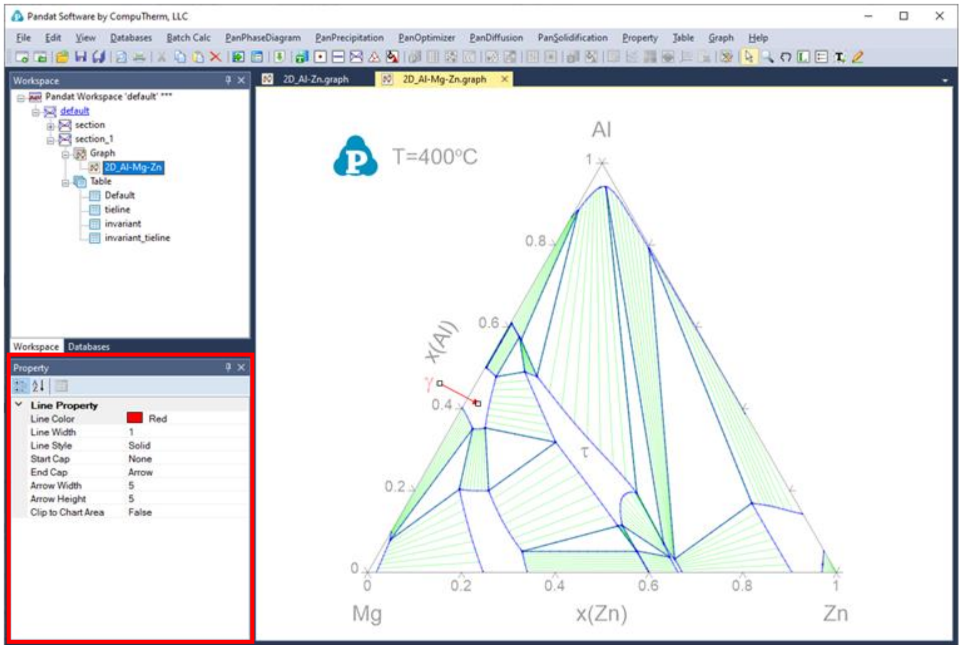
User can add texts and lines/arrows freely to the graph. The **Text Property** defines the position, content, font size, color and rotating angle of the text, as shown in the red box in Figure 2.8 when the text box is selected. The **Line Property** defines the color, width, start cap and end cap of the line as shown in the red box in Figure 2.9 when the line/arrow is selected.



Property

Position	
X	0.10491387807780202
Y	0.43715341423273624
Text Property	
Text	\g(g)
Font	Arial, 36pt
Color	🟥 Red
Angle	0
Clip to Chart Area	False

Figure 2.8 Text Property window



Property

Line Property	
Line Color	🟥 Red
Line Width	1
Line Style	Solid
Start Cap	None
End Cap	Arrow
Arrow Width	5
Arrow Height	5
Clip to Chart Area	False

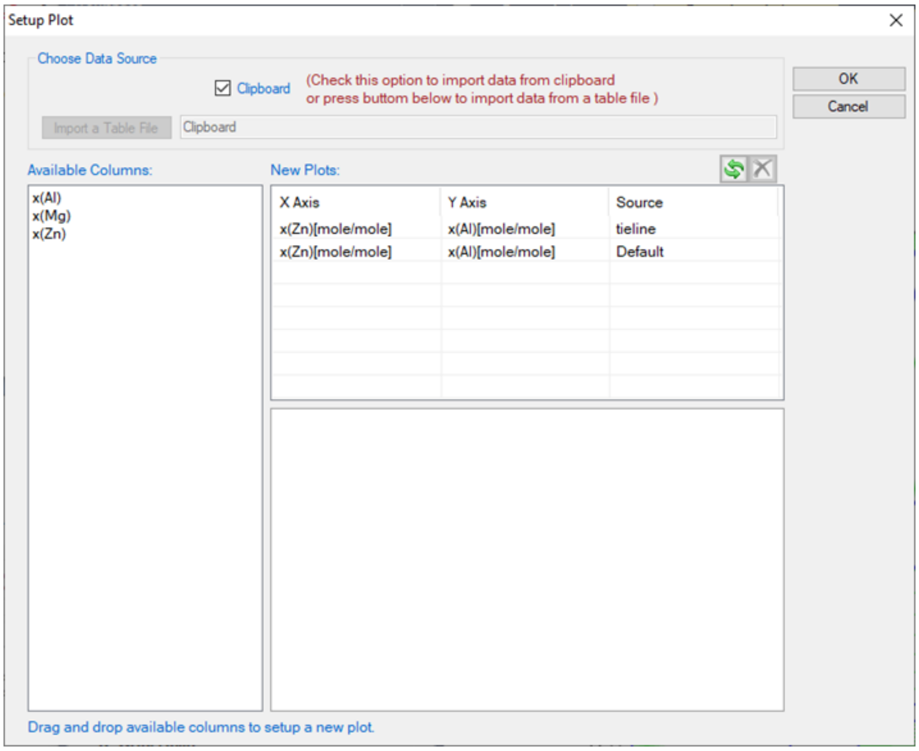
Figure 2.9 Line Property window for added line

2.3.2 Export a graph to other format

The user can output the Pandat graph to other popular formats such as emf, bmp, jpg, png, gif and tif. The command is located on the menus: **Graph → Export**, or right click the mouse on the graph and choose “Export” from the popup menu.

2.3.3 Useful icons for Graph on Toolbar

Edit Plots for the Current Graph button , allow the user to modify the plots, such as add data plots with mouse drag and drop to set up x and y of the new plot as shown in Figure 2.10, delete data plots using button , exchange x and y of the plots using button . The available columns can be imported from a file or from Clipboard if the check box in front is selected.



☑ Clipboard (Check this option to import data from clipboard or press buttom below to import data from a table file)

Clipboard

x(Al)
x(Mg)
x(Zn)

X Axis	Y Axis	Source
x(Zn)[mole/mole]	x(Al)[mole/mole]	tieline
x(Zn)[mole/mole]	x(Al)[mole/mole]	Default

Drag and drop available columns to setup a new plot.

Figure 2.10 Set up data for X and Y for a plot

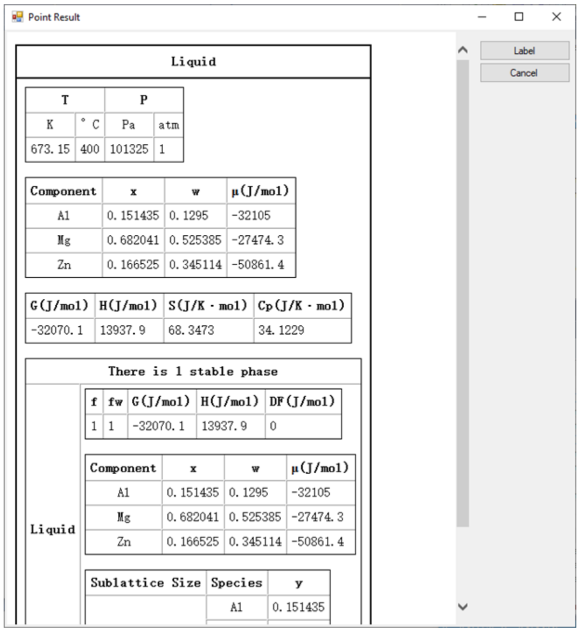
The table file to be imported can be Pandat™ table format or ASCII text format. For a general Microsoft Excel table, the user can copy the selected columns in the Excel file and check the Clipboard option, and then the column names will show up in the "Available Columns" dialog for the user to select, which is also shown in Figure 2.10. User can also copy the data from the table columns in the Pandat™ calculation results.

Select Objects button ↖, allow the user to select drawing elements in a graph such as line, arrow or text.

Zoom Mode button 🔍, use the Zoom mode to enlarge a small part of a graph. Hold the left button of the mouse and move the mouse to select a rectangular area on the graph to enlarge. The graph will zoom in to the selected area when the left button of the mouse is released. Double click this button will bring the zoom image back to the whole diagram again.

Pan Mode button ✋, when this mode is on, put the cursor on the plot and roll the mouse wheel to enlarge or shrink the graph, keeping the current center of the graph unchanged. Hold the left button of the mouse on the graph and move the mouse, the user can move the whole graph.

Label Phase Region button☑, label the graph with text. Pandat™ can not only label the normal T-x or x-x phase diagrams from calculations, but also label those user generated graphs using the table data from calculation, i.e., G-x and μ-x diagrams. The user can modify the labeled text like normal text. If the user holds the <Ctrl> key first and then click the mouse on the diagram with the ☑ function, the program will do a point calculation at the composition and temperature where the cursor locates. A new window will pop out to show the calculated result in detail as shown in Figure 2.11. The user can choose **Label** after reading or **Cancel** to close this window.



Liquid

T		P	
K	° C	Pa	atm
673.15	400	101325	1

Component	x	w	μ(J/mol)
Al	0.151435	0.1295	-32105
Mg	0.682041	0.525385	-27474.3
Zn	0.166525	0.345114	-50861.4

G(J/mol)	H(J/mol)	S(J/K · mol)	Cp(J/K · mol)
-32070.1	13937.9	68.3473	34.1229

There is 1 stable phase

Liquid

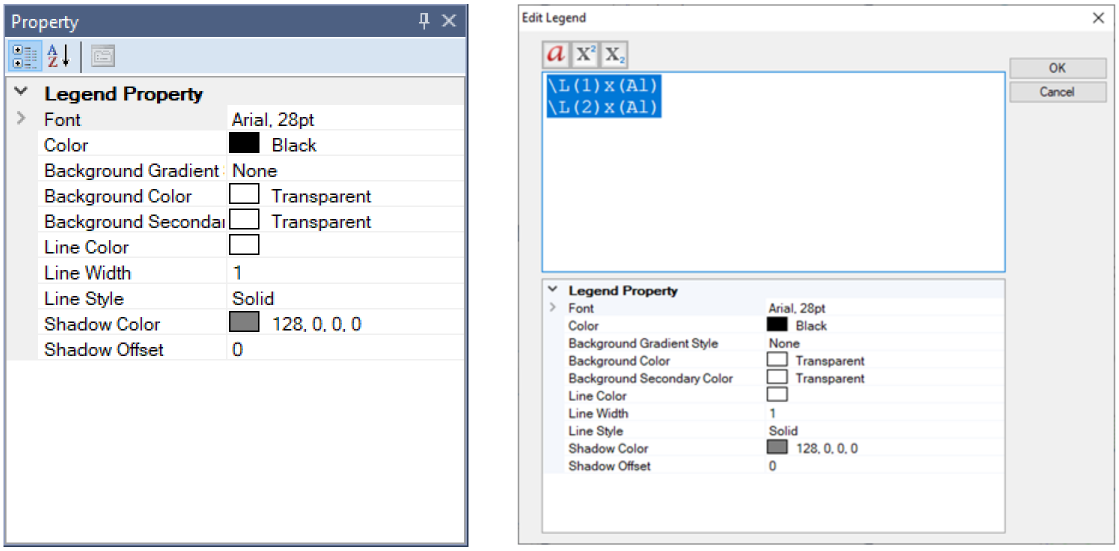
f	fw	G(J/mol)	H(J/mol)	DF(J/mol)
1	1	-32070.1	13937.9	0

Component	x	w	μ(J/mol)
Al	0.151435	0.1295	-32105
Mg	0.682041	0.525385	-27474.3
Zn	0.166525	0.345114	-50861.4

Sublattice	Size	Species	y
		Al	0.151435

Figure 2.11 Point calculation result for the combination of the “Ctrl” key and Labeling function

Add Legend for Graph button , add legend to the graph. The user can modify the legend using the Property window, as shown in Figure 2.12(a). Double click on the inserted legend will open a new Text Editor window as shown in Figure 2.12(b), and the user can input complex text, such as symbol, superscript and subscript in this windows.



Legend Property

Font	Arial, 28pt
Color	■ Black
Background Gradient	None
Background Color	☐ Transparent
Background Secondai	☐ Transparent
Line Color	☐
Line Width	1
Line Style	Solid
Shadow Color	■ 128, 0, 0, 0
Shadow Offset	0

```
\L(1)x(Al)
\L(2)x(Al)
```

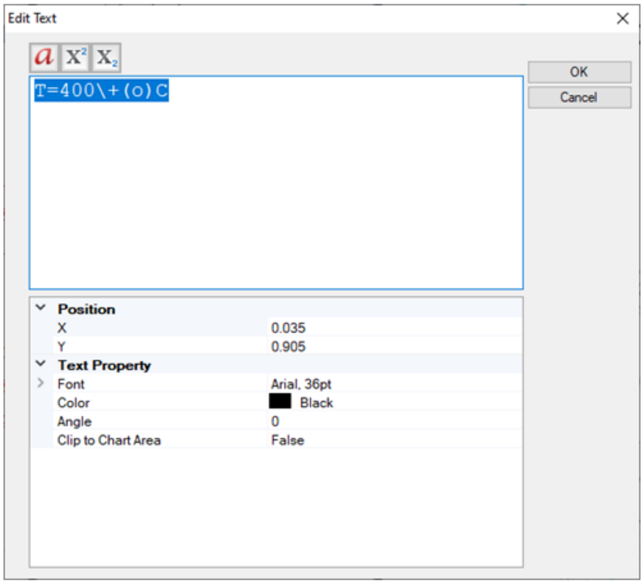
Legend Property

Font	Arial, 28pt
Color	■ Black
Background Gradient Style	None
Background Color	☐ Transparent
Background Secondary Color	☐ Transparent
Line Color	☐
Line Width	1
Line Style	Solid
Shadow Color	■ 128, 0, 0, 0
Shadow Offset	0

(a) (b)

Figure 2.12 (a) Legend property window and (b) Legend editor window

Add Text or Label button, add text to the graph. Change the text content, size, color and rotating angle in the Property window. Double click on the text also open the Text Editor window which allows user to input complex text in it as shown in Figure 2.13.



T=400\+(o)C

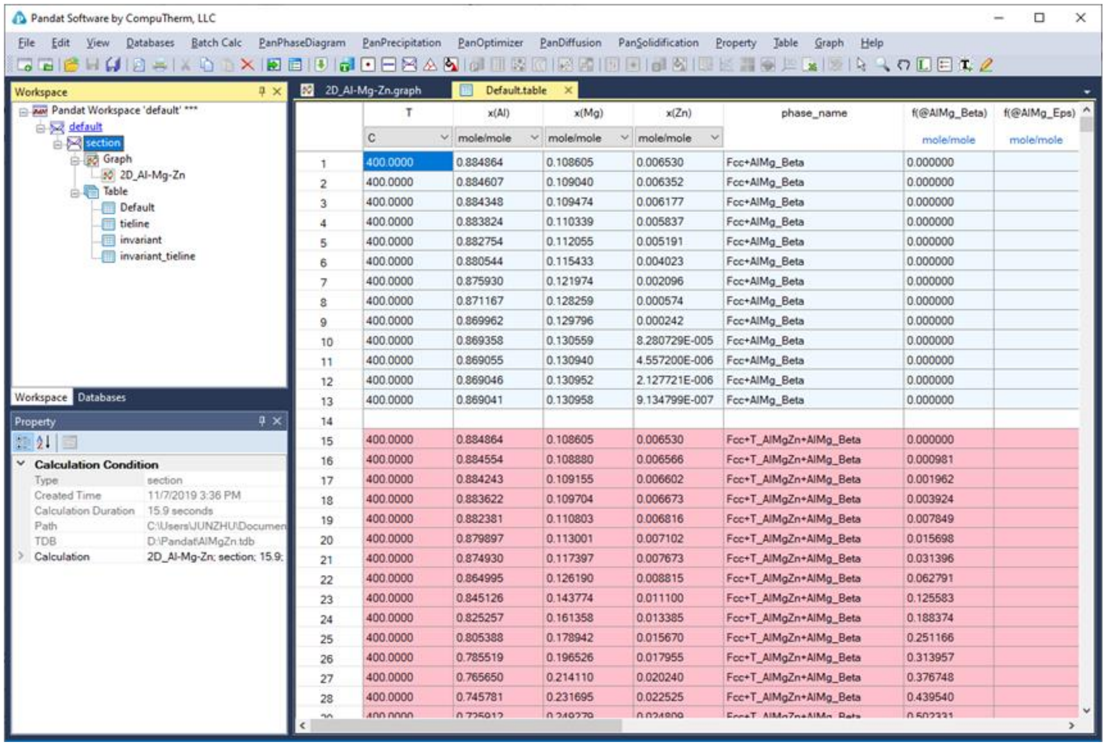
Position	
X	0.035
Y	0.905
Text Property	
Font	Arial, 36pt
Color	■ Black
Angle	0
Clip to Chart Area	False

Figure 2.13 Text editor window

Add Line button, add line with or without arrow to the graph. Change the line or arrow width and color in the Property window. The default line has one arrow at end of the line. User can set the start cap and end cap in the Line Property window as shown in Figure 2.9.

2.4 Table

The menu of Pandat™ **Table** includes: **Add a New Table**, **Import Table from File**, **Create Graph**, and **Export to Excel**. A typical table is shown as Figure 2.14. Each column of data is associated with a corresponding unit. The user can change the unit of each column and observe the instant change of the table values.



Calculation Condition

Type: section
Created Time: 11/7/2019 3:36 PM
Calculation Duration: 15.9 seconds
Path: C:\Users\JUNZHU\Documen
TDB: D:\Pandat\AlMgZn.tdb
Calculation: 2D_Al-Mg-Zn; section; 15.9;

	T	x(Al)	x(Mg)	x(Zn)	phase_name	f(@AlMg_Beta)	f(@AlMg_Eps)
	C	mole/mole	mole/mole	mole/mole		mole/mole	mole/mole
1	400.0000	0.884864	0.108605	0.006530	Fcc+AlMg_Beta	0.000000	
2	400.0000	0.884607	0.109040	0.006352	Fcc+AlMg_Beta	0.000000	
3	400.0000	0.884348	0.109474	0.006177	Fcc+AlMg_Beta	0.000000	
4	400.0000	0.883824	0.110339	0.005837	Fcc+AlMg_Beta	0.000000	
5	400.0000	0.882754	0.112055	0.005191	Fcc+AlMg_Beta	0.000000	
6	400.0000	0.880544	0.115433	0.004023	Fcc+AlMg_Beta	0.000000	
7	400.0000	0.875930	0.121974	0.002096	Fcc+AlMg_Beta	0.000000	
8	400.0000	0.871167	0.128259	0.000574	Fcc+AlMg_Beta	0.000000	
9	400.0000	0.869962	0.129796	0.000242	Fcc+AlMg_Beta	0.000000	
10	400.0000	0.869358	0.130559	8.280729E-005	Fcc+AlMg_Beta	0.000000	
11	400.0000	0.869055	0.130940	4.557200E-006	Fcc+AlMg_Beta	0.000000	
12	400.0000	0.869046	0.130952	2.127721E-006	Fcc+AlMg_Beta	0.000000	
13	400.0000	0.869041	0.130958	9.134799E-007	Fcc+AlMg_Beta	0.000000	
14							
15	400.0000	0.884864	0.108605	0.006530	Fcc+T_AlMgZn+AlMg_Beta	0.000000	
16	400.0000	0.884554	0.108880	0.006566	Fcc+T_AlMgZn+AlMg_Beta	0.000981	
17	400.0000	0.884243	0.109155	0.006602	Fcc+T_AlMgZn+AlMg_Beta	0.001962	
18	400.0000	0.883622	0.109704	0.006673	Fcc+T_AlMgZn+AlMg_Beta	0.003924	
19	400.0000	0.882381	0.110803	0.006816	Fcc+T_AlMgZn+AlMg_Beta	0.007849	
20	400.0000	0.879897	0.113001	0.007102	Fcc+T_AlMgZn+AlMg_Beta	0.015698	
21	400.0000	0.874930	0.117397	0.007673	Fcc+T_AlMgZn+AlMg_Beta	0.031396	
22	400.0000	0.864995	0.126190	0.008815	Fcc+T_AlMgZn+AlMg_Beta	0.062791	
23	400.0000	0.845126	0.143774	0.011100	Fcc+T_AlMgZn+AlMg_Beta	0.125583	
24	400.0000	0.825257	0.161358	0.013385	Fcc+T_AlMgZn+AlMg_Beta	0.188374	
25	400.0000	0.805388	0.178942	0.015670	Fcc+T_AlMgZn+AlMg_Beta	0.251166	
26	400.0000	0.785519	0.196526	0.017955	Fcc+T_AlMgZn+AlMg_Beta	0.313957	
27	400.0000	0.765650	0.214110	0.020240	Fcc+T_AlMgZn+AlMg_Beta	0.376748	
28	400.0000	0.745781	0.231695	0.022525	Fcc+T_AlMgZn+AlMg_Beta	0.439540	

Figure 2.14 Table view of the calculation results in Pandat™

2.4.1 Useful icons for Table on Toolbar

Add a New Table button, click this button or right click the mouse on the Table node in the Explore window and select "Add a New Table", a window of Table Editor as shown in Figure 2.15 will pop out. User can create a new table by dragging and dropping the available properties in the left dialog to the right dialog as shown by the red arrow in Figure 2.15, and then click "**OK**" to generate a new table with the selected properties.

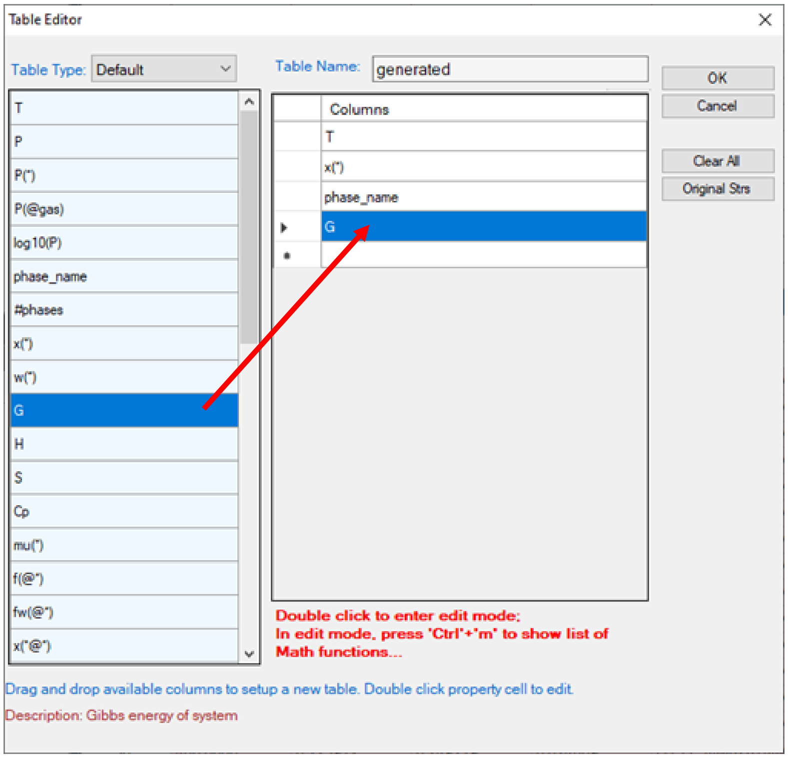


Table Type: Default

Table Name: generated

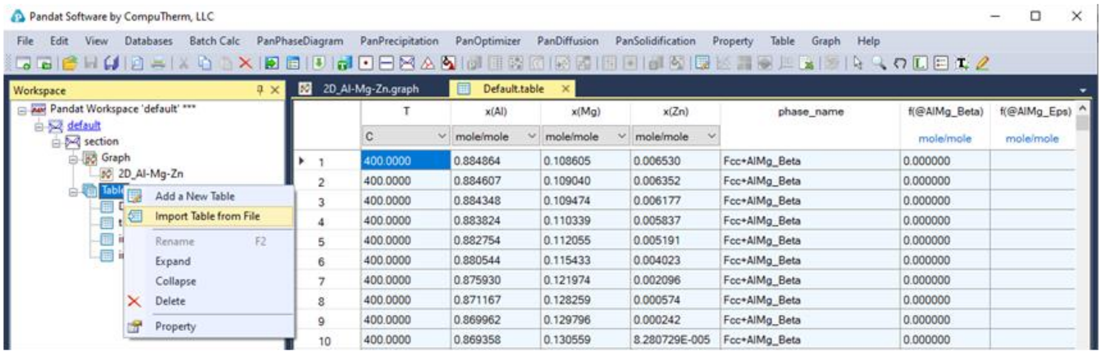
Double click to enter edit mode;
In edit mode, press 'Ctrl'+'m' to show list of Math functions...

Drag and drop available columns to setup a new table. Double click property cell to edit

Description: Gibbs energy of system

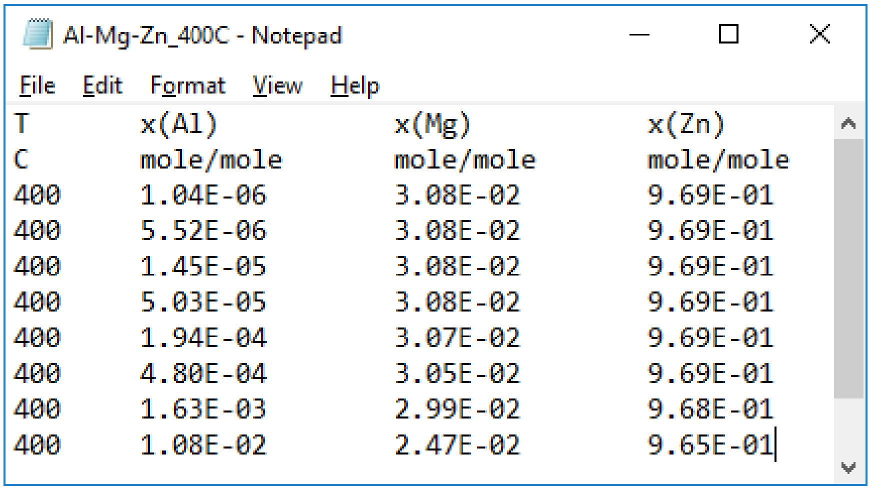
Figure 2.15 Table Editor

<u>Import Table from File</u>, User can import a customized table from an existing file. This can be done by choosing the command located on the menus: **<u>Table → Import Table from File</u>**, or right click the mouse on the Table node and choose “Import Table from File” from the popup menu as shown in Figure 2.16. Pandat™ can read data files with “.dat” and “.txt” as default file extension names. Figure 2.17 shows a typical data file for importing into Pandat™. Different columns are separated by Tabs. The first row defines the data name for each column. The second row defines the unit for the data in each column and the following rows define the data values. If the column names are the same as those in the default table, the second row (the unit row) can be blank and Pandat™ will use the same units as those in the default table.



	T	x(Al)	x(Mg)	x(Zn)	phase_name	f(@AlMg_Beta)	f(@AlMg_Eps)
	C	mole/mole	mole/mole	mole/mole		mole/mole	mole/mole
1	400.0000	0.884864	0.108605	0.006530	Fcc+AlMg_Beta	0.000000	
2	400.0000	0.884607	0.109040	0.006352	Fcc+AlMg_Beta	0.000000	
3	400.0000	0.884348	0.109474	0.006177	Fcc+AlMg_Beta	0.000000	
4	400.0000	0.883824	0.110339	0.005837	Fcc+AlMg_Beta	0.000000	
5	400.0000	0.882754	0.112055	0.005191	Fcc+AlMg_Beta	0.000000	
6	400.0000	0.880544	0.115433	0.004023	Fcc+AlMg_Beta	0.000000	
7	400.0000	0.875930	0.121974	0.002096	Fcc+AlMg_Beta	0.000000	
8	400.0000	0.871167	0.128259	0.000574	Fcc+AlMg_Beta	0.000000	
9	400.0000	0.869962	0.129796	0.000242	Fcc+AlMg_Beta	0.000000	
10	400.0000	0.869358	0.130559	8.280729E-005	Fcc+AlMg_Beta	0.000000	

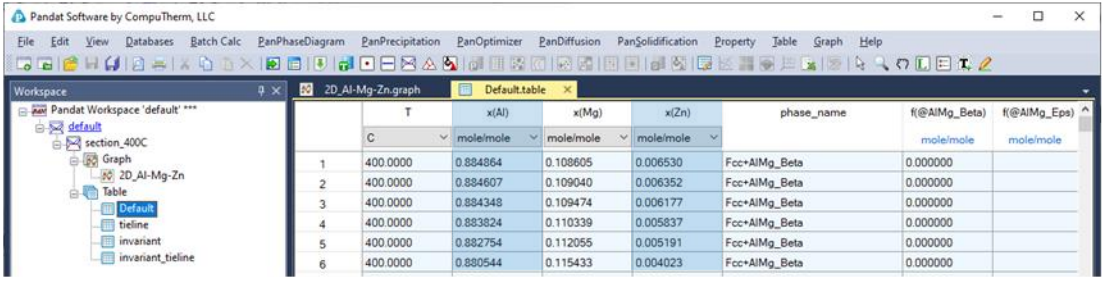
Figure 2.16 Import a table from an existing file



```
T       x(Al)           x(Mg)           x(Zn)
C       mole/mole       mole/mole       mole/mole
400     1.04E-06        3.08E-02        9.69E-01
400     5.52E-06        3.08E-02        9.69E-01
400     1.45E-05        3.08E-02        9.69E-01
400     5.03E-05        3.08E-02        9.69E-01
400     1.94E-04        3.07E-02        9.69E-01
400     4.80E-04        3.05E-02        9.69E-01
400     1.63E-03        2.99E-02        9.68E-01
400     1.08E-02        2.47E-02        9.65E-01
```

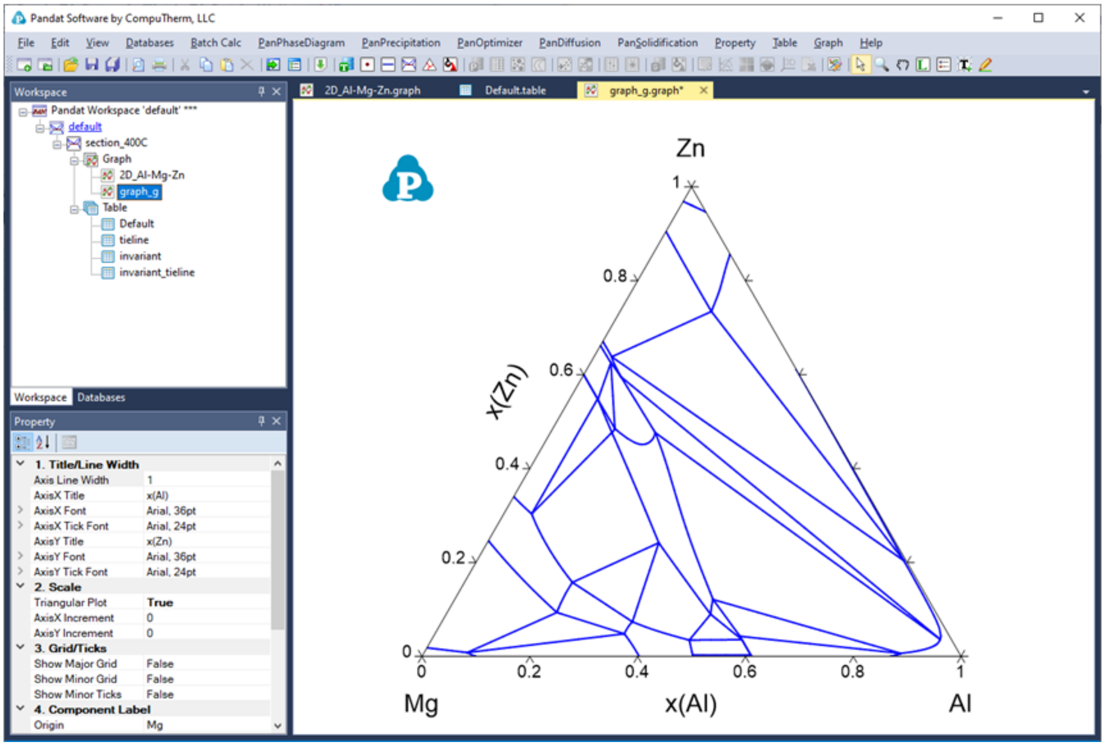
Figure 2.17 A typical data file for importing

Create Graph button , create a new graph for the selected properties. Use the <ctrl> key and the left button of the mouse to select multiple columns in the table as shown in Figure 2.18. The first selected column will be the x and the other columns will be the y's for the new plots. After click on the button, a graph will then be generated in the Pandat™ main display window as shown in Figure 2.19.



	T	x(Al)	x(Mg)	x(Zn)	phase_name	f(@AlMg_Beta)	f(@AlMg_Eps)
	C	mole/mole	mole/mole	mole/mole		mole/mole	mole/mole
1	400.0000	0.884864	0.108605	0.006530	Fcc+AlMg_Beta	0.000000	
2	400.0000	0.884607	0.109040	0.006352	Fcc+AlMg_Beta	0.000000	
3	400.0000	0.884348	0.109474	0.006177	Fcc+AlMg_Beta	0.000000	
4	400.0000	0.883824	0.110339	0.005837	Fcc+AlMg_Beta	0.000000	
5	400.0000	0.882754	0.112055	0.005191	Fcc+AlMg_Beta	0.000000	
6	400.0000	0.880544	0.115433	0.004023	Fcc+AlMg_Beta	0.000000	

Figure 2.18 Select data for creating a new graph



1. Title/Line Width	
Axis Line Width	1
AxisX Title	x(Al)
AxisX Font	Arial, 36pt
AxisX Tick Font	Arial, 24pt
AxisY Title	x(Zn)
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
2. Scale	
Triangular Plot	**True**
AxisX Increment	0
AxisY Increment	0
3. Grid/Ticks	
Show Major Grid	False
Show Minor Grid	False
Show Minor Ticks	False
4. Component Label	
Origin	Mg

Figure 2.19 A new graph created from selected columns in the table

Create Color Map button, create a new color map graph for the selected properties. Use the "ctrl" key and the left button of the mouse to select multiple columns in the table as shown in Figure 2.20. The first selected column (x(Mg)) will be the x's, the second column (x(Zn)) will be the y's and the third column (T) will be the z's for the new plot. After click on the button, a color map graph will then be generated in the Pandat™ main display window as shown in Figure 2.21, where the liquidus temperatures are represented by different colors.

	T	x(Al)	x(Mg)	x(Zn)	phase_name
	C	mole/mole	mole/mole	mole/mole	
1	382.0305	0.110828	0.000000	0.889172	Liquid+Hcp+Fcc
2	381.5659	0.110287	0.001000	0.888713	Liquid+Hcp+Fcc
3	381.0960	0.109748	0.002000	0.888252	Liquid+Hcp+Fcc
4	380.1405	0.108679	0.004000	0.887321	Liquid+Hcp+Fcc
5	378.1663	0.106569	0.008000	0.885431	Liquid+Hcp+Fcc
6	373.9677	0.102459	0.016000	0.881541	Liquid+Hcp+Fcc
7	364.5839	0.094628	0.032000	0.873372	Liquid+Hcp+Fcc
8	353.9124	0.087229	0.048000	0.864771	Liquid+Hcp+Fcc
9	348.1032	0.083663	0.056000	0.860337	Liquid+Hcp+Fcc
10	345.0816	0.081908	0.060000	0.858092	Liquid+Hcp+Fcc

Figure 2.20 Select data to create a new color map graph

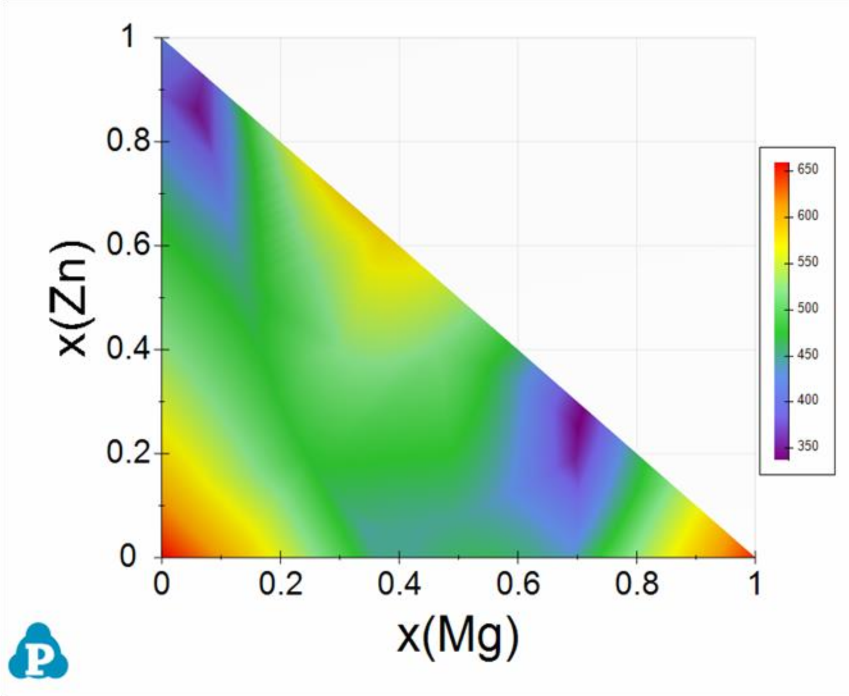


Figure 2.21 A new color map graph created from selected columns in the isotherm table from the liquidus projection calculation

Create 3D Surface Graph button , create a new 3D surface graph for the selected properties. Use the “ctrl” key and the left button of the mouse to select multiple columns in the table as shown in Figure 2.20. The first selected column will be the x’s, the second column will be the y’s and the third column will be the z’s for the new plot. After click on the button, a 3D liquidus surface graph will then be generated in the Pandat™ main display window as shown in Figure 2.22.

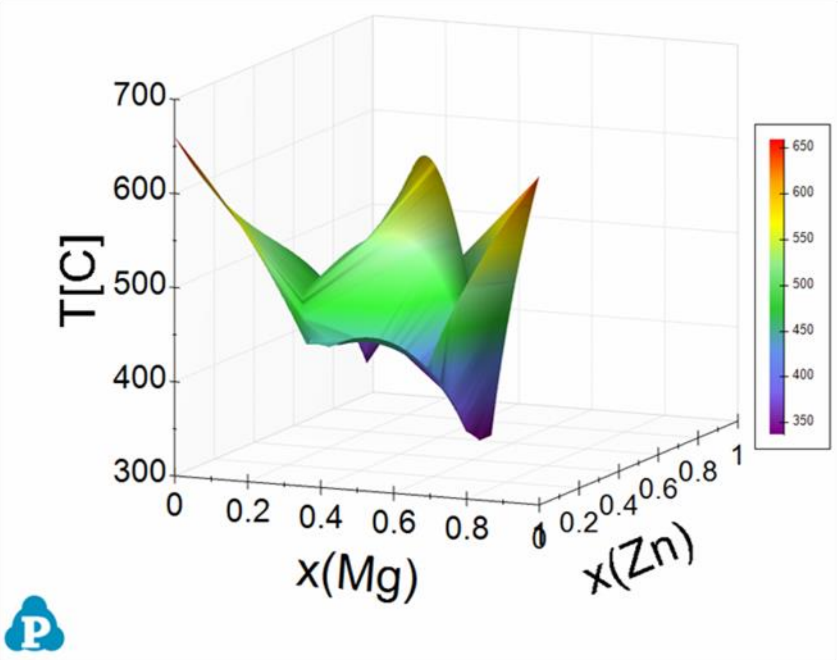
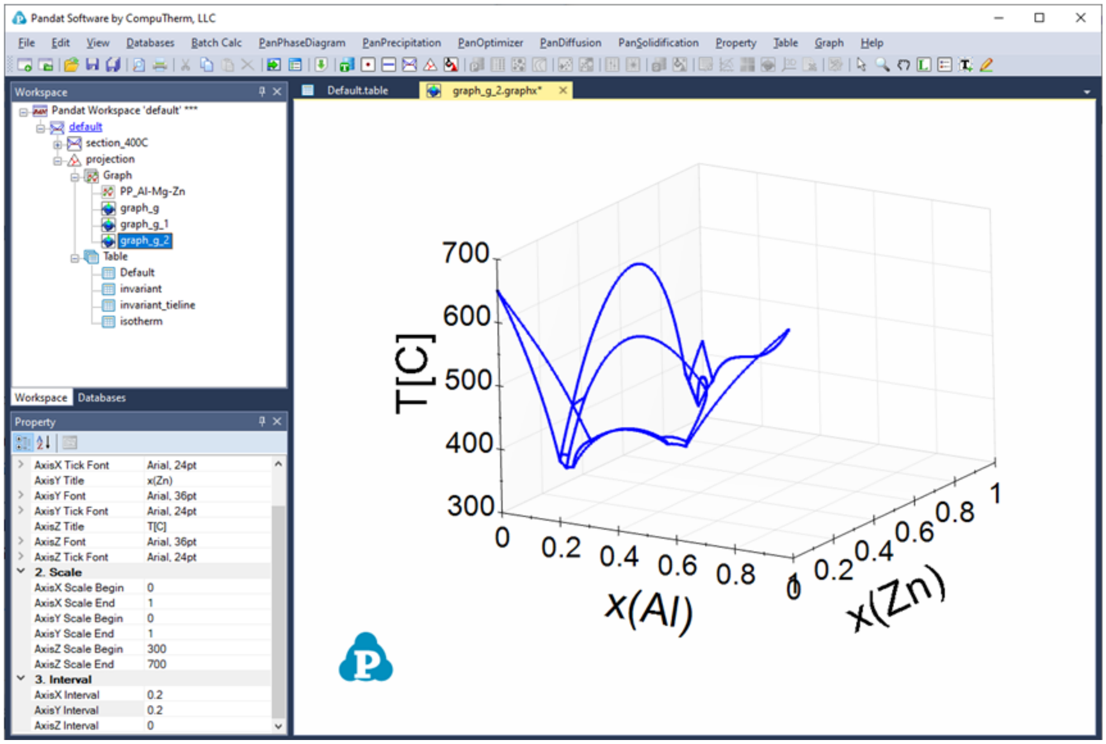


Figure 2.22 A new 3D liquidus surface graph created from selected columns in the isotherm table from the liquidus projection calculation

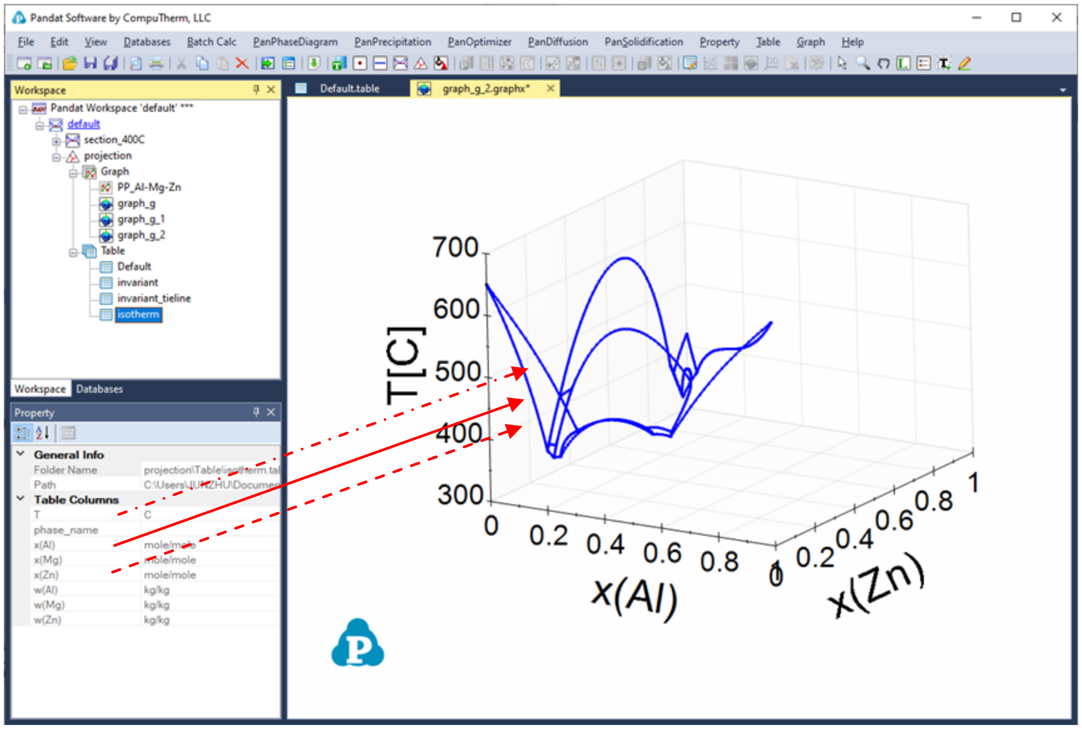
Create 3D Graph button 3D, create a new 3D graph for the selected properties. Use the "ctrl" key and the left button of the mouse to select multiple columns in the table as shown in Figure 2.20. The first selected column will be the x's, the second column will be the y's and the third column will be the z's for the new plot. After click on the 3D button, a 3D graph will then be generated in the Pandat™ main display window as shown in Figure 2.23 representing the monovariant lines of the liquidus projection.



AxisX Tick Font	Arial, 24pt
AxisY Title	x(Zn)
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
AxisZ Title	T[C]
AxisZ Font	Arial, 36pt
AxisZ Tick Font	Arial, 24pt
2. Scale	
AxisX Scale Begin	0
AxisX Scale End	1
AxisY Scale Begin	0
AxisY Scale End	1
AxisZ Scale Begin	300
AxisZ Scale End	700
3. Interval	
AxisX Interval	0.2
AxisY Interval	0.2
AxisZ Interval	0

Figure 2.23 A new 3D graph created from selected columns in the table

User can add more plots to the 3D graph. First click on the table containing the data, i.e. isotherm data in Figure 2.24, and the property window will show the column names in this table. Then select the column "x(Al)" as x-axis in the property window, drag and drop it to the graph; then hold the "Ctrl" key and select the second column "x(Zn)" as y-axis, drag and drop it to the graph; and then hold the "Shift" key, select the third column "T", drag and drop it to the graph. The new plot of the data will be added to the original 3D graph shown as Figure 2.25.



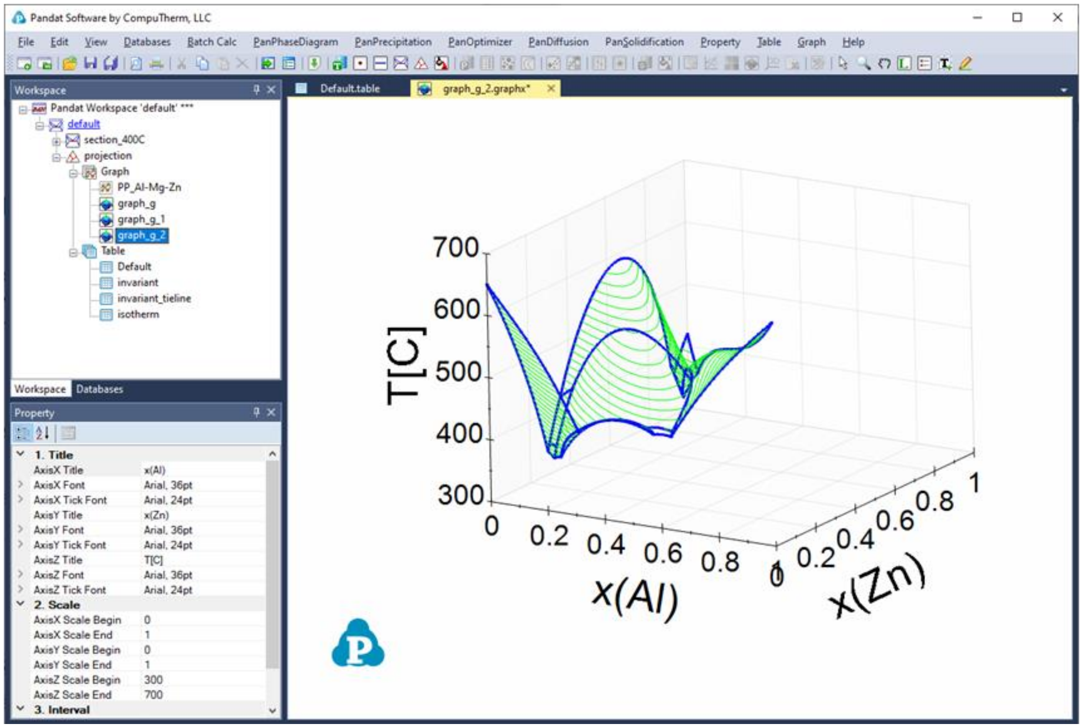
General Info

Folder Name	projection\Table\isotherm.tal
Path	C:\Users\JUNZHU\Documen

Table Columns

T	C
phase_name	
x(Al)	mole/mole
x(Mg)	mole/mole
x(Zn)	mole/mole
w(Al)	kg/kg
w(Mg)	kg/kg
w(Zn)	kg/kg

Figure 2.24 Add a plot to a 3D graph using selected columns in the table as follows: (1) Solid arrow: drag and drop, (2) Dash arrow: drag and drop with the "Ctrl" key held, (3) Dash dot arrow: drag and drop with the "Shift" key held



1. Title

AxisX Title	x(Al)
AxisX Font	Arial, 36pt
AxisX Tick Font	Arial, 24pt
AxisY Title	x(Zn)
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
AxisZ Title	T[C]
AxisZ Font	Arial, 36pt
AxisZ Tick Font	Arial, 24pt

2. Scale

AxisX Scale Begin	0
AxisX Scale End	1
AxisY Scale Begin	0
AxisY Scale End	1
AxisZ Scale Begin	300
AxisZ Scale End	700

3. Interval

Figure 2.25 3D graph with multiple plots

Export to Excel button , allow user to export the table of interest (It must be available in main display windows to activate the function button) directly to a Microsoft Excel file. Excel must be pre-installed in the user's computer.

2.4.2 Table format syntax

Pandat table column lists a series of property string switch that can be used to extract the corresponding properties from the calculation results. A property string can be simply a property name (e.g. T, P, G, H, and S) or an expression including property name and special symbols (e.g mu(Mg@Fcc)). Generally, a property string has the following format:

```
Z(component@phase:reference_phase[component])
```

Or in a simple form as

```
Z(*@*:ref_ph[*])
```

where Z is the property name and "*" represents a wild card which can be phases, components, or species. The first "*" after "(" is the name of a selected component or species. If "*" is used, it means all the components or species in the system. The second "*" represents the name of the selected phase, which must follow "@". Again, if "*" is used, it means all the phases. For example, x(*@*) means to list the composition of every element in every phase. The colon ":" is used for defining reference states. The reference phase name "`ref_ph`" must be given explicitly and the wild card "*" cannot be used for the names of reference phases. It should be pointed out that different element can have different reference state. For example, a(*@*:Fcc[Al],Hcp[Zn]) means that Al uses fcc as its reference state and Zn uses hcp as its reference state. Similarly, a(*@*:Fcc[*],Hcp[Zn]) means Hcp is selected as the reference state of Zn, while Fcc is selected for all the other components in the system.

If the property string has the following format:

```
Z(@*:ref_ph[*])
```

i.e., no component or species is specified, and the first "`*`" after "`(`" is missing, it defines the property of a phase or phases. For example, H(@Liquid) means the enthalpy of the liquid phase, and H(@*) lists enthalpies of all the phases in the system. If the reference state is not specified, it means to refer to the default reference state defined in the database which is usually the standard element reference state. When the reference state is selected, H(@Liquid:Fcc[Al],Hcp[Zn]) represents the mixing enthalpy of liquid phase referring to Fcc Al and Hcp Zn at the same temperature.

If the property string has the following format:

```
Z(:ref_ph[*])
```

i.e., both component and phase names are missing; it represents the property of the system. For example, `G(:Fcc[*])`represents the Gibbs energy of the system (equilibrium phases) referring to Fcc phase.

It is worth to pointing out that the wild card "*" is very convenient to extract properties for all the components and all the phases, especially in multicomponent, multiphase system. It should also point out that if no reference states are specified, it refers to the default reference state used in the database. Table 2.1 lists the syntaxes in the **Table** format.

Table 2.1 Table Format Syntax (commonly used properties)

Syntax	Meaning	Note and Example
`T`	Temperature	Temperature can be in Celsius, Kelvin, or Fahrenheit. The unit can be changed/selected in the row below symbol T and the values updated instantly
`phase_name`	Names of phases that are in equilibrium	Liquid+Fcc means two phases are in equilibrium, one is Liquid and the other is Fcc
`#phases`	Number of phases in equilibrium	
`f(@*), fw(@*)`	Molar fraction(s) and weight fraction(s)of a phase or phases	`f(@Fcc)`:molar fraction of Fcc phase `f(@*)`:molar fraction of every phase

		in equilibrium
`x(*), w(*)`	Nominal composition of an alloy in molar fraction or weight fraction	Fraction can be easily converted to percentage by selecting % from the unit row in the table
`x(*@*), w(*@*)`	Composition of a phase or every phase in equilibrium in molar fraction or weight fraction	`w(*@Liquid)`:composition of the Liquid phase in weight fraction `w(*@*)`:composition of every phase in equilibrium in weight fraction
`y(*@*)`	Site fraction of species in every sublattice for a specified phase or for every phase in equilibrium. If a phase has only one sublattice, it lists the composition of the phase; if a phase has two or more sublattices, it lists the site fraction of every component in every sublattice. If a component does not occupy a certain sublattice, the site fraction of this component will not be listed in that sublattice	`y(AL@*)`:site fraction of AL in every sublattice of every phase `y(*@Beta)`:site fraction of every component in every sublattice in Beta phase `y(*@*)`:site fraction of every component in every sublattice in every phase in equilibrium
`G, H, S, Cp`	Gibbs energy, enthalpy, entropy and heat capacity of the system in the equilibrium state. The equilibrium state may include one phase or a mixture of phases	The listed Gibbs energy, enthalpy, and entropy are the properties of one mole atoms refer to the default reference state defined in the database. If the Gibbs energies of pure components are from SGTE substance database, the default reference state is GHS298

`G(:ref_ph[*]),`
`H(:ref_ph[*]),`
`S(:ref_ph[*])`
	Gibbs energy, enthalpy and entropy of the system per mole of atoms referring to the given reference state.	G(:Fcc[*]) is the Gibbs energy of the system per mole of atoms referring to FCC of every element.
		H(:Fcc[Al], Hcp[Mg]) is the enthalpy per mole of atoms referring to Fcc Al and Hcp Mg.

`G_id(@*),`
`H_id(@*),`
`S_id(@*)`
	Gibbs energy, enthalpy and entropy due to ideal mixing for the given phase	S_id(@Fcc) is the entropy of the Fcc phase per mole of atoms due to ideal mixing.

`G_ex(@*),`
`H_ex(@*),`
`S_ex(@*)`
	Excess Gibbs energy, enthalpy and entropy other than ideal mixing part for the given phase	G_ex(@Fcc) is the excess Gibbs energy of the FCC phase per mole of atoms.

`mu(*)`	Chemical potential of a specified component or every component when the system reach equilibrium	`mu(Al)` is chemical potential of Al in the equilibrium system referring to the default reference state
`mu(*:ref_ph[*])`	Chemical potential of a specified component or every component when the system reach equilibrium referring to the given reference state	`mu(Al:Fcc[Al])` is chemical potential of AL in the equilibrium system referring to the Fcc Al

`a(*)`	activity of a specified component or every component when the system reach equilibrium	`a(Al)` is the activity of Al in the equilibrium system referring to the default reference state
`a(*:ref_ph[*])`, `r(*:ref_ph[*])`	activity or activity coefficient of a specified component or every component when the system reach equilibrium referring to the given reference state	`a(Al:Fcc[Al])` is the activity of Al in the equilibrium system referring to the Fcc Al
`fs, fl`	Fraction of solid (accumulated) and liquid during solidification	
`H_tot`	Total enthalpy of the system per mole of atoms. During the solidification process, `H_tot` is listed at each temperature. It is the total enthalpy of one mole atoms of the system at that temperature. It refers to the default reference state defined in the database.	For example, at 500°C there listed two phases: Liquid+Fcc, the fraction of Liquid is 0.9 and that of Fcc is 0.1, then `H_tot` is the enthalpy of 0.9 mole of Liquid plus the enthalpy of 0.1 mole of Fcc at 500°C.
`Q`	Heat evolved during solidification from the beginning temperature to the current temperature.	The beginning temperature can be set as a temperature above the liquidus if the user chooses to do so. The default setting for solidification starts at liquidus temperature
`H_Latent`	Latent heat. It is the heat released due to phase transformation only. During solidification, a small amount of liquid transformed to solid at each small temperature decrease. Latent heat listed at a certain temperature is accumulated from the beginning of solidification to the current temperature	For example, when temperature decreases from T1 to T2, a small fraction of liquid, dfL, transformed to solid, the latent heat of this small step is dfL*[H_Liquid (T2) – H_Solid (T2)]. In other words, the heat released of the Liquid due to the temperature decrease from T1 to T2 is not included in Latent heat.

Table 2.2 Table Format Syntax (less commonly used properties)

Syntax	**Meaning**	**Note and Example**
`P`	External pressure	Unit can be changed in the second row of the table, and P values updated instantly
`P(*)`	Partial pressure of species	`P(O2)` is the partial pressure of O2
`P(@gas)`	The pressure of gas phase when the system reaches equilibrium	
`reaction`	For a line calculation with decreasing temperature, the `reaction` column lists phase reaction at each temperature	

`G(@*),H(@*),S(@*),Cp(@*)`	Gibbs energy, enthalpy, entropy and heat capacity of a specified phase or every phase involved in the calculation	The listed value is for per mole of atoms. The reference state is the default reference state defined in the database

`G(@*:ref_ph[*]),`
`H(@*:ref_ph[*]),`
`S(@*:ref_ph[*]),`
`Cp(@*:ref_ph[*])`
	Gibbs energy, enthalpy, entropy and heat capacity of a specified phase or every phase involved in the calculation referring to the given reference state.	The listed value is for per mole of atoms.
		If the calculation (line calculation) is for the system, these properties for a phase are listed only in the range where the phase is stable; if the calculation is for individual phase, then these properties are listed in the entire range

`H(*@*:ref_ph),` `S(*@*:ref_ph)`	Partial molar enthalpy and entropy of a component in a phase with a given reference phase	`If reference phase is not given,` the default reference state in database is used
`G_id(@*),H_id(@*),S_id(@*)`	Reference and ideal mixing properties of a phase	`G = G_ref+G_id_mixing+G_ex` `G_id = G_ref+G_id_mixing`
`G_ex(@*),H_ex(@*),S_ex(@*)`	Excess properties of a phase	
`mu(*@*)`	Chemical potential of component(s) in a specified phase or in every phase involved in the calculation	`mu(Al@Fcc)` is chemical potential of Al in Fcc phase. If the calculation (line calculation) is for the system, these properties for a phase are listed only in the range where the phase is stable; if the calculation is for individual phase, then these properties are listed in the entire range
`mu(*@*:ref_ph[*])`	Chemical potential of component(s) in a specified phase or in every phase involved in the calculation referring to the given reference state	`mu(Al@Fcc:Fcc[*])` is chemical potential of Al in FCC phase referring to FCC state of every component.

`a(*@*), r(*@*)`	Activity and activity coefficient of component(s) in a phase referring to the default reference state in database	`a(Cu@fcc)=exp{mu(Cu@fcc)/RT}`
		`r=a/x`
		example refer to `mu(*@*)`

`a(*@*:ref_ph[*])` `r(*@*:ref_ph[*])`	Activity and activity coefficient of component(s) in a phase referring to the given reference state	`a(Cu@fcc:liquid)=exp{(mu(Cu@fcc)-mu(pure liquid Cu at same T))/RT}` example refer to `mu(*@*:ref_ph[*])`
`DF(@|*)`	Driving force of each phase entered the calculation referring to the equilibrium state of the	For example P1, P2, and P3 phases are selected in a point calculation (given an overall composition and

	system. Driving force can only apply to point calculation or line calculation	temperature), and the result shows P1 and P2 are in equilibrium at this point, then `DF(@|P1)=0, DF(@|P2)=0, and DF(@|P3)<0.` P3 is not stable, and the absolute value of `DF(@|P3)` is the minimum energy needed to make P3 stable. It should be pointed out that the equilibrium compositions of P1 and P2 are not at the overall composition, and the driving force of P3 is most likely not at this overall composition as well unless P3 is a line compound and its composition is the same as the overall composition. For a line calculation, such as at a fix temperature with varying composition, the equilibrium at each point along the line is calculated, and the driving force of each phase at each point can be listed in the table using `DF(@|*)`. Again, notice that driving force of a phase at a certain composition point is not the energy difference between this phase and the equilibrium state at this composition, it is the minimum energy needed to form this phase (most likely at another composition).
`DF(@!*)`	Driving force for each dormant phase referring to the equilibrium state of the system. Again, it only applies to point calculation or line calculation. A dormant phase does not enter a calculation, but its driving force is calculated. This is different from a suspended phase, which does not involve in the calculation at all.	For example P1, P2, and P3 phases are selected in a point calculation (given an overall composition and temperature), P4 is set as dormant phase. Again, the result shows P1 and P2 are in equilibrium at this point, then `DF(@|P1)=0, DF(@|P2)=0, and DF(@|P3)<0.` However, if you list `DF(@!P4),` it may be greater than zero. This means P4 will be stable if it is selected to enter the calculation.
`tieline`	This column will list the names of phases in equilibrium and the table is the selected tieline properties	See **Section 3.3.8** Tutorial for an example
`f_tot(@*)`	Accumulated fraction of each solid phase during solidification. By Scheil model, it is accumulated from each	$f_{tot(Liquid)} = f_l$

	solidification step. By Lever rule (equilibrium) model, it is the fraction of each phase in equilibrium at the current temperature.	$\sum_{i=1}^{n} f\_tot(Solid_i) = f_s$
`Vm, alpha_Vm, density`	Molar volume, expansion coefficient, density and molar weight of system in kg,	
`Vm(@*), density(@*)`	Molar volume and density of each phase involved in the calculation	
`n_mole, n_kg`	amount in mole and in kg	`n_mole, n_kg, n_kg(*),n_mole(@*),n_kg(*@*)`
`surface_tension(@liquid), viscosity(@liquid)`	Surface tension and viscosity of liquid phase	
`M(*@*)`	Atomic mobility of species in a phase	
`DC(*,J@*:N),`	Chemical diffusivity of species in a phase	`J`=gradient species, `N`= reference species (`N` cannot be `*`)
`DT(*@*)`	Tracer diffusivity of species in a phase	
`struct(@*)`	This is for a phase with multiple sublattice structure. It gives the structure in the form such as "`[2011]`", which means the first two sublattice have the same site fractions.	

2.4.3 Table column operations

When creating a new table in Pandat™, user can select the properties listed in the left column and drag them to the right column as shown in Figure 2.15. Pandat™ allows user perform algebraic calculations and simple logic operations on the properties and create a customized table.

Table 2.3 lists the mathematical algebraic functions available for table column expressions with examples. Nested functions are also allowed. Table 2.4 lists the logical expressions that can be used to extract a set of specific data from Pandat™ calculation results. These expressions can be applied to default table or other types of tables obtained from the calculation results. For example, user needs the first melting temperatures after a section calculation. A constraint can been easily set as "`f(@Liquid)=0`". Multiple constraints can be realized by setting one constraint in a row in the Table Editor shown in Figure 2.15.

Table 2.3 Mathematical functions for table column expressions

Function Name	**Operation**	**Examples**

+, -, *, /	addition, subtraction, multiplication and division	`H-T*S`
		`x(Al)+x(Ni)`
		`1/T`

//	Numerical derivative	`H//T` (See **Section 3.3.8** tutorial for an example)
exp	exponential function	`exp(-G/T/8.314)`
sqrt	square root	`sqrt(P(O2))`
abs	absolute value	`abs(DT(*@*))`

log, log10, ln, ln2	log and log10 are the common logarithm with base 10; ln is the natural logarithm with base e; ln2 is the binary logarithm with base 2.	`log(P(O2))`
		`log10(M(*@*))`
		`ln(a(Mg))`

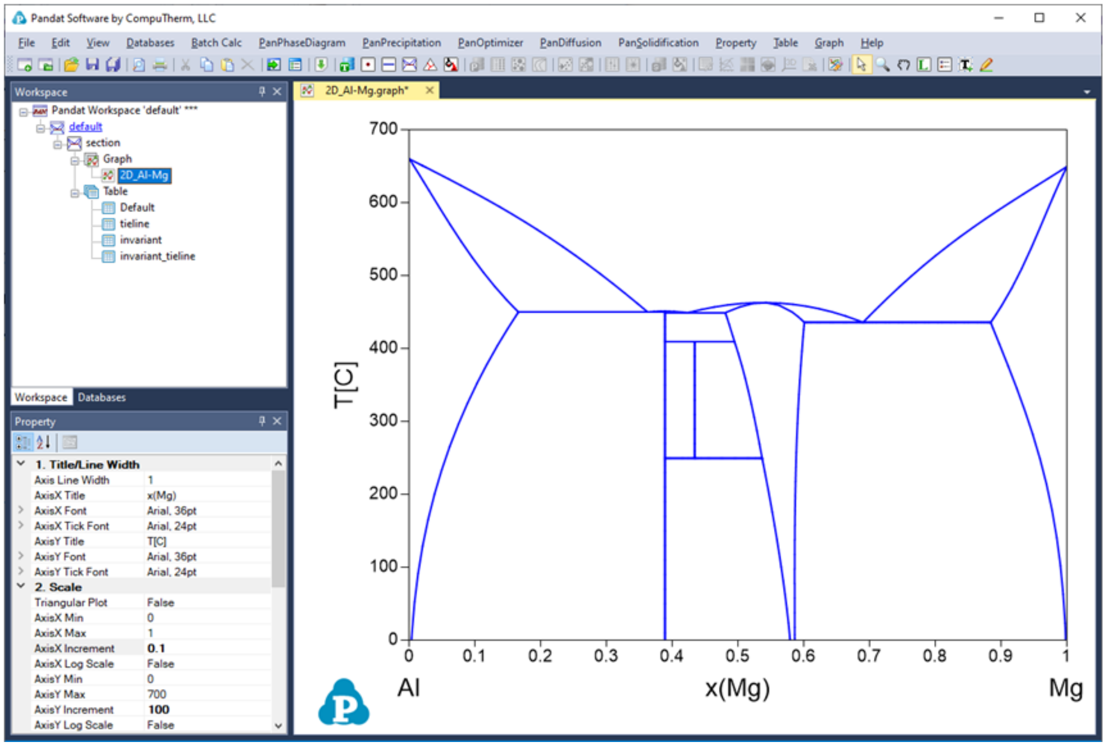
Table 2.4 Logical expression for table

Operator Name	**Comments**	**Examples**

=	equal to	`#phases=2`
		`Phase_name=liquid+fcc+hcp`
		`tieline=5` (specifying tieline density)

!=	not equal to	`phase_name!=fcc`
>	larger than	`T>1200`
<	less than	`x(Al)<0.5`
>=	larger than or equal to	`f(@Liquid)>=0`
<=	less than or equal to	`a(Al)<=0.3`

Here an example is given to demonstrate how to use the logical expression to obtain useful information from the calculated results. Figure 2.26 shows the calculated Al-Mg binary phase diagram. After the calculation, a table is generated with the constraint of `f(@Liquid)=0`, as seen in Figure 2.27. The new generated table is shown in Figure 2.28, which is a subset of the phase boundaries of Al-Mg where liquid phase exists and has phase fraction of zero, the so-call "first melting" boundary. This set of boundaries can be plotted on the Al-Mg phase diagram following the approach in **Section 2.3.3**. The first melting line is shown in red as in Figure 2.29. More examples will be presented in **Section 3.3.8**.



1. Title/Line Width	
Axis Line Width	1
AxisX Title	x(Mg)
AxisX Font	Arial, 36pt
AxisX Tick Font	Arial, 24pt
AxisY Title	T[C]
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
2. Scale	
Triangular Plot	False
AxisX Min	0
AxisX Max	1
AxisX Increment	**0.1**
AxisX Log Scale	False
AxisY Min	0
AxisY Max	700
AxisY Increment	**100**
AxisY Log Scale	False

Figure 2.26 Calculated Al-Mg binary phase diagram

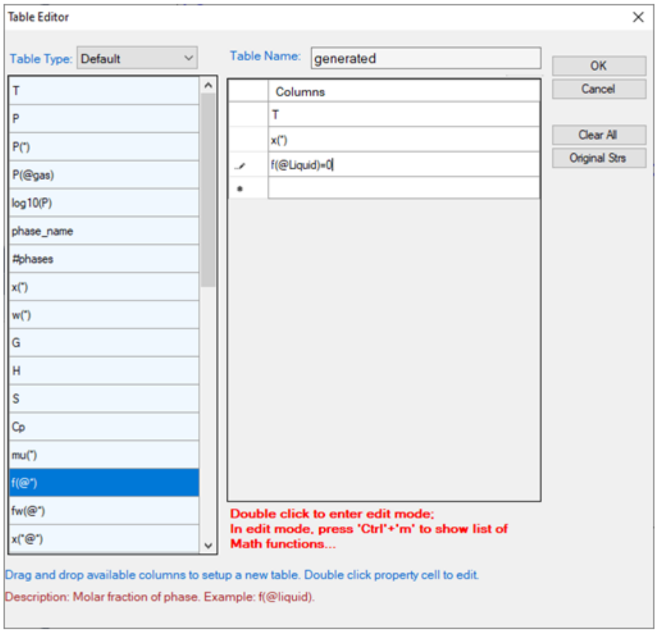


Table Type: Default

Table Name: generated

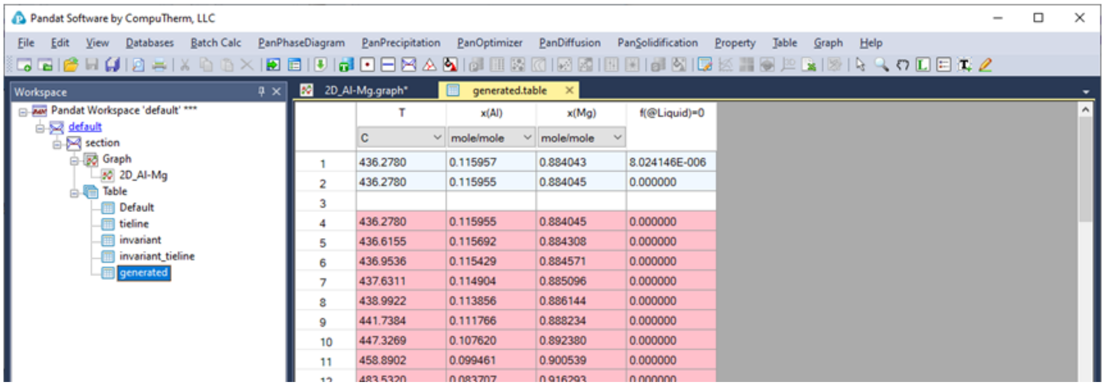
	Columns
	T
	x(*)
	f(@Liquid)=0

Double click to enter edit mode;
In edit mode, press 'Ctrl'+'m' to show list of
Math functions...

Drag and drop available columns to setup a new table. Double click property cell to edit.

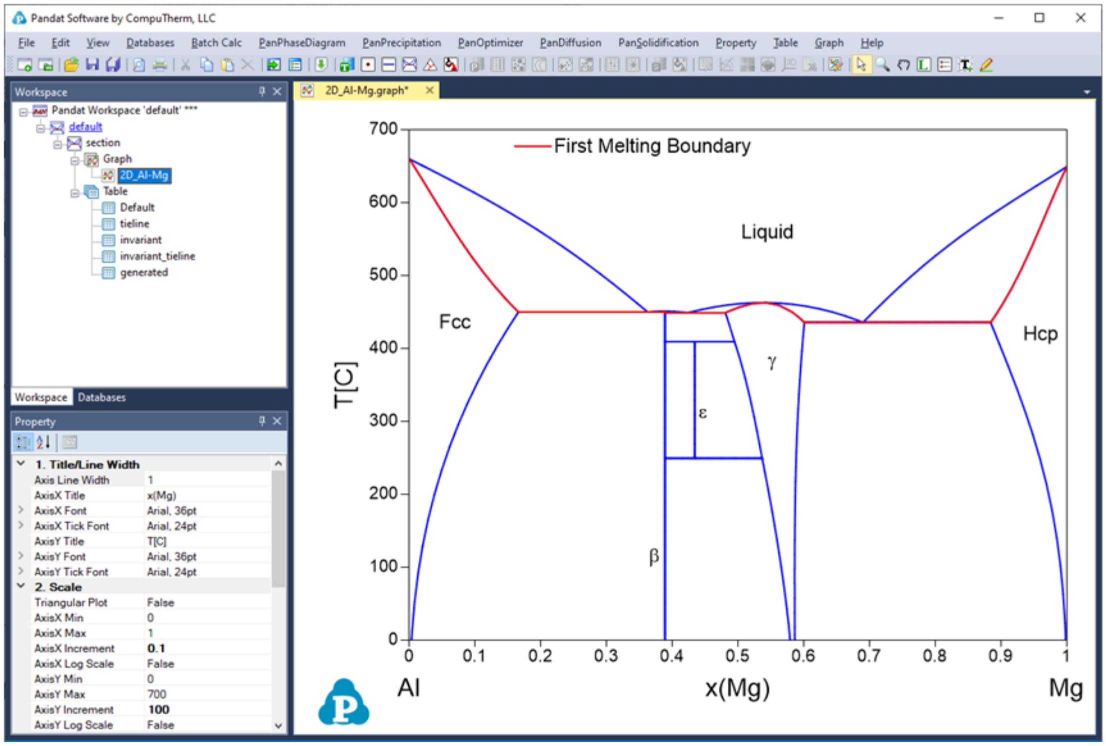
Description: Molar fraction of phase. Example: f(@liquid).

Figure 2.27 Generating a new table with a constraint of `f(@Liquid)=0`



	T	x(Al)	x(Mg)	f(@Liquid)=0
	C	mole/mole	mole/mole	
1	436.2780	0.115957	0.884043	8.024146E-006
2	436.2780	0.115955	0.884045	0.000000
3				
4	436.2780	0.115955	0.884045	0.000000
5	436.6155	0.115692	0.884308	0.000000
6	436.9536	0.115429	0.884571	0.000000
7	437.6311	0.114904	0.885096	0.000000
8	438.9922	0.113856	0.886144	0.000000
9	441.7384	0.111766	0.888234	0.000000
10	447.3269	0.107620	0.892380	0.000000
11	458.8902	0.099461	0.900539	0.000000
12	483.5320	0.083707	0.916293	0.000000

Figure 2.28 The generated table with the constraint of `f(@Liquid)=0`



1. Title/Line Width	
Axis Line Width	1
AxisX Title	x(Mg)
AxisX Font	Arial, 36pt
AxisX Tick Font	Arial, 24pt
AxisY Title	T[C]
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
2. Scale	
Triangular Plot	False
AxisX Min	0
AxisX Max	1
AxisX Increment	**0.1**
AxisX Log Scale	False
AxisY Min	0
AxisY Max	700
AxisY Increment	**100**
AxisY Log Scale	False

Figure 2.29 The first melting boundary merged on the Al-Mg phase diagram

2.5 Console Mode

In addition to the most common GUI (graphical user interface) mode, Pandat™ can also run in the console mode without opening GUI. There are two ways to activate the console mode:

(1) double click a batch file (extension with pbfx) in a folder, or

(2) run through a windows bat file. The content of an example bat file is shown below:

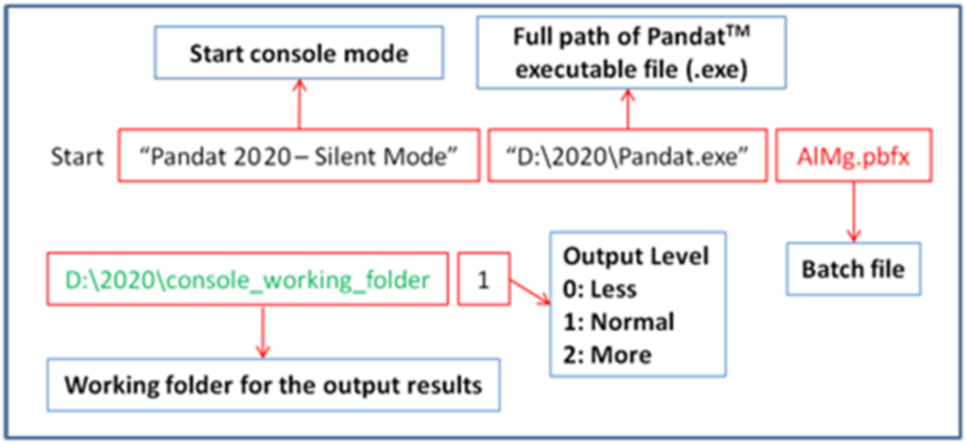


Figure 2.30 Example of the (.bat) file for console mode

The command is to start Pandat™ (with full path and titled as "Pandat 2020 - Silent Mode") and run the batch file AlMg.pbfx (in the current folder if not in full path). The last two arguments are optional. If a working folder is given ("D:\2020\console_working_folder"), a Pandat™ workspace is created in the folder and all simulation results are saved under the workspace. The simulation progress is logged in the file "pandat.log". The last argument is to control the output level with "1" the default value. The value of "2" is for more outputs and "0" for less. Please refer to example #29 in Example Book for more detail information.

3 PanPhaseDiagram

3.1 Thermodynamic Database

PanPhaseDiagram is for phase diagram and thermodynamic property calculation. Thermodynamic database is the prerequisite to fulfill such calculations. A thermodynamic database represents a set of self-consistent Gibbs-energy functions with optimized thermodynamic-model parameters for all the phases in a system. The advantage of CALPHAD method is that the separately-measured phase diagrams and thermodynamic properties can be represented by a unique "thermodynamic description" of the materials system in question. More importantly, on the basis of the known descriptions of the constituent lower-order systems, the thermodynamic description for a higher-order system can be obtained via an extrapolation method [1989Cho]. This description enables us to calculate phase diagrams and thermodynamic properties of multi-component systems that are experimentally unavailable.

In the following, thermodynamic models used to describe the disordered phase, ordered intermetallic phase, and stoichiometric phase are presented. The equations are given for a binary system, and they can be extrapolated to a multi-component system using geometric models [1975Mug, 1989Cho].

The Gibbs energy of a binary disordered solution phase can be written as:

$$G_m^{\varphi} = \sum_{i=A,B} x_i \cdot G_i^{\varphi,o} + RT \sum_{i=A,B} x_i \ln x_i + x_A \cdot x_B \sum_{\nu} L_\nu \cdot (x_A - x_B)^\nu \tag{3.1}$$

where the first, second and third terms on the right hand of the equation represent, respectively, the reference states, the entropy of ideal mixing, and the excess Gibbs energy of mixing. Here x_i is the mole fraction of a component *i*, $G_i^{\varphi,o}$ is the Gibbs energy of a pure component *i*, with an φ structure, R is the gas constant, T is the absolute temperature, L_ν is the interaction coefficient at the polynomial series of the power ν. When ν = 0, it is a regular solution model, and when ν = 0 and 1, it is a sub-regular solution model. Equation 3.1 can be extrapolated into a multi-component system using geometric models, such as the Muggianu model [1975Mug]. Ternary and higher-order interaction parameters may be necessary to describe a multi-component solution phase.

An ordered intermetallic phase is described by a variety of sublattice models, such as the compound-energy formalism [1979Ansara, 1988Ansara] and the bond-energy model [1992Oates, 1995Chen]. In these models, the Gibbs energy is a function of the sublattice species concentrations and temperature. The Gibbs energy of a binary intermetallic phase, described by a two-sublattice compound-energy formalism, $(A,B)_p:(A,B)_q$, can be written as:

$$\begin{aligned} G_m^{\varphi} = {} & \sum_{i=A,B}\sum_{j=A,B} y_i^I y_j^{II} G_{i:j}^{\varphi} + RT\Big[\frac{p}{p+q}\sum_{i=A,B} y_i^I \ln y_i^I + \frac{q}{p+q}\sum_{i=A,B} y_i^{II} \ln y_i^{II}\Big] \\ & + \sum_{j=A,B} y_A^I y_B^I y_j^{II} \sum_{v} (y_A^I - y_B^I)^v L_{A,B:j}^v + \sum_{i=A,B} y_i^I y_A^{II} y_B^{II} \sum_{v} (y_A^{II} - y_B^{II})^v L_{i:A,B}^v \\ & + y_A^I y_B^I y_A^{II} y_B^{II} L_{A,B:A,B} \end{aligned} \qquad (3.2)$$

where y_i^I and y_i^{II} are the species concentrations of a component, i, in the first and second sublattices, respectively. The first term on the right hand of the equation represents the reference state with the mechanical mixture of the stable or hypothetical compounds: A, A_pB_q, B_pA_q, and B. $G_{i:j}^{\varphi}$ is the Gibbs energy of the stoichiometric compound, $i_p j_q$, with an φ structure. The value of $G_{i:j}^{\varphi}$ can be obtained experimentally if $i_p j_q$ is a stable compound; or it can be obtained by *ab initio* calculation if $i_p j_q$ is a hypothetical compound. Sometimes, $G_{i:j}^{\varphi}$ are treated as model parameters to be obtained by optimization using the experimental data related to this phase. The second term is the ideal mixing Gibbs energy, which corresponds to the random mixing of species on the first and second sublattices. The last three terms are the excess Gibbs energies of mixing. The "L" parameters in these terms are model parameters whose values are obtained using the experimental phase-equilibrium data and thermodynamic-property data. These parameters can be temperature dependent. In this equation, a comma is used to separate species in the same sublattice, whilst a colon is used to separate species belonging to different sublattices. The compound-energy formalism can be applied to phases in a multi-component system by considering the interactions from all the constituent binaries. Additional ternary and higher-order interaction terms may also be added to the excess Gibbs energy term.

For a reciprocal system with two sublattices, sometimes the interactions among the two species on each sublattice are considered, $(A,B)_p(C,D)_q$. The interaction parameter is expressed as [2007Luk]

$$L_{AB:CD} = L^0_{AB:CD} + (y^I_A - y^I_B)L^1_{AB:CD} + (y^{II}_C - y^{II}_D)L^2_{AB:CD} \qquad (3.3)$$

Pandat treats the term $(y^I_A - y^I_B)L^1_{AB:CD}$ as the interaction on the first sublattice and the term $(y^{II}_C - y^{II}_D)L^2_{AB:CD}$ as the interaction on the second sublattice. Pandat does not use the alphabetical order of species.

The Gibbs energy of a binary stoichiometric compound A_pB_q, G^φ_m, is described as a function of temperature only:

$$G^\varphi_m = \sum_i x_i G^{\varphi,\circ}_i + \Delta_f G(A_pB_q) \qquad (3.4)$$

where x_i is the mole fraction of component i (i=p if it is A, and i=q if it is B), and $G^{\varphi,\circ}_i$ represents the Gibbs energy of component i with φ structure; $\Delta_f G(A_pB_q)$, which is normally a function of temperature, represents the Gibbs energy of formation of the stoichiometric compound. If $\Delta_f G(A_pB_q)$ is a linear function of temperature:

$$\Delta_f G(A_pB_q) = \Delta_f H(A_pB_q) - T \cdot \Delta_f S(A_pB_q) \qquad (3.5)$$

then $\Delta_f H(A_pB_q)$, and $\Delta_f S(A_pB_q)$ are the enthalpy and entropy of formation of the stoichiometric compound, respectively. Equation (3.3) can be readily extended to a multi-component stoichiometric compound phase.

The strategy of building a multi-component thermodynamic database starts with deriving the Gibbs energy of each phase in the constituent binaries. There are C_n^2 constituent binaries in an n-component alloy system, where

$$C_n^i = \frac{n!}{i!(n-i)!} \quad (3.6)$$

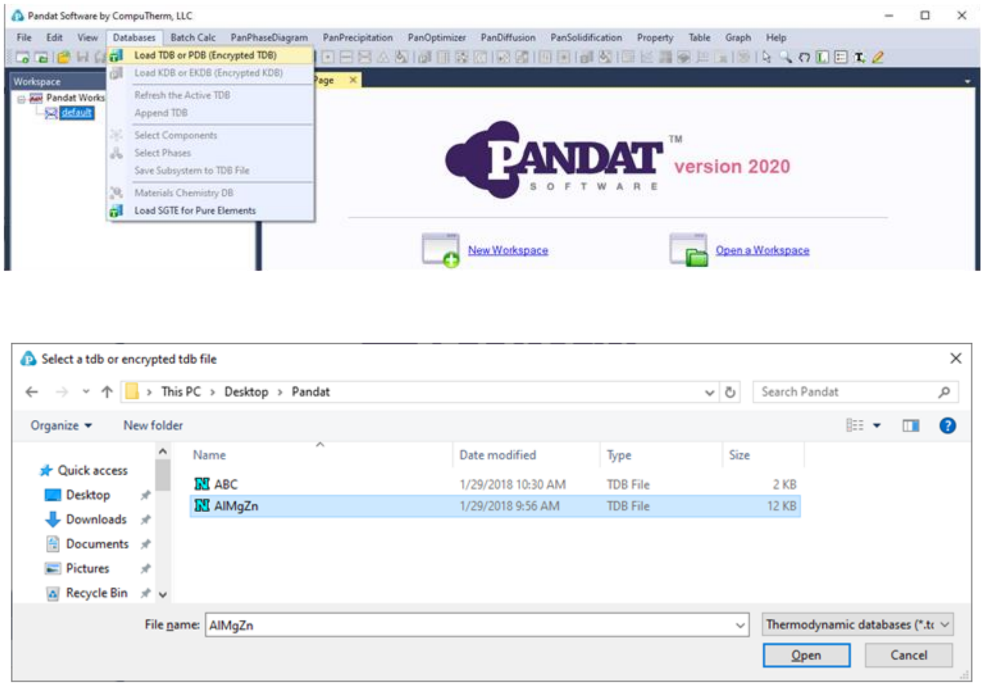
To develop a reliable database, the Gibbs energies of these binaries must be developed in a self-consistent manner and be compatible with each other. Three binaries form a ternary, and a preliminary thermodynamic description can be obtained by combining the three constituent binaries using geometric models, such as the Muggianu model [1975Mug]. In some cases, a ternary database developed in this way can describe a ternary system fairly well, while in most cases, ternary interaction parameters are necessary to better describe the ternary system. If a new phase appears in the ternary, which is not in any of the constituent binaries, a thermodynamic model is selected for this ternary phase, and its model parameters are optimized using the experimental information for this ternary phase. There are a total of C_n^3 ternary systems in an n-component system. After thermodynamic descriptions of all C_n^3 ternaries for an n-component system are established, the model parameters are simply used to describe quaternary and higher-order systems using an extrapolation approach. High-order interaction parameters are usually not necessary because although interactions between binary components are strong, in ternary systems they become weaker, and in higher-ordered systems they become negligibly weak [1997Kattner, 2004Chang]. It is worth noting that the term, “thermodynamic database” or simply “database”, is usually used in the industrial community instead of “thermodynamic description”, particularly for multi-component systems.

At CompuTherm, multi-component databases have been developed for variety of alloys, such as for Al-alloys, Co-alloys, Cu-alloys, Fe-alloys, Mg-alloys, Mo-alloys, Nb-alloys, Ni-alloys, Ti-alloys, TiAl-alloys, high entropy alloys, and solder alloys. Information for these databases is available in the "Thermodynamic Database User's Guide" from CompuTherm.

3.2 Thermodynamic Calculation

3.2.1 Load Database

Pandat™ can load both `PDB` and `TDB` database files. This command can be accessed through the toolbar icon . User can also load a database file using the Menus **<u>Database→Load TDB or PDB (Encrypted TDB)</u>** as shown in Figure 3.1. Select a database file from hard drive and click open button, or just double click the database file. Users can store the databases in any directory in the computer.



Name	Date modified	Type	Size
ABC	1/29/2018 10:30 AM	TDB File	2 KB
AlMgZn	1/29/2018 9:56 AM	TDB File	12 KB

File name: AlMgZn

Figure 3.1 Load a database from hard drive through Menus

Immediately after a database is successfully loaded, a popup window shown in Figure 3.2 will ask the user to select the components for subsequent calculations. To add a component to the list of selected components, click on the component on the list of **Available Components** on the left column, and click on the ❯ button to send them to the **Selected Components** on the right column. To select several components at one time, hold the <Ctrl> key and use mouse to select multiple components. To remove a component from selected components list, use mouse to select it, and click the ❮ button.

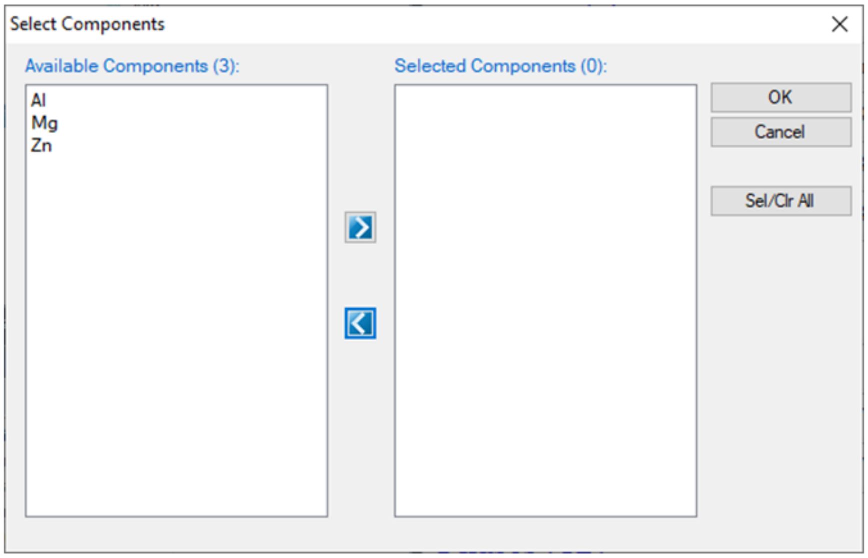
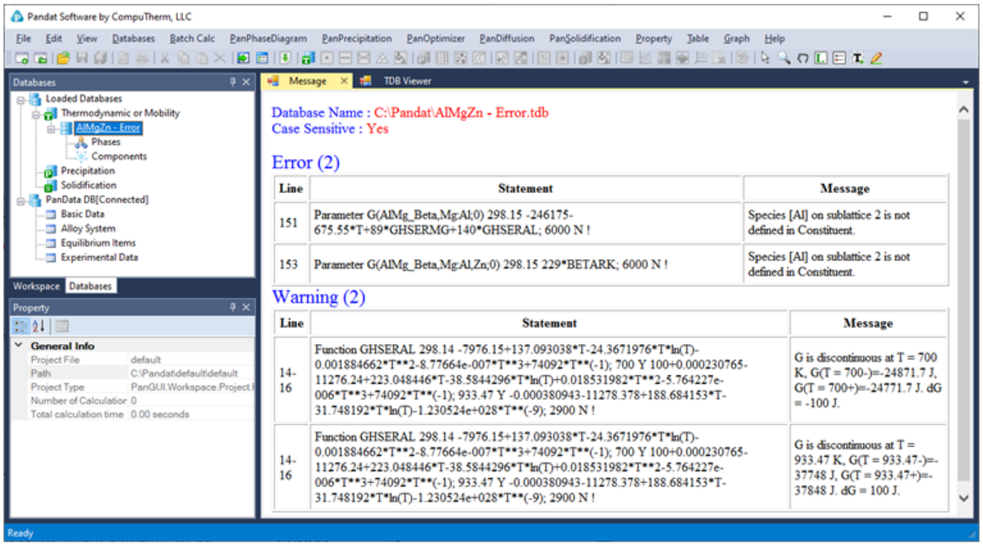


Figure 3.2 Select components for further calculation

While loading a database file, Pandat™ checks the self-consistency of the database. A message will be displayed if the database is not internally consistent such as duplicated definitions of a function, missing definition of components or species in a sublattice, and so on. There are two types of messages: Error and Warning, as shown in Figure 3.3. The warning message can be ignored but the errors must be fixed, otherwise the database cannot be loaded. It is recommended to correct both error and warning before performing calculation. If you have difficulties loading a particular **TDB** or **PDB** file, please contact CompuTherm, LLC, and we will help resolve the problem.



Project File	default
Path	C:\Pandat\default\default
Project Type	PanGUI.Workspace.Project.I
Number of Calculatior	0
Total calculation time	0.00 seconds

Database Name : C:\Pandat\AlMgZn - Error.tdb
Case Sensitive : Yes

Error (2)

Line	Statement	Message
151	Parameter G(AlMg_Beta,Mg:Al;0) 298.15 -246175-675.55*T+89*GHSERMG+140*GHSERAL; 6000 N !	Species [Al] on sublattice 2 is not defined in Constituent.
153	Parameter G(AlMg_Beta,Mg:Al,Zn;0) 298.15 229*BETARK; 6000 N !	Species [Al] on sublattice 2 is not defined in Constituent.

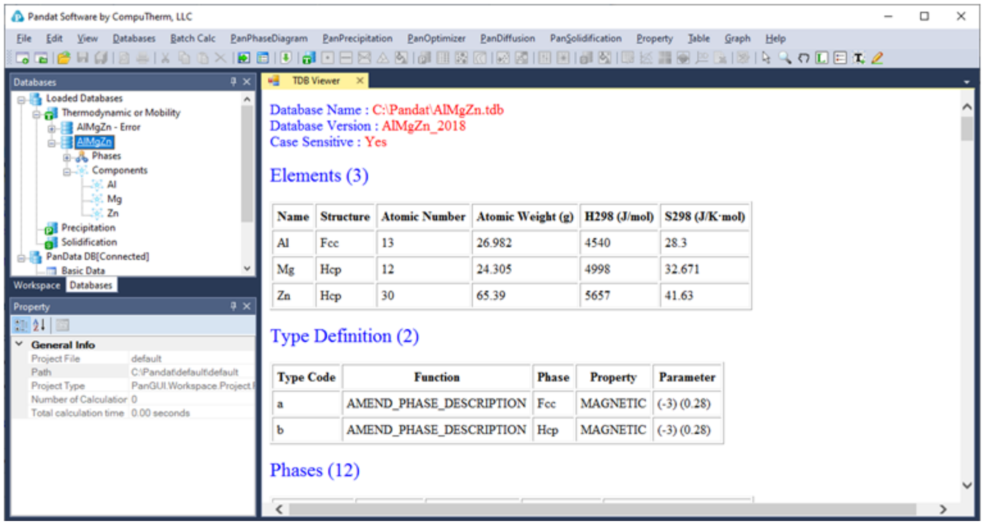
Warning (2)

Line	Statement	Message
14-16	Function GHSERAL 298.14 -7976.15+137.093038*T-24.3671976*T*ln(T)-0.001884662*T**2-8.77664e-007*T**3+74092*T**(-1); 700 Y 100+0.000230765-11276.24+223.048446*T-38.5844296*T*ln(T)+0.018531982*T**2-5.764227e-006*T**3+74092*T**(-1); 933.47 Y -0.000380943-11278.378+188.684153*T-31.748192*T*ln(T)-1.230524e+028*T**(-9); 2900 N !	G is discontinuous at T = 700 K, G(T = 700-)=-24871.7 J, G(T = 700+)=-24771.7 J. dG = -100 J.
14-16	Function GHSERAL 298.14 -7976.15+137.093038*T-24.3671976*T*ln(T)-0.001884662*T**2-8.77664e-007*T**3+74092*T**(-1); 700 Y 100+0.000230765-11276.24+223.048446*T-38.5844296*T*ln(T)+0.018531982*T**2-5.764227e-006*T**3+74092*T**(-1); 933.47 Y -0.000380943-11278.378+188.684153*T-31.748192*T*ln(T)-1.230524e+028*T**(-9); 2900 N !	G is discontinuous at T = 933.47 K, G(T = 933.47-)=-37748 J, G(T = 933.47+)=-37848 J. dG = 100 J.

Figure 3.3 A typical message when loading a database

The successfully loaded database will be automatically summarized in the TDB Viewer mode in the main Display window as shown in Figure 3.4. For a TDB format database, the summary includes elements, type definitions, phases with name and thermodynamic model, model parameters and defined functions. For a PDB format database, the model parameters and functions will not be displayed. The user can open a TDB format database with the Text Editor mode by right click of the mouse on the database name in the explorer window. The Text Editor is actually a built-in notepad for text files. User can use the Text Editor directly within Pandat™ workspace to edit the TDB database, or he/she can always use his/her favorite text editor to do it.

Multiple databases can be loaded into the same workspace but only one is activated. The current calculation will use the activated database, which is highlighted in the explorer window at Database view. The user may set the inactive database to be active with right click of the mouse as shown in Figure 3.5.



Project File: default
Path: C:\Pandat\default\default
Project Type: PanGUI.Workspace.Project.
Number of Calculation: 0
Total calculation time: 0.00 seconds

Database Name : C:\Pandat\AlMgZn.tdb
Database Version : AlMgZn_2018
Case Sensitive : Yes

Elements (3)

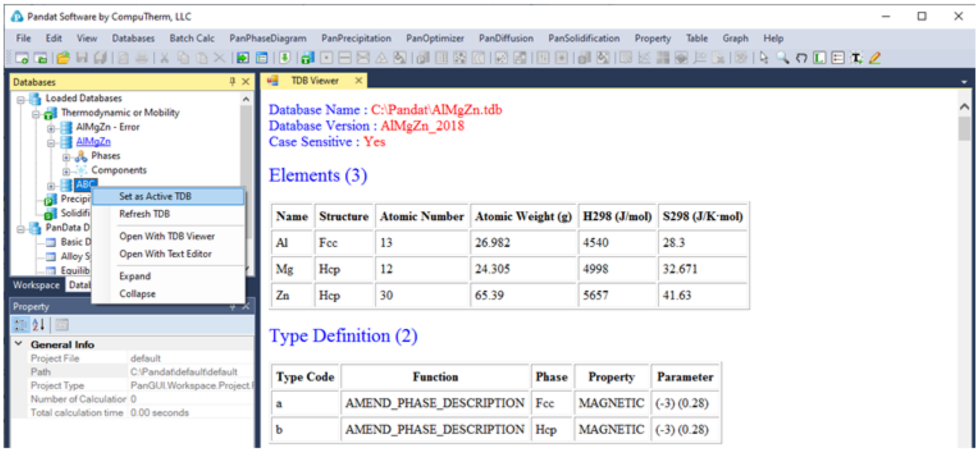
Name	Structure	Atomic Number	Atomic Weight (g)	H298 (J/mol)	S298 (J/K·mol)
Al	Fcc	13	26.982	4540	28.3
Mg	Hcp	12	24.305	4998	32.671
Zn	Hcp	30	65.39	5657	41.63

Type Definition (2)

Type Code	Function	Phase	Property	Parameter
a	AMEND_PHASE_DESCRIPTION	Fcc	MAGNETIC	(-3) (0.28)
b	AMEND_PHASE_DESCRIPTION	Hcp	MAGNETIC	(-3) (0.28)

Phases (12)

Figure 3.4 The TDB viewer mode for database summary



Project File: default
Path: C:\Pandat\default\default
Project Type: PanGUI.Workspace.Project.
Number of Calculation: 0
Total calculation time: 0.00 seconds

Database Name : C:\Pandat\AlMgZn.tdb
Database Version : AlMgZn_2018
Case Sensitive : Yes

Elements (3)

Name	Structure	Atomic Number	Atomic Weight (g)	H298 (J/mol)	S298 (J/K·mol)
Al	Fcc	13	26.982	4540	28.3
Mg	Hcp	12	24.305	4998	32.671
Zn	Hcp	30	65.39	5657	41.63

Type Definition (2)

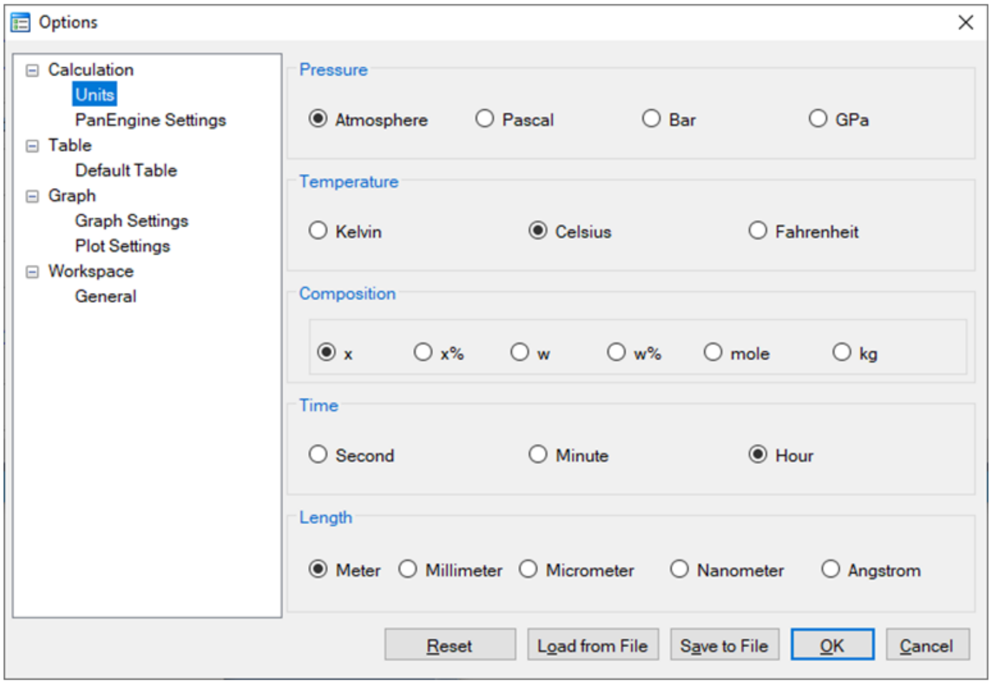
Type Code	Function	Phase	Property	Parameter
a	AMEND_PHASE_DESCRIPTION	Fcc	MAGNETIC	(-3) (0.28)
b	AMEND_PHASE_DESCRIPTION	Hcp	MAGNETIC	(-3) (0.28)

Figure 3.5 Set an inactive database to be active

3.2.2 Options

To configure the calculation options, go through the menus (**View → Options**), or click on the icon on the toolbar. A pop-up dialog box allows the user to change the units, and output formats of default Table and Graph.

Units: This dialog box allows the user to choose the units to be used in the calculation. Use the mouse left button to select a proper unit for each property and click “OK” to complete the unit setting as shown in Figure 3.6.



Pressure

● Atmosphere ○ Pascal ○ Bar ○ GPa

Temperature

○ Kelvin ● Celsius ○ Fahrenheit

Composition

● x ○ x% ○ w ○ w% ○ mole ○ kg

Time

○ Second ○ Minute ● Hour

Length

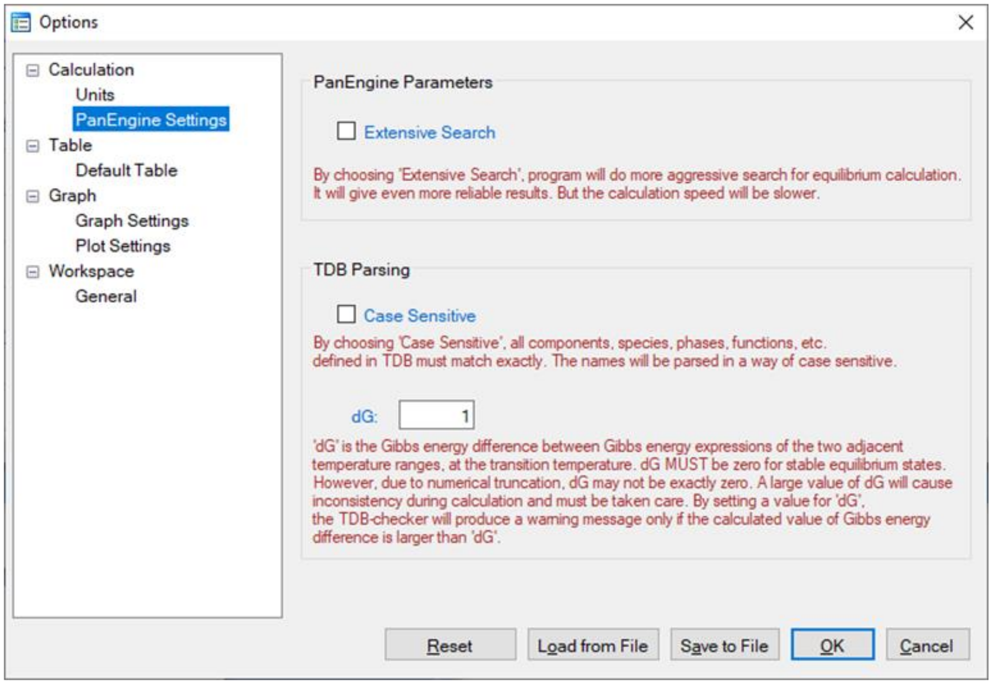
● Meter ○ Millimeter ○ Micrometer ○ Nanometer ○ Angstrom

Figure 3.6 Set units for a calculation in Options

PanEngine Settings: This dialog box allows the user to change the PanEngine Parameter and TDB Parsing parameters as shown in Figure 3.7. When “Extensive Search” is checked, PanEngine will perform a more thorough search of the global equilibrium state in case the Normal Search missed it. For majority of cases Extensive Search is not necessary and will give the same answer as that of Normal Search. The calculation will take longer time when Extensive Search is chosen. Extensive Search is recommended only when the user found metastable equilibrium in a particular calculation.

If the “Case Sensitive” box is checked, all the components, species, phases, functions, etc. defined in the TDB will be parsed in a way of case sensitive and should match exactly, in other words, the uppercase letters are treated as different from the corresponding lowercase letters.

The Gibbs energy of a pure component with a certain crystal structure is usually segmental function of temperature and is represented by different Gibbs energy expression at different temperature range. dG represents the Gibbs energy difference obtained from the two Gibbs energy expressions at adjacent temperature ranges at the transition temperature. Ideally, dG is zero if the two Gibbs energy expressions give the exact same value at the transition temperature. However, due to numerical truncation, dG is usually not zero. The default setting of dG in PanEngine is 1.0 J/mole atom. A warning message will be sent to TDB viewer if dG is greater than 1.0. A large dG will cause calculation fail, therefore should be fixed in the TDB file. User can set this value to a bigger or smaller value according to his/her tolerance.



☐ Extensive Search

By choosing 'Extensive Search', program will do more aggressive search for equilibrium calculation.
It will give even more reliable results. But the calculation speed will be slower.

☐ Case Sensitive

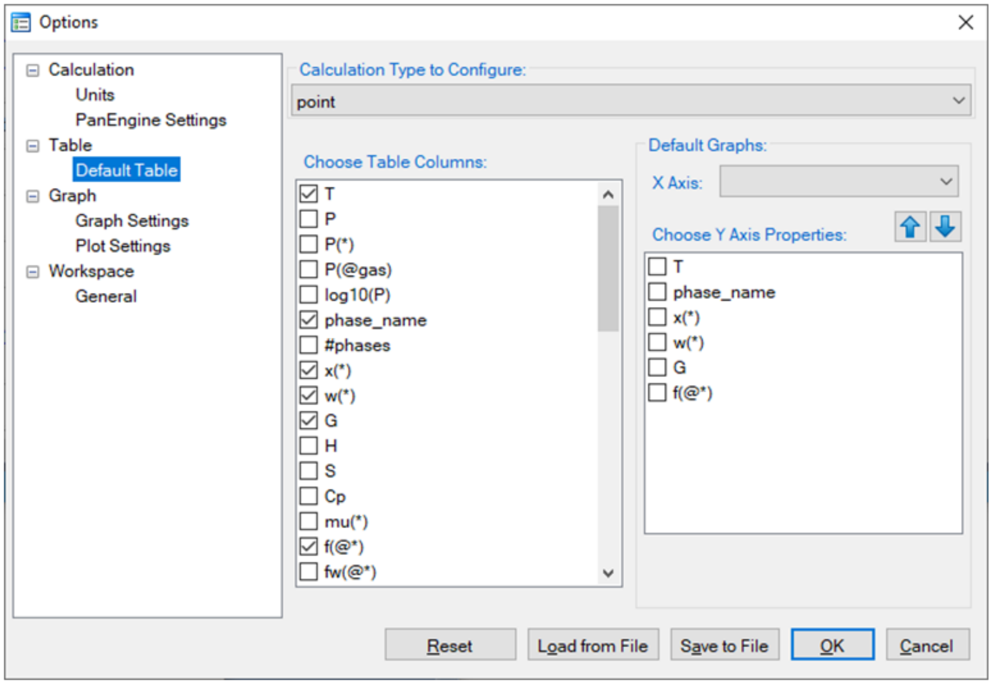
By choosing 'Case Sensitive', all components, species, phases, functions, etc.
defined in TDB must match exactly. The names will be parsed in a way of case sensitive.

dG: 1

'dG' is the Gibbs energy difference between Gibbs energy expressions of the two adjacent
temperature ranges, at the transition temperature. dG MUST be zero for stable equilibrium states.
However, due to numerical truncation, dG may not be exactly zero. A large value of dG will cause
inconsistency during calculation and must be taken care. By setting a value for 'dG',
the TDB-checker will produce a warning message only if the calculated value of Gibbs energy
difference is larger than 'dG'.

Figure 3.7 PanEngine Settings in Options

Table: This dialog box allows a user to customize the default output table with the properties the user needs. As shown in Figure 3.8, user first needs to choose the “Calculation Type to Configure” which includes point, line, section, solidification and so on. Once the Calculation Type is selected, all the possible properties for the chosen Calculation Type will be listed in the “Choose Table Columns”. The user can check the box in front of each item to select the column to be shown in the default output table. All the selected properties will be listed in the “Choose Y Axis Properties”. In this same dialog, user can also define the X axis and Y axis of the default graph that is automatically shown when a calculation finishes.



Calculation Type to Configure: point

Choose Table Columns:

☑ T
☐ P
☐ P(*)
☐ P(@gas)
☐ log10(P)
☑ phase_name
☐ #phases
☑ x(*)
☑ w(*)
☑ G
☐ H
☐ S
☐ Cp
☐ mu(*)
☑ f(@*)
☐ fw(@*)

Default Graphs:

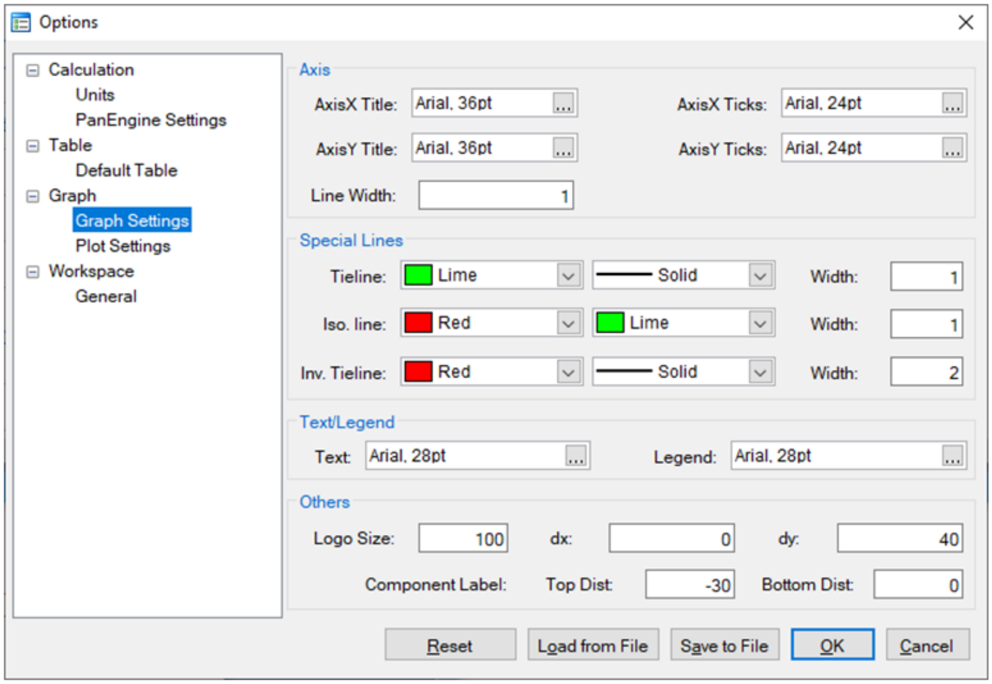
X Axis:

Choose Y Axis Properties:

☐ T
☐ phase_name
☐ x(*)
☐ w(*)
☐ G
☐ f(@*)

Figure 3.8 Set default table output and default dataset for graph output

Graph: This dialog box allows the user to set up the appearance of the output graph. As shown in Figure 3.9, user can set the font and size of the texts, color and width of the lines, color, shape and size of the symbols, and logo size and positions for the default graph. User can also set the color and width of the lines, color, shape and size of the symbols for different plots in one graph as shown in Figure 3.10.



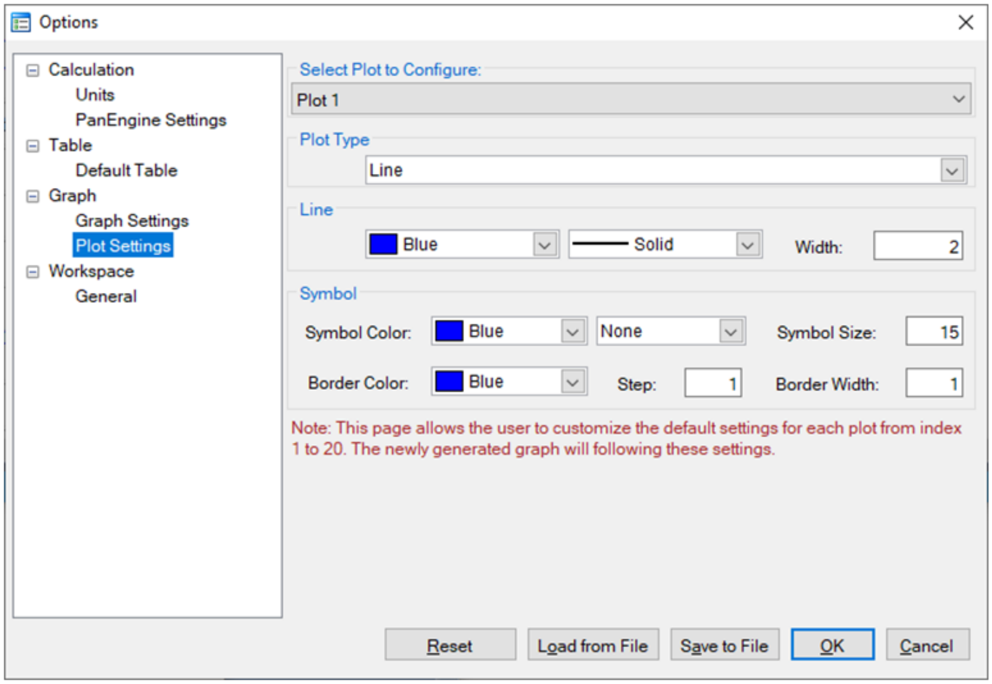
AxisX Title: Arial, 36pt
AxisX Ticks: Arial, 24pt
AxisY Title: Arial, 36pt
AxisY Ticks: Arial, 24pt
Line Width: 1

Tieline: 🟩 Lime — Solid — Width: 1
Iso. line: 🟥 Red — 🟩 Lime — Width: 1
Inv. Tieline: 🟥 Red — Solid — Width: 2

Text: Arial, 28pt
Legend: Arial, 28pt

Logo Size: 100
dx: 0
dy: 40
Component Label: Top Dist: -30
Bottom Dist: 0

Figure 3.9 Set the appearance parameters for graph



Select Plot to Configure: Plot 1

Plot Type: Line

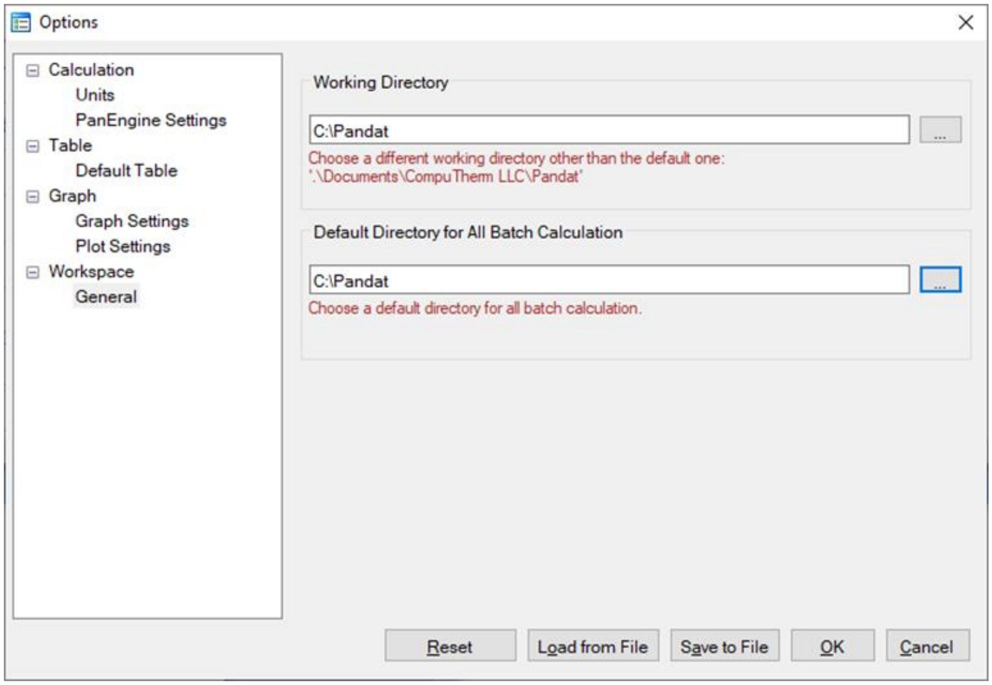
Line: 🟦 Blue — Solid — Width: 2

Symbol Color: 🟦 Blue — None
Symbol Size: 15
Border Color: 🟦 Blue
Step: 1
Border Width: 1

Note: This page allows the user to customize the default settings for each plot from index 1 to 20. The newly generated graph will following these settings.

Figure 3.10 Set the appearance parameters for each plot in the graph

Workspace: This dialog box allows the user to set up the default working directory for Pandat workspace as shown in Figure 3.11.



Working Directory: C:\Pandat

Choose a different working directory other than the default one:
'.\Documents\CompuTherm LLC\Pandat'

Default Directory for All Batch Calculation: C:\Pandat

Choose a default directory for all batch calculation.

Figure 3.11 set up the default working directory for Pandat workspace

It should be pointed out that “Options” gives users the opportunity to change the PanEngine Setting and customize the output of Default Table and Graph. However, users do not have to do anything if not necessary. By default, the most popular setting has been selected for each type of calculation.

3.3 Tutorial

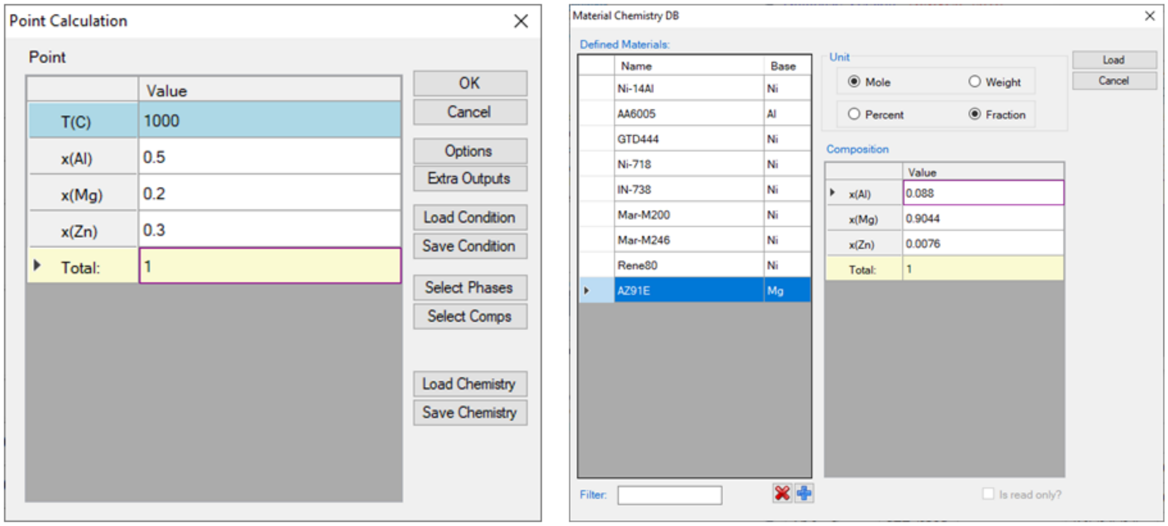
The Al-Mg-Zn is used as an example for the following calculations. TheAlMgZn.tdb is in the PanPhaseDiagram directory under Pandat™ examples. Load the database by clicking the button and select all three components.

3.3.1 Point Calculation (0D)

This function allows the user to calculate the stable phase equilibrium at a single point in a multicomponent system.

Go to **PanPhaseDiagram** on the menu bar and select **Point Calculation** or click the button on the tool bar. The dialog box for **Point Calculation** as shown in Figure 3.12(a) allows the user to set up the calculation conditions: composition and temperature. User can either input the conditions manually or use the **Load Condition** function to load from an existing batch file. User can always save the current calculation condition to a batch file by clicking the **Save Condition** button, or save the alloy composition on hard disc by clicking **Save Chemistry** button. User can load the alloy composition for the future calculation using the function **Load Chemistry** following Figure 3.12(b).

The functions of other buttons as shown in Figure 3.12(a) are given below. User can access the **Options** window again by clicking **Options** and make changes for the units**.** Please refer to the previous section for information on the **Options** window. The **Extra Outputs** button allows the user to modify the default output table and graph and add more tables and graphs as needed. A pop out window as shown in Figure 3.13(a) provides the access to the table and graph for output. User may add or delete output table/graph using the buttons ✖ and ➕, or modify the selected table/graph by clicking the “edit…” button. Please refer to the previous section for information on Table Edit. The Graph dialog is slightly different from that described in the previous section. As shown in Figure 3.13(b), data source for the graph can only be the tables generated from the calculations and there is a check box for the triangle plot. The operations for editing the graph are the same as those described in the previous section.



	Value
T(C)	1000
x(Al)	0.5
x(Mg)	0.2
x(Zn)	0.3
Total:	1

Name	Base
Ni-14Al	Ni
AA6005	Al
GTD444	Ni
Ni-718	Ni
IN-738	Ni
Mar-M200	Ni
Mar-M246	Ni
Rene80	Ni
AZ91E	Mg

● Mole ○ Weight
○ Percent ● Fraction

	Value
x(Al)	0.088
x(Mg)	0.9044
x(Zn)	0.0076
Total:	1

(a) (b)

Figure 3.12 Set alloy composition and Temperature for point calculation

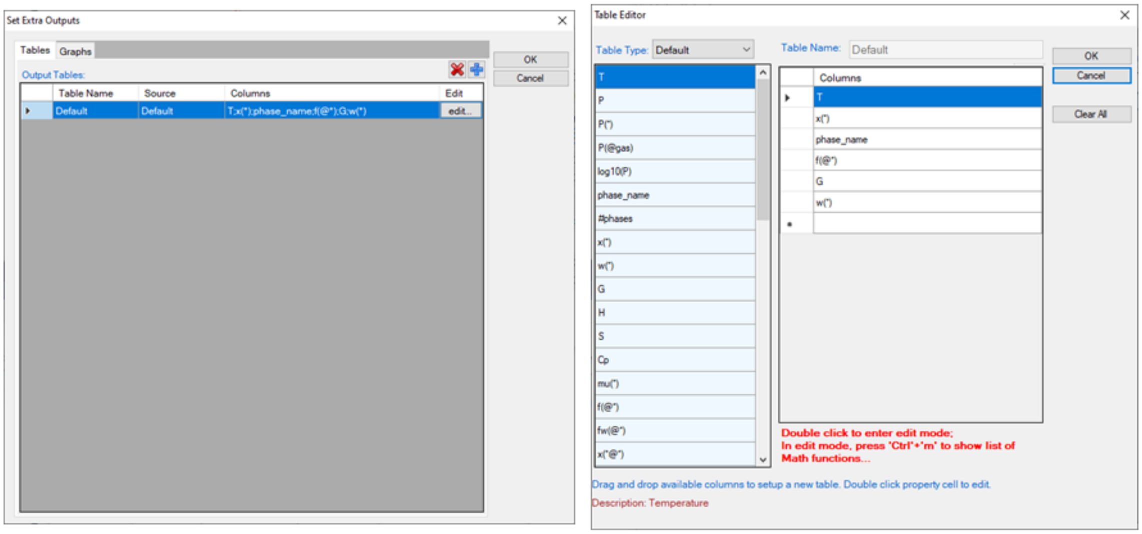


Table Name	Source	Columns	Edit
Default	Default	T;x(*);phase_name;f(@*);G;w(*)	edit...

Table Type: Default
Table Name: Default

T
P
P(*)
P(@gas)
log10(P)
phase_name
#phases
x(*)
w(*)
G
H
S
Cp
mu(*)
f(@*)
fw(@*)
x(*@*)

Columns
T
x(*)
phase_name
f(@*)
G
w(*)

Double click to enter edit mode;
In edit mode, press 'Ctrl'+'m' to show list of Math functions...

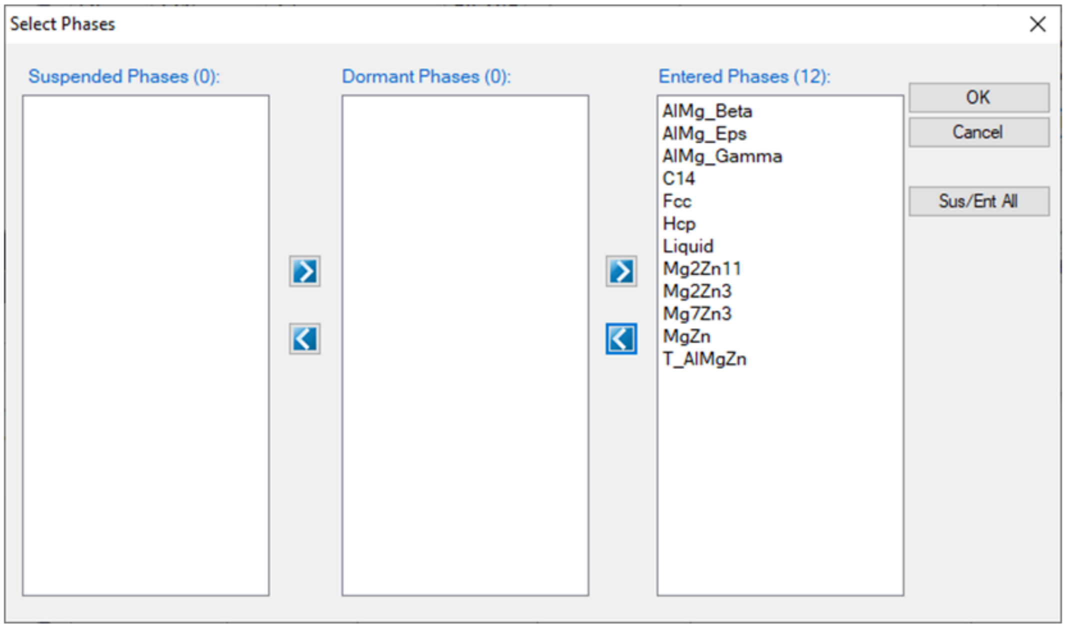
Drag and drop available columns to setup a new table. Double click property cell to edit.

Description: Temperature

(a) (b)

Figure 3.13 Set extra output table for point calculation

The **Select Phases** button in Figure 3.12(a) leads the user to a dialog which allows the user to select or deselect phases to be involved in the calculation as shown in Figure 3.14. The default setting is that all the phases in the system are selected and listed in the **Entered Phases** column, which means all the phases are involved in the equilibrium calculation. User can select the phases that will not participate in the equilibrium calculation by sending them to the **Dormant Phases** or **Suspended Phases** column using mouse to drag and drop or using the ◀ button. To select several phases at one time, hold the <Ctrl> key and use mouse to select multiple phases. The **Suspended Phases** means that the phases in that column are excluded in any calculations. The **Dormant Phases** means that the phases in that column are excluded from the equilibrium calculation but will be included for the property calculations, such as driving force, after the equilibrium calculation is finished. The **Dormant Phases** option mainly works for point calculation and line calculation. The **Suspended Phases** option is usually used for metastable phase equilibrium calculations.

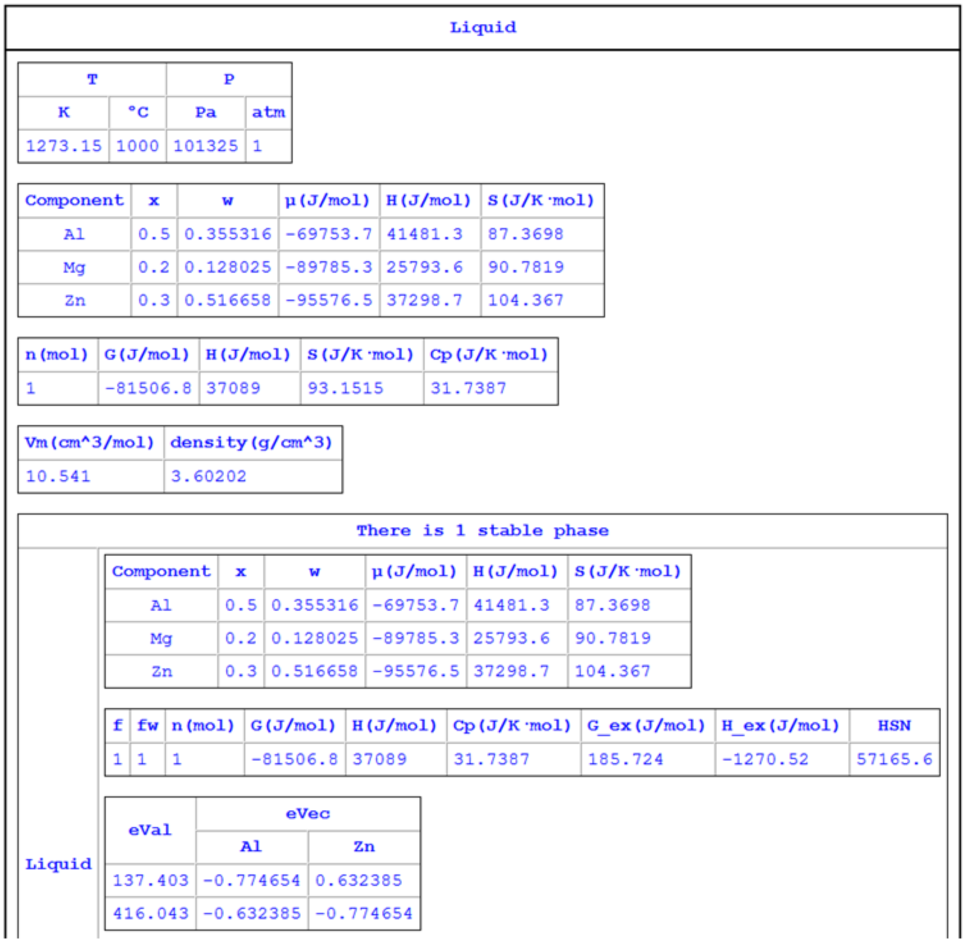


AlMg_Beta
AlMg_Eps
AlMg_Gamma
C14
Fcc
Hcp
Liquid
Mg2Zn11
Mg2Zn3
Mg7Zn3
MgZn
T_AlMgZn

Figure 3.14 Select Phases dialog

The **Select Comps** button in Figure 3.12(a) allows user to make last minute change on the component selection. Please refer to the previous section for information on the **Select Components** window.

After the calculation is completed, the calculated results are displayed in the Pandat™ main display window as shown in Figure 3.15. The listed properties include thermodynamic properties at this point, such as Gibbs energy, enthalpy, entropy and heat capacity. It also lists the stable phases and the fraction of each phase.



Liquid

T		P	
K	°C	Pa	atm
1273.15	1000	101325	1

Component	x	w	μ(J/mol)	H(J/mol)	S(J/K·mol)
Al	0.5	0.355316	-69753.7	41481.3	87.3698
Mg	0.2	0.128025	-89785.3	25793.6	90.7819
Zn	0.3	0.516658	-95576.5	37298.7	104.367

n(mol)	G(J/mol)	H(J/mol)	S(J/K·mol)	Cp(J/K·mol)
1	-81506.8	37089	93.1515	31.7387

Vm(cm^3/mol)	density(g/cm^3)
10.541	3.60202

There is 1 stable phase

Liquid

Component	x	w	μ(J/mol)	H(J/mol)	S(J/K·mol)
Al	0.5	0.355316	-69753.7	41481.3	87.3698
Mg	0.2	0.128025	-89785.3	25793.6	90.7819
Zn	0.3	0.516658	-95576.5	37298.7	104.367

f	fw	n(mol)	G(J/mol)	H(J/mol)	Cp(J/K·mol)	G_ex(J/mol)	H_ex(J/mol)	HSN
1	1	1	-81506.8	37089	31.7387	185.724	-1270.52	57165.6

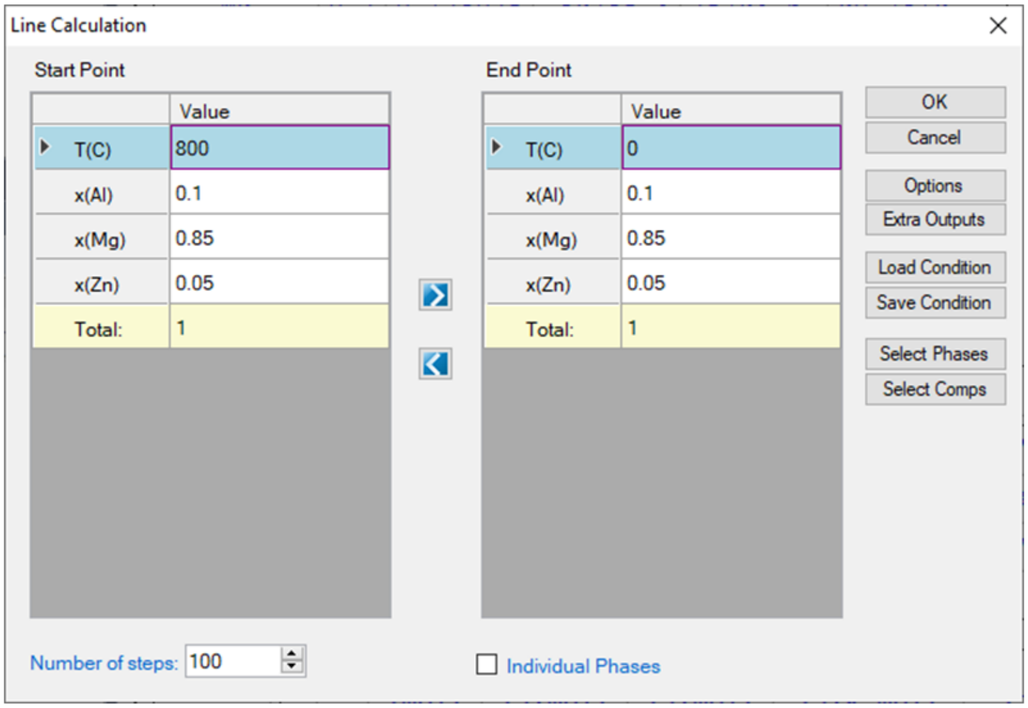
eVal	eVec	
	Al	Zn
137.403	-0.774654	0.632385
416.043	-0.632385	-0.774654

Figure 3.15 Results of point calculation

3.3.2 Line Calculation (1D)

This function allows the user to perform a series of point calculations along a line in a multicomponent system.

Go to **PanPhaseDiagram** on the menu bar and select **Line Calculation** or click the ⊟ button on the tool bar. The **Line Calculation** (1D) dialog box allows the user to set the start and end points of the line, and the number of steps to calculate along the line as shown in Figure 3.16. User can also access the **Options**, **Extra Outputs**, **Load Condition**, **Save Condition**, **Select Phases**, and **Select Comps** the same way as those in point calculation. Note that the line calculation set up in Figure 3.16 is along the line of fixing alloy chemistry with varying temperature.



Start Point

	Value
T(C)	800
x(Al)	0.1
x(Mg)	0.85
x(Zn)	0.05
Total:	1

End Point

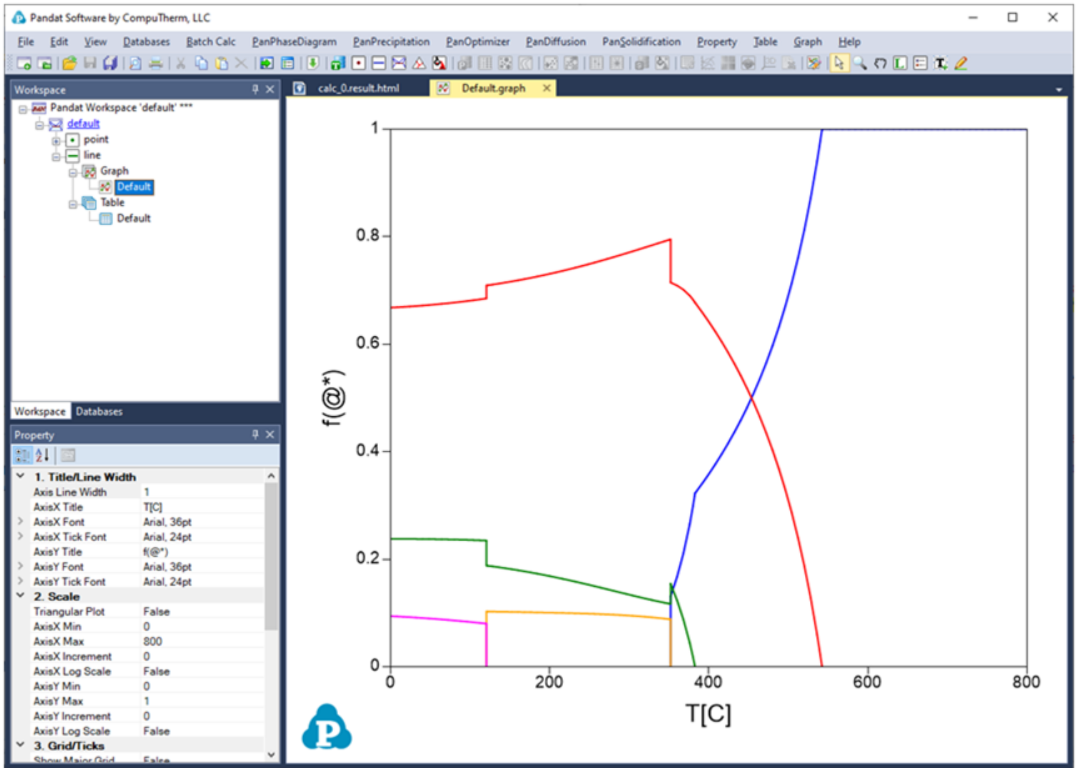
	Value
T(C)	0
x(Al)	0.1
x(Mg)	0.85
x(Zn)	0.05
Total:	1

Number of steps: 100

☐ Individual Phases

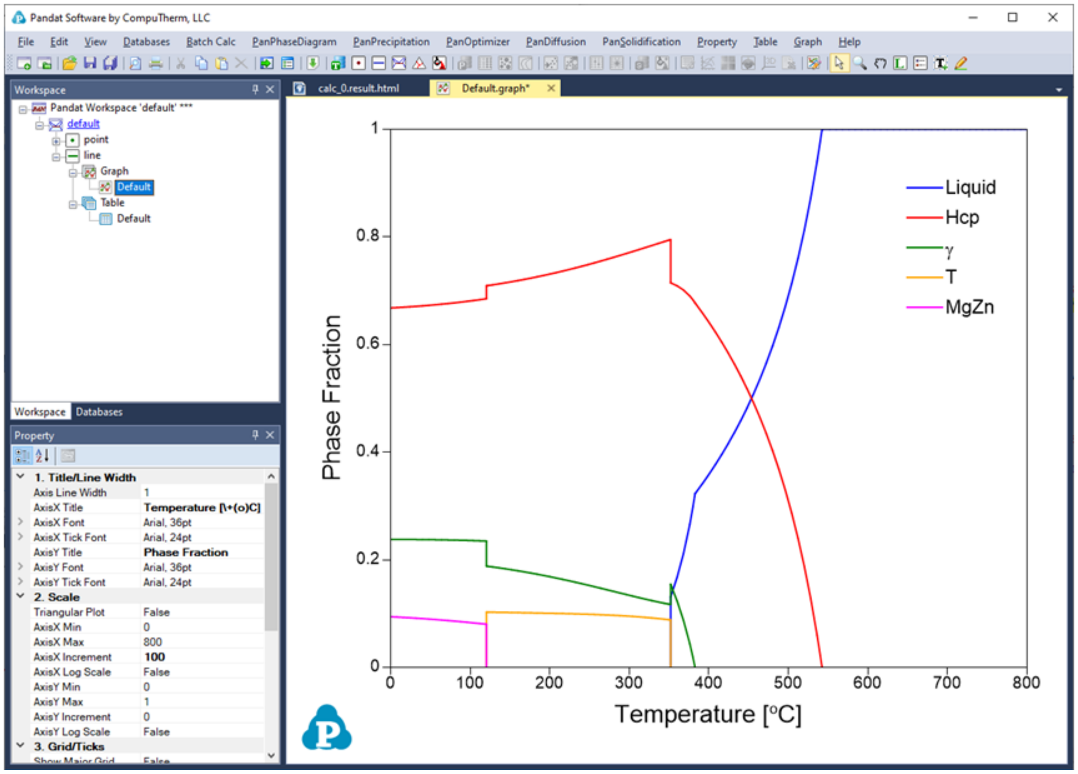
Figure 3.16 Set calculation conditions for a line calculation

The calculated results are stored in both graph and table. The default graph plots the variation of fraction of each phase with respect to temperature, as shown in Figure 3.17. User can modify the graph through the **Property** window by modifying the title, scale and add legend to get a better view as shown in Figure 3.18. In the **Explore** window, user can double click the “Default” under the “Table” tree to view the default table. User can select any columns to create new plots. Furthermore, select the “Table” and right click the mouse, user has the option to **Add a New Table** to generate new tables and then plot other figures as needed.



1. Title/Line Width	
Axis Line Width	1
AxisX Title	T[C]
AxisX Font	Arial, 36pt
AxisX Tick Font	Arial, 24pt
AxisY Title	f(@*)
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
2. Scale	
Triangular Plot	False
AxisX Min	0
AxisX Max	800
AxisX Increment	0
AxisX Log Scale	False
AxisY Min	0
AxisY Max	1
AxisY Increment	0
AxisY Log Scale	False
3. Grid/Ticks	
Show Major Grid	False

Figure 3.17 Default graph view of the line calculation result



1. Title/Line Width	
Axis Line Width	1
AxisX Title	**Temperature [\+(o)C]**
AxisX Font	Arial, 36pt
AxisX Tick Font	Arial, 24pt
AxisY Title	**Phase Fraction**
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
2. Scale	
Triangular Plot	False
AxisX Min	0
AxisX Max	800
AxisX Increment	**100**
AxisX Log Scale	False
AxisY Min	0
AxisY Max	1
AxisY Increment	0
AxisY Log Scale	False
3. Grid/Ticks	
Show Major Grid	False

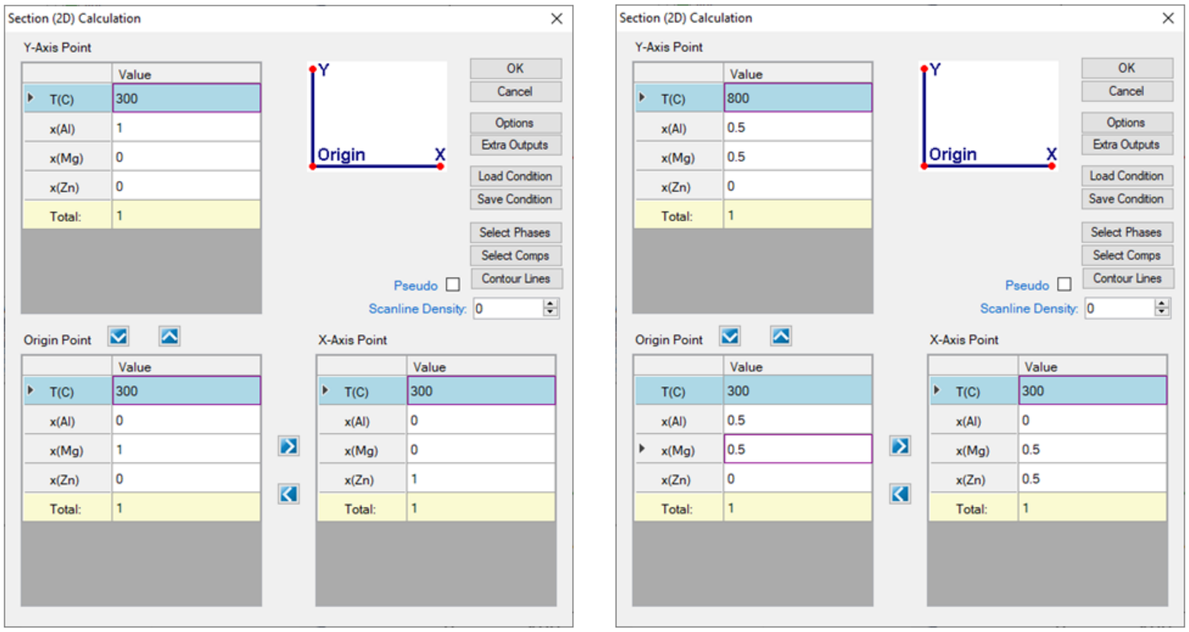
Figure 3.18 Modify the graph with a better view

It should be pointed out that user can certainly choose to fix the temperature and vary the alloy composition for a line calculation.

3.3.3 Section Calculation (2D)

This function allows user to calculate any two-dimensional section of a multicomponent system. Three non-collinear points in the calculation space are required to define a 2D section. Common 2D section diagrams are isotherms and isopleths.

Go to **PanPhaseDiagram** on the menu bar and select **Section Calculation** or click the button on the tool bar. The **Section (2D) Calculation** dialog box allows the user to set up the calculation conditions in terms of composition and temperature. Figure 3.19 shows the two most common 2D calculations for a ternary system: (a) Isotherm which is a horizontal section that fixes the temperature and (b) Isopleth which is a vertical section that uses the temperature as the Y axis.



(a)

Pseudo ☐

Scanline Density: 0

Y-Axis Point

	Value
T(C)	300
x(Al)	1
x(Mg)	0
x(Zn)	0
Total:	1

Origin Point

	Value
T(C)	300
x(Al)	0
x(Mg)	1
x(Zn)	0
Total:	1

X-Axis Point

	Value
T(C)	300
x(Al)	0
x(Mg)	0
x(Zn)	1
Total:	1

(b)

Pseudo ☐

Scanline Density: 0

Y-Axis Point

	Value
T(C)	800
x(Al)	0.5
x(Mg)	0.5
x(Zn)	0
Total:	1

Origin Point

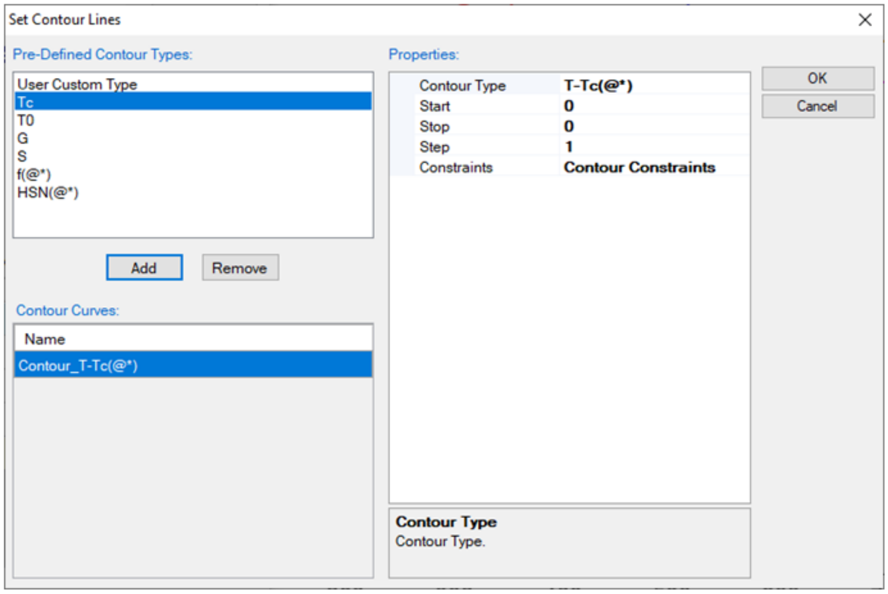
	Value
T(C)	300
x(Al)	0.5
x(Mg)	0.5
x(Zn)	0
Total:	1

X-Axis Point

	Value
T(C)	300
x(Al)	0
x(Mg)	0.5
x(Zn)	0.5
Total:	1

Figure 3.19 Set calculation conditions for section calculation

The composition at each point should be self-consistent. For example, $x(Al)+x(Mg)+x(Zn)=1$ for the Al-Mg-Zn ternary system. It is not necessary to have a correlation between the **Y-Axis** point, the **Origin** point and the **X-Axis** point. User can also access the **Options**, **Extra Outputs**, **Load Condition**, **Save Condition**, **Select Phases**, and **Select Comps** windows through this dialog box. The **Contour Lines** option allows the user to add special lines to the output results, such as Tc curve and T_0 curve as shown in Figure 3.20.



Contour_T-Tc(@*)

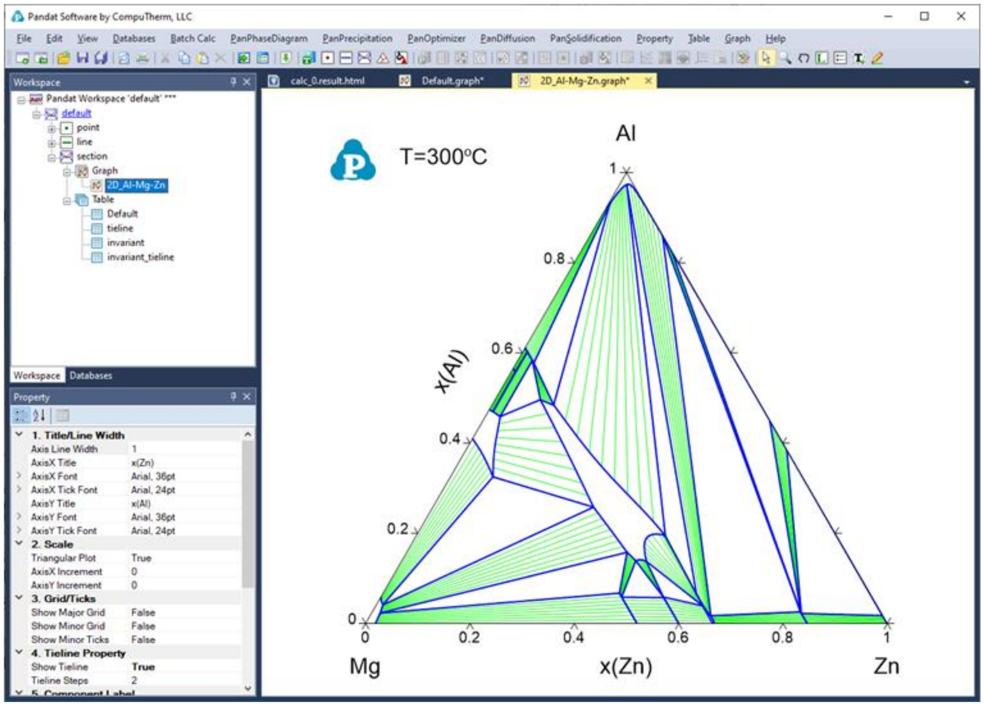
Contour Type	T-Tc(@*)
Start	0
Stop	0
Step	1
Constraints	Contour Constraints

Contour Type
Contour Type.

Figure 3.20 Contour Lines dialog

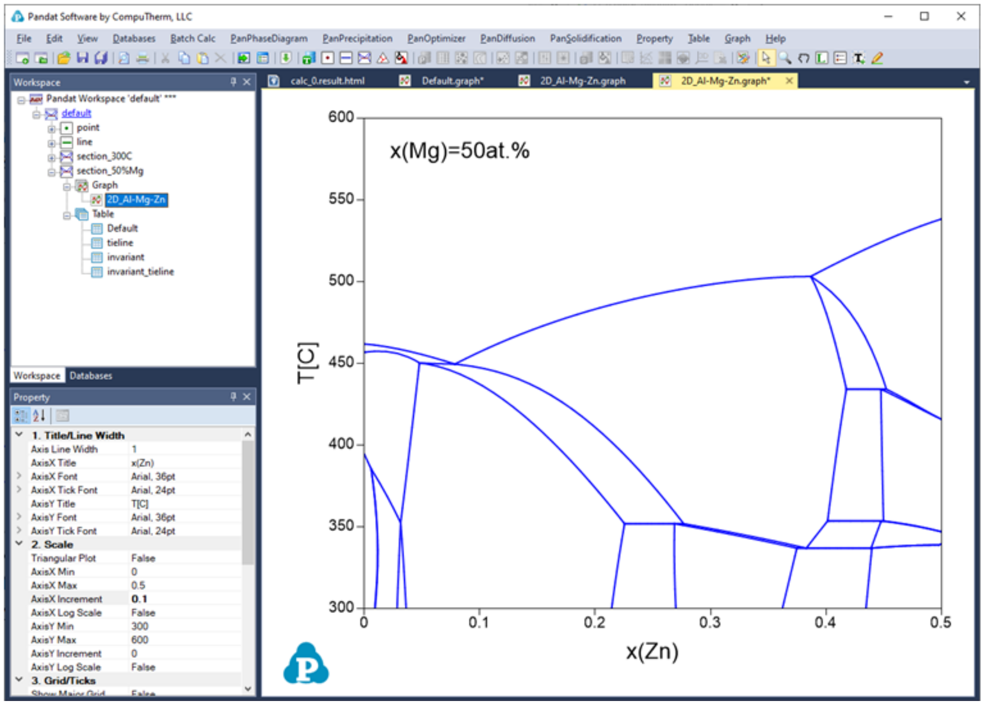
The setting on Figure 3.19(a) defines a calculation of an isothermal section for the Al-Mg-Zn ternary system at $300^{o}C$. The setting on Figure 3.19(b) defines a vertical section calculation from the middle of the Al-Mg binary to the middle of the Mg-Zn binary in the temperature range of $300\text{-}800^{o}C$. The results from a Section calculation are displayed in two types of format in the Pandat™ main window: Graph and Table. Figure 3.21 and Figure 3.22 show the graph view of the calculation results for the settings in Figure 3.19 (a) and (b), respectively. Figure 3.23 shows a table view of the isotherm calculation result. User can switch between Graph view and Table View by double clicking on the graph name or table name in the Pandat™ Explore window. Other operations on

Graph and **Table**, such as labeling and adding a legend, have been discussed in details in **Section 2.3** and **Section 2.4**.



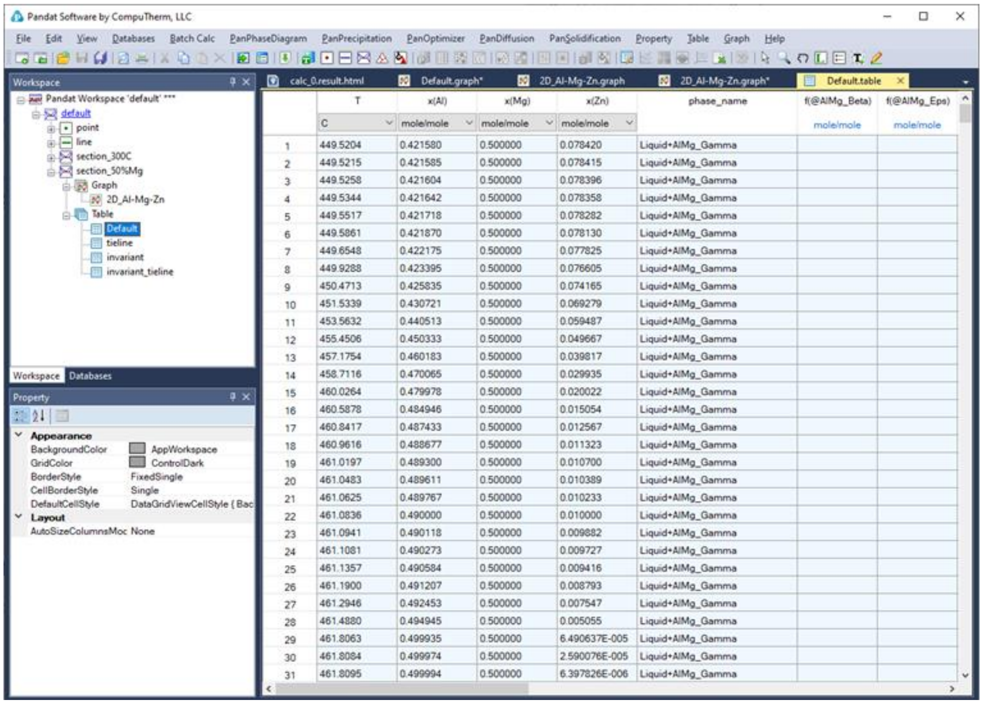
1. Title/Line Width	
Axis Line Width	1
AxisX Title	x(Zn)
AxisX Font	Arial, 36pt
AxisX Tick Font	Arial, 24pt
AxisY Title	x(Al)
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
2. Scale	
Triangular Plot	True
AxisX Increment	0
AxisY Increment	0
3. Grid/Ticks	
Show Major Grid	False
Show Minor Grid	False
Show Minor Ticks	False
4. Tieline Property	
Show Tieline	True
Tieline Steps	2
5. Component Label	

Figure 3.21 Isothermal section of the Al-Mg-Zn ternary system at 300°C



1. Title/Line Width	
Axis Line Width	1
AxisX Title	x(Zn)
AxisX Font	Arial, 36pt
AxisX Tick Font	Arial, 24pt
AxisY Title	T[C]
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
2. Scale	
Triangular Plot	False
AxisX Min	0
AxisX Max	0.5
AxisX Increment	0.1
AxisX Log Scale	False
AxisY Min	300
AxisY Max	600
AxisY Increment	0
AxisY Log Scale	False
3. Grid/Ticks	
Show Major Grid	False

Figure 3.22 Isopleth of the Al-Mg-Zn ternary system at 50 at.% of Mg



Appearance

BackgroundColor	AppWorkspace
GridColor	ControlDark
BorderStyle	FixedSingle
CellBorderStyle	Single
DefaultCellStyle	DataGridViewCellStyle { Bac

Layout

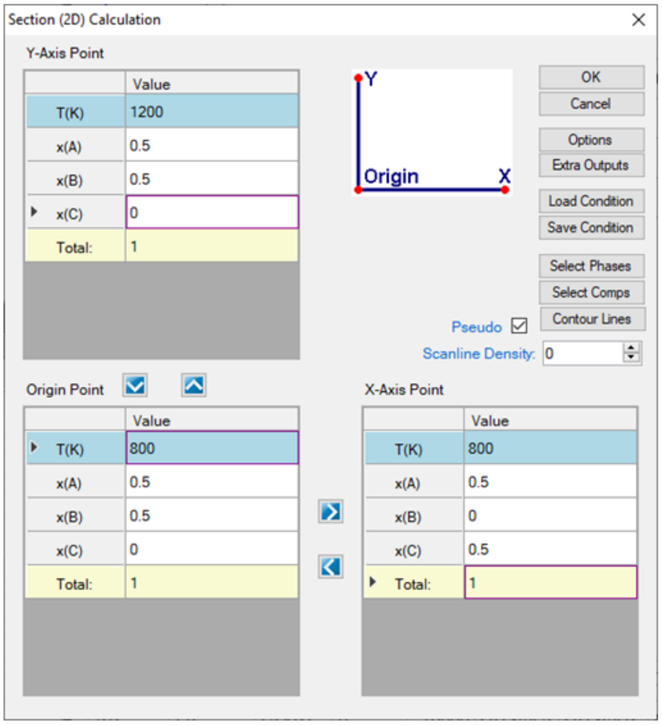
AutoSizeColumnsMoc	None

	T	x(Al)	x(Mg)	x(Zn)	phase_name	f(@AlMg_Beta)	f(@AlMg_Eps)
	C	mole/mole	mole/mole	mole/mole		mole/mole	mole/mole
1	449.5204	0.421580	0.500000	0.078420	Liquid+AlMg_Gamma		
2	449.5215	0.421585	0.500000	0.078415	Liquid+AlMg_Gamma		
3	449.5258	0.421604	0.500000	0.078396	Liquid+AlMg_Gamma		
4	449.5344	0.421642	0.500000	0.078358	Liquid+AlMg_Gamma		
5	449.5517	0.421718	0.500000	0.078282	Liquid+AlMg_Gamma		
6	449.5861	0.421870	0.500000	0.078130	Liquid+AlMg_Gamma		
7	449.6548	0.422175	0.500000	0.077825	Liquid+AlMg_Gamma		
8	449.9288	0.423395	0.500000	0.076605	Liquid+AlMg_Gamma		
9	450.4713	0.425835	0.500000	0.074165	Liquid+AlMg_Gamma		
10	451.5339	0.430721	0.500000	0.069279	Liquid+AlMg_Gamma		
11	453.5632	0.440513	0.500000	0.059487	Liquid+AlMg_Gamma		
12	455.4506	0.450333	0.500000	0.049667	Liquid+AlMg_Gamma		
13	457.1754	0.460183	0.500000	0.039817	Liquid+AlMg_Gamma		
14	458.7116	0.470065	0.500000	0.029935	Liquid+AlMg_Gamma		
15	460.0264	0.479978	0.500000	0.020022	Liquid+AlMg_Gamma		
16	460.5878	0.484946	0.500000	0.015054	Liquid+AlMg_Gamma		
17	460.8417	0.487433	0.500000	0.012567	Liquid+AlMg_Gamma		
18	460.9616	0.488677	0.500000	0.011323	Liquid+AlMg_Gamma		
19	461.0197	0.489300	0.500000	0.010700	Liquid+AlMg_Gamma		
20	461.0483	0.489611	0.500000	0.010389	Liquid+AlMg_Gamma		
21	461.0625	0.489767	0.500000	0.010233	Liquid+AlMg_Gamma		
22	461.0836	0.490000	0.500000	0.010000	Liquid+AlMg_Gamma		
23	461.0941	0.490118	0.500000	0.009882	Liquid+AlMg_Gamma		
24	461.1081	0.490273	0.500000	0.009727	Liquid+AlMg_Gamma		
25	461.1357	0.490584	0.500000	0.009416	Liquid+AlMg_Gamma		
26	461.1900	0.491207	0.500000	0.008793	Liquid+AlMg_Gamma		
27	461.2946	0.492453	0.500000	0.007547	Liquid+AlMg_Gamma		
28	461.4880	0.494945	0.500000	0.005055	Liquid+AlMg_Gamma		
29	461.8063	0.499935	0.500000	6.490637E-005	Liquid+AlMg_Gamma		
30	461.8084	0.499974	0.500000	2.590076E-005	Liquid+AlMg_Gamma		
31	461.8095	0.499994	0.500000	6.397826E-006	Liquid+AlMg_Gamma		

Figure 3.23 Table view for the 300°C isotherm calculation results

3.3.4 Pseudo Binary Section

Sometimes a ternary isoplethal section is so special that all the tie-lines are with this section to form a pseudo binary section. To calculate this type of section, a special algorithm is designed in Pandat™ and a special keyword "`pseudo`" is required. In the folder where Pandat™ software is installed: Pandat 2020 Examples`/PanPhaseDiagram/Pseudo_Binary/`, there is an example `A-B-C` system with "`Pseudo_Binary.tdb`". After load the database file, click on "`Section Calculation`". Set the calculation condition and check the "`Pseudo`" box, as shown in Figure 3.24. The calculated pseudo binary section is shown in Figure 3.25.


Section (2D) Calculation

Y-Axis Point

	Value
T(K)	1200
x(A)	0.5
x(B)	0.5
x(C)	0
Total:	1

Origin Point

	Value
T(K)	800
x(A)	0.5
x(B)	0.5
x(C)	0
Total:	1

X-Axis Point

	Value
T(K)	800
x(A)	0.5
x(B)	0
x(C)	0.5
Total:	1

Pseudo ☑

Scanline Density: 0

Figure 3.24 Set calculation condition for a pseudo-binary section

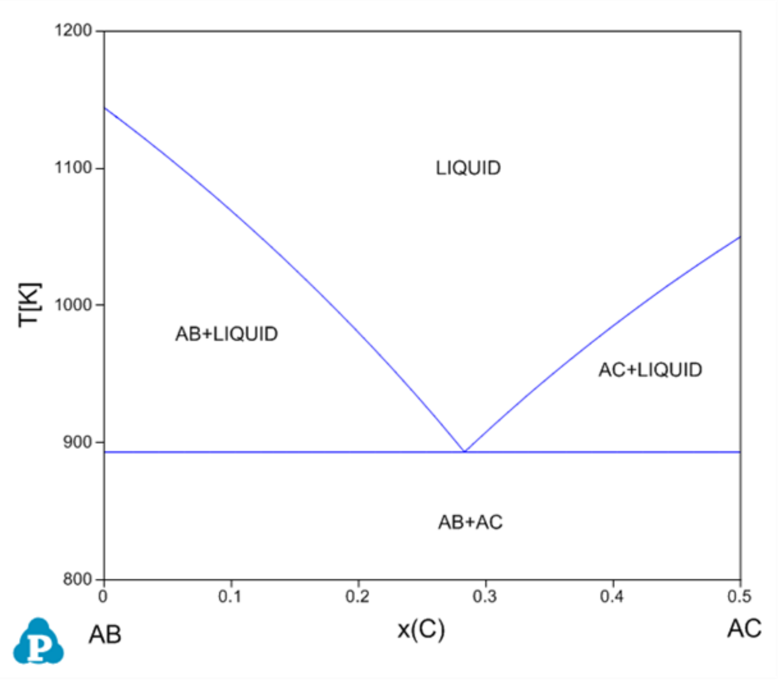


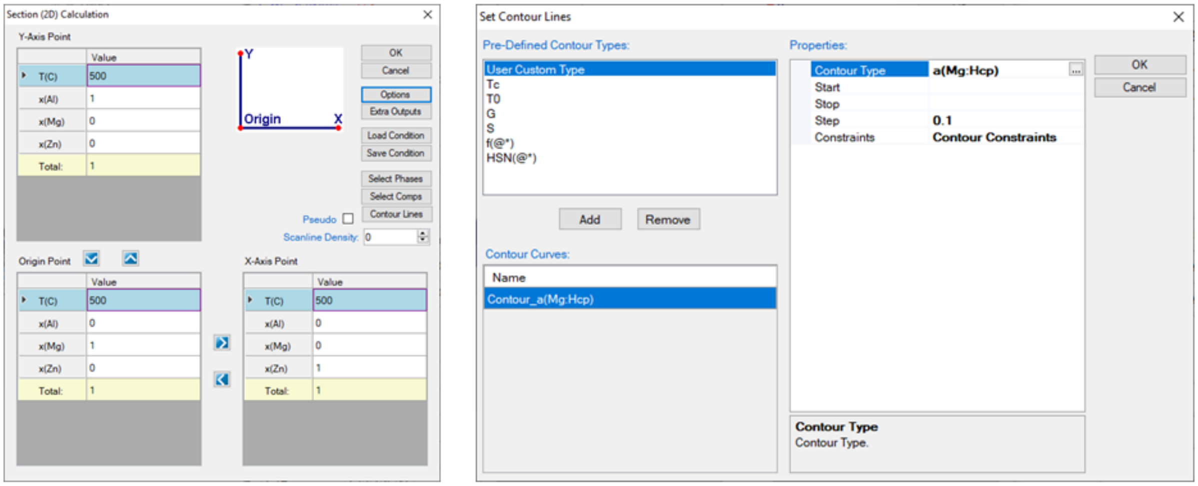
Figure 3.25 A pseudo-binary section in a ternary A-B-C system

3.3.5 Contour Diagram

Contour diagram shows how a property changes in a 2D or 3D diagram [2015Che]. The most commonly used contour diagram is the ternary isothermal lines superimposed on a liquidus projection. Another example is the activity contour diagram. Pandat™ extends contour diagram to many other properties including thermodynamic properties, physical properties and any combination of them. In the following, we will give a few examples of useful contour diagrams. Please keep in mind that Pandat™ can plot many other contour diagrams beyond these examples.

3.3.5.1 Activity Contour Diagram

Let’s use the contour diagram of Mg activity in Al-Mg-Zn as the first example. Figure 3.26(a) shows the input window for calculating the isothermal section of Al-Mg-Zn at 500°C. In this input window, there is a button “Contour Lines”. Click on the “Contour Lines” button, a new window “Set Contour Lines” will pop out, as shown in Figure 3.26(b). Click on “Add” button and change the “Contour Type” to “a(Mg:Hcp)”, which means that the contour diagram is for the activity of Mg with reference state of Hcp. There are three initials related to which values of the contour lines to be calculated: “Start”, “Stop” and “Step”. In this example, “Start” and “Stop” can be left as empty and Pandat™ will search for all possible values. User can set values for “Start” and “Stop” for specific range of the contour lines. However, the value of “Step” must be given. Another condition “Constraints” will be explained later. Figure 3.26(b) sets the initial condition to calculate the contour lines for the activity of Mg referring to Mg in Hcp phase with the step size of 0.1. Click “OK” in this window and also in the “Section (2D) Calculation” window to proceed with the calculation. The calculated isothermal diagram with the contour lines of activity of Mg is shown in Figure 3.27 after labeling.



Y-Axis Point

	Value
T(C)	500
x(Al)	1
x(Mg)	0
x(Zn)	0
Total:	1

Pseudo ☐

Scanline Density: 0

Origin Point

	Value
T(C)	500
x(Al)	0
x(Mg)	1
x(Zn)	0
Total:	1

X-Axis Point

	Value
T(C)	500
x(Al)	0
x(Mg)	0
x(Zn)	1
Total:	1

Pre-Defined Contour Types:

- User Custom Type
- Tc
- T0
- G
- S
- f(@*)
- HSN(@*)

Properties:

Contour Type	a(Mg:Hcp)
Start	
Stop	
Step	0.1
Constraints	Contour Constraints

Contour Curves:

Name
Contour_a(Mg:Hcp)

Contour Type
Contour Type.

(a) 2D Diagram input window (b) Contour Diagram input window

Figure 3.26 Input windows for contour diagram of activity of Mg at 500°C

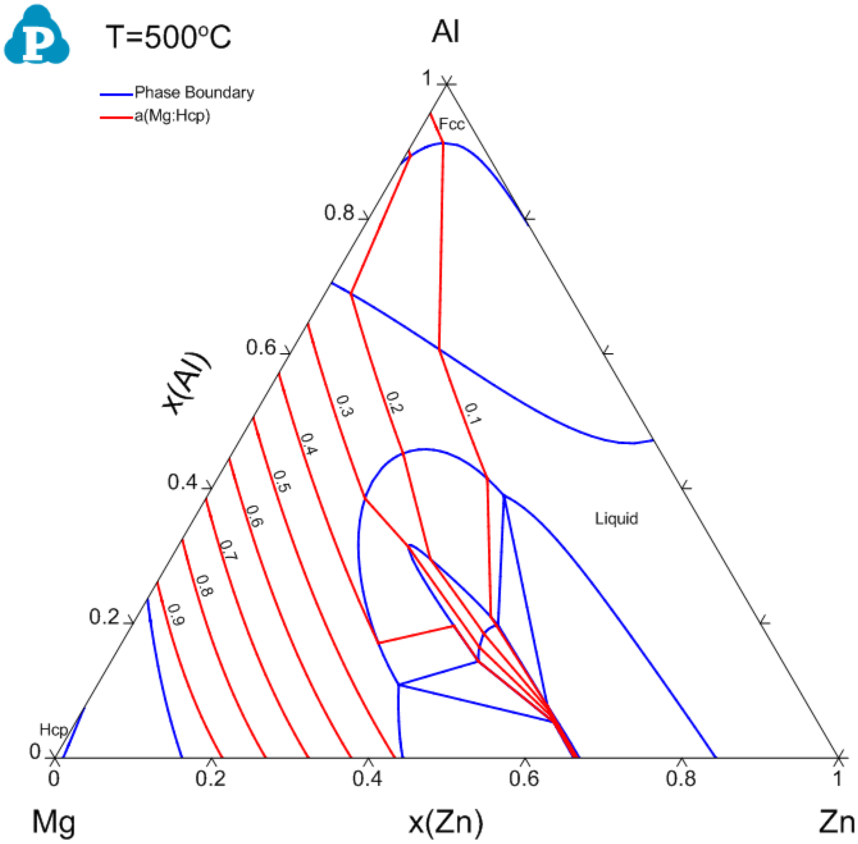


Figure 3.27 Contour diagram of activity of Mg in the isothermal section of Al-Mg-Zn at 500°C

If we want to calculate the contour lines of the Mg activity only in the liquid phase, it can be achieved by setting a constraint in the contour diagram input condition. In Figure 3.26(b), click on "`Contour Constraints`", a small button ... will show up. Click on it, we will have a window of "`Set Contour Constraints`" as shown in Figure 3.29. Add "`f(@Liquid)=1`" as the constraint in this window and then click "`OK`" to return to "`Set Contour Lines`" window as in Figure 3.29. This will set a constraint on the contour line calculation that only the contour lines with "`f(@Liquid)=1`" will be calculated. Figure 3.30 is the calculated phase diagram with the contour diagram of `a(Mg)` only in the liquid phase region in the isothermal section of Al-Mg-Zn at 500°C.

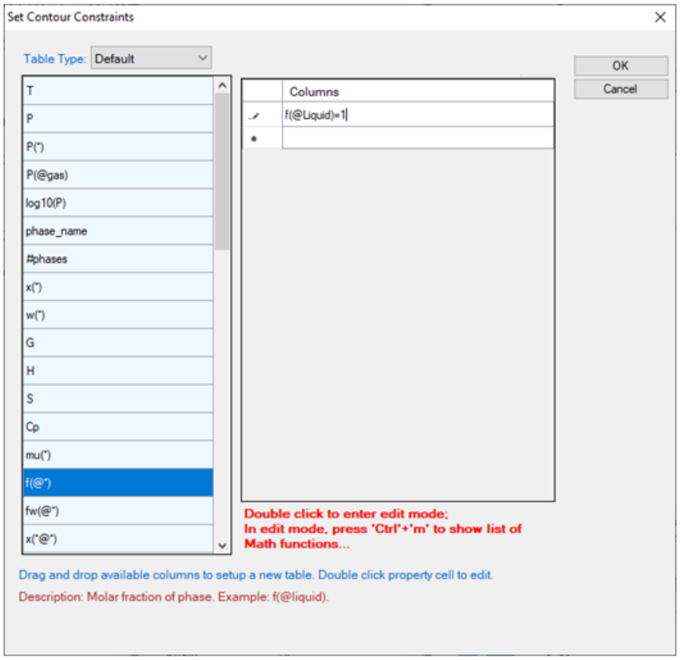


Table Type: Default

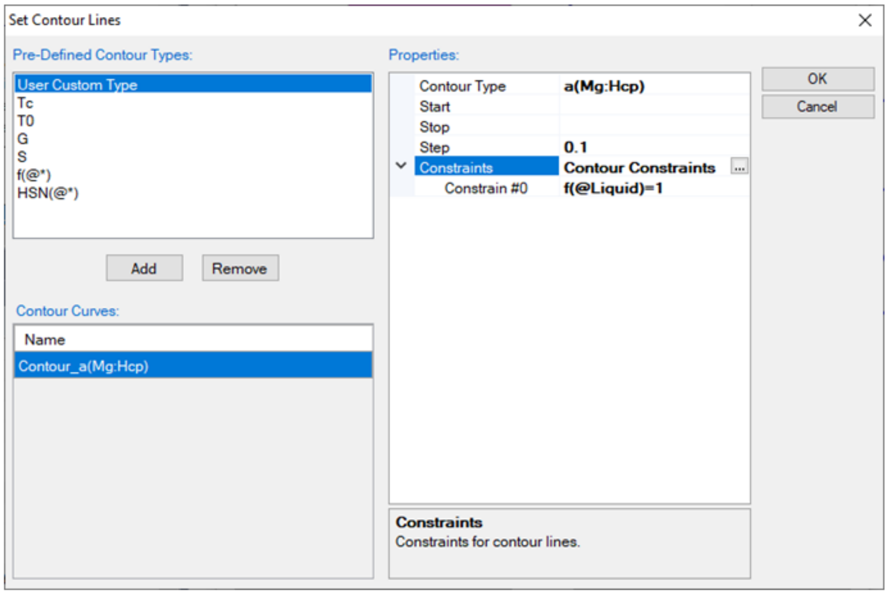
f(@Liquid)=1

Double click to enter edit mode;
In edit mode, press 'Ctrl'+'m' to show list of Math functions...

Drag and drop available columns to setup a new table. Double click property cell to edit.

Description: Molar fraction of phase. Example: f(@liquid).

Figure 3.28 Set contour constraints window



Contour_a(Mg:Hcp)

Properties	
Contour Type	a(Mg:Hcp)
Start	
Stop	
Step	0.1
Constraints	Contour Constraints
Constrain #0	f(@Liquid)=1

Constraints
Constraints for contour lines.

Figure 3.29 Input windows for setting constraints for the contour diagram

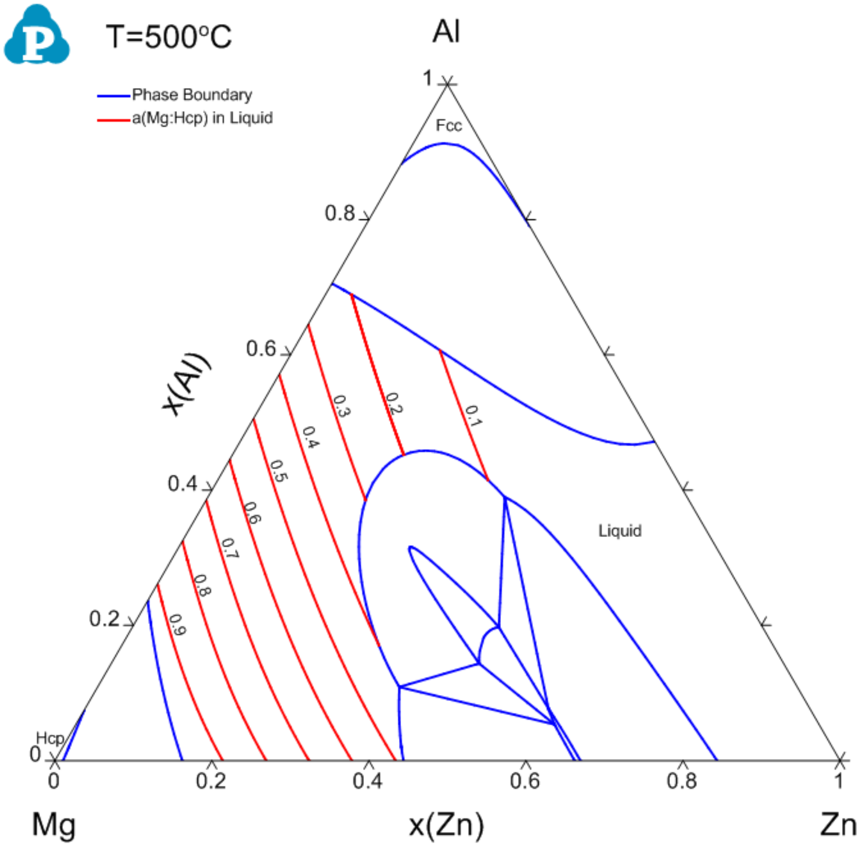
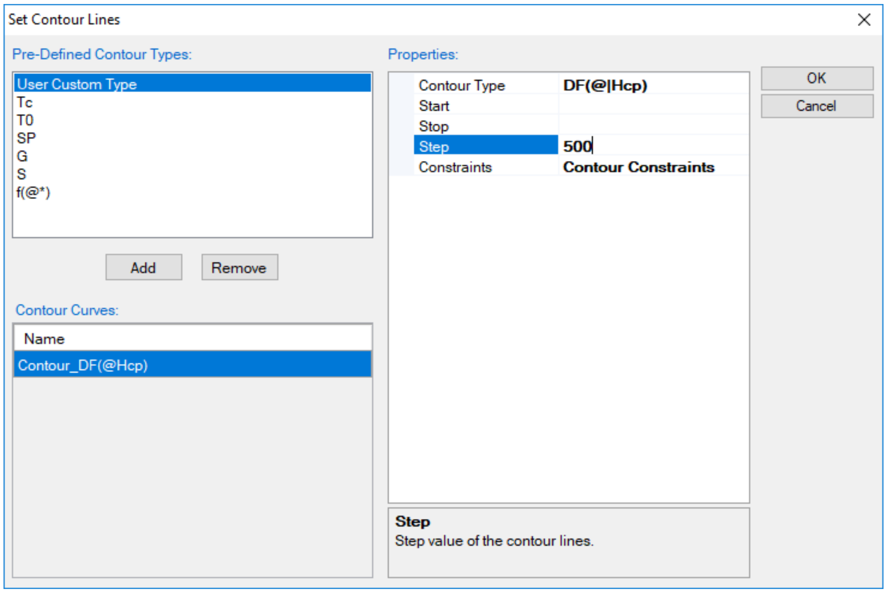


Figure 3.30 Contour diagram of activity of Mg only in liquid phase in the isothermal section of Al-Mg-Zn at 500°C

3.3.5.2 Driving Force Contour Diagram

Contour diagram is also useful in viewing the stability of a phase comparing to the equilibrium state. Figure 3.31 shows the driving force contour lines of the `Hcp` phase in the Al-Mg-Zn system at 500°C. The contour type is defined as `DF(@|Hcp)` as shown in Figure 3.31 (see Table 2.2 for the definition of `DF`). Since `Hcp` phase may not be stable in all the phase regions in this isothermal section, in between "`@`" and "`Hcp`" a vertical bar symbol "`|`" is added to specify that the phase `Hcp` is in the "`entered`" status. From Figure 3.32, we see that `Hcp` phase has less driving force to be stable in the central region of the compositional triangle.



Contour_DF(@Hcp)

Contour Type	DF(@|Hcp)
Start	
Stop	
Step	500
Constraints	Contour Constraints

Step
Step value of the contour lines.

Figure 3.31 Set driving force contour

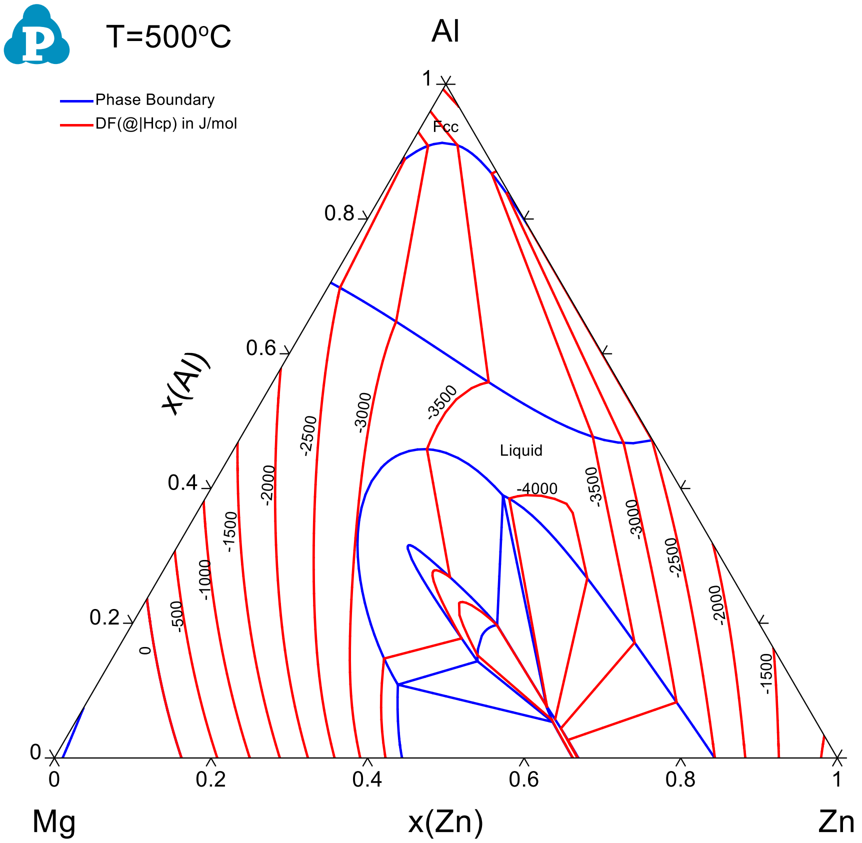


Figure 3.32 Contour diagram of the driving force of the Hcp phase relative to the equilibrium phases in Al-Mg-Zn at 500°C

3.3.5.3 Partial Molar Property Diagram

Partial molar properties such as partial molar enthalpy and entropy of a component can also be calculated as a contour diagram along with the phase diagram. The red curves in Figure 3.33 and Figure 3.34 are the calculated contour curves of the partial molar enthalpy and entropy of Zn in the liquid phase for the Al-Zn system. The constraints in both calculations are `f(@Liuid)>0` since the calculation is for the stable liquid phase only.

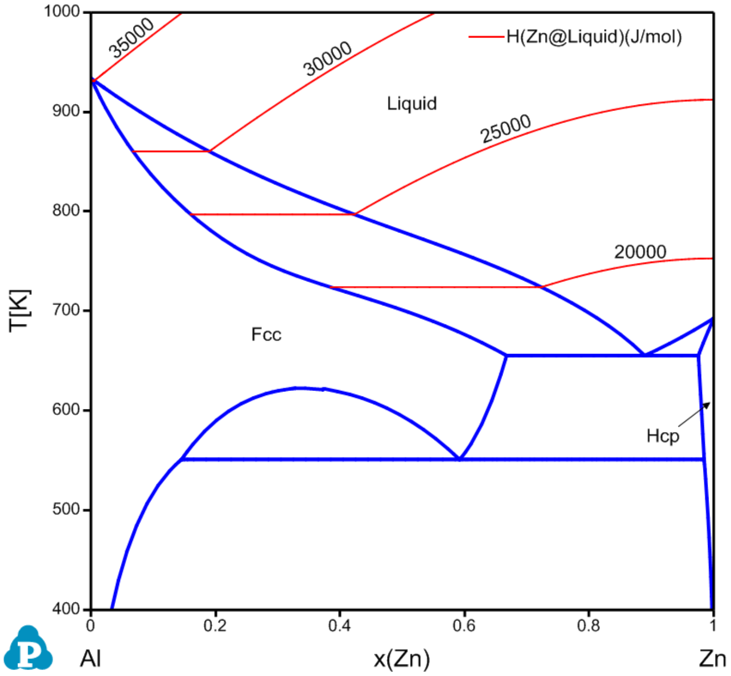


Figure 3.33 Contour diagram of the partial molar enthalpy of Zn in the liquid phase of Al-Zn system.

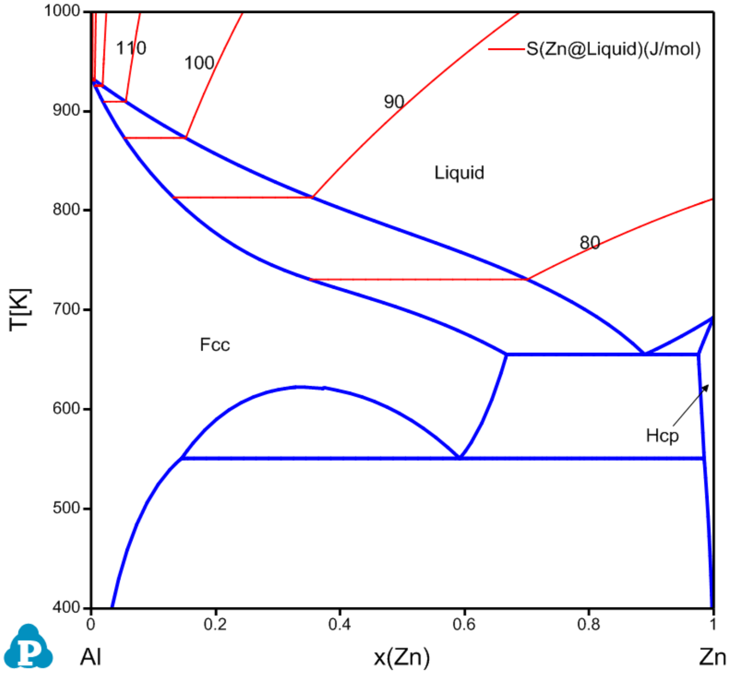


Figure 3.34 Contour diagram of the partial molar entropy of Zn in the liquid phase of Al-Zn system.

3.3.5.4 Excess Molar Property Diagram

Sometimes we have interest in the excess properties, such as excess Gibbs free energy, excess enthalpy and excess entropy of a phase. These properties are available from the property definitions of `G_ex`, `H_ex` and `S_ex` in a contour diagram. Figure 3.35, Figure 3.36 and Figure 3.37 show the calculated contour curves for the excess properties of liquid in the Mg-Zn system.

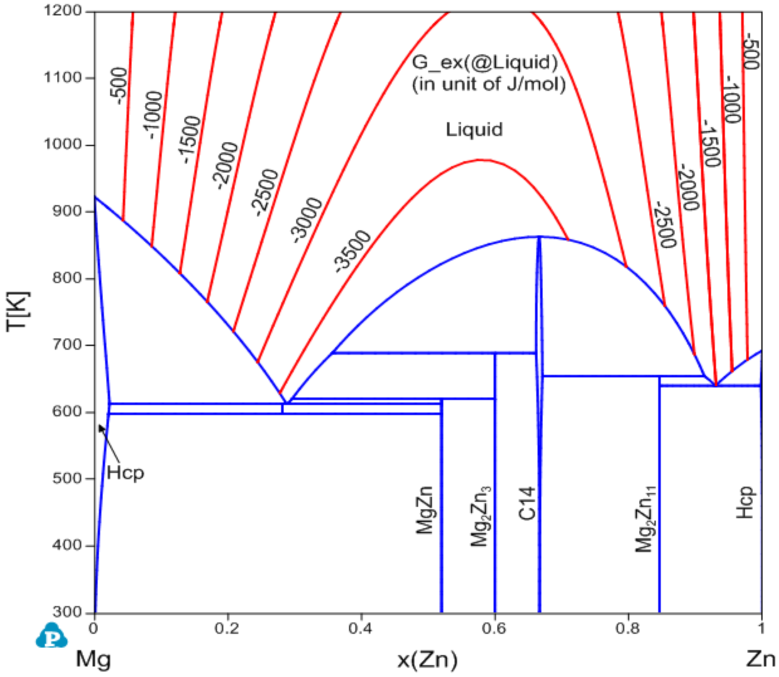


Figure 3.35 Contour diagram of the excess Gibbs free energy in the liquid phase of Mg-Zn system.

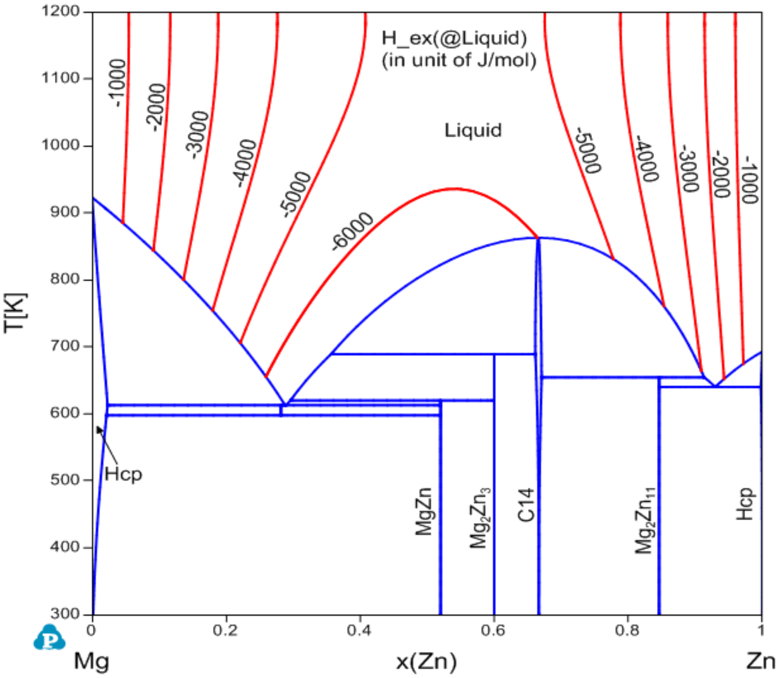


Figure 3.36 Contour diagram of the excess enthalpy in the liquid phase of Mg-Zn system.

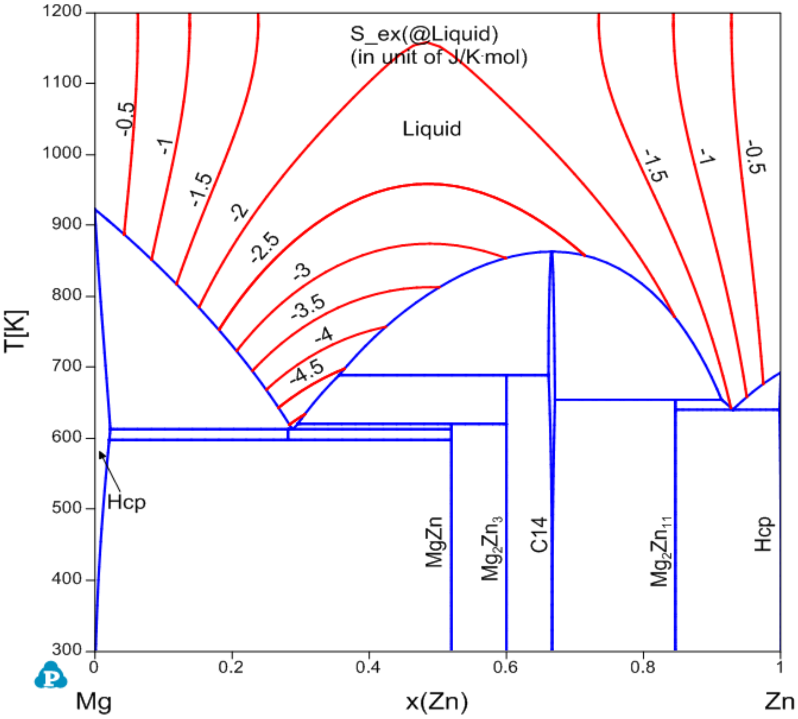
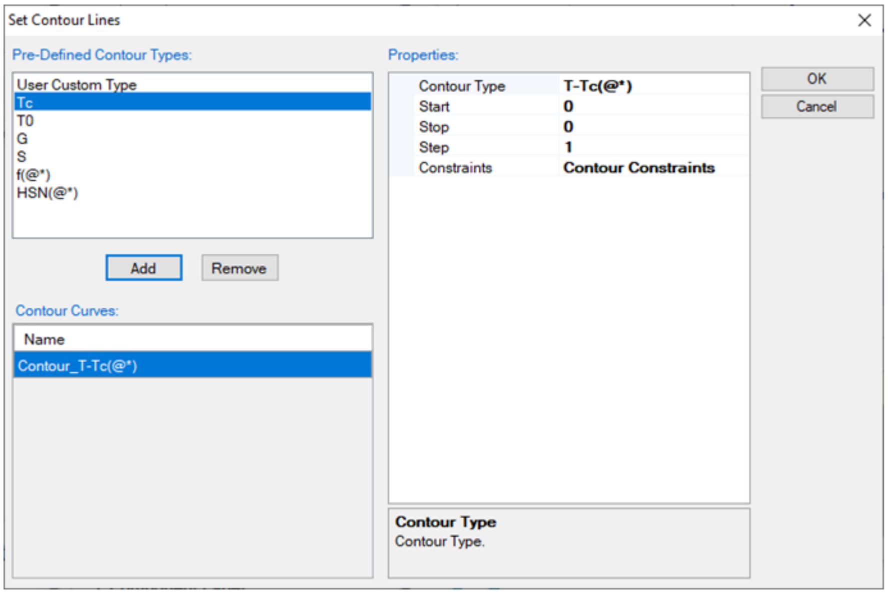


Figure 3.37 Contour diagram of the excess entropy in the liquid phase of Mg-Zn system.

3.3.5.5 User Defined Contour Diagram

Contour diagram can be any type of customized properties defined by the user using a mathematical expression. Contour diagram can therefore be used to plot some special property lines. For example, we want to calculate Curie temperature `Tc` curves in the Fe-Cr system. A `Tc` curve can be considered as a special contour line when `T` equals to `Tc`, which means the constraint: `T-Tc=0` is set on the `Tc` curve. Figure 3.38 is the input window for calculating the `Tc` contour curves. Since the constraint is `T-Tc(@*)=0`, the “`Start`” and “`Stop`” values are both set to be `zero`, and “`Step`” value is ignored. `@*` means in every phase. Figure 3.39 is the calculated Fe-Cr phase diagram with the `Tc` curves of the `Bcc` phase.



Contour_T-Tc(@*)

Contour Type	T-Tc(@*)
Start	0
Stop	0
Step	1
Constraints	Contour Constraints

Contour Type
Contour Type.

Figure 3.38 Input windows for `Tc` curves in Fe-Cr system

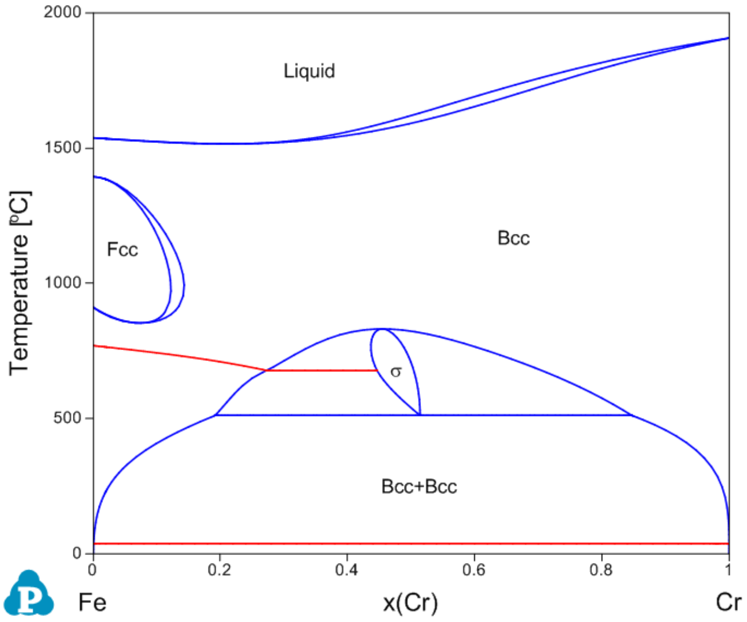


Figure 3.39 Phase diagram of Fe-Cr with Curie temperature curves (in red color) of Bcc phase

A second order transition curve could also be calculated as a contour curve. Fe-Al binary system [2009Sun] is given as an example here. Figure 3.40 is the calculated Fe-Al binary phase diagram with Tc curves and the second order transition curves. The Tc curves can be calculated the same way as that shown in this section for the Fe-Cr system.

The calculation of the second order transition needs special contour property definition. For the Bcc/B2, the contour property is defined as

```
abs(y(Fe#2@BCC_4SL)-y(Fe#3@BCC_4SL))
```

which represents the absolute value of the difference between the site fractions of Fe on the 2nd and 3rd sublattices. The "`start`" and "`stop`" values are set to be "`0.05`", which avoids the numerical difficulty in calculation and gives a very good approximation of the order/disorder transition curves.

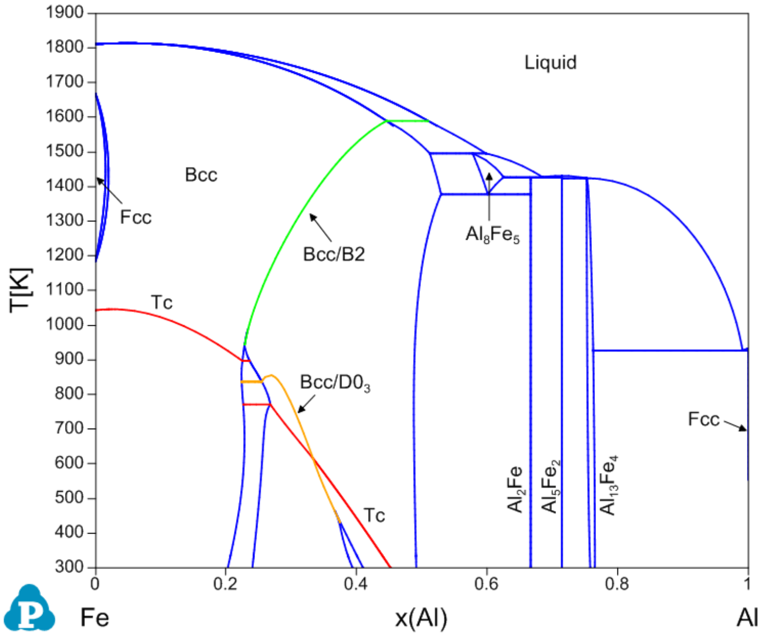


Figure 3.40 Phase Diagram of Fe-Al with the Tc curves and the 2nd order transition curves between Bcc and B2 and between B2 and $D0_3$.

The contour property for the second order transition between B2 and $D0_3$ is defined as

```
abs(y(Fe#3@BCC_4SL)-y(Fe#4@BCC_4SL))
```

with the "`start`" and "`stop`" values of "`0.05`". A constraint is also added in this contour calculation to make sure that the first and second sublattices have the same site fractions,

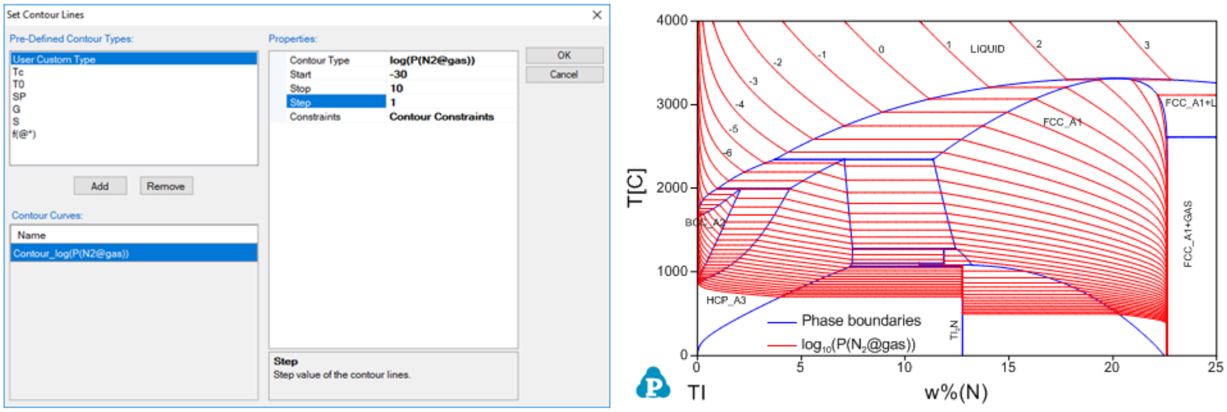
```
abs(y(Fe#1@BCC_4SL)-y(Fe#2@BCC_4SL))<0.001
```

Pandat™ batch file is written in the language of `XML`(*`Extensible Markup Language`*). The less-than "<" and great-than ">" characters are reserved as the `XML` special characters. In an `XML` file, the less-than "<" and great-than ">" symbols are written as "`<`" and "`>`". Above constraint is written in a Pandat batch file as

```
abs(y(Fe#1@BCC_4SL)-y(Fe#2@BCC_4SL))&lt;0.001
```

3.3.5.6 Partial Pressure Contour Diagram

The following example shows how to calculate the contour lines for the partial pressure of the gas phase in the Ti-N system [1996Zen]. Figure 3.41 (a) is the input condition window and Figure 3.41 (b) is the calculated phase diagram of Ti-N with the contour lines of log(P(N_2@gas)) (pressure unit is Pa), which is the common logarithm of the partial pressure of N_2 in gas. Figure 3.41 (c) is another input condition window and Figure 3.41 (d) is the calculated phase diagram of Ti-N with the contour lines of log(P(@gas)), which is the common logarithm of the total pressure of gas with the gas species N, N_2, N_3 and Ti.

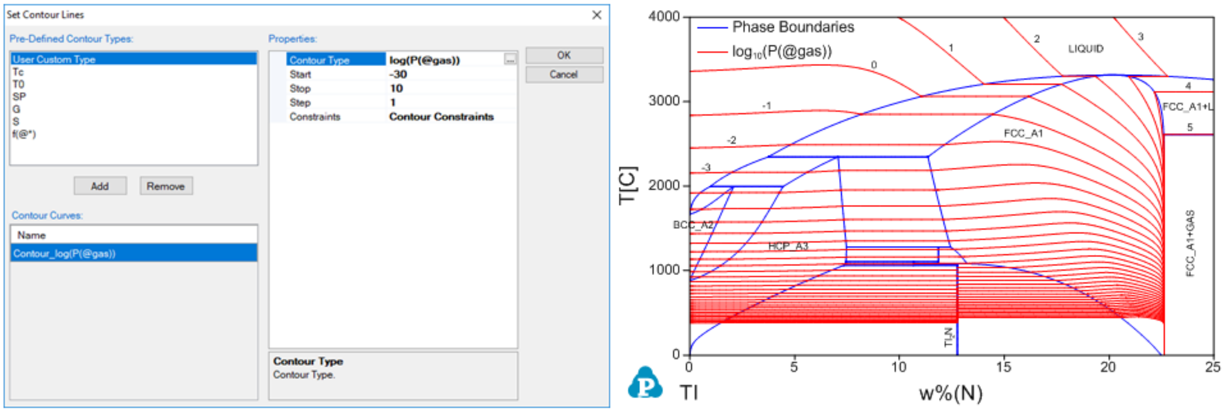


Contour_log(P(N2@gas))

Contour Type log(P(N2@gas))
Start -30
Stop 10
Step 1
Constraints Contour Constraints

Step
Step value of the contour lines.

(a) Input condition (b) log(P(N_2@gas)) contour



Contour_log(P(@gas))

Contour Type log(P(@gas))
Start -30
Stop 10
Step 1
Constraints Contour Constraints

Contour Type
Contour Type.

(c) Input condition (d) (log(P(@gas)) contour

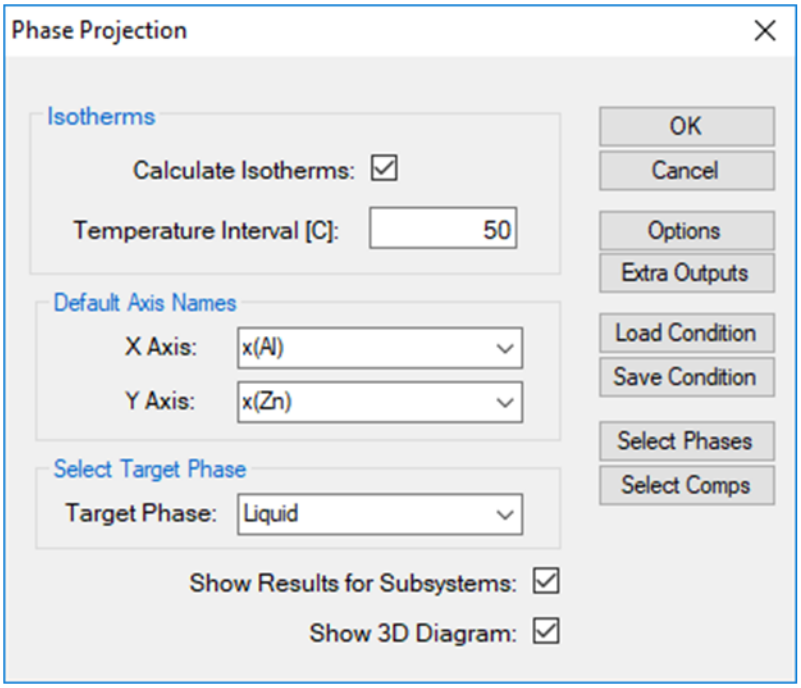
Figure 3.41 Contour diagrams of partial pressure of gas in the Ti-N system

More examples can be found in the Pandat example folder: `/PanPhaseDiagram/Contour/`.

3.3.6 Phase Projection

This function permits the calculation of a phase projection diagram for a system with two or more components. PanEngine automatically searches the univariant phase projection lines.

Go to **PanPhaseDiagram** on the menu bar and select **Phase Projection** or Click the button on the tool bar. The **Phase Projection** dialog box shown in Figure 3.42 allows the user to calculate projection of any phase in the system. If “Liquid” is selected as Target Phase, liquidus projection for the system is calculated. Isothermal curves involving the selected phase in a ternary system can also be calculated by checking the box **Calculate Isotherms**. The density of isothermal curves depends on the scale of **Temperature Interval**. A larger value for the temperature interval leads to fewer isothermal curves but with faster speed of calculation. The default **Compositional Range** is full range for each component. User can define the default output graph by selecting the X and Y axis. User can also access the **Options**, **Extra Outputs**, **Load Condition**, **Save Condition**, **Select Phases**, and **Select Comps** windows through this dialog box. If the **Show Results for Subsystems** box is checked, the output files will include the results for the subsystems together with the multicomponent system. Be aware that the output table will be huge if the box is checked for a calculation with a higher order multi-component system. User can choose the specific phase for projection calculation in the **Target Phase** dialog, such as Fcc phase. If “*” is selected, the projection for all the phases will be calculated. If the **Show 3D Diagram** box is checked, there will be an extra 3D diagram showing the calculation results as well as the original 2D diagram. For the 3D diagram, user can rotate the diagram by holding the left button of mouse and move it around.



Phase Projection

Isotherms

Calculate Isotherms: ☑

Temperature Interval [C]: 50

Default Axis Names

X Axis: x(Al)

Y Axis: x(Zn)

Select Target Phase

Target Phase: Liquid

Show Results for Subsystems: ☑

Show 3D Diagram: ☑

Figure 3.42 Phase projection calculation setting dialog

The results from a liquidus projection calculation are displayed in two types of format in the Pandat™ main window: Graph and Table. Figure 3.43 to Figure 3.46 show the 2D and 3D graph view, default table and isotherm table for the liquidus projection calculation results, respectively. Users can switch between Graph view to Table View by double clicking on the graph name or the table name in the Pandat™ Workspace window. Extensive operations on Graph and Table, such as labeling and adding legend, have been discussed in details in **Section 2.3** and **Section 2.4**.

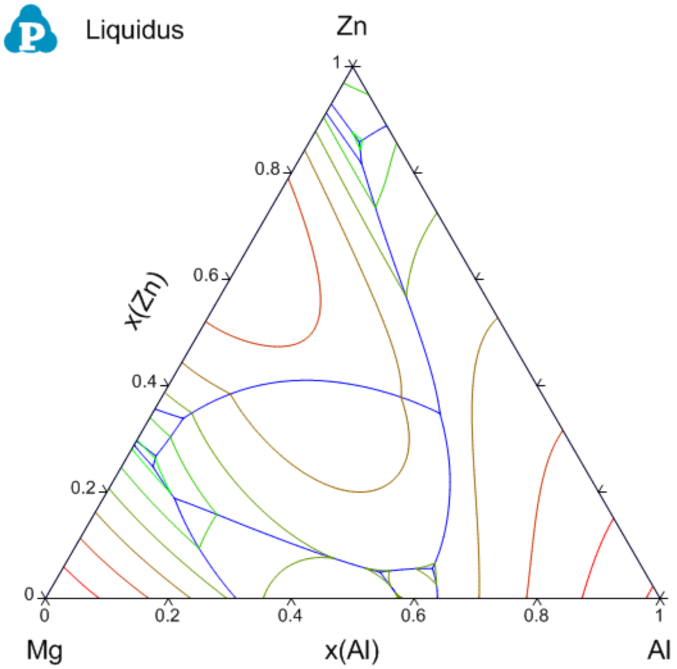


Figure 3.43 Liquidus projection in 2D of the Al-Mg-Zn ternary system

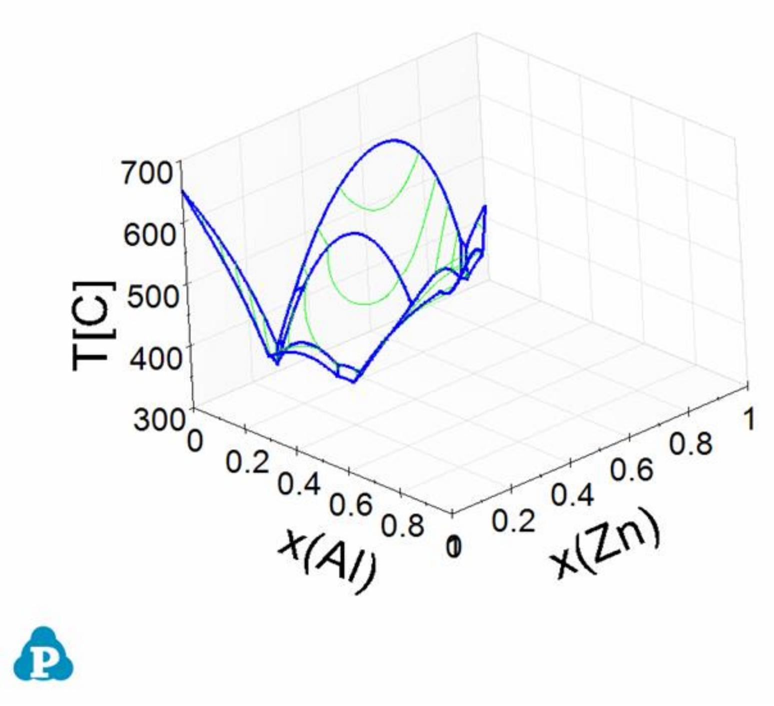
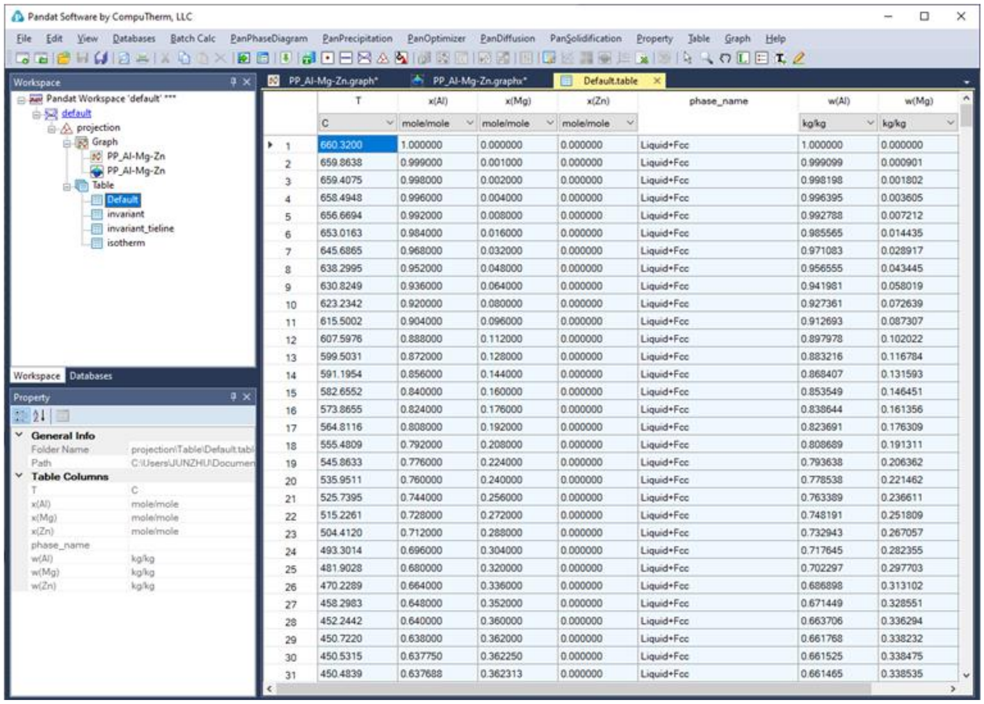


Figure 3.44 Liquidus projection in 3D of the Al-Mg-Zn ternary system



General Info

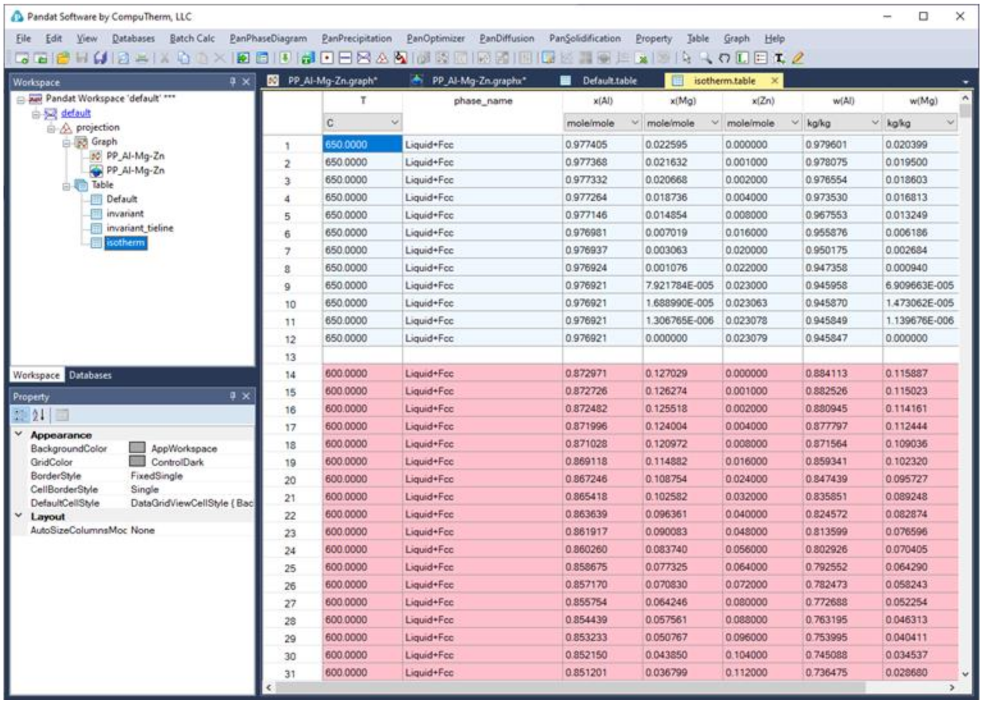
Folder Name	projection\Table\Default.tabl
Path	C:\Users\JUNZHU\Documen

Table Columns

T	C
x(Al)	mole/mole
x(Mg)	mole/mole
x(Zn)	mole/mole
phase_name	
w(Al)	kg/kg
w(Mg)	kg/kg
w(Zn)	kg/kg

	T	x(Al)	x(Mg)	x(Zn)	phase_name	w(Al)	w(Mg)
	C	mole/mole	mole/mole	mole/mole		kg/kg	kg/kg
1	660.3200	1.000000	0.000000	0.000000	Liquid+Fcc	1.000000	0.000000
2	659.8638	0.999000	0.001000	0.000000	Liquid+Fcc	0.999099	0.000901
3	659.4075	0.998000	0.002000	0.000000	Liquid+Fcc	0.998198	0.001802
4	658.4948	0.996000	0.004000	0.000000	Liquid+Fcc	0.996395	0.003605
5	656.6694	0.992000	0.008000	0.000000	Liquid+Fcc	0.992788	0.007212
6	653.0163	0.984000	0.016000	0.000000	Liquid+Fcc	0.985565	0.014435
7	645.6865	0.968000	0.032000	0.000000	Liquid+Fcc	0.971083	0.028917
8	638.2995	0.952000	0.048000	0.000000	Liquid+Fcc	0.956555	0.043445
9	630.8249	0.936000	0.064000	0.000000	Liquid+Fcc	0.941981	0.058019
10	623.2342	0.920000	0.080000	0.000000	Liquid+Fcc	0.927361	0.072639
11	615.5002	0.904000	0.096000	0.000000	Liquid+Fcc	0.912693	0.087307
12	607.5976	0.888000	0.112000	0.000000	Liquid+Fcc	0.897978	0.102022
13	599.5031	0.872000	0.128000	0.000000	Liquid+Fcc	0.883216	0.116784
14	591.1954	0.856000	0.144000	0.000000	Liquid+Fcc	0.868407	0.131593
15	582.6552	0.840000	0.160000	0.000000	Liquid+Fcc	0.853549	0.146451
16	573.8655	0.824000	0.176000	0.000000	Liquid+Fcc	0.838644	0.161356
17	564.8116	0.808000	0.192000	0.000000	Liquid+Fcc	0.823691	0.176309
18	555.4809	0.792000	0.208000	0.000000	Liquid+Fcc	0.808689	0.191311
19	545.8633	0.776000	0.224000	0.000000	Liquid+Fcc	0.793638	0.206362
20	535.9511	0.760000	0.240000	0.000000	Liquid+Fcc	0.778538	0.221462
21	525.7395	0.744000	0.256000	0.000000	Liquid+Fcc	0.763389	0.236611
22	515.2261	0.728000	0.272000	0.000000	Liquid+Fcc	0.748191	0.251809
23	504.4120	0.712000	0.288000	0.000000	Liquid+Fcc	0.732943	0.267057
24	493.3014	0.696000	0.304000	0.000000	Liquid+Fcc	0.717645	0.282355
25	481.9028	0.680000	0.320000	0.000000	Liquid+Fcc	0.702297	0.297703
26	470.2289	0.664000	0.336000	0.000000	Liquid+Fcc	0.686898	0.313102
27	458.2983	0.648000	0.352000	0.000000	Liquid+Fcc	0.671449	0.328551
28	452.2442	0.640000	0.360000	0.000000	Liquid+Fcc	0.663706	0.336294
29	450.7220	0.638000	0.362000	0.000000	Liquid+Fcc	0.661768	0.338232
30	450.5315	0.637750	0.362250	0.000000	Liquid+Fcc	0.661525	0.338475
31	450.4839	0.637688	0.362313	0.000000	Liquid+Fcc	0.661465	0.338535

Figure 3.45 Default table view for the liquidus projection calculation results



Appearance

BackgroundColor	AppWorkspace
GridColor	ControlDark
BorderStyle	FixedSingle
CellBorderStyle	Single
DefaultCellStyle	DataGridViewCellStyle { Bac

Layout

AutoSizeColumnsMoc	None

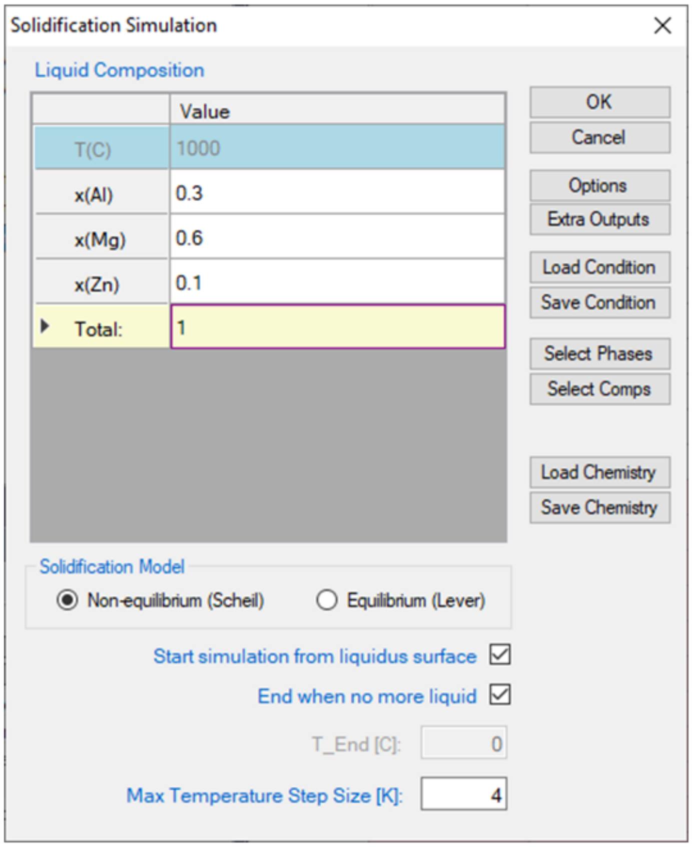
	T	phase_name	x(Al)	x(Mg)	x(Zn)	w(Al)	w(Mg)
	C		mole/mole	mole/mole	mole/mole	kg/kg	kg/kg
1	650.0000	Liquid+Fcc	0.977405	0.022595	0.000000	0.979601	0.020399
2	650.0000	Liquid+Fcc	0.977368	0.021632	0.001000	0.978075	0.019500
3	650.0000	Liquid+Fcc	0.977332	0.020668	0.002000	0.976554	0.018603
4	650.0000	Liquid+Fcc	0.977264	0.018736	0.004000	0.973530	0.016813
5	650.0000	Liquid+Fcc	0.977146	0.014854	0.008000	0.967553	0.013249
6	650.0000	Liquid+Fcc	0.976981	0.007019	0.016000	0.955876	0.006186
7	650.0000	Liquid+Fcc	0.976937	0.003063	0.020000	0.950175	0.002684
8	650.0000	Liquid+Fcc	0.976924	0.001076	0.022000	0.947358	0.000940
9	650.0000	Liquid+Fcc	0.976921	7.921784E-005	0.023000	0.945958	6.909663E-005
10	650.0000	Liquid+Fcc	0.976921	1.688990E-005	0.023063	0.945870	1.473062E-005
11	650.0000	Liquid+Fcc	0.976921	1.306765E-006	0.023078	0.945849	1.139676E-006
12	650.0000	Liquid+Fcc	0.976921	0.000000	0.023079	0.945847	0.000000
13							
14	600.0000	Liquid+Fcc	0.872971	0.127029	0.000000	0.884113	0.115887
15	600.0000	Liquid+Fcc	0.872726	0.126274	0.001000	0.882526	0.115023
16	600.0000	Liquid+Fcc	0.872482	0.125518	0.002000	0.880945	0.114161
17	600.0000	Liquid+Fcc	0.871996	0.124004	0.004000	0.877797	0.112444
18	600.0000	Liquid+Fcc	0.871028	0.120972	0.008000	0.871564	0.109036
19	600.0000	Liquid+Fcc	0.869118	0.114882	0.016000	0.859341	0.102320
20	600.0000	Liquid+Fcc	0.867246	0.108754	0.024000	0.847439	0.095727
21	600.0000	Liquid+Fcc	0.865418	0.102582	0.032000	0.835851	0.089248
22	600.0000	Liquid+Fcc	0.863639	0.096361	0.040000	0.824572	0.082874
23	600.0000	Liquid+Fcc	0.861917	0.090083	0.048000	0.813599	0.076596
24	600.0000	Liquid+Fcc	0.860260	0.083740	0.056000	0.802926	0.070405
25	600.0000	Liquid+Fcc	0.858675	0.077325	0.064000	0.792552	0.064290
26	600.0000	Liquid+Fcc	0.857170	0.070830	0.072000	0.782473	0.058243
27	600.0000	Liquid+Fcc	0.855754	0.064246	0.080000	0.772688	0.052254
28	600.0000	Liquid+Fcc	0.854439	0.057561	0.088000	0.763195	0.046313
29	600.0000	Liquid+Fcc	0.853233	0.050767	0.096000	0.753995	0.040411
30	600.0000	Liquid+Fcc	0.852150	0.043850	0.104000	0.745088	0.034537
31	600.0000	Liquid+Fcc	0.851201	0.036799	0.112000	0.736475	0.028680

Figure 3.46 Isotherms table for the liquidus projection calculation results

3.3.7 Solidification Simulation

Two simple models, equilibrium solidification and Scheil solidification, have been integrated into Pandat™ for calculating solidification pathways. The equilibrium model, also called the lever rule model, assumes that complete diffusion occurs in both liquid and solid phases, and the compositions of solid and liquid always follow the phase boundaries defined by the equilibrium phase diagram. The fractions of liquid and solid can be calculated through the lever rule. In contrast, Scheil solidification assumes that no diffusion occurs in the solid phases, that the composition of liquid phase is uniform (infinite diffusivity in liquid) and that local equilibrium at the solid-liquid interface is always maintained. The **Solidification Simulation** function calculates the solidification path of an alloy using either the lever rule or Scheil model as being decided by the user.

Go to **PanPhaseDiagram** on the menu bar and select **Solidification Simulation** or click the button on the tool bar. The dialog box as shown in Figure 3.47 allows the user to set up the alloy composition for the solidification simulation. User can choose the simulation under either **Non-Equilibrium(Scheil)** or **Equilibrium (Lever Rule)** condition. There are two check boxes at the bottom of the input dialog: **Start simulation from liquidus surface**, and **End when no more liquid**. If both boxes were checked, the solidification simulation will be carried out in the temperature range when solid start to form from liquid (liquidus surface) to the point when liquid just completely disappear. Pandat™ software will find these two points automatically. If one or both of the check boxes are not checked, user will need to define the start or/and the end temperature for the solidification simulation proceeds.



	Value
T(C)	1000
x(Al)	0.3
x(Mg)	0.6
x(Zn)	0.1
Total:	1

Solidification Model

● Non-equilibrium (Scheil) ○ Equilibrium (Lever)

Start simulation from liquidus surface ☑

End when no more liquid ☑

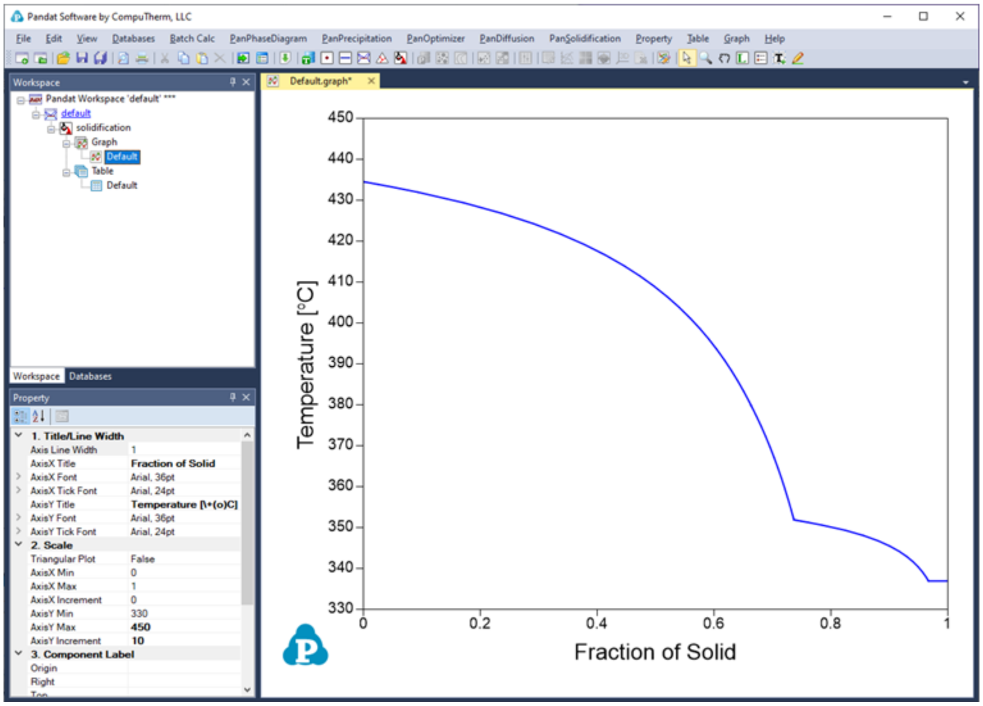
T_End [C]: 0

Max Temperature Step Size [K]: 4

Figure 3.47 Set calculation conditions for solidification simulation

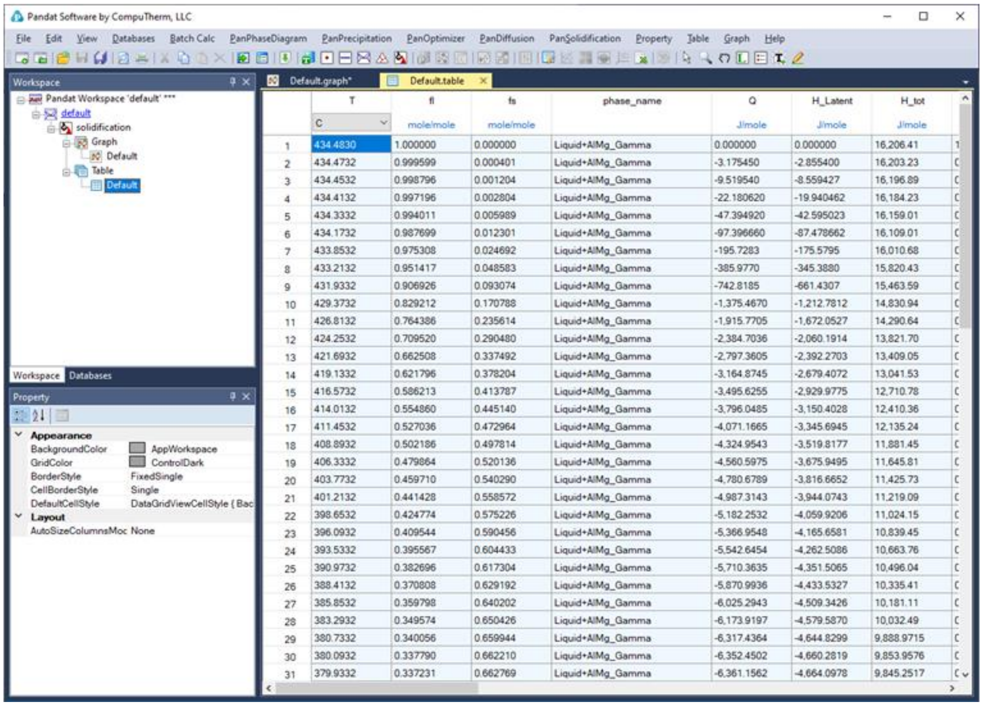
The results are displayed in either Graph View or Table View. Figure 3.48 and Figure 3.49 show the graph view and table view for the solidification simulation results with the calculation condition shown in Figure 3.47. Extensive operations on Graph and Table, such as labeling and adding legend, have been discussed in details in **Section 2.3** and **Section 2.4**.

PanSolidification, a new module introduced in Pandat 2020, is considered the back diffusion in the solid phase during solidification. Detailed description on PanSolidification module is in **section** 7.



1. Title/Line Width	
Axis Line Width	1
AxisX Title	**Fraction of Solid**
AxisX Font	Arial, 36pt
AxisX Tick Font	Arial, 24pt
AxisY Title	**Temperature [\+(o)C]**
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
2. Scale	
Triangular Plot	False
AxisX Min	0
AxisX Max	1
AxisX Increment	0
AxisY Min	330
AxisY Max	**450**
AxisY Increment	**10**
3. Component Label	
Origin	
Right	

Figure 3.48 Graph view of the solidification simulation result



Appearance	
BackgroundColor	AppWorkspace
GridColor	ControlDark
BorderStyle	FixedSingle
CellBorderStyle	Single
DefaultCellStyle	DataGridViewCellStyle { Bac
Layout	
AutoSizeColumnsMoc	None

	T	fl	fs	phase_name	Q	H_Latent	H_tot
	C	mole/mole	mole/mole		J/mole	J/mole	J/mole
1	434.4830	1.000000	0.000000	Liquid+AlMg_Gamma	0.000000	0.000000	16,206.41
2	434.4732	0.999599	0.000401	Liquid+AlMg_Gamma	-3.175450	-2.855400	16,203.23
3	434.4532	0.998796	0.001204	Liquid+AlMg_Gamma	-9.519540	-8.559427	16,196.89
4	434.4132	0.997196	0.002804	Liquid+AlMg_Gamma	-22.180620	-19.940462	16,184.23
5	434.3332	0.994011	0.005989	Liquid+AlMg_Gamma	-47.394920	-42.595023	16,159.01
6	434.1732	0.987699	0.012301	Liquid+AlMg_Gamma	-97.396660	-87.478662	16,109.01
7	433.8532	0.975308	0.024692	Liquid+AlMg_Gamma	-195.7283	-175.5795	16,010.68
8	433.2132	0.951417	0.048583	Liquid+AlMg_Gamma	-385.9770	-345.3880	15,820.43
9	431.9332	0.906926	0.093074	Liquid+AlMg_Gamma	-742.8185	-661.4307	15,463.59
10	429.3732	0.829212	0.170788	Liquid+AlMg_Gamma	-1,375.4670	-1,212.7812	14,830.94
11	426.8132	0.764386	0.235614	Liquid+AlMg_Gamma	-1,915.7705	-1,672.0527	14,290.64
12	424.2532	0.709520	0.290480	Liquid+AlMg_Gamma	-2,384.7036	-2,060.1914	13,821.70
13	421.6932	0.662508	0.337492	Liquid+AlMg_Gamma	-2,797.3605	-2,392.2703	13,409.05
14	419.1332	0.621796	0.378204	Liquid+AlMg_Gamma	-3,164.8745	-2,679.4072	13,041.53
15	416.5732	0.586213	0.413787	Liquid+AlMg_Gamma	-3,495.6255	-2,929.9775	12,710.78
16	414.0132	0.554860	0.445140	Liquid+AlMg_Gamma	-3,796.0485	-3,150.4028	12,410.36
17	411.4532	0.527036	0.472964	Liquid+AlMg_Gamma	-4,071.1665	-3,345.6945	12,135.24
18	408.8932	0.502186	0.497814	Liquid+AlMg_Gamma	-4,324.9543	-3,519.8177	11,881.45
19	406.3332	0.479864	0.520136	Liquid+AlMg_Gamma	-4,560.5975	-3,675.9495	11,645.81
20	403.7732	0.459710	0.540290	Liquid+AlMg_Gamma	-4,780.6789	-3,816.6652	11,425.73
21	401.2132	0.441428	0.558572	Liquid+AlMg_Gamma	-4,987.3143	-3,944.0743	11,219.09
22	398.6532	0.424774	0.575226	Liquid+AlMg_Gamma	-5,182.2532	-4,059.9206	11,024.15
23	396.0932	0.409544	0.590456	Liquid+AlMg_Gamma	-5,366.9548	-4,165.6581	10,839.45
24	393.5332	0.395567	0.604433	Liquid+AlMg_Gamma	-5,542.6454	-4,262.5086	10,663.76
25	390.9732	0.382696	0.617304	Liquid+AlMg_Gamma	-5,710.3635	-4,351.5065	10,496.04
26	388.4132	0.370808	0.629192	Liquid+AlMg_Gamma	-5,870.9936	-4,433.5327	10,335.41
27	385.8532	0.359798	0.640202	Liquid+AlMg_Gamma	-6,025.2943	-4,509.3426	10,181.11
28	383.2932	0.349574	0.650426	Liquid+AlMg_Gamma	-6,173.9197	-4,579.5870	10,032.49
29	380.7332	0.340056	0.659944	Liquid+AlMg_Gamma	-6,317.4364	-4,644.8299	9,888.9715
30	380.0932	0.337790	0.662210	Liquid+AlMg_Gamma	-6,352.4502	-4,660.2819	9,853.9576
31	379.9332	0.337231	0.662769	Liquid+AlMg_Gamma	-6,361.1562	-4,664.0978	9,845.2517

Figure 3.49 Table view of the solidification simulation result

3.3.8 Table Column Functions

Examples are given in this section show how to use the table column property names and functions to obtain more information from the calculated results.

3.3.8.1 Activity and activity coefficient

The activity of a component j, a_j, is defined by

$$\mu_j = \mu_j^{\circ} + RTlna_j$$

where μ_j is the chemical potential of the component j in equilibrium state and μ_j° is the chemical potential of this component at its reference state. For example, the activity of component Al in the liquid Al-Mg system referring the Al in Fcc phase is calculated by

$$a_{Al} = e^{\frac{\mu_{Al}^{liquid} - \mu_{Al}^{\circ,fcc}}{RT}}$$

The corresponding Table column name is `a(Al@Liquid:Fcc[Al])`, or `a(Al@Liquid:Fcc)`.

If a reference state is not specified in Table column name, the default reference state in the database is taken as the reference state. For example, `a(Al@Liquid)` is calculated by

$$a_{Al} = e^{\frac{\mu_{Al}^{liquid}}{RT}}$$

Activity coefficient is defined as

$$\gamma_j = \frac{a_j}{x_j}$$

which is available from Table by defining Table column name similar to that of activity. Table column name for the activity coefficient of Al in liquid is `r(Al@Liquid:Fcc[Al])`, or `r(Al@Liquid:Fcc)`.

Figure 3.50 to Figure 3.53 show the screen images for creating a table of activity and activity coefficient from a line calculation result at 1000K in the Al-Mg-Zn ternary system. The two end points are at `x(Mg)=0.2,x(Al)=0.8` and `x(Mg)=0.2,x(Zn)=0.8.` The liquid phase is the stable phase under this condition. The setting in Figure 3.50 is to choose Fcc Al, Fcc Mg, and Hcp Zn as the reference state.

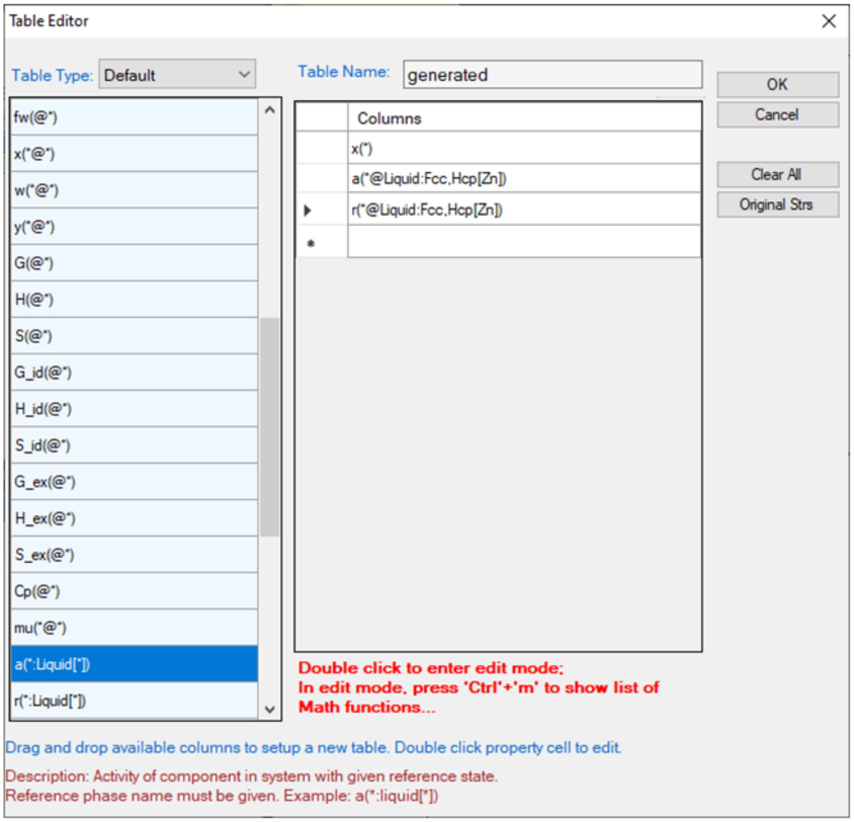


Table Type: Default

Table Name: generated

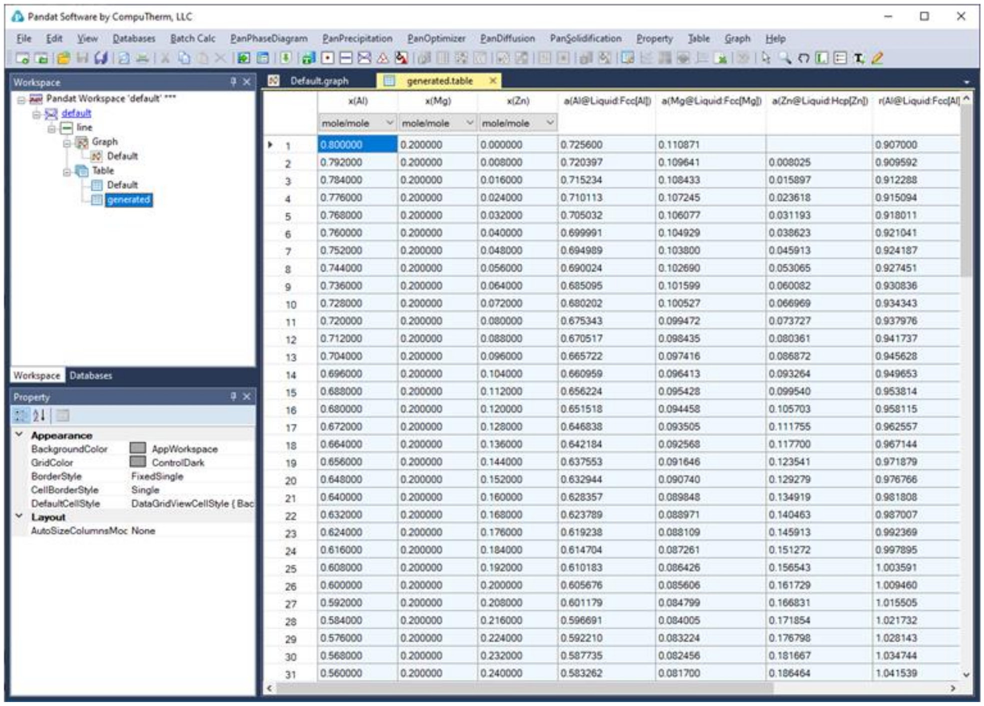
	Columns
	x(*)
	a(*@Liquid:Fcc,Hcp[Zn])
▶	r(*@Liquid:Fcc,Hcp[Zn])
*	

Double click to enter edit mode;
In edit mode, press 'Ctrl'+'m' to show list of Math functions...

Drag and drop available columns to setup a new table. Double click property cell to edit.

Description: Activity of component in system with given reference state.
Reference phase name must be given. Example: a(*:liquid[*])

Figure 3.50 Table editor for creating activity and activity coefficient table



	x(Al)	x(Mg)	x(Zn)	a(Al@Liquid:Fcc[Al])	a(Mg@Liquid:Fcc[Mg])	a(Zn@Liquid:Hcp[Zn])	r(Al@Liquid:Fcc[Al]
	mole/mole	mole/mole	mole/mole				
1	0.800000	0.200000	0.000000	0.725600	0.110871		0.907000
2	0.792000	0.200000	0.008000	0.720397	0.109641	0.008025	0.909592
3	0.784000	0.200000	0.016000	0.715234	0.108433	0.015897	0.912288
4	0.776000	0.200000	0.024000	0.710113	0.107245	0.023618	0.915094
5	0.768000	0.200000	0.032000	0.705032	0.106077	0.031193	0.918011
6	0.760000	0.200000	0.040000	0.699991	0.104929	0.038623	0.921041
7	0.752000	0.200000	0.048000	0.694989	0.103800	0.045913	0.924187
8	0.744000	0.200000	0.056000	0.690024	0.102690	0.053065	0.927451
9	0.736000	0.200000	0.064000	0.685095	0.101599	0.060082	0.930836
10	0.728000	0.200000	0.072000	0.680202	0.100527	0.066969	0.934343
11	0.720000	0.200000	0.080000	0.675343	0.099472	0.073727	0.937976
12	0.712000	0.200000	0.088000	0.670517	0.098435	0.080361	0.941737
13	0.704000	0.200000	0.096000	0.665722	0.097416	0.086872	0.945628
14	0.696000	0.200000	0.104000	0.660959	0.096413	0.093264	0.949653
15	0.688000	0.200000	0.112000	0.656224	0.095428	0.099540	0.953814
16	0.680000	0.200000	0.120000	0.651518	0.094458	0.105703	0.958115
17	0.672000	0.200000	0.128000	0.646838	0.093505	0.111755	0.962557
18	0.664000	0.200000	0.136000	0.642184	0.092568	0.117700	0.967144
19	0.656000	0.200000	0.144000	0.637553	0.091646	0.123541	0.971879
20	0.648000	0.200000	0.152000	0.632944	0.090740	0.129279	0.976766
21	0.640000	0.200000	0.160000	0.628357	0.089848	0.134919	0.981808
22	0.632000	0.200000	0.168000	0.623789	0.088971	0.140463	0.987007
23	0.624000	0.200000	0.176000	0.619238	0.088109	0.145913	0.992369
24	0.616000	0.200000	0.184000	0.614704	0.087261	0.151272	0.997895
25	0.608000	0.200000	0.192000	0.610183	0.086426	0.156543	1.003591
26	0.600000	0.200000	0.200000	0.605676	0.085606	0.161729	1.009460
27	0.592000	0.200000	0.208000	0.601179	0.084799	0.166831	1.015505
28	0.584000	0.200000	0.216000	0.596691	0.084005	0.171854	1.021732
29	0.576000	0.200000	0.224000	0.592210	0.083224	0.176798	1.028143
30	0.568000	0.200000	0.232000	0.587735	0.082456	0.181667	1.034744
31	0.560000	0.200000	0.240000	0.583262	0.081700	0.186464	1.041539

Property

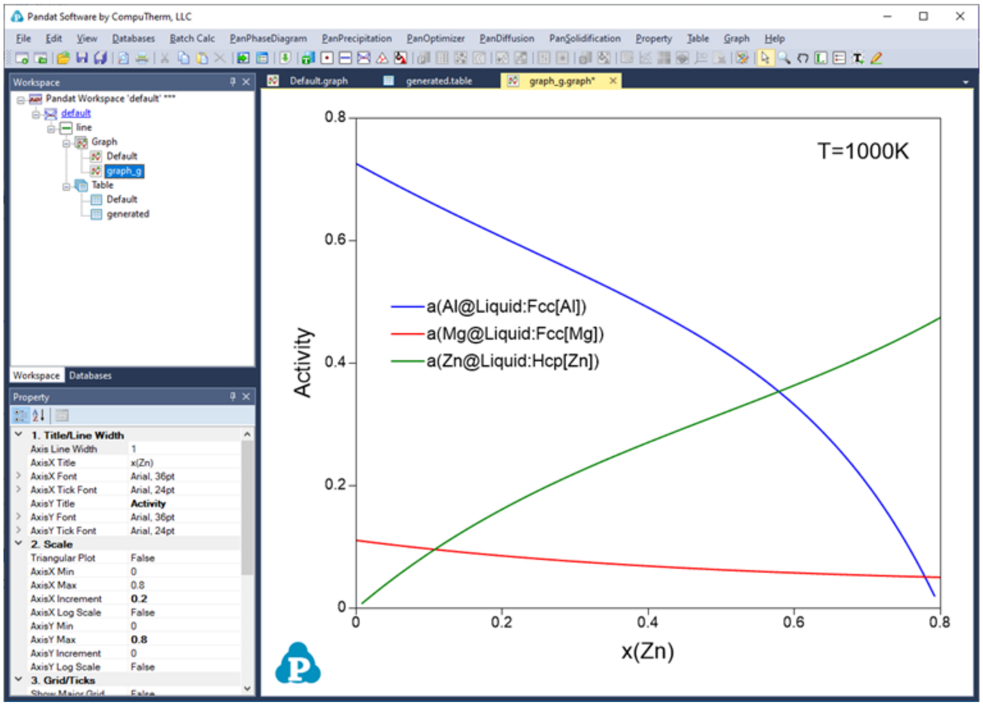
Appearance

BackgroundColor	▨ AppWorkspace
GridColor	▨ ControlDark
BorderStyle	FixedSingle
CellBorderStyle	Single
DefaultCellStyle	DataGridViewCellStyle { Bac

Layout

AutoSizeColumnsMoc	None

Figure 3.51 Table of activity and activity coefficient



Property

1. Title/Line Width

Axis Line Width	1
AxisX Title	x(Zn)
AxisX Font	Arial, 36pt
AxisX Tick Font	Arial, 24pt
AxisY Title	**Activity**
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt

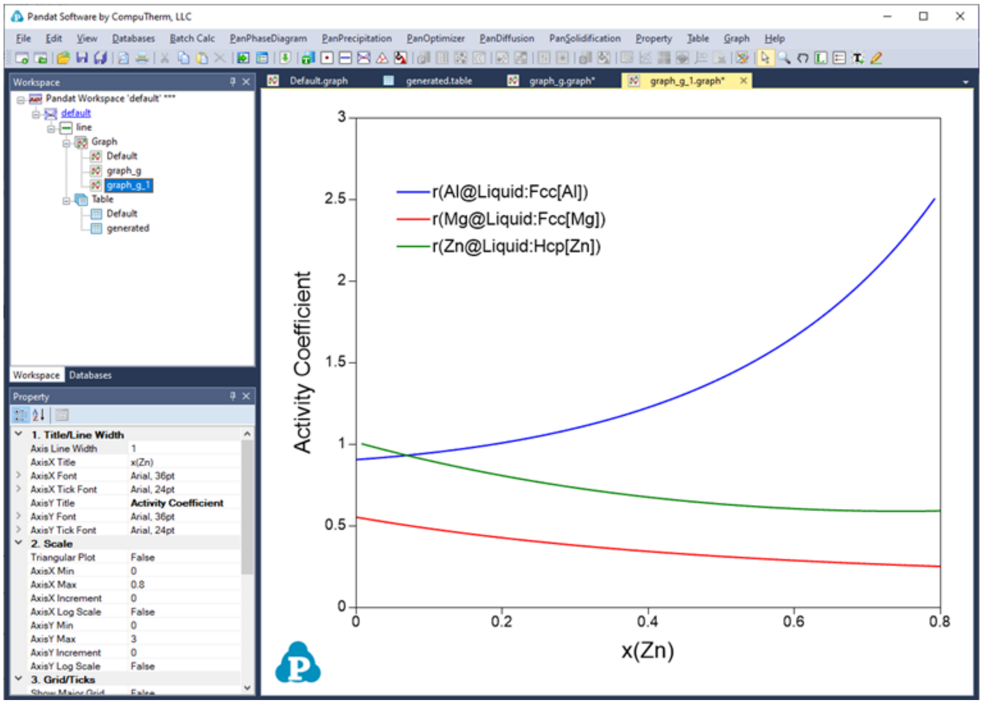
2. Scale

Triangular Plot	False
AxisX Min	0
AxisX Max	0.8
AxisX Increment	**0.2**
AxisX Log Scale	False
AxisY Min	0
AxisY Max	**0.8**
AxisY Increment	0
AxisY Log Scale	False

3. Grid/Ticks

Show Major Grid	False

Figure 3.52 Graph of activity vs. x(Zn)



1. Title/Line Width	
Axis Line Width	1
AxisX Title	x(Zn)
AxisX Font	Arial, 36pt
AxisX Tick Font	Arial, 24pt
AxisY Title	**Activity Coefficient**
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
2. Scale	
Triangular Plot	False
AxisX Min	0
AxisX Max	0.8
AxisX Increment	0
AxisX Log Scale	False
AxisY Min	0
AxisY Max	3
AxisY Increment	0
AxisY Log Scale	False
3. Grid/Ticks	
Show Major Grid	False

Figure 3.53 Graph of activity coefficient vs. x(Zn)

3.3.8.2 Tielines

A special column property name "`tieline`" is introduced to create a table of tielines from the calculated results. It can be combined with other column constraints to select a special set of tielines.

Figure 3.54 is a 3D ternary phase diagram calculated from the database file "`ABC.tdb`" which is provided in the Pandat Examples. This system has three binary eutectic reactions. To show the invariant tielines in these binaries, set the "Show Invariant Tieline" in the Property window as "true", then the invariant lines will be plotted on it as shown in Figure 3.55.

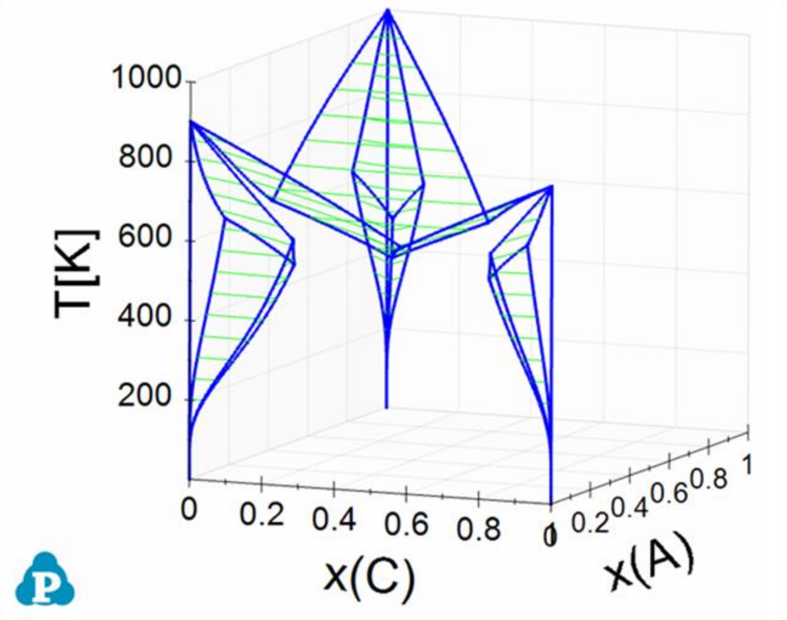
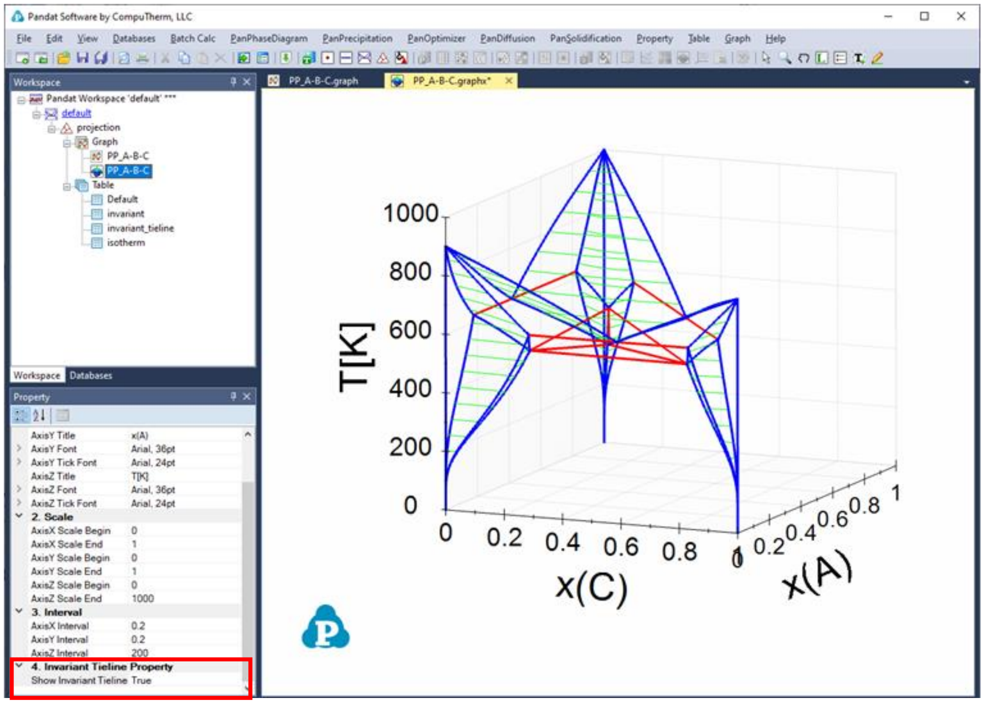


Figure 3.54 3D phase projection of a simple ternary system with eutectic reaction in every binary system



AxisY Title	x(A)
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
AxisZ Title	T[K]
AxisZ Font	Arial, 36pt
AxisZ Tick Font	Arial, 24pt
2. Scale	
AxisX Scale Begin	0
AxisX Scale End	1
AxisY Scale Begin	0
AxisY Scale End	1
AxisZ Scale Begin	0
AxisZ Scale End	1000
3. Interval	
AxisX Interval	0.2
AxisY Interval	0.2
AxisZ Interval	200
4. Invariant Tieline Property	
Show Invariant Tieline	True

Figure 3.55 3D phase projection with three binary eutectic and one ternary eutectic tielines shown as red

The ternary univariant lines (L+Bcc+Fcc, L+Bcc+Hcp, and L+Fcc+Hcp, magenta color) connects these reactions can be highlighted as follows. First, create a new table as shown in Figure 3.56. The purpose of the new table is to extract the boundary line(s) that connect Liquid, and the other two solid phases, and the fraction of Liquid on this boundary line is 1. After the table is created, select this new table in the Explore window, and drag x(C) from the Property window to the Main Display window, and drop it as the x-axis; press “Ctrl” and then drag x(A) from the Property window to the Main Display window, and drop it as the y-axis; press “Shift” and then drag T from the Property window to the Main Display window, and drop it as the z-axis. This line showing the gradually change from the peritectic reaction to the eutectic reaction is then highlighted (green color), as shown in Figure 3.57.

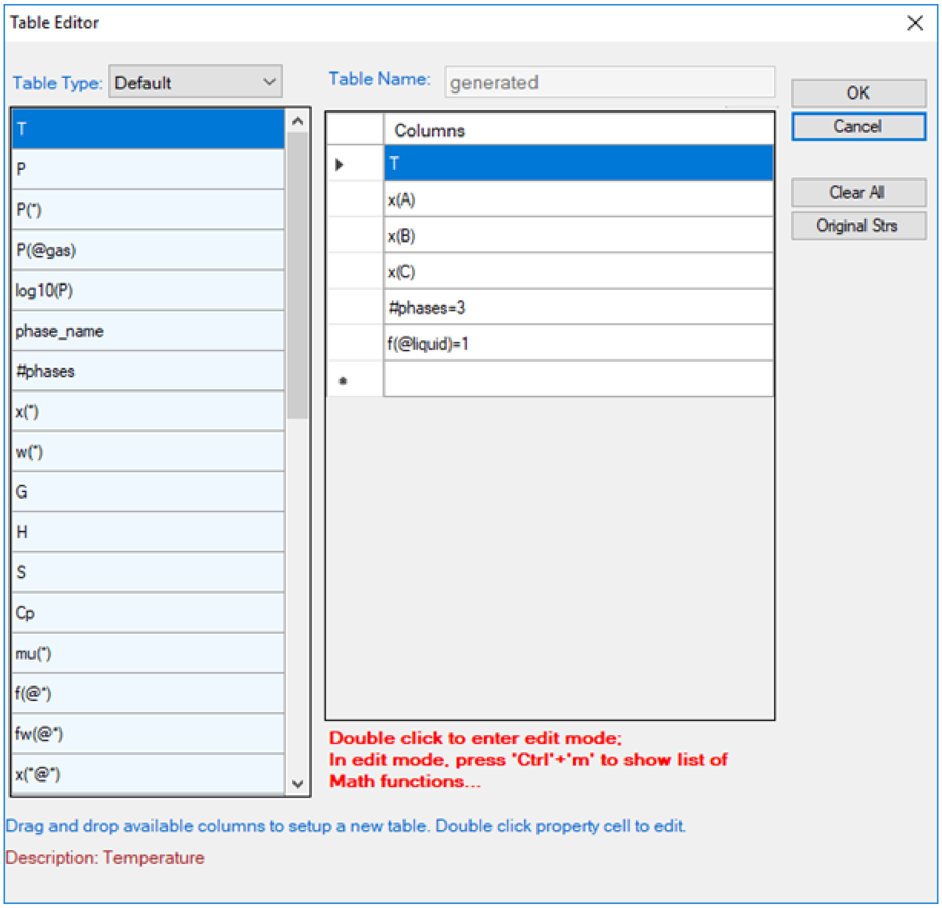


Table Type: Default

Table Name: generated

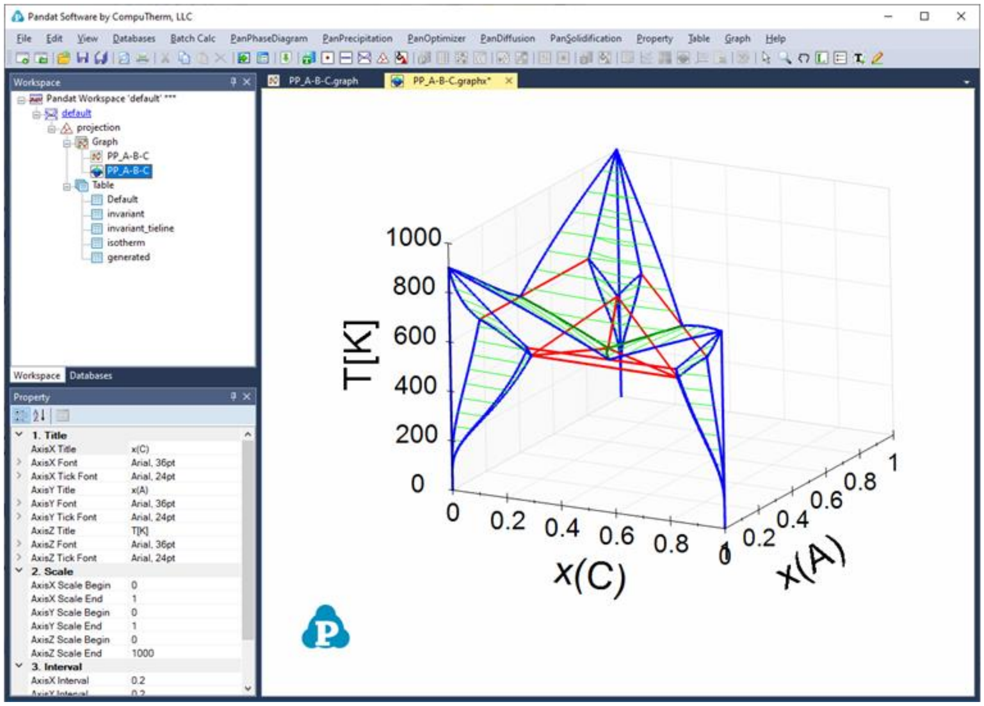
Columns
T
x(A)
x(B)
x(C)
#phases=3
f(@liquid)=1

Double click to enter edit mode;
In edit mode, press 'Ctrl'+'m' to show list of Math functions...

Drag and drop available columns to setup a new table. Double click property cell to edit.

Description: Temperature

Figure 3.56 Create a new table to extract the ternary univariant lines



1. Title	
AxisX Title	x(C)
AxisX Font	Arial, 36pt
AxisX Tick Font	Arial, 24pt
AxisY Title	x(A)
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
AxisZ Title	T[K]
AxisZ Font	Arial, 36pt
AxisZ Tick Font	Arial, 24pt
2. Scale	
AxisX Scale Begin	0
AxisX Scale End	1
AxisY Scale Begin	0
AxisY Scale End	1
AxisZ Scale Begin	0
AxisZ Scale End	1000
3. Interval	
AxisX Interval	0.2
AxisY Interval	0.2

Figure 3.57 The ternary univariant lines (green lines) connecting the two invariant reactions in the two binaries

Figure 3.58 shows how to create 4 new tables to plot the 3D diagram in Figure 3.59, which shows the ternary three-phase equilibrium tie-triangle volume. The 4 tables include a set of the tie-triangles by setting its density as "tieline=5" and the phase lines for the liquid, Bcc, Fcc phases by setting the fraction of the corresponding phase to be 1.

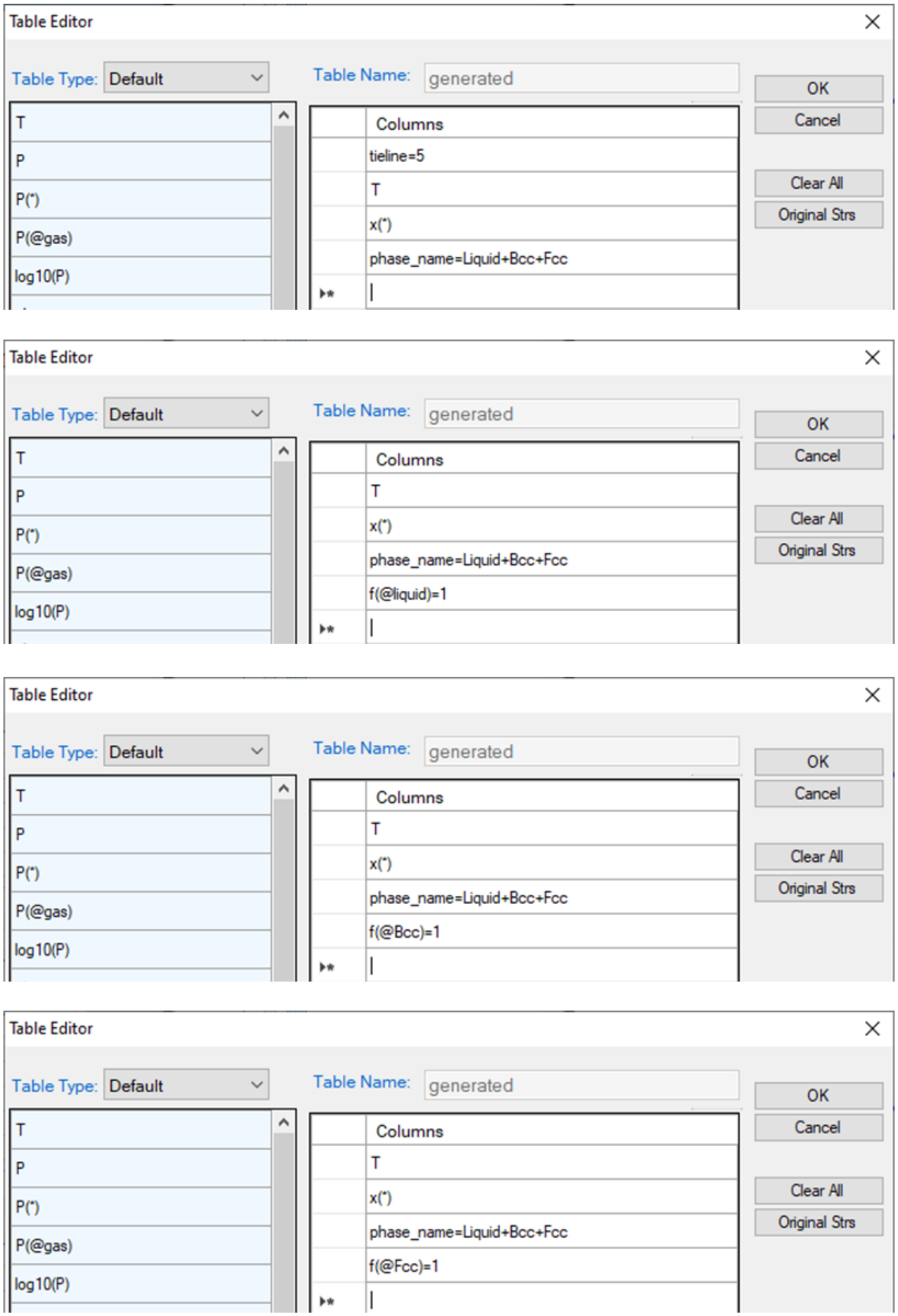


Table Type: Default
Table Name: generated

Columns:
tieline=5
T
x(*)
phase_name=Liquid+Bcc+Fcc

Table Type: Default
Table Name: generated

Columns:
T
x(*)
phase_name=Liquid+Bcc+Fcc
f(@liquid)=1

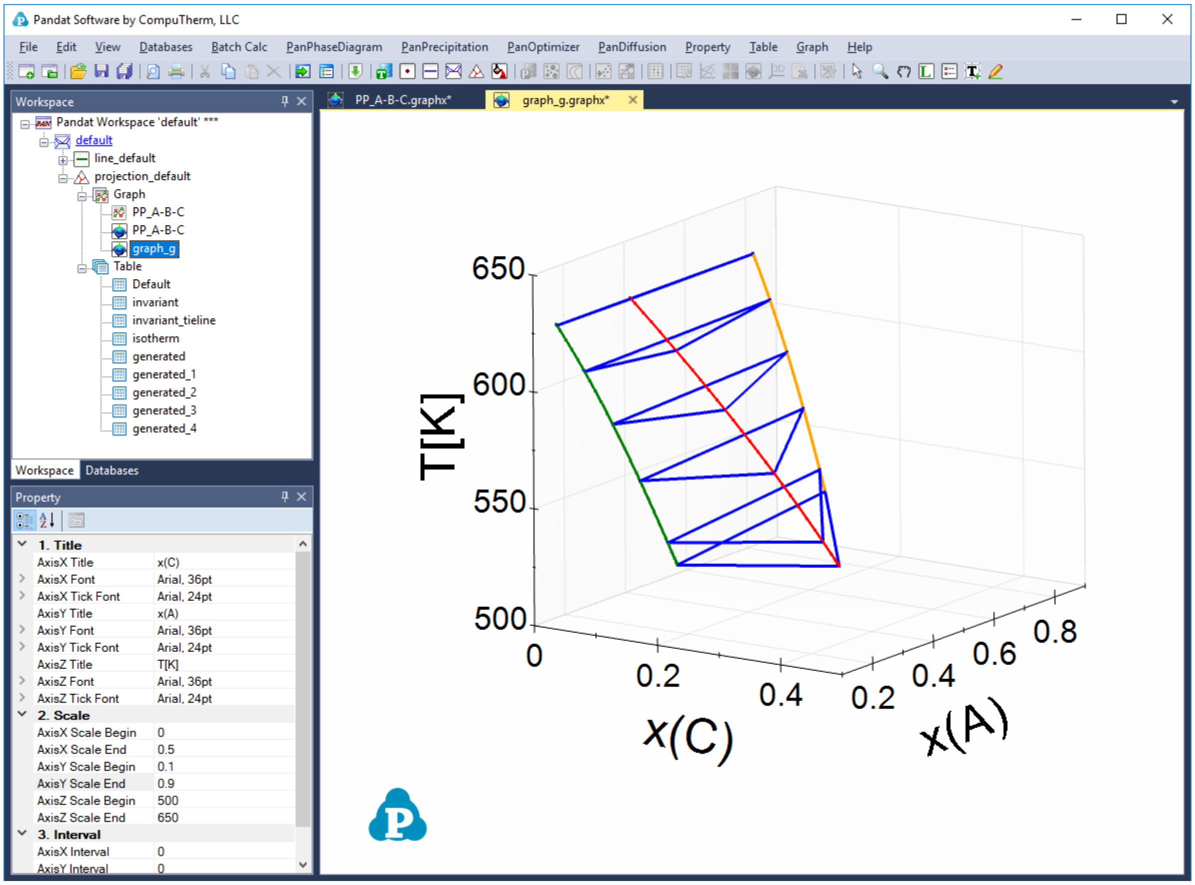
Table Type: Default
Table Name: generated

Columns:
T
x(*)
phase_name=Liquid+Bcc+Fcc
f(@Bcc)=1

Table Type: Default
Table Name: generated

Columns:
T
x(*)
phase_name=Liquid+Bcc+Fcc
f(@Fcc)=1

Figure 3.58 Create tables to extract tie-triangles and the three edges of the three-phase volume.



1. Title	
AxisX Title	x(C)
AxisX Font	Arial, 36pt
AxisX Tick Font	Arial, 24pt
AxisY Title	x(A)
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
AxisZ Title	T[K]
AxisZ Font	Arial, 36pt
AxisZ Tick Font	Arial, 24pt
2. Scale	
AxisX Scale Begin	0
AxisX Scale End	0.5
AxisY Scale Begin	0.1
AxisY Scale End	0.9
AxisZ Scale Begin	500
AxisZ Scale End	650
3. Interval	
AxisX Interval	0
AxisY Interval	0

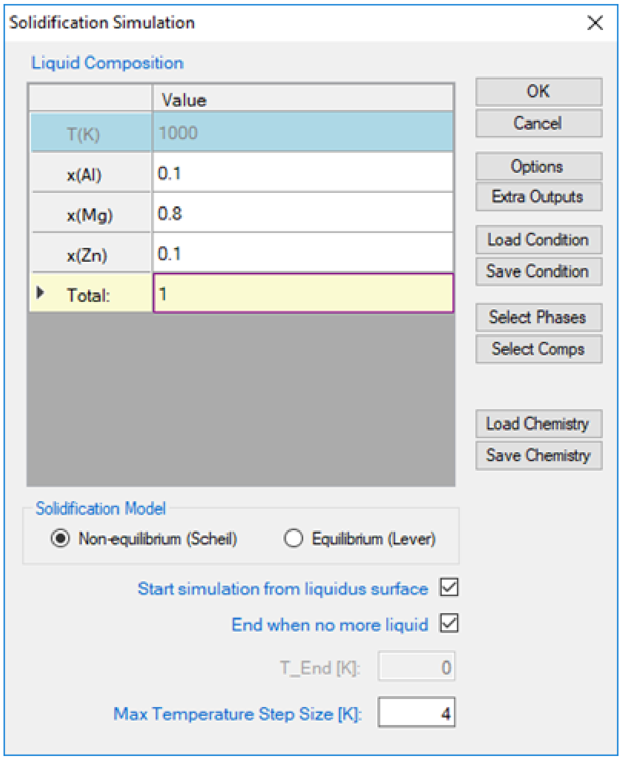
Figure 3.59 3D diagram of the three-phase volume.

3.3.8.3 Numerical derivative

The derivative $\frac{dY}{dZ}$ can be calculated numerically from the two columns of Y and Z. The operator for numerical derivative is "`//`", double slashes. The numerical derivative of $\frac{dY}{dZ}$ is written in the form of "`Y//Z`" as the column name. Only one numerical derivative operator is allowed in one column. In other words, user cannot type in "`Y//Z//X`".The derivative "`Y//Z`" will be parsed into three columns in the new table: "`Y`", "`Z`" and "`Y//Z`", which makes it easy for the user to view the original data set "`Y`", "`Z`" and choose to plot either $\frac{dY}{dZ}$ vs `Z` or $\frac{dY}{dZ}$ vs `Y`.

The example given here is to find the "effective heat capacity" of the system during solidification (`H_tot//T`). A system of Al-Mg-Zn is chosen and the composition is shown in Figure 3.60. After Scheil simulation is done, a new table is created with the definition of the column names shown in Figure 3.61.

Figure 3.62 is the newly generated table. Select the columns “`T`” and “`H_tot//T`”, we have the $\frac{dH\_tot}{dT}$ vs `T` diagram as in Figure 3.63. This diagram shows the effective heat capacity change during the solidification by Scheil simulation. There are two peaks in Figure 3.63, which represent roughly the phase transformation from liquid to Hcp+γ and that from liquid to Hcp+τ, respectively.



	Value
T(K)	1000
x(Al)	0.1
x(Mg)	0.8
x(Zn)	0.1
Total:	1

Solidification Model
● Non-equilibrium (Scheil) ○ Equilibrium (Lever)

Start simulation from liquidus surface ☑
End when no more liquid ☑
T_End [K]: 0
Max Temperature Step Size [K]: 4

Figure 3.60 Solidification simulation condition.

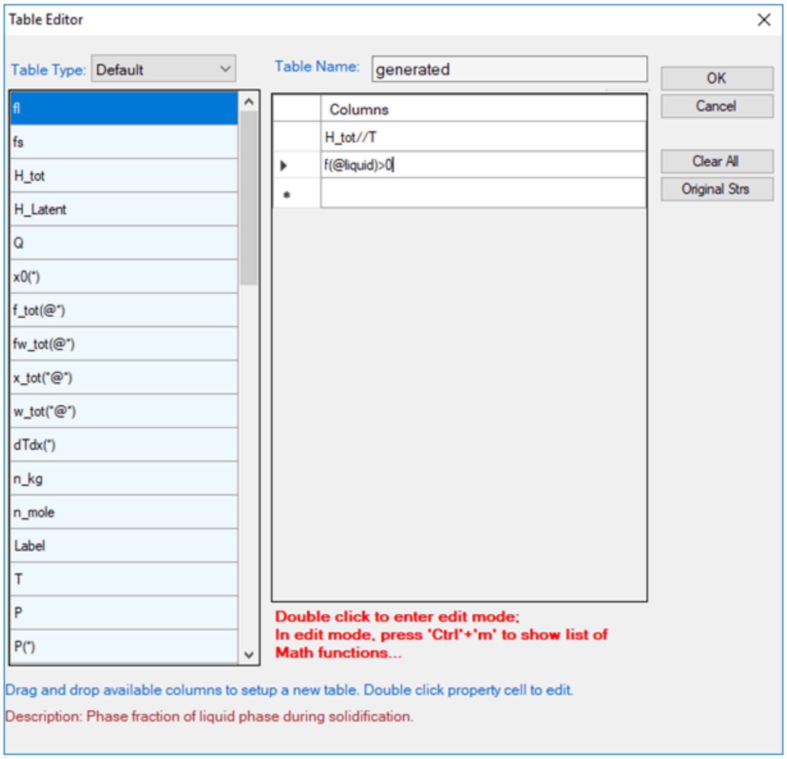


Table Type: Default

Table Name: generated

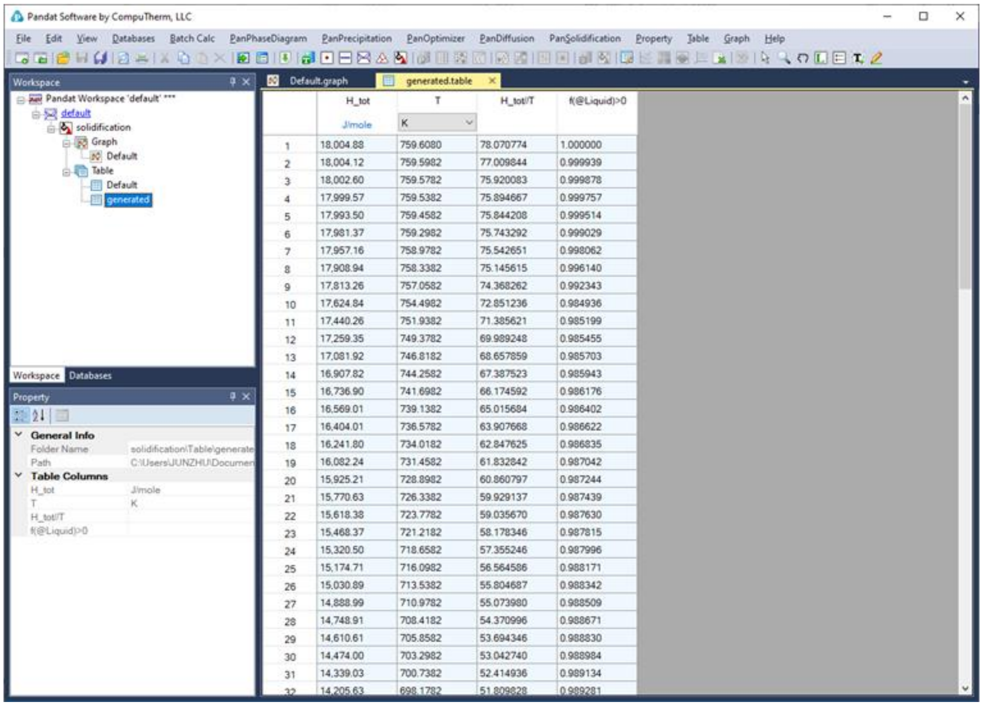
	Columns
	H_tot//T
▶	f(@liquid)>0
*	

Double click to enter edit mode;
In edit mode, press 'Ctrl'+'m' to show list of Math functions...

Drag and drop available columns to setup a new table. Double click property cell to edit.

Description: Phase fraction of liquid phase during solidification.

Figure 3.61 Create a table for the numerical derivative of `H_tot` w.r.t. `T`.

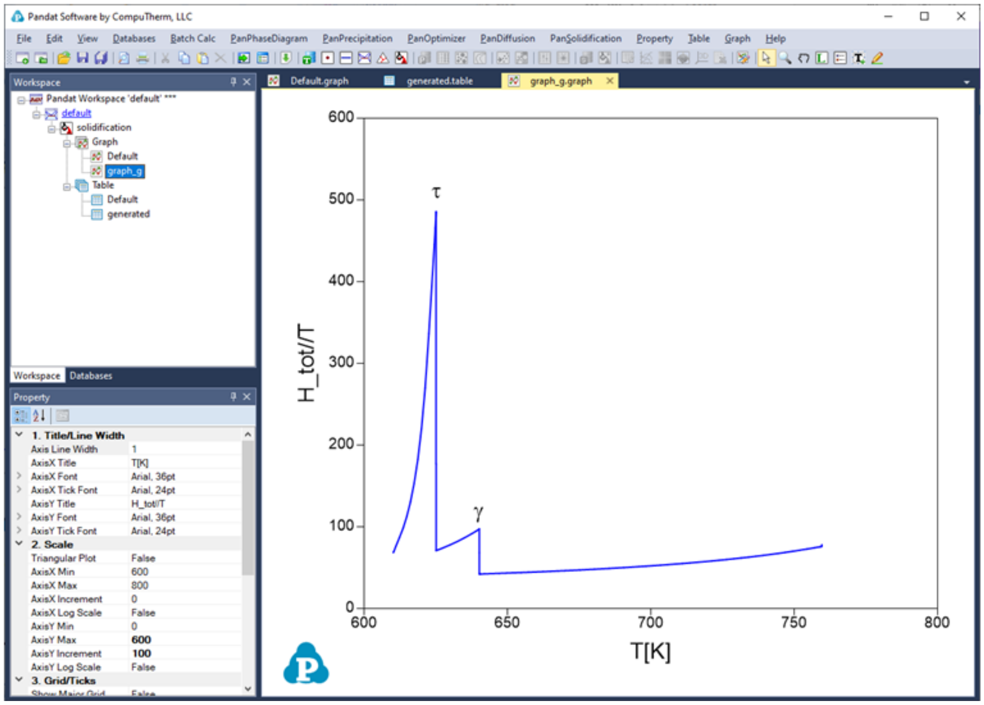


General Info
Folder Name: solidification\Table\generate
Path: C:\Users\JUNZHU\Documen

Table Columns
H_tot: J/mole
T: K
H_tot//T
f(@Liquid)>0

	H_tot	T	H_tot//T	f(@Liquid)>0
	J/mole	K		
1	18,004.88	759.6080	78.070774	1.000000
2	18,004.12	759.5982	77.009844	0.999939
3	18,002.60	759.5782	75.920083	0.999878
4	17,999.57	759.5382	75.894667	0.999757
5	17,993.50	759.4582	75.844208	0.999514
6	17,981.37	759.2982	75.743292	0.999029
7	17,957.16	758.9782	75.542651	0.998062
8	17,908.94	758.3382	75.145615	0.996140
9	17,813.26	757.0582	74.368262	0.992343
10	17,624.84	754.4982	72.851236	0.984936
11	17,440.26	751.9382	71.385621	0.985199
12	17,259.35	749.3782	69.989248	0.985455
13	17,081.92	746.8182	68.657859	0.985703
14	16,907.82	744.2582	67.387523	0.985943
15	16,736.90	741.6982	66.174592	0.986176
16	16,569.01	739.1382	65.015684	0.986402
17	16,404.01	736.5782	63.907668	0.986622
18	16,241.80	734.0182	62.847625	0.986835
19	16,082.24	731.4582	61.832842	0.987042
20	15,925.21	728.8982	60.860797	0.987244
21	15,770.63	726.3382	59.929137	0.987439
22	15,618.38	723.7782	59.035670	0.987630
23	15,468.37	721.2182	58.178346	0.987815
24	15,320.50	718.6582	57.355246	0.987996
25	15,174.71	716.0982	56.564586	0.988171
26	15,030.89	713.5382	55.804687	0.988342
27	14,888.99	710.9782	55.073980	0.988509
28	14,748.91	708.4182	54.370996	0.988671
29	14,610.61	705.8582	53.694346	0.988830
30	14,474.00	703.2982	53.042740	0.988984
31	14,339.03	700.7382	52.414936	0.989134
32	14,205.63	698.1782	51.809828	0.989281

Figure 3.62 The table for the numerical derivative of `H_tot` w.r.t. `T`.



1. Title/Line Width	
Axis Line Width	1
AxisX Title	T[K]
AxisX Font	Arial, 36pt
AxisX Tick Font	Arial, 24pt
AxisY Title	H_tot/T
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
2. Scale	
Triangular Plot	False
AxisX Min	600
AxisX Max	800
AxisX Increment	0
AxisX Log Scale	False
AxisY Min	0
AxisY Max	**600**
AxisY Increment	**100**
AxisY Log Scale	False
3. Grid/Ticks	
Show Major Grid	False

Figure 3.63 plot of effective heat capacity change during the solidification

3.3.9 Append Database

On top of the original database (*.tdb or *.pdb) loaded from Pandat GUI, user can append a custom-made database (*.tdb) by select the **Append TDB** function from the **Databases** menu as shown in Figure 3.64.

Using this function, user can (1) replace the value of an existing parameter, (2) add value to an existing parameter, (3) add new parameters to an existing phase, (4) add new phases to the original database, and (5) add user-defined properties. In the following, the hypothetical A-B system will be used as example to explain the **Append TDB** function in detail.

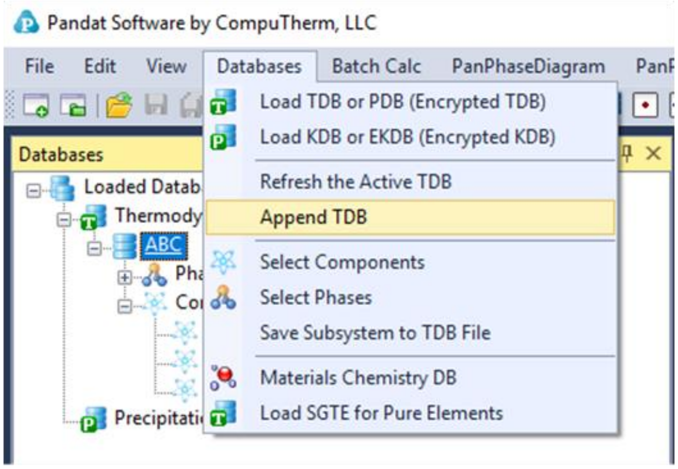


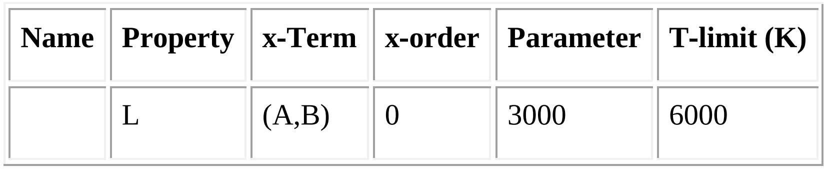
Figure 3.64 Append TDB function under the Databases menu

3.3.9.1 Replace the Value of an Existing Parameter

In this example, we are going to replace the interaction parameter of the liquid phase: G(Liquid,A,B;0) within the original AB_original.tdb database. Load the AB_original.tdb from the **Databases** menu by selecting the **Load TDB or PDB** function. The interaction parameter of G(Liquid,A,B;0) described in the original database is expressed as:

```
Parameter G(Liquid,A,B;0) 298 3000; 6000 N !
```

In the TDB Viewer, one can see the original value of G(Liquid,A,B;0)=3000.



Name	Property	x-Term	x-order	Parameter	T-limit (K)
	L	(A,B)	0	3000	6000

In the AB_replace parameter.tdb, only the interaction parameter for G(Liquid,A,B;0) is defined, but with a different value:

```
Parameter G(Liquid,A,B;0) 298 -2000; 6000 N !
```

Load the AB_replace parameter.tdb via the **Append TDB** function, one can see from the TDB Viewer that the interaction parameter of G(Liquid,A,B;0) is replaced with the value (-2000) from the appended database.

Name	Property	x-Term	x-order	Parameter	T-limit (K)
Liquid	L	(A,B)	0	-2000	6000

The calculated phase diagrams using both original database and original + appended databases are shown in Figure 3.65.

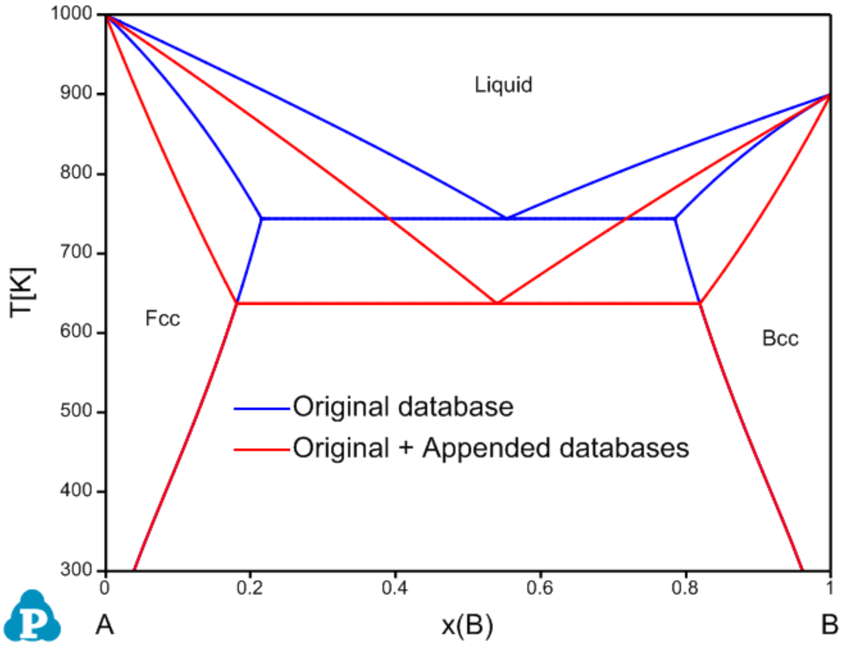


Figure 3.65 Calculated A-B phase diagram using both original database and original + appended databases

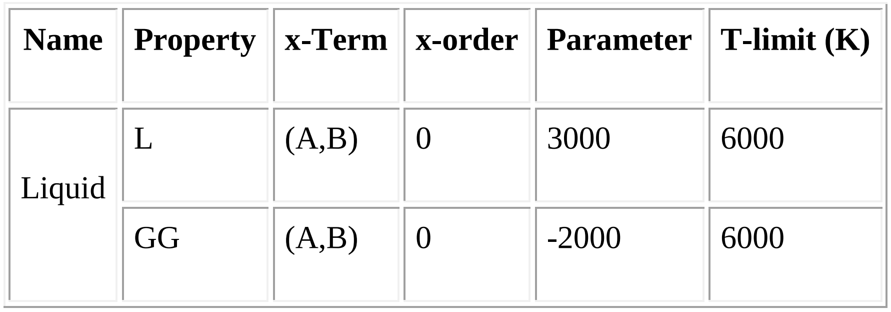
3.3.9.2 Add Value to an Existing Parameter

In this example, we are going to modify the interaction parameter of the liquid phase G(Liquid,A,B;0) within the original AB_original.tdb database by adding a value to it. As shown in the AB_modify parameter.tdb, the interaction parameter is expressed as GG(Liquid,A,B;0), which means adding this assigned value to the original value rather than replacing it.

```
Parameter GG(Liquid,A,B;0) 298 -2000; 6000 N !
```

As shown in the above section 3.3.9.1, the original value of the G(Liquid,A,B;0) interaction parameter is +3000. When we append the AB_modify parameter.tdb to the original database, the value of -2000 will be added to the original value

+3000 for the G(Liquid,A,B;0) interaction parameter. As shown in the TDB viewer below, one extra term “GG” is listed. For this case, the total value of the interaction parameter of G(Liquid,A,B;0) will be modified to be 3000 + (-2000) = +1000.



Name	Property	x-Term	x-order	Parameter	T-limit (K)
Liquid	L	(A,B)	0	3000	6000
	GG	(A,B)	0	-2000	6000

The calculated phase diagrams using both original database and original + appended databases are shown in Figure 3.66.

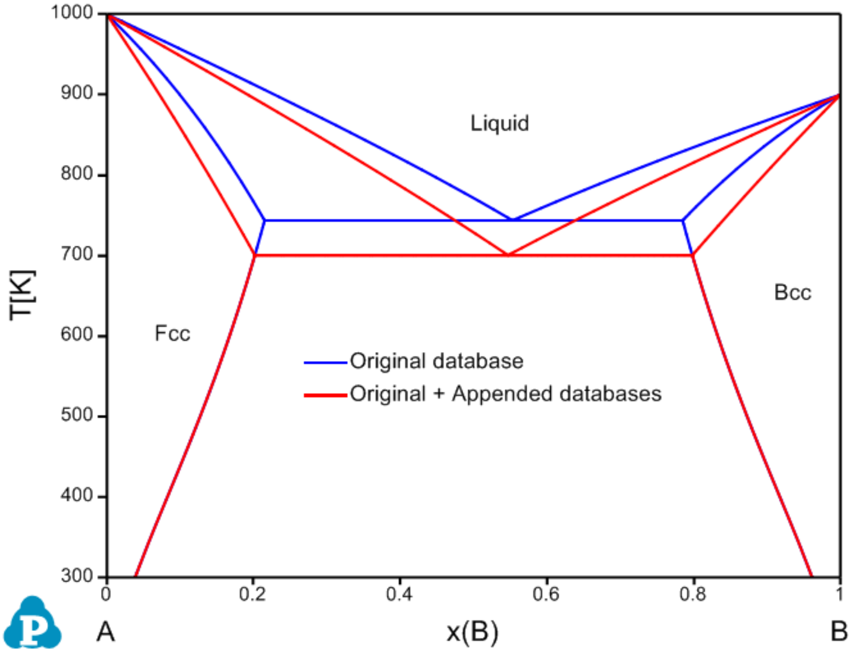
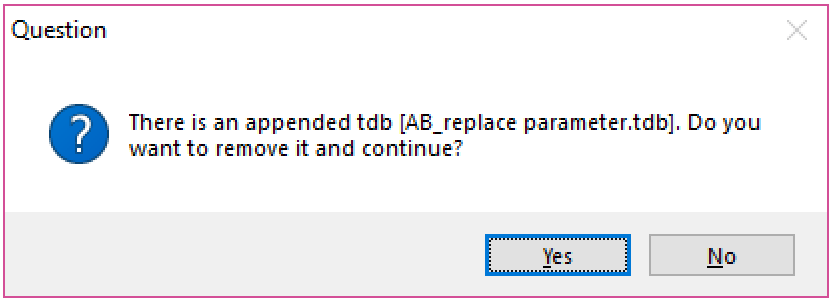


Figure 3.66 Calculated A-B phase diagram using both original database and original + appended databases with adjusted parameters

Note that, the **Append TDB** function allows user to append only one database to the original database. When user wants to append another database to the original database, the previously appended database will need to be removed first. Pandat™ will notify the user as shown in Figure 3.67 and user need to click **Yes** to confirm.



There is an appended tdb [AB_replace parameter.tdb]. Do you want to remove it and continue?

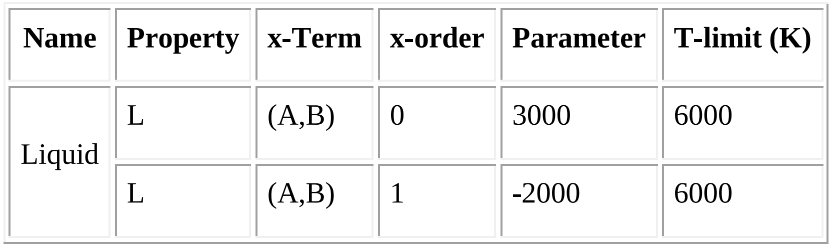
Figure 3.67 Append database confirmation

3.3.9.3 Add New Parameter to an Existing Phase

In addition to replace or modify the existing parameters for an existing phase in the original database, one can also add new parameters to this phase. In the AB_Original.tdb database, there is only one interaction parameter for the Liquid phase G(Liquid,A,B;0). Using the Append TDB function, we can add more interaction parameters to the Liquid phase. As shown in the AB_new parameter.tdb, another interaction parameter for the liquid phase, G(Liquid,A,B;1), is given as:

```
Parameter G(Liquid,A,B;1) 298 -2000; 6000 N !
```

Load the original AB_original.tdb and then load the AB_new parameter.tdb via the **Append TDB** function. As shown in the TDB viewer, the new interaction parameter (x-order value is 1) is added.



Name	Property	x-Term	x-order	Parameter	T-limit (K)
Liquid	L	(A,B)	0	3000	6000
	L	(A,B)	1	-2000	6000

The calculated phase diagrams using both original database and original + appended databases are shown in Figure 3.68.

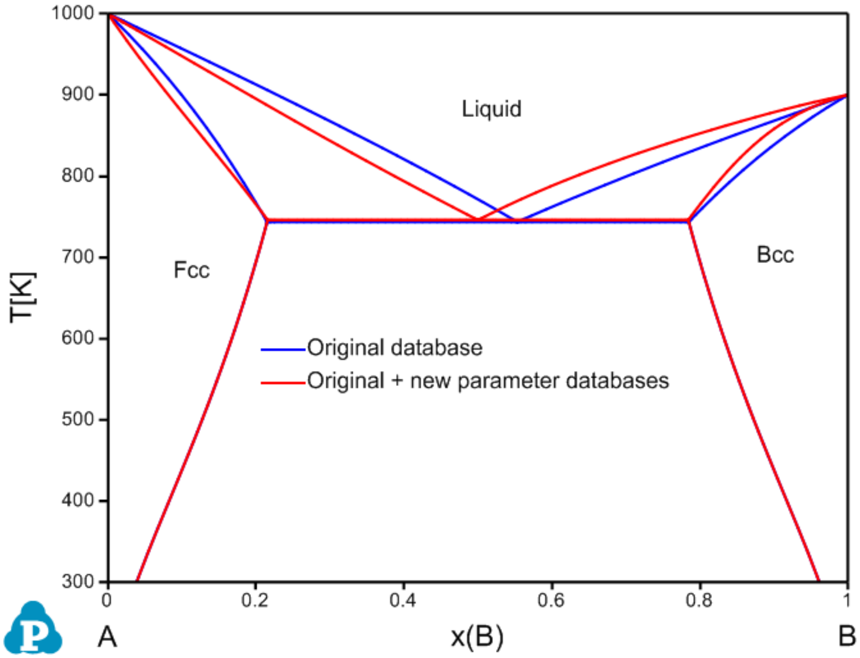


Figure 3.68 Calculated A-B phase diagram using both original database and original + appended databases with new parameters

3.3.9.4 Add New Phases to the Original Database

In addition to modify the parameters for existing phases within the original database, one can also add new phases via the **Append TDB** function. A new phase AB is introduced in the AB_new phase.tdb, which is described as:

```
Phase AB % 2 0.5 0.5 !

Constituent AB :A:B:!

      Parameter G(AB,A:B;0) 298.15 -10000+6*T; 6000 N !
```

Load the AB_original.tdb first and then load the AB_new phase.tdb via the **Append TDB** function. As shown in the TDB Viewer, a new AB phase is introduced.

Name	Property	x-Term	x-order	Parameter	T-limit (K)
AB	L0	(A)(B)	0	-10000+6*T	6000

The calculated phase diagrams using both original database and original + appended databases are shown in Figure 3.69.

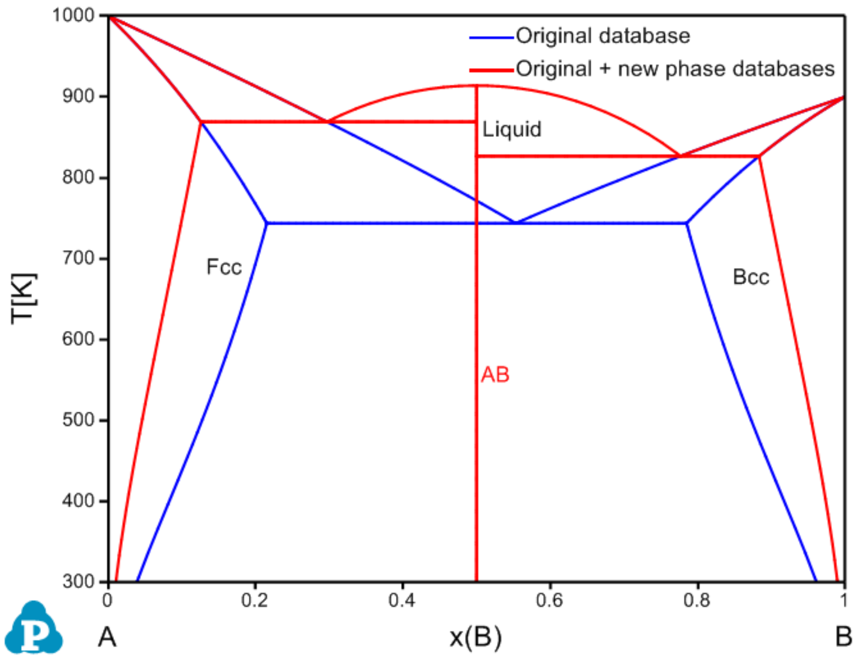


Figure 3.69 Calculated A-B phase diagram using both original database and original + appended databases with new phase

3.3.9.5 Add User-defined Properties to the Original Database

As is well known, the CALPHAD method has now been used to describe various types of phase properties in addition to thermodynamic properties. Mobility databases, molar volume databases and other thermo-physical property databases can be developed via similar route as that of developing a thermodynamic database. The **Append TDB** function allows a user to add user-defined properties to an original database. In this example, we add molar volume to AB_Original.tdb via the **Append TDB** function. The molar volume parameters of A and B within the Bcc, Fcc, and Liquid phases are described in the AB_property.tdb database as listed below:

```
Parameter Vm(Bcc,A;0) 298.15  +7.4e-6*exp(1e-6*T); 3000 N !

Parameter Vm(Bcc,B;0) 298.15  +8.4e-6*exp(1e-6*T); 3000 N !

Parameter Vm(Fcc,A;0) 298.15  +7.0e-6*exp(1e-6*T); 3000 N !

Parameter Vm(Fcc,B;0) 298.15  +8.0e-6*exp(1e-6*T); 3000 N !

Parameter Vm(Liquid,A;0) 298.15  +8.0e-6*exp(1e-6*T); 3000 N !
```

```
Parameter Vm(Liquid,B;0) 298.15  +9.0e-6*exp(1e-6*T); 3000 N !
```

Load the original database AB_original.tdb and then append the AB_property.tdb database via the **Append TDB** function. The currently combined AB_original + AB_property database enables us to calculate molar volume of the A-B binary system in addition to the phase diagram. The molar volume contour lines are shown in Figure 3.70 (refer to **Section 3.3.5** for calculating contour diagrams). Moreover, density and linear thermal expansion coefficient can also be calculated with this AB_original + AB_property database.

Please note that, various types of user-defined properties including but not limited to atomic mobility, molar volume, viscosity, surface tension can all be combined with the original thermodynamic database via the **Append TDB** function.

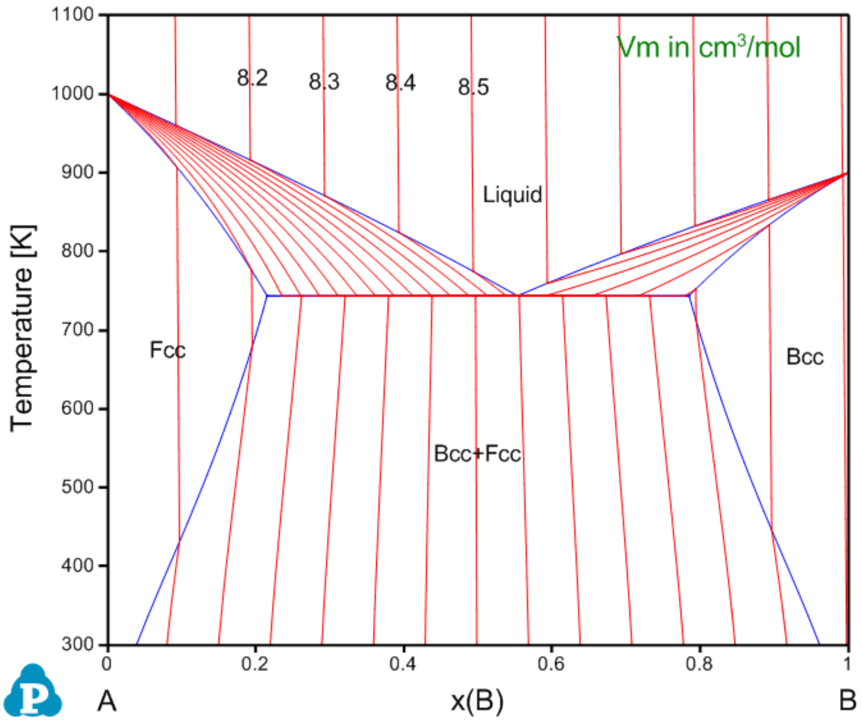


Figure 3.70 Calculated A-B phase diagram using both original database and original + appended databases with specific property

3.3.10 User-defined Property

This section is an extension of the above **Append database** section to develop and add user-defined-property database to the original database. Pandat allows user to define any property of a phase in a format similar to that of the Gibbs energy describing a disordered solution phase. Let *U* be the user-defined property and it is expressed as:

$$U = \sum_{i=1}^{c} x_i U_i^o + \sum_{i=1}^{c-1} \sum_{j=i+1}^{c} x_i x_j \sum_{k} (x_i - x_j)^k L_{ij}^k$$

where x_i is the molar fraction of component *i* and U_i^0 is the property of the pure component *i*, L_{ij}^k is the kth order interaction parameter between components *i* and *j*.

User can also define special properties associated with the properties of phases in the original database. Any phase property available from Pandat Table can be used for user-defined property, such as G, H, mu, and ThF. However, the star symbol in a property, like mu(*), cannot be used. User may refer to **section** 8 for more properties in detail.

3.3.11 Advanced Features

In this section, we are going to cover some advanced features of the PanPhaseDiagram module.

3.3.11.1 Local Equilibrium

In default, Pandat always calculates global stable phase equilibria. Even some phases are suspended, the calculated phase equilibria are still global stable ones for those “Entered” phases. The current version of Pandat enables us to calculate a “real” local equilibrium. The Al-Zn binary system is used as an example to demonstrate how to calculate the local phase equilibrium between the Fcc and Hcp phases. Note that, there is not GUI for the local equilibrium function and user has to run it through the batch file (.pbfx).

As shown below, a point with initial values needs to be defined in the batch file.

```
<point>
      <statespace>
            T value="500"/>
            <P value="1"/>
            <n component="Al" value="0.5"/>
            <n component="Zn" value="0.5"/>
      </statespace>

      <initial_value>
            <mu species="Al" value="-16000" />
            <mu species="Zn" value="-22000" />

            <phase_point phase_name="Fcc">
                  <y species="Al" sublattice="1" value="0.9" />
                  <y species="Zn" sublattice="1" value="0.1" />
            </phase_point>

            <phase_point phase_name="Hcp">
                  <y species="Al" sublattice="1" value="0.01" />
                  <y species="Zn" sublattice="1" value="0.99" />
            </phase_point>
      </initial_value>
</point>
```

In addition to the point with initial values, equilibrium type needs to be set as “local” (as shown below)

```
<condition>
      <equilibrium_type type="local"/>
</condition>
```

Figure 3.71 is the calculated stable Al-Zn binary phase diagram with the local-equilibrium between Fcc and Hcp phases.

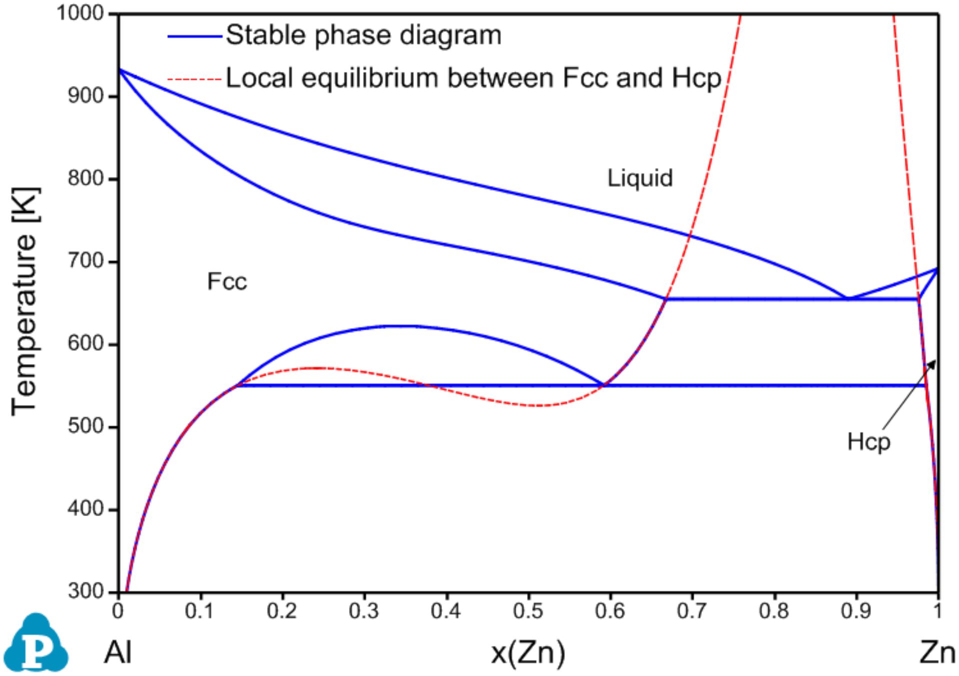


Figure 3.71 Calculated Al-Zn stable phase diagram with local-equilibrium between Fcc and Hcp phases

3.3.11.2 Hessian matrix of Gibbs energy

Pandat can calculate the determinant of Hessian matrix of Gibbs energy of a phase and the eigenvalues and eigenvectors of the Hessian matrix.

Since there is one dependent molar fraction for the molar fraction variables$(x_1, x_2, \cdots, x_n)$, one of the components is selected as the dependent one. Without loss of generality, x_n is selected as the one, i.e., the last component is considered as the solvent. Then, the second derivatives of Gibbs free energy of a phase form the Hessian matrix, which is an $(n-1) \times (n-1)$ symmetrical matrix.

$$HSN = \begin{pmatrix} \frac{\partial^2 G}{\partial x_1 \partial x_1} & \frac{\partial^2 G}{\partial x_1 \partial x_2} & \frac{\partial^2 G}{\partial x_1 \partial x_3} & \cdots & \frac{\partial^2 G}{\partial x_1 \partial x_{n-1}} \\ \frac{\partial^2 G}{\partial x_2 \partial x_1} & \frac{\partial^2 G}{\partial x_2 \partial x_2} & \frac{\partial^2 G}{\partial x_2 \partial x_3} & \cdots & \frac{\partial^2 G}{\partial x_2 \partial x_{n-1}} \\ \frac{\partial^2 G}{\partial x_3 \partial x_1} & \frac{\partial^2 G}{\partial x_3 \partial x_2} & \frac{\partial^2 G}{\partial x_3 \partial x_3} & \cdots & \frac{\partial^2 G}{\partial x_3 \partial x_{n-1}} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 G}{\partial x_{n-1} \partial x_1} & \frac{\partial^2 G}{\partial x_{n-1} \partial x_2} & \frac{\partial^2 G}{\partial x_{n-1} \partial x_3} & \cdots & \frac{\partial^2 G}{\partial x_{n-1} \partial x_{n-1}} \end{pmatrix}$$

Its determinant is given by

$$|HSN| = \begin{vmatrix} \frac{\partial^2 G}{\partial x_1 \partial x_1} & \frac{\partial^2 G}{\partial x_1 \partial x_2} & \frac{\partial^2 G}{\partial x_1 \partial x_3} & \cdots & \frac{\partial^2 G}{\partial x_1 \partial x_{n-1}} \\ \frac{\partial^2 G}{\partial x_2 \partial x_1} & \frac{\partial^2 G}{\partial x_2 \partial x_2} & \frac{\partial^2 G}{\partial x_2 \partial x_3} & \cdots & \frac{\partial^2 G}{\partial x_2 \partial x_{n-1}} \\ \frac{\partial^2 G}{\partial x_3 \partial x_1} & \frac{\partial^2 G}{\partial x_3 \partial x_2} & \frac{\partial^2 G}{\partial x_3 \partial x_3} & \cdots & \frac{\partial^2 G}{\partial x_3 \partial x_{n-1}} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 G}{\partial x_{n-1} \partial x_1} & \frac{\partial^2 G}{\partial x_{n-1} \partial x_2} & \frac{\partial^2 G}{\partial x_{n-1} \partial x_3} & \cdots & \frac{\partial^2 G}{\partial x_{n-1} \partial x_{n-1}} \end{vmatrix}$$

The determinant of Hessian matrix for phase `f` is available from “`HSN(@f)`”. The value of “`HSN(@f)`” is independent of the selection of the solvent component.

A Hessian matrix has real eigenvectors and each eigenvalue has a corresponding eigenvector. The eigenvalues and their eigenvectors are available from “`eVal(#*@f)`” and “`eVec(*#*@f)`”. Above Hessian matrix has eigenvalues of “`eVal(#1@f)`”, `eVal(#2@f)`”, ⋯ ,“`eVal(#n-1@f)`”. Each eigenvalue has an eigenvector. For example, `eVal(#1@f)` has an eigenvector of (`eVec(C`$_1$`#1@f)`, `eVec(C`$_2$`#1@f)`, ⋯ , `eVec(C`$_{n-1}$`#1@f)`), where `C`$_k$ is the name of the `k`th component.

Table 3.1 Functions that can be used in database and Table operation

Function	Meaning
`sin(x), cos(x), tan(x), tan2(y,x)`	Trigonometric functions. tan2(y,x)=tan(y/x)
`asin(x), acos(x), atan(x), atan2(y,x)`	Arcus functions. atan2(y,x)= atan(y/x)
`sinh(x), cosh(x), tanh(x)`	Hyperbolic functions
`asinh(x), acosh(x), atanh(x)`	Arcus hyperbolic functions
`Log2(x), log10(x), ln(x)`	Logarithm functions to base 2, 10 or e
`exp(x)`	exponential function
`abs(x)`	absolute value
`sqrt(x)`	square root
`rint(x)`	round to integral value
`sign(x)`	sign function
`HSN(@*)`	determinant of Hessian matrix of Gibbs free energy of a phase
`eVal(#*@*)`	eigenvalues of Hessian matrix of Gibbs free energy of a phase. * after # represents the eigenvalue index
`eVec(*#*@*)`	eigenvectors for the eigenvalues of Hessian matrix of Gibbs free energy of a phase. * before # represents the component of eigenvector. * after # represents the eigenvalue index.

The “solvent” component can be defined while using “Thermodynamic Property” calculation, or defined in Pandat Batch file. If “solvent” component is not defined, Pandat will choose the first component (the smallest atomic number) as the default “solvent” component.

4 PanOptimizer

PanOptimizer is a module of Pandat™ software designed for optimizing thermodynamic, kinetic and thermo-physical model parameters using experimental data. The module allows users to develop their own databases or model parameters for customized applications. This module is also easy to master by students who want to learn thermodynamic modeling.

4.1 Features of PanOptimizer

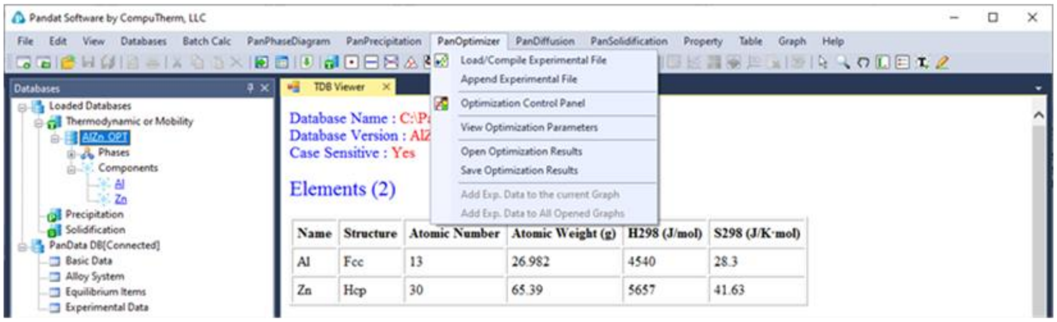
Derived from the maximum likelihood principle, when the discrepancies between model-calculated and experimental values are assumed to be independent, identically distributed with a normal distribution function, a set of model parameters with the best fit to the given experimental data can be obtained by the least square method. In the real world the experimental data may come from different sub-populations for which an independent estimate of the error variance is available. In this case, a better estimate than the ordinary least squares (OLS) can be obtained using weighted least squares (WLS), also called generalized least squares (GLS), then the sum of the squares can be written as

$$\frac{1}{2}\sum_{j=1}^{m} w_j \left[y_j - \phi(x;T_j,c_j) \right]^2 \tag{4.1}$$

The idea is to assign each observation a weight factor that reflects the uncertainty of the measurement. According to our previous experiences this method is efficient and reliable in the optimization of model parameters and develop variety of databases.

4.2 PanOptimizer Functions

The major functions included in the PanOptimizer menu are shown in Figure 4.1:



Database Name : C:\P
Database Version : AlZ
Case Sensitive : Yes

Elements (2)

Name	Structure	Atomic Number	Atomic Weight (g)	H298 (J/mol)	S298 (J/K·mol)
Al	Fcc	13	26.982	4540	28.3
Zn	Hcp	30	65.39	5657	41.63

Figure 4.1 The PanOptimizer Menu

The shortcut of the three commonly used functions **Load/Compile Experimental File**, **Rough Search** and **Optimization Control Panel** are also displayed in the Toolbar as shown in Figure 4.2.

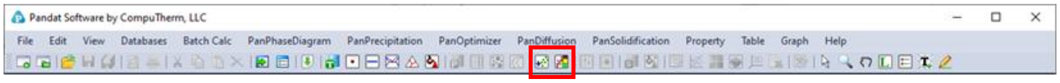


Figure 4.2 PanOptimizer toolbar

The functionality of each function is given below:

- **Load/Compile Experimental File**: Load/Compile experimental data file for model parameter optimization
- **Append Experimental File**: Append more experimental data from different data file
- **Rough Search**: Global/Local search of initial values of model parameters for obtaining the phase diagram topology of a system
- **Optimization Control Panel**: Allow user to set boundaries for the model parameters to be optimized, select experimental data to be used, and assign weight to each set of experimental data
- **View Optimization Parameters**: View/Edit model parameters to be optimized
- **Open Optimization Results**: Open the saved intermediate optimization results including the model parameters and experimental data

- **Save Optimization Results**: Save the intermediate optimization results during the optimization process including the model parameters and experimental data

4.3 Step by Step Instruction for Optimization

In general, user should follow a few steps below to perform the model parameter optimization.

4.3.1 Step 1: File preparation

4.3.1.1 Prepare the thermodynamic database file (.TDB)

In order to do the optimization, user must first define the model parameters to be optimized in the thermodynamic database (.tdb). The model parameters to be optimized can be defined in Pandat™ workspace where all the built-in keywords are automatically highlighted. It can also be done through outside text editor such as "Notepad". Each model parameter that needs to be optimized is defined by the keyword "`Optimization`". The format of defining a model parameter is:

```
Optimization [parameter name][low bound][initial value][high bound] N !
```

A definition sample for liquid phase in binary Al-Zn system is given as follows

```
$ Keyword          Name          Low Bound    Init. Value High Bound

Optimization       LIQ_AA        0            0;          60000       N !

Optimization       LIQ_AAT       -20          0;          20          N !

Optimization       LIQ_BB        -60000       0;          60000       N !

Optimization       LIQ_BBT       -20          0;          20          N !

Phase Liquid % 1 1 !

Constituent Liquid : Al, Zn : !
```

```
Optimization G(Liquid,Al;0)     298.15  G_Al_LIQUID;          6000 N !
Optimization G(Liquid,Zn;0)     298.15  G_Zn_LIQUID;          6000 N !
Optimization G(Liquid,Al,Zn;0)  298.15  LIQ_AA + LIQ_AAT*T;   6000 N !
Optimization G(Liquid,Al,Zn;1)  298.15  LIQ_BB + LIQ_BBT*T;   6000 N !
```

Two modes of optimization are allowed in the current version: one is “bounded” optimization and the other one is “no bound” optimization. Even though the low and high bounds will be in effect in the bounded optimization only, they are required for definition of model parameters in a `TDB` file. The model parameters can be named at users’ choices. It is suggested that the name is related to the phase to be optimized. Note: User may use “`%`” to denote the major species in a sublattice of a phase in a `TDB` file. PanOptimizer will automatically assign the initial values for the major species denoted by “`%`”. The following example means Zn is the major species in the first sublattice of the Hcp phase:

```
Phase Hcp % 2 1 0.5 !
Constituent Hcp: Al, Zn%: Va:!
```

4.3.1.2 Prepare the experimental file (.POP)

Users need to provide their own experimental data file for optimization of model parameters. The most widely accepted format for experimental data file in the CALPHAD society is a `POP` file. PanOptimizer accepts most of the keywords in the `POP` format and adds a few special keywords. In a `POP` file, a phase can have four statuses: ENTERED, FIXED, DORMANT, and SUSPEND. The first two statuses were used most frequently. When phases are in the ENTERED status, PanOptimizer does not require user to input any initial values for calculation since the truly stable phase equilibria will be found automatically in this case with the built-in global optimization algorithm. On the other hand, for those phases in FIXED or DORMANT status, the initial values should be provided by the user. Example POP files are provided in the installation dictionary of Pandat™.

4.3.2 Step 2: Carry out optimization

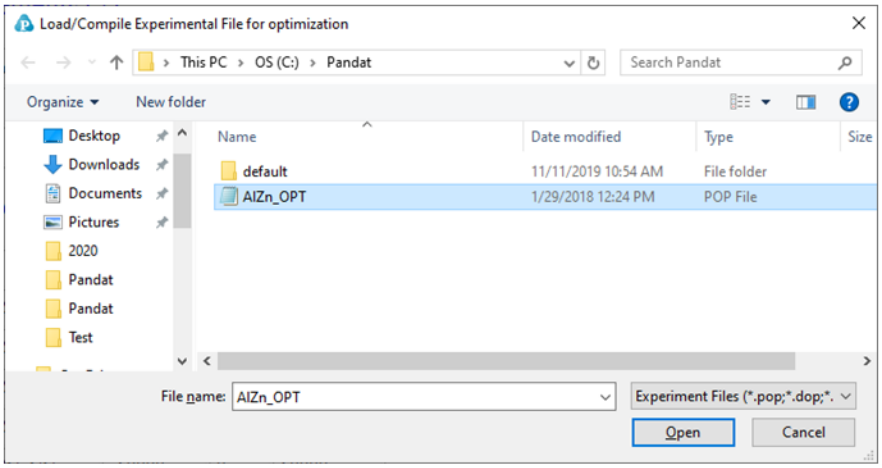
Once above files have been prepared, user is ready to carry out optimization:

4.3.2.1 Load thermodynamic database file

First of all, the database file (`.TDB`) containing the phases to be modeled is loaded by click the button. This database file defines the model type and model parameters of each phase in the system. The model definition is consistent with the currently accepted format in the CALPHAD society, and the model parameters can be real numbers or variables to be optimized.

4.3.2.2 Load and compile experimental file

After loading a `TDB` file with defined model parameters to be optimized, users should then load and compile the experimental `POP` file. Go to PanOptimizer menu and choose **Load/Compile Experimental File**, user can then select the `POP` file already prepared as shown in Figure 4.3. User can also choose **Append Experimental File** to append new experimental data stored in a separate file to the currently opened `POP` file.



Name	Date modified	Type	Size
default	11/11/2019 10:54 AM	File folder	
AlZn_OPT	1/29/2018 12:24 PM	POP File	

File name: AlZn_OPT

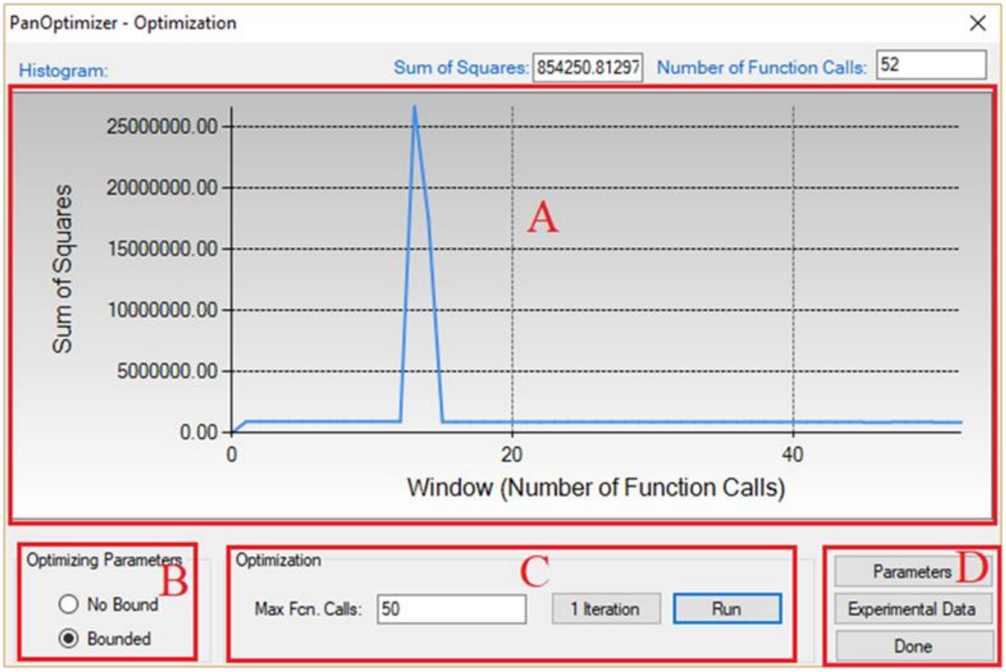
Experiment Files (*.pop;*.dop;*.

Figure 4.3 Dialog window of loading an experimental file

4.3.2.3 Perform Optimization

Once the `TDB` file and the experimental `POP` file are loaded, user is ready to do the optimization. In the current version of PanOptimizer, the optimization is controlled through the optimization control panel as shown in Figure 4.4.

There are four control areas in the optimization control panel. They are: Histogram (A), Bound/Unbound Variables (B), Optimization (C), and Optimization Results (D).



Sum of Squares: 854250.81297

Number of Function Calls: 52

Optimizing Parameters: ○ No Bound ● Bounded

Max Fcn. Calls: 50

Figure 4.4 The optimization control panel.

4.3.2.4 Histogram (A)

Histogram is for displaying and tracing the history of the discrepancy between model-calculated values and experimental data, which is characterized by the Sum of Squares displayed during the whole optimization procedure. The histogram plots the sum of squares *vs.* the number of function calls. The exact value of the sum of squares in the current step can be found at the up-right corner of this area.

4.3.2.5 Free Bound/Unbound Variables (B)

The user can choose the model parameters to be optimized in either the bounded or the unbounded mode. In the bounded mode, the low and high bounds defined in a `TDB` file will take into effects.

4.3.2.6 Optimization (C)

The goal of the optimization process is to obtain an optimal set of model parameters so that the model calculated results can best fit the given experimental measurements. The optimization process can be controlled by choosing **1 Iteration** or **Run**. With **1 Iteration**, the maximum number of function calls is set to be `2(N+2)`, where `N` is the number of model parameters to be optimized. The user can click **Run** mode several times until the optimal solution is found or the designated maximum number of function calls is reached.

Here we take the binary Al-Zn system as an optimization example. The `TDB` and `POP` files are available at the installing directory of Pandat™ "`/Pandat_Examples/PanOptimizer/`". In this example, there are totally 11 parameters to be optimized and all the initial values are set to be zero. The available experimental data include:

- mixing enthalpy of liquid phase at 953K
- invariant reaction at 655K: Liquid → Fcc + Hcp
- invariant reaction at 550K: Fcc#2 → Fcc#1 + Hcp
- tie-lines: Fcc#1+Fcc#2, Liquid + Fcc, Liquid + Hcp and Hcp + Fcc

Before the optimization, user may want to check the calculated results using the initial set of model parameters without optimization. Phase diagram calculation can be done through 2-D section calculation, and enthalpy calculation can be done through the 1-D line calculation. Figure 4.5 shows the calculated Al-Zn phase diagram and enthalpy of mixing for liquid phase at

953K along with the given experimental data, respectively. The parameters before optimization result in large discrepancies between the calculated values and the experimental measurements. Optimization of these model parameters (initially set as zero) is needed.

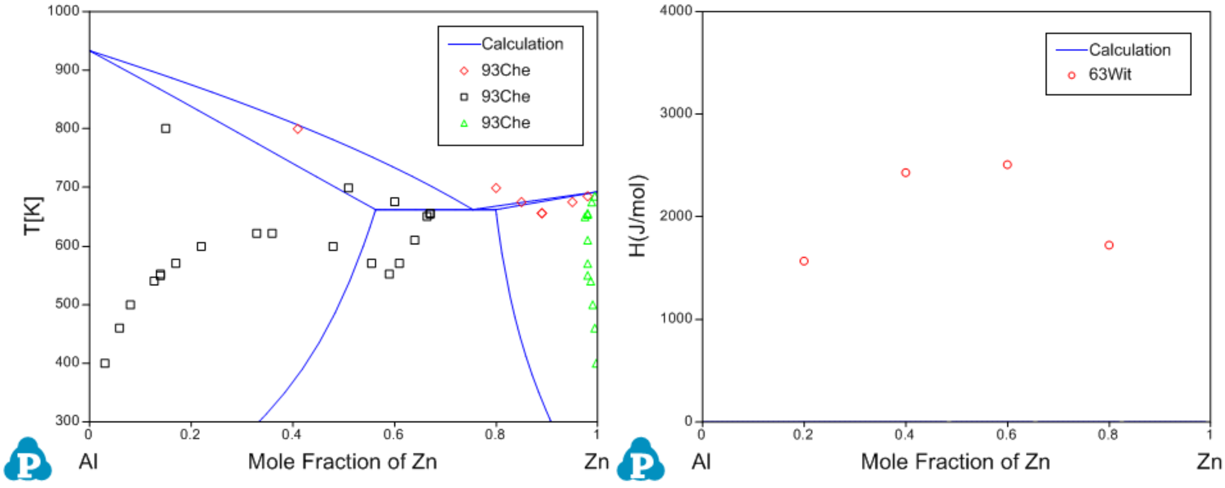
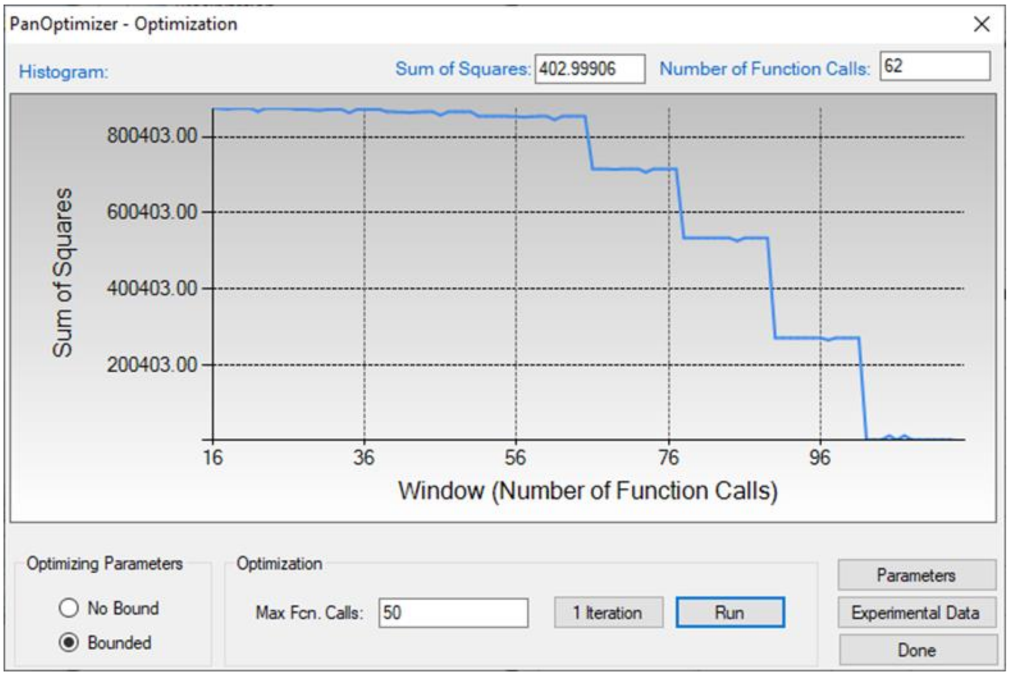


Figure 4.5 Comparisons between calculated results and experimental data before the optimization

By clicking **Run** twice (two rounds), and each run performs 50 function calls, the sum of squares decreases from 854251 to 403 as shown in Figure 4.6. After another round of **Run**, the sum of squares decreases from 403 to 3.15 as shown in Figure 4.7. Now, we can do the real time calculation using the instantly obtained optimized parameters. The two comparisons in Figure 4.8 show excellent agreements between the calculated results and the measured data. By selecting the command from PanOptimizer menu: **PanOptimizer → Add Exp. Data to the current Graph**, user can add the corresponding experimental data defined in the pop file directly to the calculated diagram for comparison.


PanOptimizer - Optimization

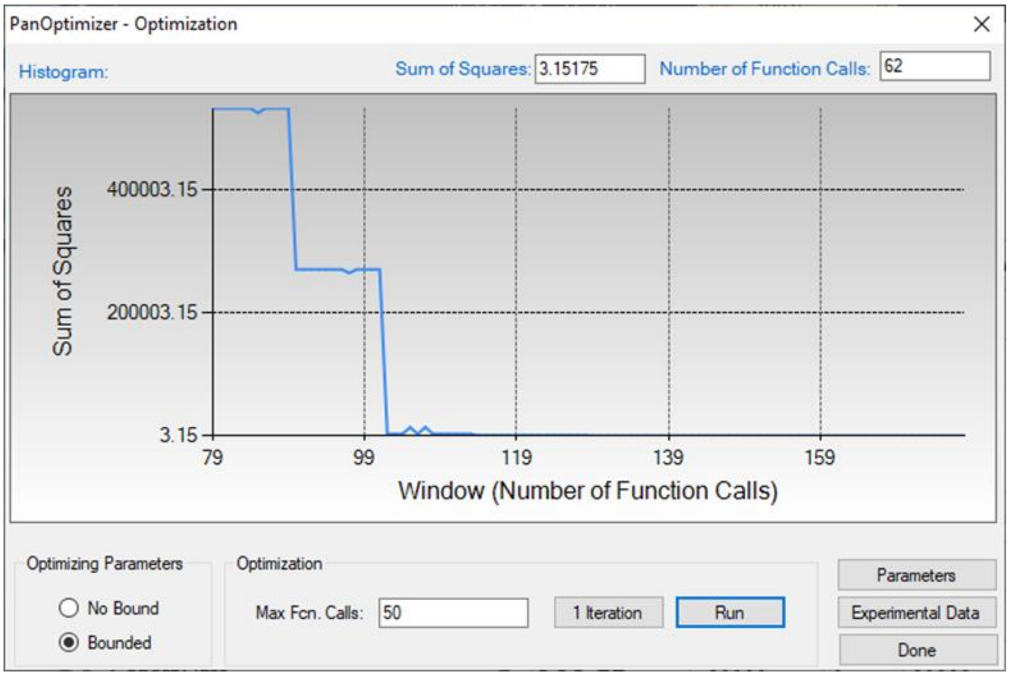
Sum of Squares: 402.99906

Number of Function Calls: 62

Optimizing Parameters: ○ No Bound ● Bounded

Max Fcn. Calls: 50

Figure 4.6 The sum of squares after two rounds of optimization


PanOptimizer - Optimization

Sum of Squares: 3.15175

Number of Function Calls: 62

Optimizing Parameters: ○ No Bound ● Bounded

Max Fcn. Calls: 50

Figure 4.7 The sum of squares after another two rounds of optimization

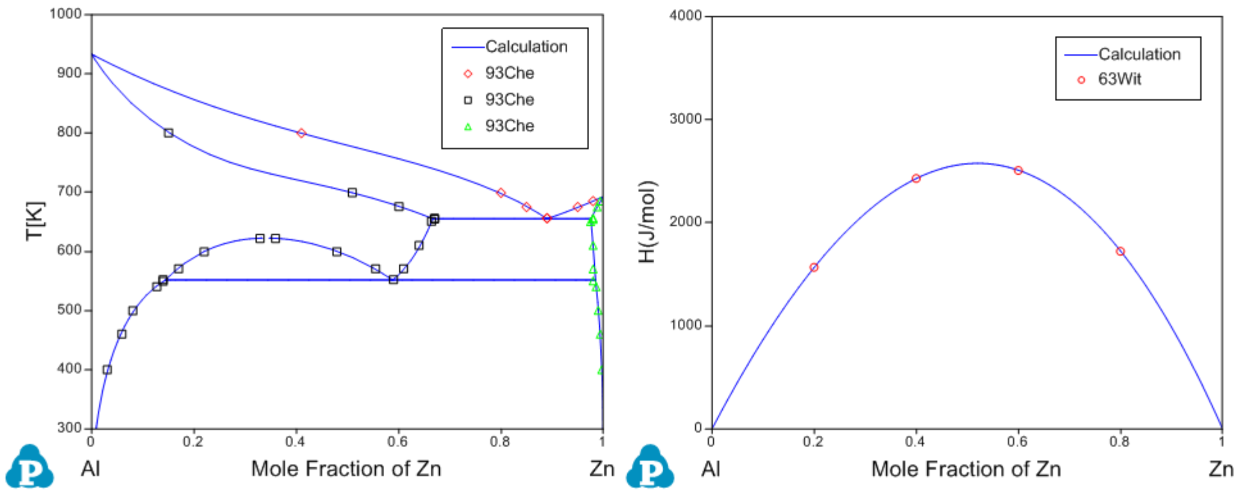
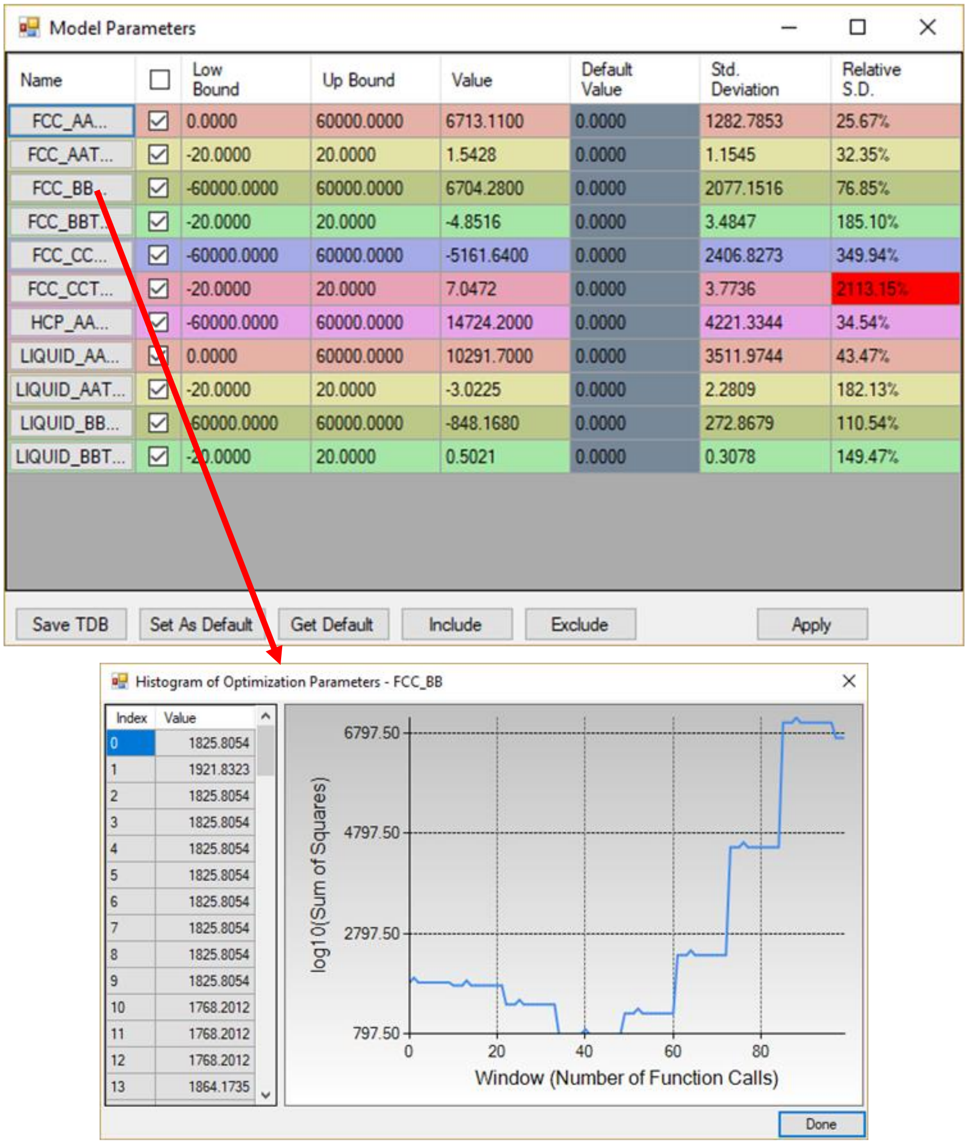


Figure 4.8 Comparisons between the calculated results and the experimental data after optimization

4.3.2.7 Optimization Results (D)

During optimization, user can check model parameters through the **Parameters** button as shown in Figure 4.4. For each model parameter, user can change its low bound, upper bound and initial value in the dialog window as shown in Figure 4.9. User can **Include** or **Exclude** a certain parameter in the optimization through the “check box” in front of the parameter. If a set of optimized parameters is satisfactory, user can save this set of values as default ones through **Set Default** shown in Figure 4.9. Otherwise, user can reject this set of values and go back to previous default values through **Get Default**. User also can save the `TDB` file with the optimized model parameters through **Save TDB**. The standard deviation and relative standard deviation (RSD) of each parameter are computed during optimization. The parameter evolution during the last 100 iterations can be tracked by clicking the parameter name in the table as indicated in Figure 4.9. It should be noted that any changes on model parameters made by user will take into effect only after the “**Apply**” button is clicked.

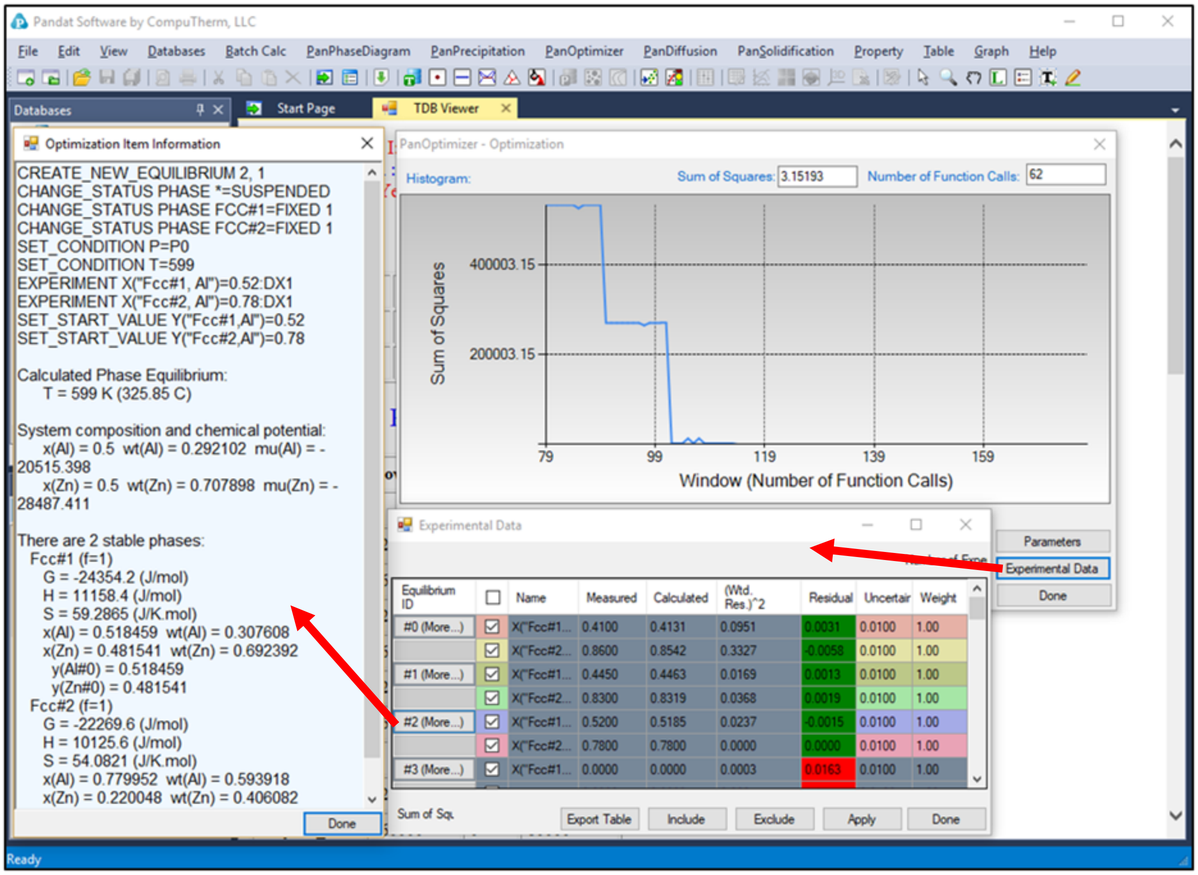


Name	☐	Low Bound	Up Bound	Value	Default Value	Std. Deviation	Relative S.D.
FCC_AA...	☑	0.0000	60000.0000	6713.1100	0.0000	1282.7853	25.67%
FCC_AAT...	☑	-20.0000	20.0000	1.5428	0.0000	1.1545	32.35%
FCC_BB...	☑	-60000.0000	60000.0000	6704.2800	0.0000	2077.1516	76.85%
FCC_BBT...	☑	-20.0000	20.0000	-4.8516	0.0000	3.4847	185.10%
FCC_CC...	☑	-60000.0000	60000.0000	-5161.6400	0.0000	2406.8273	349.94%
FCC_CCT...	☑	-20.0000	20.0000	7.0472	0.0000	3.7736	2113.15%
HCP_AA...	☑	-60000.0000	60000.0000	14724.2000	0.0000	4221.3344	34.54%
LIQUID_AA...	☑	0.0000	60000.0000	10291.7000	0.0000	3511.9744	43.47%
LIQUID_AAT...	☑	-20.0000	20.0000	-3.0225	0.0000	2.2809	182.13%
LIQUID_BB...	☑	60000.0000	60000.0000	-848.1680	0.0000	272.8679	110.54%
LIQUID_BBT...	☑	-20.0000	20.0000	0.5021	0.0000	0.3078	149.47%

Index	Value
0	1825.8054
1	1921.8323
2	1825.8054
3	1825.8054
4	1825.8054
5	1825.8054
6	1825.8054
7	1825.8054
8	1825.8054
9	1825.8054
10	1768.2012
11	1768.2012
12	1768.2012
13	1864.1735

Figure 4.9 Dialog windows of Model Parameters and Histogram of Optimization Parameters

By clicking the **Experimental Data** button on Figure 4.7, a table which lists the calculated values together with the experimental data will pop out as shown in Figure 4.10. This table allows user to view how well the current optimized parameters describe each set of experimental data. If the discrepancy is found to be large and not satisfied for a certain set of data, a larger weight factor for this set of data can be given in the next round of optimization. Through the column of "**Residual**" shown in Figure 4.10, user can see different color after each comparison. The green means satisfactory results are achieved, while the red color means large deviation remaining. Again, user can **Include** or **Exclude** a certain experimental data set for the optimization through the check box in front of each experimental data **Name**. Also, more detailed experimental data information can be viewed by clicking the experimental data ID in the table.



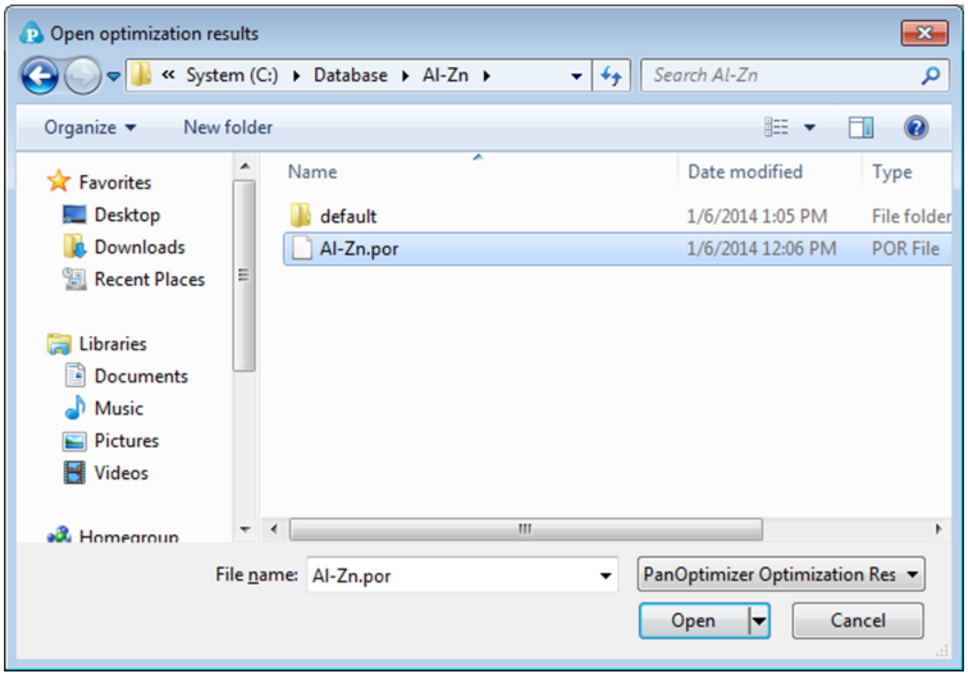
```
CREATE_NEW_EQUILIBRIUM 2, 1
CHANGE_STATUS PHASE *=SUSPENDED
CHANGE_STATUS PHASE FCC#1=FIXED 1
CHANGE_STATUS PHASE FCC#2=FIXED 1
SET_CONDITION P=P0
SET_CONDITION T=599
EXPERIMENT X("Fcc#1, Al")=0.52:DX1
EXPERIMENT X("Fcc#2, Al")=0.78:DX1
SET_START_VALUE Y("Fcc#1,Al")=0.52
SET_START_VALUE Y("Fcc#2,Al")=0.78

Calculated Phase Equilibrium:
    T = 599 K (325.85 C)

System composition and chemical potential:
    x(Al) = 0.5  wt(Al) = 0.292102  mu(Al) = -
20515.398
    x(Zn) = 0.5  wt(Zn) = 0.707898  mu(Zn) = -
28487.411

There are 2 stable phases:
  Fcc#1 (f=1)
    G = -24354.2 (J/mol)
    H = 11158.4 (J/mol)
    S = 59.2865 (J/K.mol)
    x(Al) = 0.518459  wt(Al) = 0.307608
    x(Zn) = 0.481541  wt(Zn) = 0.692392
     y(Al#0) = 0.518459
     y(Zn#0) = 0.481541
  Fcc#2 (f=1)
    G = -22269.6 (J/mol)
    H = 10125.6 (J/mol)
    S = 54.0821 (J/K.mol)
    x(Al) = 0.779952  wt(Al) = 0.593918
    x(Zn) = 0.220048  wt(Zn) = 0.406082
```

Equilibrium ID	☐	Name	Measured	Calculated	(Wtd. Res.)^2	Residual	Uncertair	Weight
#0 (More...)	☑	X("Fcc#1...	0.4100	0.4131	0.0951	0.0031	0.0100	1.00
	☑	X("Fcc#2...	0.8600	0.8542	0.3327	-0.0058	0.0100	1.00
#1 (More...)	☑	X("Fcc#1...	0.4450	0.4463	0.0169	0.0013	0.0100	1.00
	☑	X("Fcc#2...	0.8300	0.8319	0.0368	0.0019	0.0100	1.00
#2 (More...)	☑	X("Fcc#1...	0.5200	0.5185	0.0237	-0.0015	0.0100	1.00
	☑	X("Fcc#2...	0.7800	0.7800	0.0000	0.0000	0.0100	1.00
#3 (More...)	☑	X("Fcc#1...	0.0000	0.0000	0.0003	0.0163	0.0100	1.00

Figure 4.10 Dialog windows of Experimental Data and Optimization Item Information

4.3.3 Step 3: Save/Open Optimization Results

During optimization, the user may save and load optimization file through **Save Optimization Results** and **Open Optimization Results** (see Figure 4.11). The optimization results file has the extension name of *POR* that can only be read by PanOptimizer. Intermediate optimization results can be saved and restored through these two operations. These functions are very useful especially when a user is optimizing model parameters for a complicated system. The user can always go back to a certain middle stage and restart from there. This will save user's time by avoiding some repeated work.



Name	Date modified	Type
default	1/6/2014 1:05 PM	File folder
Al-Zn.por	1/6/2014 12:06 PM	POR File

File name: Al-Zn.por

Figure 4.11 Dialog window of open the saved optimization results

4.4 User-defined Property Optimization

The parameters for physical property, kinetic property, and user-defined property can also be optimized with respect to experimental data just like the parameters in a thermodynamic database. User can refer to section 8.4 for the format to define user-defined property in a database. Similar to the optimization of thermodynamic model parameters, user needs to define the parameters to be optimized in the database and prepare a pop file with corresponding experimental data. An example for the parameter definition in the database is shown below.

```
$Thermal conductivity of pure element in the Fcc phase

PARAMETER ThCond(Fcc,Al;0) 298.15  +311.72511-0.09661*T-13510.26/T; 3000 N !

PARAMETER ThCond(Fcc,Cu;0) 298.15  +417.28065-0.06598*T+944.065/T; 3000 N !
```

```
$Thermal conductivity interaction parameters for Fcc phase to be optimized
OPTIMIZATION      Fcc_TC           0          0;      60000 N !
OPTIMIZATION      Fcc_TCT        -50      -24.6;      0     N !
OPTIMIZATION      Fcc_TC_1    -60000          0;      0     N !
OPTIMIZATION      Fcc_TCT_1        0         28;      50    N !
PARAMETER ThCond(Fcc,Al,Cu;0) 298.15  +Fcc_TC+Fcc_TCT*T; 3000 N !
PARAMETER ThCond(Fcc,Al,Cu;1) 298.15  +Fcc_TC_1+Fcc_TCT_1*T; 3000 N !
```

And an example pop file for the experimental data is shown below.

```
$Thermal Conductivity of the Fcc phase at 1000K
TABLE_HEAD
CREATE_NEW_EQUILIBRIUM @@,1
CHANGE_STATUS PHASE * = S
CHANGE_STATUS PHASE Fcc = FIX 1
SET_CONDITION T=1000, P = P0, X(Fcc,Cu) = @1
EXPERIMENT ThCond(Fcc)= @3 : @4
TABLE_VALUES
$ x(Cu)     x(Al)       TC          DTC
0.05        0.95        194         50
0.1         0.9         295         50
0.2         0.8         750         50
0.8         0.2         3116        50
0.9         0.1         2122        50
0.95        0.05        1343        50
TABLE_END
```

The optimization procedure is the same as that for thermodynamic parameters. User may refer to the previous section for details and get the optimization result step by step.

5 PanPrecipitation

A module of Pandat™ software, which is seamlessly integrated with the thermodynamic calculation engine – PanEngine for the necessary thermodynamic input and mobility data, is designed for the simulation of precipitation kinetics during heat treatment process. 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). For this reason, precipitation simulations for highly complex alloys under arbitrary heat treatment conditions can be accomplished with only a few operations. Figure 5.1 shows the three-layered architecture of this modeling tool.

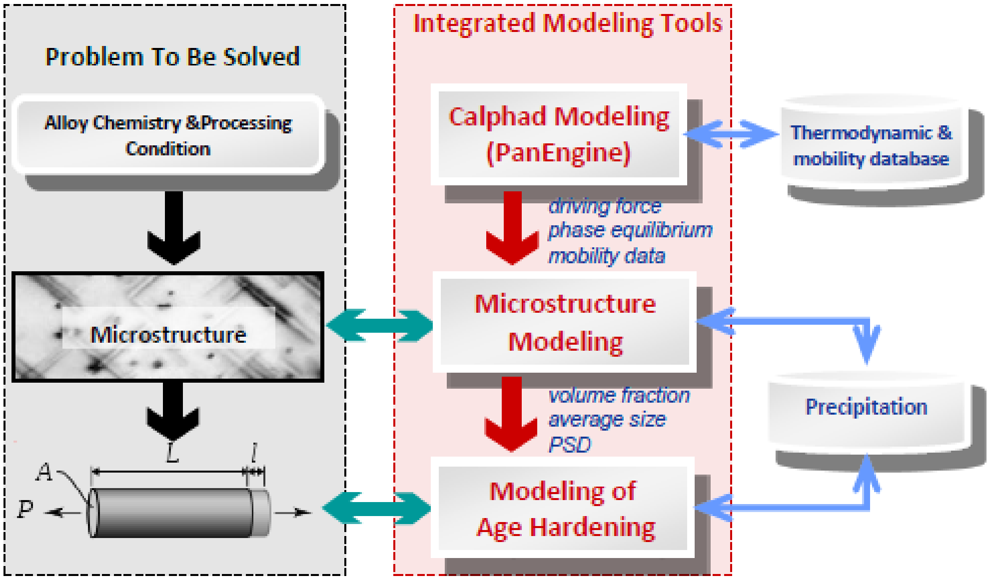


Figure 5.1 The three-layered architecture of the integrated modeling tool

5.1 Features of PanPrecipitation

5.1.1 Overall Design

➢ Concurrent nucleation, growth/dissolution, and coarsening of precipitates

- Temporal evolution of average particle size and number density
- Temporal evolution of particle size distribution
- Temporal evolution of volume fraction and composition of precipitates

5.1.2 Data Structure

PanPrecipitation is a purely object-oriented module written in C++ with generic data structures like PanEngine, balancing performance, maintainability and scalability. The basic data structure for storing precipitation information in the system of interest is schematically shown in Figure 5.2.

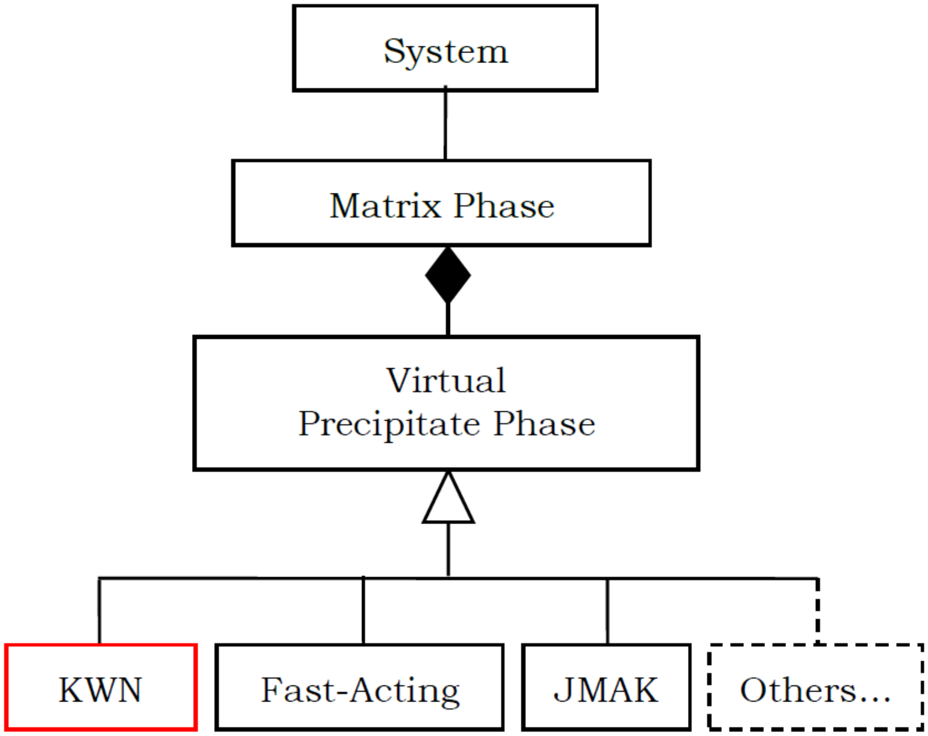


Figure 5.2 Data structure of system information in PanPrecipitation

In general, a system contains a matrix phase and a number of precipitate phases. Different precipitate phases may behave differently, which should be described by different kinetic models. On the other hand, the calculation speed is directly related to the complexity of the model. It therefore requires multi-level models for different purposes. The current PanPrecipitation module includes two built-in models: the Kampmann/Wagner Numerical (KWN) model and the Fast-Acting model. One unique advantage is that this generic data structure allows easy integration of other precipitation models with the PanPrecipitation module as shown in Figure 5.2. This gives users great flexibility in choosing the proper kinetic models, including their own user-defined models, for custom applications.

Based on the above data structure, input parameters for the matrix and its precipitate phases are organized in “Extensible Markup Language” (XML) format, which is a standard markup language and well-known for its extendibility. In accordance with the XML syntax, a set of well-formed tags are specially designed to define the kinetic model for each precipitate phase and its corresponding model parameters such as interfacial energy, molar volume, nucleation type, and morphology type. In PanPrecipitation, two kinetic models known as the KWN and Fast-Acting were implemented and available for user’s choice. Both models can be used to simulate the co-precipitation of phases with various morphologies (sphere and lens), with concurrent processes of nucleation, growth and coarsening. With the selection of the KWN model, the particle size distributions (PSD) of various precipitate phases can be obtained in addition to the temporal evolution of the average size and volume fraction as obtained from the Fast-Acting model. Therefore, the KWN model is recommended by default.

5.1.3 Kinetic Models

In PanPrecipitation, KWN model is based on the Kampmann and Wagner’s work as implemented in a numerical framework, and extended to handle both homogeneous and heterogeneous nucleation, dealing with various morphologies for the simulation of precipitation kinetics of multi-component alloys under arbitrary heat treatment conditions. The following is a brief introduction to the KWN model along with its sub-models for nucleation, growth and coarsening.

Specifically, in the KWN model the continuous PSD is divided into a large number of size classes. The program takes a simulation step at every sample time hit. To maintain both accuracy and efficiency between two adjacent simulation steps, a fifth-order Runge-Kutta scheme is used to generate an adaptive step size based on the continuity equation.

Please note that all the variables used in the equations in this section are summarized in Tables 5.1-5.4. Please refer to Tables 5.2-5.4 and examples in Section 5.1.4 for setting up these variables in the KDB files.

5.1.3.1 Nucleation

(a) Homogeneous nucleation

At each simulation step, the number of new particles is first calculated using classical nucleation theory and then these new particles are allocated to an appropriate size class. The transient nucleation rate is given by,

$$J = N_v Z \beta^* exp\left(-\frac{\Delta G^*}{k_B T}\right) exp\left(-\frac{\tau}{t}\right) \tag{5.1}$$

The pre-exponential terms in equation (5.1) are: N_v, the nucleation site density, Z , the Zeldovich factor and β^*, the atomic attachment rate. t is the time, τ the incubation time for nucleation, k_B the Boltzmann constant and T the temperature.

The nucleation barrier is defined as $\Delta G^* = \frac{4\pi}{3}(R^*)^2 \sigma_{\alpha\beta}$ where R^* is the radius of the critical nucleus and $R^* = -\frac{2\sigma_{\alpha\beta}}{\Delta G_{vol}}$. The nucleation barrier can be written as,

$$\Delta G^* = \frac{16\pi}{3} \frac{(\sigma_{\alpha\beta})^3}{(\Delta G_V + \Delta G_S)^2} \tag{5.2}$$

ΔG_V is the chemical driving force per volume for nucleation and calculated directly from thermodynamic database with $\Delta G_V = \frac{\Delta G_m}{V_m}$, ΔG_S is the elastic strain energy per volume of precipitate. $\sigma_{\alpha\beta}$ is the interfacial energy of the matrix/particle interface. For a spherical nucleus,

$$Z = \frac{V_\alpha}{2\pi N_A {R^*}^2}\sqrt{\frac{\sigma_{\alpha\beta}}{k_B T}} \tag{5.3}$$

$$\beta^* = \frac{4\pi {R^*}^2}{a^4} D_{eff} \tag{5.4}$$

$$\tau = \frac{1}{2Z^2\beta^*} \tag{5.5}$$

Where V_α is the molar volume of the matrix, and a is the lattice constant of the precipitate phase and D_{eff} is the effective diffusivity $D_{eff} = \left[\sum_{i=1}^{n}\frac{(C_{pi}-C_{0i})^2}{C_{0i}D_{0i}}\right]^{-1}$ and is defined by [2004Svo], where C_{pi} is the mean concentration in the precipitate and C_{0i} is the mean concentration in the matrix phase. D_{0i} is the matrix diffusion coefficient of the component i.

The calculation of the elastic strain energy is given by Nabarro [1940Nab] for a homogeneous inclusion in an isotropic matrix,

$$\Delta G_S = \frac{2}{3}\mu\Delta^2 f(A_R) \tag{5.6}$$

Where μ is the shear modulus of the matrix. Thus the elastic strain energy is proportional to the square of the volume misfit Δ^2. The function $f(A_R)$ provided in [1940Nab] is a factor that takes into account the shape effects. For a given volume, a sphere $(A_R = 1)$ has the highest strain energy while a thin plate $(A_R \to 0)$ has a very low strain energy, and a needle shape $(A_R \to \infty)$ lies between the two. Therefore the equilibrium shape of precipitates will be reached by balancing the opposing effects of interfacial energy and strain energy. When Δ is small, interfacial energy effect should dominate and the precipitates should be roughly spherical.

In homogeneous nucleation, the number of potential nucleation sites can be estimated by,

$$N_v = N_f \frac{N_A}{V_\alpha} \tag{5.7}$$

Where N_A is the Avogadro number. The value of nucleation site parameter N_f is an adjustable parameter and usually chosen close to solute concentration for homogeneous nucleation.

(b) Heterogeneous nucleation

For heterogeneous nucleation on dislocations, grain boundaries (2-grain junctions), grain edges (3-grain junctions) and grain corners (4-grain junctions), the potential nucleation sites N_v and the nucleation barrier ΔG^* must be adjusted accordingly.

There are two ways to account for heterogeneous nucleation in PanPrecipitation. One way is to treat nucleation site parameter N_f in equation (5.7) as phenomenological parameters and replace equation (5.2) by a user-defined equation. An example is given at **section 5.1.4.4**. The other way is to theoretically estimate the potential nucleation sites and calculate the nucleation barrier by assuming an effective interfacial energy for each nucleation site. For nucleation on grain boundaries, edges or corners, the nucleation barrier can be calculated by [55Cle],

$$\Delta G^* = \frac{4}{27}\frac{\left(b\sigma_{\alpha\beta} - a\sigma_{\alpha\alpha}\right)^3}{(c\Delta G_{vol})^2} \tag{5.8}$$

Where $\sigma_{\alpha\beta}$ is the interfacial energy and $\sigma_{\alpha\alpha}$is the grain boundary energy and a, b, c are geometrical parameters, which are evaluated for grain boundaries, edges and corners. By introducing a contact angle, the grain boundary energy can be calculated from $\sigma_{\alpha\alpha} = 2\cos\theta\sigma_{\alpha\beta}$. An effective interfacial energy σ_{eff} is then introduced and the nucleation barrier is given as $\Delta G^* = \frac{16\pi}{3}\frac{\left(\sigma_{eff}\right)^3}{(\Delta G_{vol})^2}$ with

$$\sigma_{eff} = \frac{b\sigma_{\alpha\beta} - a\sigma_{\alpha\alpha}}{c^{\frac{2}{3}}}\left(\sqrt[3]{\frac{1}{36\pi}}\right) \tag{5.9}$$

The effective interfacial energy σ_{eff} can be applied in the framework of classical nucleation theory. One can verify that the homogenous nucleation equations are recovered with $a = 0, b = 4\pi, c = \frac{4\pi}{3}$.

The potential nucleation sites on grain boundaries can be estimated from the densities for grain boundary area, grain edge and grain corner, which depend on the shape and size of grain in the matrix phase,

$$N_i = \rho_i \left(\frac{N_A}{V_\alpha}\right)^{i/3} \qquad i = 3, 2, 1, 0 \tag{5.10}$$

and

$$N_v = N_f N_i \qquad i = 3, 2, 1, 0 \tag{5.11}$$

where ρ_i are nucleation densities, $i = 3$ for bulk nucleation, $i = 2$ for grain boundary nucleation, $i = 1$ for grain edge or dislocation nucleation and $i = 0$ for grain corner nucleation. The nucleation densities for grain boundary, edge or corner are dependent on the grain size D and the aspect ratio $A = H/D$ in tetrakaidecahedron shape,

$$\rho_i = f_i(A) D^{3-i} \qquad i = 2, 1, 0 \tag{5.12}$$

where $f_i(A)$ is a function of A and can be estimated for each case.

For nucleation on dislocations, the potential nucleation sites can be calculated from equation (5.11) if a dislocation density $\rho_1 = \rho_d$ is given.

(c) Estimation of interfacial energy

The interphase boundary energy between the matrix and a precipitate phase or interfacial energy is the most critical kinetic parameter in the precipitation simulation. The generalized broken bond (GBB) method is used to estimate the interfacial energy for different alloys and temperatures,

$$\sigma_{sphere,dff} = 0.329 \alpha_{SCF} \beta_{diff} (N_A V_\alpha^2)^{-1/3} \Delta H_{sol} \tag{5.13}$$

The prefixed structure factor of 0.329 reflects the average proportion of broken bonds due to precipitations for *fcc* and *bcc* matrix. ΔH_{sol} is the solution enthalpy and calculated from thermodynamic database. α_{SCF} is a correction factor for the size of the precipitate particle. β_{dff} is a correction factor for diffuse interfaces. It is a function of $\frac{T}{T_C}$ with T_C being the highest or critical temperature at which two phases are present in the system. At T_C, the composition of matrix and precipitate phases is the same and the interface energy equals to zero. At $T = 0K$, an ideal sharp interface is present. T_C can be provided by the user in the kdb file. If T_C is unknown and not provided, $\beta_{dff} = 1$. Such an example is given in **section 5.1.4.2**.

Table 5.1 Summary of equations for nucleation models

Symbol	**Equation**	**Description**
J	$J = N_v Z \beta^* exp\left(-\frac{\Delta G^*}{k_B T}\right) exp\left(-\frac{\tau}{t}\right)$	The transient nucleation rate
N_v	$N_v = N_f N_i$ and $N_i = \rho_i \left(\frac{N_A}{V_\alpha}\right)^{i/3}$ $i = 3, 2, 1, 0$	Potential nucleation sites
Z	$\frac{V_\alpha}{2\pi N_A {R^*}^2}\sqrt{\frac{\sigma}{k_B T}}$	Zeldovich factor
β^*	$\frac{4\pi {R^*}^2}{a^4} D_{eff}$	Atomic attachment rate
τ	$\frac{1}{2Z^2\beta^*}$	Incubation time
ΔG^*	$\frac{16\pi}{3}\frac{\left(\sigma_{eff}\right)^3}{(\Delta G_{vol})^2}$	Nucleation barrier energy
R^*	$-\frac{2\sigma_{eff}}{\Delta G_{vol}}$	Critical nucleation radius
ΔG_{vol}	$\Delta G_V + \Delta G_S$	Volume energy change during nucleation. ΔG_V is the chemical driving force per volume and ΔG_S is the elastic strain energy
ΔG_S	$\Delta G_S = \frac{2}{3}\mu \Delta^2 f(A_R)$	Elastic strain energy. The volume misfit Δ and particle aspect ratio A_R are given in kdb file
σ_{eff}	$\frac{b\sigma_{\alpha\beta} - a\sigma_{\alpha\alpha}}{c^{\frac{2}{3}}}\left(\sqrt[3]{\frac{1}{36\pi}}\right)$	Effective interfacial energy
$\sigma_{\alpha\beta}$	$0.329\alpha_{SCF}\beta_{diff}(N_A V_{m\alpha}^2)^{-1/3}\Delta H_{sol}$	The estimated interfacial energy based on GBB method
D_{eff}	$\left[\sum_{i=1}^{n}\frac{\left(C_{pi} - C_{0i}\right)^2}{C_{0i} D_{0i}}\right]^{-1}$	Effective diffusivity for multi-component alloys

5.1.3.2 Growth

Two kinds of growth models are implemented in current PanPrecipitation module:

(a) Simplified Growth model

The growth of existing particles for each size class is computed by assuming diffusion-controlled growth, where the Gibbs-Thomson size effect is also taken into account. The growth model for multi-component alloys proposed by Morral and Purdy [1994Mor] is adopted in PanPrecipitation and modified to handle the growth/dissolution of various precipitate phases with different morphologies. The motion rate of the curved interface, e.g., the interface of a spherical or lens-like precipitate is given by,

$$v = \frac{dR}{dt} = \frac{K}{R}\left(\frac{2\sigma V_m}{R^*} - \frac{2\sigma V_m}{R}\right) \tag{5.14}$$

where R is the radius of the interface. R^* is the radius of the critical nucleus and $K = \frac{1}{\left(\Delta C^{\alpha\beta}\right]\left[M\right]^{-1}\left[\Delta C^{\alpha\beta}\right)}$. $\left(\Delta C^{\alpha\beta}\right]$ and $\left[\Delta C^{\alpha\beta}\right)$ are the row and column vector of the solute concentration difference between α (matrix phase) and β (precipitate phase), and $\left[M\right]$ is the chemical mobility matrix. One can verify that the equation (5.14) can be further simplified and written as,

$$v = \frac{dR}{dt} = \frac{K}{R}\Delta G_m^* \tag{5.15}$$

where K is the kinetic parameter, and ΔG_m^* is the transformation driving force defined as $\Delta G_m^* = \Delta G_m - \Delta G_T$ with ΔG_m being the molar chemical driving force and $\Delta G_T = \frac{2\sigma V_m}{R}$ compensating the energy difference due to the Gibbs-Thompson effect.

(b) SFFK (Svoboda-Fischer-F-Kozeschnik) Model

The SFFK model [2004Svo] presents a set of linear equations describing the rate of change of radius and chemical composition of each precipitate in the system. Let the system consist of a matrix and a number of precipitates. The composition of each precipitate phase is not without boundary, it is determined by the complex lattice structure of the precipitate and the thermodynamic model used to describe the phase. The constraints can be written as,

$$\sum_{i=1}^{n} a_{ij} C_i = U_j, (j = 1, ..., p) \tag{5.16}$$

where the parameters a_{ij} take on the values 0 or 1.

For the description of the state of a closed system under constant temperature and pressure, the state parameters q_i can be chosen. Then under several assumptions for the geometry of the system and/or coupling of process, the total Gibbs energy *G* of the system can be expressed by means of the state parameters, and the rate of the total Gibbs energy dissipation *Q* can be expressed by means of $\dot{q}_i$. In the case of *Q* being a positive definite quadratic form of the rates $\dot{q}_i$, the evolution of the system is given by the requirement of the maximum of the total Gibbs energy dissipation *Q* constrained by $\dot{G} + Q = 0$ and by additional constrains which stem from the physical nature of the problem. Such a treatment is based on the thermodynamic extreme principle, which was formulated by Onsager in 1931 [1931Ons1, 1931Ons2].

Let $\mu_{0i}(i = 1, ..., n)$ be the chemical potential of component i in the matrix and $\mu_i(i = 1, ..., n)$ be the chemical potential of component i in the precipitate. All chemical potentials can be expressed as functions of the concentrations C_i. The total Gibbs energy of the system, *G*, is given by,

$$G = \sum_{i=1}^{n} N_{0i}\mu_{0i} + \frac{4\pi R^3}{3}(\lambda + \sum_{i=1}^{n} C_i \mu_i) + 4\pi R^2 \sigma \tag{5.17}$$

where σ is the interfacial energy and λ accounts from the contribution of the elastic energy and plastic work due to volume change of precipitates.

The evolution of the system corresponds to the maximum total dissipation rate Q and constrained $\dot{G}+Q=0$ where,

$$\dot{G}=\frac{\partial G}{\partial R}\dot{R}+\sum_{i=1}^{n}\frac{\partial G}{\partial C_i}\dot{C}_i \tag{5.18}$$

The problem can then be expressed by a set of linear equations. By solving the linear equation $Ay=B$, one can obtain the particle growth rate as well as the composition change rate of each precipitate phase. The detail description of the SFFK model can be found in reference [2004Svo].

(c) Morphology evolution

The driving force for the evolution of the aspect ratio of the precipitate stems from the anisotropic misfit strain of the precipitate and from the orientation dependence of the interface energy. The SFFK model was modified to account for shape factor and its evolution during precipitation process [2006Koz, 2008Svo]. In the model, the precipitate shape is approximated by a family of cylinders having a length L and a diameter D as shown in Figure 5.3. The aspect ratio A_R is used to describe the precipitate shape given by $A_R = L/D$. The quantity R is the equivalent precipitate radius of the spherical shape with the same volume of the cylindrical precipitate. With this definition, small values of A_R represent discs, whereas large values of A_R represent needles as shown in Figure 5.3.

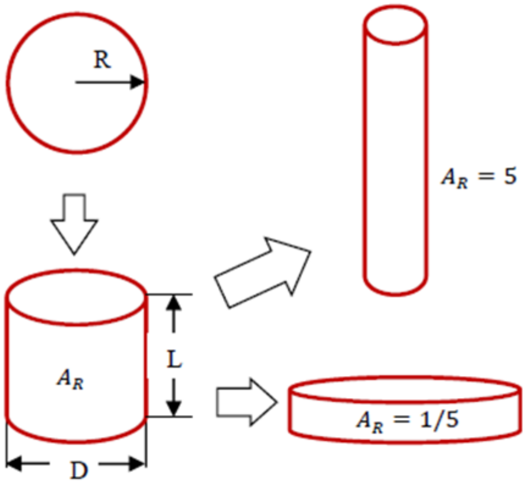


Figure 5.3 Schematic plot illustrating aspect ratio

In PanPrecipitation, the aspect ratio A_R of a precipitate phase can be treated as either a constant or a variable during evolution. In the former case, a set of shape factors are calculated based on A_R and the growth models are adjusted accordingly [2006Koz]. The shape factor S relating the surface of the cylindrical precipitate to the spherical precipitate is given by,

$$S = \frac{S_{cylinder}}{S_{sphere}} = 0.7631 {A_R}^{1/3} + 0.3816 {A_R}^{-2/3} \tag{5.19}$$

The shape factor K for interface migration of the precipitate is given by $K = 0.2912 {A_R}^{2/3} + 0.5824 {A_R}^{-1/3}$. The shape factor I for diffusion inside the precipitate is given by $I = 0.4239 {A_R}^{4/3} + 0.6453 {A_R}^{-2/3}$. The shape factor O for diffusion outside the precipitate is given by $O = 1.0692 {A_R}^{2/3}$.

In the latter case, the original SFFK model was modified and the evolution equations are described by a set of independent parameters including the effective radius (R), mean chemical composition (C_{ki}) and the aspect ratio A_R of each precipitate phase. The evolution rates of these parameters $\dot{R},\ \dot{C}_{ki}\ and\ \dot{A}_R$ are obtained by solving the linear equation $Ay = B$ [2008Svo]. In the modified SFFK, the shape evolution is determined by the anisotropic misfit strain of the precipitate and by the orientation dependence of the interface energy. The total Gibbs energy of the system, G, is given by,

$$G = \sum_{i=1}^{n} N_{0i}\mu_{0i} + \sum_{k=1}^{m} \frac{4\pi R_k^3}{3}\left(\lambda_k\left(A_{R_k}\right) + \sum_{i=1}^{n} c_{ki}\mu_{ki}\right)$$

$$+\sum_{k=1}^{m} 4\pi R_k^2 \frac{\beta_k^2}{8}\left(\sigma_k^L + 2A_{Rk}\sigma_k^D\right) \tag{5.20}$$

The first term is the chemical part of the Gibbs energy of the matrix, the second term corresponds to the stored elastic energy and the chemical part of the Gibbs energy of the precipitates and the third term represents the total precipitate/matrix interface energy. The subscripts “0” denote quantities related to the matrix, e.g., N_{0i} is the number of moles of component i in the matrix and μ_{0i} its chemical potential in the matrix. The quantity $\lambda_k\left(A_{R_k}\right)$ accounts for the contribution of elastic strain energy due to the volume misfit between the precipitate and the matrix and is calculated from equation (5.6).μ_{ki} are the values of chemical potentials in the precipitates corresponding to c_{ki}. In the model, there are two interface energies that must be assigned: σ_k^D at the mantle of the cylinder and σ_k^L at the bottom and top of the cylinder. The shape factor $\beta_k = \sqrt[3]{\frac{16}{3A_{R_k}}}$ is obtained by calculating equivalent radius of a sphere $R_k = D_k/\beta_k$ with the same volume of cylinder.

5.1.3.3 Precipitation Strengthening Model

The precipitation hardening arises from the interactions between dislocations and precipitates. Specifically, the dispersed precipitate particles act as pinning points or obstacles and impede the movement of dislocations through the lattice, and therefore strengthen the material. In general, either a dislocation would pass the obstacles by cutting through the small and weak particles (the shearing mechanism) or it would have to by-pass the strong impenetrable precipitates (the by-passing mechanism). The shearing mechanism is believed to predominate in lightly aged alloys with fine coherent precipitates or zones, while the by-passing mechanism is more characteristic of over-aged alloys with coarser precipitates.

Following an usual approach to determine the critical resolved shear stress at which a dislocation overcomes the obstacles in the slip plane, the response equation can be derived and written as [1979Ger,1998Des],

$$\sigma_P = \frac{M\bar{F}}{bL} \tag{5.21}$$

where M is the Taylor factor, $\bar{F}$ the mean obstacle strength, b the Burgers vector, and L the average particle spacing on the dislocation line. It has been shown that the Friedel statistics gives fairly good results in the calculation of the average particle spacing [1998Des]. Accordingly, this statistics is adopted and equation (5.21) becomes [1998Des],

$$\sigma_P = \frac{M}{b\sqrt{2\beta G b^2}}\sqrt{\frac{3V_f}{2\pi}}\frac{\bar{F}^{3/2}}{\bar{R}} \tag{5.22}$$

where G is the shear modulus, β a constant close to 0.5, V_f the particle volume fraction and $\bar{R}$ the mean particle size.

The calculation of the mean obstacle strength $\bar{F}$ in equation (5.22) is determined by the obstacle size distribution and the obstacle strength:

$$\bar{F} = \frac{\sum_i N_i F_i}{\sum_i N_i} \tag{5.23}$$

where N_i is the obstacle number density of the size class R_i and F_i is the corresponding obstacle strength, which is related to the size of the obstacles and how the obstacles are overcome (particle shearing or particle by-passing).

In the case of particle shearing for weak obstacles, a rigorous expressions of the obstacle strength is quite complex and depends on different strengthening mechanisms (*e.g.*, chemical strengthening, modulus hardening, coherency strengthening, ordering strengthening and so on). Therefore, we will not consider the detailed mechanisms involved. Instead, a more general model proposed by Gerold [1979Ger] is used in the present study and the obstacle strength of a precipitate of radius R is given by,

$$F = kGbR \tag{5.24}$$

where k is a constant and G is the shear modulus.

On the other hand, the obstacle strength is constant and independent of particle radius R in the case of particle by-passing [1979Ger],

$$F = 2\beta Gb^2 \tag{5.25}$$

where β is a constant close to 0.5. From equations (5.24) and (5.25), one can find that the critical radius for the transition of the shearing and the by-passing mechanism is $R_C = \frac{2\beta b}{k}$. By treating R_C an adjustable parameter as suggested by Myhr *et al.* [2001Myh], the equations (5.24) and (5.25) can be written as,

$$F_i = \begin{cases} 2\beta Gb^2\left(\dfrac{R_i}{R_C}\right) & \text{if } R_i < R_C \text{ (weak particles)} \\ 2\beta Gb^2 & \text{if } R_i \geq R_C \text{ (strong particles)} \end{cases} \tag{5.26}$$

Combining equations (5.22), (5.23) and (5.26) gives the yield strength contributed by a particle of radius R_i,

$$\sigma_{P,i} = \begin{cases} k_P \dfrac{\sqrt{V_f}}{\bar{R}}\left(\dfrac{\sum_i N_i \dfrac{R_i}{R_C}}{\sum_i N_i}\right)^{3/2} & \text{if } R_i < R_C \text{ (weak particles)} \\ k_P \dfrac{\sqrt{V_f}}{\bar{R}} & \text{if } R_i \geq R_C \text{ (strong particles)} \end{cases} \tag{5.27}$$

where $k_P = 2\beta GbM\sqrt{\frac{3}{2\pi}}$. This leads to the expression for the yield strength arising from precipitation hardening in the general case where both shearable (weak) and non-shearable (strong) particles are present,

$$\sigma_P = \sum_i \sigma_{P,i} \tag{5.28}$$

Equations (5.27) and (5.28) yield the relationships $\sigma_P \sim \sqrt{V_f \bar{R}}$ and $\sigma_P \sim \frac{\sqrt{V_f}}{\bar{R}}$, respectively, in the two extreme case of pure shearing (*i.e.*, all particles are small and shearable) and pure by-passing (*i.e.*, all particles are bigger than the critical radius and non-shearable). The two relationships are consistent with the usual expressions derived from the classical models.

Besides the precipitate hardening σ_P, the other two major contributions should be considered in the calculation of the overall yield: 1) σ_0, the baseline contribution including lattice resistance σ_i, work-hardening σ_{WH} and grain boundaries hardening σ_{GB}; 2) σ_{SS}, the solid solution strengthening. If all three contributions can be estimated individually, the overall yield strength of the material can thus be obtained according to the rule of additions. Several types of these rules have been proposed to account for contributions from different sources [1975Koc, 1985Ard]. A general form is written as [1985Ard],

$$\sigma^q = \sum \sigma_i^q \tag{5.29}$$

when $q = 1$, it is a linear addition rule and it becomes the Pythagorean superposition rule when $q = 2$. The value of q can also be adjusted between 1 and 2 in terms of experimental data. When applying to aluminum alloys, the linear addition rule has been shown to be the appropriate one [1985Ard, 1998Des, 2001Myh, 2003Esm] and therefore the overall yield strength is given by the following equation,

$$\sigma = \sigma_0 + \sigma_{SS} + \sigma_P \tag{5.30}$$

where $\sigma_0 = \sigma_i + \sigma_{\mathrm{WH}} + \sigma_{\mathrm{GB}}$; it does not change during precipitation process. σ_{SS} is the solid solution strengthening term, which depends on the mean solute concentration of each alloying element [1964Fri, 2001Myh],

$$\sigma_{SS} = \sum_j a_j W_j^{2/3} \tag{5.31}$$

where W_j is the weight percentage of the j^{th} alloying element in the solid solution matrix phase and a_j is the corresponding scaling factor. σ_P is the precipitation hardening term defined by equation (5.28). By applying a regression formula [1991Gro, 2001Myh], the yield strength σ in MPa can be converted to hardness HV in VPN as,

$$HV = A\sigma + B \tag{5.32}$$

where A and B are treated as fitting parameters in terms of experimental data.

5.1.3.4 Precipitation hardening model with multiple particle groups

The calculation of precipitation strengthening σ_p in equation (5.30) can be extended to multiple particle groups with different strengthening mechanism,

$$\sigma_p = \sum_g f_g \sum_j W_j \sigma_p^j \tag{5.33}$$

Where g is the size group defined by a particle size range and f_g is the volume fraction of the group. j is the strengthening mechanism in each size group. $W_j = \frac{\sum_{i,R_i>R_C} N_i}{\sum_i N_i}$ is the weight fraction of the mechanism with R_C the critical radius for transition from one mechanism to another.

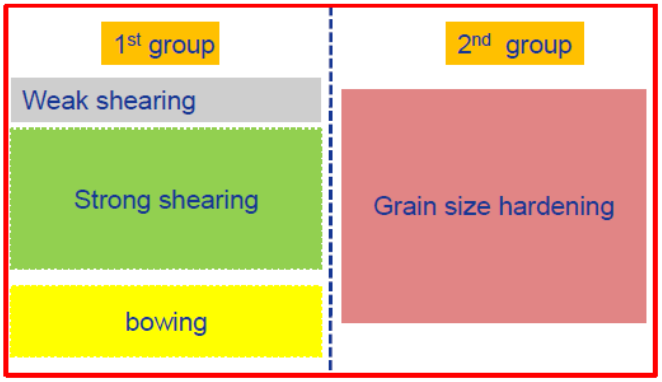


Figure 5.4 Schematic plot for strengthening groups

As an example shown in Figure 5.4, the first group has three mechanisms "weak shearing", "strong shearing" and "bowing" while the second group has only one mechanism. This is very typical in the γ' strengthened Ni-based superalloys. The big primary γ' acts to limit grain growth during solution treatment and enhances grain boundary strengthening while the tertiary/secondary γ' particles strengthen materials through the weak/strong shearing and bowing mechanisms. In [2015Gal], Galindo-Nava proposed an unified model for weak/strong shearing and bowing mechanisms. The transitions from weak to strong shearing and to bowing are automatically taken care. The unified critical resolved shear stress $\tau_{shearing}$ is calculated as,

$$\tau_{shearing} = \frac{\gamma_{APB} l_1}{2b(\Lambda_1 - 2R)} \tag{5.34}$$

Where l_1 is the length of the leading dislocation cutting the precipitates and defined as,

$$l_1 = \begin{cases} 2R & \text{if } R<R_C \text{ (weak pair-coupling)} \\ 2\sqrt{R^2 - (R - R_C)^2} & \text{if } R\geq R_C \text{ (strong pair-coupling)} \end{cases} \tag{5.35}$$

with the critical radius defined as,

$$R_C = \frac{\mu b^2}{2\gamma_{APB}} \tag{5.36}$$

Where μ is the shear modulus and b is the magnitude of the Burgers vector. In Equation (5.34), the mean distance Λ_1 is given by $\Lambda_1 = max\left(L\sqrt{\frac{T_{ten}}{\gamma_{APB}R}}, L - l_1\right)$ with $T_{ten} = \frac{\mu b^2}{2}$ and $L = R\sqrt{\frac{2\pi}{3V_f}}$.

The Orowan yield stress is given by,

$$\sigma_{bowing} = M\frac{3\mu b}{2L} \tag{5.37}$$

Where M is the Taylor orientation factor. The total yield strengthen due to precipitation hardening can be calculated by equation (5.33).

5.1.4 The Precipitation Database Syntax and Examples

The precipitation database (.KDB) uses the XML format, which defines the kinetic model for each precipitate phase and its corresponding model parameters such as interfacial energy, molar volume, nucleation type, morphology type, and so on.

In the KDB, a series of alloys can be defined. Each alloy has a matrix phase with one or multiple precipitate phases. A sample kdb structure is shown as follows,

```
<Alloy name="Fe-Mn-C">
 <MatrixPhase name="Bcc">
  <ParameterTable type="kinetic" name="Parameters for Bcc"> </ParameterTable >
  <PrecipitatePhase name="Cementite_GB" phase_name="Cementite" model="kwn"
   morphology="Sphere" nucleation="Grain_Boundary" growth="simp">
   <ParameterTable type="kinetic" name="Parameters for Cementite">
    <Parameter type="Molar_Volume" value="6E-6" description="Molar Volume" />
    <Parameter type="Interfacial_Energy" value="0.2" description=
      "Interfacial Energy" />
    </ParameterTable >
```

```
  </PrecipitatePhase >
  <PrecipitatePhase name="M7C3_GB" phase_name="M7C3" model="kwn"
   morphology="Sphere" nucleation="Grain_Boundary"  growth="simp">
   <ParameterTable type="kinetic" name="Parameters for M7C3">
    <Parameter type="Molar_Volume" value="6E-6" description="Molar Volume" />
    <Parameter type="Interfacial_Energy" value="0.1" description=
      "Interfacial Energy" />
    </ParameterTable >
   </PrecipitatePhase >
   </MatrixPhase >
</Alloy >
```

In this sample KDB, an alloy “`Fe-Mn-C`” is defined with the matrix phase “`Bcc`”, which has two precipitate phases “`Cementite_GB`” and “`M7C3_GB`”. The precipitate name, kinetic model, morphology, as well as nucleation and growth model can be defined for each precipitate phase. Available options for the kinetic models and morphology are given in Table 5.2. A set of parameters for each phase, such as molar volume, interfacial energy, and so on, can be defined in “`ParameterTable`”. The kinetic and mechanical model parameters that can be defined under “`ParameterTable`” are listed in Table 5.3 and Table 5.4.

Table 5.2 Model options in kdb

Name	**Options**	**Description**
model	KWN, Fast-Acting(FA)	Refer to Figure 5.2
morphology	Sphere, Cylinder	Refer to Figure 5.3. The aspect ratio A_R and shape factors are set to 1 automatically when "Sphere" is selected.
nucleation	Modified_Homogeneous, Grain_Boundary, Grain_Edge, Grain_Corner, Dislocation	Refer to Table 5.1. Both homogeneous and heterogeneous nucleation can be considered by "Modified_Homogeneous". In this case, the values of N_v and ΔG^*must be manually adjusted through Nf, ΔGv and ΔGS as discussed in Table 5.3.
growth	Simplified, SFFK, SFFK_Shape_Evolution	A constant value of The aspect ratio A_R can be assigned for "Simplified" and "SFFK". Choose "SFFK_Shape_Evolution" for shape evolution, which means AR varies during particle growth.
phase_name		Each "PrecipitatePhase" has a "name" and "phase_name". "phase_name" must be consistent with the name in tdb/pdb. The "phase_name" tag can be empty if "name" and "phase_name" are same.

Table 5.3 Kinetic model parameters in kdb

Name	**Unit**	**Description**	**Equation**
Molar_Volume	m³/mole	Molar volume of matrix or precipitate phase `<Parameter type="Molar_Volume" value="6E-6" description="Molar Volume" />`	V_m in (5.2) and V_α in (5.3)
Grain_Size	m	The grain size of the matrix phase `<Parameter type="Grain_Size" value="1e-4" description="Grain size, default value = 1e-4m" />`	D in (5.12)
Dislocation_Density	m^{-2}	The dislocation density in the matrix phase `<Parameter type="Dislocation_Density" value="1e13" description="Dislocation density, Default value  =1.0e12/m^-2" />`	ρ_i in (5.10)
Grain_Aspect_Ratio	N/A	The aspect ratio for the matrix grain `<Parameter type="Grain_Aspect_Ratio" value="1.0" description="grain aspect ratio, default value = 1.0" />`	A in (5.12)
Contact_Angle	degree	Contact angle of nucleus on grain boundary, default value = 90 degree	$\sigma_{\alpha\alpha} = 2\cos\theta\sigma_{\alpha\beta}$ in (5.8)
Aspect_Ratio	N/A	The aspect ratio of the precipitate phase. The value of A_R is evolving if "SFFK_Shape_Evolution" is chosen as	A_R in (5.19)

		growth model. `<Parameter type="A_R" value="1" description="Initial aspect ratio" />`	

Interfacial_Energy	J/m^2	Interfacial energy
		`<Parameter type="Interfacial_Energy" value="0.2" description="Interfacial Energy" />`
		User keyword “IPB_CAC(*)” to get the calculated interfacial energy:
		`<Parameter type="Interfacial_Energy" value="IPB_CALC(*)" description="Interfacial Energy" />`
			$\sigma_{\alpha\beta}$ in (5.2) and (5.13)

Interfacial_Energy_L	J/m^2	Interfacial energy in L direction `<Parameter type="Interfacial_Energy_L" value="0.05" description="Interfacial Energy in L direction" />`	Used in “SFFK_Shape_Evolution” model
Antiphase_Boundary_Energy	J/m^2	Antiphase boundary energy	γ_{APB} in (5.34) and (5.36)
Atomic_Spacing	m	Usually use lattice constant `<Parameter type="Atomic_Spacing" value="7.6E-10" description="Atomic Spacing" />`	a in equations (5.4)
Nucleation_Site_Parameter	N/A	Homogeneous: choose a value close to solute concentration; Heterogeneous: choose a value close to nucleation density when “`Modified_Homogeneous`” option is chosen for nucleation model. Otherwise, use the model automatically estimate the nucleation density and default value of 1.0 can be used. Such an example is given in **section 5.1.4.5**.	N_f in (5.7) and (5.11)
Driving_Force_Factor	N/A	A factor adjusting chemical driving force obtained by thermodynamic calculation	A pre-factor applied to ΔG_V in equation (5.2)
Strain_Energy	J/m^3	The elastic strain energy per volume of precipitate offsetting the calculated value by equation (5.5)	
Volume_Misfit	N/A	The volume misfit	Δ in (5.6)
Kinetic_Parameter_Factor	N/A	A factor adjusting kinetic parameter obtained by thermodynamic and mobility calculation	A pre-factor applied to adjust K in equation (5.14)
Effective_Diffusivity_Factor	N/A	A factor adjusting effective diffusivity for nucleation obtained by mobility calculation	A pre-factor applied to adjust D_{eff} in equation (5.4)
Steady_State_Nucleation_Rate	N/A	0: transient nucleation rate; 1: steady state nucleation rate;	$\exp(\frac{-\tau}{t})$ in equation (5.1)

Table 5.4 Mechanical model parameters defined in kdb

Name	**Unit**	**Description**	**Equation**
Shear_Modulus	Pa	The shear modulus of the matrix phase	μ in (5.6) and (5.36)
Burgers_Vector	m	The Burgers vector of the matrix phase	b in(5.36)
Taylor_Factor	N/A	The Taylor factor of the matrix phase	M in (5.37)
Solution_Strengthening_Factor	N/A	scaling factor of alloying element for solution strengthening	a_j in equation (5.31)
Strength_Parameter	N/A	Strengthening parameter due to precipitation hardening	k_p in equation (5.27)
Shearing_Critical_Radius	m	Critical radius shifting from shearing to looping mechanism	R_C in equation (5.27)
Intrinsic_Strength	MPa	The baseline contribution including lattice resistance, work-hardening and grain boundaries hardening.	σ_0 in equation (5.30)
Hardness_Factor	N/A	The yield strength in MPa can be converted to hardness in VPN based on eq (5.31)	A in equation (5.32)
Hardness_Constant	VPN	The yield strength in MPa can be converted to hardness in VPN based on eq (5.31)	B in equation (5.32)

Table 5.5 Symbol and syntax for retrieving system quantities

Name	**Unit (SI)**	**Comments**
time	second	Time
T	K	Temperature
vft		Total Transformed Volume Fraction: $vft = \sum_p vf_p$ where vf_p is the transformed volume fraction of p phase
x(comp), w(comp)		Overall alloy composition

Table 5.6 Symbol and syntax for retrieving quantities of precipitate phases

Name	**Unit (SI)**	**Comments**
s(@phase)	m	Average size/radius of equivalent sphere particles
D(@phase)	m	Diameter of cylinder
L(@phase)	m	Length/Height of cylinder
A_R(@phase)	m	Aspect ratio of cylinder
nd(@phase)	#m^{-3}	Number density
nr(@phase)	m^{-3}sec^{-1}	Nucleation rate
vf(@phase)		Volume fraction of specified phase
x(comp@phase), w(comp@ phase)		Instant composition of the matrix or precipitate phases
IPB_CALC(@phase)	J/m^2	Model calculated interfacial energy
dgm(@phase)	J/mole	Nucleation driving force of phase(s)
vf_range(@phase,lb,ub)		The volume fraction for different particle groups defined by a size range [lb, ub] such as primary, secondary and tertiary in Ni-based super alloys, for example `vf_range(@L12_FCC,0.5e-8, 0.5e-7)`
s_range(@phase,lb,ub)		average size for different particle groups defined by a size range [lb, ub], for example `s_range(@L12_FCC,0.5e-8, 0.5e-7)`

Table 5.7 Symbol and syntax for retrieving quantities of particle size distribution (PSD)

Name	**Unit**	**Comments**
time		The PSDs are saved for the user-specified times; the PSD for the last time step is automatically saved. Using ***time* = *t*** to get the PSD for time "*t*".
psd_id		The PSD consists of a certain number of cells (size classes); ***psd_id*** gets the cell id.
psd_s(@phase)	m	The characteristic size of a precipitate phase for each cell.
psd_nd(@phase)	$\#m^{-3}$	The number density of a precipitate phase for each cell.
psd_gr(@phase)	m/sec	The growth rate of a precipitate phase for each cell.
psd_ns(@phase)		Normalized size of the cell $psd\_ns(@phase) = \frac{psd\_s(@phase)}{s(@phase)}$
psd_nnd(@phase)		Normalized number density of the cell $psd\_nnd(@phase) = \frac{psd\_nd(@phase)}{nd(@phase)}$
psd_df(@phase)		The distribution function: $psd\_df(@phase) = \frac{s(@phase)}{psd\_w(@phase)} psd\_nnd(@phase)$ with $psd\_w(@phase)$ being the cell width
psd_cvf(@phase)		Cumulative volume fraction of phase(s). Example: psd_cvf(@L12_FCC).

Table 5.8 Symbol and syntax for retrieving mechanical properties

Name	**Unit (SI)**	**Comments**
sigma_y	MPa	Overall yield strength. Example: sigma_y
hv	vpn	Overall microhardness. Example: hv
sigma_i	MPa	Intrinsic yield strength. Example: sigma_i.
sigma_ss	MPa	Yield strength due to solution strengthening. Example: sigma_ss.
sigma_p(@*)	MPa	Yield strength due to precipitation hardening. Example: sigma_p(@Mg5Si6).

Table 5.9 Constants of mathematics and physics

Name	**Comments**
_K	Boltzmann constant
_PI	Archimedes' constant.
_R	Molar gas constant.
_NA	Avogadro constant.
_E	Natural Logarithmic Base.

Table 5.10 Mathematical operators

Name	**Comments**
+	Addition
-	Subtraction
*	Multiplication
/	Division
^	Exponentiation

Table 5.11 Mathematical Functions

Name	**Comments**
exp(x)	Exponential
ln(x)	Natural Logarithm of x
log2(x)	Base 2 Logarithm of x
log10(x)	Base 10 Logarithm of x

sqrt(x)	Square root of x
abs(x)	Absolute value of x
sin(x)	Sine of x
cos(x)	Cosine of x
tan(x)	Tangent of x
asin(x)	Inverse sine of x
acos(x)	Inverse cosine of x
atan(x)	Inverse tangent of x

A few examples are given below to explain the content of the precipitation database in detail. In the reference folder, test batch files (.pbfx) are prepared with .kdb files for running example simulations.

5.1.4.1 An example kdb file for Ni-14Al (at%) alloy

Reference Folder: $Pandat_Installation_Folder\Pandat 2020 Examples \PanPrecipitation\Ni-14%Al\Ni-14Al_Precipitation.kdb

This precipitation database defines the kinetic parameters for the $L1_2$_Fcc (γ’) phase in the Ni-Al binary system at the Ni-rich side. The matrix phase is Fcc_A1 (γ) phase. The detail explanations of kinetic parameters are listed in Table 5.3. This precipitation database can be used for multi-component Ni-based superalloys as well, but some of the key parameters, such as the interfacial energy, and/or nucleation site parameter, may need to be calibrated accordingly. The molar volume and atomic spacing for various types of crystal structures can be found or estimated following reference of ASM handbook. The interfacial energy between γ and γ’ for nickel alloys is usually in the range of 0.02-0.035 J/m^2, it is given as a constant in this example. Interfacial energy can be estimated as discussed in 5.1.3.1(c), and an example is given in the following section 5.1.4.2.

```
<Alloy name="NI-14Al_KWN">
<MatrixPhase name="Fcc">
  <ParameterTable type="kinetic" name="Parameters for gamma">
   <Parameter type="Molar_Volume" value="7.1E-6" description="Molar Volume" />
  </ParameterTable >
<PrecipitatePhase name="L12_FCC" model="KWN" morphology="Sphere"
  nucleation="Modified_Homo" growth="SFFK">
  <ParameterTable type="kinetic" name="Parameters for Gamma_prime">
   <Parameter type="Molar_Volume" value="7.1E-6" description="Molar Volume" />
   <Parameter type="Interfacial_Energy" value="0.025" description=
     "Interfacial Energy" />
   <Parameter type="Atomic_Spacing" value="3.621E-10" description=
     "Atomic Spacing" />
   <Parameter type="Nucleation_Site_Parameter" value="0.001" description=
     "Nucleation Site Parameter" />
  </ParameterTable >
</PrecipitatePhase >
</MatrixPhase >
</Alloy >
```

5.1.4.2 An example kdb file for Ni-14Al (at%) alloy using the calculated interfacial energy

Reference Folder: $Pandat_Installation_Folder\Pandat 2020 Examples \PanPrecipitation\Ni-14%Al_IPB_CALC\Ni-14Al_Precipitation.kdb

In .kdb file, use keyword “`IPB_CALC(*)`” to get the calculated interfacial energy. The value can also be an expression, such as: `value="1.2 * IPB_CALC(*)"`. The optional parameter “`Interfacial_Energy_Tc`” is used to define the temperature at which γ’ forms from γ congruently, and T_C represents the congruent point. In many cases this point does not exist. This parameter is optional and users should not give an arbitrary value to this parameter since it will lead to unrealistic results. In this example, this parameter is commented out in the Ni-14Al_Precipitation.kdb kinetic database. This means the correction factor β_{dff} in Eq. (5.13) is set to be 1.

```
<Parameter type="Interfacial_Energy" value = "IPB_CALC(*)" description =
"Interfacial Energy" />
```

5.1.4.3 An example kdb file for AA6005 Al alloy

Reference Folder: $Pandat_Installation_Folder\Pandat 2020 Examples \PanPrecipitation\AA6005_yield_strength\AA6xxx.kdb

This precipitation database defines the kinetic parameters for the Mg_5Si_6 (β’) phase within the Al-Mg-Si alloys at the Al-rich side. The matrix phase is Fcc_A1-(Al) phase. This example AA6xxx.kdb can be used for most of the AA6xxx and AA3xx series of alloys. Again, some of the key kinetic parameters may need to be slightly revised according to the chemical compositions. Note that, the strengthening model is also included, which enables us to simulate the yield strength (σ) as well as its contributions (σ_i, σ_{ss}, σ_p). Using the equation (5.30), the hardness can then be obtained as well. Table 5.4 lists the strengthening model parameters defined in the precipitation database. These model parameters are adjustable and obtained via optimization to describe available experimental data.

```
<Alloy name="AA6xxx">
 <MatrixPhase name="Fcc">
    <ParameterTable type="Strength" name="Parameters for Fcc">
      <Parameter type="Solution_Strengthening_Factor" name="Si" value="66.3"
        description="solid solution strengthening scaling factor" />
      <Parameter type="Solution_Strengthening_Factor" name="Mg" value="29"
```

```
      description="solid solution strengthening scaling factor" />
    <Parameter type="Solution_Strengthening_Factor" name="Cu" value="46.4"
      description="solid solution strengthening scaling factor" />
    <Parameter type="Solution_Strengthening_Factor" name="Li" value="20"
      description="solid solution strengthening scaling factor" />
    <Parameter type="Intrinsic_Strength" value="10" description=
      "intrinsic strength" />
    <Parameter type="Hardness_Factor" value="0.33" description=
      "intrinsic strength" />
    <Parameter type="Hardness_Constant" value="16" description=
      "intrinsic strength" />
  </ParameterTable >
  <ParameterTable type="kinetic" name="Parameters for (Al)">
    <Parameter type="Molar_Volume" value="1.0425E-5" description=
     "Molar Volume" />
  </ParameterTable >
<PrecipitatePhase name="Mg5Si6" model="KWN" morphology="sphere"
  nucleation="Modified_Homo" growth="SFFK">
  <VariableTable name="Variables replacing built-in variables">
    <Parameter type="Nucleation_Barrier_Energy" value="7.475e-12/dgm(*)^2"
      description="Nucleation_Barrier_Energy" />
  </VariableTable >
  <ParameterTable type="kinetic" name="Parameters for kinetic model">
    <Parameter type="Molar_Volume" value="3.9e-5"
      description="Molar Volume" />
    <Parameter type="Interfacial_Energy" value="0.4"
      description="Interfacial Energy" />
    <Parameter type="Atomic_Spacing" value="4.05E-10"
```

```
          description="Atomic Spacing" />
        <Parameter type="Nucleation_Site_Parameter" value="0.3e-5"
          description="Nucleation Site Parameter" />
        <Parameter type="Steady_State_Nucleation_Rate" value="1"
          description="Indicate whether or not steady state nucleation rate" />
        <Parameter type="Driving_Force_Factor" value="1.0"
          description="Driving Force Factor" />
        <Parameter type="Kinetic_Parameter_Factor" value="3.0"
          description="a factor for kinetic parameter" />
        <Parameter type="Effective_Diffusivity_Factor" value="3"
          description="a factor for effective diffusivity" />
      </ParameterTable >
      <ParameterTable type="strength" name="Parameters for
        strengthening models">
        <Parameter type="Strength_Parameter" value="1.1e-5"
          description="th k_ppt in the equation" />
        <Parameter type="Shearing_Critical_Radius" value="5.0e-9"
          description="Critical size of shifting from shearing to looping" />
      </ParameterTable >
    </PrecipitatePhase >
  </MatrixPhase >
</Alloy >
```

5.1.4.4 An example for heterogeneous nucleation:

Reference Folder: $Pandat_Installation_Folder\Pandat 2020 Examples \PanPrecipitation\AA6005_yield_strength\AA6xxx.kdb

There are two parameters need to be adjusted in order to consider heterogeneous nucleation. In this example, the heterogeneous nucleation sites and barrier energy are adjusted manually by user:

(a) Nucleation_Site_Parameter; in the above example of AA6005 alloy, the value of 0.3e-5 was chosen based on experimental data.

(b) Re-define the nucleation barrier energy. In this example, the nucleation barrier energy for the heterogeneous nucleation is manually adjusted. For homogeneous nucleation, the nucleation barrier energy is defined by equation (5.2) with $\Delta G^* = \frac{16\pi}{3}\frac{(\sigma_{\alpha\beta})^3}{(\Delta G_V)^2} = \frac{16\pi}{3}\frac{(\sigma_{\alpha\beta})^3}{\left(\frac{\Delta G_m}{V_m}\right)^2} = \frac{16\pi}{3}\frac{{V_m}^2(\sigma_{\alpha\beta})^3}{(\Delta G_m)^2} = \frac{16\pi}{3}\frac{{V_m}^2(\sigma_{\alpha\beta})^3}{dgm(*)^2}$

Taking Vm=3.9e-5 and σ=0.4 in the kdb file as shown in **section 5.1.4.3**, we get the nucleation barrier energy for the homogeneous nucleation as 1.63e-9/ dgm(*)^2. For heterogeneous, the nucleation barrier energy is ~2-3 order smaller than that of homogeneous nucleation. In this example, a value "7.475e-12/dgm(*)^2" is used. This value is optimized by using experimental data.

```
<VariableTable name="Variables replacing built-in variables">

  <Parameter type="Nucleation_Barrier_Energy" value="7.475e-12/dgm(*)^2"

    description="Nucleation_Barrier_Energy"/>

</VariableTable >
```

Where dgm(*) is the calculated thermodynamic driving force, which will be update at every simulation steps.

5.1.4.5 Another example for heterogeneous nucleation:

Reference Folder: $Pandat_Installation_Folder\Pandat 2020 Examples \PanPrecipitation\Fe-Mn-C_Heterogeneous_Nucleation\PanFe.kdb

In the example of **section 5.1.4.4**, the heterogeneous nucleation sites and nucleation barrier energy were treated as adjustable parameters and were given manually by the user based on available experimental data. In this example, the potential heterogeneous nucleation sites and nucleation barrier energy are estimated by theoretical models as discussed in **section 5.1.3.1(b)** depending on the selected nucleation type.

```
<PrecipitatePhase name="Cementite_GB" phase_name="Cementite" model="kwn"
  morphology="Sphere" nucleation = "Grain Boundary" growth="simp">
<PrecipitatePhase name="Cementite_Dislocation" phase_name="Cementite"
  model="kwn" morphology="Sphere" nucleation="Dislocation" growth="simp">
```

The nucleation type can be specified when defining a precipitate phase. In this example, two different type of heterogeneous nucleation are defined for "`Cementite`" phase: one at "`Grain_Boundary`" and the other at "`Dislocation`".

5.1.4.6 An example kdb file for a Mg-based AZ91 alloy considering shape factor and shape evolution

Reference Folder: $Pandat_Installation_Folder\Pandat 2020 Examples \PanPrecipitation\AZ91_Morphology\AZ91.kdb

✓ **Consider shape factor but shape factor not evolve (AZ91_200C.pbfx)**

```
<PrecipitatePhase name="ALMG_GAMMA" model="kwn"
morphology="Cylinder" nucleation="Modified_Homo" growth="sffk">
```

In this case, the morphology must be set to "`morphology="Cylinder"`" and the keyword "Aspect_Ratio" or "A_R" is used to set the aspect ratio of the particles:

```
<Parameter type="A_R" value="0.15" description="aspect ratio" />
```

In this example, the Aspect Ratio is set as a constant during the particle evolution.

✓ **Shape evolution (AZ91_200C_shape_evolution.pbfx)**

```
<PrecipitatePhase name="ALMG_GAMMA" model="KWN" morphology="Cylinder"
    nucleation="Modified_Homo" growth="SFFK_Shape_Evolution">
```

In order to consider shape evolution, the morphology must be set to "`morphology="Cylinder"`" and the growth model should be set to "`growth="SFFK_Shape_Evolution"`".

In this case, the aspect ratio value set in “`<Parameter type="A_R" value="1" description="Initial aspect ratio" />`” will be used as a starting value and evolves during precipitation process.

There are two sets of parameters that can control the shape evolution. The first set includes the interfacial energies of the two different directions:

```
<Parameter type="Interfacial_Energy" value="0.25" description=
    "Interfacial Energy" />
<Parameter type="Interfacial_Energy_L" value="0.05" description=
    "Interfacial Energy in L direction"/>
```

The second set includes the anisotropic misfit strain of the precipitate and its model parameters can be defined as follows:

```
<Parameter type="Shear_Modulus" value="30e9" description=
    "the shear modulus, in Pa"/>
<Parameter type="Volume_Misfit" value="0.02" description=
    "the volume misfit"/>
```

It should note that user can set parameters for either interfacial energy or strain energy or both to control the shape evolution.

5.1.4.7 An example to show how to set an initial microstructure for simulation

Reference Folder: $Pandat_Installation_Folder\Pandat 2020 Examples \PanPrecipitation\Ni-16%Al_Dissolution\Al-Ni.ini

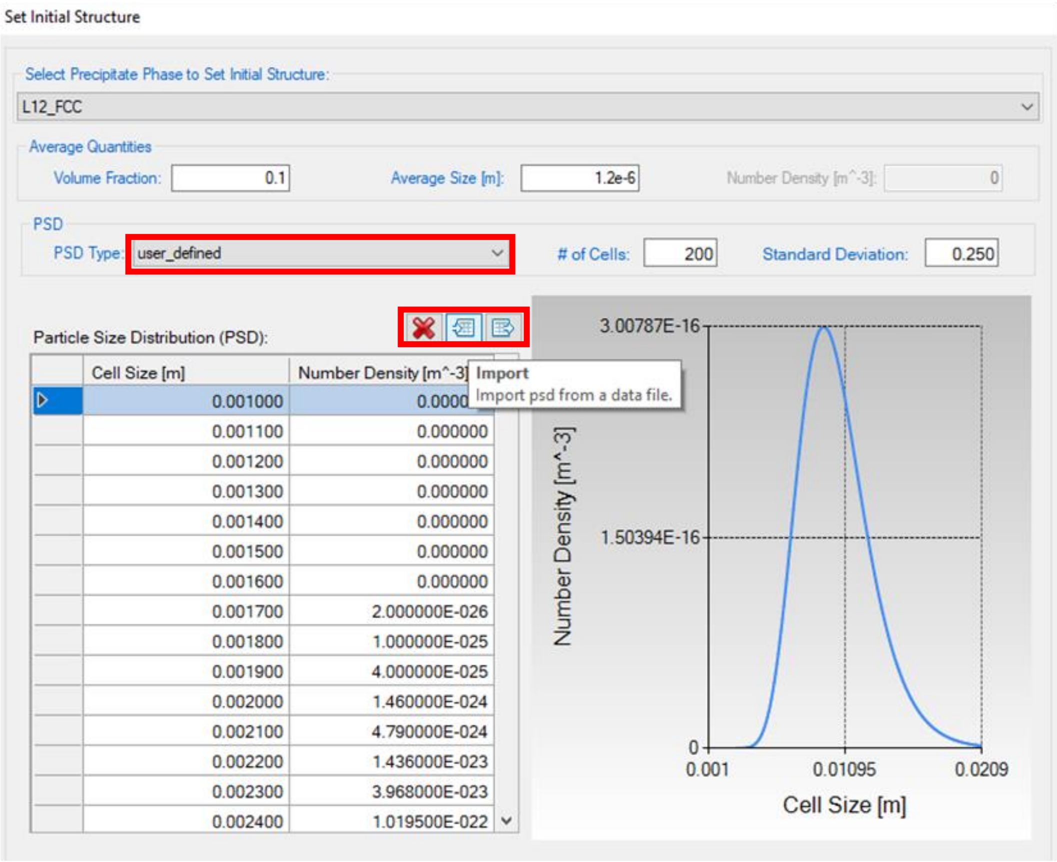
This example is to demonstrate how to set up the initial microstructure for dissolution simulation. In this example, the alloy composition is Ni-16Al at.%, which is isothermally annealed at 1444K for 100 seconds. The alloy composition and heat treatment condition is given in Ni-16Al_dissolution.pbfx. Initially, there is 10% (volume fraction) $L1_2$_Fcc (γ’) phase with average particle size 1.2μm. The initial microstructure is set in Al-Ni.ini as shown below:

```
<Condition name="C1">
```

```
  <MatrixPhase name="Fcc">
    <PrecipitatePhase name="L12_FCC">
      <Parameter name="size" value="1.2e-6" description="average size" />
      <Parameter name="volume_fraction" value="0.1" description=
        "volume fraction" />
      <Parameter name="particle_size_distribution" value="2" number_cells =
        "200" sigma="0.25" description="initial psd shape: 0-uniform;
        1-normal; 2-lognormal;10: user-defined psd" />
      <psd>
          <cell size="1.2E-08" number_density="170191212760.267" />
          <cell size="2.4E-08" number_density="199242482086.767" />
          <cell size="3.6E-08" number_density="232879833831.677" />
          <cell size="4.8E-08" number_density="271760886495.754" />
          <cell size="6E-08" number_density="316626417716.63" />
          ……
      </psd>
    </PrecipitatePhase >
  </MatrixPhase >
</Condition>
```

The "`<psd>` " section can be empty if uniform, normal or lognormal distribution is selected and the initial PSD is automatically generated based on the defined number_cells and standard deviation sigma. If the "`<psd>` " section is given, the provided psd data will be used and the defined `initial psd shape` (uniform, normal or lognormal distribution) is neglected.

User can also define the initial structure from GUI. User first chooses the target phase to set the initial structure and then set the average quantities including the volume fraction and average size. The PSD type can be "uniform", "normal", "log_normal" or "user_defined". When "normal" and "log_normal" are selected, the PSD data will be generated and the corresponding plot is shown on the right panel. In order to load a user defined PSD, the user can set PSD type to be “user_defined” and then load the PSD data file by clicking the import button. An example PSD data file “psd_test.dat” can be found in the folder: $Pandat_Installation_Folder\Pandat 2020 Examples\PanPrecipitation\Ni-16%Al_Dissolution\.



L12_FCC

Volume Fraction: 0.1
Average Size [m]: 1.2e-6
Number Density [m^-3]: 0

PSD Type: user_defined
\# of Cells: 200
Standard Deviation: 0.250

Cell Size [m]	Number Density [m^-3]
0.001000	0.0000
0.001100	0.000000
0.001200	0.000000
0.001300	0.000000
0.001400	0.000000
0.001500	0.000000
0.001600	0.000000
0.001700	2.000000E-026
0.001800	1.000000E-025
0.001900	4.000000E-025
0.002000	1.460000E-024
0.002100	4.790000E-024
0.002200	1.436000E-023
0.002300	3.968000E-023
0.002400	1.019500E-022

Figure 5.5 Dialog to define the initial structure from GUI

5.2 PanPrecipitation Functions

The current version of **PanPrecipitation** menu includes the following major functions: **Load Precipitation Database**, **Select Alloy Parameter**, **Precipitation Simulation**, and **TTT Simulation**.

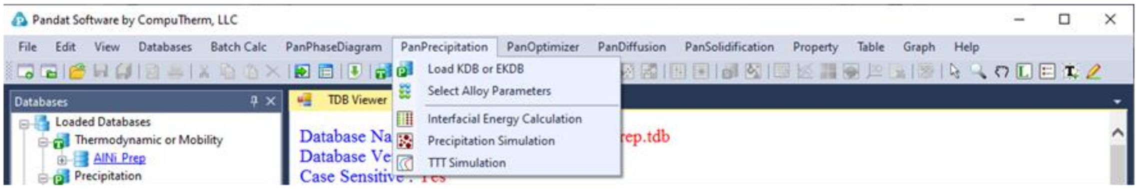


Figure 5.6 Menu functions of PanPrecipitation

The shortcut of the two commonly used functions **Load Precipitation Database** and **Precipitation Simulation** are also displayed in the Toolbar as shown in Figure 5.7.

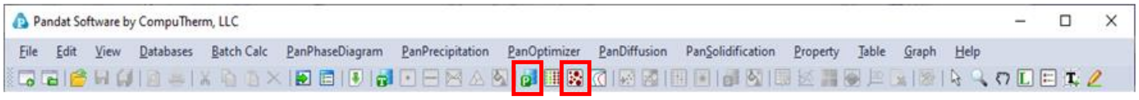


Figure 5.7 Toolbar buttons of PanPrecipitation

- **Load Precipitation Database**: Load a precipitation database into PanPrecipitation module for simulation.
- **Select Alloy Parameters**: Select an alloy parameter available in precipitation database for simulation.
- **Select Precipitate Phases**: Select one or more precipitate phases available in precipitation database for simulation.
- **Precipitation Simulation**: Perform the precipitation simulation.

5.3 Tutorial

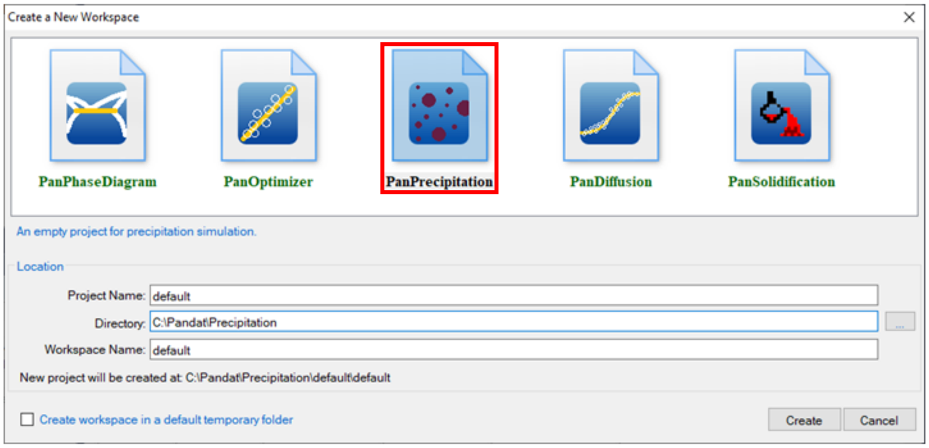
In this tutorial, the Ni -14 at% Al alloy is taken as an example to demonstrate the functionalities provided by PanPrecipitation. The four files mentioned in this section (“`AlNi_Prep.tdb`”, “`Ni-14Al_Precipitation.kdb`”, “`Ni-14Al_Exp.dat`” and “`Ni-14Al_Precipitation.pbfx`”) can be found in the installation folder of Pandat. In general, user should follow four steps to carry out a precipitation simulation:

5.3.1 Step 1: Create a Workspace

Let’s start this tutorial by “creating a workspace”. By clicking the button on the toolbar, the **“Create a New Workspace”** popup window will open. User can choose the “**PanPrecipitation**” icon and define the location (project name, directory and/or workspace name), then click the “**Create**” button to create a precipitation workspace. User can also create a default precipitation workspace by double-click the “**PanPrecipitation**” icon as shown in Figure 5.8.

5.3.2 Step 2: Load Thermodynamic and Mobility Database

The next step is to load the database, which is `AlNi_Prep.tdb` in this example. Different from the normal thermodynamic database, this database also contains mobility data for the matrix phase (Fcc) in addition to the thermodynamic model parameters. Both are needed for carrying out precipitation simulation. By clicking the button on the toolbar, a popup window will open, allowing user to select the database file. User may select the TDB file and click on **Open** button or just double click on the TDB file to load it into the PanPrecipitation module as shown in Figure 5.9.



An empty project for precipitation simulation.

Location

Project Name: default

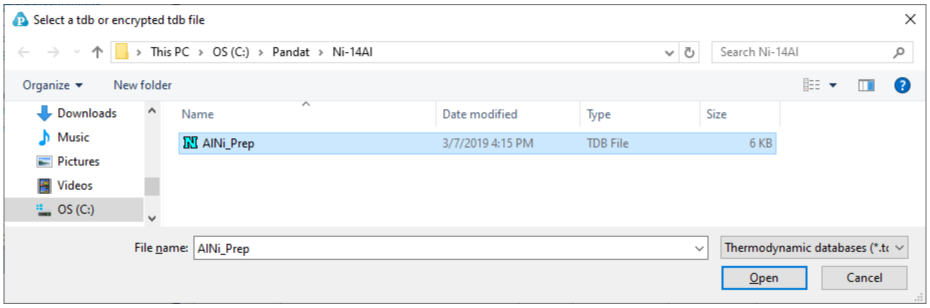
Directory: C:\Pandat\Precipitation

Workspace Name: default

New project will be created at: C:\Pandat\Precipitation\default\default

☐ Create workspace in a default temporary folder

Figure 5.8 Dialog window for creating a workspace



Name	Date modified	Type	Size
AlNi_Prep	3/7/2019 4:15 PM	TDB File	6 KB

File name: AlNi_Prep

Thermodynamic databases (*.t

Figure 5.9 Dialog window for loading thermodynamic and mobility database

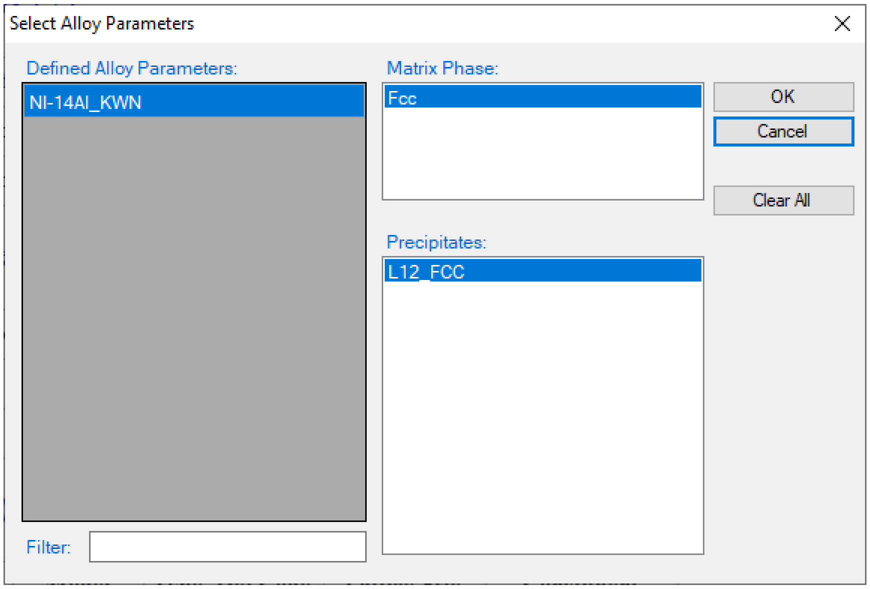
5.3.3 Step 3: Load Precipitation Database

A precipitation database is required for precipitation simulation. Such a database contains kinetic parameters which are alloy dependent. Each alloy is composed of one matrix phase and a number of precipitate phases. To organize these parameters in a more intuitive way, the standard XML format is adopted and a set of well-formed tags are deliberately designed to define the kinetic model (KWN or Fast_Acting) for each precipitate phase and its corresponding model parameters such as interfacial energy, molar volume, nucleation type, and morphology type.

In this example, the Ni-14Al_Precipitation.kdb is prepared. This file can be opened by click 📂 button in the toolbar and be viewed in the Pandat workspace or through third-party external editors, such as NotePad, WordPad etc. The advantage to open this file in Pandat workspace is that all the key words will be highlighted which makes it easy to read. In this example, the matrix phase for this alloy is “Fcc”, which has one precipitate phase “L12_FCC”. The “KWN” model with “Sphere” morphology and “Modified Homogeneous” nucleation type are selected for precipitation simulation. There are five model parameters: Molar_Volume, Interfacial_Energy, Atomc_Spacing, Nucleation_Site_Parameter, and Driving_Force_Factor. These parameters have been developed for the Ni-14Al alloy in this particular example; these parameters need to be optimized for different alloys in terms of experimental data.

Please note that, two sets of model parameters are given in the Ni-14Al_Precipitation.kdb file for two models: KWN or Fast_Acting models. User may select either one for the simulation as is shown in Figure 5.10.

To load a precipitation database, user should navigate the command through menu **PanPrecipitation → Load Precipitation Database**, or click icon from the toolbar. After Ni-14Al_Precipitation.kdb is chosen, a dialog box pops out automatically for user to select the model, i.e., Ni-14Al_FAST or Ni-14Al_KWN, for the simulation. As shown in Figure 5.10, the “Ni-14Al_KWN” is chosen in this example. The **Matrix Phase** window allows user to select the matrix phase and the **Precipitates** window allows user to choose one or more precipitate phases of interest for simulation. To select several phases at one time, press and hold the <Ctrl> key.



Defined Alloy Parameters: NI-14Al_KWN

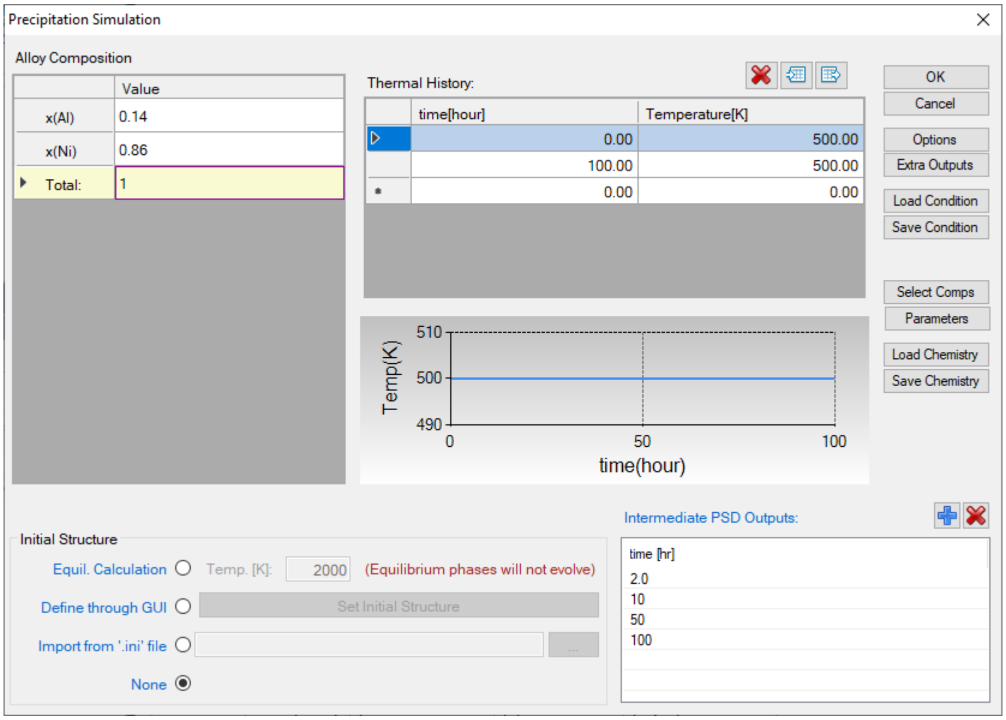
Matrix Phase: Fcc

Precipitates: L12_FCC

Figure 5.10 Dialog box for selecting alloy parameter

5.3.4 Step 4: Precipitation Simulation

After successfully loading both thermodynamic/mobility and precipitation databases, the function for precipitation simulation is then being activated. To perform a precipitation simulation, choose from Pandat GUI menu **<u>PanPrecipitation → Precipitation Simulation</u>**, or click icon from the toolbar. A dialog box entitled "Precipitation Simulation", as shown in Figure 5.11, pops out for user's inputs to set up the simulation conditions: alloy composition and thermal history.



Precipitation Simulation

Alloy Composition

	Value
x(Al)	0.14
x(Ni)	0.86
Total:	1

Thermal History:

	time[hour]	Temperature[K]
▷	0.00	500.00
	100.00	500.00
*	0.00	0.00

Initial Structure

Equil. Calculation ○ Temp. [K]: 2000 (Equilibrium phases will not evolve)

Define through GUI ○ Set Initial Structure

Import from '.ini' file ○

None ●

Intermediate PSD Outputs:

time [hr]
2.0
10
50
100

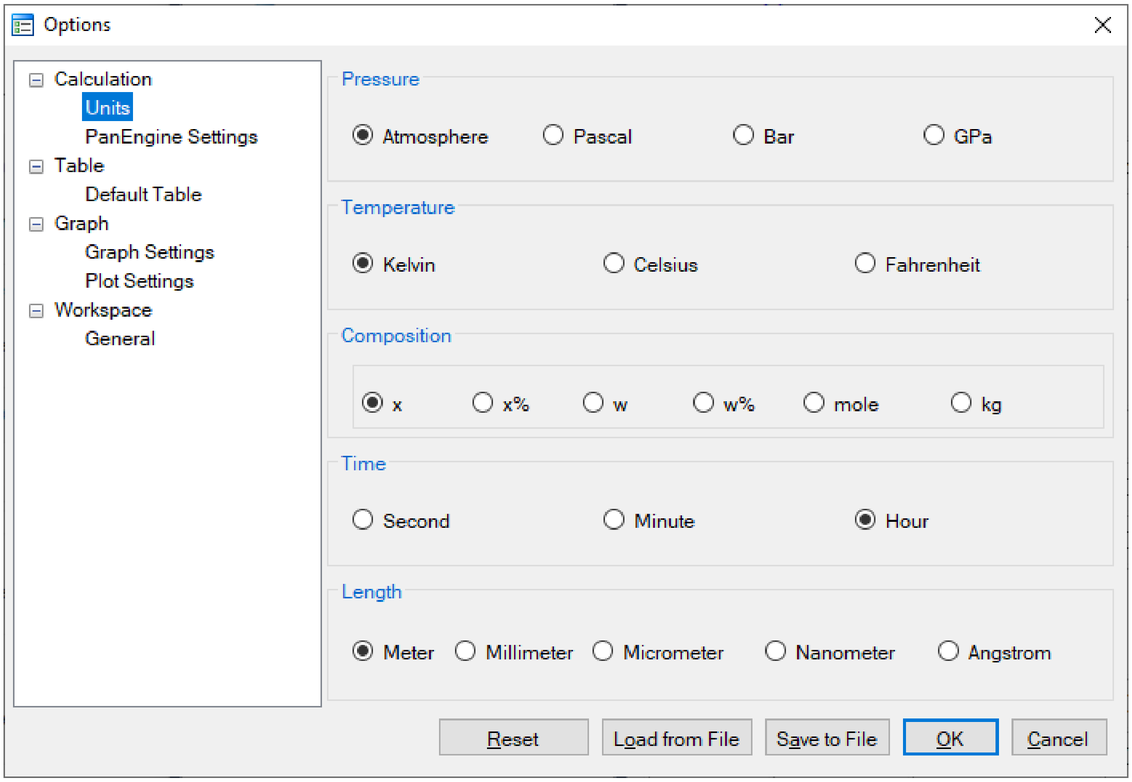
Figure 5.11 Dialog box for setting precipitation simulation conditions

<u>Alloy Composition:</u> User can set alloy composition by typing in or use the **<u>Load Chemistry</u>** function. User can also save the alloy composition through **<u>Save Chemistry</u>**. This is especially useful when working on a multi-component system, so that user does not need to type in the chemistry every time.

<u>Thermal History:</u> Arbitrary heat treatment schedule can be inputted, with a linear *<u>Time</u>*-*<u>Temperature</u>* relationship (i.e., constant cooling or heating rate) at each two consecutive rows. *<u>Time</u>* at the first row must be zero representing the initial time. The thermal history set up in the Figure 5.11 represents an isothermal heat treatment for 100 hours at 500°C. If the temperatures in the two rows are different, it represents constant cooling or heating. Multi-stages of heat treatment can be set by adding more rows in the Thermal History column.

<u>Set intermediate PSD outputs:</u> Based on the specified intermediate PSD outputs, psd tables are automatically generated and the psd plot for the final time step will be created. As shown in Figure 5.11, the intermediate PSD outputs are set up at 2, 10, 50, and 100 hours, respectively.

User can access the Options window by clicking the **Options** button. The **Calculation Options** window allows user to change the units for pressure, temperature, time and composition required in the simulation (as shown in Figure 5.12). User can also define the output **Table** and **Graph** within the **Output Options** window (as shown in Figure 5.13).



Pressure
● Atmosphere ○ Pascal ○ Bar ○ GPa

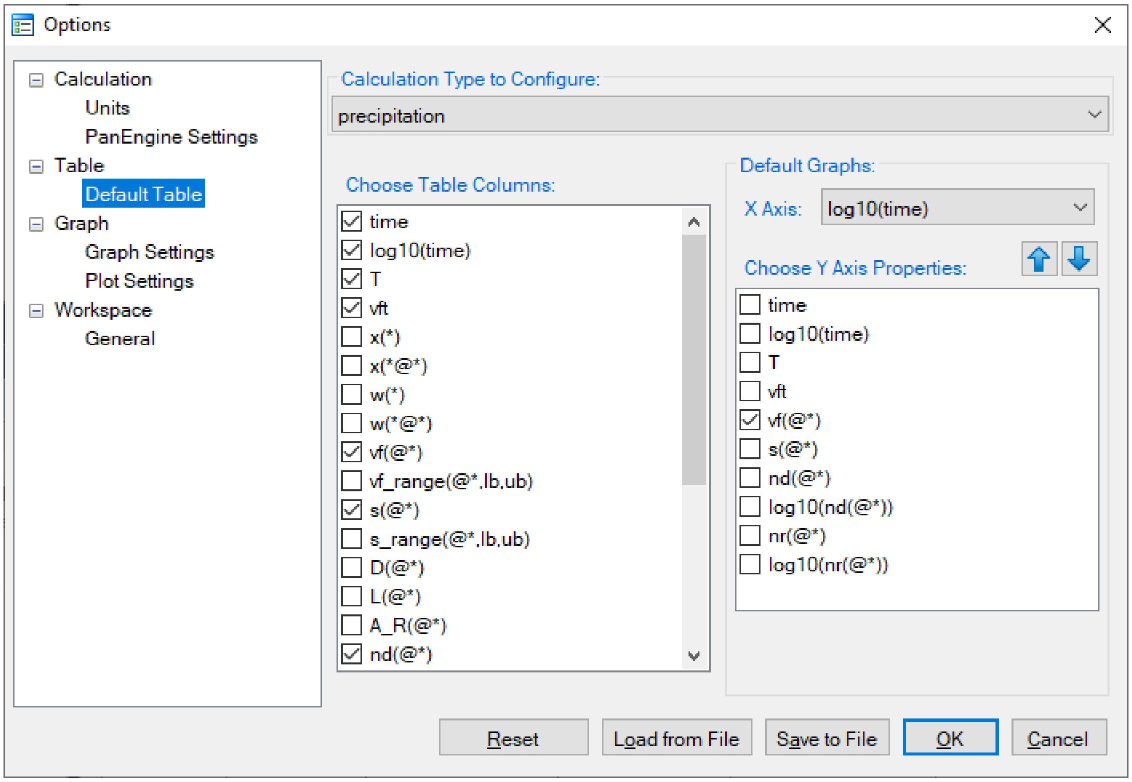
Temperature
● Kelvin ○ Celsius ○ Fahrenheit

Composition
● x ○ x% ○ w ○ w% ○ mole ○ kg

Time
○ Second ○ Minute ● Hour

Length
● Meter ○ Millimeter ○ Micrometer ○ Nanometer ○ Angstrom

Figure 5.12 Dialog box for setting simulation units



Calculation Type to Configure: precipitation

Choose Table Columns:

☑ time
☑ log10(time)
☑ T
☑ vft
☐ x(*)
☐ x(*@*)
☐ w(*)
☐ w(*@*)
☑ vf(@*)
☐ vf_range(@*,lb,ub)
☑ s(@*)
☐ s_range(@*,lb,ub)
☐ D(@*)
☐ L(@*)
☐ A_R(@*)
☑ nd(@*)

Default Graphs:

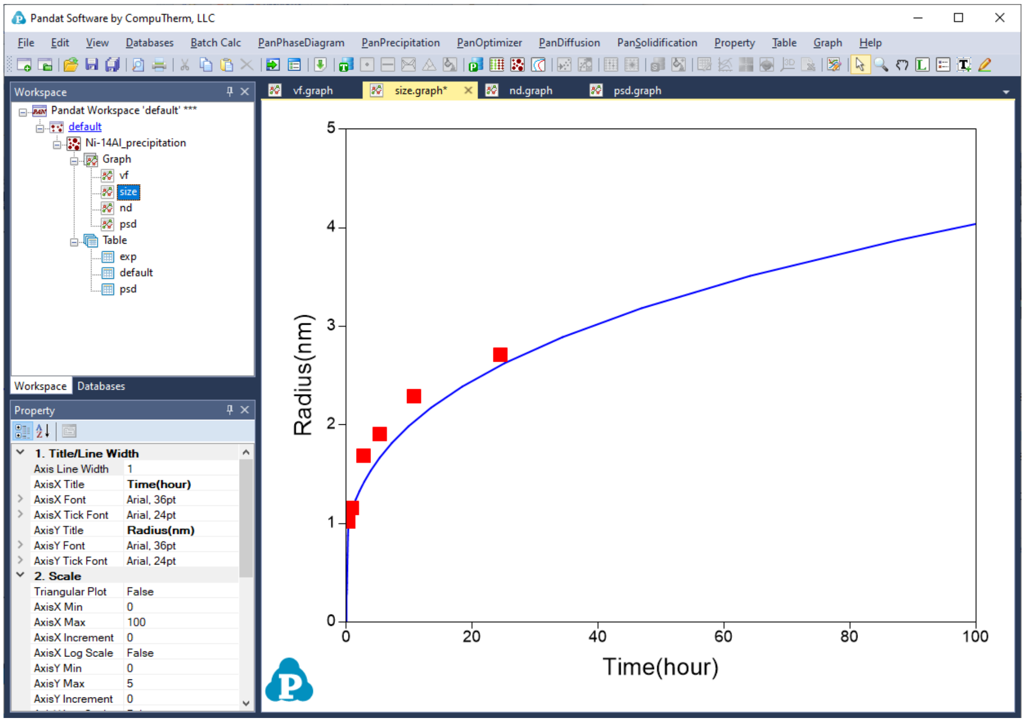
X Axis: log10(time)

Choose Y Axis Properties:

☐ time
☐ log10(time)
☐ T
☐ vft
☑ vf(@*)
☐ s(@*)
☐ nd(@*)
☐ log10(nd(@*))
☐ nr(@*)
☐ log10(nr(@*))

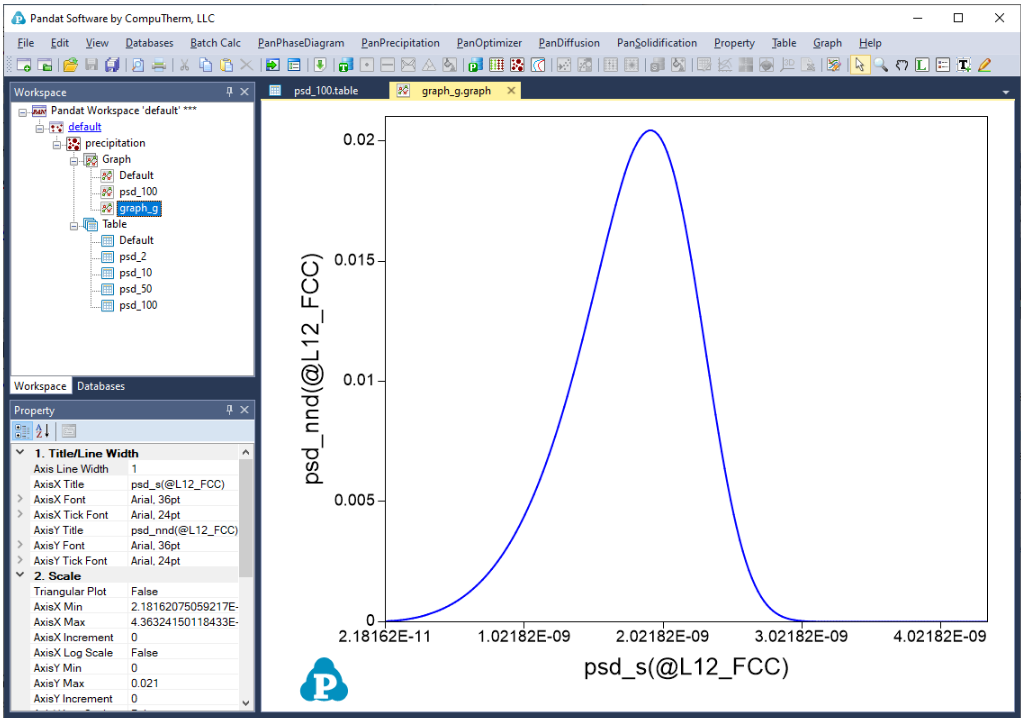
Figure 5.13 Dialog box for setting simulation outputs

In **Precipitation Simulation** window (as shown in Figure 5.11), click **OK** to run the simulation. After the simulation is completed, its results are displayed in two types of formats in the Pandat™ Explorer window: Graph and Table. By default, the graphs plotting average size evolution and PSD at 100 hours are displayed in the Pandat™ main window as shown in Figure 5.14 and Figure 5.15, respectively. To view detailed simulation results, user can switch from Graph view to Table View by clicking tabs in the Pandat™ Explorer window.



1. Title/Line Width	
Axis Line Width	1
AxisX Title	**Time(hour)**
AxisX Font	Arial, 36pt
AxisX Tick Font	Arial, 24pt
AxisY Title	**Radius(nm)**
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
2. Scale	
Triangular Plot	False
AxisX Min	0
AxisX Max	100
AxisX Increment	0
AxisX Log Scale	False
AxisY Min	0
AxisY Max	5
AxisY Increment	0

Figure 5.14 Default graph plotting average size changes



1. Title/Line Width	
Axis Line Width	1
AxisX Title	psd_s(@L12_FCC)
AxisX Font	Arial, 36pt
AxisX Tick Font	Arial, 24pt
AxisY Title	psd_nnd(@L12_FCC)
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
2. Scale	
Triangular Plot	False
AxisX Min	2.18162075059217E-
AxisX Max	4.36324150118433E-
AxisX Increment	0
AxisX Log Scale	False
AxisY Min	0
AxisY Max	0.021
AxisY Increment	0

Figure 5.15 Calculated PSD at 100 hour

User can customize the output results with Pandat batch file. Experimental data may be imported as a separate table using the syntax below:

```
<table source="Ni-14Al_Exp.dat" name="exp"/>
```

The experimental data file should be in the same folder where the batch file locates, otherwise a full path is needed for the experimental file as shown below:

```
<table source="D:\Pandat\Precipitation\Ni-14Al_Exp.dat" name="exp"/>
```

And the experimental data can be plotted together with the calculated results using the syntax below to obtain a diagram as shown in Figure 5.14.

```
<graph name="size">
  <plot table_name="default" xaxis="t/3600" yaxis="s(*)*1e9"/>
  <plot type="point" table_name="exp" xaxis="t(hr)" yaxis="radius(nm)"/>
</graph>
```

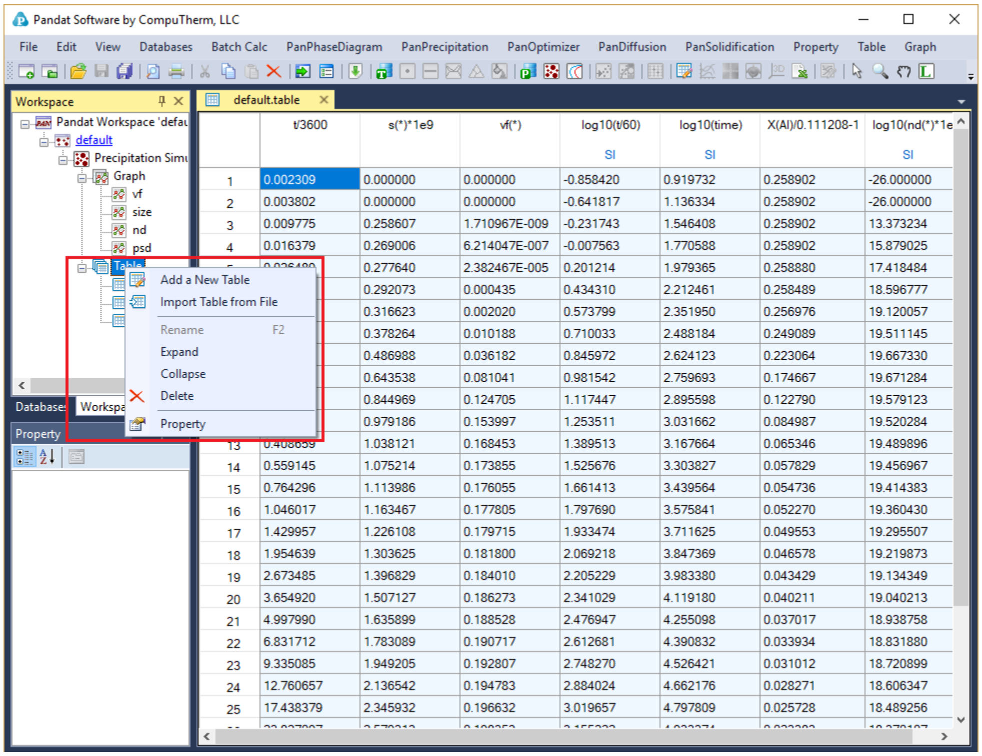
5.3.5 Step 5: Customize Simulation Results

As all other calculations available in Pandat™, upon the completion of the precipitation simulation, a default table with related kinetic properties (such as time, total transformed volume fraction, average size of each precipitate phase, number density of each precipitate phase and nucleation rate of each precipitate phase) is automatically generated and a default graph for average size changes is displayed Figure 5.15.

However, it should be emphasized that, in addition to the default tables, variety of properties, such as temperature, volume fraction of each individual precipitate phase, instant composition of matrix phase and also size distribution related information if the KWN model is used for simulation, can be retrieved through "**Add a new table**".

5.3.6 Add a new table

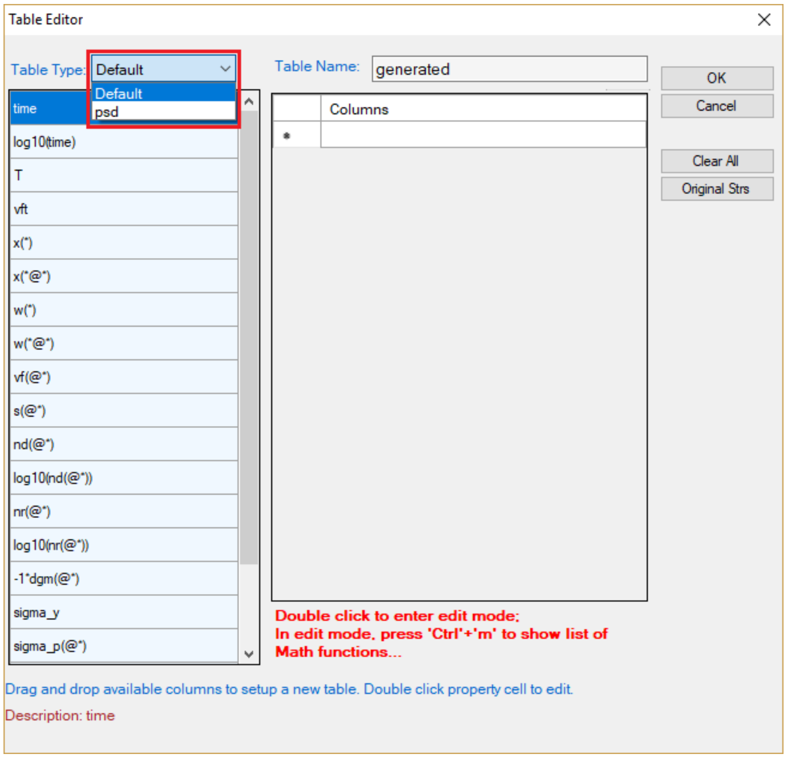
Add a new table function can be activated by the following ways: (1) selecting the "Table" node in the Explore Window, then right click the mouse and select "Add a New Table" option (as shown in Figure 5.16); or (2) choose "Add or Edit a Table” from the “Table” menu. This function allows user to create a new table at their own choices.



	t/3600	s(*)*1e9	vf(*)	log10(t/60) SI	log10(time) SI	X(Al)/0.111208-1	log10(nd(*)*1e SI
1	0.002309	0.000000	0.000000	-0.858420	0.919732	0.258902	-26.000000
2	0.003802	0.000000	0.000000	-0.641817	1.136334	0.258902	-26.000000
3	0.009775	0.258607	1.710967E-009	-0.231743	1.546408	0.258902	13.373234
4	0.016379	0.269006	6.214047E-007	-0.007563	1.770588	0.258902	15.879025
		0.277640	2.382467E-005	0.201214	1.979365	0.258880	17.418484
		0.292073	0.000435	0.434310	2.212461	0.258489	18.596777
		0.316623	0.002020	0.573799	2.351950	0.256976	19.120057
		0.378264	0.010188	0.710033	2.488184	0.249089	19.511145
		0.486988	0.036182	0.845972	2.624123	0.223064	19.667330
		0.643538	0.081041	0.981542	2.759693	0.174667	19.671284
		0.844969	0.124705	1.117447	2.895598	0.122790	19.579123
		0.979186	0.153997	1.253511	3.031662	0.084987	19.520284
13	0.408659	1.038121	0.168453	1.389513	3.167664	0.065346	19.489896
14	0.559145	1.075214	0.173855	1.525676	3.303827	0.057829	19.456967
15	0.764296	1.113986	0.176055	1.661413	3.439564	0.054736	19.414383
16	1.046017	1.163467	0.177805	1.797690	3.575841	0.052270	19.360430
17	1.429957	1.226108	0.179715	1.933474	3.711625	0.049553	19.295507
18	1.954639	1.303625	0.181800	2.069218	3.847369	0.046578	19.219873
19	2.673485	1.396829	0.184010	2.205229	3.983380	0.043429	19.134349
20	3.654920	1.507127	0.186273	2.341029	4.119180	0.040211	19.040213
21	4.997990	1.635899	0.188528	2.476947	4.255098	0.037017	18.938758
22	6.831712	1.783089	0.190717	2.612681	4.390832	0.033934	18.831880
23	9.335085	1.949205	0.192807	2.748270	4.526421	0.031012	18.720899
24	12.760657	2.136542	0.194783	2.884024	4.662176	0.028271	18.606347
25	17.438379	2.345932	0.196632	3.019657	4.797809	0.025728	18.489256

Figure 5.16 Dialog of add a new table

The basic layout of the window of “**Add a new table**” is shown in Figure 5.17. There are two major parts in this window. The left part is the available variables and contents. User first chooses the type of the tables from the “**Table Type**” drop-down list as highlighted in Figure 5.17, to show the list of available variables. The right part is the generated table field. User can drag the available variables from the left column to the right side by clicking and holding the left mouse button.



Double click to enter edit mode;
In edit mode, press 'Ctrl'+'m' to show list of Math functions...

Drag and drop available columns to setup a new table. Double click property cell to edit.

Description: time

Figure 5.17 Dialog window of table editor

5.3.7 Table Format Syntax

Moreover, mathematical calculation over these properties is allowed in PanPrecipitation. Accordingly, a variety of property diagrams can be generated based on the customized tables, which offers users an excellent flexibility for different applications. A detailed description of table format is given below. Figure 5.18 shows the dialog window of table editor for customized new table. The symbol “*” can be used to get quantities of all the phases or all components. As an example, s(*) retrieves the average size of phase L12_FCC, which is equivalent to s(L12_FCC).

Figure 5.19Figure 5.19 shows the dialog window of table editor for user to get a psd table by specifying time. For example, the psd table at 100 hours can be obtained by setting “time = 360000”. Note that the default unit for time is second.

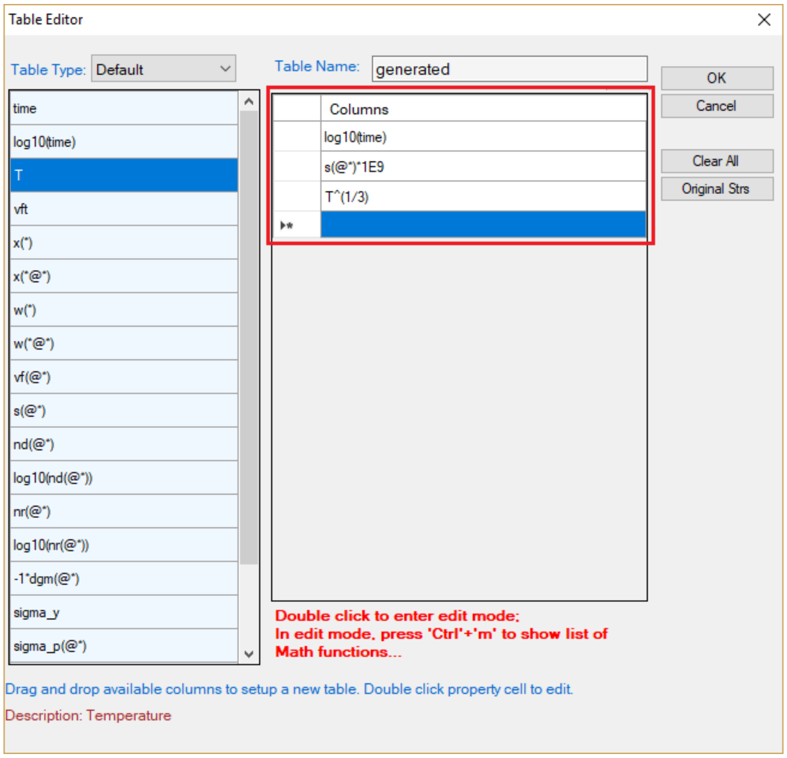


Table Type: Default

Table Name: generated

Columns
log10(time)
s(@*)*1E9
T^(1/3)

Double click to enter edit mode;
In edit mode, press 'Ctrl'+'m' to show list of Math functions...

Drag and drop available columns to setup a new table. Double click property cell to edit.

Description: Temperature

Figure 5.18 Dialog window of table editor for customized new table

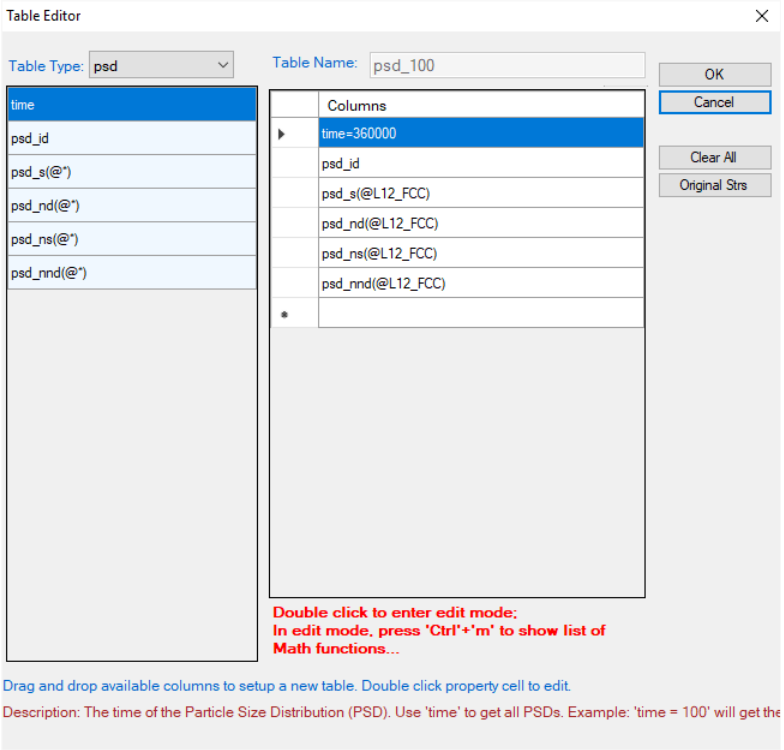


Table Type: psd

Table Name: psd_100

Columns
time=360000
psd_id
psd_s(@L12_FCC)
psd_nd(@L12_FCC)
psd_ns(@L12_FCC)
psd_nnd(@L12_FCC)

Double click to enter edit mode;
In edit mode, press 'Ctrl'+'m' to show list of Math functions...

Drag and drop available columns to setup a new table. Double click property cell to edit.

Description: The time of the Particle Size Distribution (PSD). Use 'time' to get all PSDs. Example: 'time = 100' will get the

Figure 5.19 Dialog to get a psd table at a specified time

6 PanDiffusion

PanDiffusion is a module of Pandat™ software designed to simulate kinetic processes dominated by elemental diffusion. PanDiffusion provides a rich variety of applications including particle dissolution, carburization, decarburization, homogenization, phase transformation, diffusion couple, and so on.

PanDiffusion is seamlessly integrated with the user-friendly Pandat™ Graphical User Interface (PanGUI) as well as thermodynamic calculation engine, PanEngine. The interface between PanDiffusion and PanEngine is managed through PanDataNet. The implementation of PanEngine guarantees reliable input data, such as chemical potential, phase equilibrium and mobility. Figure 6.1 shows an overall architecture of the PanDiffusion module.

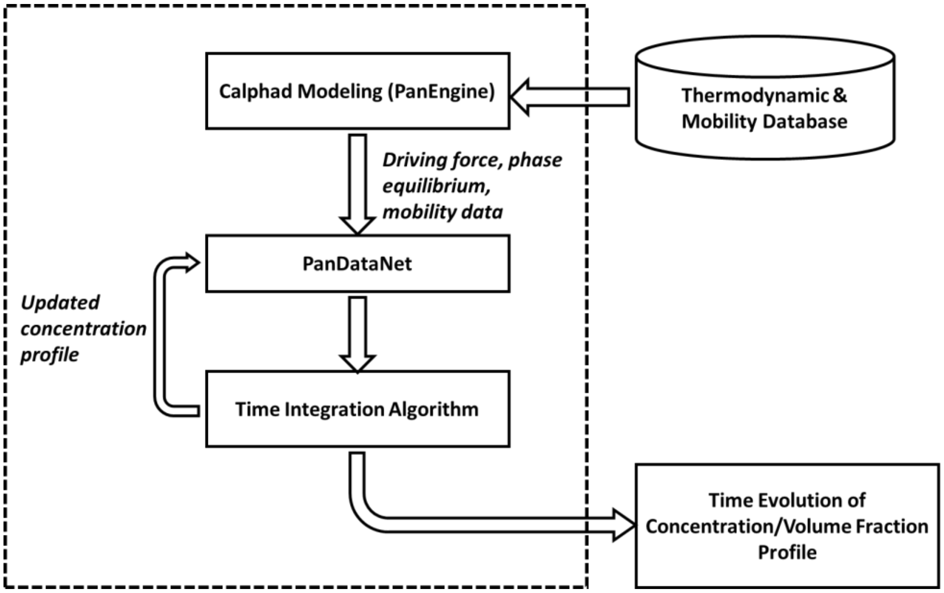


Figure 6.1 An overall architecture of the PanDiffusion module

6.1 Features of PanDiffusion

6.1.1 Overall Design

- Time evolution of composition profile, phase volume fraction, and phase composition.
- Multiple selections of thermal history, boundary condition and geometry.
- Applications including particle dissolution, carburization, decarburization, homogenization, phase transformation, and diffusion couple.

6.1.2 Kinetic Model

Figure 6.2 shows a schematic plot of a composition profile in a diffusion couple. In the simulation, the sample is divided by grids with equal width. The numbers, 1, 2, 3, …, n, indicate grid id. The solid black and dashed red lines means inter-grid interface. What is more, the red dashed line between (i-1)-th and i-th grids indicates the position of a sharp interface of this diffusion couple. Inter-grid flux is calculated following Fick's first law. Composition of each grid, which is indicated by solid blue line in Figure 6.2, is calculated following Fick's second law. The discrete composition profile represents a continuous composition profile of grey dashed line. Chemical potential, mobility, phase equilibrium and related properties are updated for each grid after calculating the composition.

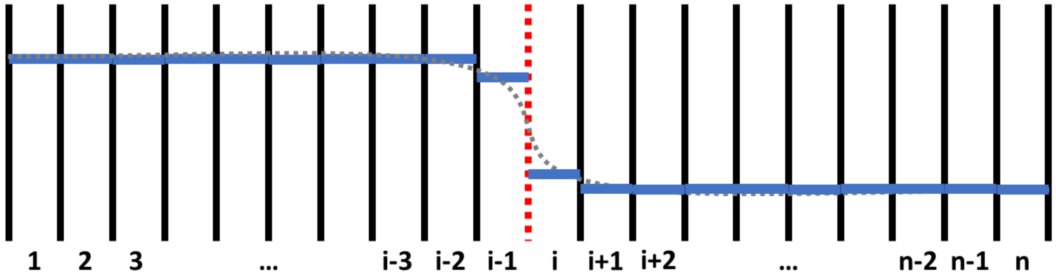


Figure 6.2 A schematic plot of a composition profile in a diffusion couple

6.1.2.1 Flux Model

The evolution of each grid's composition is controlled by the inter-grid flux which is calculated based on absolute reaction rate theory [1941Gla]. At the lattice-fixed frame of reference, the flux is:

$$J_k = -\frac{M_k RT}{V_m \Delta z}\sqrt{x_k^i x_k^{i+1}} * 2\sinh(\frac{\Delta\mu_k}{2RT}) \tag{6.1}$$

Where J_k is the flux of k-th element between the grid i and the grid $i+1$. M_k is effective mobility, R is the gas constant, T is temperature in Kelvin, V_m is molar volume, Δz is the thickness of grid interface and in most cases calculated as average grid size, x_k^i and x_k^{i+1} are molar fraction of k-th element at the grid i and the grid $i+1$, $\Delta\mu_k$ is the chemical potential difference of k-th element between the grid i and the grid $i+1$. The sinh is the hyperbolic sine function. For convenience of calculation, a composition profile is observed at a volume-fixed frame of reference, and the flux of substitute element is transformed to $J_k^V = J_k - x_k \sum J_k$.

Then the amount of k-th element (n_k) of each grid can be updated according Fick's 2nd law:

$$\frac{dn_k}{dt} = -\iint_S \vec{J}_k^V \cdot d\vec{S} \tag{6.2}$$

Where unit normal vectors point outward from the grid.

6.2 Get Started

6.2.1 Step 1: Create a PanDiffusion Project

Users can create a PanDiffusion project through menu "**File → Create a New Workspace**" or "**File → Add a New Project**" in an existing workspace. The "Module Window" pops out for user to choose a module for the new project as shown in Figure 6.3. Choose "PanDiffusion" module for diffusion simulation, and the PanDiffusion project will be created after user click on **Create** button or double click on the PanDiffusion icon.

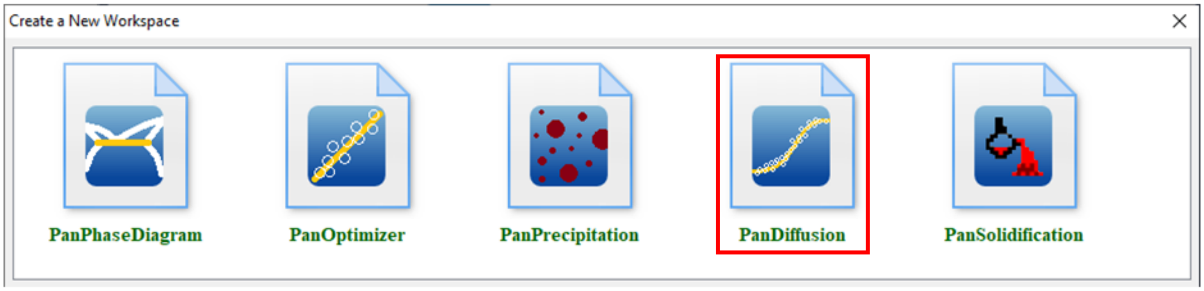


Figure 6.3 Creating a PanDiffusion workspace

6.2.2 Step 2: Load Thermodynamic and Mobility Database

The next step is to load the database, which is FeCrNi.tdb in this example. Different from the normal thermodynamic database, this database also contains mobility data for the phases of interest in addition to the thermodynamic model parameters. Both are needed for carrying out diffusion simulation. By clicking the button on the toolbar, a popup window will open, allowing user to select the database file.

6.2.3 Step 3: Start PanDiffusion Module

Perform diffusion simulation through manual bar **PanDiffusion**->**Diffusion Simulation** or tool bar as shown in Figure 6.4 and Figure 6.5.

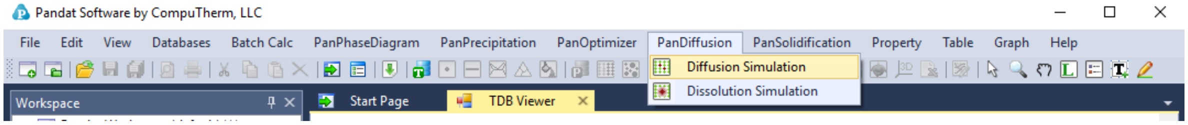


Figure 6.4 Menu functions of PanDiffusion

The shortcut of this is also displayed in the Toolbar as shown in Figure 6.5.

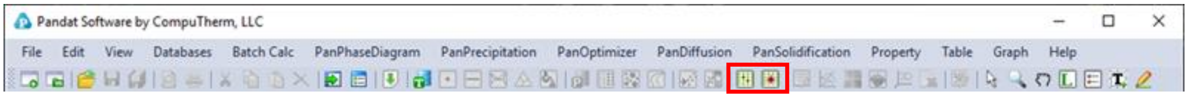


Figure 6.5 Toolbar buttons of PanDiffusion

6.3 Tutorial 1: Diffusion Couple with Uniform Composition Input

In this tutorial, the diffusion simulation on a diffusion couple with uniform composition at each side (as shown in Figure 6.6) is carried out. The annealing temperature is 1000°C and the duration is 2 hours. “Region_1” represents the left-hand side of this diffusion couple, and “Region_2” represents the right-hand side of this diffusion couple. Each region is 100µm and the simulation box is discretized to 100 grids.

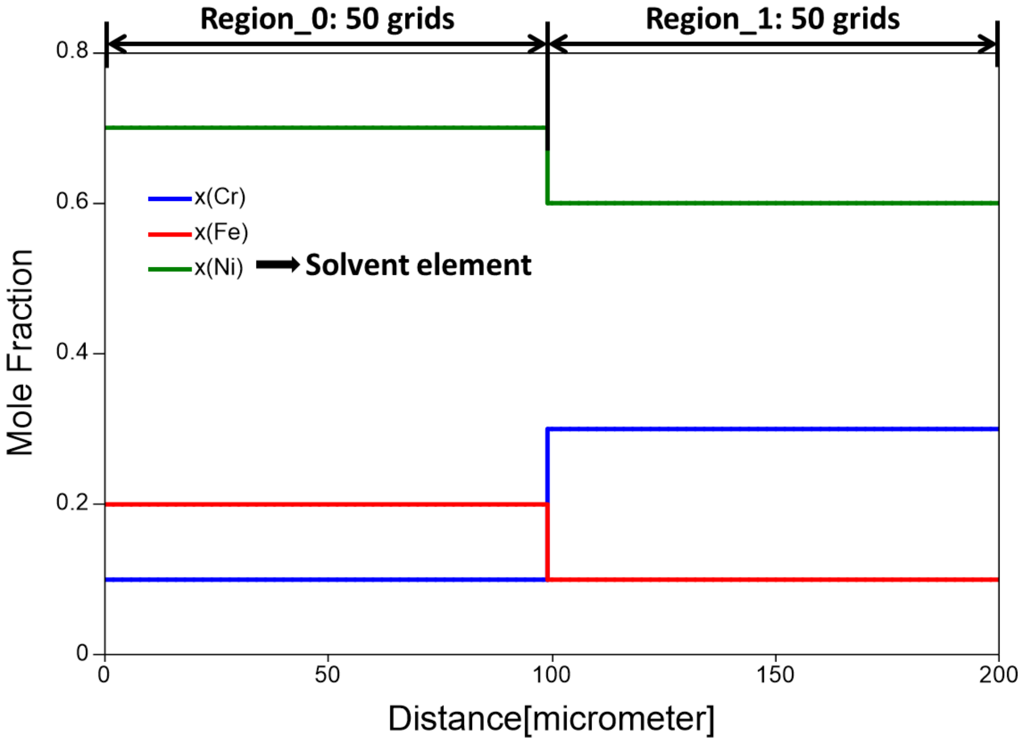
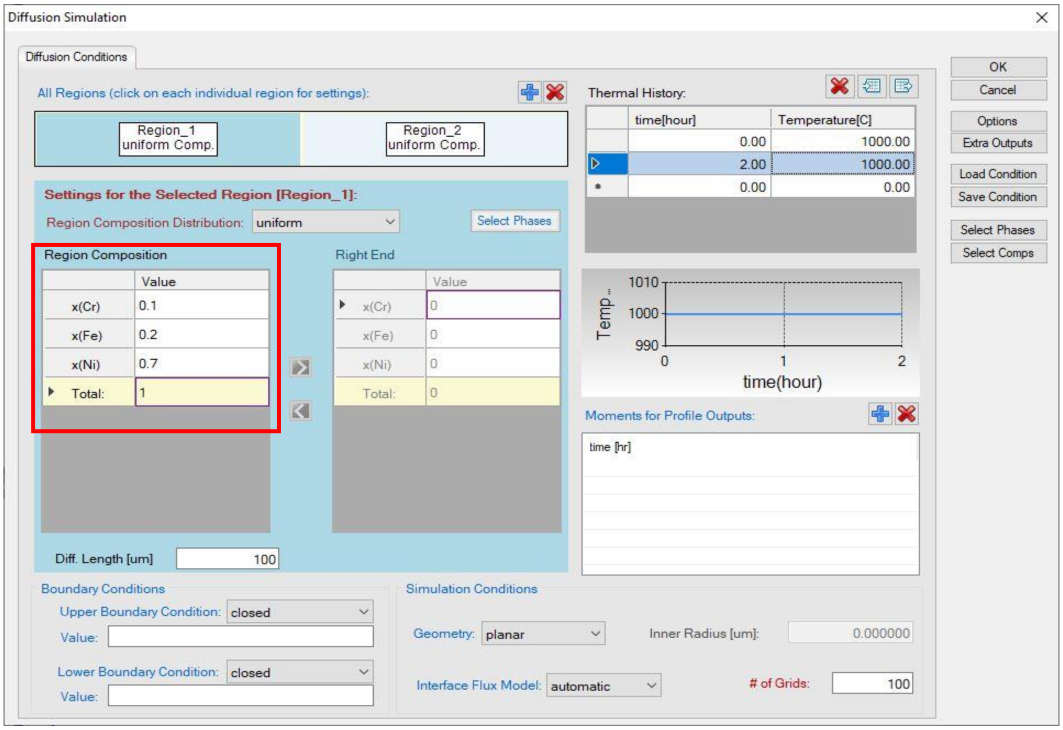


Figure 6.6 Initial conditions of the diffusion couple simulation.

6.3.1 Set up initial condition for diffusion simulation

In order to set the above conditions in PanDiffusion, click through the menu “**<u>PanDiffusion → Diffusion Simulation</u>**” or click the ▦ button on the tool bar, a popup window will show and allow users to set up calculation conditions (as shown in Figure 6.7 and Figure 6.8).

Click Region_1 to set up the composition of the left-hand side as shown in Figure 6.7, and click Region_2 to set up composition of the right-hand side as shown in Figure 6.8. Details regarding the interface design will be described in Section 6.5. Constant annealing temperature is set as 1000°C, and annealing time is 2 hours.



Settings for the Selected Region [Region_1]:

Region Composition Distribution: uniform

Region Composition

	Value
x(Cr)	0.1
x(Fe)	0.2
x(Ni)	0.7
Total:	1

Right End

	Value
x(Cr)	0
x(Fe)	0
x(Ni)	0
Total:	0

Diff. Length [um] 100

time[hour]	Temperature[C]
0.00	1000.00
2.00	1000.00
0.00	0.00

Upper Boundary Condition: closed

Value:

Lower Boundary Condition: closed

Value:

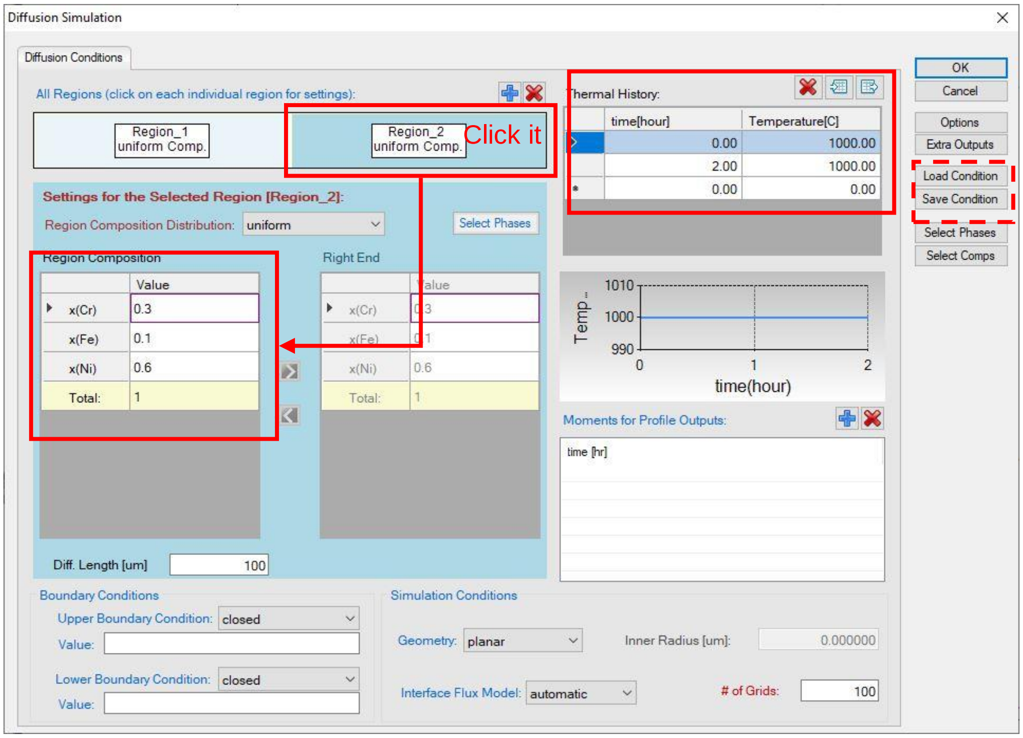
Geometry: planar

Inner Radius [um]: 0.000000

Interface Flux Model: automatic

# of Grids: 100

Figure 6.7 Dialog window for user to set the composition of Region_1



Diffusion Simulation

Diffusion Conditions

All Regions (click on each individual region for settings):

Region_1 uniform Comp.

Region_2 uniform Comp.

Settings for the Selected Region [Region_2]:

Region Composition Distribution: uniform

Region Composition

	Value
x(Cr)	0.3
x(Fe)	0.1
x(Ni)	0.6
Total:	1

Right End

	Value
x(Cr)	0.3
x(Fe)	0.1
x(Ni)	0.6
Total:	1

Diff. Length [um]: 100

Thermal History:

time[hour]	Temperature[C]
0.00	1000.00
2.00	1000.00
0.00	0.00

Moments for Profile Outputs:

time [hr]

Boundary Conditions

Upper Boundary Condition: closed

Value:

Lower Boundary Condition: closed

Value:

Simulation Conditions

Geometry: planar

Inner Radius [um]: 0.000000

Interface Flux Model: automatic

# of Grids: 100

Figure 6.8 Dialog window for user to set the composition of Region_2 and diffusion simulation conditions

As is highlighted by the dashed box, the simulation condition can be saved to a ".pbfx" file by selecting "Save Condition". The saved condition can be loaded by clicking "Load Condition" for the future usage. When a condition is loaded from ".pbfx" file, the settings in the GUI are updated accordingly.

6.3.2 Simulation results

Click **OK** button in Figure 6.8 to start the simulation after the initial condition is set properly. The simulation result is displayed in Figure 6.9.

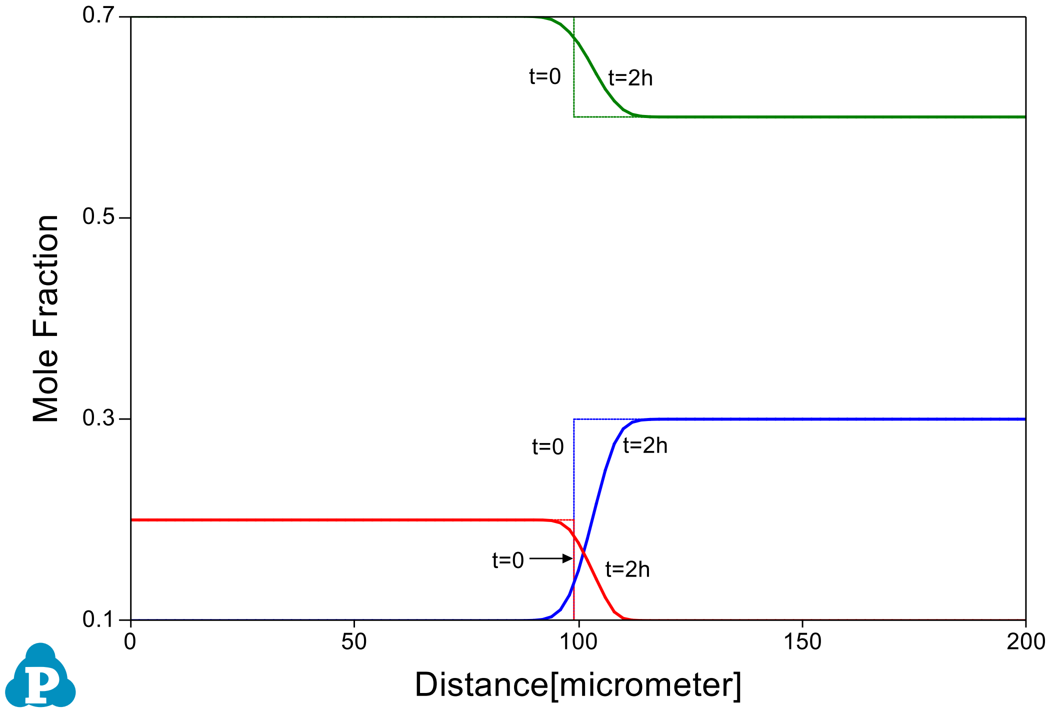


Figure 6.9 Output graph showing the initial and final composition profiles.

In this case, only the initial and final composition profiles are presented: the dotted lines with sharp interface are for the initial stage and the solid lines with smooth interface are for the final stage.

6.3.3 Customize Simulation Results

As all other calculations available in Pandat™, upon the completion of the diffusion simulation, a default table of properties (such as time, temperature, grid size, distance, composition distribution, volume fraction and chemical potential) is automatically generated and a default graph of composition profiles is displayed. User can refer to sections 2.3 and 2.4 to learn how to customize simulated graph and table.

6.4 Tutorial 2: Diffusion Simulation with Composition Profile Input

In this tutorial, the Fe-Ni-Cr alloy is taken as an example to demonstrate a diffusion simulation with a composition profile input. The format of input file is discussed in section 6.6.3. The database file mentioned in this section, "FeCrNi.tdb", can be found in the installation folder of Pandat™. In general, user should follow the following steps to carry out a diffusion simulation:

6.4.1 Set up initial condition for diffusion simulation

Figure 6.10 demonstrates the conditions of this simulation. The initial composition profile from the input file is displayed in this figure. The length of the profile is 200um and is discretized to 100 grids.

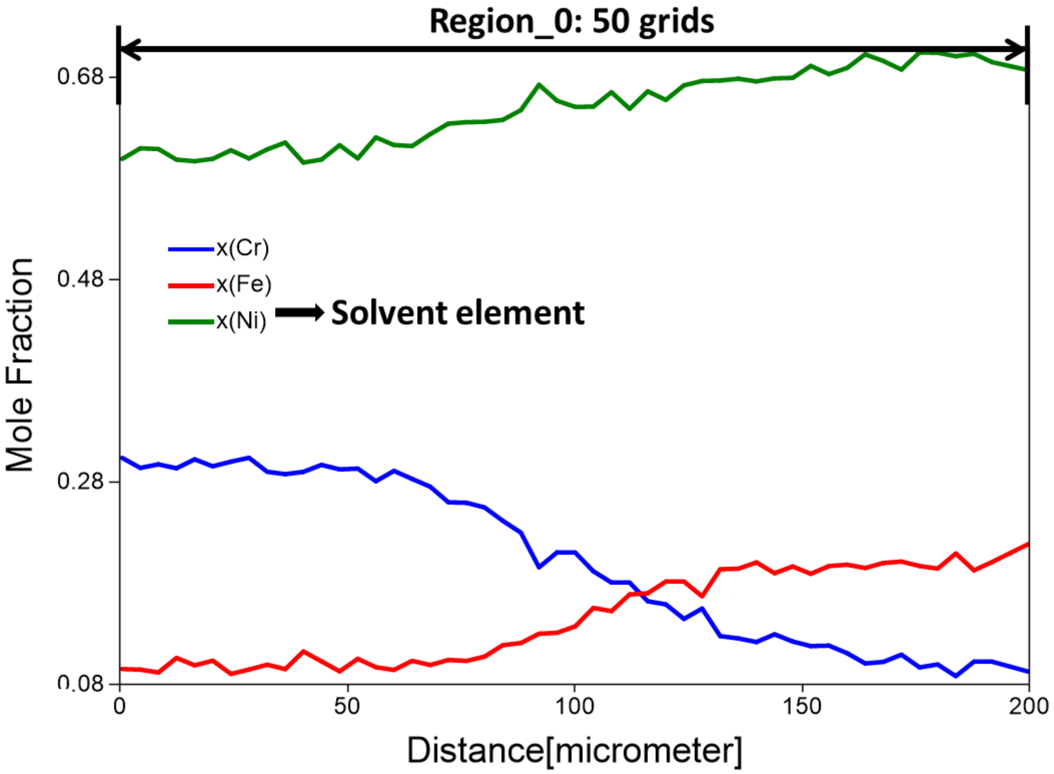
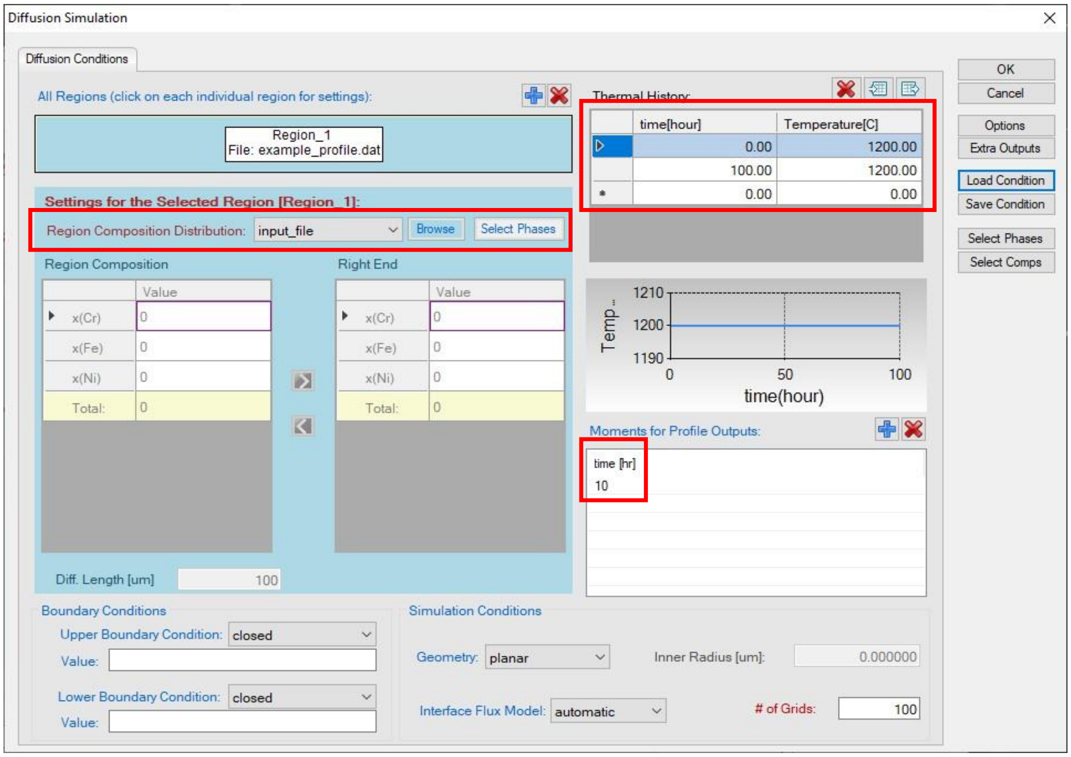


Figure 6.10 Initial conditions of the diffusion simulation with a composition profile input.

To set the above conditions in PanDiffusion, click through on the tool bar, or from the menu "**PanDiffusion → Diffusion Simulation**" a popup window as shown in Figure 6.8 will allow users to set up calculation conditions. In Figure 6.11, "Region_2" is deleted firstly. Please refer to section 6.6.4 on how to delete a region. In the remaining "Region_1", select "input_file" from "Region Composition Distribution", and click "Browse" to load a .dat (or .txt) file which contains composition profile. Annealing time (100 hours in total) and annealing temperature (1200°C) are set. Add an intermediate output at 10 h in the "Moments of Profile Outputs" to observe simulation process. Please refer to section 6.6.8 on how to add a moment of profile output.



Region_1
File: example_profile.dat

Settings for the Selected Region [Region_1]:

Region Composition Distribution: input_file

time[hour]	Temperature[C]
0.00	1200.00
100.00	1200.00
0.00	0.00

Region Composition

	Value
x(Cr)	0
x(Fe)	0
x(Ni)	0
Total:	0

Right End

	Value
x(Cr)	0
x(Fe)	0
x(Ni)	0
Total:	0

Diff. Length [um] 100

Moments for Profile Outputs:

time [hr]
10

Boundary Conditions
Upper Boundary Condition: closed
Value:
Lower Boundary Condition: closed
Value:

Simulation Conditions
Geometry: planar
Inner Radius [um]: 0.000000
Interface Flux Model: automatic
# of Grids: 100

Figure 6.11 Dialog window for user to input diffusion simulation conditions and composition of Region_1.

6.4.2 Simulation results

Click **OK** button in Figure 6.11 to start the simulation after the initial condition is set properly. The simulation result is displayed in Figure 6.12. Please refer to section 2.3 of this user manual to add text, legend, and change the appearance of the figure.

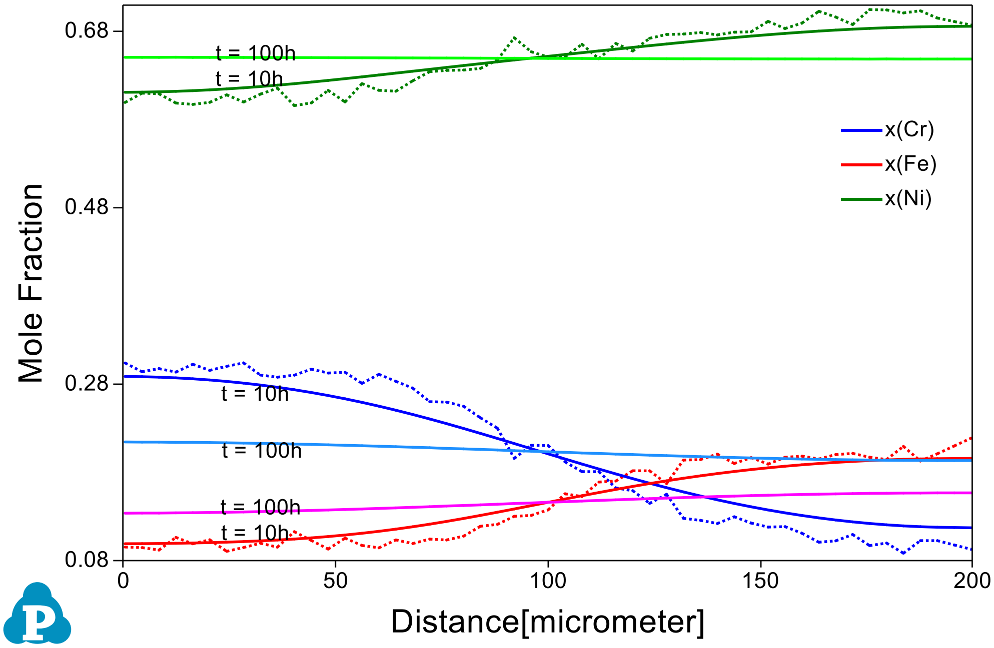


Figure 6.12 Output graph showing the initial and final composition profiles

As is seen in this figure, the initial serrated composition profiles were smoothed out after 10 hours of annealing at 1200°C, and the material is homogenized after 100 hours of annealing.

6.5 Tutorial 3: Dissolution Simulation

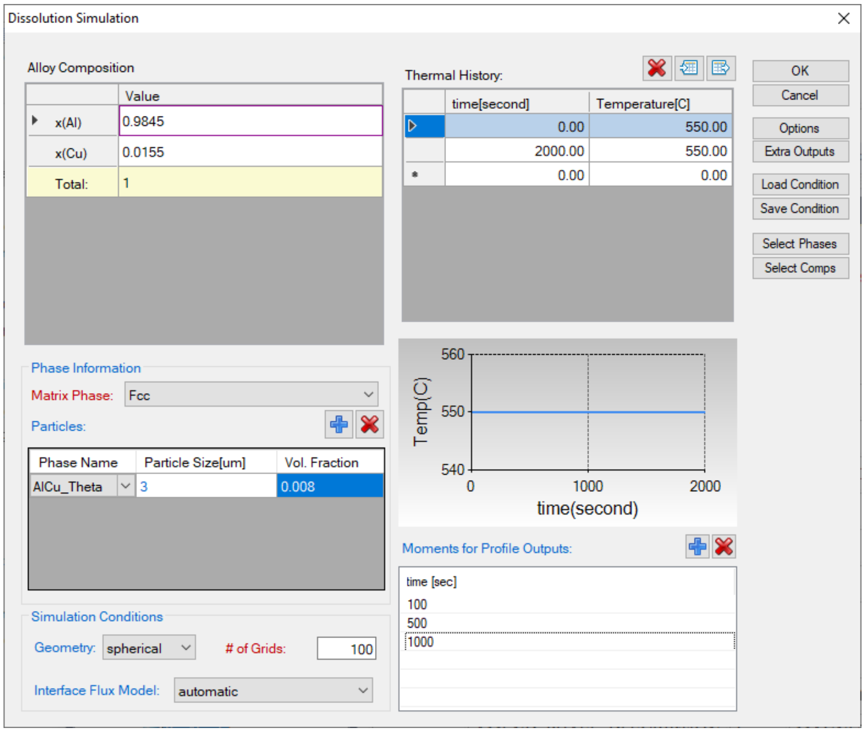
In this tutorial, the Al-Cu alloy is taken as an example to demonstrate a dissolution simulation. The GUI of dissolution is discussed in section 6.7. In general, user should follow the following steps to carry out a dissolution simulation:

6.5.1 Set up initial condition for dissolution simulation

The particle is assumed to be spherical and have a radius of 3 um, and its volume fraction is 0.008. The overall composition of the system is 98.45Al-1.55Cu (at%). The simulation box is digitized to 100 grids.

To set the above conditions in PanDiffusion, click ▦ on the tool bar, or from the menu "**PanDiffusion → Dissolution Simulation**" a popup window as shown in Figure 6.13 will allow users to set up calculation conditions. In "Alloy Composition" section, the overall composition of Al-Cu alloy is set to 98.45Al-1.55Cu (at%). In "Phase Information" section, set "Matrix Phase" as Fcc. In "Particles" subsection, click ✚ bottom to add a particle, set "Phase Name" as AlCu_Theta, set "Particle Size" as 3 um, and set "Vol. Fraction" as 0.008. In "Simulation Conditions" Section, set "Geometry" as spherical, and set "# of Grids" as 100. In "Thermal History" section, temperature is set as 550°C, and heat treatment duration is set as 2000 seconds.

Add additional intermediate outputs at 100s, 500s and 1000s in the section "Moments for Profile Outputs", then click "OK" to start the calculation



Alloy Composition

	Value
x(Al)	0.9845
x(Cu)	0.0155
Total:	1

Thermal History:

	time[second]	Temperature[C]
	0.00	550.00
	2000.00	550.00
*	0.00	0.00

Phase Information

Matrix Phase: Fcc

Particles:

Phase Name	Particle Size[um]	Vol. Fraction
AlCu_Theta	3	0.008

Simulation Conditions

Geometry: spherical

# of Grids: 100

Interface Flux Model: automatic

Moments for Profile Outputs:

time [sec]
100
500
1000

Figure 6.13 Dialog window for user to input dissolution simulation conditions.

6.5.2 Simulation results

Click **OK** button in Figure 6.14 to start the simulation after the initial condition is set properly. The simulation results are displayed in Figure 6.15 and Figure 6.15. Please refer to **Section 2.3** of this user manual to add text, legend, and change the appearance of the figure. Figure 6.14 shows the particle size change with time, from 3µm (radius) at beginning to zero after annealing at 550°C for ~1000 seconds. Figure 6.15 shows diffusion between particle and matrix and the composition profiles at 0s, 100s, 500s, 1000s, and 2000s. It is seen from Figure 6.15 that the particles are completely dissolved after annealing for 2000s.

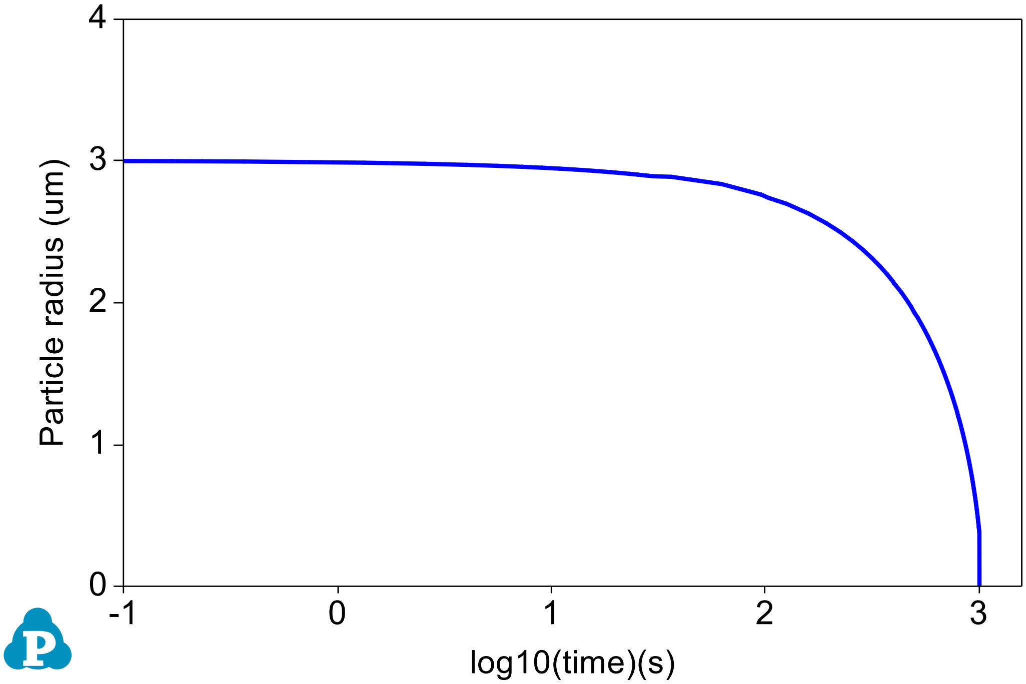


Figure 6.14 Output graph showing the time evolution of particle radius

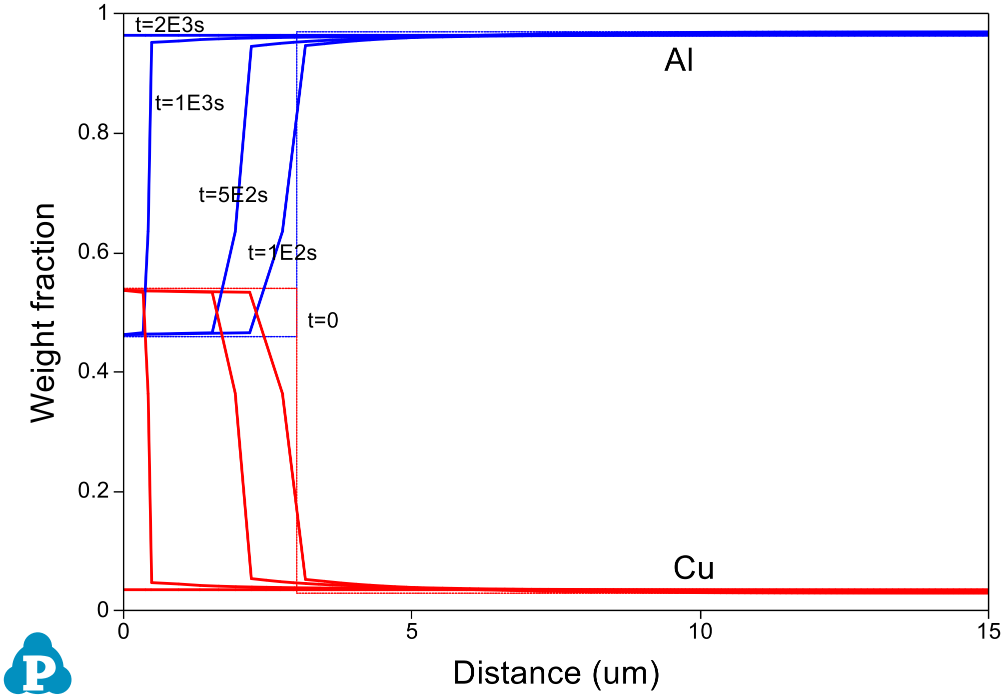


Figure 6.15 Output graph showing the time evolution of composition profile.

6.6 Settings in General Simulation GUI

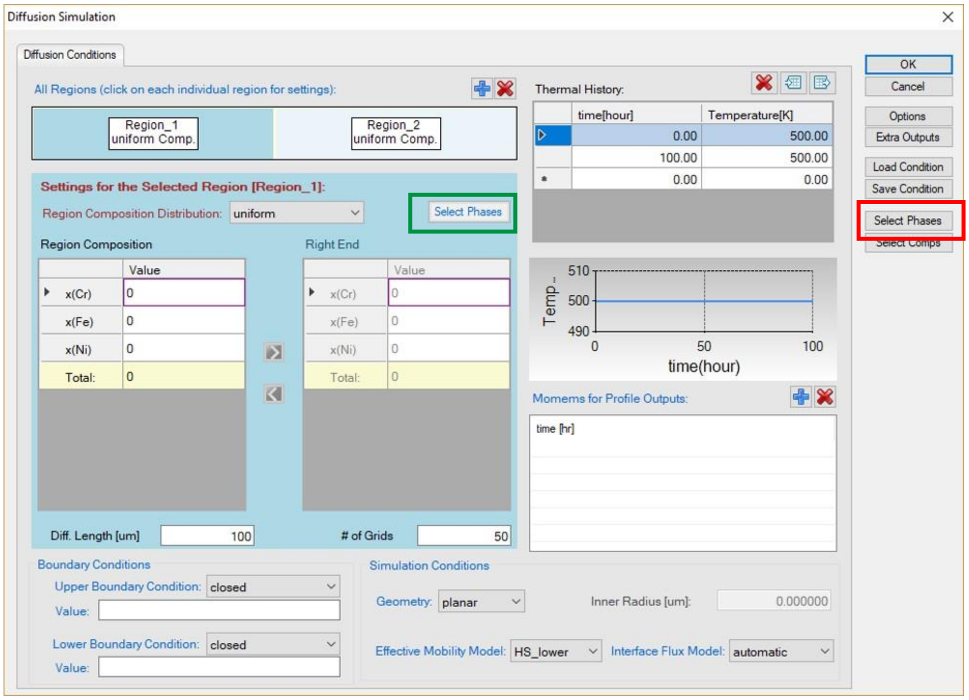
User can perform variety of diffusion simulations by PanDiffusion module. All types of simulations, except for particle dissolution, share the same general graphic user interface (GUI) to set up simulation conditions. This GUI can be accessed through manual bar **PanDiffusion**->**Diffusion Simulation**, or by clicking ▦ on the Toolbar. The speial GUI for dissolution simulation can be accessed through **PanDiffusion**->**Dissolution Simulation**, or by clicking ▣ on the Toolbar. We will present the features of the general GUI ▦ in this section.

6.6.1 Set Units

In the GUI of PanDiffusion, unit settings can be accessed through "**Options**->**Calculation**->**Units**". Please refer to section 3.2.2 for details.

6.6.2 Select Phases

By clicking "**Select Phases**" as highlighted by the **red box** in Figure 6.16, user can select phases involved in the diffusion simulation on the system level. By default, all the phases in the alloy system are selected, while user can deselect some of them as wishes. In addition, user can also select phases for each region by clicking "**Select Phases**" as highlighted by the **green box** in Figure 6.16. By default, phase selection for each region follows the global setting in the system level.



Region Composition Distribution: uniform

	Value
x(Cr)	0
x(Fe)	0
x(Ni)	0
Total:	0

Right End

	Value
x(Cr)	0
x(Fe)	0
x(Ni)	0
Total:	0

Diff. Length [um] 100

# of Grids 50

time[hour]	Temperature[K]
0.00	500.00
100.00	500.00
0.00	0.00

Upper Boundary Condition: closed

Value:

Lower Boundary Condition: closed

Value:

Geometry: planar

Inner Radius [um]: 0.000000

Effective Mobility Model: HS_lower

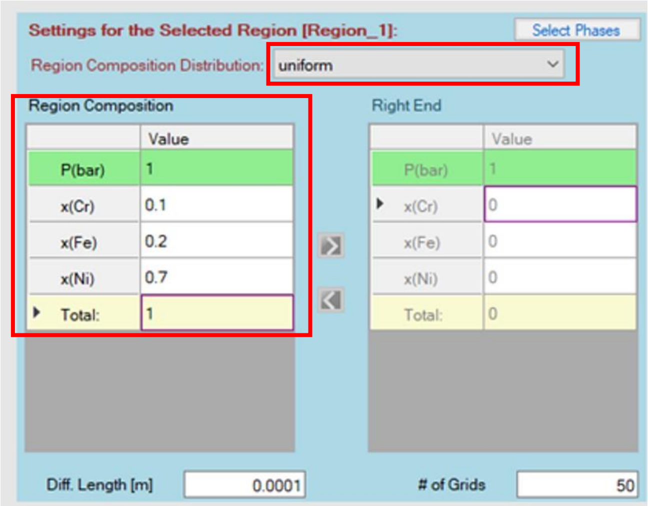
Interface Flux Model: automatic

Figure 6.16 Select phases in a system and/or in a region

6.6.3 Set Initial Composition Profile

In the GUI of PanDiffusion, initial composition profile is assigned region-by-region. In each region, composition profile can be:

- Uniform: the composition of each element in the selected Region is a constant. When "uniform" is selected, a homogenous "Region Composition" can be set.



Region Composition Distribution: uniform

Region Composition

	Value
P(bar)	1
x(Cr)	0.1
x(Fe)	0.2
x(Ni)	0.7
Total:	1

Right End

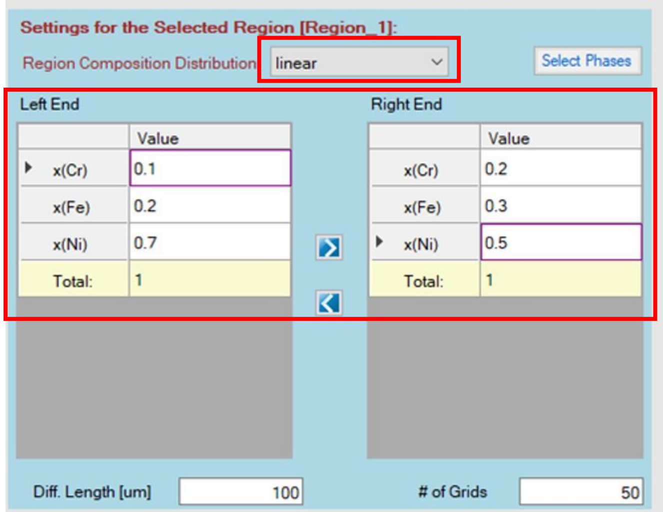
	Value
P(bar)	1
x(Cr)	0
x(Fe)	0
x(Ni)	0
Total:	0

Diff. Length [m] 0.0001

# of Grids 50

Figure 6.17 "Uniform" composition of a Region

- Linear: a linear composition interpolation is set from the left edge to the right edge of the selected Region. When "linear" is selected, both "Left End" and "Right End" compositions need to be set.



Settings for the Selected Region [Region_1]:

Region Composition Distribution: linear

Left End

	Value
x(Cr)	0.1
x(Fe)	0.2
x(Ni)	0.7
Total:	1

Right End

	Value
x(Cr)	0.2
x(Fe)	0.3
x(Ni)	0.5
Total:	1

Diff. Length [um]: 100

# of Grids: 50

Figure 6.18 "Linear" composition of a region

- Input_file: Load composition profile from a tab-delimited .dat (or.txt) file with the following two kinds of formats:

  Format (I): the distance is specified for each element, which is usually the case when using experimental data. The 1st row contains the name of each column, the 2nd row contains the unit definition, and value starts from the 3rd row.

distance(Cr)	x(Cr)	distance(Ni)	x(Ni)
meter	x	meter	x
3.92E-07	0.307	3.90E-07	0.693

  Format (II): the distance is specified in the 1st column, the composition of every element correspond to the same distance. This format is usually obtained by digitalizing data from literature. The 1st row contains the name of each column, the 2nd row contains the unit definition, and value starts from the 3rd row.

```
distance(*)      x(Cr)      x(Ni)
meter            x          x
3.92E-07         0.307      0.693
```

The unit of distance can be: meter (or m), millimeter (or mm), micrometer (or um), nanometer (or nm) and angstrom. The unit of composition can be: x for mole fraction, x% for mole percentage, w for weight fraction, and w% for weight percentage. Note that, the units in the input file will override setting in “Options->Calculation->Units” and the input file is case insensitive.

6.6.4 Delete and Add a Region

In the GUI of PanDiffusion, there are two Regions by default. In the following cases, single region is recommended:

- Only one input composition profile
- Carburization, decarburization, or other surface flux process, with a homogeneous initial composition profile
- Homogenization of a linear composition profile

The redundant region can be removed by first selecting the Region, then clicking ✖ button as shown in Figure 6.. If diffusion is among three or more Regions, Regions can also be added one by one by clicking ✚ .

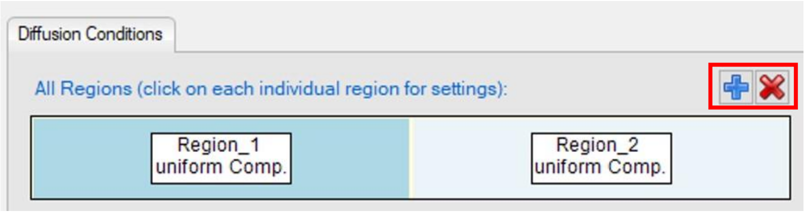
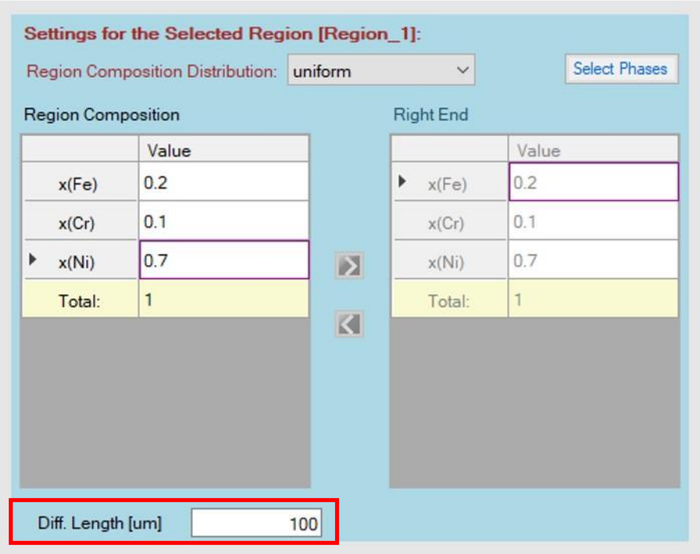


Figure 6.19 Add or delete a region

6.6.5 Set Regional Length

In the GUI of PanDiffusion, “Diff. Length” is the length of a region.


Settings for the Selected Region [Region_1]:

Region Composition Distribution: uniform

Region Composition

	Value
x(Fe)	0.2
x(Cr)	0.1
x(Ni)	0.7
Total:	1

Right End

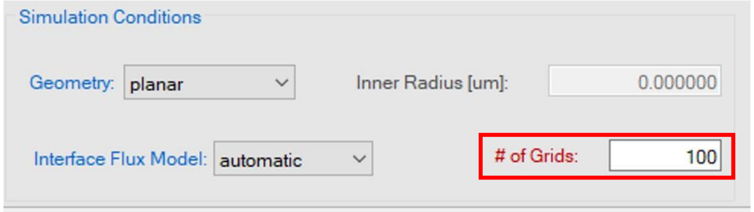
	Value
x(Fe)	0.2
x(Cr)	0.1
x(Ni)	0.7
Total:	1

Diff. Length [um] 100

Figure 6.19 Length in a region

6.6.6 Set # of Grids

In the GUI of PanDiffusion, number of grids is set for the entire simulation box and is distributed automatically to each region.


Simulation Conditions

Geometry: planar

Inner Radius [um]: 0.000000

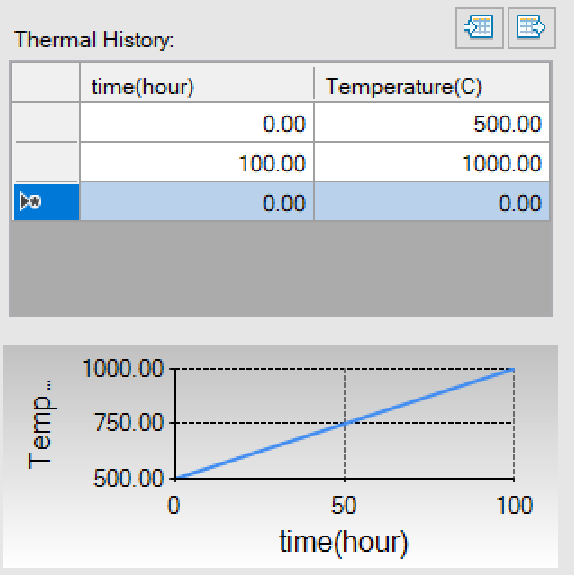
Interface Flux Model: automatic

# of Grids: 100

Figure 6.20 Number of grids

6.6.7 Set Thermal History

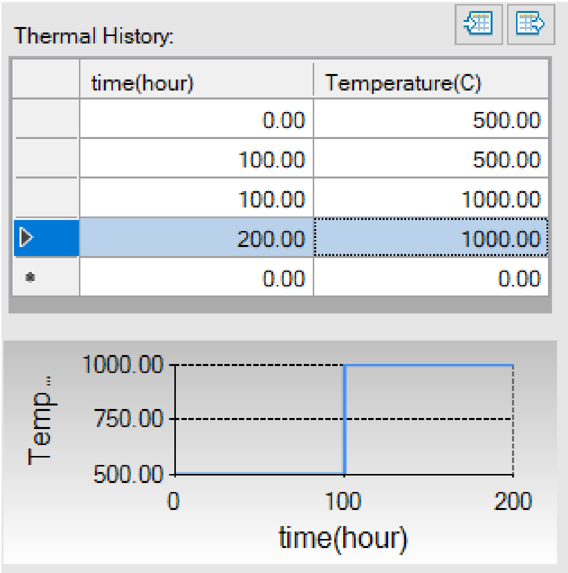
In the GUI of PanDiffusion, “Thermal History” controls temperature and the duration at each temperature. The setting in Figure 6. indicates that the temperature increases linearly from 500°C to 1000°C by 100 hours (5°C/hour).


Thermal History:

	time(hour)	Temperature(C)
	0.00	500.00
	100.00	1000.00
▷*	0.00	0.00

Figure 6.21 A linear increment of temperature

The setting shown in Figure 6. means that the sample is held at 500°C for 100 hours, and then the furnace temperature is **suddenly** increased to 1000°C and held there for another 100 hours.

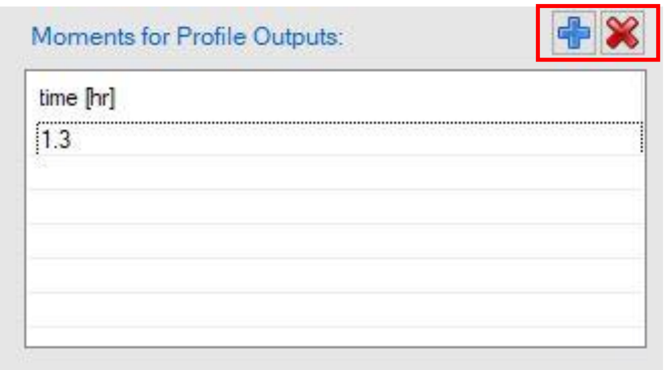

Thermal History:

	time(hour)	Temperature(C)
	0.00	500.00
	100.00	500.00
	100.00	1000.00
▷	200.00	1000.00
*	0.00	0.00

Figure 6.22 A step-like thermal history.

6.6.8 Add Moments for Profile Outputs

For a calculation set up through GUI of PanDiffusion, two moments of profiles, initial and final, will be provided by default. To add more intermediate moments of profiles, click ➕ besides the “Moments for Profile Outputs”, and edit time of the expected moment.

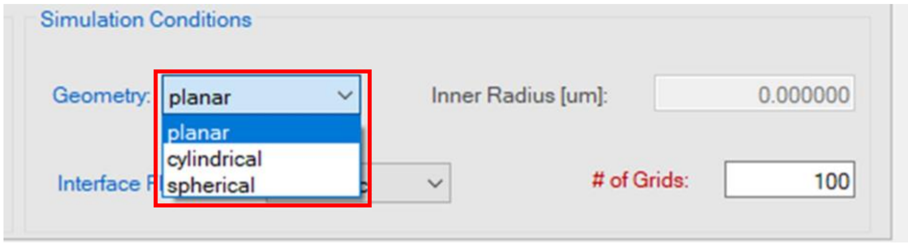

Moments for Profile Outputs:

time [hr]
1.3

Figure 6.23 Add a moment for profile output at 1.3 hour.

6.6.9 Set Geometry

In the GUI of PanDiffusion, “Geometry” under “Simulation Conditions” decides the shape of inter-grid interface. By default, “planar” is used for most diffusion couple simulations. When particle homogenization or transformation is performed, “spherical” or “cylindrical” could be selected depending on the problem of interest.


Simulation Conditions

Geometry: planar

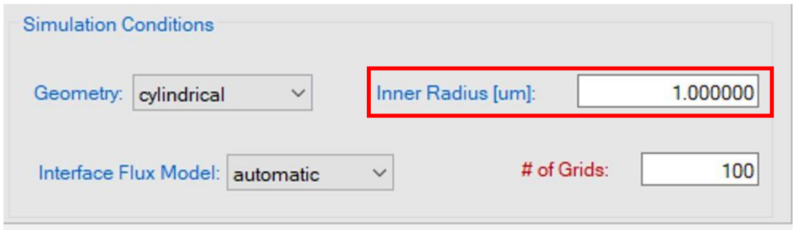
Inner Radius [um]: 0.000000

# of Grids: 100

Figure 6.24 Select the geometry

6.6.10 Set Inner Radius

When geometry other than “planar” is selected, user can set inner radius of cell, to simulate for a tube or shell geometry. When “cylindrical” geometry is selected, and the inner radius is non-zero, tube geometry is set up. When “spherical” geometry is selected, and the inner radius is non-zero, shell geometry is set up.



Simulation Conditions

Geometry: cylindrical

Inner Radius [um]: 1.000000

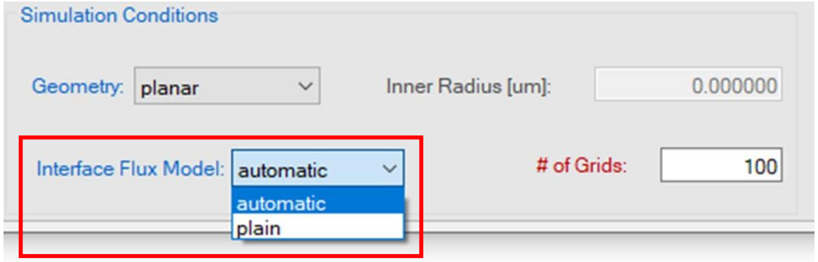
Interface Flux Model: automatic

# of Grids: 100

Figure 6.25 Set Inner Radius

6.6.11 Set Interface Flux Model

In the GUI of PanDiffusion, “Interface Flux Model” under “Simulation Conditions” decides how the grid composition evolves. When “automatic” is selected by default, sharp interface between two distinct phases is calculated with interface-fixed reference and local equilibrium applied at the interface. When “plain” is selected, sharp interface between two distinct phases is calculated in volume-fixed reference.



Simulation Conditions

Geometry: planar

Inner Radius [um]: 0.000000

Interface Flux Model: automatic

# of Grids: 100

Figure 6.26 Select interface flux model

6.6.12 Set Boundary Conditions

There are “Upper Boundary Condition” and “Lower Boundary Condition” in PanDiffusion. Their definitions are illustrated in the following figure:

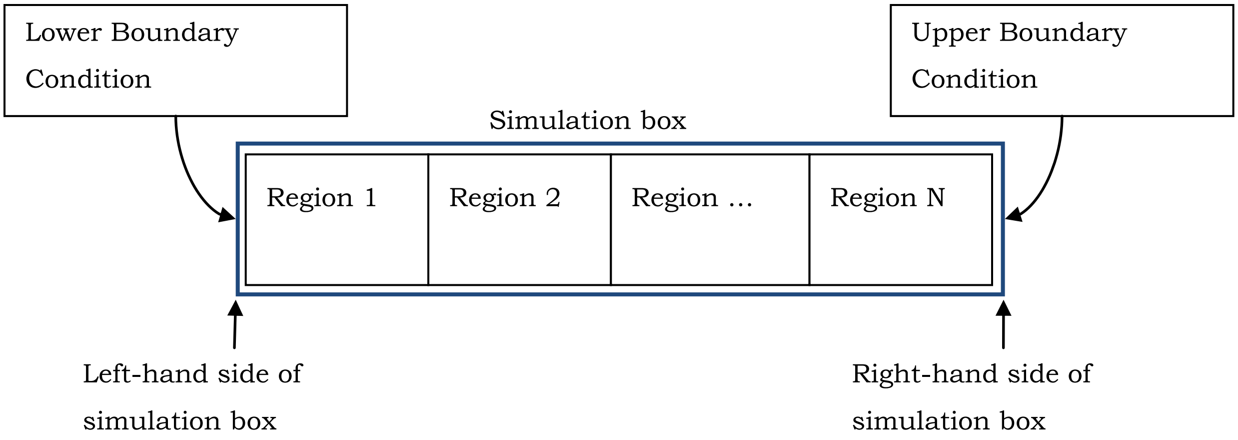
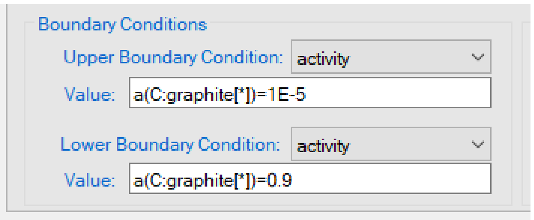


Figure 6.27 Definition of boundary conditions

Fixed activity at boundaries can be set following the format:



Upper Boundary Condition: activity

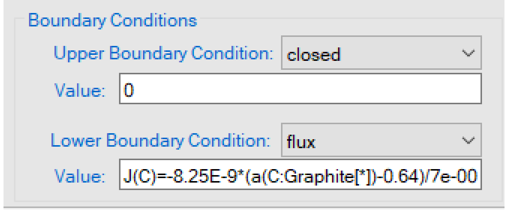
Value: a(C:graphite[*])=1E-5

Lower Boundary Condition: activity

Value: a(C:graphite[*])=0.9

Figure 6.29 Set fixed activity as a boundary condition

Mass flux expression at boundaries can be set following the format:



Upper Boundary Condition: closed

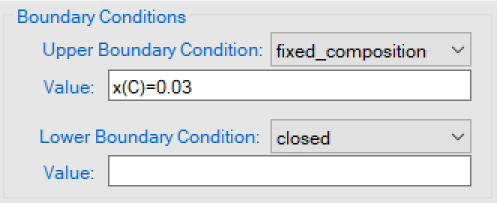
Value: 0

Lower Boundary Condition: flux

Value: J(C)=-8.25E-9*(a(C:Graphite[*])-0.64)/7e-00

Figure 6.28 Set mass flux expression as a boundary condition

Fixed composition of boundaries can be set following the format:



Upper Boundary Condition: fixed_composition

Value: x(C)=0.03

Lower Boundary Condition: closed

Value:

Figure 6.29 Set fixed composition as a boundary condition

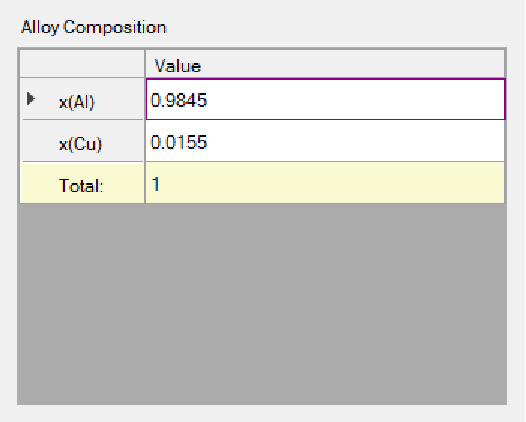
6.7 Settings in Dissolution Simulation GUI

The features of general GUI for diffusion simulation have been demonstrated in Section 6.6. In this section, we will present the features of the special GUI for dissolution simulation.

Settings for units, number of grids, geometry, interface flux model, thermal history and output profiles follow the same way as those in general GUI. The phases are selected globally in dissolution GUI. There is no regional setting in dissolution simulation. The global phase setting follows the same way as the general GUI.

6.7.1 Set Alloy Composition

In the dissolution GUI, overall composition of an alloy is set in the following section:



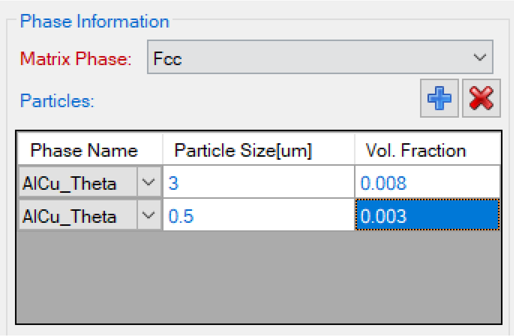
Alloy Composition

	Value
x(Al)	0.9845
x(Cu)	0.0155
Total:	1

Figure 6.30 Alloy composition in dissolution simulation GUI.

6.7.2 Set Matrix and Particle Information

Matrix phase and particle phases are explicitly selected in the "Phase Information" section. There can be more than one particle phases. For each particle phase, particle radius and volume fraction need to be set up.



Matrix Phase: Fcc

Particles:

Phase Name	Particle Size[um]	Vol. Fraction
AlCu_Theta	3	0.008
AlCu_Theta	0.5	0.003

Figure 6.31 Matrix and particle information in dissolution simulation.

7 PanSolidification

PanSolidification is a module of Pandat™ software designed to simulate solidification behavior under a variety of conditions with different cooling rates. It is an extension of the Scheil model taking into consideration of back diffusion in the solid, secondary dendrite arm coarsening, and the formation of eutectic structure.

It is seamlessly integrated with the user-friendly Pandat™ Graphical User Interface (PanGUI) as well as thermodynamic calculation engine, PanEngine. The implementation of PanEngine guarantees reliable input data, such as chemical potential, phase equilibrium and mobility. Figure 7.1 shows an overall architecture of the PanSolidification module.

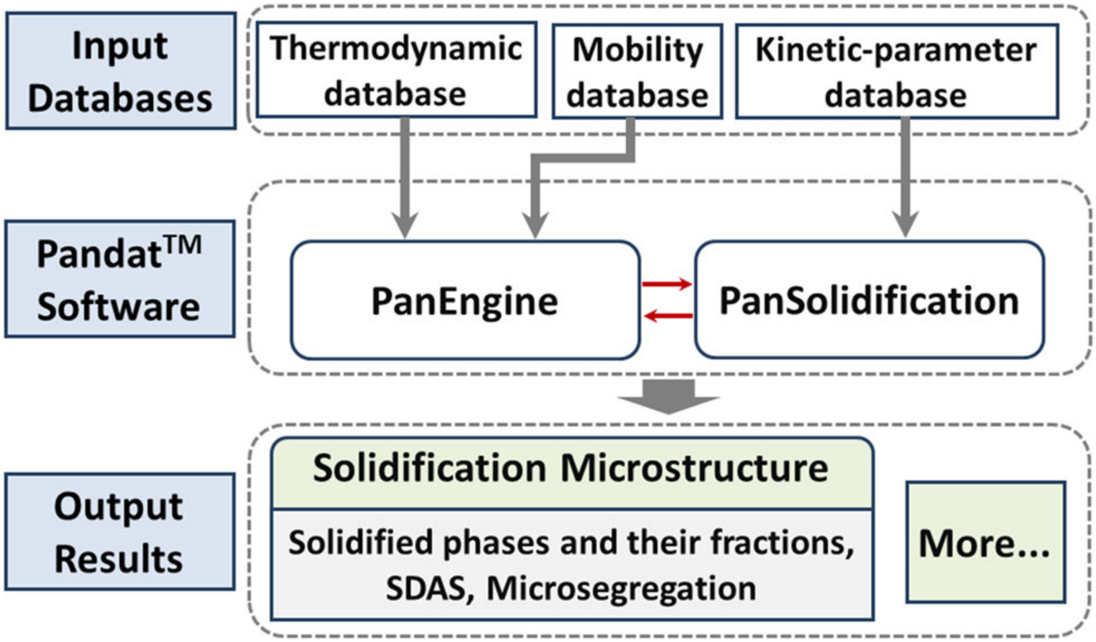


Figure 7.1 An overall architecture of the PanSolidification module

7.1 Features of PanSolidification

7.1.1 Overall Design

- The system composition profile, phase fraction, and phase concentration evolution during solidification
- Secondary dendrite arm spacing (SDAS) evolution during solidification.
- Back diffusion during the entire solidification process.

7.1.2 Data Structure

Thermodynamic and mobility parameters are stored in TDB file, and the kinetic parameters for undercooling and coarsening effects are stored in an SDB file in "Extensible Markup Language" (XML) format, which is a standard markup language and well-known for its extendibility. In accordance with the XML syntax, a set of well-formed tags are specially designed to define the back diffusion model for the morphology of primary phase and its corresponding model parameters such as interfacial energy, latent heat, coarsening geometric factor, dendrite tip factor, solute trapping parameter, solid diffusivity factor and boundary layer factor.

7.1.3 Numerical Model

The PanSolidification module, which is developed by coupling a solidification micro-model with PanEngine, is basically a modified Scheil model incorporating back-diffusion, undercooling, and dendrite arm coarsening. Figure 7.2 shows a sketch of dendrite, with a big solid trunk as the primary dendrite arm and fine secondary dendrite arms symmetrically distributed at the sides; the SDAS is indicated as λ_2. A one-dimensional morphology within the interdendritic region of secondary arms is usually used to describe the solidification processing (as enlarged and shown at the bottom part of Figure 7.2). Because of the symmetry of the dendrite arms, there is no mass flow through the arm center. Therefore, only one half of the arm spacing is considered.

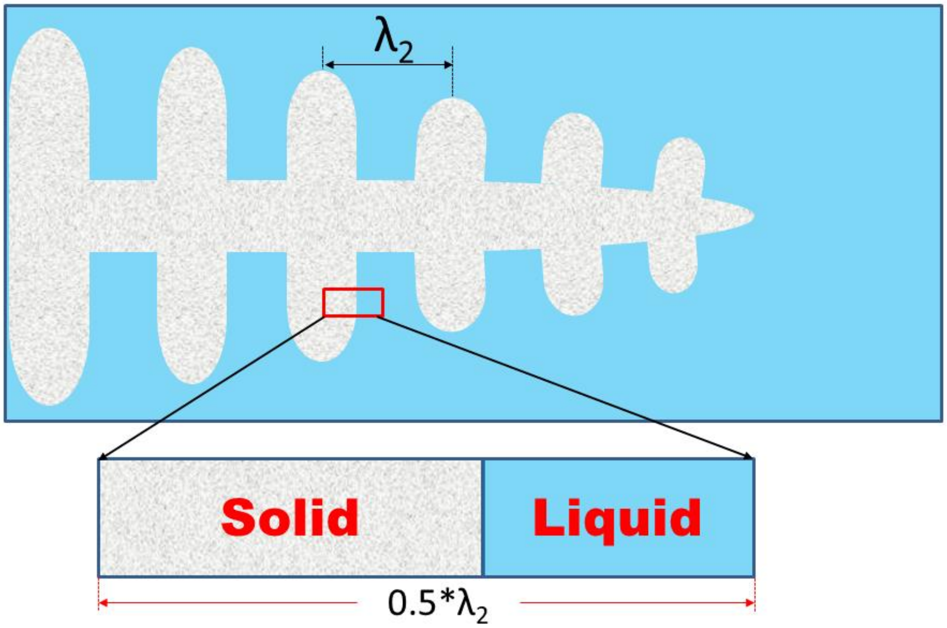


Figure 7.2 A schematic diagram of dendrites in the solid and liquid region

7.1.3.1 Back diffusion in the solid

The evolution of the concentration profile for component *i* in the considered dendrite arm is shown schematically in Figure 7.3. C_L^i and C_S^i are compositions of component *i* within the liquid and solid phases (given the unit of wt.% in this work), respectively. *V* is the velocity of S/L interface. During the time interval Δt, the S/L interface advances Δx_s (due to solidification) and the length of the solidification region increases by ΔL (due to the SDAS coarsening). For the current solidification simulation at each time step, three major tasks are carried out: (1) calculate the composition of each component at the S/L interface including the undercooling effects and local-equilibrium conditions; (2) solve the diffusion equations within the solid phase; (3) update the length scale to conserve mass balance for every component. More detailed description on the back diffusion can be found in some textbooks [1974Fle, 1985Kur].

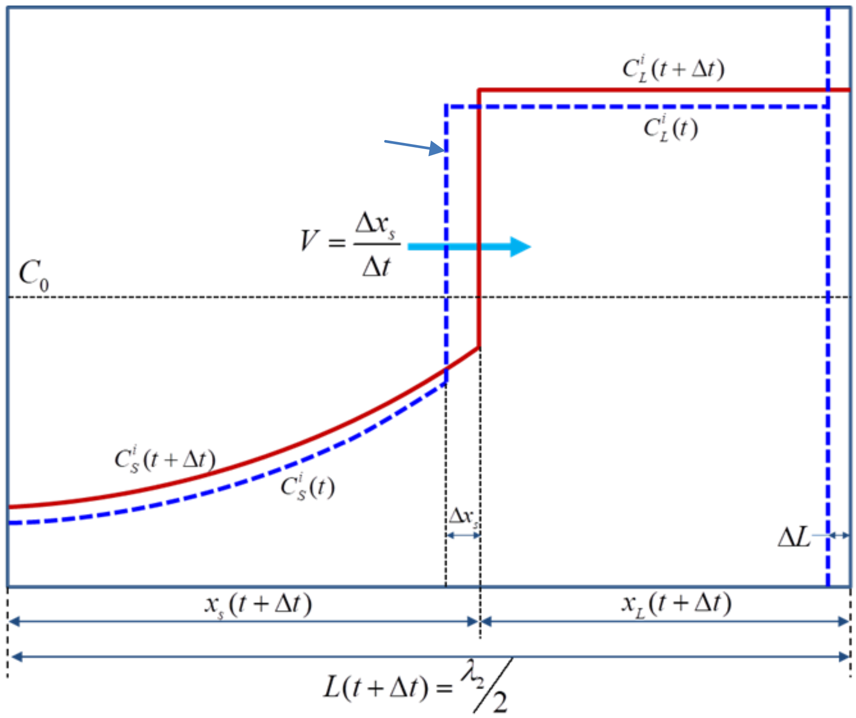


Figure 7.3 A schematic plot showing the composition distribution of component *i* in a dendrite arm at time t and *t*+Δ*t*.

7.1.3.2 Micro-model for dendrite arm coarsening

The initial SDAS is about twice of the dendrite tip radius: $\lambda_0 \cong 2r_T$ and r_T is described as a function of initial alloy composition, growth rate, and independent of temperature gradient

$$r_T^2 = \frac{2\gamma D_L T_0 \delta}{V \Delta T_0 k_e \Delta H_f} \tag{7.1}$$

where V, ΔT_0, k_e are the interface solidification velocity, freezing temperature range, and equilibrium partition coefficient, respectively. δ is a constant being dependent on the harmonic of the perturbation.

The dendrite arm spacing needs to be known since it sets the diffusion distances in the liquid and solid phases. Owing to the re-melting and re-solidification mechanism, dendrite arm coarsening contributes significantly to homogenization during solidification. The calculation of coarsening is described as below [1986Roo]:

$$\lambda^3 - \lambda_0^3 = \int_0^t gMdt \tag{7.2}$$

λ_0 is the initial SDAS obtained from the calculated dendrite tip radius as described in above equation 7.2, and λ is the model predicted SDAS at a certain time. M is coarsening parameter which is proportional to $\lambda^{1/3}$, t is time and g is the geometry factor representing the influence of the dendrite geometry.

For a binary system, the coarsening parameter M is defined as [1990Roo]:

$$M = \frac{\gamma D_L T}{\Delta H_f m_L^v (1-k_v) C_L^v} \tag{7.3}$$

For a multicomponent system, the coarsening parameter must be calculated separately for each alloying element. Then, the following model is used to take into consideration all the solute elements:

$$M = \frac{1}{\sum_{j=1}^{n} 1/M_j} \tag{7.4}$$

All phase equilibrium related quantities needed in the above equations (such as m_L and k_e) are directly calculated via PanEngine [2009Cao] at each time step by assuming the local equilibrium at the liquid/solid interface.

7.1.4 The Solidification Kinetic Database Syntax and Examples

The Solidification kinetic database (.SDB) uses the XML format, which defines the back diffusion model for the morphology of primary phase and its corresponding model parameters such as interfacial energy, latent heat, coarsening geometric factor, dendrite tip factor, solute trapping parameter, solid diffusivity factor, boundary layer factor, and so on.

In the SDB, a series of alloys can be defined. A sample SDB file is given below,

```
<Alloy name="Mg alloys">
```

```
    <solvent name="Mg"/>
    <primary_phase name="Hcp"/>
    <ParameterTable name="">
      <Parameter name="coordinate" value="0" description = "geometry of
        dendrite. 0 for plate; 1 for cylinder; 2 for sphere" />
      <Parameter name="interfacial_energy" value="0.065"  description =
        "interfacial energy, unit = J/m^2"/>
      <Parameter name="latent_heat" value="5.5e8"  description =
        "latent heat, unit=J/m^3"/>
      <Parameter name="solute_trapping_parameter" value="1e-9"  description =
        "solute trapping parameter, unit=m"/>
      <Parameter name="sound_velocity" value="1000"  description =
        "sound velocity, unit=m/s"/>
      <Parameter name="coarsening_geometric_factor" value="40"  description =
        "No unit"/>
      <Parameter name="dendrite_tip_factor" value="1"  description =
        "No unit"/>
      <Parameter name="solid_diffusivity_factor" value="0.2"  description =
        "No unit"/>
      <Parameter name="boundary_layer_factor" value="1"  description =
        "No unit"/>
    </ParameterTable>
  </Alloy>
</sdb>
```

In this sample SDB, “Mg alloys” is defined as the name of the alloy, the primary phase is thus set as “Hcp” phase. A set of parameters for each phase, such as interfacial energy, latent heat and so on, can be defined in “ParameterTable”.

The kinetic model parameters that can be defined under “ParameterTable” are listed in Table 7.1.

Table 7.1 Kinetic model parameters in sdb

Name	**Unit**	**Description**
Coordinate	N/A	Describe the geometry of dendrite for back diffusion model. `<Parameter name="coordinate" value="0" description = "geometry of dendrite. 0 for plate; 1 for cylinder; 2 for sphere" />`
Interfacial_Energy	J/m^2	Interfacial energy `<Parameter name="interfacial_energy" value="0.065" description = "interfacial energy, unit = J/m^2"/>`
Latent_heat	J/m^3	Latent Heat of the alloy `<Parameter name="latent_heat" value="5.5e8"  description = "latent heat, unit=J/m^3"/>`
Solute_Trapping_Parameter	N/A	Solute trapping parameter `<Parameter name="solute_trapping_parameter" value="1e-9" description = "solute trapping parameter, unit=m"/>`
Sound_velocity	N/A	Sound velocity `<Parameter name="sound_velocity" value="1000"  description = "sound velocity, unit=m/s"/>`
Coarsening_Geometric_Factor	N/A	A factor adjusting adjust the coarsen speed of the dendrite. `<Parameter  name="coarsening_geometric_factor"  value="40" description = "No unit"/>`

7.2 Tutorial

7.2.1 Step 1: Create a PanSolidification Project

Users can create a PanSolidification project through menu “**File → Create a New Workspace**” or “**File → Add a New Project**” in an existing workspace. The “Module Window” pops out for user to choose a module for the new project as shown in Figure 7.4. Choose “PanSolidification” module for Solidification simulation, and the PanSolidification project will be created after user click on **Create** button or double click on the PanSolidification icon.

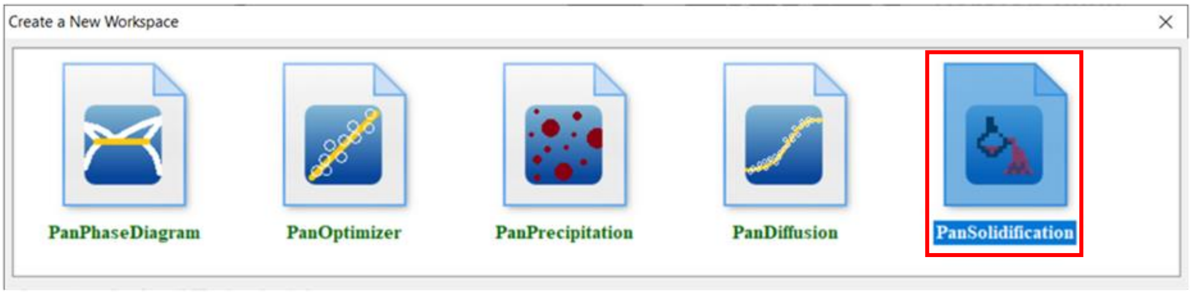
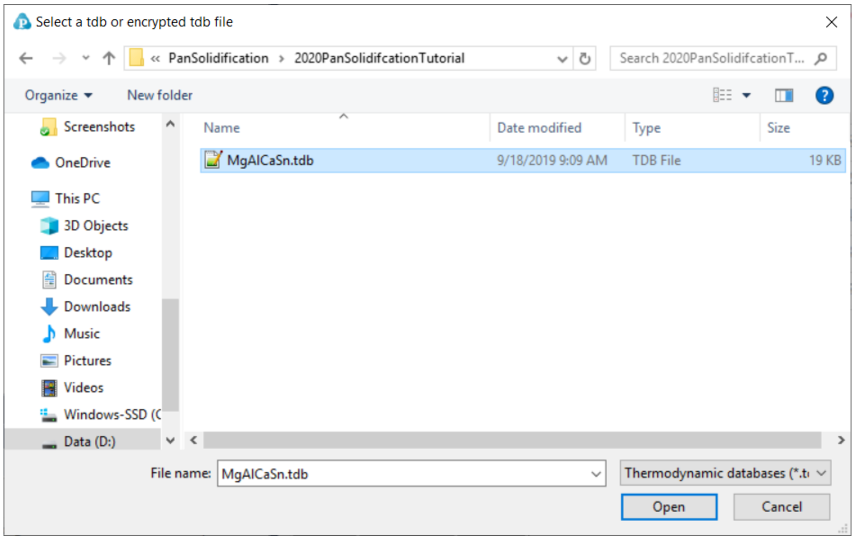


Figure 7.4 Creating a PanSolidification workspace

7.2.2 Step 2: Load Thermodynamic and Mobility Database

The next step is to load the database, which is `MgAlCaSn.tdb` in this example. Different from the normal thermodynamic database, this database also contains mobility model parameters for the phases of interest in addition to the thermodynamic model parameters. Both are needed for carrying out solidification simulation. By clicking the button on the toolbar, a pop-up window as shown in Figure 7.5 will open, allowing user to select the database file. And Click “Open” to select the database, then a window as Figure 7.6 will pop up for user to select components for PanSolidification simulation.

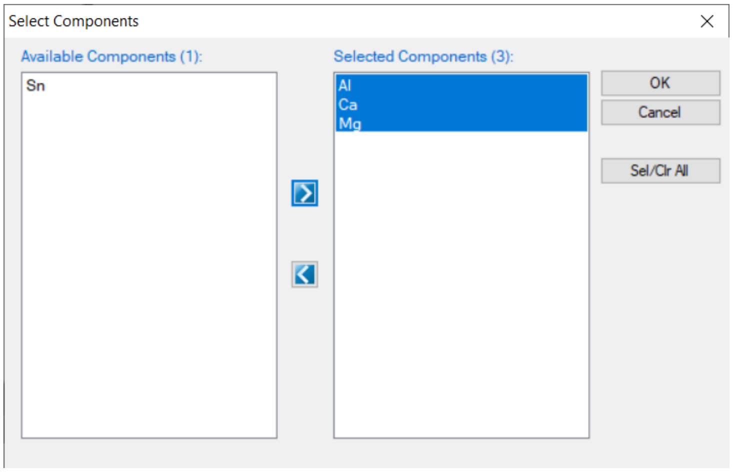


Name	Date modified	Type	Size
MgAlCaSn.tdb	9/18/2019 9:09 AM	TDB File	19 KB

File name: MgAlCaSn.tdb

Thermodynamic databases (*.t

Figure 7.5 Dialog window for loading thermodynamic and mobility database.



Available Components (1):

Sn

Selected Components (3):

Al
Ca
Mg

Figure 7.6 Dialog window for components selection.

7.2.3 Step 3: Load Solidification Kinetic Database

A solidification kinetic database is required for solidification simulation. Such a database contains kinetic parameters which are alloy dependent. To organize these parameters in a more intuitive way, the standard XML format is adopted and a set of well-formed tags are deliberately designed to define back diffusion model for the morphology of primary phase (which could be plate, cylinder and sphere) and its corresponding model parameters such as interfacial energy, latent heat, coarsening geometric factor, dendrite tip factor, solute trapping parameter, solid diffusivity factor and boundary layer factor.

In this example, the `MgAlloys.sdb` is prepared. To load a solidification database, user should navigate the command through menu **PanSolidification → Load SDB**, or click icon from the toolbar. After `MgAlloys.sdb` is chosen, a dialog box pops out automatically for user to select the alloy for the simulation. As shown in Figure 7.7, Mg alloys is contained in this SDB file.

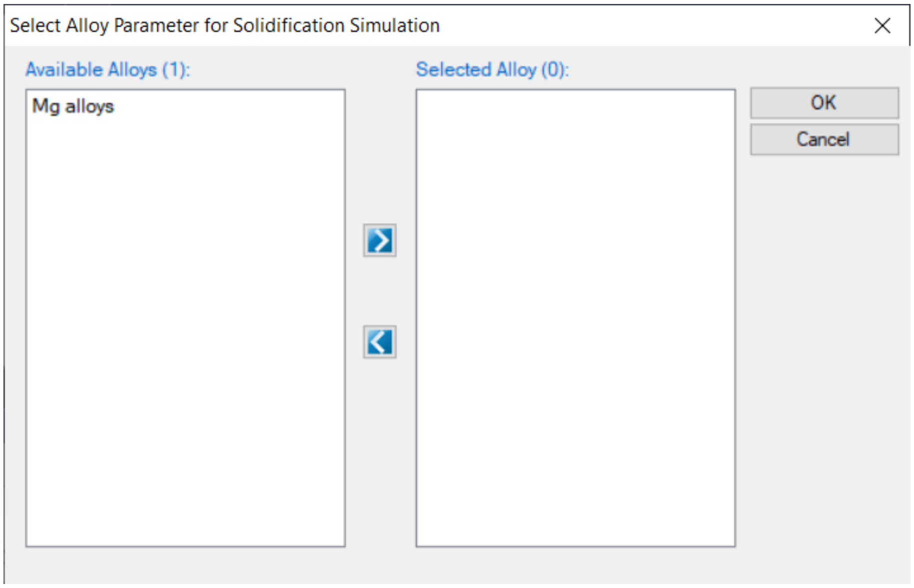


Figure 7.7 Dialog box for selecting alloy parameter.

7.2.4 Step 4: Solidification Simulation

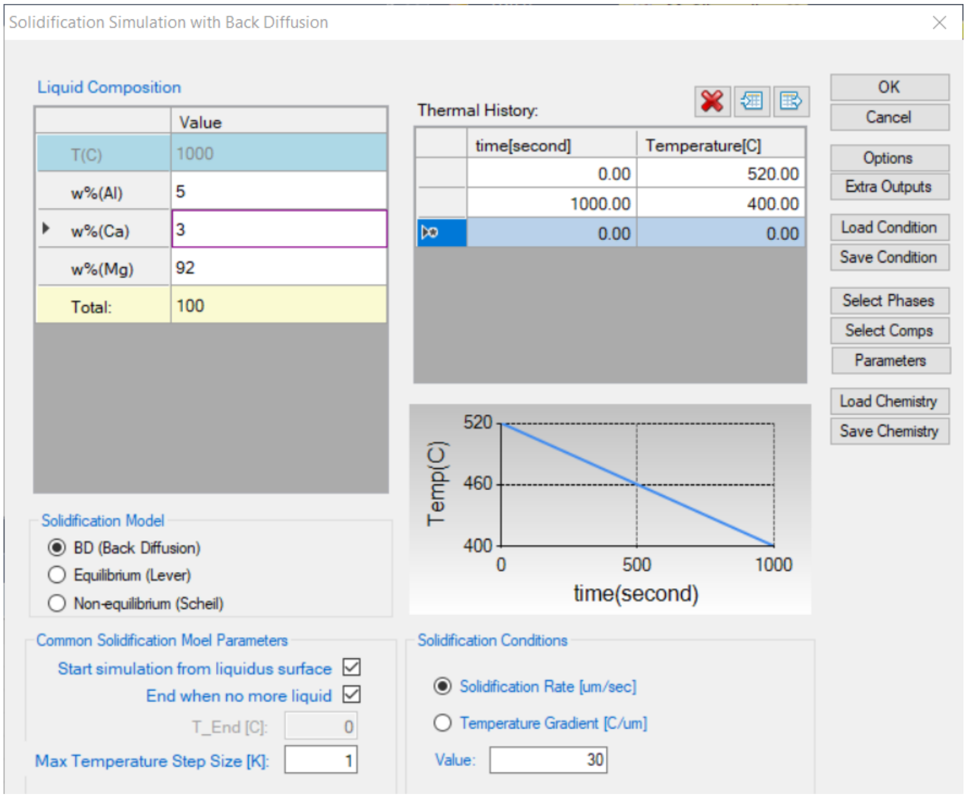
Perform solidification simulation through menu bar **PanSolidification ->Solidification Simulation with Back Diffusion** or click icon from the tool bar. A dialog box entitled "Solidification Simulation with Back Diffusion", as shown in Figure 7.8, pops out for user's inputs to set up the simulation conditions: alloy composition and solidification conditions. When setting the solidification conditions, users need to be careful about the units used for the conditions. Click **Option**, a window as shown in Figure 7.9 will pops out for units setting.

Alloy Composition: User can set alloy composition by typing in or use the **Load Chemistry** function. User can also save the alloy composition through

Save Chemistry. This is especially useful when working on a multi-component system, so that user does not need to type in the chemistry every time.

Solidification Conditions: The **Cooling Rate** of solidification can be defined through **Thermal History** window. The cooling rate determined by cooling curves can also be imported by click the icon as shown in Figure 7.8. The **Solidification Rate** and **Temperature Gradient** can be defined from the interface. As the **Cooling Rate (CR)**, **Solidification Rate (V)** and **Temperature Gradient (G)** has a relationship of **CR = G*V**, user may choose to provide either **Solidification Rate** or **Temperature Gradient**.

User can also define the output **Table** and **Graph** within the **Output Options** window.



Liquid Composition

	Value
T(C)	1000
w%(Al)	5
w%(Ca)	3
w%(Mg)	92
Total:	100

Thermal History:

time[second]	Temperature[C]
0.00	520.00
1000.00	400.00
0.00	0.00

Solidification Model

● BD (Back Diffusion)
○ Equilibrium (Lever)
○ Non-equilibrium (Scheil)

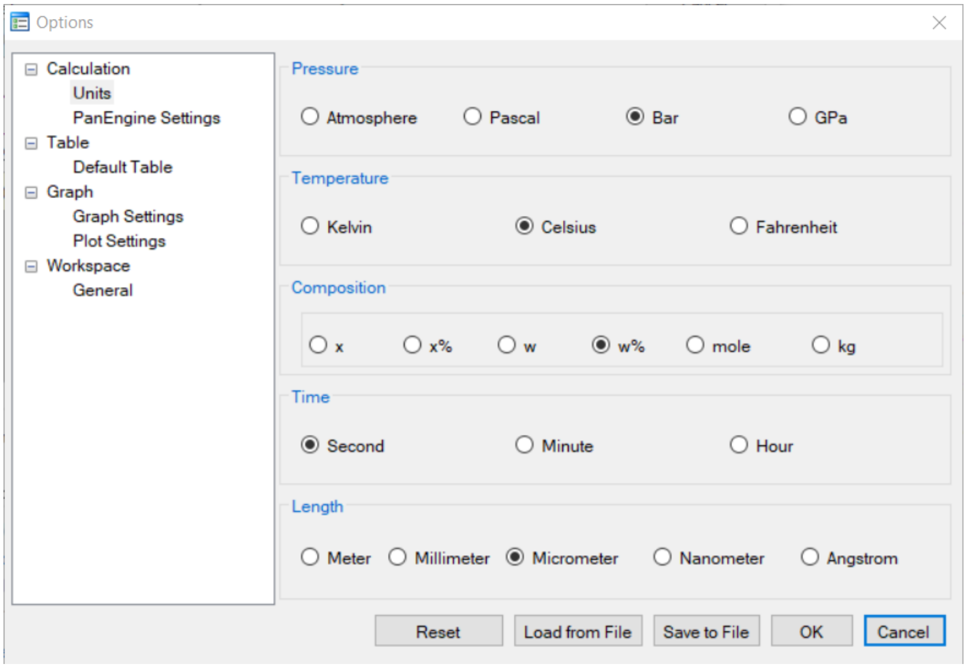
Common Solidification Moel Parameters

Start simulation from liquidus surface ☑
End when no more liquid ☑
T_End [C]: 0
Max Temperature Step Size [K]: 1

Solidification Conditions

● Solidification Rate [um/sec]
○ Temperature Gradient [C/um]
Value: 30

Figure 7.8 Dialog box for setting solidification simulation conditions



Pressure
○ Atmosphere ○ Pascal ● Bar ○ GPa

Temperature
○ Kelvin ● Celsius ○ Fahrenheit

Composition
○ x ○ x% ○ w ● w% ○ mole ○ kg

Time
● Second ○ Minute ○ Hour

Length
○ Meter ○ Millimeter ● Micrometer ○ Nanometer ○ Angstrom

Figure 7.9 Dialog box for setting units.

7.2.5 Step 5: Customize Simulation Results

As all other calculations available in Pandat™, upon the completion of the solidification simulation, a default table with related solidification related properties (time, temperature, secondary dendrite arm spacing, solid and liquid phase fractions, etc.) is automatically generated and a default graph for temperature (T) vs solid fraction (fs) is displayed as shown in Figure 7.10. User can refer to sections 2.3 and 2.4 to learn how to customize simulated graph and table.

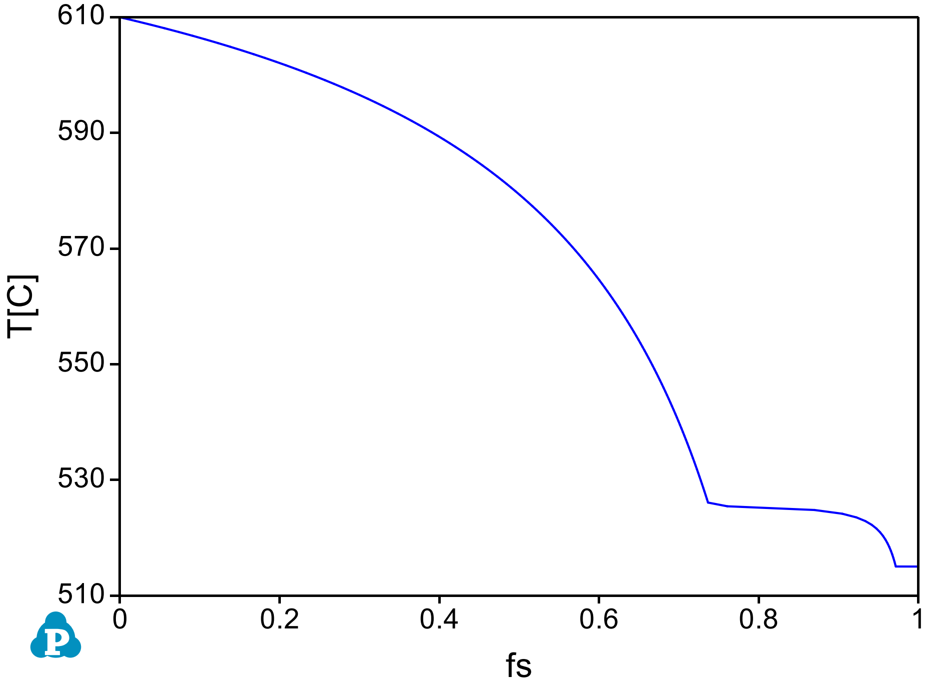


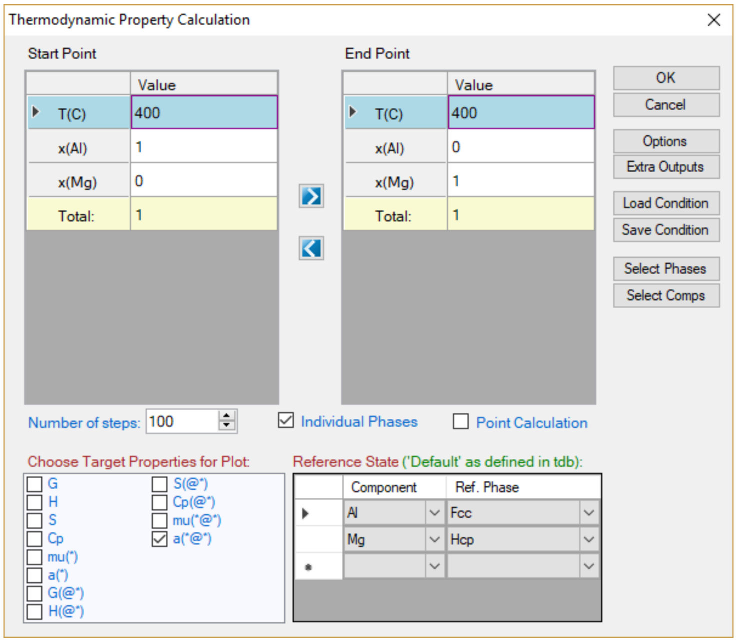
Figure 7.10 Default graph plotting Temperature vs f_s during solidification.

8 Property

Property calculation has been added into Pandat™ and is characterized in three categories, thermodynamic property, physical property and kinetic property. The database format and the equations for these properties are described below.

8.1 Thermodynamic Property

The **Thermodynamic Property** function is used to calculate thermodynamic properties, such as Gibbs energy, enthalpy, entropy, chemical potential, activity, etc. It is under the **PanPhaseDiagram** module. User can access this function through the menu (**Property → Thermodynamic Property**) after the thermodynamic database is loaded. A popup window will allow user to input calculation conditions as shown in Figure 8.1.



Start Point

	Value
T(C)	400
x(Al)	1
x(Mg)	0
Total:	1

End Point

	Value
T(C)	400
x(Al)	0
x(Mg)	1
Total:	1

Number of steps: 100
☑ Individual Phases
☐ Point Calculation

Choose Target Properties for Plot:

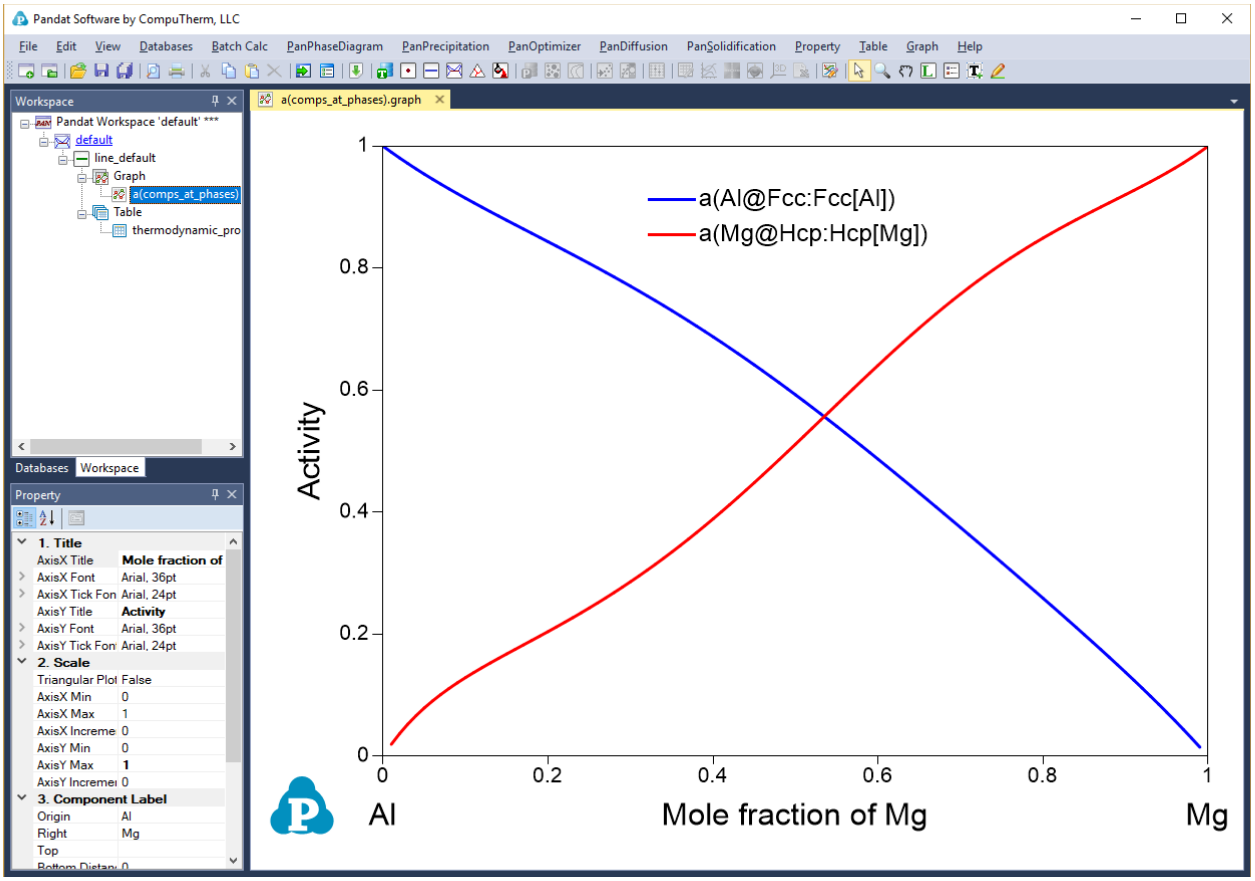
☐ G
☐ H
☐ S
☐ Cp
☐ mu(*)
☐ a(*)
☐ G(@*)
☐ H(@*)
☐ S(@*)
☐ Cp(@*)
☐ mu(*@*)
☑ a(*@*)

Reference State ('Default' as defined in tdb):

Component	Ref. Phase
Al	Fcc
Mg	Hcp

Figure 8.1 Thermodynamic Property calculation dialog

The calculation is set as a line calculation with the desired thermodynamic properties output. User may select the thermodynamic properties as needed by checking the boxes in front of each property as shown in Figure 8.1 and specify the reference state for each element. The selected property will be calculated and graph plotted as shown in Figure 8.2. If two or more thermodynamic properties are selected, they will be plotted separately. Experienced user can also get these results directly from the **Line Calculation** in the **PanPhaseDiagram** module with proper syntax using self-defined table.



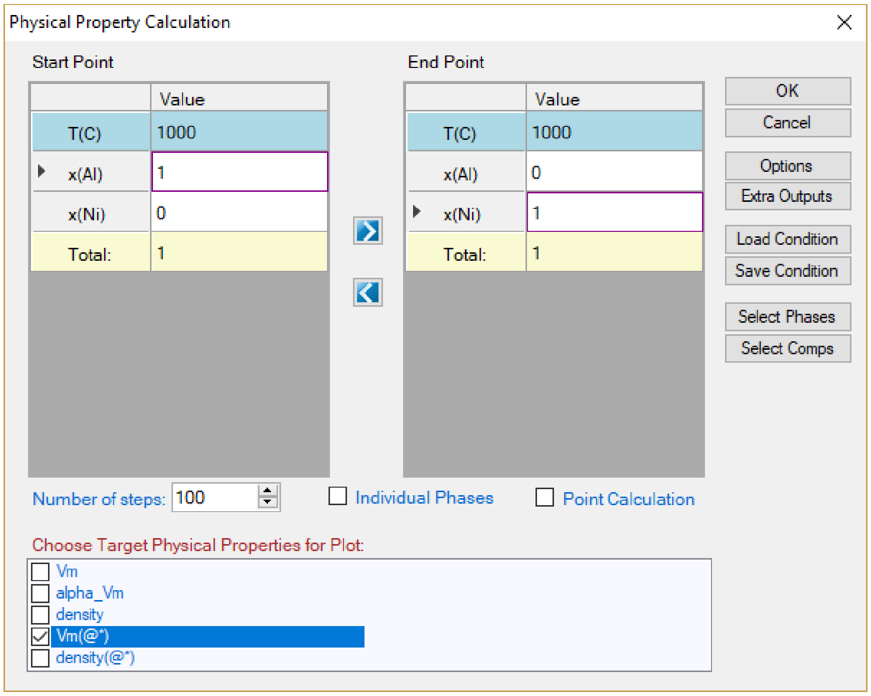
1. Title	
AxisX Title	**Mole fraction of**
AxisX Font	Arial, 36pt
AxisX Tick Fon	Arial, 24pt
AxisY Title	**Activity**
AxisY Font	Arial, 36pt
AxisY Tick Font	Arial, 24pt
2. Scale	
Triangular Plot	False
AxisX Min	0
AxisX Max	1
AxisX Increme	0
AxisY Min	0
AxisY Max	**1**
AxisY Increme	0
3. Component Label	
Origin	Al
Right	Mg
Top	
Bottom Distan	0

Figure 8.2 Thermodynamic Property calculation results

8.2 Physical Property

Physical property calculation implemented in Pandat™ allows user to calculate the molar weight, molar volume, density, surface tension and viscosity. The interface is similar to the Thermodynamic property calculation as shown in Figure 8.3. User can set up the calculation condition as a line calculation and select the properties to be calculated. The default graph is the calculated property as shown in Figure 8.4 as an example. Again, if two or more properties are selected, all of them will be plotted one by one.

The detailed calculation method for each property and the format of the database file are described in the following sections.



Physical Property Calculation

Start Point

	Value
T(C)	1000
x(Al)	1
x(Ni)	0
Total:	1

End Point

	Value
T(C)	1000
x(Al)	0
x(Ni)	1
Total:	1

Number of steps: 100

☐ Individual Phases ☐ Point Calculation

Choose Target Physical Properties for Plot:

☐ Vm
☐ alpha_Vm
☐ density
☑ Vm(@*)
☐ density(@*)

Figure 8.3 Physical property calculation dialog

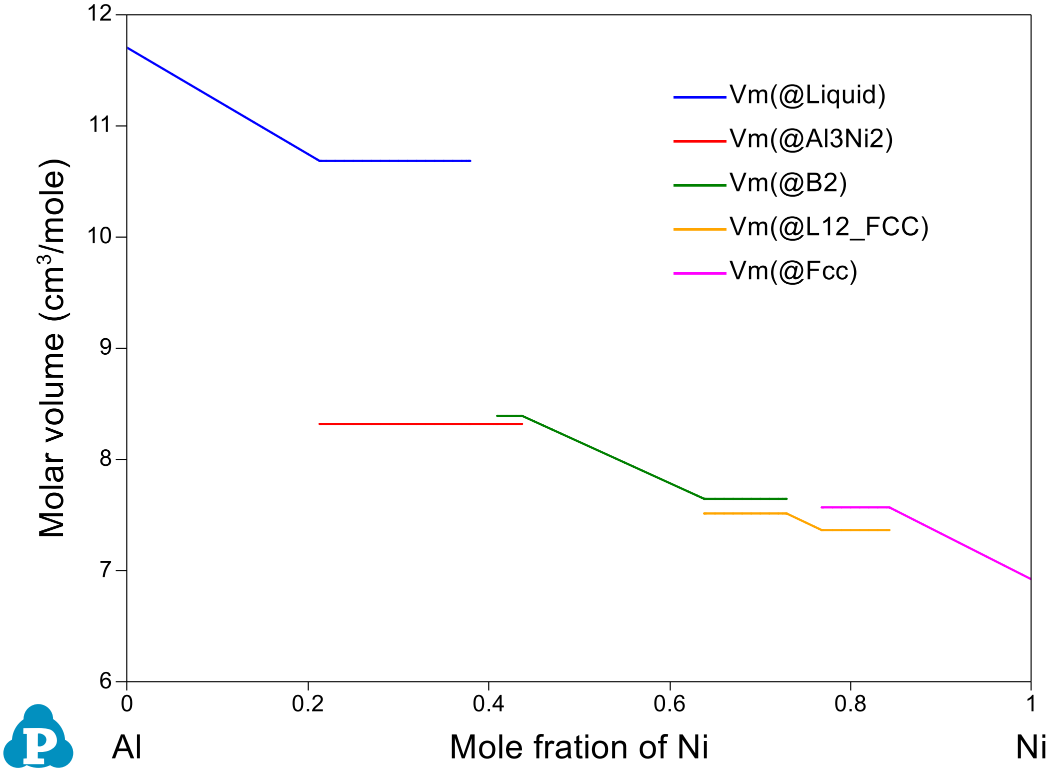


Figure 8.4 Physical property calculation results

8.2.1 Molar Weight and Phase Weight Fraction

The molar weight for a phase is calculated from the atomic weights of the elements involved in the phase. The unit is kg/mol-atoms. Since atomic weights of elements have been included in Pandat, no input is required in the database `TDB` file.

For example, an Fcc phase in Al-Cu binary system with $x_{Al} = 0.9$ and $x_{Cu} = 0.1$, its molecular weight is

$$
\begin{aligned}
MW^{fcc} &= x_{Al} M_{Al} + x_{Cu} M_{Cu} = 0.9 \times 26.982 \times 10^{-3} + 0.1 \times 63.546 \times 10^{-3} \\
&= 30.6384 \times 10^{-3} (kg / mol - atoms)
\end{aligned}
\tag{8.1}
$$

8.2.2 Molar Volume and Phase Volume Fraction

The molar volume can be calculated by Pandat™ if the model parameters are properly defined in the database file. The molar volume of a pure component is described as a function of temperature and pressure, and the excess molar volume of a phase is described in the format similar to that of excess Gibbs energy. The unit of molar volume is $m^3/mol-atoms$. In the database (.TDB) file, the format of molar volume is:

```
PARAMETER Vm(Fcc,Al;0) 298.15 +9.7743e-006*exp(6.91213e-005*T+1.62267e-011*T**3+0.413484*T**(-1)); 3000 N !
PARAMETER Vm(Fcc,Fe;0) 298.15  +6.72092e-006*exp(6.97895e-005*T); 3000 N !
PARAMETER Vm(Fcc,Al,Fe:Va;0) 298.15  -3e-6; 3000 N !
```

The calculation of molar volume for a phase is

$$V_m = \sum x_i V_{m_i}^o + \sum x_i x_j V_{m_{ij}} (x_i - x_j)^k \tag{8.2}$$

where $V_{m_{ij}}$ is the parameter for the excess molar volume of this phase.

Molar volume of a system with phase mixture is calculated by

$$V_m = \sum f^\phi V_m^\phi \tag{8.3}$$

where f^ϕ and V_m^ϕ are the molar fraction and molar volume for phase ϕ.

Note that, if a phase is described by a compound-energy-formalism (CEF) with multi-sublattices, the molar volume is automatically described as a function of T, P, and site fraction (y) following the format of the Gibbs energy. This will introduce many end members in the molar volume and may lead to instability in the calculated molar volume. In reality, molar volume should be a function of mole fraction (x) instead of site fraction (y), it is thus recommended to define the molar volume of a phase separately from its Gibbs energy if the phase is described by the CEF model. This can be realized through the user-defined molar volume property (section 3.3.8).

Using the Al-Ni binary system as an example, type “VARIABLE_X” is defined as property “V_m”:

```
Type_Definition v GES AMEND_PHASE_DESCRIPTION * VARIABLE_X Vm !
```

which means any phase with the Type_Defination "v" will use mole fractions as the variables of Vm. Here are examples to define the molar volume parameters for the Liquid and L12_FCC phases:

```
Phase Liquid %v 1 1 !

Parameter Vm(Liquid,Al;0) 298.15    +V_Al_Liquid; 3000 N !

Parameter Vm(Liquid,Ni;0) 298.15    +V_Ni_liquid; 3000 N !


Phase L12_FCC %v 2 0.75 0.25 !

Parameter Vm(L12_FCC,Al;0) 298.15    +0.935*V_Al_fcc; 3000 N !

Parameter Vm(L12_FCC,Ni;0) 298.15    +0.935*V_Ni_fcc; 3000 N !
```

In this case, the molar volume of L12_FCC is calculated as:

$$V_m = 0.935 * x_{Al} * V_{Al}^{fcc} + 0.935 * x_{Ni} * V_{Ni}^{fcc} \tag{8.4}$$

although the L12_FCC phase is described by CEF model with two sublattices. Please refer to the example #28 in the example book for detail information.

8.2.3 Density

Density is calculated from molar volume and the molar weight. It requires the molar volume parameters in database. The unit for density is kg/m^3. Density of a phase is defined as

$$d^{\varphi} = \frac{W_m^{\varphi}}{V_m^{\varphi}} \tag{8.5}$$

The density of a system with phase mixture is calculated from the molar weight and the molar volume of the mixture:

$$d = \frac{W_m}{V_m} \tag{8.6}$$

8.2.4 Viscosity

A function to calculate viscosity of liquid phase is added into current Pandat™. The model used for describing the viscosity of liquid phase is semi-empirical relation presented in the paper by Seetharaman and Du [1994See],

$$\eta = A \exp\left(\frac{\Delta G^*}{RT}\right) \tag{8.7}$$

with

$$A = \frac{hN}{V} \tag{8.8}$$

where V is the molar volume of the melt, h the Plank's constant, N the Avogadro's number. ΔG^* is the Gibbs energy of activation, and can be calculated by

$$\Delta G^* = \sum x_i \Delta G_i^o + \Delta^m G_{mix} + 3RT \sum\sum x_i x_j \tag{8.9}$$

where x_i and x_j are the molar fractions of component i and j, ΔG_i^o, Gibbs energy of activation of component i, and $\Delta^m G_{mix}$, Gibbs energy of mixing. The calculation of molar volume is given in above sections. The parameter for the activation energy of a pure component in database `TDB` file has the format

```
Parameter ActivationEnergy(Liquid,Al;0) 298.15 15051+13.519*T; 2000 N !
```

8.2.5 Surface Tension

Current Pandat has another new function to calculate surface tension of liquid phase. The model for calculating surface tension of liquid is the semi-empirical relationship proposed by Yeum et al. [1989Yeu] to estimate the surface tensions of binary alloys based on the model of Butler [1932But].

$$\sigma = \sigma_i + \frac{RT}{S_i} \ln \frac{a_i^{'}}{a_i} \tag{8.10}$$

where σ_i, $a_i^{'}$ and a_i are the surface tension, activity at the surface and activity in the bulk of component i. And S_i is the surface monolayer area,

$$S_i = bN^{1/3}V_i^{2/3} \tag{8.11}$$

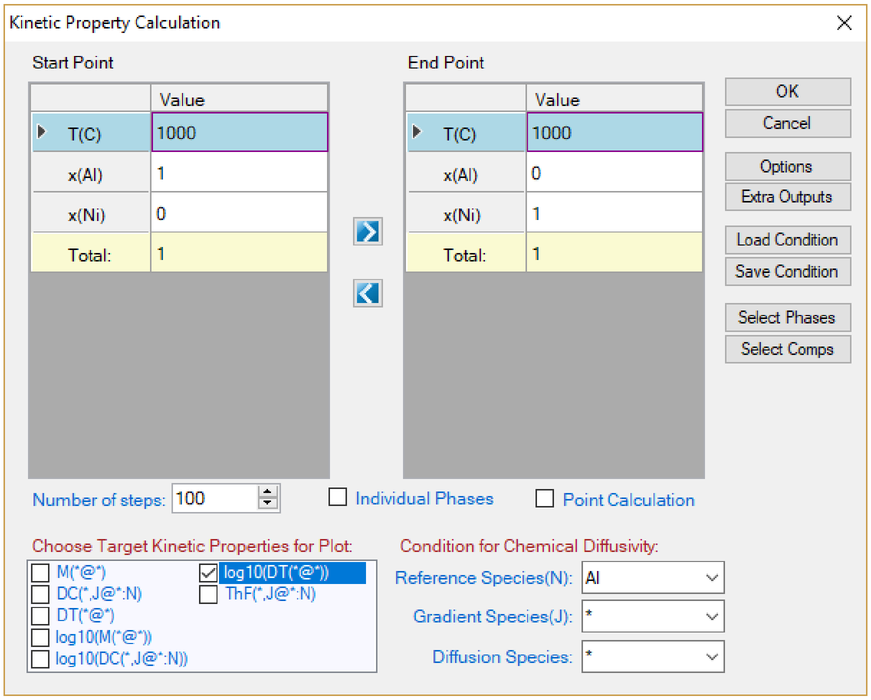
where b is geometric factor, N the Avogadro's number, and V_i molar volume of component i. This approach was extended to calculate surface tensions of multicomponent liquid alloys [1997Zha]. The calculation of molar volume is the same as given in **section 8.2.2**. The ratio of the coordination number for the surface atoms to that for the atoms in the bulk phase, b, is represented by a parameter `beta`, described in database (`.tdb`) file in the format as

```
Parameter Beta(Liquid,Al;0) 298.15  0.83;  2000  N !
```

8.3 Kinetic Property

Diffusivity related properties can be calculated from Pandat™ as long as the corresponding species mobility parameters are available in the database. User can input the calculation condition through the interface shown in Figure 8.5 and select the desired properties for output. The default graph is the selected property as shown in Figure 8.6. If two or more properties are selected, they will be plotted separately.

Details on the kinetic models for the multicomponent diffusion are referred to the literature [1982Ågr, 1992And]. Only the key equations related to the properties of mobility, tracer diffusivity and chemical diffusivity are given in the below sections.



Start Point

	Value
T(C)	1000
x(Al)	1
x(Ni)	0
Total:	1

End Point

	Value
T(C)	1000
x(Al)	0
x(Ni)	1
Total:	1

Number of steps: 100

☐ Individual Phases ☐ Point Calculation

Choose Target Kinetic Properties for Plot:

☐ M(*@*)
☐ DC(*,J@*:N)
☐ DT(*@*)
☐ log10(M(*@*))
☐ log10(DC(*,J@*:N))
☑ log10(DT(*@*))
☐ ThF(*,J@*:N)

Condition for Chemical Diffusivity:

Reference Species(N): Al
Gradient Species(J): *
Diffusion Species: *

Figure 8.5 Kinetic Property calculation dialog

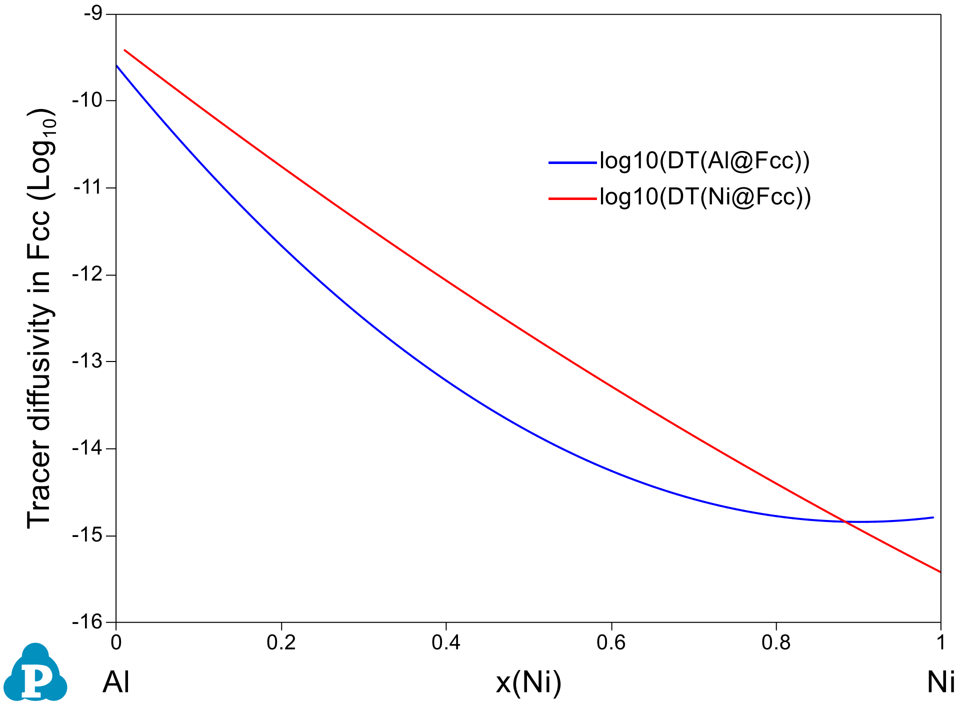


Figure 8.6 Calculated diffusivity in the Al-Ni system

8.3.1 Atomic Mobility

In order to simulate diffusivity related properties such as chemical diffusivities of components, atomic mobility data of species in phases are required and stored in the database. Mobility of species *k* is related to its activation energy (Q_k) by

$$M_k = M_k^{\circ} e^{-Q_k/RT} \tag{8.12}$$

where M_k° is a frequency factor, *R* is the gas constant and *T* the temperature in Kelvin. Define MQ_k as

$$MQ_k = RT\ln M_k = RT\ln M_k^{\circ} - Q_k \tag{8.13}$$

Then, atomic mobility can be calculated from MQ_k. MQ_k is a function of composition, temperature and pressure and can be expressed as Redlich-Kister type of polynomial expansion as for the excess Gibbs energy [1982Ågr]. Each polynomial coefficient is stored in database. For example, the coefficient for term contributed to Al from Ni in Fcc phase ($MQ_{Al}^{Ni,\circ}$) is described in `TDB` file as follows,

```
Parameter MQ(Fcc&Al,Ni;0) 298.15 -285517+R*T*Ln(0.0007933); 6000 N !
```

In Pandat, atomic mobility of species can be obtained through table operation with field of "`M(*@*)`". For example, `M(Al@Fcc)` represents the atomic mobility of Al in Fcc phase.

8.3.2 Tracer Diffusivity

Tracer diffusivity of a species *k* is directly related to its atomic mobility by

$$D_k^* = RTM_k \tag{8.14}$$

where *R* is the gas constant and *T* the temperature. Tracer diffusivity can be obtained in Pandat™ from table with field of "`DT(*@*)`". For example, the tracer diffusivity of Al in Fcc can be extracted from calculation result with the table field of “`DT(Al@Fcc)`”. The natural logarithm of the tracer diffusivity is available with “`logDT(*@*)`”.

8.3.3 Chemical Diffusivity

Chemical diffusivity of species *k*, D_{kj}^{n}, could be calculated by

$$D_{kj}^{n} = D_{kj} - D_{kn} \quad \text{(when } j \text{ is substitutional)} \tag{8.15}$$

$$D_{kj}^{n} = D_{kj} \quad \text{(when } j \text{ is interstitial)} \tag{8.16}$$

and

$$D_{kj} = \sum_{i \in S} (\delta_{ik} - u_k) u_i M_i \frac{\partial \mu_i}{\partial u_j} + \sum_{i \notin S} \delta_{ik} u_i y_{Va} M_i \frac{\partial \mu_i}{\partial u_j} \tag{8.17}$$

where *S* represents the set of the substitutional species, δ_{ik} .is the Kronecker delta, and μ_i is the chemical potential of species *i*. u_k is defined as

$$u_k = \frac{x_k}{\sum_{i \in S} x_j} \tag{8.18}$$

Chemical diffusivity of species *k* in phase p can be obtained in Pandat™ with the table field of “DC(k,j@p:n)”, where j and n are the gradient species and the reference species, respectively. Its corresponding natural logarithm is “logDC(k,j@p:n)”.

8.4 User defined properties

Pandat allows user to define any property of a phase or a system following some simple syntax rules. The **user-defined-property** database can be added to the original database, either TDB or PDB files, through **Append database** function**.** (Please refer to **Section 3.3.9** for the detailed description on **Append database** function). Users can also add the **user-defined-property** parameters into their home-developed TDB files to develop a combined database for **User-defined property** calculations.

Three methods are implemented in Pandat to add **User-defined-properties**, depending on the nature of the properties. Key words `Phase_Property;` `System_Property` and `Property` are used in the syntax respectively.

Phase Property is used to define a property of a phase with a similar expression which describes the Gibbs energy of a disordered solution phase. Let *U* be the user-defined phase property and it is expressed as:

$$U = \sum_{i=1}^{c} x_i U_i^o + \sum_{i=1}^{c-1} \sum_{j=i+1}^{c} x_i x_j \sum_k (x_i - x_j)^k L_{ij}^k \tag{8.19}$$

where x_i is the molar fraction of component *i* and U_i^0 is the property of the pure component *i*, L_{ij}^k is the *k*th order interaction parameter between components *i* and *j*. The syntax used in the TDB file are:

```
Type_Definition z PHASE_PROPERTY U 1 !
```

```
Type_Definition v GES AMEND_PHASE_DESCRIPTION * VARIABLE_X U !
```

In this definition, “v” is the identifier, “*” means any phase, and VARIABLE_X is the key word indicating X as the variable. The meaning of this definition is that any phase with the identifier “v” will use mole fractions (*x*) as the variables for property U.

System Property is used to define a property of a system with more than one phase. For a property in a system with multi-phase mixture, the property of the system is the weighted average of that of each phase. By default, the arithmetic mean is applied to a user defined Phase Property in a multi-phase system. For example, the user defines **Phase Property U** in a system with α and β two-phase mixture. The property of U of this system is calculated by

$$U = f_\alpha U_\alpha + f_\beta U_\beta \tag{8.20}$$

If the simple arithmetic mean does not apply, more complicated expression can be defined by User through Command **System Property**. For example, the value of the system property can be calculated through the function:

$$U_{\alpha+\beta} = f_\alpha U_\alpha + f_\beta U_\beta - f_\alpha f_\beta \sum_{i=0} M_i (f_\alpha - f_\beta)^i \tag{8.21}$$

where $U_{\alpha+\beta}$ is the user defined property of U in α+β two phase region. U_α and U_β is the property U in α and β phase respectively; f_α and f_β are the phase fraction of α and β phase respectively. M_i are the i^{th} order of the additional parameters which are used to describe additional effects on the user defined property U.

The syntax for the **System Property** used in the TDB file is:

```
System_Property Sys_U 1 !

Parameter L(Sys_U, Alpha, Beta;0)  298.15  M0; 3000 N !

Parameter L(Sys_U, Alpha, Beta;1)  298.15  M1; 3000 N !
```

Using command **Property,** user can also define special properties associated with phases in the original database. Any phase property available from Pandat Table can be used for user-defined property, such as G, H, mu, and ThF. However, the star symbol in a property, like `mu(*)`, cannot be used.

The syntax for the **Property** used in the TDB file is:

```
Property GFcc_GLiq  298.15  G(@Fcc)-G(@Liquid); 6000 N !
```

8.4.1 User-defined Molar Volume Database

The molar volume (V_m) is one of the pre-defined properties in Pandat. The molar volume of a pure component is described as a function of temperature and pressure, and the excess molar volume of a phase is usually described in the format similar to that used to describe the excess Gibbs energy of the phase. Note that, if a phase is described by a compound-energy-formalism (CEF) with multi-sublattices, the molar volume is automatically described as a function of T, P, and site fraction (y) following the format of the Gibbs energy. This will introduce many end members in the molar volume and may lead to incontinuity in the calculated molar volume. In reality, molar volume should be a function of mole fraction (x) instead of site fraction (y), it is thus recommended to define the molar volume of a phase separately from its Gibbs energy if the phase is described by the CEF model. This can be realized through the user-defined molar volume property.

In brief, the molar volume of element i with crystal structure φ can be expressed as:

$$V_i^{\varphi}(T) = V_0 \exp\left(\int_{T_0}^{T} 3\alpha dT\right) \tag{8.22}$$

where V_0 is the molar volume under atmospheric pressure at the reference temperature T_0. And α is the coefficient of linear thermal expansion (CLE). The volume of a phase with crystal structure φ can then be obtained via the Redlich-Kister polynomial:

$$V^{\varphi}(T) = \sum_i x_i V_i^{\varphi} + V_m^{ex} \tag{8.23}$$

where x_i is the mole fraction of element i and V_m^{ex} is the excess molar volume. Using ternary system as an example, the V_m^{ex} can be expressed by:

$$V_m^{ex} = \sum_{i=1}^{c-1} \sum_{j=i+1}^{c} x_i x_j \sum_k (x_i - x_j)^k L_{ij}^k + x_i x_j x_p L_{i,j,p} \tag{8.24}$$

The terms $L_{i,j}^k$ and $L_{i,j,k}$ are the interaction parameters from the constituent binary and the ternary systems, respectively. The standard unit of molar volume is m^3/mol.atom.

The molar volume database also enables us to calculate the density based on the relationship of $\rho = M/V_m$ (ρ is the mass density, M is the molar mass, and V_m is the molar volume).

Here we use the Al-Ni binary system as an example to demonstrate the calculation of molar volume through user-defined property. Please refer to the AlNi_Vm.tdb for details. In the beginning of the database file, a Type_Definition is given as below:

```
Type_Definition v GES AMEND_PHASE_DESCRIPTION * VARIABLE_X Vm !
```

In this definition, “v” is the identifier, “*” means any phase, and VARIABLE_X is the key word indicating X as the variable. The meaning of this definition is that any phase with the identifier “v” will use mole fractions (x) as the variables for V_m. Here are examples to define the molar volume parameters for the Fcc and L12_FCC phases in the Al-Ni system:

```
Phase Fcc %(v 1 1 !

Constituent Fcc: Al,Ni:!

      Parameter Vm(Fcc,Al;0)         298.15      +V_Al_fcc; 3000 N !

      Parameter Vm(Fcc,Ni;0)         298.15      +V_Ni_fcc; 3000 N !

      Parameter Vm(Fcc,Al,Ni;0)      298.15      -2.85e-6; 3000 N !


Phase L12_FCC %v 2 0.75 0.25 !

Constituent L12_FCC: Al,Ni:Al,Ni:!

      Parameter Vm(L12_FCC,Al;0)     298.15      +V_Al_fcc; 3000 N !

      Parameter Vm(L12_FCC,Ni;0)     298.15      +V_Ni_fcc; 3000 N !

      Parameter Vm(L12_FCC,Al,Ni;0)  298.15      -3.2e-6; 3000 N !
```

Even though the L12_FCC phase is modeled by CEF model with two sublattices, four end members, and 13 interaction parameters, its molar volume property can be described as a function of x_i like a solution phase through user-defined property. In other words, the molar volume of L12_Fcc is:

$$V_m^{L12} = x_{Al} \times V_{Al_{fcc}} + x_{Ni} \times V_{Ni_{fcc}} - 3.2 \times 10^{-6} x_{Al} x_{Ni} \qquad (8.25)$$

Figure 8.7 shows the calculated Al-Ni binary phase diagram with molar volume contour lines. Please refer to AlNi_Vm.pbfx and **section 3.3.5** for details on the calculation of contour diagrams.

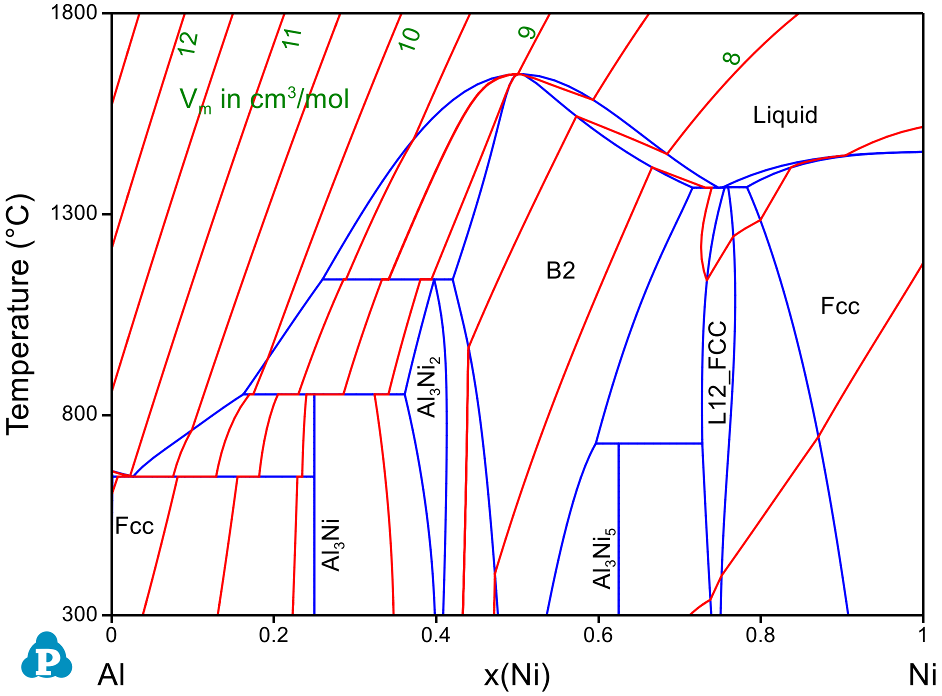


Figure 8.7 Al-Ni binary phase diagram with the calculated contour lines of molar volume (cm^3/mol).

The lattice constant, or lattice parameter, refers to the physical dimension of unit cells in a crystal lattice. For FCC crystal structure, the lattice constant can be calculated by:

$$a = \left(\frac{4}{6.02\times10^{23}} V_m\right)^{1/3} \tag{8.26}$$

An example is given for the calculation of lattice constant in Ni-Al binary at Ni-rich corner. The calculated lattice constant agrees with the experimental data well as is shown in Figure 8.8. Please refer to `AlNi_lattice.pbfx` for details. It should point out that the unit of Vm in the above equation is cm^3/mol.

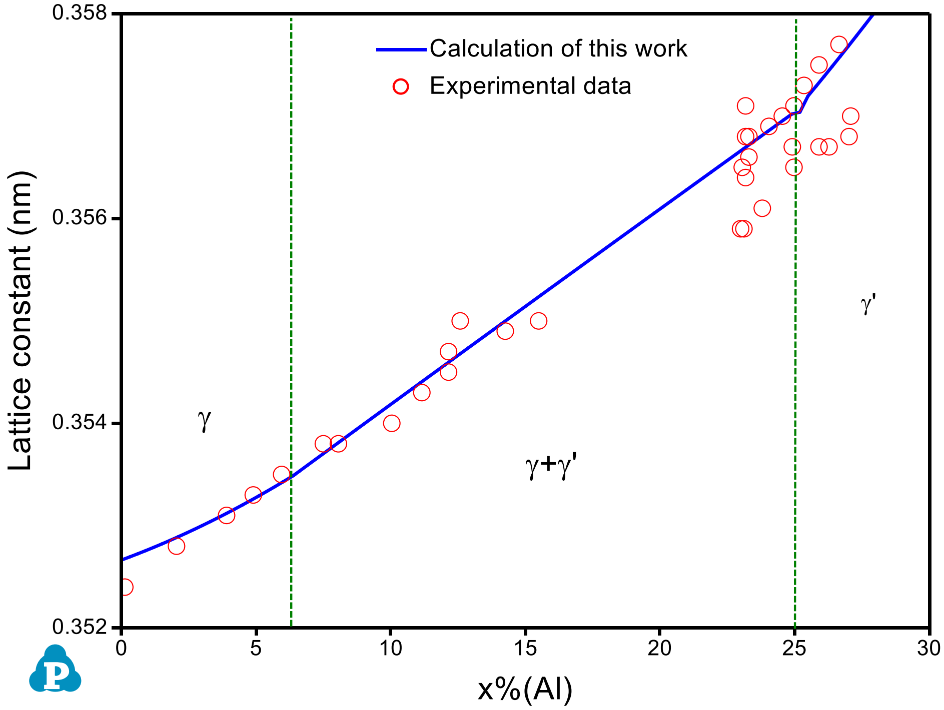


Figure 8.8 Comparison of calculated and measured lattice constants of the γ and γ’ phases in Ni-Al binary alloys at room temperature

8.4.2 Thermal Resistivity and Thermal Conductivity

Thermal conductivity of a pure element or a stoichiometric phase at temperature above 273 K is described as a function of temperature using the following equation:

$$\kappa = A + BT + CT^{-1} + DT^{2} \tag{8.27}$$

where κ is the thermal conductivity and T is the temperature in Kelvin. This function can reasonably fit most of the experimental thermal conductivity data of elements at temperature above 273 K.

The **thermal conductivity** of solid solution phase can be calculated from **thermal resistivity**, which is the reciprocal of thermal conductivity. According to the Nordheim rule, the thermal resistivity (ρ) of a solid solution phase can be described by the following Redich–Kister polynomials:

$$\rho_{AB}^{\alpha} = x_A\rho_A + x_B\rho_B + x_A x_B \sum_{i=0} L_i (x_A - x_B)^i \tag{8.28}$$

where ρ_{AB}^{α} is the thermal resistivity of the α solution phase in the A-B system. x_j and ρ_j are the mole fraction and thermal resistivity of pure elements j, respectively. L_i are the i^{th} order interaction parameters which are used to describe the effect of solute elements on the thermal resistivity. In general, the interaction parameter can be expressed as:

$$L_i = a_i + b_i T + c_i T^{-1} \tag{8.29}$$

where the parameters a_i, b_i and c_i are evaluated based on the experimental data.

The interface scattering parameters is introduced to describe the effect of the second phase on the thermal resistivity in two-phase region. The thermal resistivity of the two-phase region is described as following:

$$\rho_{\alpha+\beta} = f_\alpha\rho_\alpha + f_\beta\rho_\beta - f_\alpha f_\beta \sum_{i=0} M_i (f_\alpha - f_\beta)^i \tag{8.30}$$

where $\rho_{\alpha+\beta}$ is the thermal resistivity of the alloys in $\alpha+\beta$ two-phase region, f_p and ρ_p (p = α, β) are the mole fraction and thermal resistivity of the phase p, respectively. M_i, which can be considered to be linearly temperature dependent, is the i^{th} interface scattering parameter and and can be evaluated from the experimental data. The thermal conductivity of alloy system and the value of each phase can be obtained by using the reciprocal of the thermal resistivity values through output option.

In this example, thermal resistivity of the Al-Mg binary alloys is described using the user-defined property function.

As shown in the AlMg_ThCond.tdb, the thermal resistivity **ThRss** property is first defined as user-defined property since it hasn't been pre-defined in the current Pandat software.

```
Type_Definition z PHASE_PROPERTY ThRss 1 !
```

In accordance, the following definition is also needed to add this property to the original database.

```
Type_Definition e GES AMEND_PHASE_DESCRIPTION * VARIABLE_X ThRss !
```

As is seen, the thermal resistivity of the Fcc phase or the Hcp phase follows the same format as that of Gibbs energy for a disordered solution phase.

```
Parameter ThRss(Liquid,Al;0)  298.15     1/ThCond_Al_Liq; 3000 N !

Parameter ThRss(Liquid,Mg;0)  298.15     1/ThCond_Mg_Liq; 3000 N !

Parameter ThRss(Fcc,Al;0)     298.15     1/ThCond_Al_Fcc; 3000 N !

Parameter ThRss(Fcc,Mg;0)     298.15     1/ThCond_Mg_Hcp; 3000 N !

Parameter ThRss(Fcc,Al,Mg;0) 298.15    0.02566-1.3333e-05*T+14.5*T^(-1);

    3000 N !

Parameter ThRss(Hcp,Al;0)     298.15     1/ThCond_Al_Fcc; 3000 N !

Parameter ThRss(Hcp,Mg;0)     298.15     1/ThCond_Mg_Hcp; 3000 N !

Parameter ThRss(Hcp,Al,Mg;0) 298.15    0.02140-1.3669e-05*T+12.7158*T^(-1);

    3000 N !

Parameter ThRss(Hcp,Al,Mg;1) 298.15    0; 3000 N !

Parameter ThRss(Hcp,Al,Mg;2) 298.15    0.14825-7.7706e-05*T+25.3031*T^(-1);

    3000 N !
```

Thermal resistivity of the intermetallic phases with narrow solid solubility rage in the phase diagrams is treated like that of a stoichiometric compound phase, i.e., it is composition independent and is described as below:

```
Parameter ThRss(AlMg_Beta,*;0) 298.15   1/42; 6000 N !

Parameter ThRss(AlMg_Eps,*;0) 298.15   1/42; 6000 N !

Parameter ThRss(AlMg_Gamma,*;0) 298.15   -0.03267+2.7412e-05*T+20.722*T^(-1);
6000 N !
```

In order to describe the thermal resistivity within two-phase region, a system property, Sys_ThRss, is then defined by the command:

```
System_Property Sys_ThRss 1 !
Parameter L(Sys_ThRss, Fcc, AlMg_Beta;0)  298.15  0.005; 3000 N !
Parameter L(Sys_ThRss, Hcp, AlMg_Gamma;0)  298.15  0; 3000 N !
Parameter L(Sys_ThRss, Hcp, AlMg_Gamma;1)  298.15  0.01; 3000 N !
```

After the thermal resistivity has been properly modeled for each phase, the thermal conductivity of each phase and that of the system can be directly calculated and outputed by using extra output in Pandat defined as `1/ThRss(@*)` and `1/Sys_ThRss`, respectively. The comparisons between the calculated and measured thermal conductivities of the Al-Mg alloys are shown in Figure 8.9 to Figure 8.11. This example demonstrates that the user-defined property function is very powerful and flexible to allow users define various types of properties. The property can be a function of any phase properties that can be calculated by PanPhaseDiagram module.

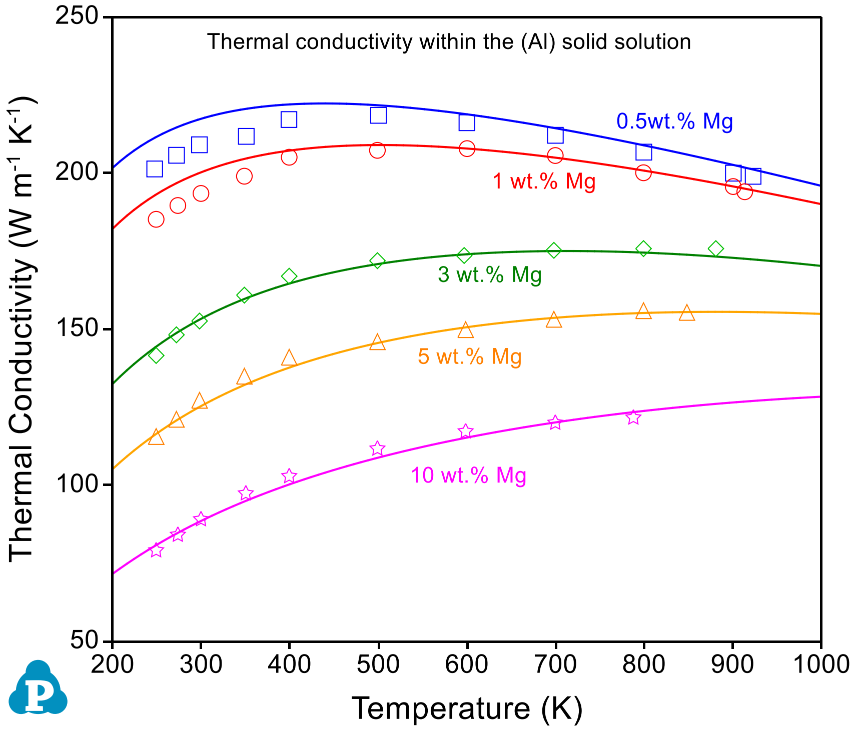


Figure 8.9 Comparison between the calculated and measured thermal conductivities in the (Al) solid solution in the Al-Mg binary system

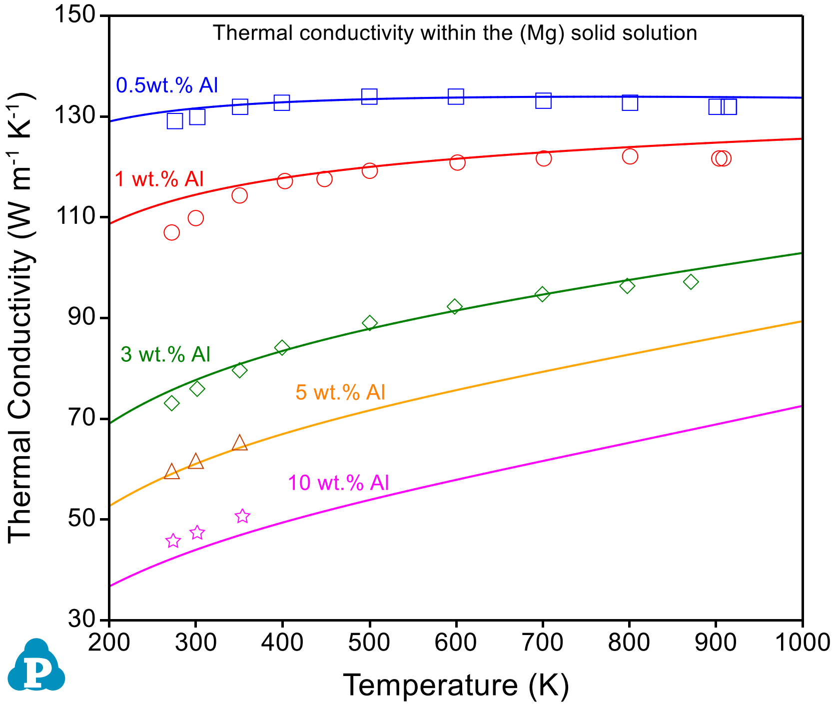


Figure 8.10 Comparison of the calculated and measured thermal conductivities in the (Mg) solid solution in the Al-Mg binary system

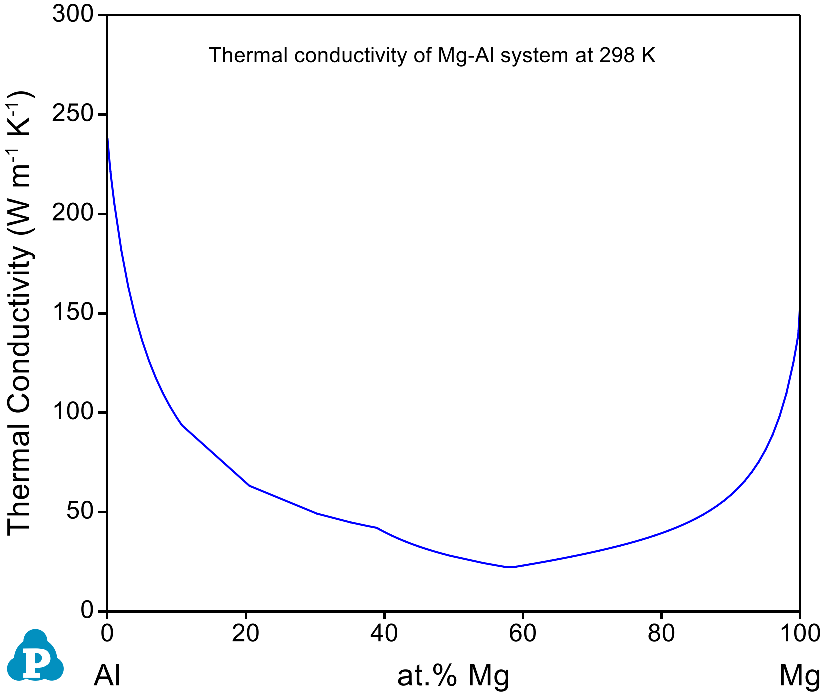


Figure 8.11 Calculated thermal conductivities of Mg-Al system at 298 K.

8.4.3 Calculation of T_0 Curve Using User-defined Property

T_0 curve is the trace of a series of points in a two-phase field at which the Gibbs energy of the two phases are identical. In this example, the original database is ABC.tdb, and the T_0-curve property is defined in the Appended database ABC_T0.tdb. In the ABC_T0.tdb file, the T_0-curves of Bcc/Liquid and Fcc/Liquid phases are defined as:

```
Property GFcc_GLiq 298.15 G(@Fcc)-G(@Liquid); 6000 N !

Property GBcc_GLiq 298.15 G(@Bcc)-G(@Liquid); 6000 N !
```

Where "Property" is the key word for user-defined property and `G(@Bcc)`, `G(@Fcc)`, `G(Liquid)` are the Gibbs free energies of the Bcc, Fcc, and Liquid phases, respectively. Note that, the Bcc, Fcc and Liquid are defined in the ABC.tdb. In this particular case, the above "Property" can be directly defined in the ABC.tdb, i.e., the ABC.tdb and ABC_T0.tdb can be combined into one database. This example demonstrates that user-defined property can be separated from the original database. This design makes it possible to obtain user-defined properties even the original database is in encrypted pdb format.

In this example, the **GBcc_GLiq** property is defined as the Gibbs free energy difference between the Bcc phase and the Liquid phase, and **GFcc_GLiq** property is defined as the Gibbs free energy difference between the Fcc phase and the Liquid phase.

Using the **Contour** function (Section 3.3.5), we can calculate contour maps of these user-defined properties and plot them on the calculated phase diagram. When we set the calculation condition as **GBcc_GLiq=0**, the T_0 curve for Bcc/Liquid is obtained as is shown by the green line in Figure 8.12. Similarly, by setting **GFcc_GLiq=0,** we obtain the T_0 curve for Fcc/Liquid as is shown by the red line in Figure 8.12.

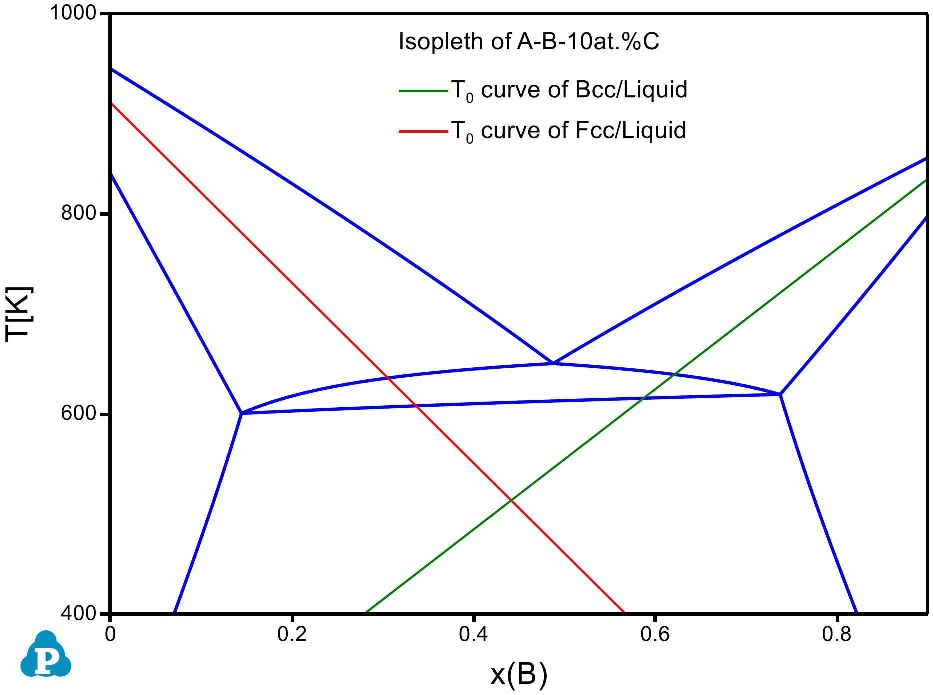


Figure 8.12 Calculated isopleth of A-B-10at.%C with T_0 curves of Bcc/Liquid and Fcc/Liquid phases

User can run the ABC_T0.pbfx batch file to obtain Figure 8.12. Two points should be addressed for this batch file:

- Both the "`start`" and "`stop`" values should set to be zero for the contour mapping as following to get the T_0 line.

```
<contour name="Contour_T0_Fcc_Liq" property="GFcc_GLiq" start ="0" stop ="0" step="1"/>

<contour name="Contour_T0_BCC_Liq" property="GBcc_GLiq" start ="0" stop ="0" step="1"/>
```

- To obtain the T_0 curve, each phase needs to be considered individually, thus the equilibrium type is set to be "`individual`"

```
<individual_phase value="true"/>

<equilibrium_type type="individual"/>
```

8.4.4 Calculation of Spinodal Curve Using User-defined Property

A Spinodal curve is where the determinant of the Hessian of Gibbs free energy with respect to composition is zero. For a phase with c-components, above condition is expressed as

$$\begin{vmatrix} \frac{\partial^2 G}{\partial x_2^2} & \cdots & \frac{\partial^2 G}{\partial x_2 \partial x_c} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 G}{\partial x_c \partial x_2} & \cdots & \frac{\partial^2 G}{\partial x_c^2} \end{vmatrix} = 0 \qquad (8.31)$$

where the molar fraction of component 1 is chosen as the dependent variable. The second derivative of G w.r.t. molar fractions can be calculated from the thermodynamic factors:

$$\frac{\partial^2 G}{\partial x_j \partial x_k} = \mathrm{ThF}(x_j, x_k) - \mathrm{ThF}(x_1, x_k) - \mathrm{ThF}(x_j, x_1) + \mathrm{ThF}(x_1, x_1) \quad (j,k=2,3,\ldots,c) \; (8.32)$$

Example #1: Spinodal curve of Fcc phase in the Al-Zn binary system

In this example, the spinodal curve of the Fcc phase in the Al-Zn binary system is calculated through user-defined property. A user-defined property `d2GdxZn2` for the Fcc phase is defined in `AlZn_Spinodal.tdb` as:

```
Property d2GdxZn2 298.15 ThF(Zn,Zn@Fcc)-ThF(Al,Zn@Fcc)-ThF(Zn,Al@Fcc)+
ThF(Al,Al@Fcc); 6000 N !
```

where `ThF(Zn,Zn@Fcc)`, `ThF(Al,Zn@Fcc)`, `ThF(Zn,Al@Fcc)`, and `ThF(Al,Al@Fcc)` are the thermodynamic factors of Fcc phase. Since the value of `d2GdxZn2` is usually a large number, we define the Hessian function, HSN, as `d2GdxZn2` multiplied by a factor 1e-4:

```
Property HSN 298.15 1e-4*d2GdxZn2; 6000 N !
```

As shown in the `AlZn_Spinodal.pbfx`, the `AlZn_Spinodal.tdb` is appended to the `AlMgZn.tdb`. The spinodal line is calculated through contour mapping by using following conditions:

```
<contour name="Spinodal" property="HSN" start="0" stop="0" step="1"/>
```

```
<equilibrium_type type="individual"/>
```

The calculated Fcc Spinodal is shown in Figure 8.13 with the stable Al-Zn binary phase diagram.

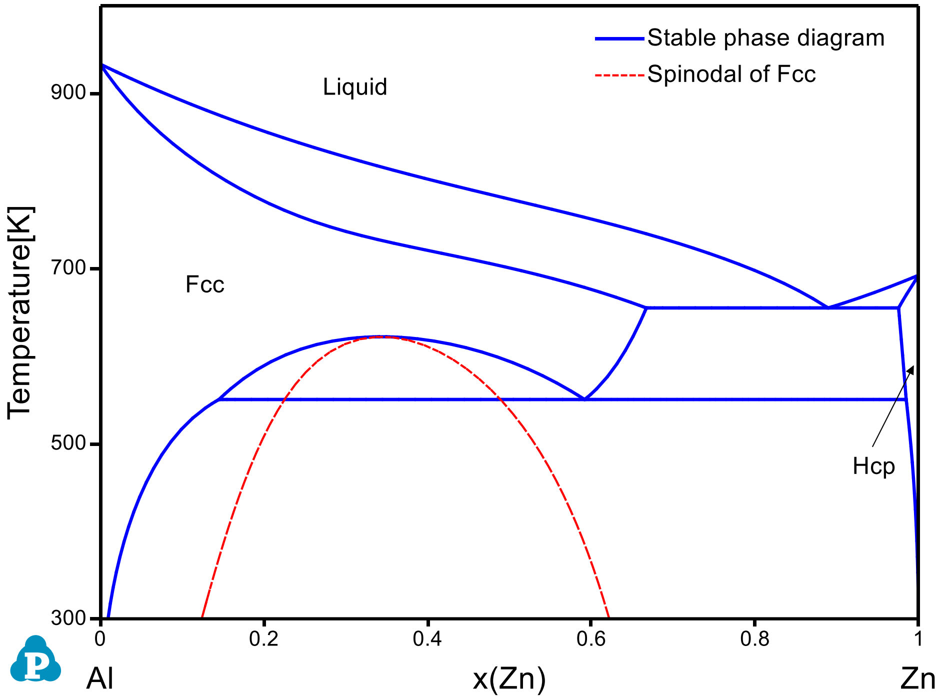


Figure 8.13 Calculated spinodal curve of the Fcc phase within the Al-Zn binary system

Example #2: Spinodal curve of Fcc phase in the X-Y-Z ternary system

In this example, the original database is XYZ.tdb, and the user-defined `HSN` property is defined in `XYZ_Spinodal.tdb` as described below:

```
Property d2Gdx2 298.15 ThF(Y,Y@Fcc)-ThF(X,Y@Fcc)-ThF(Y,X@Fcc)+ThF(X,X@Fcc);
6000 N !

Property d2Gdy2 298.15 ThF(Z,Z@Fcc)-ThF(X,Z@Fcc)-ThF(Z,X@Fcc)+ThF(X,X@Fcc);
6000 N !

Property d2Gdxy 298.15 ThF(Y,Z@Fcc)-ThF(X,Z@Fcc)-ThF(Y,X@Fcc)+ThF(X,X@Fcc);
6000 N !

Property HSN 298.15 1e-10*(d2Gdx2 * d2Gdy2 - d2Gdxy * d2Gdxy); 6000 N !
```

Note that the `HSN` property within the XYZ ternary system is derived and described as a function of the thermodynamic factor `ThF`. A factor of 1e-10 is used to scale the `HSN` property since the numerical value of HSN is very big.

Again the spinodal lines are calculated through contour mapping. Details can be found in `XYZ_Isotherm_Spinodal.pbfx` and `XYZ_Isopleth_Spinodal.pbfx`. Figure 8.14 and Figure 8.15 show the calculated spinodal curves superimposed on the stable phase diagrams:

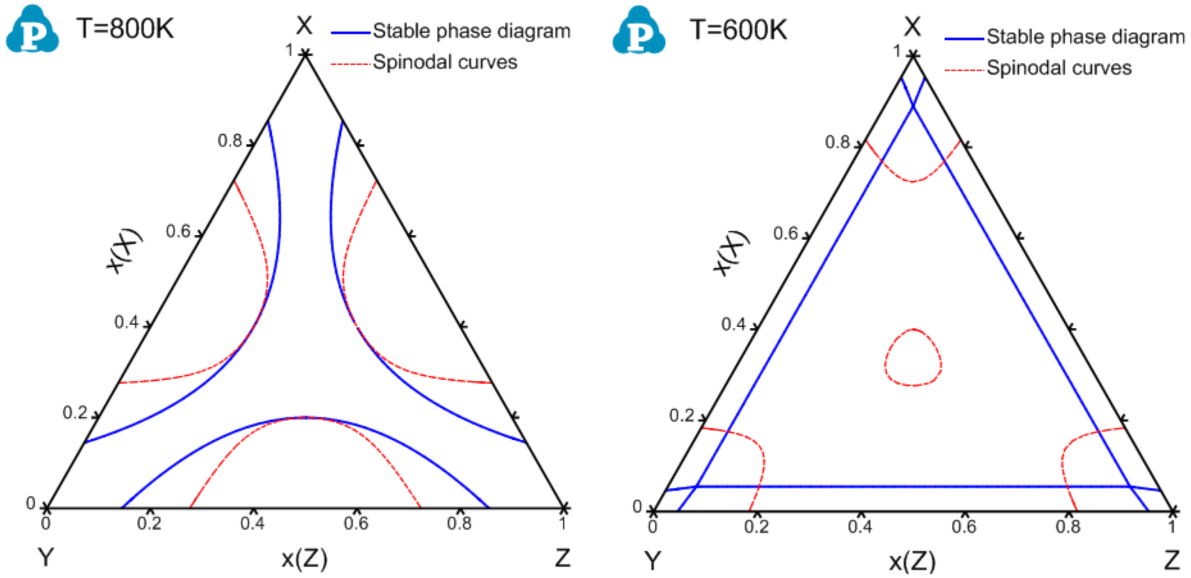


Figure 8.14 Calculated isothermal sections of the X-Y-Z system at 800 and 600K with spinodal curves, respectively

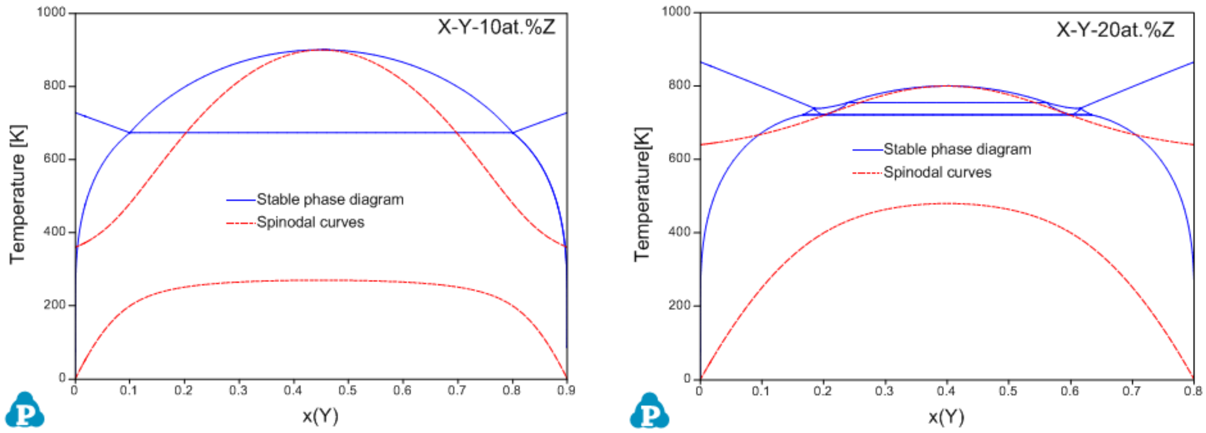


Figure 8.15 Calculated isopleths within the X-Y-Z system for 10 and 20 at.%Z with spinodal curves, respectively

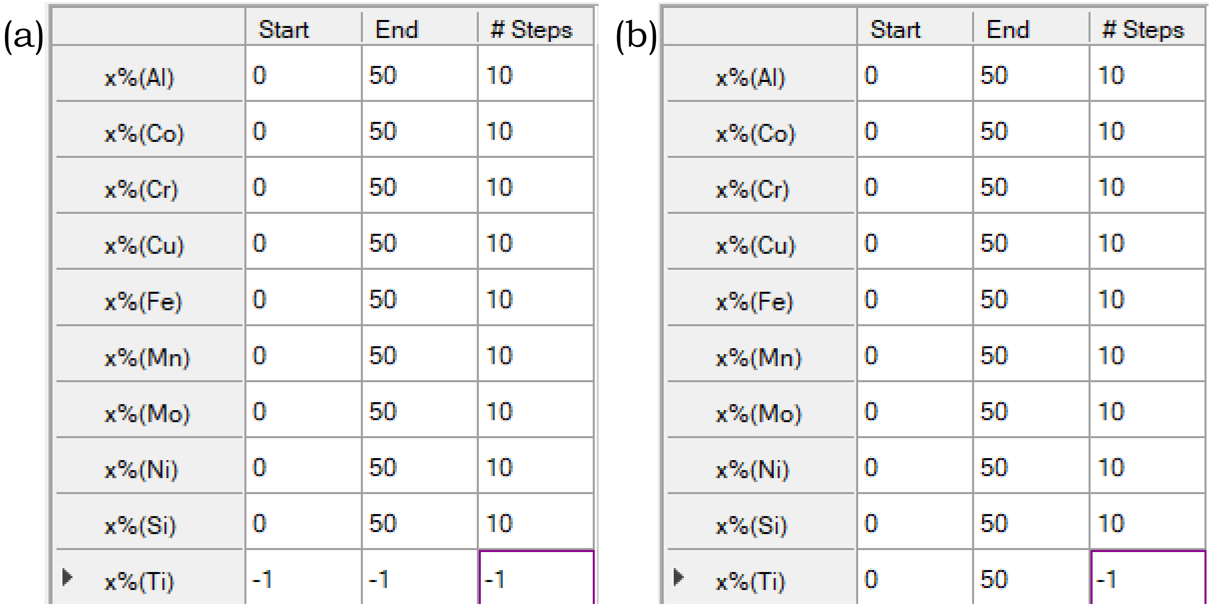
9 High-Throughput-Calculation

The High-Throughput-Calculation (HTC) function has been implemented in Pandat™ for the PanPhaseDiagram, PanPrecipitation, and PanSolidification modules. It can perform thousands of calculations in a user defined compositional space by a simple setting. Alloy compositions that satisfy user defined criteria can then be identified through mining the thousands of simulated results. This function allows user to develop alloys with certain properties through design. There are two methods to define alloy compositions for HTC: one is to setup the composition range of each component and its steps through user-interface; the other one is to load the user-defined composition data file. These two methods will be explained in detail in this section. Note that, the current HTC function can carry out 0D-point calculation and solidification simulation using both the Scheil and Lever-rule models in the PanPhaseDiagram module. In the PanPrecipitation module, HTC can be carried out for all defined/imported alloys under one or multiple heat-treatment conditions. The HTC function is also available in the newly developed PanSolidification module for alloys under different cooling rates. The tutorial of the HTC function in different modules will be given in this section as well. Other types of simulations will be continuously developed in the future.

9.1 Alloy Composition Setup

9.1.1 Setting Composition Range and Steps

The composition setup dialog for the HTC function in different modules is the same. As shown in Figure 9.1, the composition range of each component can be defined by using the **Start** and **End** values. The **#steps** define the composition increment from the **Start** value. Note that the **End** value will always be selected even it may not be the same as the last value calculated by the defined composition increment. In this example, the composition of Ti is set as the balance by right-click the row of Ti (a) or typing in the Ti composition rang and “-1” for steps (b).



(a)

	Start	End	# Steps
x%(Al)	0	50	10
x%(Co)	0	50	10
x%(Cr)	0	50	10
x%(Cu)	0	50	10
x%(Fe)	0	50	10
x%(Mn)	0	50	10
x%(Mo)	0	50	10
x%(Ni)	0	50	10
x%(Si)	0	50	10
▶ x%(Ti)	-1	-1	-1

(b)

	Start	End	# Steps
x%(Al)	0	50	10
x%(Co)	0	50	10
x%(Cr)	0	50	10
x%(Cu)	0	50	10
x%(Fe)	0	50	10
x%(Mn)	0	50	10
x%(Mo)	0	50	10
x%(Ni)	0	50	10
x%(Si)	0	50	10
▶ x%(Ti)	0	50	-1

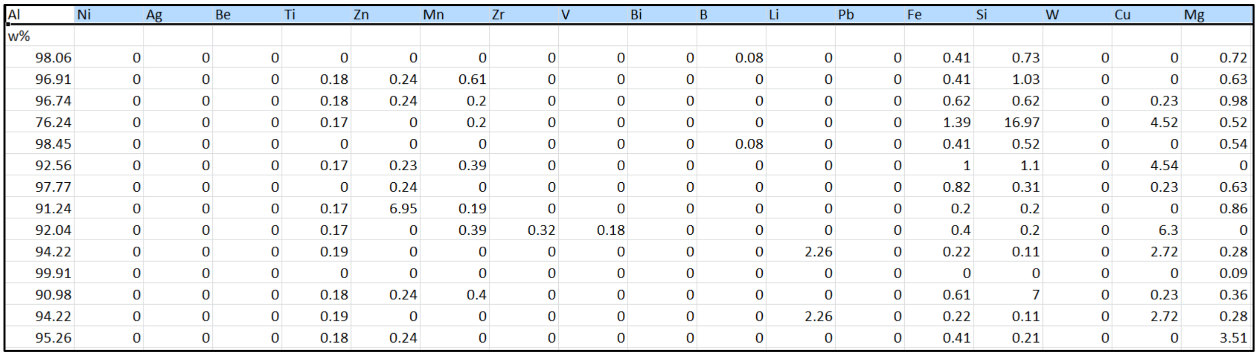
Figure 9.1 HTC composition setup dialog

9.1.2 Import Alloy Compositions

Pandat also allows user to import alloy compositions for HTC through a data file. This is a more flexible and efficient way to perform HTC for a group of multi-component alloys which may contain different alloying elements. The format of a data file (.txt or .dat) is simple. Figure 9.2 shows an example which contains a group of Al-rich alloys. The first row shows all alloying elements involved in these alloys. The first column of the second row defines the unit of the alloy composition. Then alloy compositions are given from the third row forward. There are a few points to emphasize here:

1. The element in the first column is automatically treated as “balance” element, such as Al in this example. No matter what values are given in the first column, those values will be recalculated after the compositions of all other components are read in.
2. The first row lists all the elements used in the alloys. The compositions of some of them can be zero in a certain alloy.

3. If an alloying element is not available in the database used to perform HTC, this element will be kicked out in the calculation and its composition will be automatically added to that of the “balance” element.



Al	Ni	Ag	Be	Ti	Zn	Mn	Zr	V	Bi	B	Li	Pb	Fe	Si	W	Cu	Mg
w%																	
98.06	0	0	0	0	0	0	0	0	0	0.08	0	0	0.41	0.73	0	0	0.72
96.91	0	0	0	0.18	0.24	0.61	0	0	0	0	0	0	0.41	1.03	0	0	0.63
96.74	0	0	0	0.18	0.24	0.2	0	0	0	0	0	0	0.62	0.62	0	0.23	0.98
76.24	0	0	0	0.17	0	0.2	0	0	0	0	0	0	1.39	16.97	0	4.52	0.52
98.45	0	0	0	0	0	0	0	0	0	0.08	0	0	0.41	0.52	0	0	0.54
92.56	0	0	0	0.17	0.23	0.39	0	0	0	0	0	0	1	1.1	0	4.54	0
97.77	0	0	0	0	0.24	0	0	0	0	0	0	0	0.82	0.31	0	0.23	0.63
91.24	0	0	0	0.17	6.95	0.19	0	0	0	0	0	0	0.2	0.2	0	0	0.86
92.04	0	0	0	0.17	0	0.39	0.32	0.18	0	0	0	0	0.4	0.2	0	6.3	0
94.22	0	0	0	0.19	0	0	0	0	0	0	2.26	0	0.22	0.11	0	2.72	0.28
99.91	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.09
90.98	0	0	0	0.18	0.24	0.4	0	0	0	0	0	0	0.61	7	0	0.23	0.36
94.22	0	0	0	0.19	0	0	0	0	0	0	2.26	0	0.22	0.11	0	2.72	0.28
95.26	0	0	0	0.18	0.24	0	0	0	0	0	0	0	0.41	0.21	0	0	3.51

Figure 9.2 Example of composition file for multi-component Al-rich alloys

9.2 HTC Tutorial in PanPhaseDiagram

In this example, we will demonstrate how to calculate liquidus, solidus, and solidification ranges for a number of Al-Mg-Zn alloys via the HTC function by setting composition range and steps.

1. Load proper database and choose the Al-Mg-Zn system.
2. Choose the HTC function from the **Batch Calc → High Throughput Calculation (HTC)** (as shown in Figure 9.3).

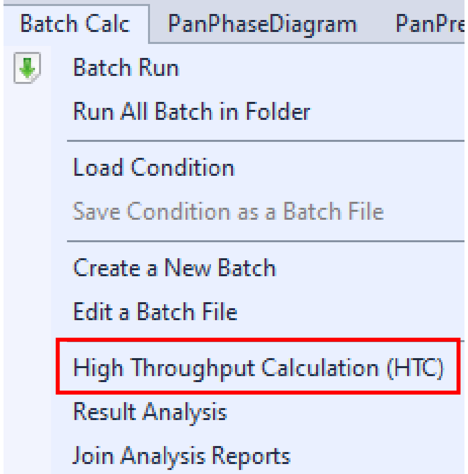
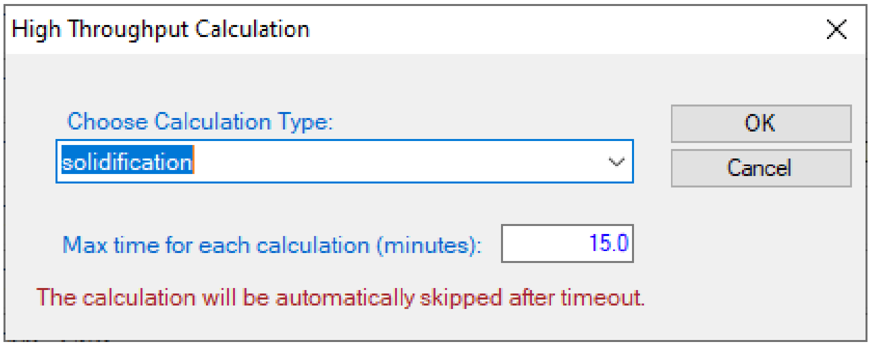


Figure 9.3 HTC function under the “Batch Calc” menu

3. Choose the calculation type from the drop-down list of HTC pop-up window and select “*Solidification*”.



Choose Calculation Type: solidification

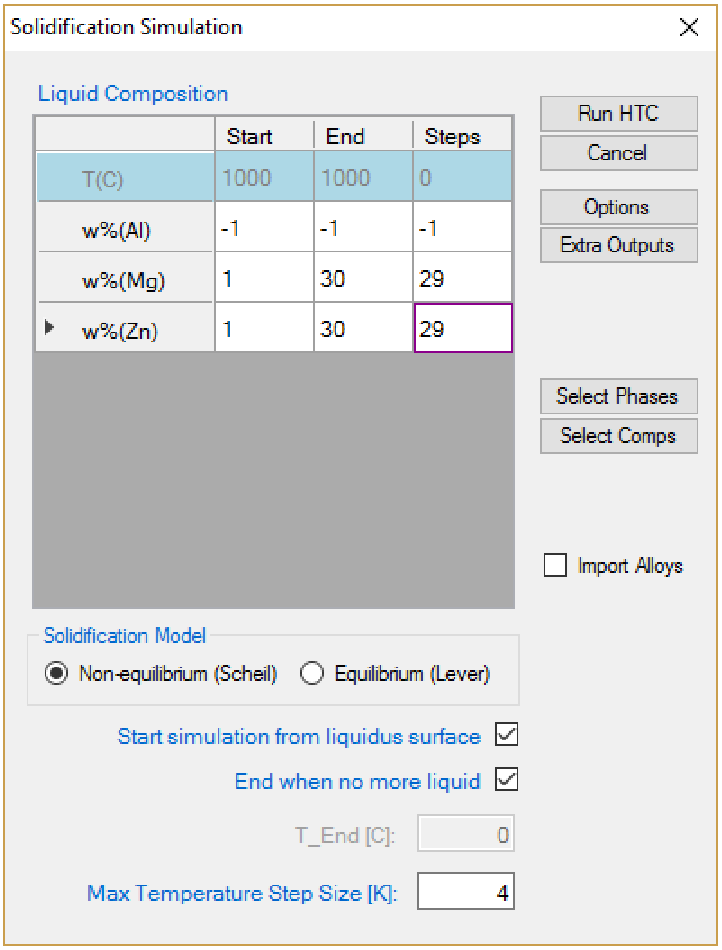
Max time for each calculation (minutes): 15.0

The calculation will be automatically skipped after timeout.

Figure 9.4 Dialog to choose calculation type of HTC

4. Define the compositional space for HTC simulation.

After step 3, a window pops out as shown in Figure 9.5. In this setting, the compositions of both Mg and Zn vary from 1 to 30 wt.% in a double composition loops. The "Steps" is set to 29, which means the composition increases by 1 wt% at each step. The total number of calculations is 30×30=900 in this setting. The composition of Al is set as balance by typing "-1" for steps or right-click the row of Al. No "**Start**" or "**End**" values are required for the balance component, which is Al in this case. After setup the compositional space for HTC and choose the proper solidification model, user can click "**Run HTC**" button to perform HTC simulations, which is 900 calculations in this case.



Liquid Composition

	Start	End	Steps
T(C)	1000	1000	0
w%(Al)	-1	-1	-1
w%(Mg)	1	30	29
w%(Zn)	1	30	29

☐ Import Alloys

Solidification Model

● Non-equilibrium (Scheil) ○ Equilibrium (Lever)

Start simulation from liquidus surface ☑

End when no more liquid ☑

T_End [C]: 0

Max Temperature Step Size [K]: 4

Figure 9.5 Dialog to setup compositional space for HTC

5. Save the current workspace after all calculations are finished. It is suggested that user saves the current workspace immediately after the

HTC calculation. This allows all the calculated results saved in the workspace for future use.

6. Choose "**Result Analysis**" from the "**Batch Calc**" menu. User can use this commend to analyze the calculated results for a group of alloys and choose a certain property from each calculation for comparison.

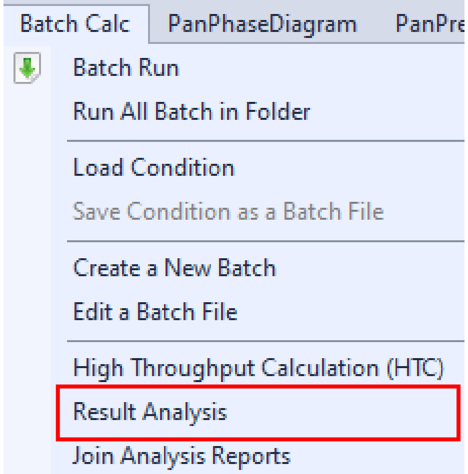
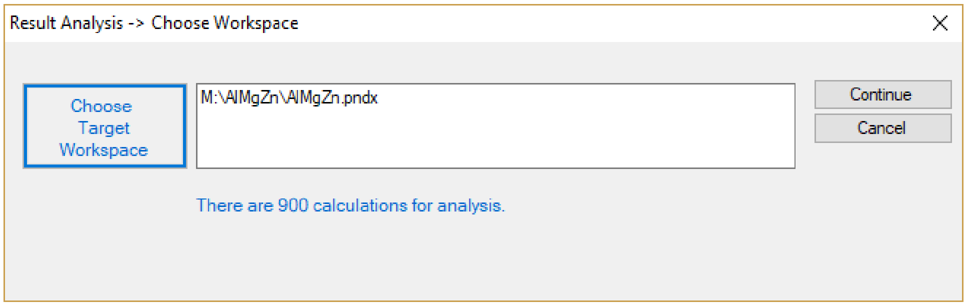


Figure 9.6 "Result Analysis" function under the "Batch Calc" menu

7. Open the workspace saved previously for "**Result Analysis**". User can perform several HTC calculations and save all the workspaces. User can then analyze the results of the selected HTC calculation by opening the corresponding workspace as shown in Figure 9.7.

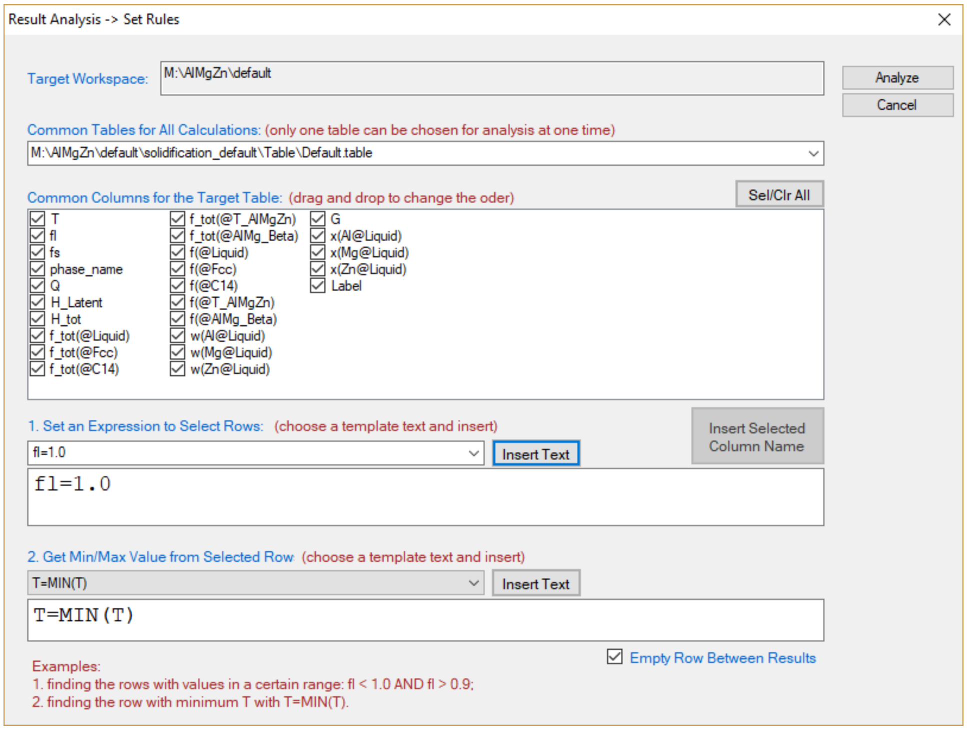


M:\AlMgZn\AlMgZn.pndx

There are 900 calculations for analysis.

Figure 9.7 "Result Analysis" popup dialog to choose target workspace

8. Define the criteria of the properties as filters for result analysis.



Target Workspace: M:\AlMgZn\default

Common Tables for All Calculations: (only one table can be chosen for analysis at one time)
M:\AlMgZn\default\solidification_default\Table\Default.table

Common Columns for the Target Table: (drag and drop to change the oder)

- ☑ T
- ☑ fl
- ☑ fs
- ☑ phase_name
- ☑ Q
- ☑ H_Latent
- ☑ H_tot
- ☑ f_tot(@Liquid)
- ☑ f_tot(@Fcc)
- ☑ f_tot(@C14)
- ☑ f_tot(@T_AlMgZn)
- ☑ f_tot(@AlMg_Beta)
- ☑ f(@Liquid)
- ☑ f(@Fcc)
- ☑ f(@C14)
- ☑ f(@T_AlMgZn)
- ☑ f(@AlMg_Beta)
- ☑ w(Al@Liquid)
- ☑ w(Mg@Liquid)
- ☑ w(Zn@Liquid)
- ☑ G
- ☑ x(Al@Liquid)
- ☑ x(Mg@Liquid)
- ☑ x(Zn@Liquid)
- ☑ Label

1. Set an Expression to Select Rows: (choose a template text and insert)
fl=1.0
```
fl=1.0
```

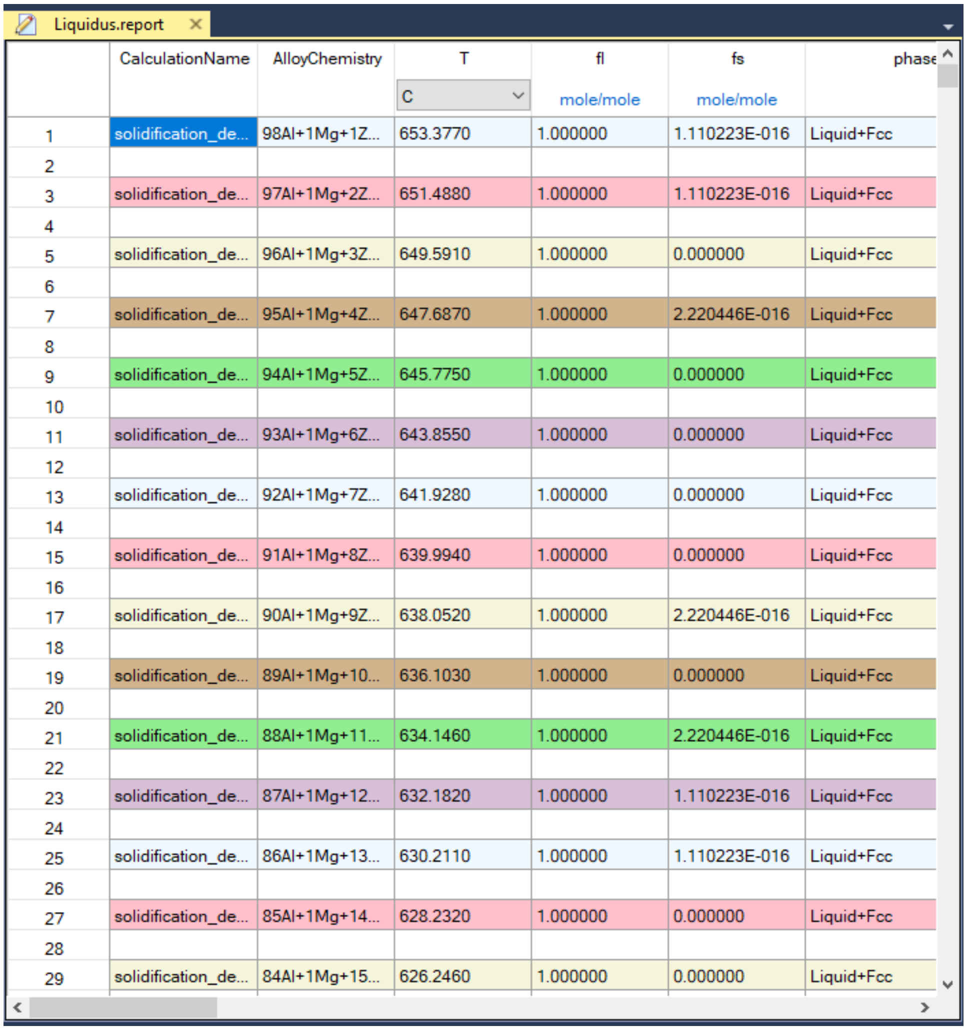
2. Get Min/Max Value from Selected Row (choose a template text and insert)
T=MIN(T)
```
T=MIN(T)
```

☑ Empty Row Between Results

Examples:
1. finding the rows with values in a certain range: fl < 1.0 AND fl > 0.9;
2. finding the row with minimum T with T=MIN(T).

Figure 9.8 “Result Analysis” popup dialog to define the criteria of the properties

In Figure 9.8, the “Target Workspace” shows the workspace selected by the user for results analysis. It should point out that there can be more than one table in each calculation, the “Common Tables for All Calculations” allows user to choose the table for analysis. In the “Common Columns for the Target Table” window, names for all the output properties available in the selected table are listed. User can choose the properties to be listed in the “Analysis Report”. As shown in Figure 9.9, temperature and the alloy composition will be listed in the “Analysis Report” in this case. Since the purpose of HTC is to compare a special target property for the several hundred/thousands of calculations, the “Set an Expression to Select Rows” at the bottom of the window allows user define the criteria. In Figure 9.9, this criterion is $f_L=1$, i.e. the fraction of liquid is 1. With this filter, only the row satisfies this criterion will be listed in the “Analysis Report”. It should point out that several criteria can be set in the “Set an Expression to Select Rows”. Click “Analyze” to create the “Analysis Report” as shown in Figure 9.9. In this table, each row lists the liquidus temperature for the corresponding alloy composition. The liquidus temperatures for 900 alloys are listed in the same report which allows a quick comparison of liquidus temperature for different alloy composition. User can also plot 3D colormap and surface diagrams using the data in this report as shown in Figure 9.10.



	CalculationName	AlloyChemistry	T	fl	fs	phase
			C	mole/mole	mole/mole	
1	solidification_de...	98Al+1Mg+1Z...	653.3770	1.000000	1.110223E-016	Liquid+Fcc
2						
3	solidification_de...	97Al+1Mg+2Z...	651.4880	1.000000	1.110223E-016	Liquid+Fcc
4						
5	solidification_de...	96Al+1Mg+3Z...	649.5910	1.000000	0.000000	Liquid+Fcc
6						
7	solidification_de...	95Al+1Mg+4Z...	647.6870	1.000000	2.220446E-016	Liquid+Fcc
8						
9	solidification_de...	94Al+1Mg+5Z...	645.7750	1.000000	0.000000	Liquid+Fcc
10						
11	solidification_de...	93Al+1Mg+6Z...	643.8550	1.000000	0.000000	Liquid+Fcc
12						
13	solidification_de...	92Al+1Mg+7Z...	641.9280	1.000000	0.000000	Liquid+Fcc
14						
15	solidification_de...	91Al+1Mg+8Z...	639.9940	1.000000	0.000000	Liquid+Fcc
16						
17	solidification_de...	90Al+1Mg+9Z...	638.0520	1.000000	2.220446E-016	Liquid+Fcc
18						
19	solidification_de...	89Al+1Mg+10...	636.1030	1.000000	0.000000	Liquid+Fcc
20						
21	solidification_de...	88Al+1Mg+11...	634.1460	1.000000	2.220446E-016	Liquid+Fcc
22						
23	solidification_de...	87Al+1Mg+12...	632.1820	1.000000	1.110223E-016	Liquid+Fcc
24						
25	solidification_de...	86Al+1Mg+13...	630.2110	1.000000	1.110223E-016	Liquid+Fcc
26						
27	solidification_de...	85Al+1Mg+14...	628.2320	1.000000	0.000000	Liquid+Fcc
28						
29	solidification_de...	84Al+1Mg+15...	626.2460	1.000000	0.000000	Liquid+Fcc

Figure 9.9 Analysis report file of liquidus temperature T_L

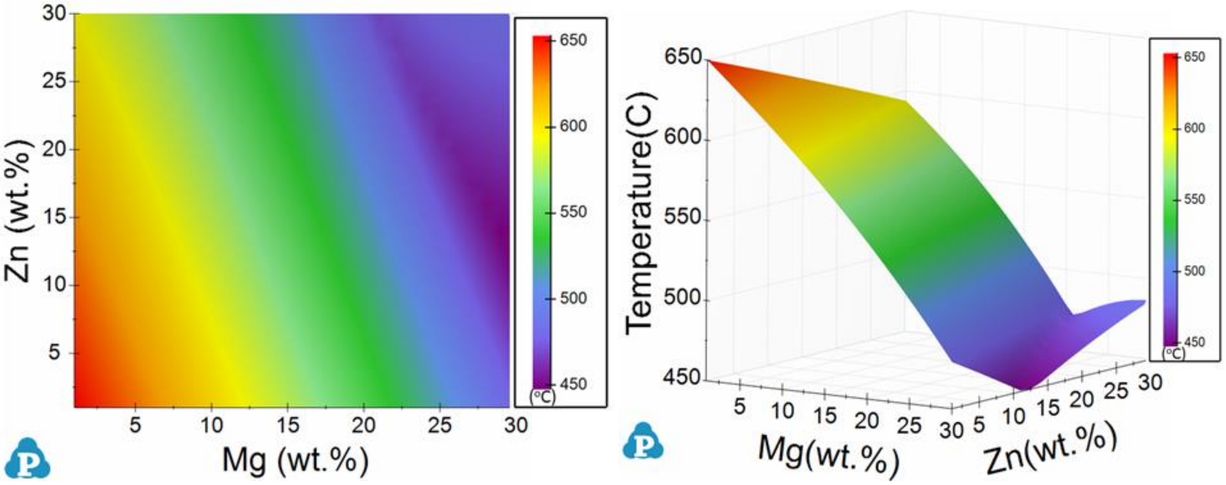
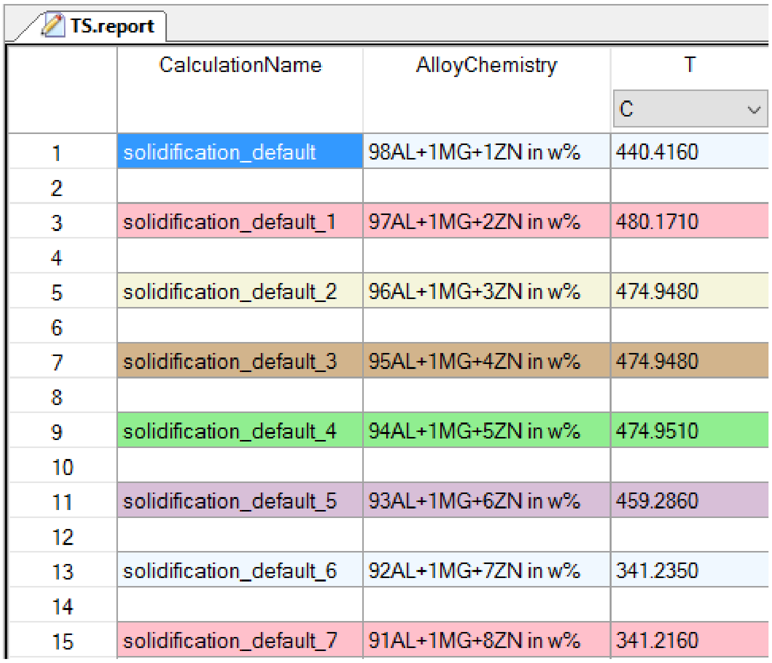


Figure 9.10 3D diagrams of the liquidus temperatures: colormap (left) and 3D surface (right)

9. Save the obtained T_L report file via “**File → Save Current File As**”.
10. Now repeat the steps of 1-8 to obtain the T_S report file and save it.



	CalculationName	AlloyChemistry	T
			C
1	solidification_default	98AL+1MG+1ZN in w%	440.4160
2			
3	solidification_default_1	97AL+1MG+2ZN in w%	480.1710
4			
5	solidification_default_2	96AL+1MG+3ZN in w%	474.9480
6			
7	solidification_default_3	95AL+1MG+4ZN in w%	474.9480
8			
9	solidification_default_4	94AL+1MG+5ZN in w%	474.9510
10			
11	solidification_default_5	93AL+1MG+6ZN in w%	459.2860
12			
13	solidification_default_6	92AL+1MG+7ZN in w%	341.2350
14			
15	solidification_default_7	91AL+1MG+8ZN in w%	341.2160

Figure 9.11 Analysis report file of solidus temperature T_S

11. Combine the two analysis reports. Note that user can also easily export the obtained report file to excel (**Table → Export to Excel**) for further editing and then import the modified file back to Pandat™ to create plot. For example, we can export the T_L and T_S reports to excel files and then

combine them to obtain the solidification range ($\Delta T = T_L - T_S$). By importing the modified table data, one can plot the contour mapping of the solidification range as shown in Figure 9.12.

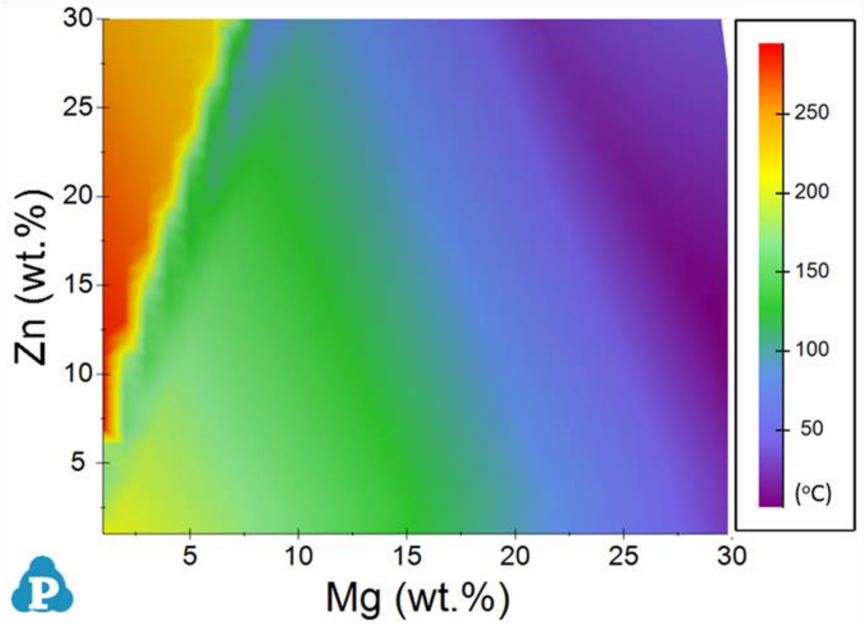
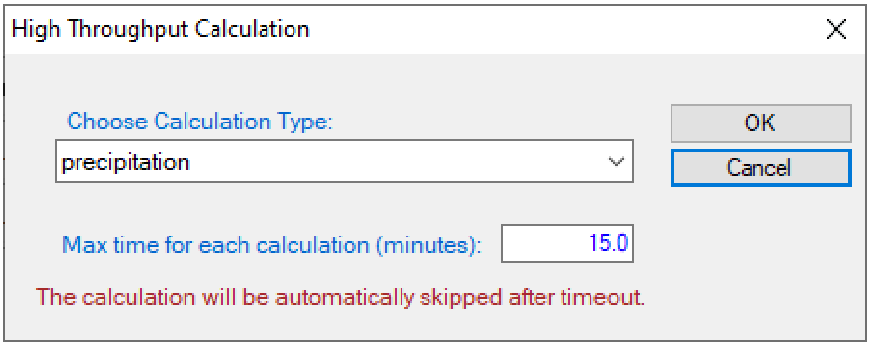


Figure 9.12 The color map of solidification range for Al-rich alloys using the Scheil model

9.3 HTC Tutorial in PanPrecipitation

In this example, we will demonstrate how to find the peak yield strength of the AA6005 alloy with varying both composition and heat-treatment temperature.

1. Load proper thermodynamic + mobility database and select Al, Mg, Si three components.
2. Load proper kinetic-parameter database to select the matrix phase and precipitates.
3. Choose the HTC function from the **Batch Calc → High Throughput Calculation (HTC)**.
4. Choose the calculation type from the drop-down list of HTC pop-up window and select "*Precipitation*".



Choose Calculation Type: precipitation

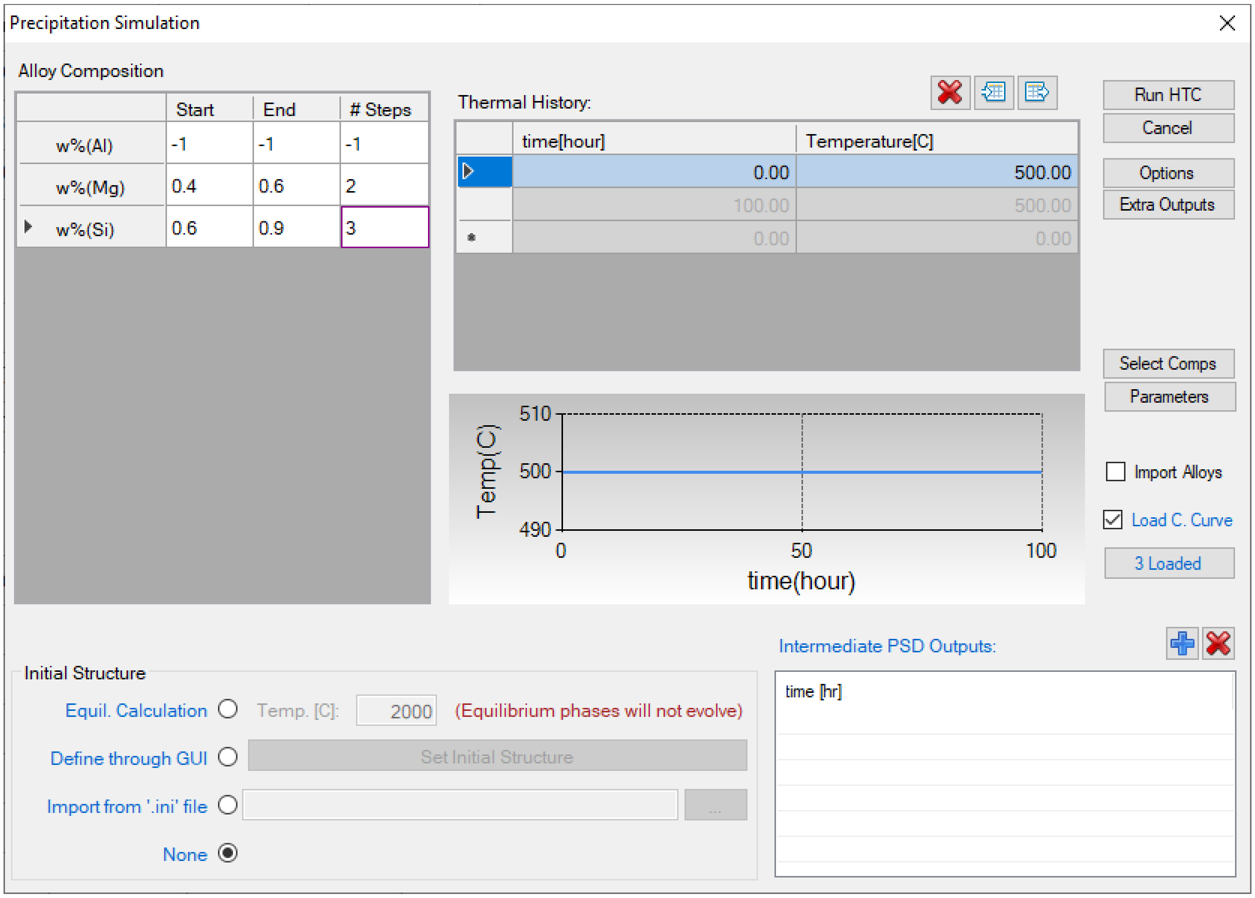
Max time for each calculation (minutes): 15.0

The calculation will be automatically skipped after timeout.

Figure 9.13 Dialog to choose calculation type of HTC

5. Define the compositional space for HTC simulation. As shown in Figure 9.14, the compositions of Mg and Si varying within the ranges of 0.4-0.6, and 0.6-0.9 (wt.%), respectively.
6. Define the thermal history for HTC simulation. User can define/import one thermal history by using the "**Thermal History**" dialog in Figure 9.14 or select the "**Load C. Curve**" and click the "**Import CC**" button to browse and load the predefined cooling curves (.txt or .dat). The example format of cooling curve file can be found in Figure 9.21 in section 9.x.x. In this example cooling curves, isothermal aging for 20 hours at three temperatures 190, 182, and 170°C are defined individually.

7. In addition to use the default output, user can also customize the outputs using the "**Extra Outputs**" function. In this example, the extra output with time, T - temperature, w(*) - alloy composition, and sigma_y (yield strength) is generated.
8. After setup the compositional space for HTC and define/import the proper thermal history, user can click "**Run HTC**" button to perform HTC simulations.



Alloy Composition

	Start	End	# Steps
w%(Al)	-1	-1	-1
w%(Mg)	0.4	0.6	2
w%(Si)	0.6	0.9	3

Thermal History:

	time[hour]	Temperature[C]
▷	0.00	500.00
	100.00	500.00
*	0.00	0.00

☐ Import Alloys

☑ Load C. Curve

3 Loaded

Initial Structure

Equil. Calculation ○ Temp. [C]: 2000 (Equilibrium phases will not evolve)

Define through GUI ○ Set Initial Structure

Import from '.ini' file ○

None ●

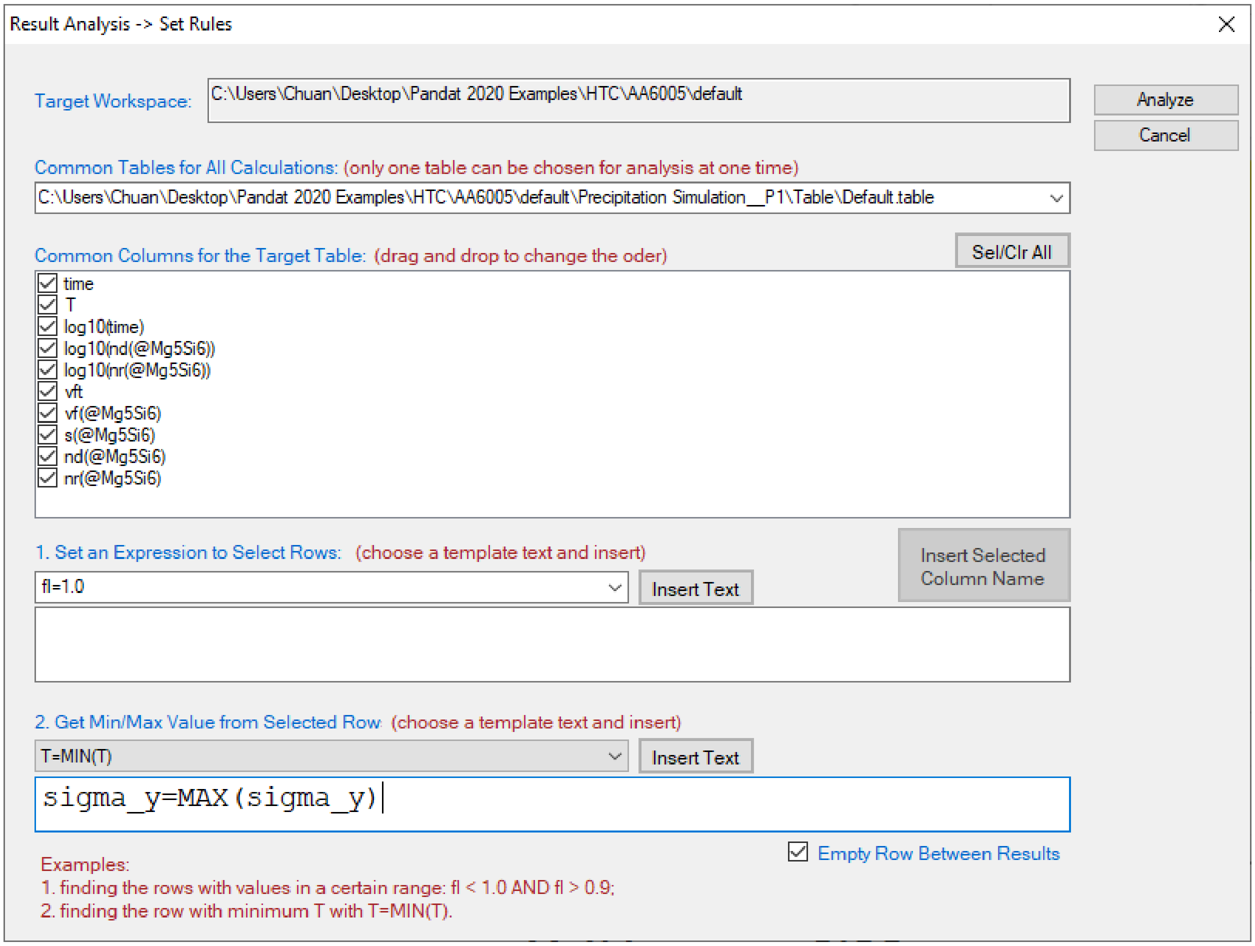
Intermediate PSD Outputs:

time [hr]

Figure 9.14 Dialog to setup compositional space and thermal history for precipitation HTC

9. Save the current workspace after all calculations are finished and run "**Result Analysis**" from the "**Batch Calc**" menu. User can use this commend to analyze the calculated results for a group of alloys and pick a certain property from each calculation for comparison. As shown in the following Figure 9.15, the following rule is used to obtain the maximum

yield strength of each alloy under thee different heat treatment conditions.



Result Analysis -> Set Rules

Target Workspace: C:\Users\Chuan\Desktop\Pandat 2020 Examples\HTC\AA6005\default

Common Tables for All Calculations: (only one table can be chosen for analysis at one time)
C:\Users\Chuan\Desktop\Pandat 2020 Examples\HTC\AA6005\default\Precipitation Simulation__P1\Table\Default.table

Common Columns for the Target Table: (drag and drop to change the oder)
- ☑ time
- ☑ T
- ☑ log10(time)
- ☑ log10(nd(@Mg5Si6))
- ☑ log10(nr(@Mg5Si6))
- ☑ vft
- ☑ vf(@Mg5Si6)
- ☑ s(@Mg5Si6)
- ☑ nd(@Mg5Si6)
- ☑ nr(@Mg5Si6)

1. Set an Expression to Select Rows: (choose a template text and insert)
fl=1.0

2. Get Min/Max Value from Selected Row (choose a template text and insert)
T=MIN(T)

sigma_y=MAX(sigma_y)

☑ Empty Row Between Results

Examples:
1. finding the rows with values in a certain range: fl < 1.0 AND fl > 0.9;
2. finding the row with minimum T with T=MIN(T).

Figure 9.15 Criteria for precipitation results analysis

Figure 9.16 shows the obtained peak yield strength distribution within the defined composition space considering all three heat treatment conditions. User can run “**Result Analysis**” on this save workspace and dig out more information using other rules. For example, user can plot peak yield strength distribution in the composition space for one particular heat treatment condition.

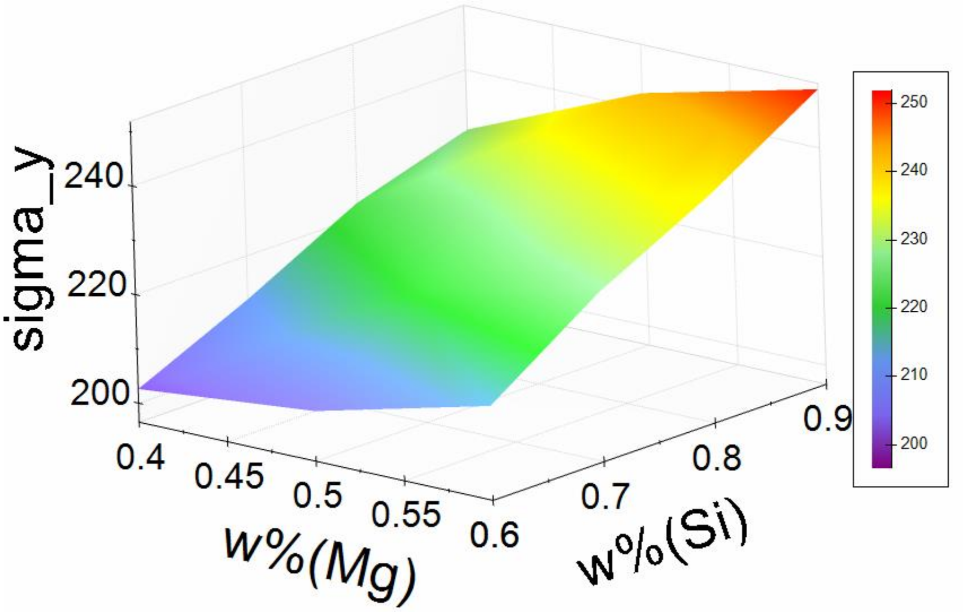
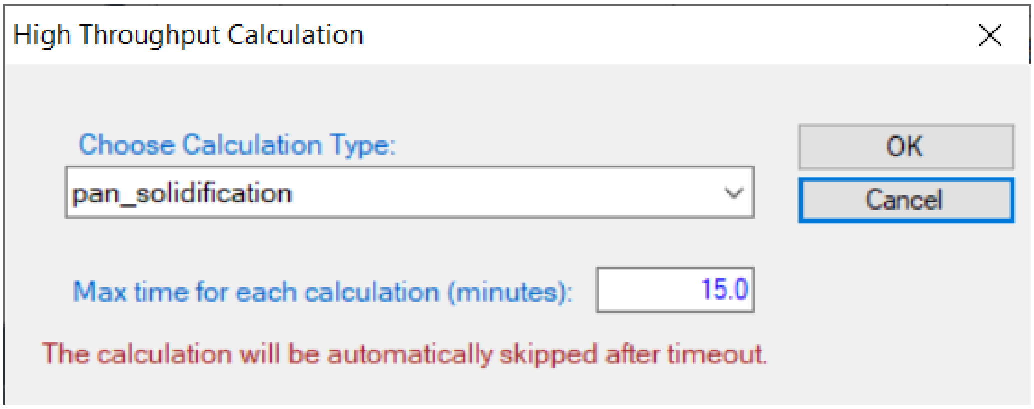


Figure 9.16 The maximum yield strength distribution within the defined compositional space

9.4 HTC Tutorial in PanSolidification

Hot tearing or hot cracking is a serious defect occurred in welding and casting solidification. Cracking usually generated at the end stage of solidification along grain boundaries. Prof. Kou [2005Kou] proposed a criterion to describe the crack susceptibility by using a simple crack susceptibility index (CSI), which is the maximum value of $|dT/d(f_s)^{1/2}|$ at $f_s^{1/2} < 0.99$. The CSI criterion has been successfully applied to several Al-based alloy systems. In this example, we will demonstrate how to use HTC function in PanSolidification module to produce a susceptibility map in the Al-Cu-Mg ternary system.

1. Create a workspace and select PanSolidification module. Save the workspace in a user assigned folder different from that of the default workspace. The HTC calculation results will be saved automatically under this folder.
2. Load proper thermodynamic + mobility database and select Al, Cu, Mg three components.
3. Load proper solidification kinetic-parameter database (.sdb) to select the solidification alloy system.
4. Choose the HTC function from the **Batch Calc → High Throughput Calculation (HTC)**.
5. Choose the calculation type from the drop-down list of HTC pop-up window and select "*pan_solidification*".



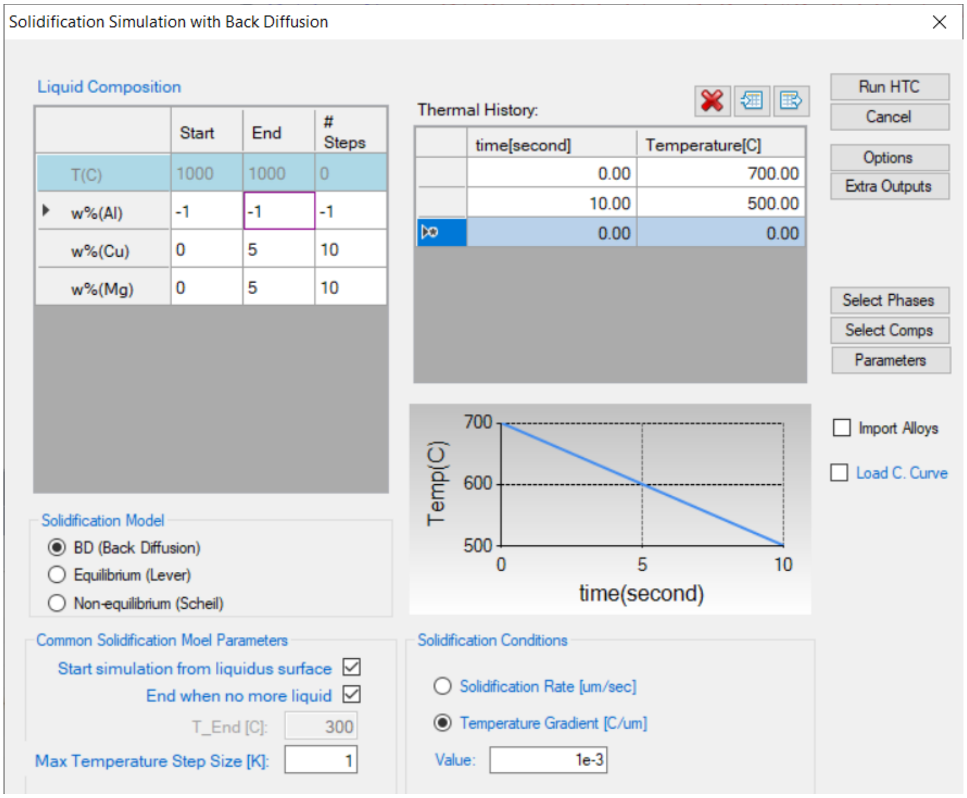
Choose Calculation Type: pan_solidification

Max time for each calculation (minutes): 15.0

The calculation will be automatically skipped after timeout.

Figure 9.17 Dialog to choose calculation type of HTC in PanSolidification

6. Define the compositional space for HTC simulation. As shown in Figure 9.18, the compositions of Cu and Mg varying within the ranges of 0-5, and 0-5 (wt.%), respectively.
7. Define the solidification conditions for HTC simulation. User can define/import cooling rate (the example is 20 K/s) by using the "**Thermal History**" dialog in Figure 9.18 or select the "**Load C. Curve**" and click the "**Import CC**" button to browse and load the predefined cooling curves (.txt or .dat). The example format of cooling curve file can be found in Figure 9.21. Besides the cooling rate, the solidification rate or temperature gradient is also needed to be defined.


Solidification Simulation with Back Diffusion

Liquid Composition

	Start	End	# Steps
T(C)	1000	1000	0
w%(Al)	-1	-1	-1
w%(Cu)	0	5	10
w%(Mg)	0	5	10

Thermal History:

time[second]	Temperature[C]
0.00	700.00
10.00	500.00
0.00	0.00

Solidification Model

● BD (Back Diffusion)
○ Equilibrium (Lever)
○ Non-equilibrium (Scheil)

Common Solidification Moel Parameters

Start simulation from liquidus surface ☑
End when no more liquid ☑
T_End [C]: 300
Max Temperature Step Size [K]: 1

Solidification Conditions

○ Solidification Rate [um/sec]
● Temperature Gradient [C/um]
Value: 1e-3

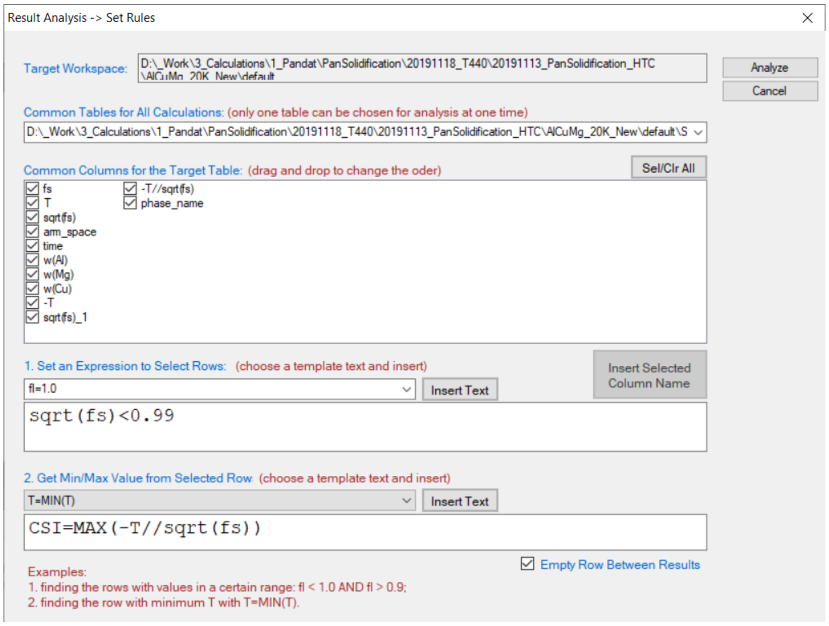
☐ Import Alloys
☐ Load C. Curve

Figure 9.18 Dialog to setup compositional space and solidification conditions for PanSolidification HTC.

8. In addition to use the default output, user can also customize the outputs using the "**Extra Outputs**" function. In this example, we defined the following extra output: time; T – temperature; w(*) – alloy composition; fs – solid phase fraction; sqrt(fs) – the square root value of the solid

phase fraction; and -T//sqrt(fs) – the CSI index $|dT/d(f_S)^{1/2}|$ because T//sqrt(fs) is a negative value.

9. After setup the compositional space for HTC and define/import the proper thermal history (as shown in Figure 9.18), user can click “**Run HTC**” button to perform HTC simulations.
10. Run “**Result Analysis**” from the “**Batch Calc**” menu. User can use this commend to analyze the calculated results for a group of alloys and pick a certain property from each calculation for comparison. As shown in the following Figure 9.19, the criterion is to output the MAX(-T//sqrt(fs)) at each composition point.
11. Figure 9.20 shows the obtained crack susceptibility map for Al-Cu-Mg alloys with cooling rate of 20 K/s. User can run “**Result Analysis**” on this save workspace and dig out more information using other rules.



Target Workspace: D:_Work\3_Calculations\1_Pandat\PanSolidification\20191118_T440\20191113_PanSolidification_HTC\AlCuMg_20K_New\default

Common Tables for All Calculations: (only one table can be chosen for analysis at one time)

D:_Work\3_Calculations\1_Pandat\PanSolidification\20191118_T440\20191113_PanSolidification_HTC\AlCuMg_20K_New\default\S

Common Columns for the Target Table: (drag and drop to change the oder)

☑ fs
☑ T
☑ sqrt(fs)
☑ arm_space
☑ time
☑ w(Al)
☑ w(Mg)
☑ w(Cu)
☑ -T
☑ sqrt(fs)_1
☑ -T//sqrt(fs)
☑ phase_name

1. Set an Expression to Select Rows: (choose a template text and insert)

fl=1.0

```
sqrt(fs)<0.99
```

2. Get Min/Max Value from Selected Row (choose a template text and insert)

T=MIN(T)

```
CSI=MAX(-T//sqrt(fs))
```

☑ Empty Row Between Results

Examples:
1. finding the rows with values in a certain range: fl < 1.0 AND fl > 0.9;
2. finding the row with minimum T with T=MIN(T).

Figure 9.19 Criteria for Cracking Susceptibility Index setting from solidification results analysis.

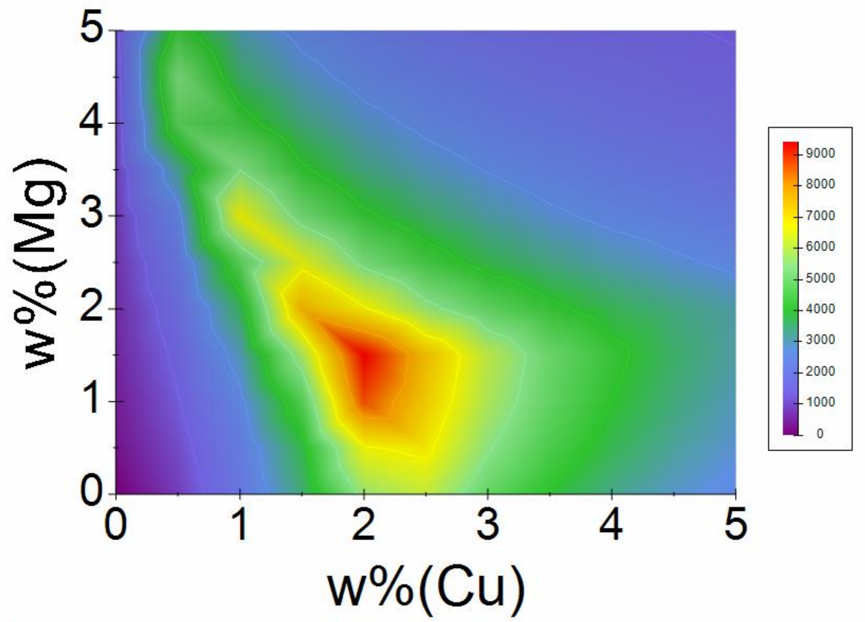


Figure 9.20 Al-Cu-Mg crack susceptibility map with cooling rate of 20 K/s.

9.5 Run HTC in Console Mode

In order to facilitate the integration of PanPrecipitation with a third-party software package such as *iSight* or *DEFORM*, a new feature is developed so that the software can call PanPrecipitation for multiple simulations with different conditions. In this case, PanPrecipitation run in a console mode rather than in a regular GUI mode. This would significantly reduce the overhead from creating and maintaining many GUI components. In this mode, the simulation is performed through a script file or Pandat batch file (.pbfx file). After the simulation is done, the results are saved as ASCII files, which can then be loaded by third-party software package for subsequent simulations.

A typical application of this function is to run HTC of an alloy at various cooling profiles. The command to run this type of precipitation HTC is:

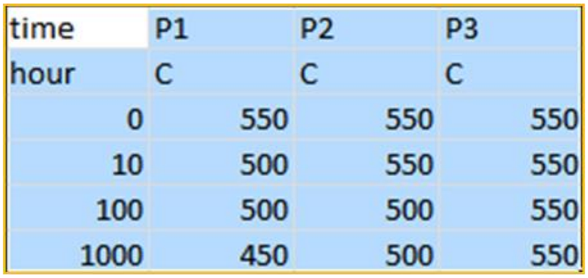
```
Pandat.exe   Ni-14Al.pbfx   “D:\ConsoleMode\results”   cooling_curve.txt   1
```

There are four arguments passed to **Pandat.exe** in order to run HTC:

a) **Ni-14Al.pbfx**: batch file name, which defines all the simulation conditions such as unit, alloy chemistry, output format, etc.; The heat treatment schedule will be replaced by the 3rd argument if there is cooling curve file attached;

b) **"D:\ConsoleMode\results"**: working folder for Pandat HTC. A default workspace will be created automatically when running Pandat each time. The old workspace will be removed in this folder. If the user wants to keep the workspace and its results, all the files in this folder should be backed up before running HTC each time. Or the user may specify a different working folder for each HTC calculation;

c) **cooling_curve.txt**: the files defining cooling curves for different points. The file format is Tab Delimited text file.



time	P1	P2	P3
hour	C	C	C
0	550	550	550
10	500	550	550
100	500	500	550
1000	450	500	550

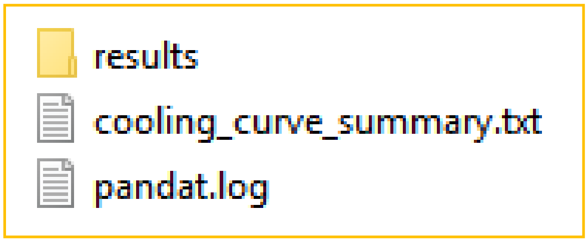
Figure 9.21 The example file format defining cooling curves for different points

The following is the structure of the working folder (see Figure 9.22):

1. **Workspace folder**: contains all the results for each simulation;

2. **"cooling_curve_summary.txt"**: the summary file which contains the results for the final step of each simulation; if there are multiple tables in pbfx file, only the results from the last table is summarized; the file format is Tab Delimited text file;

3. **pandat.log**: which logs the simulation progress; the level can be controlled by the last argument as shown above.



results
cooling_curve_summary.txt
pandat.log

Figure 9.22 The structure of the working folder.

Please refer to **Pandat Examples\ConsoleMode** for more detail information.

10 References

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