Pandat 2025

Example book

CompuTherm LLC

Contents

1 PanPhaseDiagram Examples

Example 1.1 Al-Mg Binary Phase Diagram

Purpose: Learn to calculate and use a binary phase diagram

Module: PanPhaseDiagram

Thermodynamic Database: `AlMgZn.tdb`

Batch file: `Example_#1.1.pbfx`

Calculation Procedures:

- Load `AlMgZn.tdb` following the procedure in Pandat User's Guide 3.2.1, and select `Al` and `Mg` two components;
- Perform section (2D) calculation following the procedure in Pandat User's Guide 3.3.3;
- Set Calculation Condition as shown in Figure 1.1.1;

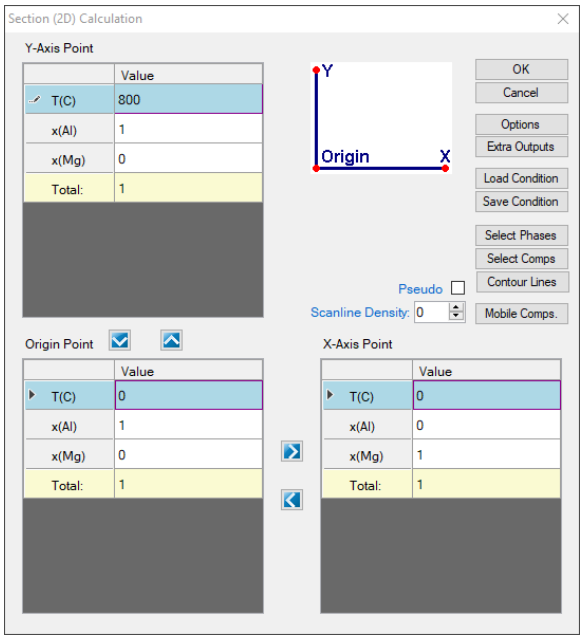


Figure 1.1.1: 2D calculation with composition from pure Al to pure Mg and temperature from 0°C to 800°C

Post Calculation Operation:

- Label phase field following the procedure in Pandat User's Guide 2.3.3;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Zoom the interested area following the procedure in Pandat User's Guide 2.3.3;

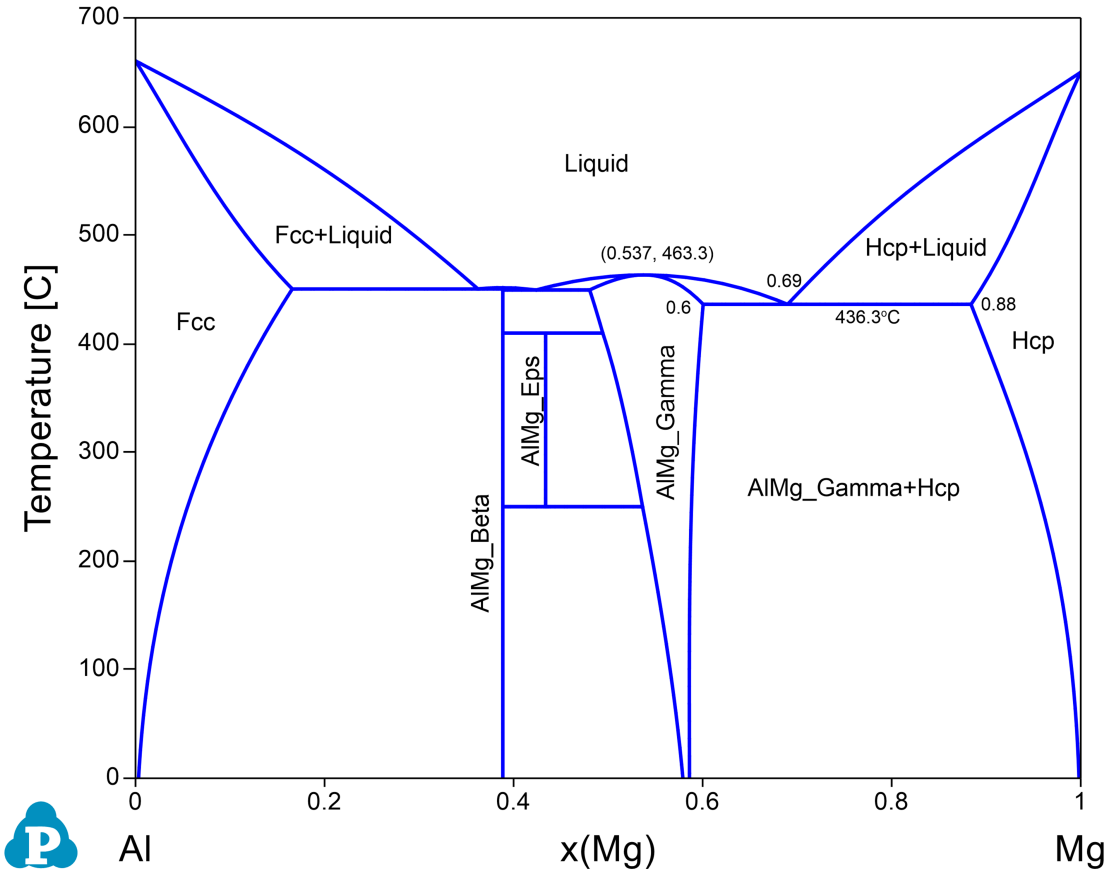


Figure 1.1.2: Calculated Al-Mg binary phase diagram

Information obtained from this calculation:

- Phase stability as a function of composition and temperature;
- Congruent melting temperature and composition of a phase. For example the congruent melting temperature of the `AlMg_Gamma` phase is at `463.3°C` and `x(Mg)=0.537`;

- Invariant reaction temperatures and phase compositions. For example the three phase equilibrium: `Liquid->AlMg_Gamma+Hcp` is at `436.3°C`, the composition, `x(Mg)`, of each phase at equilibrium is indicated in Figure 1.1.2. Details on the invariant reactions can be found in the "**`invariant`**" table as shown in Figure 1.1.1, and composition of each phase involved in the invariant reaction can be found in the "**`invariant_tieline`**" tables as shown in Figure 1.1.4.

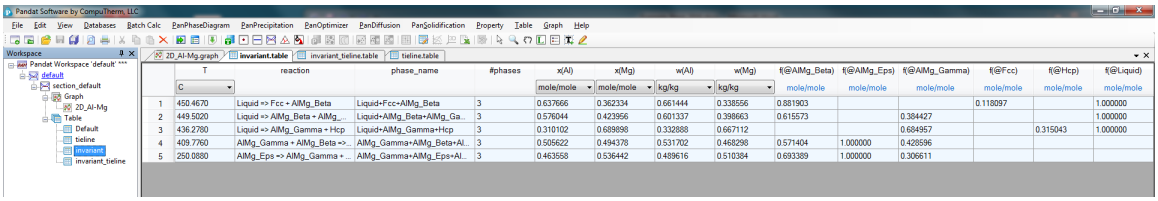
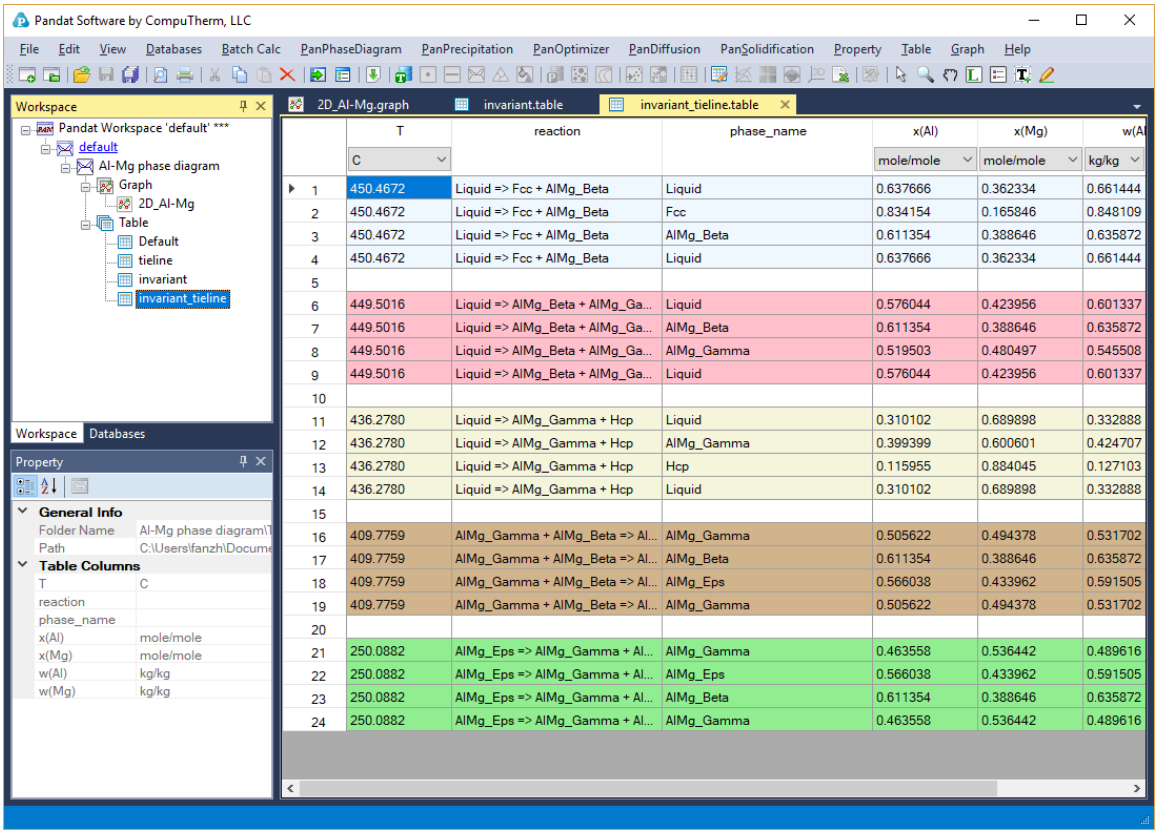


Figure 1.1.3: The invariant table showing all the three-phase equilibrium in the Al-Mg binary system



	T	reaction	phase_name	x(Al)	x(Mg)	w(Al
	C			mole/mole	mole/mole	kg/kg
1	450.4672	Liquid => Fcc + AlMg_Beta	Liquid	0.637666	0.362334	0.661444
2	450.4672	Liquid => Fcc + AlMg_Beta	Fcc	0.834154	0.165846	0.848109
3	450.4672	Liquid => Fcc + AlMg_Beta	AlMg_Beta	0.611354	0.388646	0.635872
4	450.4672	Liquid => Fcc + AlMg_Beta	Liquid	0.637666	0.362334	0.661444
5						
6	449.5016	Liquid => AlMg_Beta + AlMg_Ga...	Liquid	0.576044	0.423956	0.601337
7	449.5016	Liquid => AlMg_Beta + AlMg_Ga...	AlMg_Beta	0.611354	0.388646	0.635872
8	449.5016	Liquid => AlMg_Beta + AlMg_Ga...	AlMg_Gamma	0.519503	0.480497	0.545508
9	449.5016	Liquid => AlMg_Beta + AlMg_Ga...	Liquid	0.576044	0.423956	0.601337
10						
11	436.2780	Liquid => AlMg_Gamma + Hcp	Liquid	0.310102	0.689898	0.332888
12	436.2780	Liquid => AlMg_Gamma + Hcp	AlMg_Gamma	0.399399	0.600601	0.424707
13	436.2780	Liquid => AlMg_Gamma + Hcp	Hcp	0.115955	0.884045	0.127103
14	436.2780	Liquid => AlMg_Gamma + Hcp	Liquid	0.310102	0.689898	0.332888
15						
16	409.7759	AlMg_Gamma + AlMg_Beta => Al...	AlMg_Gamma	0.505622	0.494378	0.531702
17	409.7759	AlMg_Gamma + AlMg_Beta => Al...	AlMg_Beta	0.611354	0.388646	0.635872
18	409.7759	AlMg_Gamma + AlMg_Beta => Al...	AlMg_Eps	0.566038	0.433962	0.591505
19	409.7759	AlMg_Gamma + AlMg_Beta => Al...	AlMg_Gamma	0.505622	0.494378	0.531702
20						
21	250.0882	AlMg_Eps => AlMg_Gamma + Al...	AlMg_Gamma	0.463558	0.536442	0.489616
22	250.0882	AlMg_Eps => AlMg_Gamma + Al...	AlMg_Eps	0.566038	0.433962	0.591505
23	250.0882	AlMg_Eps => AlMg_Gamma + Al...	AlMg_Beta	0.611354	0.388646	0.635872
24	250.0882	AlMg_Eps => AlMg_Gamma + Al...	AlMg_Gamma	0.463558	0.536442	0.489616

Figure 1.1.4: The invariant_tieline table showing the composition of each phase involved in the invariant reaction in the Al-Mg binary system

Example 1.2 Phase Fraction as a Function of Composition

Purpose: Learn to calculate and use a phase fractions vs. composition plot

Module: PanPhaseDiagram

Thermodynamic Database: `AlMgZn.tdb`

Batch file: `Example_#1.2.pbfx`

Figure 1.2.1 is the `Al-Mg` binary phase diagram, which clearly shows the single phase region, two-phase region, three-phase equilibrium. However if you want to know the fraction of a stable phase in a two-phase field at a certain temperature, you need to draw a horizontal line at this temperature and calculate it by line (1D) calculation. In this example, we calculate the fraction of each phase as a function of composition, `x(Mg)`, at `300°C` (the red dash line).

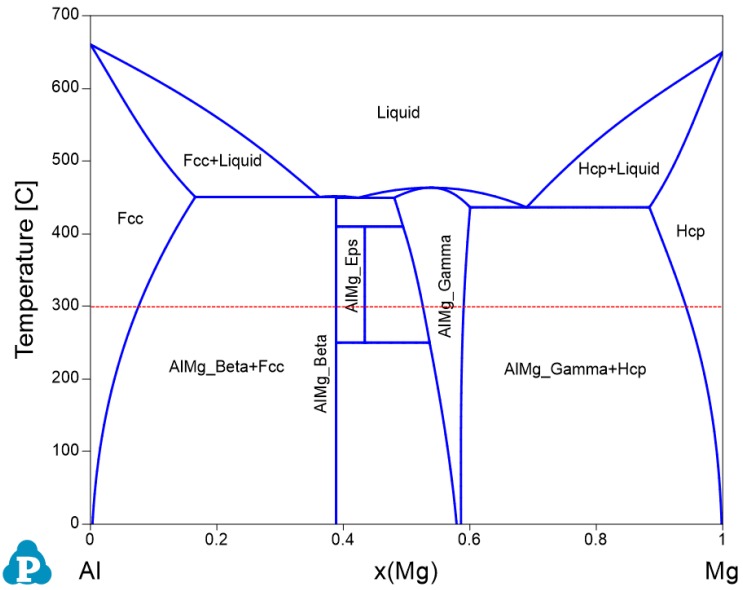


Figure 1.2.1: Al-Mg binary phase diagram

Calculation Procedures:

- Load `AlMgZn.tdb` following the procedure in Pandat User's Guide 3.2.1, and select `Al` and `Mg` two components;
- Perform 1D calculation following the procedure in Pandat User's Guide 3.3.2;
- Set Calculation Condition as shown in Figure 1.2.2;

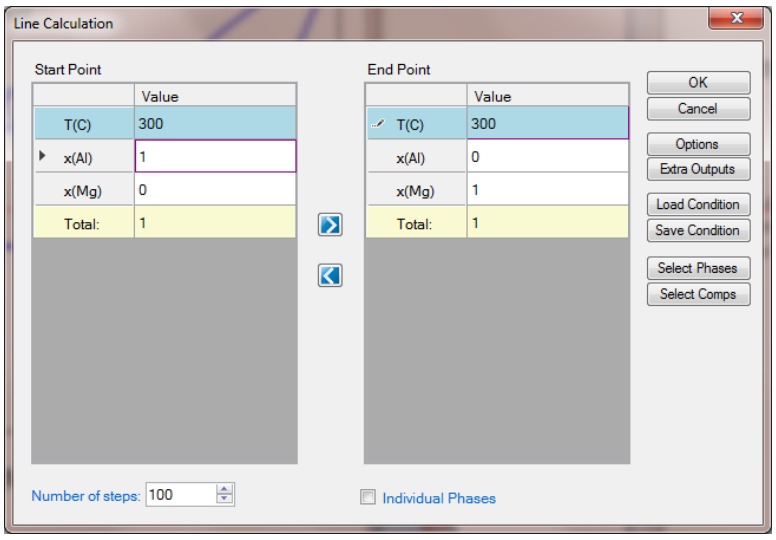


Figure 1.2.2: 1D calculation from pure Al to pure Mg at 300 °C

Post Calculation Operation:

- Add legend for graph following the procedure in Pandat User's Guide 2.3.3;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;

Information obtained from this calculation:

- The composition range that a phase is stable at the selected temperature;
- In a single phase field, the fraction of the stable phase is 1;
- In a two-phase field, the fraction of one phase decrease from 1 to 0, while the other increase from 0 to 1 as shown in Figure 1.2.3
- Details on the fraction of each phase as a function of composition can also be found in the Default table as shown in Figure 1.2.4;

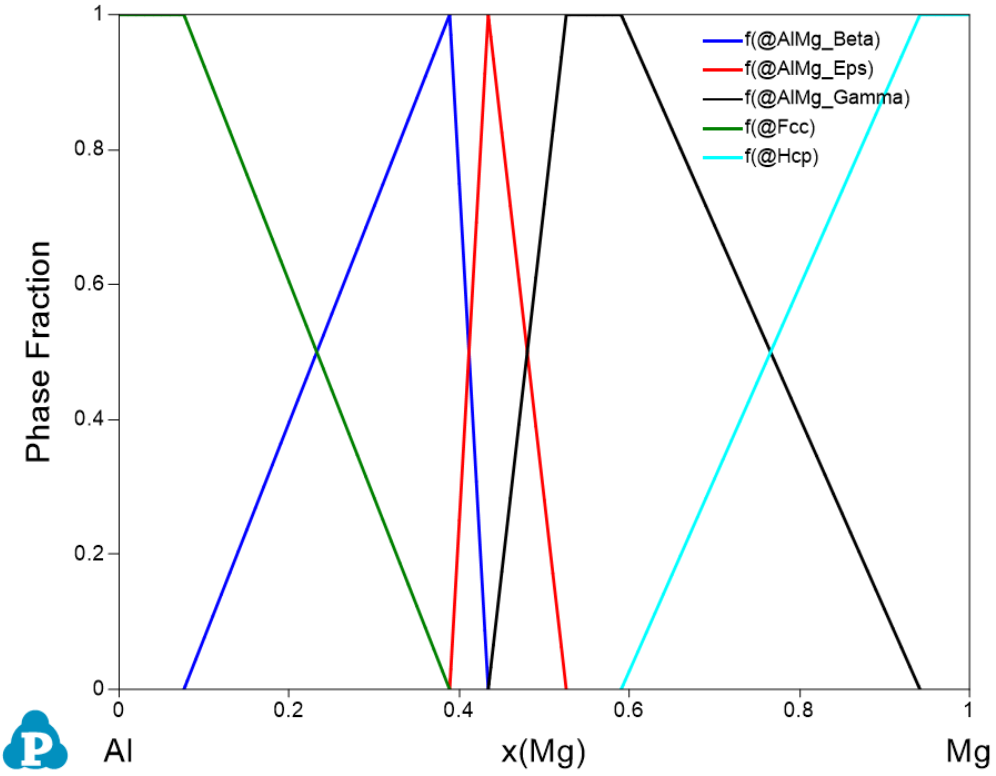


Figure 1.2.3: Phase fraction variation as a function of composition

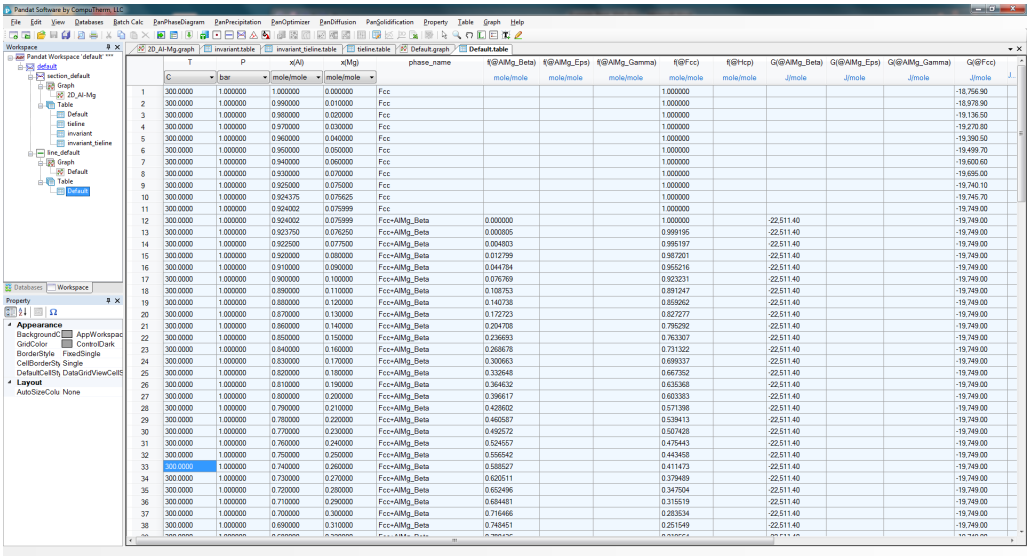


Figure 1.2.4: Default table showing phase fraction variation as a function of composition

Example 1.3 Phase Fraction as a Function of Temperature

Purpose: Learn to calculate and use a phase fractions vs. temperature plot

Module: PanPhaseDiagram

Thermodynamic Database: `AlMgZn.tdb`

Batch file: `Example_#1.3.pbfx`

In Example 1.2 : Phase Fraction as a Function of Composition, we have calculated the fraction of each phase as a function of composition. In most cases, people would like to know phase transformation when temperature varies. In this example, we calculate the fraction of phases as a function of temperature for an AlMg binary alloy with composition of *x*(Mg)=0.3 (the red dash line in Figure 1.3.1). Such a calculation is especially valuable for a multi-component alloy.

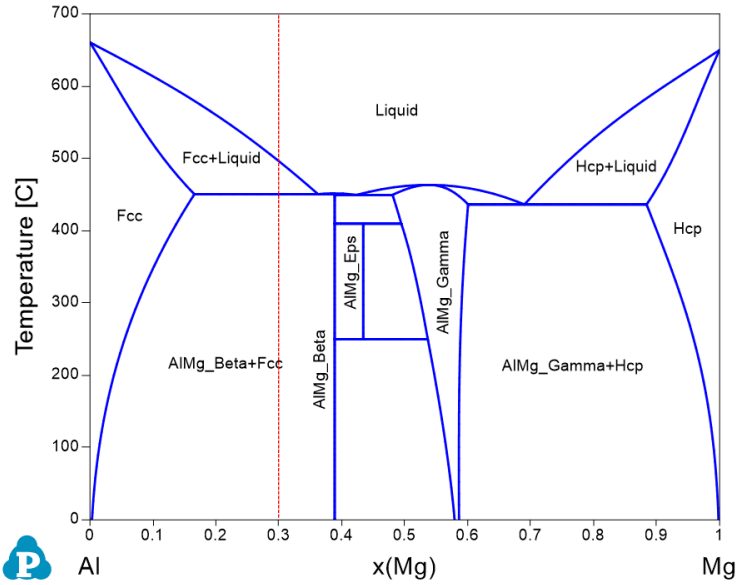


Figure 1.3.1: Al-Mg binary phase diagram

Calculation Procedures:

- Load `AlMgZn.tdb` following the procedure in Pandat User's Guide 3.2.1, and select `Al` and `Mg` two components;
- Perform 1D calculation following the procedure in Pandat User's Guide 3.3.2;
- Set Calculation Condition as shown in Figure 1.3.2;

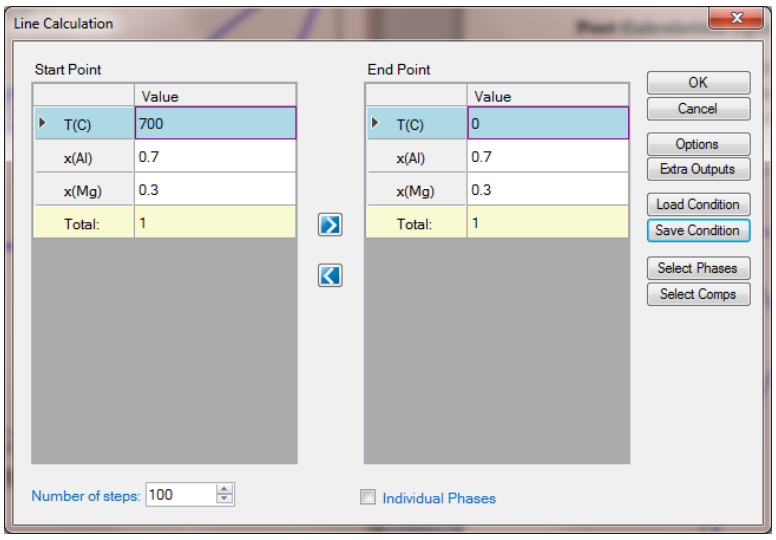


Figure 1.3.2: 1D calculation from 700°C to 0°C for an Al-Mg alloy with *x*(Mg)=0.3

Post Calculation Operation:

- Add legend for graph following the procedure in Pandat User's Guide 2.3.3;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;

Information obtained from this calculation:

- Liquid is the only stable phase at high temperature until 496.1 °C, which is the liquidus temperature;
- Below liquidus, Fcc phase forms and its fraction increases while that of the Liquid phase decreases until the eutectic temperature 450.47 °C;
- At eutectic temperature 450.47 °C, Liquid is disappeared (drops to 0% from 68.3%), fraction of the `AlMg_Beta` phase jumps from 0% to 60.21% and that of the `Fcc` phase jumps from 31.7% to 39.79%;
- Details on the fraction of each phase as a function of temperature can also be found in the Default table as shown in Figure 1.3.4;

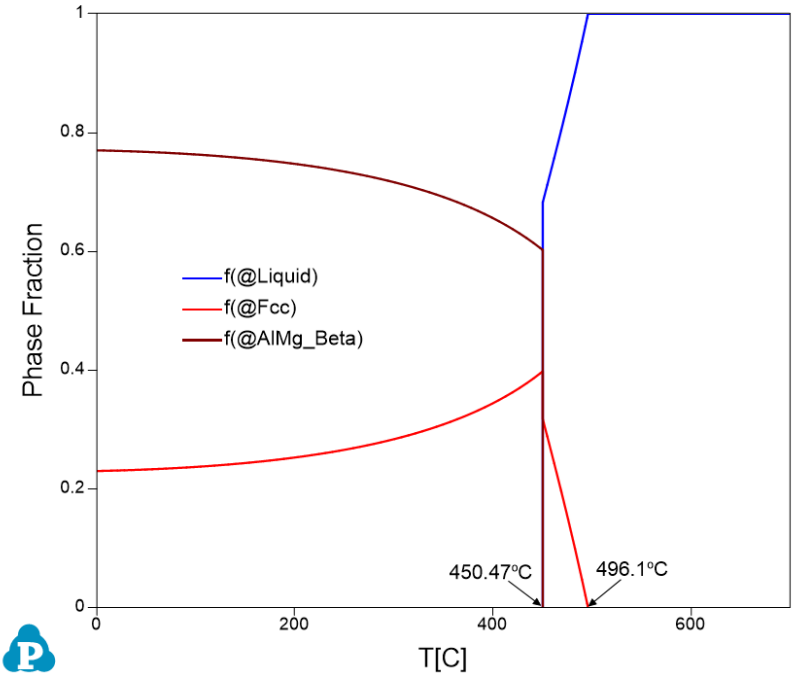


Figure 1.3.3: Phase fraction variation as a function of composition

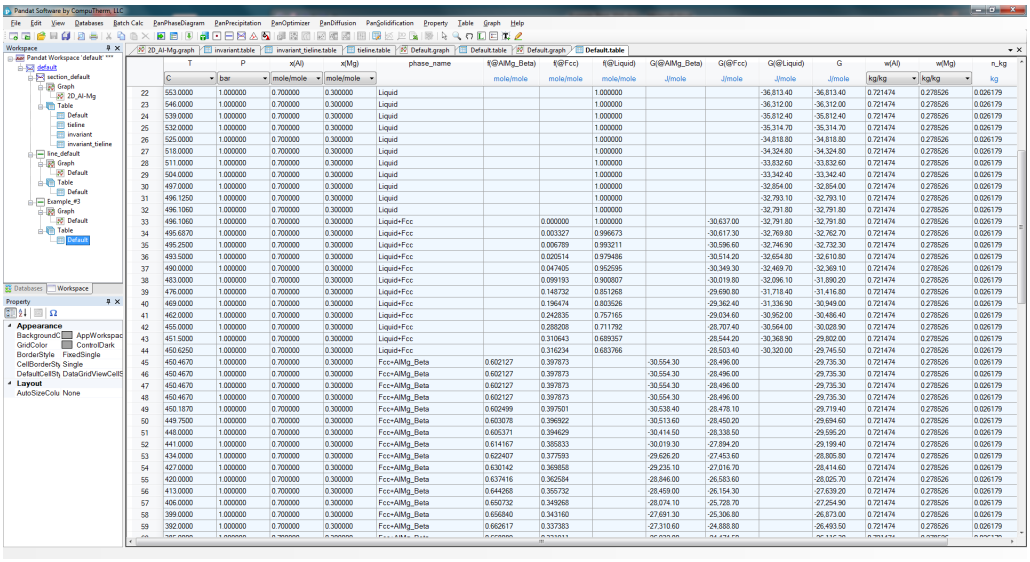


Figure 1.3.4: Default table showing phase fraction variation as a function of temperature

Example 1.4 Point Calculation at Fixed Temperature and Composition

Purpose: Learn to calculate and get detailed phase stability information at a given temperature and composition

Module: PanPhaseDiagram

Thermodynamic Database: `AlMgZn.tdb`

Batch file: `Example_#1.4.pbfx`

From the `Al-Mg` phase diagram shown in Figure 1.4.1, we know that two phases, `AlMg_Beta+Fcc`, are stable at the point indicated by Φ (the cross of the two dash lines). Other than that, no detail information about this point can be read directly from this phase diagram. In this example, we perform a Point Calculation to obtain the detail information at the selected point.

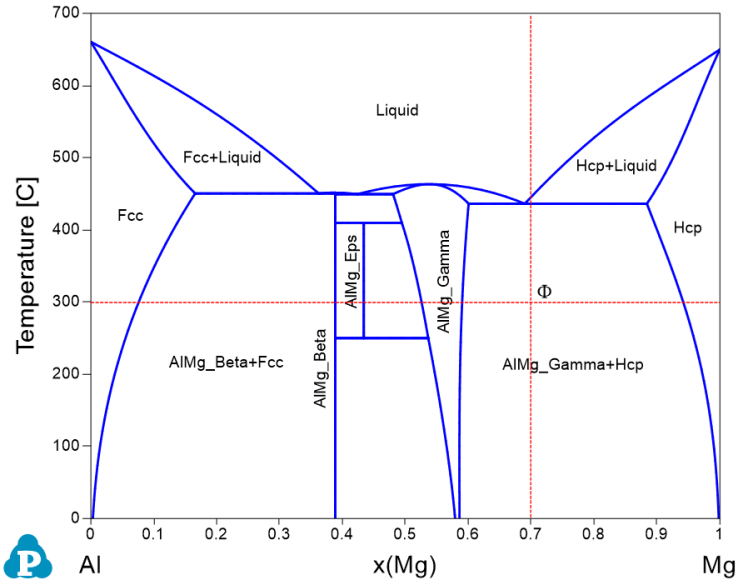


Figure 1.4.1: Al-Mg binary phase diagram

Calculation Procedures:

- Load `AlMgZn.tdb` following the procedure in Pandat User's Guide 3.2.1 , and select `Al` and `Mg` two components;
- Perform 0D calculation following the procedure in Pandat User's Guide 3.3.1;
- Set Calculation Condition as shown in Figure 1.4.2;

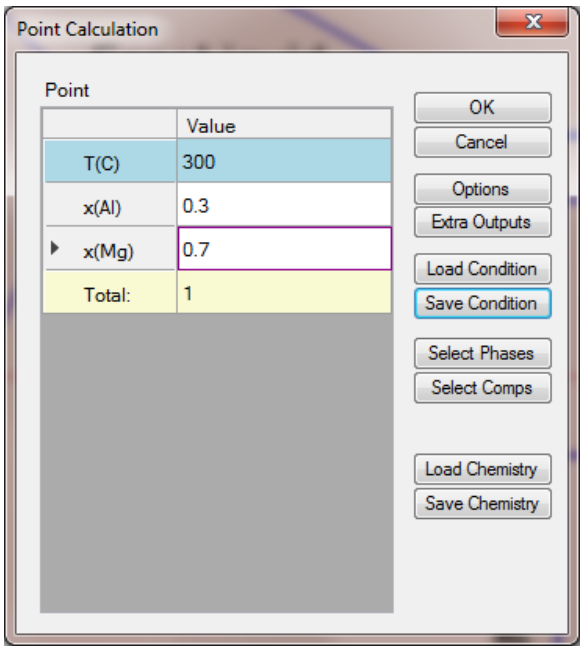


Figure 1.4.2: Point Calculation for an alloy with 30 at% Al and 70 at% of Mg at 300°C

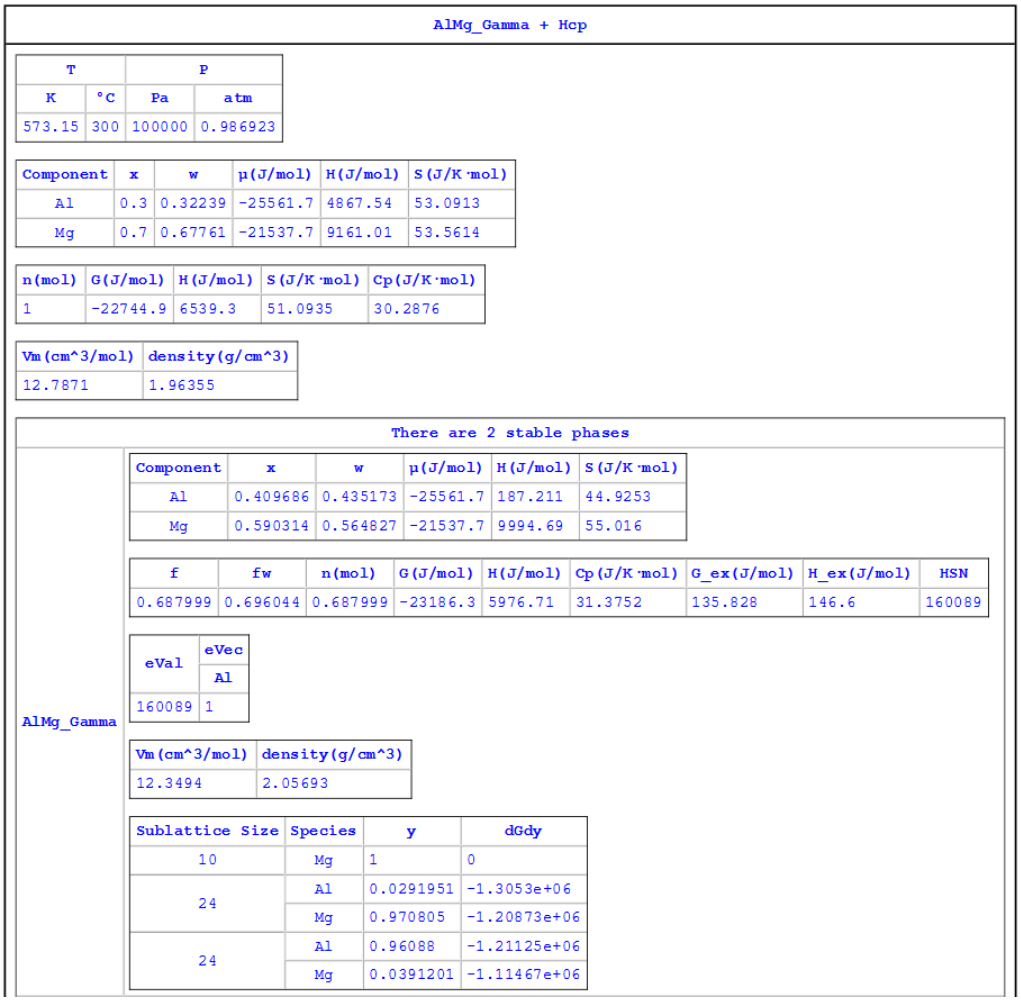
Calculation Method 2 from labeling:

- After the Al-Mg phase diagram is calculated, click L on the Labeling mode, then put the cursor at the selected point and press **`Ctrl`** button, click the mouse.

Information obtained from this calculation:

- Two phases, `AlMg_Gamma` and `Hcp`, are stable at the given condition (temperature and composition);
- The `G, H, S,` and `Cp` of the system at the given composition and temperature are -22744.9 J/mol, 6539.3 J/mol, 51.0935 J/K·mol, and 30.2876 J/K·mol, respectively;
- The equilibrium composition of `AlMg_Gamma` is x(Al) = 0.409686, x(Mg) = 0.590314;
- The mole fraction of `AlMg_Gamma` is 0.687999 (weight fraction is 0.696044);
- The `G, H, Cp,` G^{ex}, and H^{ex} of `AlMg_Gamma` at equilibrium composition are -23186.3 J/mol, 5976.71 J/mol, 31.3752 J/K·mol, 135.828 J/mol, and 146.6 J/mol, respectively;
- The site fraction of `AlMg_Gamma` are: y_{Mg}^{I} =1, y_{Al}^{II} =0.0291951, y_{Mg}^{II} =0.970805, y_{Al}^{III} =0.96088, y_{Mg}^{III}=0.0391201;

- The equilibrium composition of `Hcp` is x(Al) = 0.058129, x(Mg) = 0.941871;
- The mole fraction of `Hcp` phase is 0.312001 (weight fraction is 0.303956);
- The `G`, `H`, `Cp`, G^{ex}, and H^{ex} of `Hcp` at equilibrium composition are -21771.6 J/mol, 7779.87 J/mol, 27.8893 J/K·mol, 179.735 J/mol, and 184.813 J/mol, respectively;
- The site fraction of `Hcp` is the same as its composition since it is essentially one sublattice model, the second sublattice is occupied by vacancy.



AlMg_Gamma + Hcp

T		P	
K	°C	Pa	atm
573.15	300	100000	0.986923

Component	x	w	μ(J/mol)	H(J/mol)	S(J/K·mol)
Al	0.3	0.32239	-25561.7	4867.54	53.0913
Mg	0.7	0.67761	-21537.7	9161.01	53.5614

n(mol)	G(J/mol)	H(J/mol)	S(J/K·mol)	Cp(J/K·mol)
1	-22744.9	6539.3	51.0935	30.2876

Vm(cm^3/mol)	density(g/cm^3)
12.7871	1.96355

There are 2 stable phases

AlMg_Gamma

Component	x	w	μ(J/mol)	H(J/mol)	S(J/K·mol)
Al	0.409686	0.435173	-25561.7	187.211	44.9253
Mg	0.590314	0.564827	-21537.7	9994.69	55.016

f	fw	n(mol)	G(J/mol)	H(J/mol)	Cp(J/K·mol)	G_ex(J/mol)	H_ex(J/mol)	HSN
0.687999	0.696044	0.687999	-23186.3	5976.71	31.3752	135.828	146.6	160089

eVal	eVec
	Al
160089	1

Vm(cm^3/mol)	density(g/cm^3)
12.3494	2.05693

Sublattice Size	Species	y	dGdy
10	Mg	1	0
24	Al	0.0291951	-1.3053e+06
	Mg	0.970805	-1.20873e+06
24	Al	0.96088	-1.21125e+06
	Mg	0.0391201	-1.11467e+06

Figure 1.4.3: Calculated results for an alloy with 30 at% Al and 70 at% of Mg at 300°C

Example 1.5 Isotherm of Al-Mg-Zn at 500°C

Purpose: Learn to calculate and use an isothermal section in a ternary system

Module: PanPhaseDiagram

Thermodynamic Database: `AlMgZn.tdb`

Batch file: `Example_#1.5.pbfx`

A complete phase diagram of a ternary system should be described by a triangular prism in a 3D space with each edge of the triangle base representing the composition axis of each component and the vertical axis the temperature. Due to the complexity of many ternary systems, phase stability of a ternary system is usually described by Isothermal sections parallel to the triangle base (constant temperature) and isoplethal sections vertical to the triangle base plane. In this example, we will calculate an isothermal section of Al-Mg-Zn at 500°C.

Calculation Procedures:

- Load `AlMgZn.tdb` following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Perform 2D calculation following the procedure in Pandat User's Guide 3.3.3;
- Set Calculation Condition as shown in Figure 1.5.1;

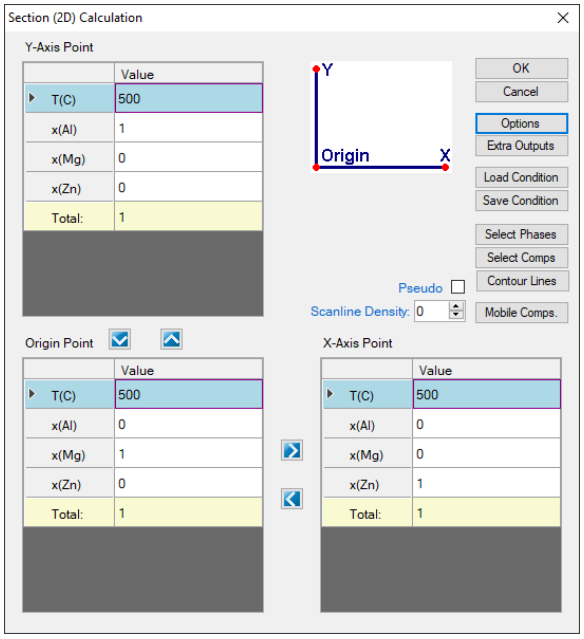


Figure 1.5.1: 2D calculation of an isotherm of Al-Mg-Zn at 500°C

Post Calculation Operation:

- Label phase field following the procedure in Pandat User's Guide 2.3.3;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Add tie-lines following the procedure in Pandat User's Guide 2.3.1;

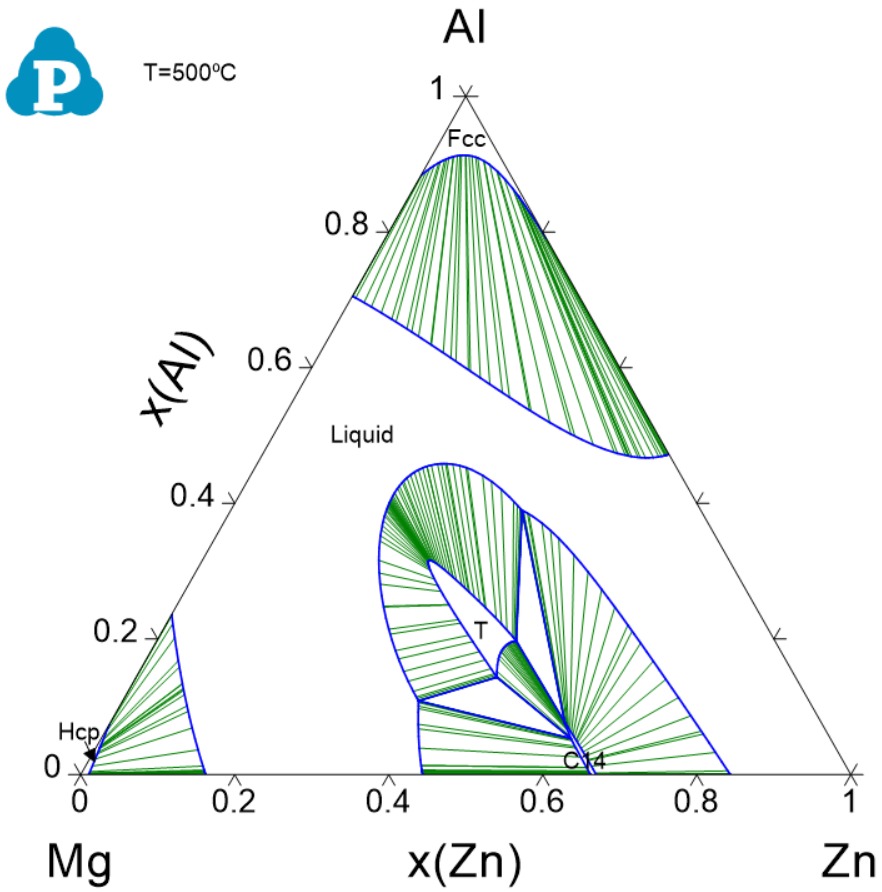


Figure 1.5.2: Calculated isotherm of Al-Mg-Zn at 500 °C

Information obtained from this calculation:

- Phase stability in different composition areas, single phase, two-phase, and three-phase regions, can be viewed clearly at this temperature;
- Equilibrium between two phases is connected by tie- lines, and the equilibrium compositions of the two phases can be read at the end points of the tie-line; Details on the tie-lines can be found in **`Table->tieline`** as shown in Figure 1.5.3. In this table, the compositions of the two phases connected by each tieline are listed for all the calculated tielines;
- Three-phase equilibrium is shown by the tie-triangle. The composition of each phase in the three-phase equilibrium is listed in invariant_tieline table, as shown in Figure 1.5.4.

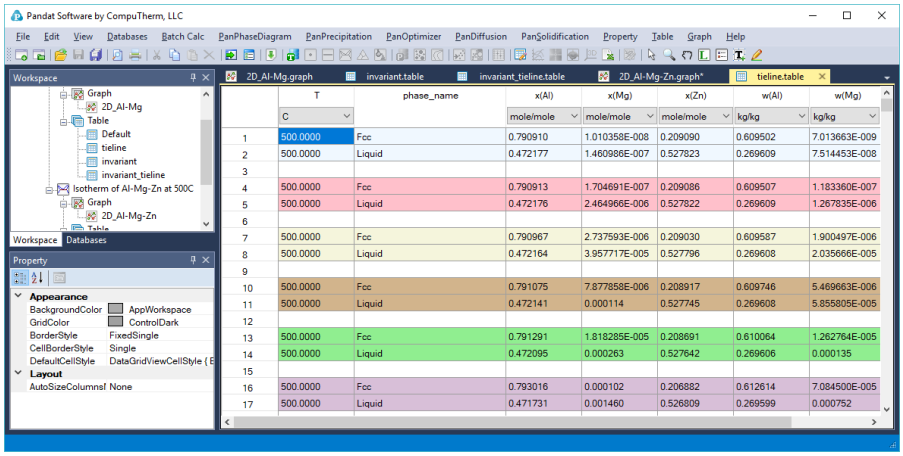


Figure 1.5.3: The tieline table showing the detailed information of calculated tieline

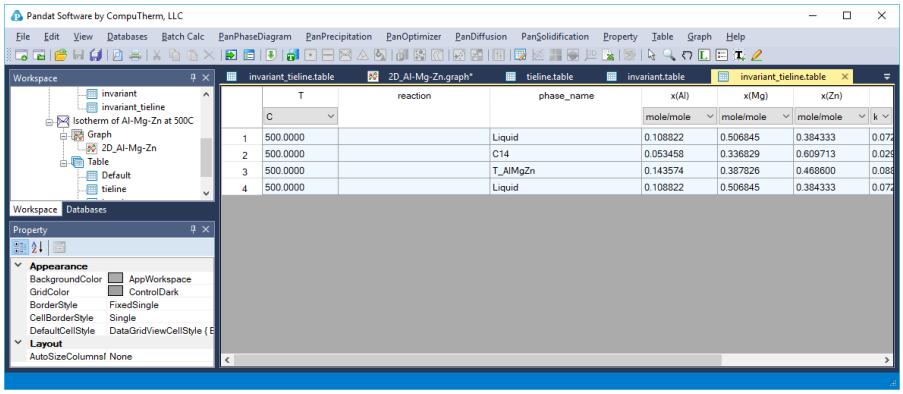


Figure 1.5.4: The invariant_tieline table showing the composition of each phase in the invariant reaction

Example 1.6 Isopleth of Al-Mg-Zn at 15 at% Zn

Purpose: Learn to calculate and use an isoplethal section in a ternary system

Module: PanPhaseDiagram

Thermodynamic Database: `AlMgZn.tdb`

Batch file: `Example_#1.6.pbfx`

As mentioned in Example 1.5 : Isotherm of Al-Mg-Zn at 500°C, isopleths are sections vertical to the triangle base plane of the triangular prism. An isopleth is important in understanding phase relationship in a ternary system when temperature is a variable. In this example, we will calculate an isoplethal section in the Al-Mg-Zn ternary parallel to Al-Mg binary with 15 at% of Zn.

Calculation Procedures:

- Load `AlMgZn.tdb` following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Perform 2D calculation following the procedure in Pandat User's Guide 3.3.3;
- Set Calculation Condition as shown in Figure 1.6.1;

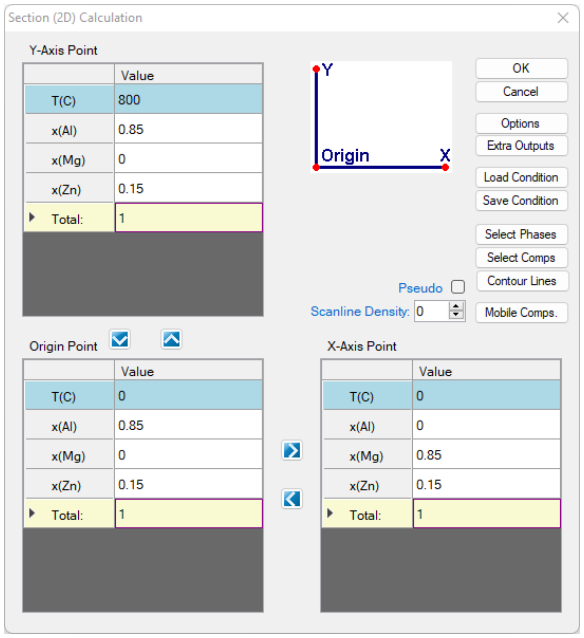


Figure 1.6.1: 2D calculation of an isopleth parallel to Al-Mg binary with 15 at% Zn

Post Calculation Operation:

- Label phase field following the procedure in Pandat User's Guide 2.3.3;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;

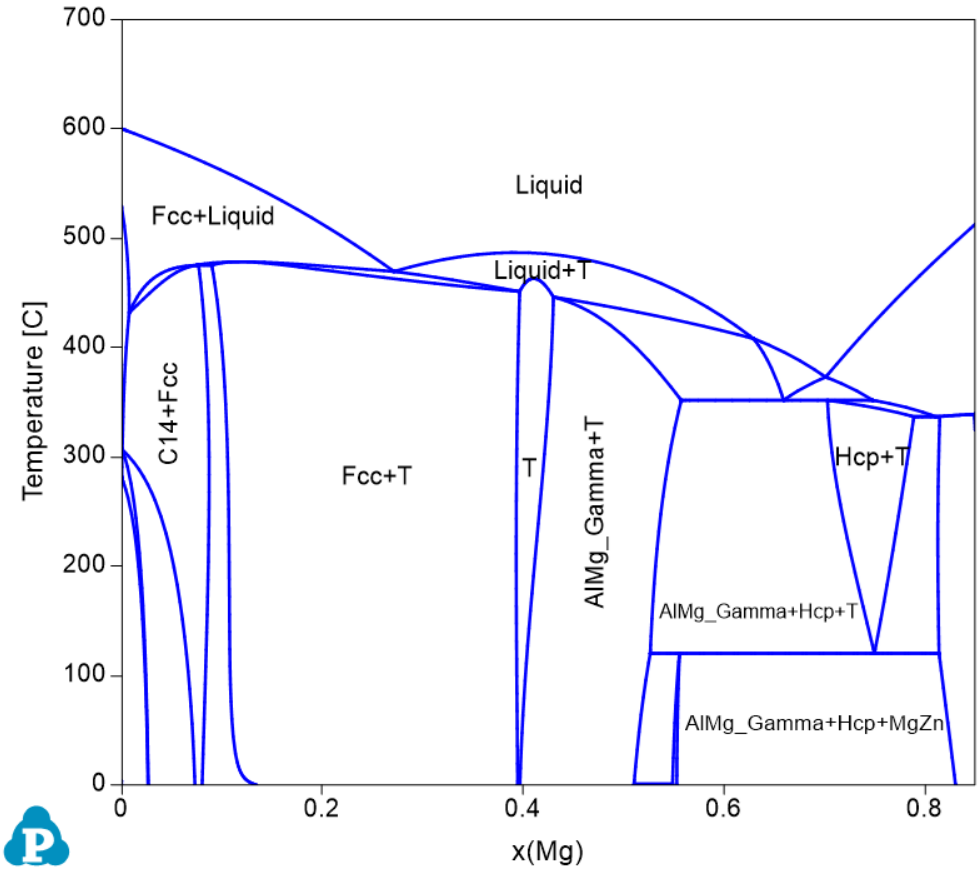


Figure 1.6.2: Calculated isopleth parallel to Al-Mg binary with 15 at% Zn

Information obtained from this calculation:

- Phase stability as a function of composition of Mg and temperature. Single phase, two-phase, and three-phase regions, can be viewed clearly at different composition and temperature;
- Tie-lines cannot be viewed on an isopleth since they are usually not on the same isoplethal plane except for a pseudo-binary. The tieline information is listed in tieline Table as shown in Figure 1.6.3.

- The invariant reactions and the phase composition for every phase in the invariant reaction are listed in invariant_tieline table as shown in Figure 1.6.4.

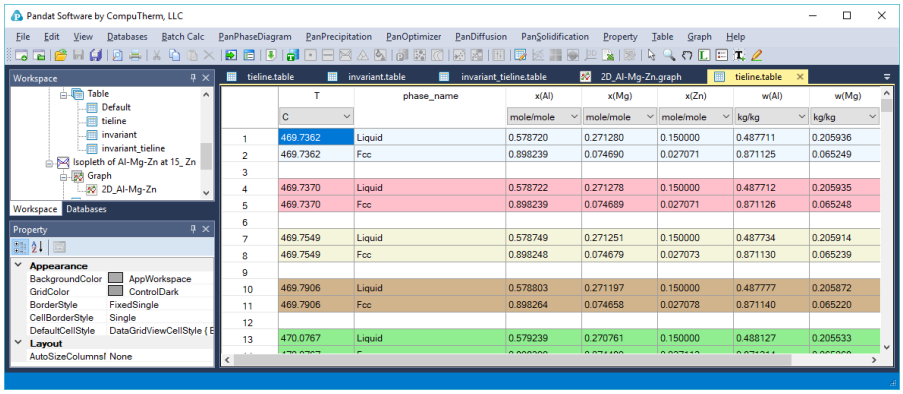


Figure 1.6.3: The tieline table showing the detailed information of calculated tieline

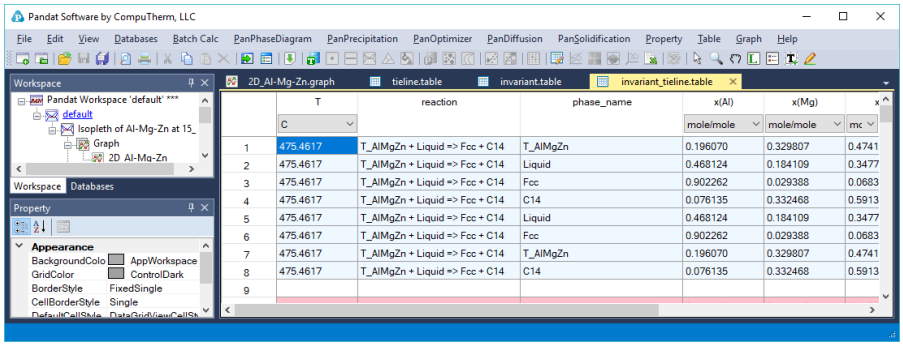


Figure 1.6.4: The invariant_tieline table showing composition of each phase involved in the invariant reaction

Example 1.7 Liquidus Projection of Al-Mg-Zn

Purpose: Learn to calculate and use a liquidus projection in a ternary system

Module: PanPhaseDiagram

Thermodynamic Database: `AlMgZn.tdb`

Batch file: `Example_#1.7.pbfx`

As mentioned in Example 1.5 : Isotherm of Al-Mg-Zn at 500°C and Example 1.6 : Isopleth of Al-Mg-Zn at 15 at% Zn, isotherms and isopleths are two types of phase diagrams used to view the phase relationship in a ternary system. Another type of phase diagrams commonly used to understand a ternary system is the liquidus projection which is the projection of the liquid surface onto the base triangle plane. In this example, we will calculate the liquidus projection of Al-Mg-Zn ternary system.

Calculation Procedures:

- Load `AlMgZn.tdb` following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Perform phase projection following the procedure in Pandat User's Guide 3.3.6;
- Set Calculation Condition as shown in Figure 1.7.1;

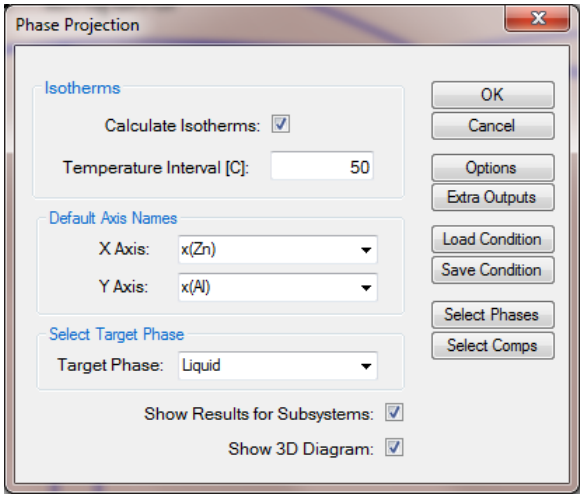


Figure 1.7.1: Phase projection calculation setting dialog

Post Calculation Operation:

- Label phase field following the procedure in Pandat User's Guide 2.3.3;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Label the isothermal lines by put the cursor on each line and then press F2;

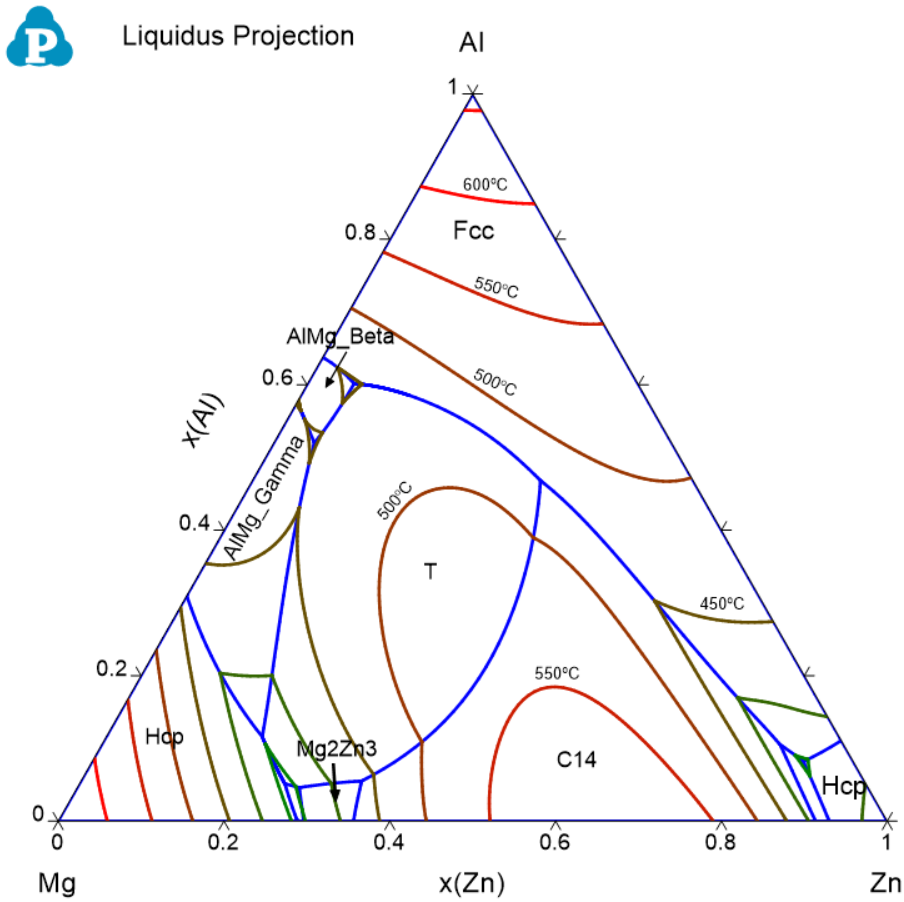


Figure 1.7.2: Calculated liquidus projection of the Al-Mg-Zn system

Information obtained from this calculation:

- The phase name labeled in each region indicates the primary solidified phase from liquid when the given alloy composition falls in that region;
- The univariant liquid projection lines (blue lines) trace the composition of the liquid phase for the three-phase equilibrium among the liquid and the other two phases separated by the liquid projection line;

- The isothermal lines (from red to green with temperature descending) represent the liquidus temperatures. The liquidus temperature for all the compositions along each line is identical;
- Each triple point at the intersection of three projection lines represents a invariant reaction (four phases in a ternary system) involving the liquid phase. All the invariant reactions are listed in invariant table as shown in Figure 1.7.3. The composition of each phase involved in the invariant reaction is listed in invariant_tieline table as shown in in Figure 1.7.4.

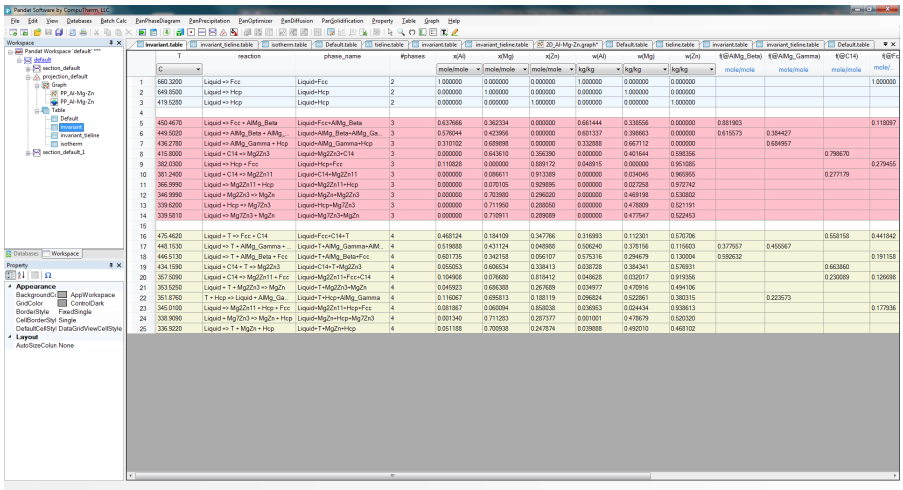


Figure 1.7.3: Invariant table showing all the invariant reactions involving liquid phase

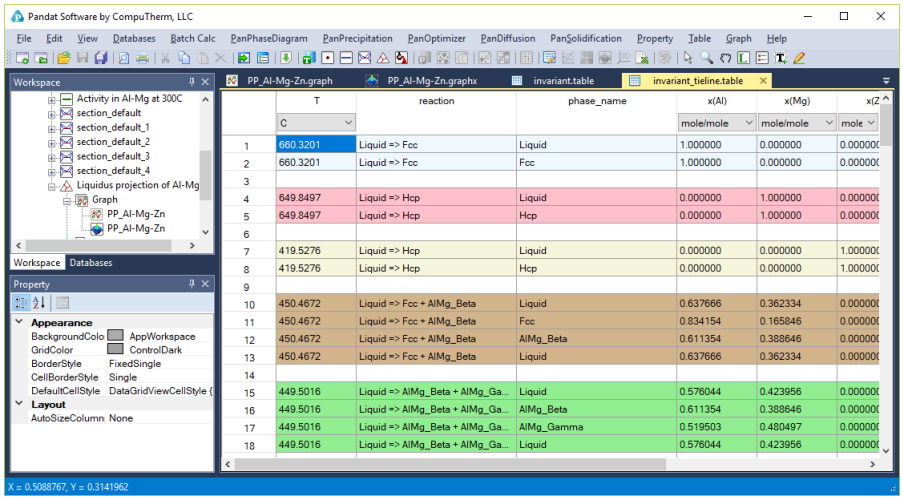


Figure 1.7.4: Invariant_tieline table showing composition of each phase involved in the invariant reaction

Example 1.8 Solidification Simulation by Scheil Model and Lever Rule

Purpose: Learn to perform solidification simulation for a given alloy composition

Module: PanPhaseDiagram

Thermodynamic Database: `AlMgZn.tdb`

Batch file: `Example_#1.8.pbfx`

Pandat has two models for solidification simulation, one based on Lever rule and the other Scheil model. Lever rule assumes infinite slow cooling so that equilibrium is reached at every step of solidification. Scheil model assumes fast cooling and fast diffusion in the liquid so that liquid maintains uniform composition, no diffusion in the solid and local equilibrium is reached between liquid and solid at the interface. In this example we will perform two solidification simulations using the two models for an alloy with 40 at% of Al, 50 at% of Mg and 10 at% of Zn. We will then compare the simulation results by plotting them on the same plot.

Calculation Procedures:

- Load `AlMgZn.tdb` following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Perform solidification simulation following the procedure in Pandat User's Guide 3.3.7;
- Set Calculation Condition as shown in Figure 1.8.1 , check "Scheil" for the first calculation and "Lever" for the second calculation

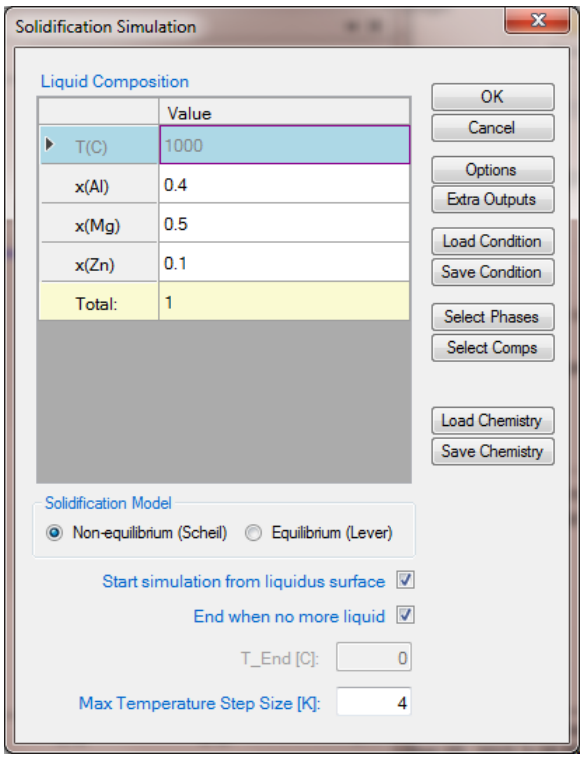


Figure 1.8.1: Input the alloy composition for solidification simulation

Post Calculation Operation:

- Add text and arrow on the plot following the procedure in Pandat User's Guide 2.3.3;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;

Information obtained from this calculation:

- Figure 1.8.2 shows the fraction of solid as a function of temperature from Scheil simulation. Solidification starts at 457°C and ends at 336.9°C, the freezing range is 120.1°C;
- The primary solidified phase is T_AlMgZn phase, AlMg_Gamma starts to solidify at 447.5°C and Hcp starts to solidify at 351.8°C. Put the cursor on the line segment, a tool tip will pop out showing the phase(s) solidified in that composition and temperature range (Figure 1.8.2). Press 'F2' to label it;

- Detail information for the simulation, such as solidification start temperature for a certain phase, the total fraction of each solid at different temperatures, latent heat, and total heat evolved can be found in the Default Table as shown in Figure 1.8.3;
- Certain properties can be selected from the Default table and plotted. Figure 1.8.4 shows the fraction of each solid phase as a function of temperature, and Figure 1.8.5 shows the Latent heat and total heat evolution as a function of temperature;
- Figure 1.8.6 shows the lever rule simulation which follows equilibrium calculation. It therefore shows a very narrow solidification range, starting from 457°C and ending at 437°C;
- Only two phases solidified from lever rule simulation, i.e., T_AlMgZn phase and AlMg_ Gamma phase;
- Details on the fraction of solid phase, heat evolution, and so on can also be found in the Default table;
- Figure 1.8.7 shows the overlapped plots from Scheil simulation and Lever rule simulation. To merge two plots together, we first open the plot from Lever rule simulation as shown in Figure 1.8.6, right click the mouse and choose "**Copy Data**", then open the plot from Scheil simulation as shown in Figure 1.8.2, right click the mouse and choose "**Paste Data**". The two plots from Lever rule simulation and Scheil simulation are merged in the same diagram as shown in Figure 1.8.7;

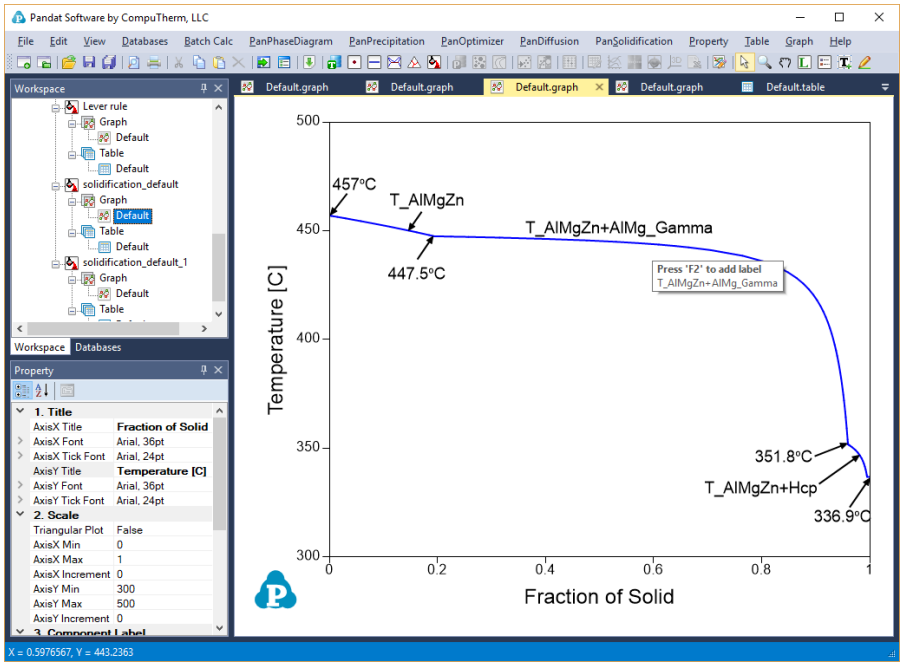


Figure 1.8.2: Fraction of solid as a function of temperature from Scheil simulation

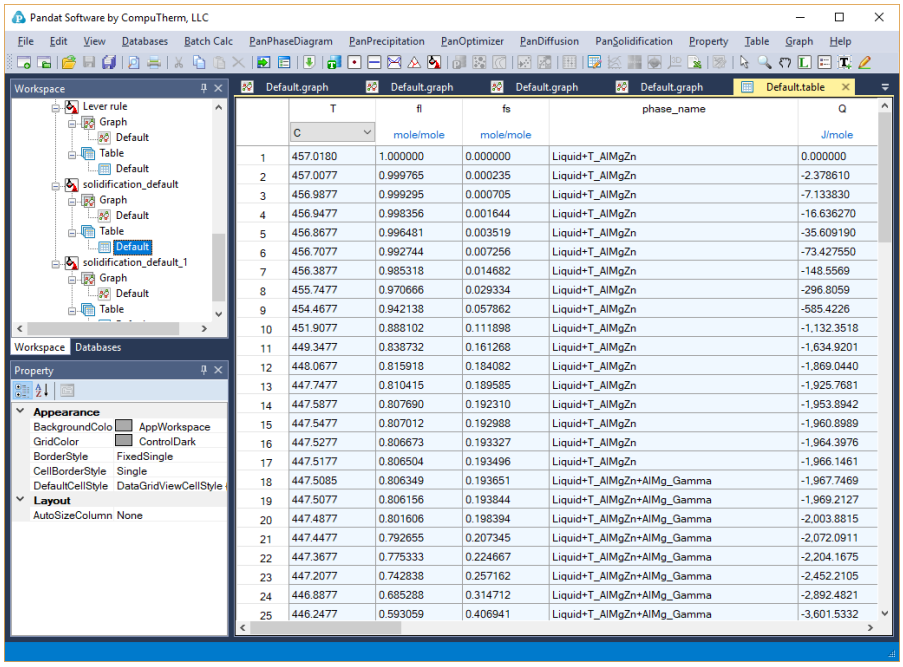


Figure 1.8.3: Detailed solidification information listed in the Default table

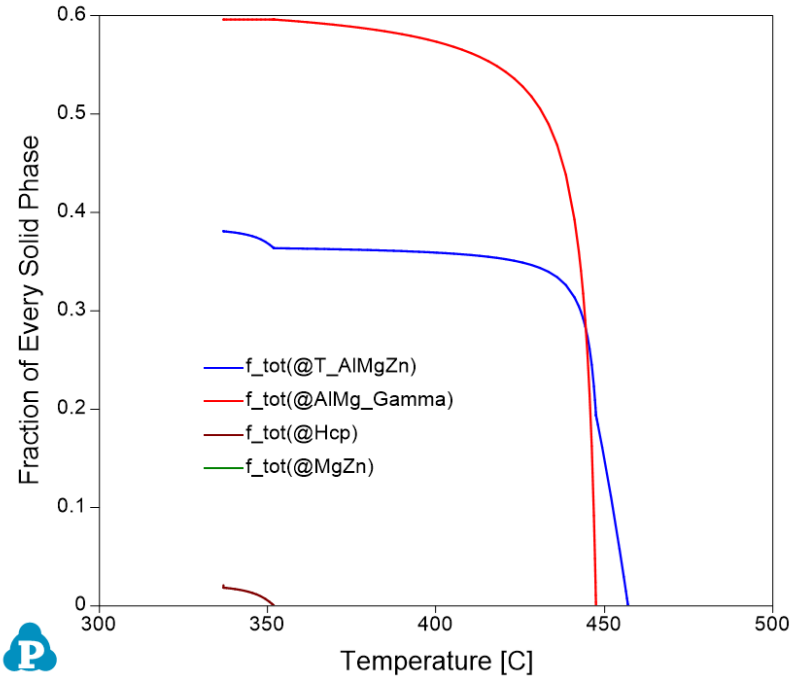


Figure 1.8.4: Fraction of each solid phase as a function of temperature

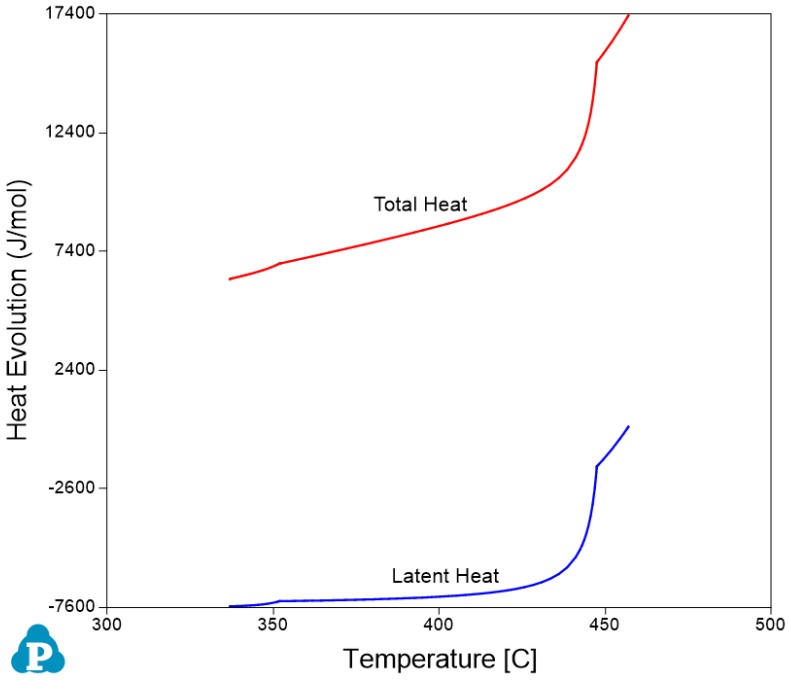


Figure 1.8.5: Heat evolution as a function of temperature

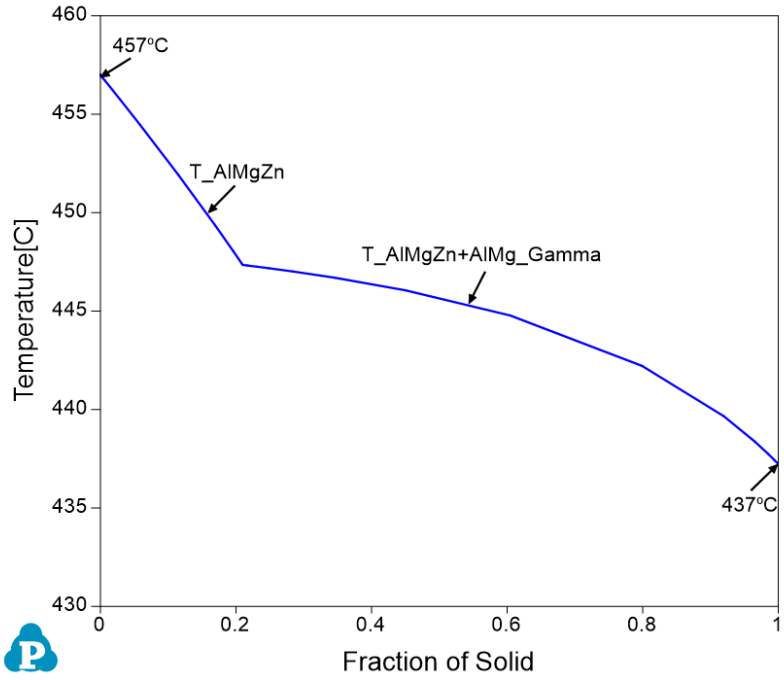


Figure 1.8.6: Fraction of solid as a function of temperature by Lever rule simulation

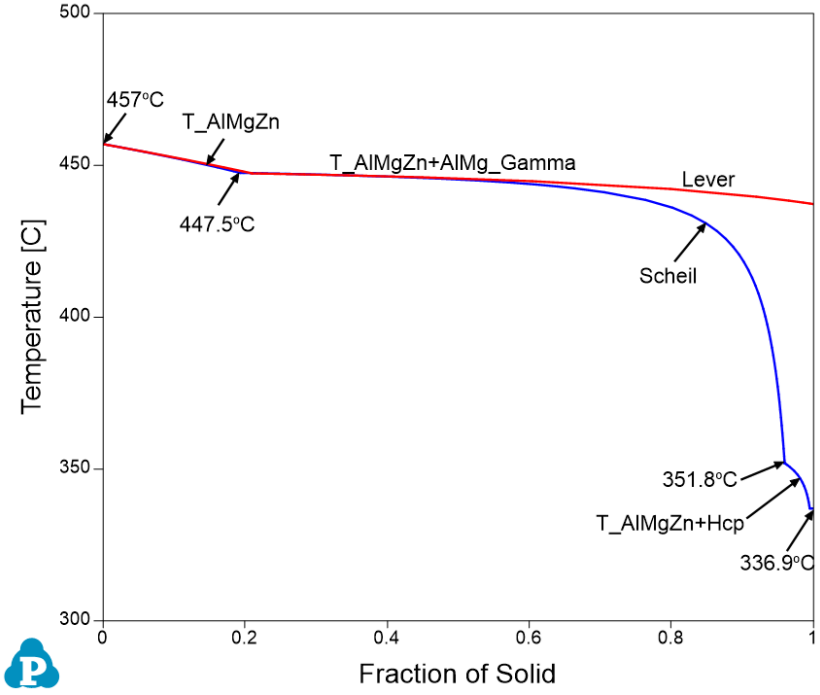


Figure 1.8.7: Merge the Scheil and Lever simulation results together

Example 1.9 Calculation of Gibbs Energy Curves

Purpose: Learn to calculate the Gibbs energy of a system or individual phase

Module: PanPhaseDiagram

Thermodynamic Database: `AlMgZn.tdb`

Batch file: `Example_#1.9.pbfx`

Figure 1.9.1 is the `Al-Mg` binary phase diagram. In this example, we learn to calculate the Gibbs energy of the system and the Gibbs energy of each phase as a function of composition, `x(Mg)`, at 300°C (the red dash line).

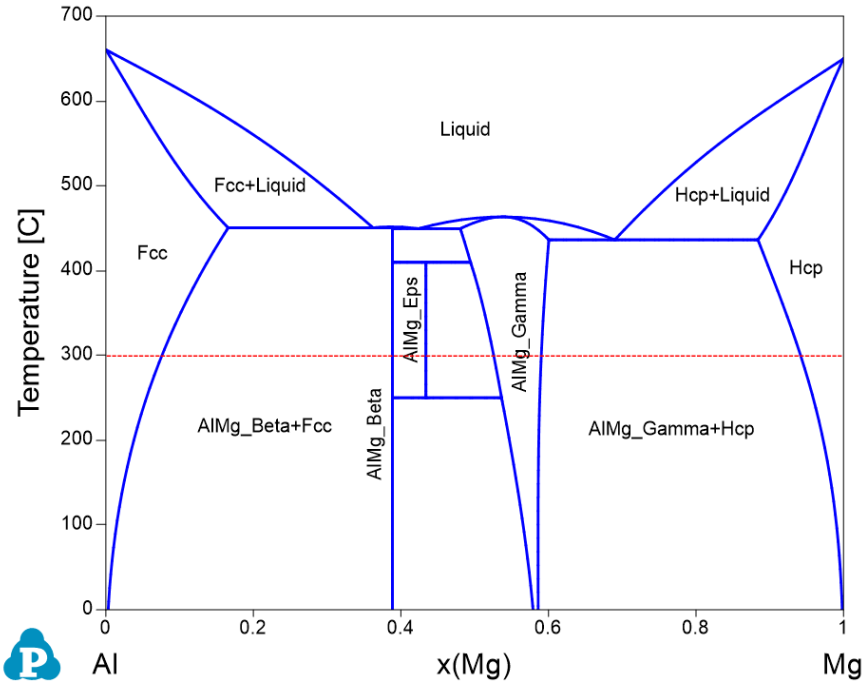


Figure 1.9.1: Al-Mg binary phase diagram

Calculation Method 1, From menu bar "Property":

- Load `AlMgZn.tdb` following the procedure in Pandat User's Guide 3.2.1, and select `Al` and `Mg` two components;
- Click "**`Property`**" on the menu bar and select "**`Thermodynamic Property`**";

- Set Calculation Condition as shown in Figure 1.9.2. The property selected is `G`, and the reference states are set as `Fcc` for `Al` and `Hcp` for `Mg`, the Gibbs energy of the system (stable phases in each composition range) will be calculated as shown by Figure 1.9.4;
- If the "**`Individual Phases`**" is checked, and `G(@*)` is selected instead of `G`, the Gibbs energy curve of every phase as a function of composition will be calculated as shown by Figure 1.9.5;

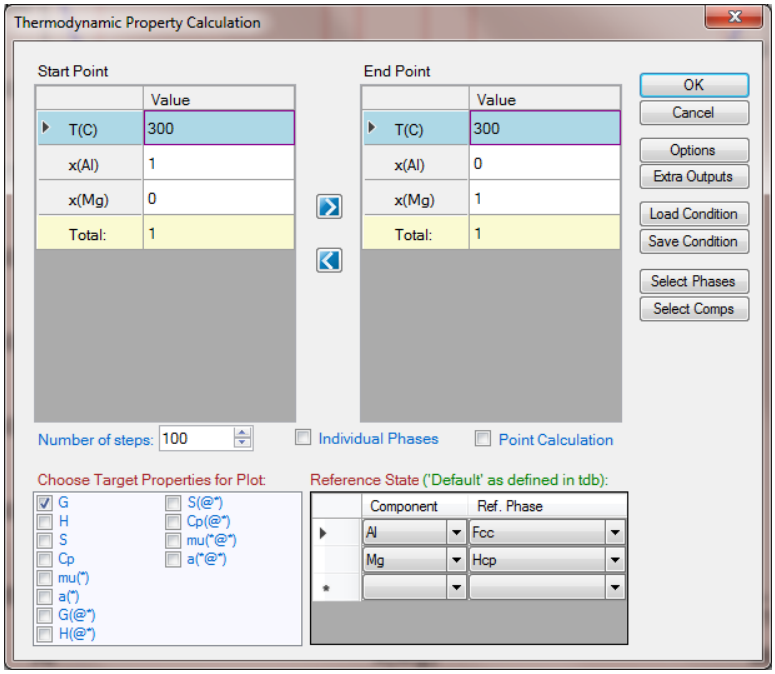


Figure 1.9.2: Calculation of the Gibbs energy for individual phases or the system from "Property" calculation

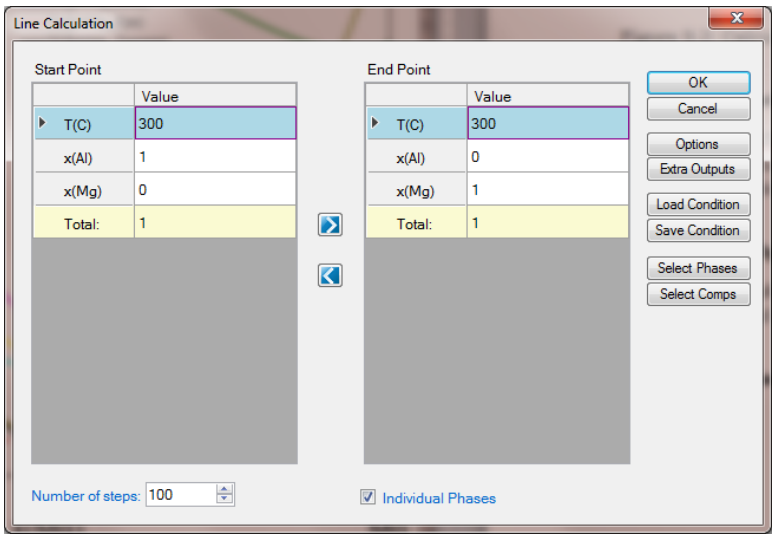


Figure 1.9.3: Calculation of the Gibbs energy for individual phases by Line calculation

Calculation Method 2, from Line calculation function in PanPhaseDiagram module:

- Load `AlMgZn.tdb` following the procedure in Pandat User's Guide 3.2.1, and select `Al` and `Mg` two components;
- Click "**`PanPhaseDiagram`**" on the menu bar and select "**`Line Calculation`**";
- Set Calculation Condition as shown in Figure 1.9.3, check the "**`Individual Phases`**";

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Add text and arrow on the plot following the procedure in Pandat User's Guide 2.3.3;

Information obtained from this calculation:

- Figure 1.9.4 shows the Gibbs energy of the system as a function of `x(Mg)`, i.e., the Gibbs energy at each composition represents the Gibbs energy of the stable phase(s) at that composition;
- Figure 1.9.5 shows the Gibbs energy curve of every individual phase as a function of x(Mg)
- Detail Gibbs energy values can be found in the "**`thermodynamic property`**" table

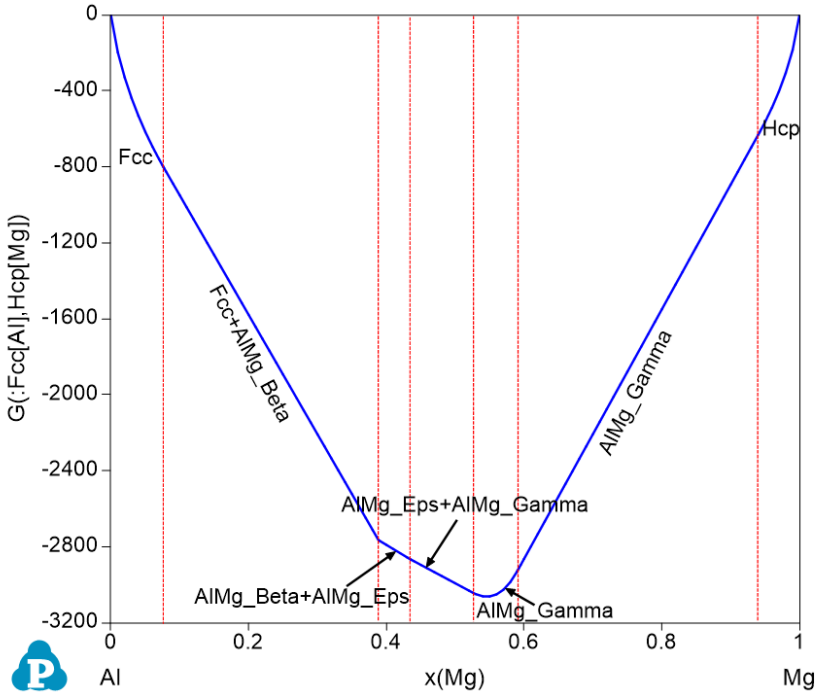


Figure 1.9.4: Calculated Gibbs energy of the system

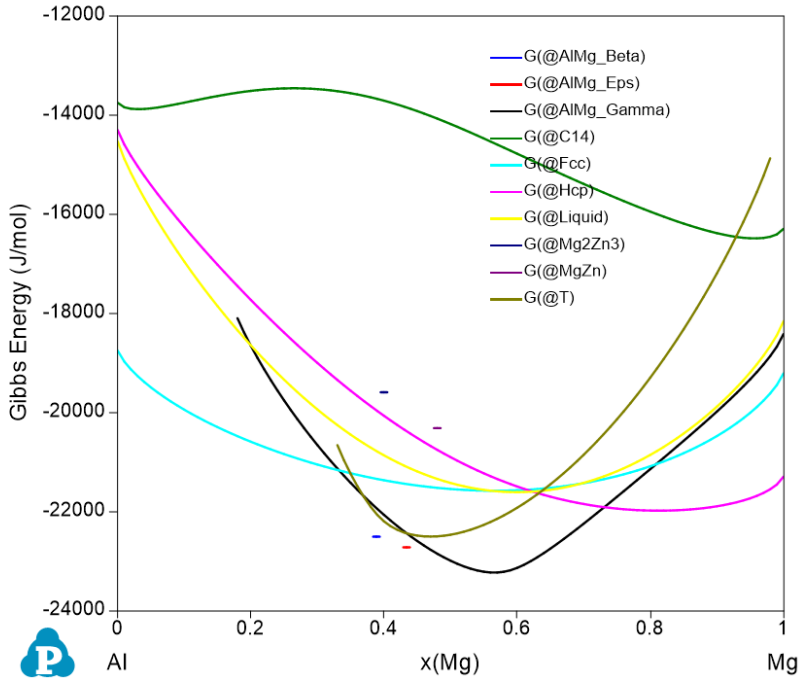


Figure 1.9.5: Calculated Gibbs energy of each individual phase by Line calculation

Example 1.10 Calculation of Activity at Constant Temperature

Purpose: Learn to calculate activities of components in a system

Module: PanPhaseDiagram

Thermodynamic Database: `AlMgZn.tdb`

Batch file: `Example_#1.10.pbfx`

Figure 1.10.1 is the `Al-Mg` binary phase diagram. In this example, we learn to calculate the activity of `Al` and `Mg` as a function of composition, `x(Mg)`, at 300°C (the red dash line).

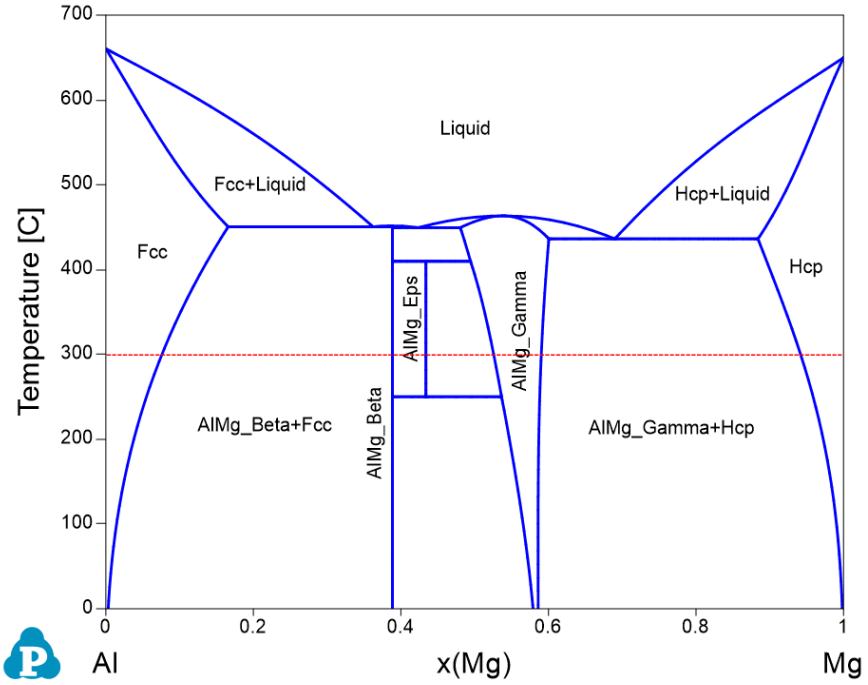


Figure 1.10.1: Al-Mg binary phase diagram

Calculation Method 1, From menu bar "Property":

- Load `AlMgZn.tdb` following the procedure in Pandat User's Guide 3.2.1, and select `Al` and `Mg` two components;
- Click "**`Property`**" on the menu bar and select "**`Thermodynamic Property`**";

- Set Calculation Condition as shown in Figure 1.10.2. The property selected is `a(*)`, and the reference states are set as `Fcc` for `Al` and `Hcp` for `Mg`; `(*)` means the activity of every component (both Al and Mg in this case);

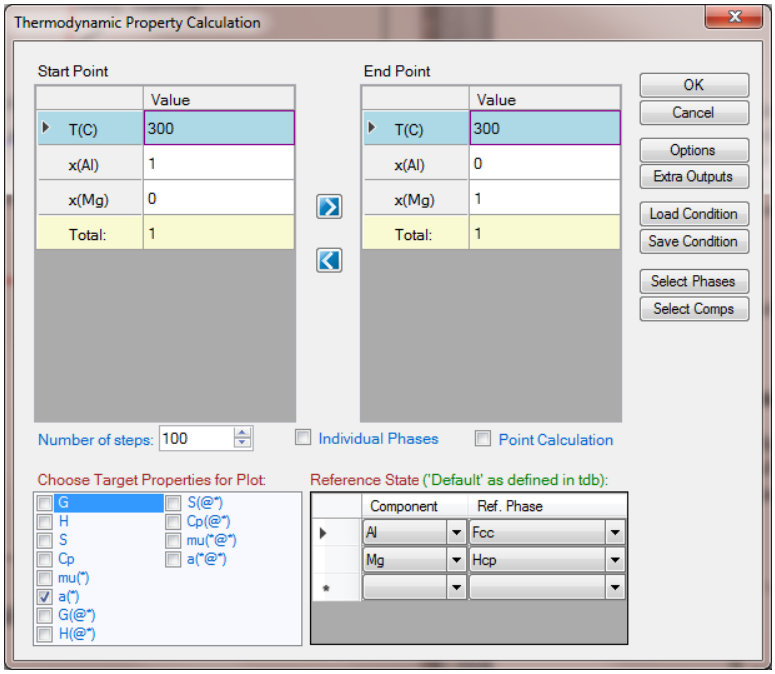


Figure 1.10.2: Calculation of the activity of Al and Mg from "Property" calculation

Calculation Method 2, From menu bar "PanPhaseDiagram":

- Load `AlMgZn.tdb` following the procedure in Pandat User's Guide 3.2.1, and select `Al` and `Mg` two components;
- Click "**`PanPhaseDiagram`**" on the menu bar and select "**`Line Calculation`**";
- Add the new table following the procedure in Pandat User's Guide 2.4.1;;

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Add text and arrow on the plot following the procedure in Pandat User's Guide 2.3.3;

Information obtained from this calculation:

- Figure 1.10.3 shows the activities of `Al` and `Mg` as a function of `x(Mg)` using `Fcc Al` and `Hcp Mg` as reference states;

- Activity of `Al` is `1` at `x(Al)=1` (`x(Mg)=0`) since it is pure `Fcc Al` at this temperature and `Fcc` is used as the reference state; Activity of `Al` decreases with the increase `x(Mg)` and becomes zero at `x(Mg)=1`;
- Activity of `Mg` is 0 at `x(Al)=1` (`x(Mg)=0`) and increases with the increase `x(Mg)` and becomes 1 at `x(Mg)=1`;
- Activity of either component is constant in a two-phase field.

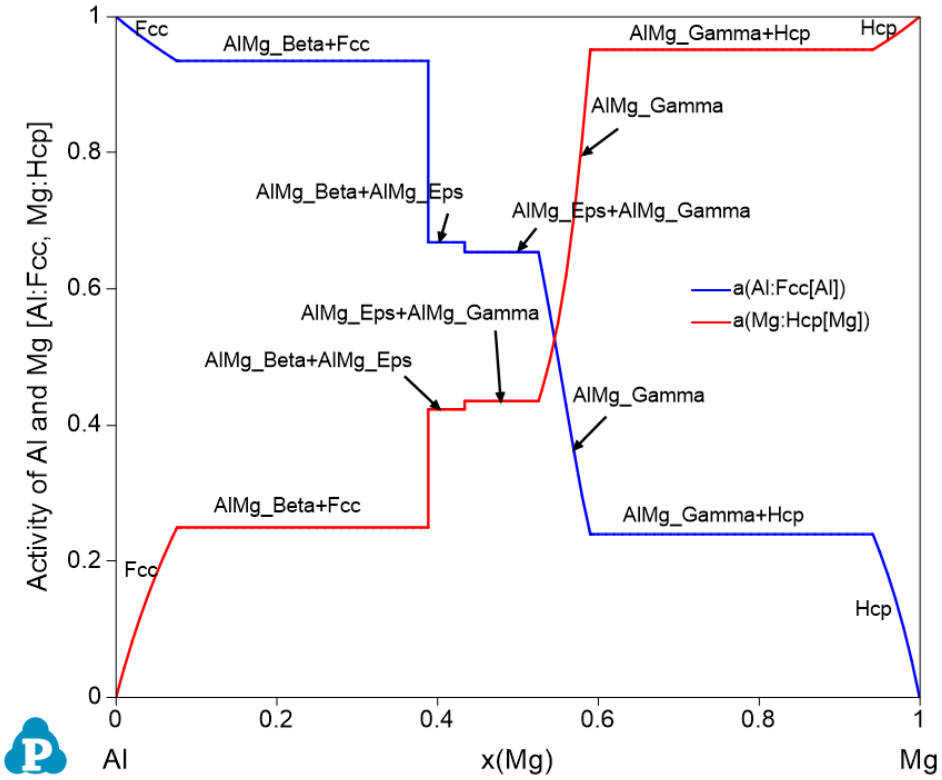


Figure 1.10.3: Activities of Al and Mg in Al-Mg binary at 300°C

Example 1.11 Calculation of Activity at Constant Composition

Purpose: Learn to calculate activities of components as a function of temperature

Module: PanPhaseDiagram

Thermodynamic Database: `AlMgZn.tdb`

Batch file: `Example_#1.11.pbfx`

Figure 1.11.1 is the `Al-Mg` binary phase diagram. In this example, we learn to calculate the activity of Al and Mg as a function of temperature at a fixed composition (the red dash line).

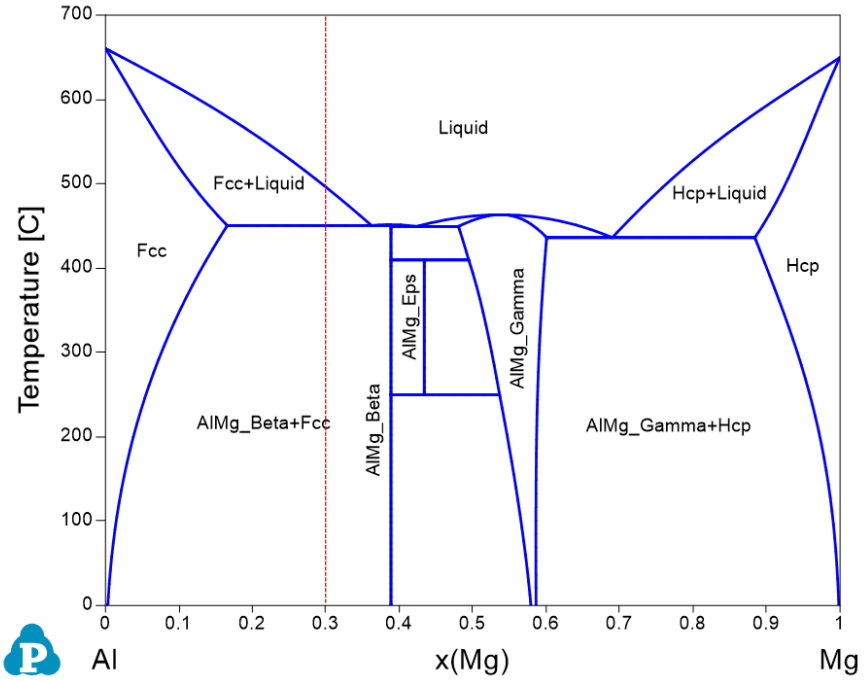


Figure 1.11.1: Al-Mg binary phase diagram

Calculation Method 1, From menu bar "Property":

- Load `AlMgZn.tdb` following the procedure in Pandat User's Guide 3.2.1, and select `Al` and `Mg` two components;
- Click "**`Property`**" on the menu bar and select "**`Thermodynamic Property`**";
- Set Calculation Condition as shown in Figure 1.11.2. The property selected is `a(*)`, and the reference states are set as `Liquid` for both `Al` and `Mg`;

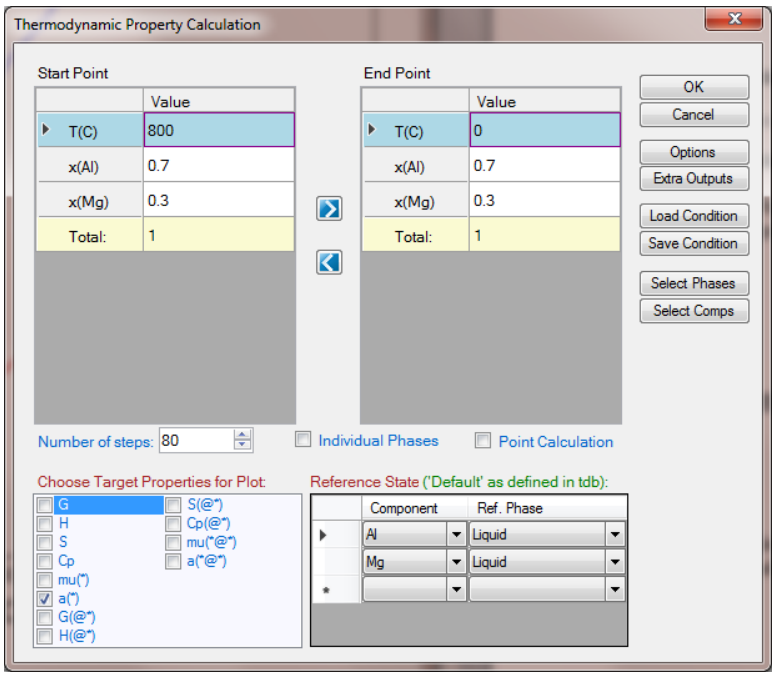


Figure 1.11.2: Calculation of the activity of Al and Mg from "Property" calculation

Calculation Method 2, From menu bar "PanPhaseDiagram":

- Load `AlMgZn.tdb` following the procedure in Pandat User's Guide 3.2.1, and select `Al` and `Mg` two components;
- Click "**`PanPhaseDiagram`**" on the menu bar and select "**`Line Calculation`**";
- Add the new table following the procedure in Pandat User's Guide 2.4.1;;

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Add text and arrow on the plot following the procedure in Pandat User's Guide 2.3.3;

Information obtained from this calculation:

- Figure 1.11.3 shows the activities of `Al` and `Mg` as a function of temperature using `Liquid Al` and `Liquid Mg` as reference states;
- In the `Liquid` phase field at high temperature, activities of both `Al` and `Mg` decrease as temperature decreases;

- In the `Fcc+Liquid` two-phase field, the activity of `Al` decreases as temperature decreases, but the activity of `Mg` increases as temperature decreases. This is because in this two-phase field the activity of each component follows its activity along the liquidus line. The composition of `Mg` increases along the liquidus line with decreasing temperature, which makes its activity increase;
- In the `AlMg_Beta+Fcc` two-phase field, activities of both `Al` and `Mg` decrease with the decrease of temperature refer to the `Liquid Al` and `Mg` reference states;

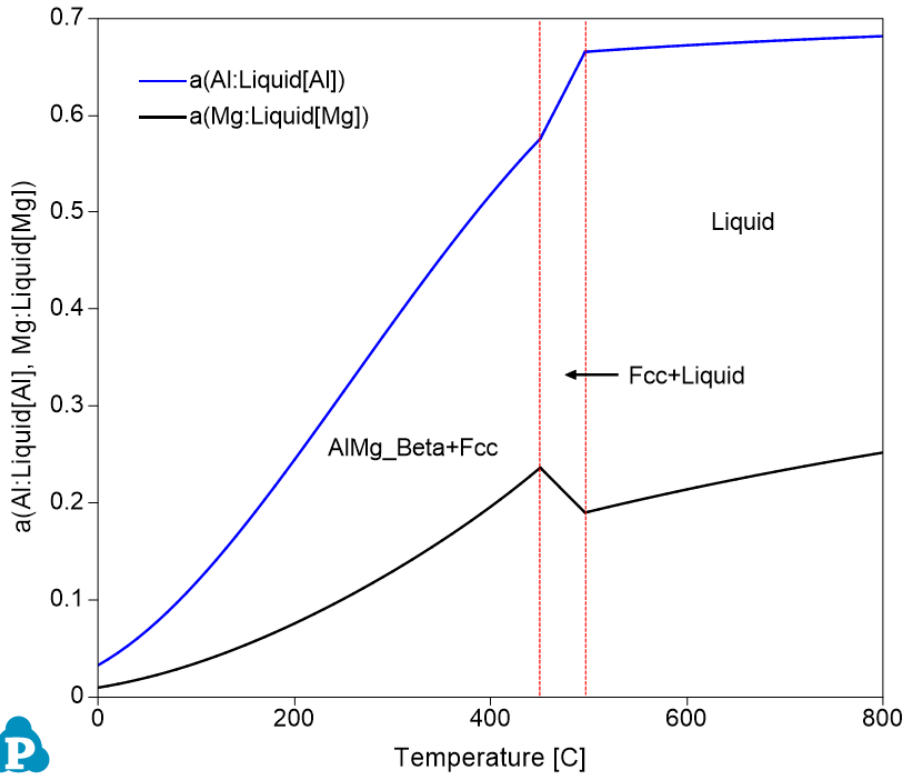


Figure 1.11.3: Activities of Al and Mg at 70% at% Al and 30 at% Mg as a function of temperature

Example 1.12 Calculation of Molar Volume and Density at Fixed Temperature

Purpose: Learn to calculate physical properties in a system

Module: PanPhaseDiagram

Thermodynamic and molar volume Database: `AlMg_MV.tdb`

Batch file: `Example_#1.12.pbfx`

Figure 1.12.1 is the `Al-Mg` binary phase diagram. In this example, we learn to calculate the molar volume and density of the system as a function of `x(Mg)` at 300°C (the red dash line).

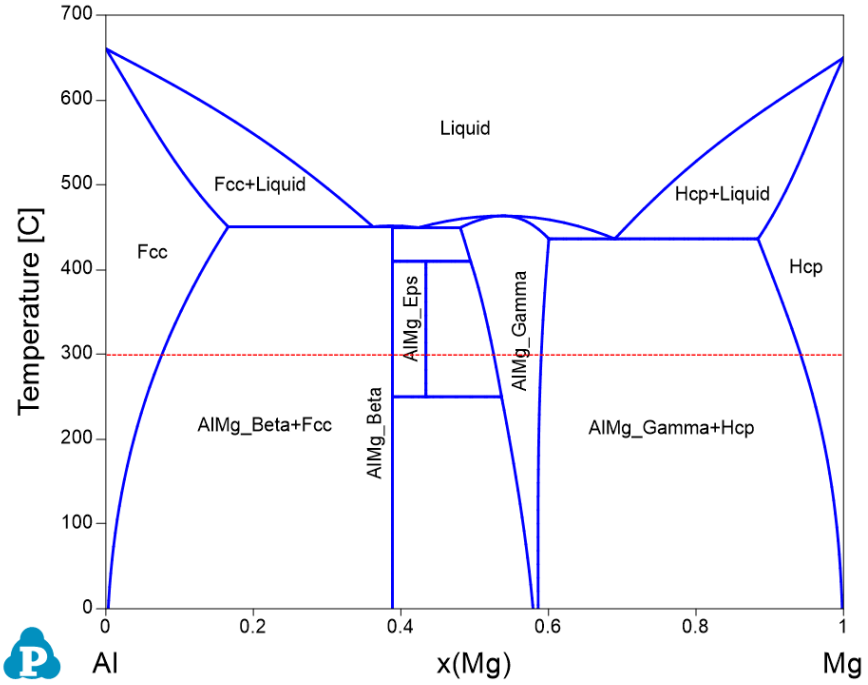


Figure 1.12.1: Al-Mg binary phase diagram

Calculation Method 1, From menu bar "Property":

- Load `AlMg_MV.tdb` following the procedure in Pandat User's Guide 3.2.1, and select `Al` and `Mg` two components;
- Click "**`Property`**" on the menu bar and select "**`Physical Property`**";
- Set Calculation Condition as shown in Figure 1.12.2. The property selected is `Vm` (molar volume) and density;

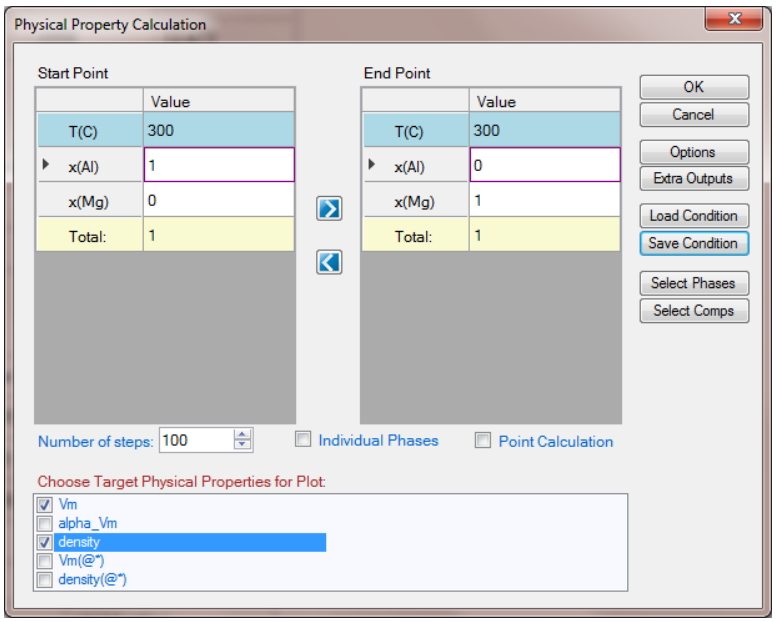


Figure 1.12.2: Setup calculation of molar volume and density from pure Al to pure Mg at 300 °C

Calculation Method 2, From menu bar "PanPhaseDiagram":

- Load `AlMg_MV.tdb` following the procedure in Pandat User's Guide 3.2.1, and select `Al` and `Mg` two components;
- Click "**`PanPhaseDiagram`**" on the menu bar and select "**`Line Calculation`**";
- Add the new table following the procedure in Pandat User's Guide 2.4.1, and select Table Type as "**`Physical_Property`**"

Information obtained from this calculation:

- Figure 1.12.3 shows the calculated molar volume which increases with the increase of Mg content;
- Figure 1.12.4 is the calculated density which shows the opposite trend as that of the molar volume;
- Details information can be found in the physical_property Table as shown in Figure 1.12.5;

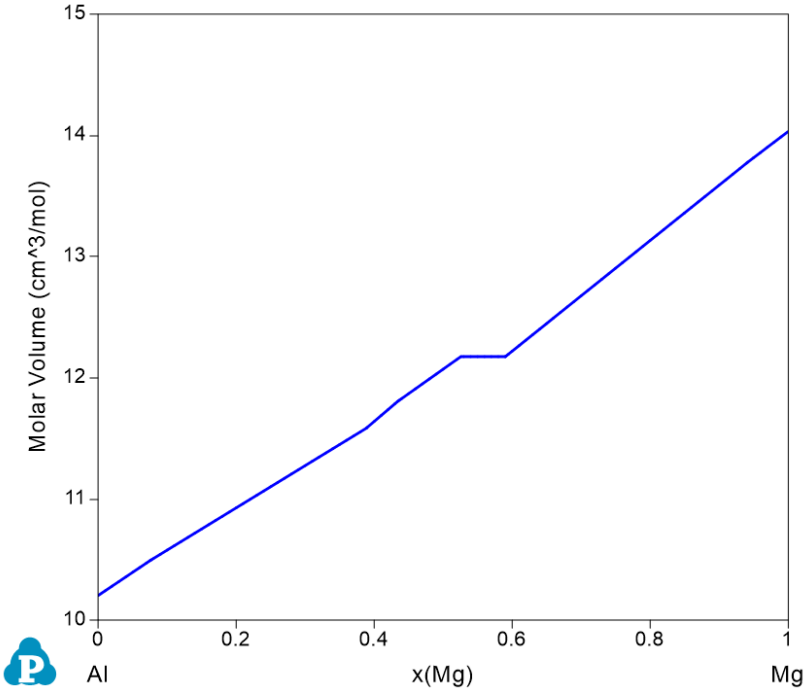


Figure 1.12.3: Calculated molar volume of the system from pure Al to pure Mg in Al-Mg binary at 300 °C

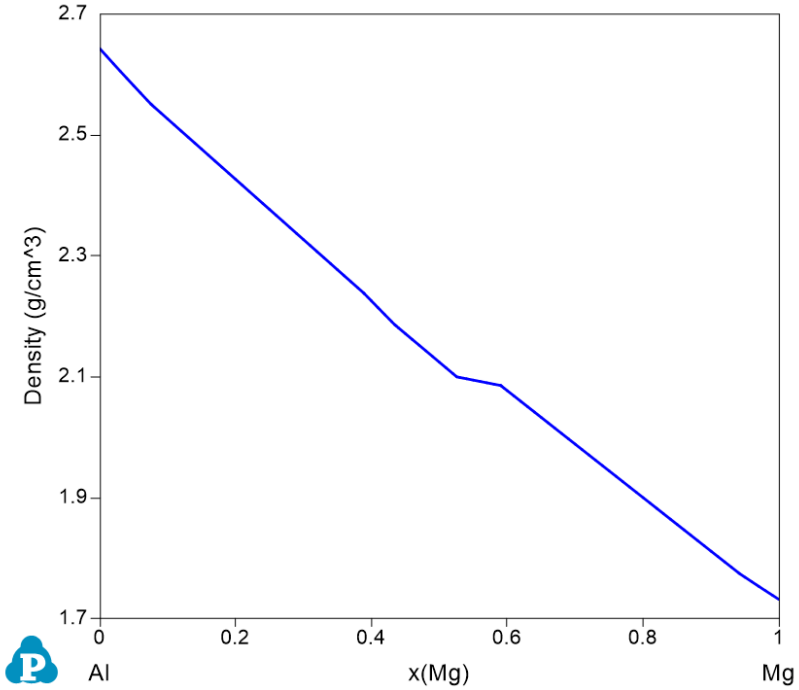
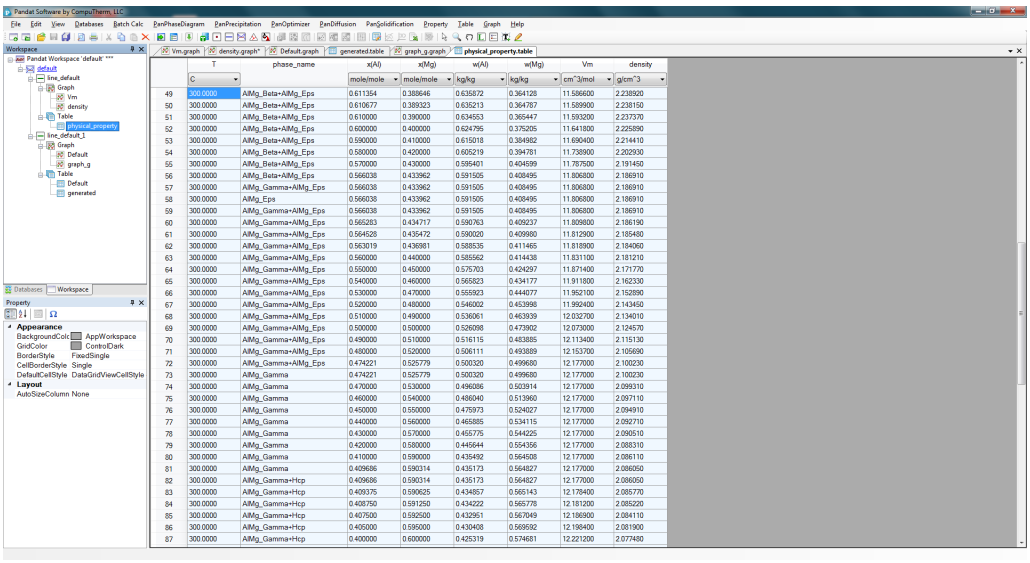


Figure 1.12.4: Calculated density from pure Al to pure Mg in Al-Mg binary at 300 °C



	T	phase_name	x(Al)	x(Mg)	w(Al)	w(Mg)	Vm	density
	C		mole/mole	mole/mole	kg/kg	kg/kg	cm^3/mol	g/cm^3
49	300.0000	AlMg_Beta+AlMg_Eps	0.611354	0.388646	0.635872	0.364128	11.586600	2.238920
50	300.0000	AlMg_Beta+AlMg_Eps	0.610677	0.389323	0.635213	0.364787	11.589900	2.238150
51	300.0000	AlMg_Beta+AlMg_Eps	0.610000	0.390000	0.634553	0.365447	11.593200	2.237370
52	300.0000	AlMg_Beta+AlMg_Eps	0.600000	0.400000	0.624795	0.375205	11.641800	2.225890
53	300.0000	AlMg_Beta+AlMg_Eps	0.590000	0.410000	0.615018	0.384982	11.690400	2.214410
54	300.0000	AlMg_Beta+AlMg_Eps	0.580000	0.420000	0.605219	0.394781	11.738900	2.202930
55	300.0000	AlMg_Beta+AlMg_Eps	0.570000	0.430000	0.595401	0.404599	11.787500	2.191450
56	300.0000	AlMg_Beta+AlMg_Eps	0.566038	0.433962	0.591505	0.408495	11.806800	2.186910
57	300.0000	AlMg_Gamma+AlMg_Eps	0.566038	0.433962	0.591505	0.408495	11.806800	2.186910
58	300.0000	AlMg_Eps	0.566038	0.433962	0.591505	0.408495	11.806800	2.186910
59	300.0000	AlMg_Gamma+AlMg_Eps	0.566038	0.433962	0.591505	0.408495	11.806800	2.186910
60	300.0000	AlMg_Gamma+AlMg_Eps	0.565283	0.434717	0.590763	0.409237	11.809800	2.186190
61	300.0000	AlMg_Gamma+AlMg_Eps	0.564528	0.435472	0.590020	0.409980	11.812900	2.185480
62	300.0000	AlMg_Gamma+AlMg_Eps	0.563019	0.436981	0.588535	0.411465	11.818900	2.184060
63	300.0000	AlMg_Gamma+AlMg_Eps	0.560000	0.440000	0.585562	0.414438	11.831100	2.181210
64	300.0000	AlMg_Gamma+AlMg_Eps	0.550000	0.450000	0.575703	0.424297	11.871400	2.171770
65	300.0000	AlMg_Gamma+AlMg_Eps	0.540000	0.460000	0.565823	0.434177	11.911800	2.162330
66	300.0000	AlMg_Gamma+AlMg_Eps	0.530000	0.470000	0.555923	0.444077	11.952100	2.152890
67	300.0000	AlMg_Gamma+AlMg_Eps	0.520000	0.480000	0.546002	0.453998	11.992400	2.143450
68	300.0000	AlMg_Gamma+AlMg_Eps	0.510000	0.490000	0.536061	0.463939	12.032700	2.134010
69	300.0000	AlMg_Gamma+AlMg_Eps	0.500000	0.500000	0.526098	0.473902	12.073000	2.124570
70	300.0000	AlMg_Gamma+AlMg_Eps	0.490000	0.510000	0.516115	0.483885	12.113400	2.115130
71	300.0000	AlMg_Gamma+AlMg_Eps	0.480000	0.520000	0.506111	0.493889	12.153700	2.105690
72	300.0000	AlMg_Gamma+AlMg_Eps	0.474221	0.525779	0.500320	0.499680	12.177000	2.100230
73	300.0000	AlMg_Gamma	0.474221	0.525779	0.500320	0.499680	12.177000	2.100230
74	300.0000	AlMg_Gamma	0.470000	0.530000	0.496086	0.503914	12.177000	2.099310
75	300.0000	AlMg_Gamma	0.460000	0.540000	0.486040	0.513960	12.177000	2.097110
76	300.0000	AlMg_Gamma	0.450000	0.550000	0.475973	0.524027	12.177000	2.094910
77	300.0000	AlMg_Gamma	0.440000	0.560000	0.465885	0.534115	12.177000	2.092710
78	300.0000	AlMg_Gamma	0.430000	0.570000	0.455775	0.544225	12.177000	2.090510
79	300.0000	AlMg_Gamma	0.420000	0.580000	0.445644	0.554356	12.177000	2.088310
80	300.0000	AlMg_Gamma	0.410000	0.590000	0.435492	0.564508	12.177000	2.086110
81	300.0000	AlMg_Gamma	0.409686	0.590314	0.435173	0.564827	12.177000	2.086050
82	300.0000	AlMg_Gamma+Hcp	0.409686	0.590314	0.435173	0.564827	12.177000	2.086050
83	300.0000	AlMg_Gamma+Hcp	0.409375	0.590625	0.434857	0.565143	12.179400	2.085770
84	300.0000	AlMg_Gamma+Hcp	0.408750	0.591250	0.434222	0.565778	12.181200	2.085220
85	300.0000	AlMg_Gamma+Hcp	0.407500	0.592500	0.432951	0.567049	12.186900	2.084110
86	300.0000	AlMg_Gamma+Hcp	0.405000	0.595000	0.430408	0.569592	12.198400	2.081900
87	300.0000	AlMg_Gamma+Hcp	0.400000	0.600000	0.425319	0.574681	12.221200	2.077480

Figure 1.12.5: The physical_property table showing the stable phases varying with the composition and the calculated molar volume and density

Example 1.13 Calculation of Molar Volume and Density at Fixed Composition

Purpose: Learn to calculate physical properties in a system

Module: PanPhaseDiagram

Thermodynamic and molar volume Database `AlMg_MV.tdb`

Batch file: `Example_#1.13.pbfx`

Figure 1.13.1 is the `Al-Mg` binary phase diagram. In this example, we learn to calculate the molar volume and density of the system as a function of temperature at a fixed composition (the red dash line).

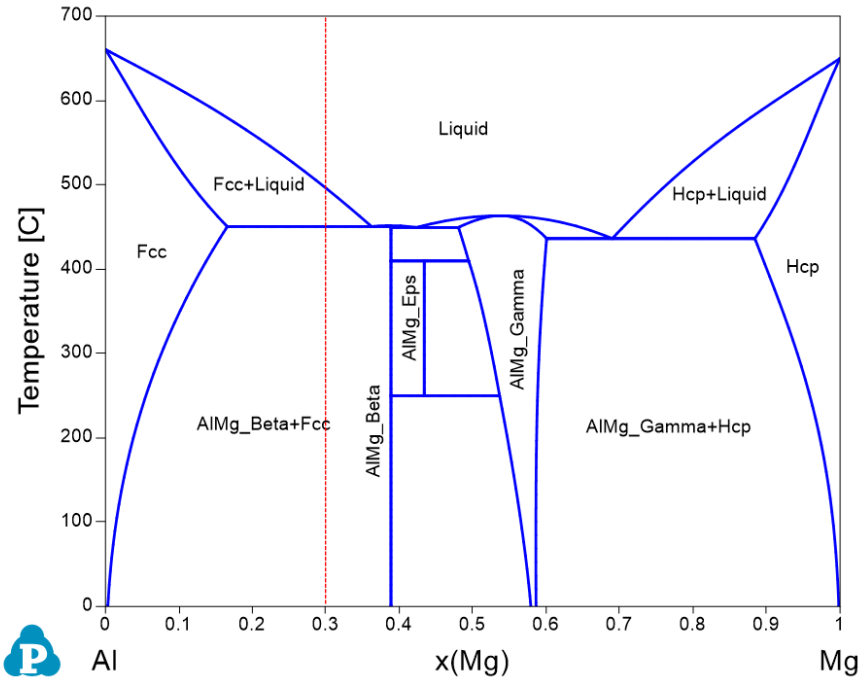


Figure 1.13.1: Al-Mg binary phase diagram

Calculation Method 1, From menu bar "Property":

- Load `AlMg_MV.tdb` following the procedure in Pandat User's Guide 3.2.1, and select `Al` and `Mg` two components;
- Click "**`Property`**" on the menu bar and select "**`Physical Property`**";

- Set Calculation Condition as shown in Figure 1.13.2. The property selected is `Vm` (molar volume) and density;

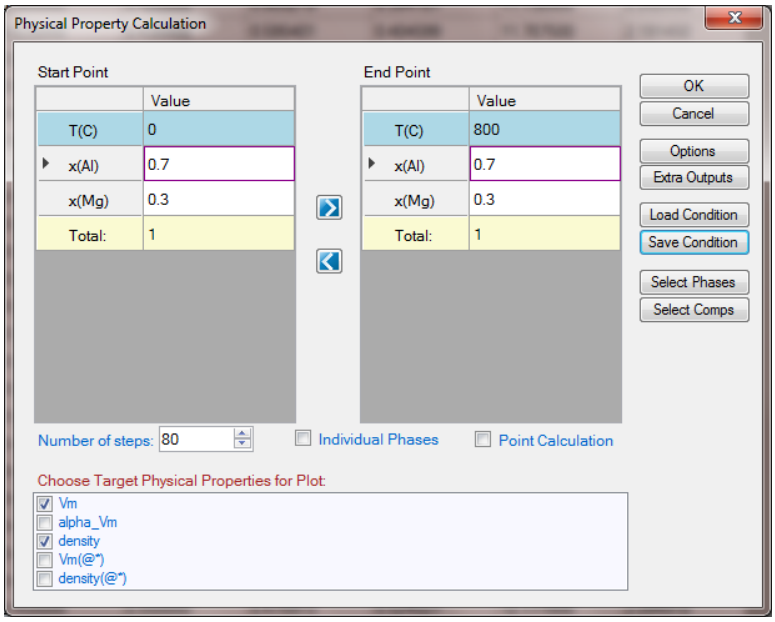


Figure 1.13.2: Setup calculation of molar volume and density from 0 to 800 °C at a fixed composition

Calculation Method 2, From menu bar "PanPhaseDiagram":

- Load `AlMg_MV.tdb` following the procedure in Pandat User's Guide 3.2.1, and select `Al` and `Mg` two components;
- Click "**`PanPhaseDiagram`**" on the menu bar and select "**`Line Calculation`**";
- Add the new table following the procedure in Pandat User's Guide 2.4.1, and select Table Type as "**`Physical_Property`**"

Information obtained from this calculation:

- Figure 1.13.3 Calculated molar volume of the system in Al-Mg binary from 0 to 800°C at a fixed composition
- Figure 1.13.4 is the calculated density which shows the opposite trend as that of the molar volume;
- Details information can be found in the physical_property Table.

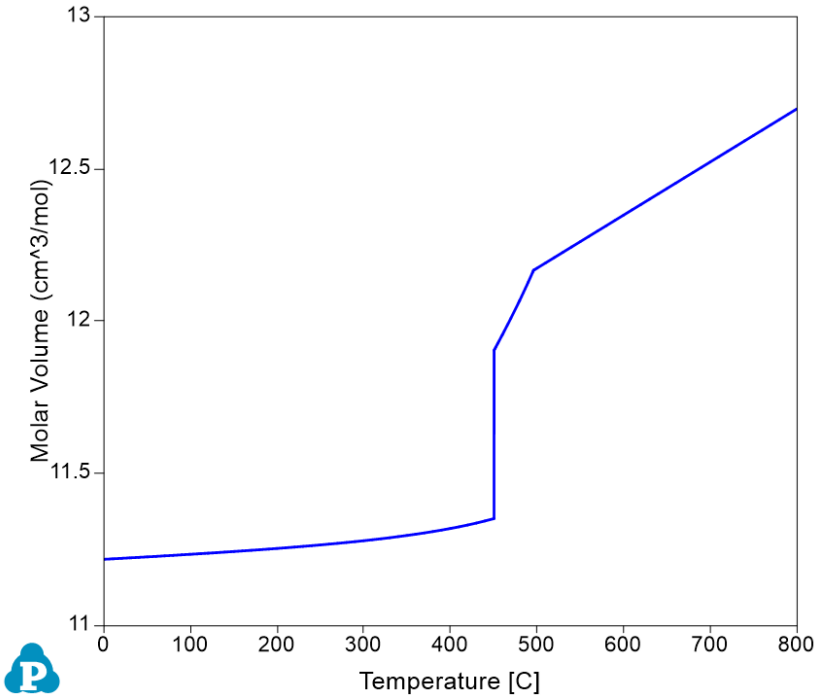


Figure 1.13.3: Calculated molar volume of the system in Al-Mg binary from 0 to 800°C at a fixed composition

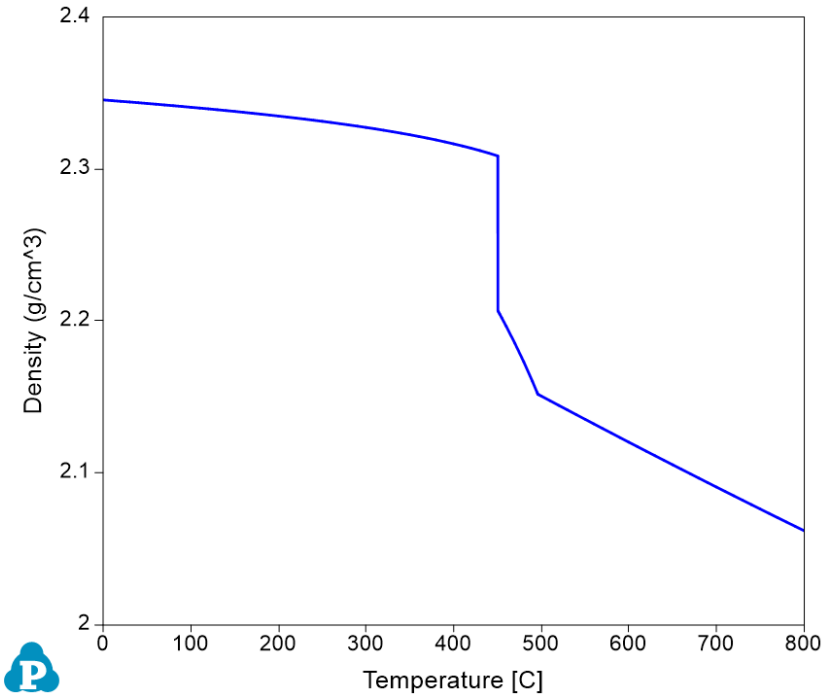


Figure 1.13.4: Calculated density of the system in Al-Mg binary from 0 to 800°C at a fixed composition

Example 1.14 Density Contour Diagram

Purpose: Learn to calculate density contour diagram. In this example, the density contour lines will be plotted in the Al-Mg binary phase diagram so that density at different temperatures and compositions can be viewed together with phase stability.

Module: PanPhaseDiagram

Thermodynamic and molar volume Database `AlMg_MV.tdb`

Batch file: `Example_#1.14.pbfx`

Calculation Procedures:

- Load `AlMg_MV.tdb` following the procedure in Pandat User's Guide 3.2.1, and select `Al` and `Mg` two components;
- First set up the calculation condition as shown in Figure 1.14.1 in the same way as we did to calculate Al-Mg binary phase diagram (see Example 1.1 : Al-Mg Binary Phase Diagram), then click "**`Contour Lines`**" to open the contour line dialog as shown in Figure 1.14.2;

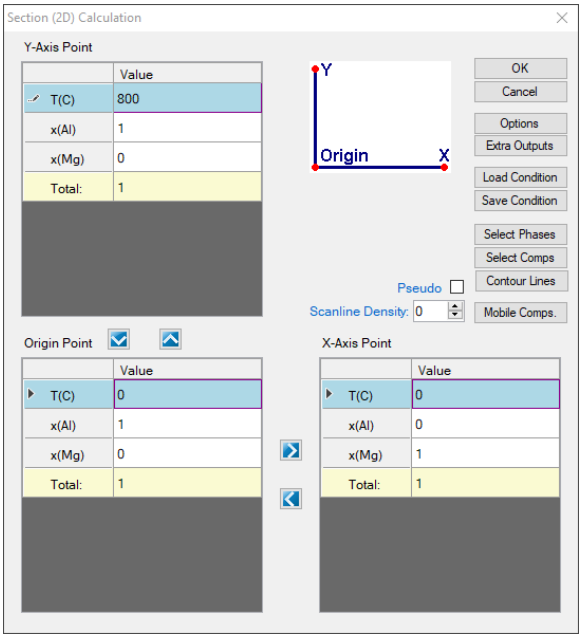


Figure 1.14.1: Setup calculation for the Al-Mg binary phase diagram, then press "Contour Lines"

- Choose “**Density**” and click **Add**. the contour type of density will be added as shown in Figure 1.14.2, then press OK;

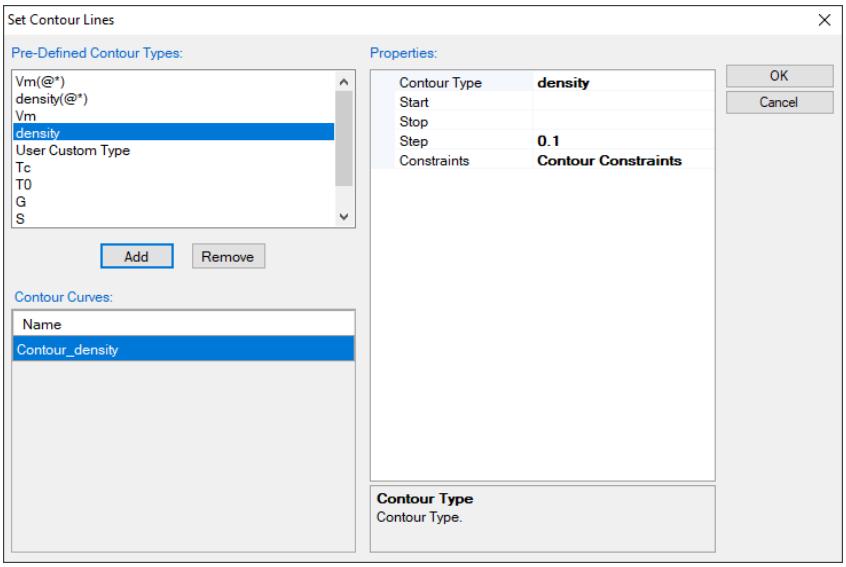


Figure 1.14.2: Add “density” contour lines in the "set contour lines" window

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User’s Guide 2.3.1;
- Label each line by putting the cursor on each line and wait for the tool tip to pop out, then press F2;

Information obtained from this calculation:

- Figure 1.14.3 shows the density contour diagram, i.e., plotting density contour lines on top of the Al-Mg binary phase diagram. The density on the same red line is constant;
- Density contour diagram is very useful in alloy design. Given the requirements on stable phases and alloy density, the alloy compositions can be identified from this one diagram;

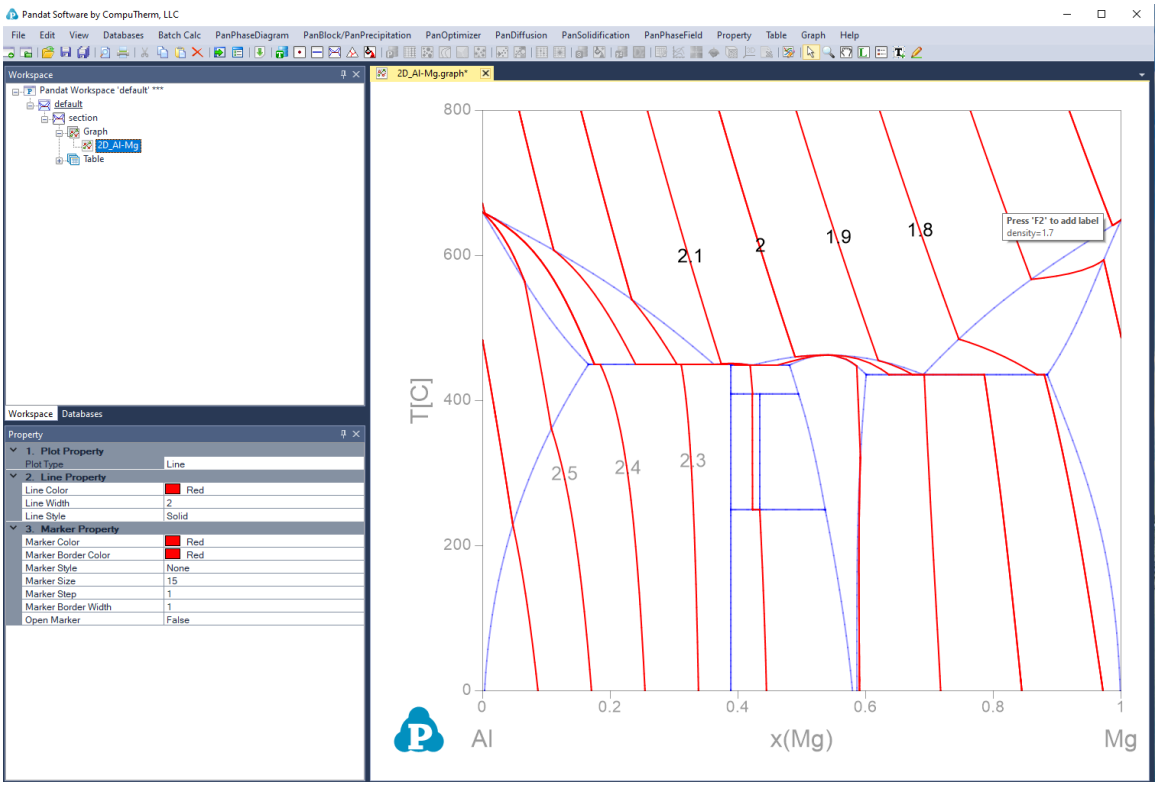


Figure 1.14.3: Density contour diagram for the Al-Mg binary system

Example 1.15 Activity Contour Diagram

Purpose: Learn to calculate activity contour diagram. In this example, the activity contour lines of Mg will be calculated and plotted on the isothermal section of the Al-Mg-Zn ternary system at 500 °C.

Module: PanPhaseDiagram

Thermodynamic Database: `AlMgZn.tdb`

Batch file: `Example_#1.15.pbfx`

Calculation Procedures:

- Load `AlMgZn.tdb` following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- First set up the calculation condition as shown in Figure 1.15.1 in the same way as we did to calculate Al-Mg-Zn isotherm (see Example 1.5 : Isotherm of Al-Mg-Zn at 500°C), then click "**`Contour Lines`**" to open the contour line dialog as shown in Figure 1.15.2;

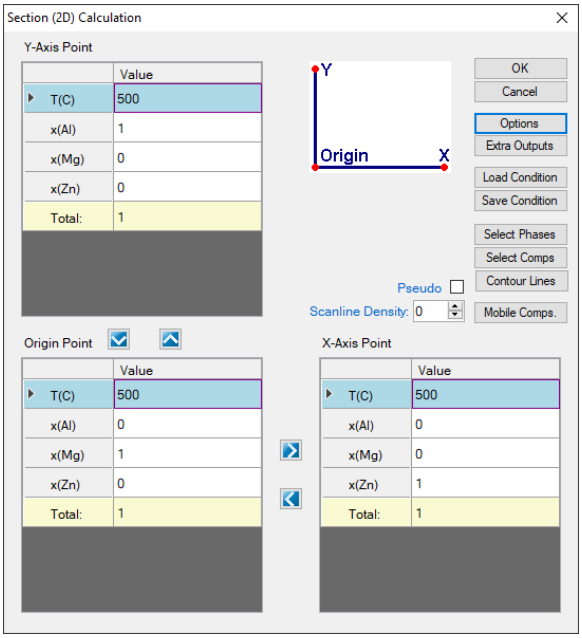


Figure 1.15.1: Setup calculation for an isotherm in the Al-Mg-Zn ternary at 500°C, then press "Contour Lines"

- Choose "**User Custom Type**" and click **Add**Type in "a(Mg:Hcp)" for the Contour Type in the "**Properties**" window as shown in Figure 1.15.2, then press OK;

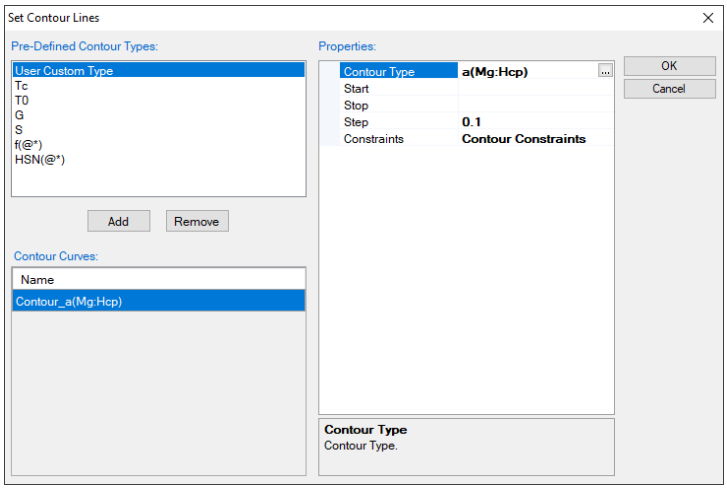


Figure 1.15.2: Type in "a(Mg:Hcp)" for the Contour Type in the "Properties" window, it is to calculate the activity of Mg contour lines using Hcp Mg as reference state

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Label each line by putting the cursor on each line and wait for the tool tip to pop out, then press F2;

Information obtained from this calculation:

- Figure 1.15.3 shows the activity contour diagram of Mg at 500 °C. The variation of Mg activity in the composition triangle is clearly seen at this temperature;
- Activity contour lines can also be plotted only in the selected phase field, such as in the Liquid phase field, in the Liquid+Fcc phase field. An example is given in Pandat User's Guide 3.3.5.1;

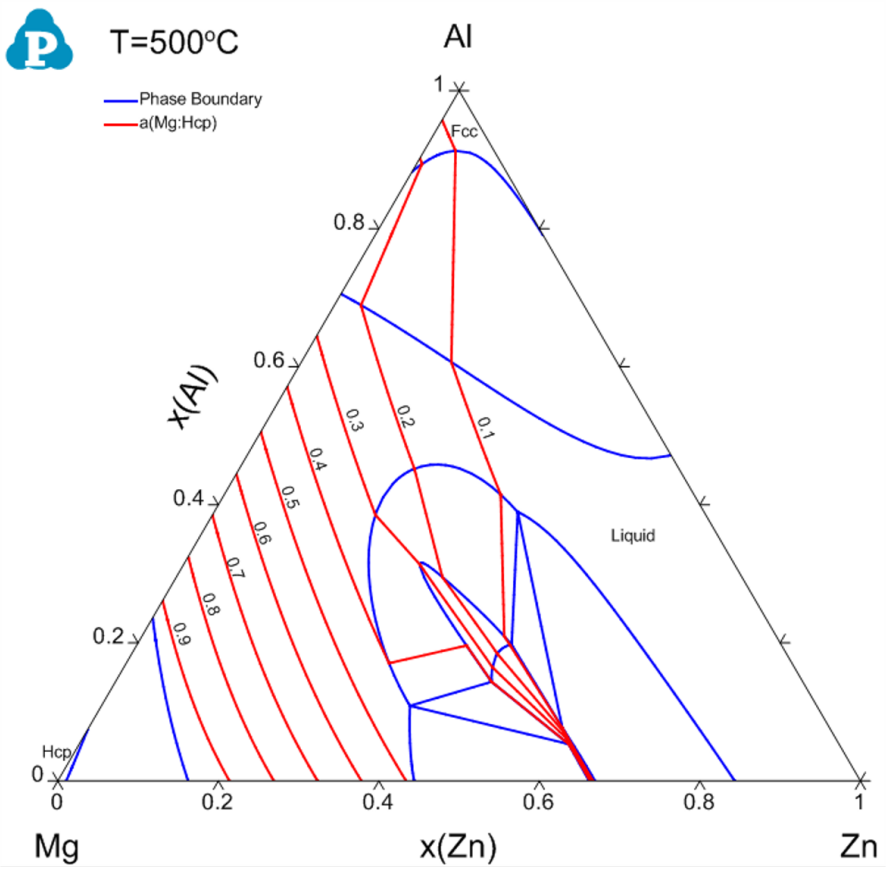


Figure 1.15.3: Activity contour diagram of Mg in the Al-Mg-Zn ternary at 500 °C

Example 1.16 Pressure Contour Diagram

Purpose: Learn to calculate pressure contour diagram. In this example, the pressure contour lines of total pressure and partial pressure of N2 in the Ti-N system will be calculated and plotted on the Ti-N binary phase diagram.

Module: PanPhaseDiagram

Thermodynamic Database: `TiN_Gas_Pressure.tdb`

Batch file: `Example_#1.16.pbfx`

Calculation Procedures:

- Load `TiN_Gas_Pressure.tdb` following the procedure in Pandat User's Guide 3.2.1, and select both Ti, Ni components;
- First set up the calculation condition as shown in Figure 1.16.1 for calculating Ti-N binary phase diagram, then click "**`Contour Lines`**" to open the contour line dialog as shown in Figure 1.16.2;

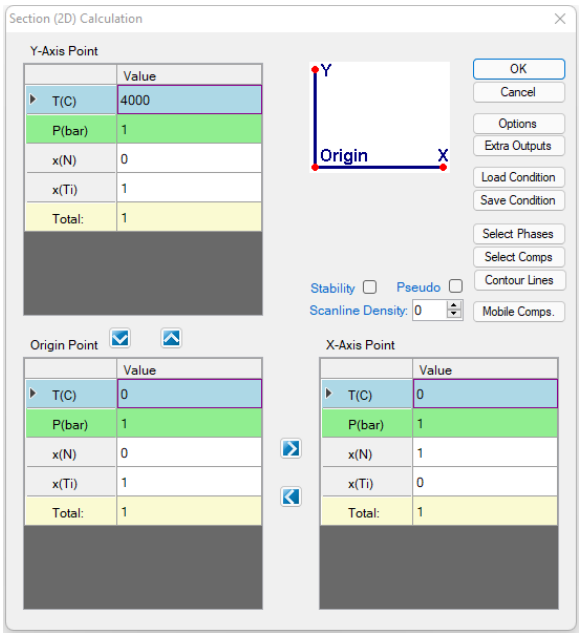


Figure 1.16.1: Setup calculation for Ti-N binary phase diagram, then click "Contour Lines"

- Choose “**User Custom Type**” and click **Add**Type in “`log(P(@gas))`” for the Contour Type in the “**Properties**” window as shown in Figure 1.16.2, then press OK;

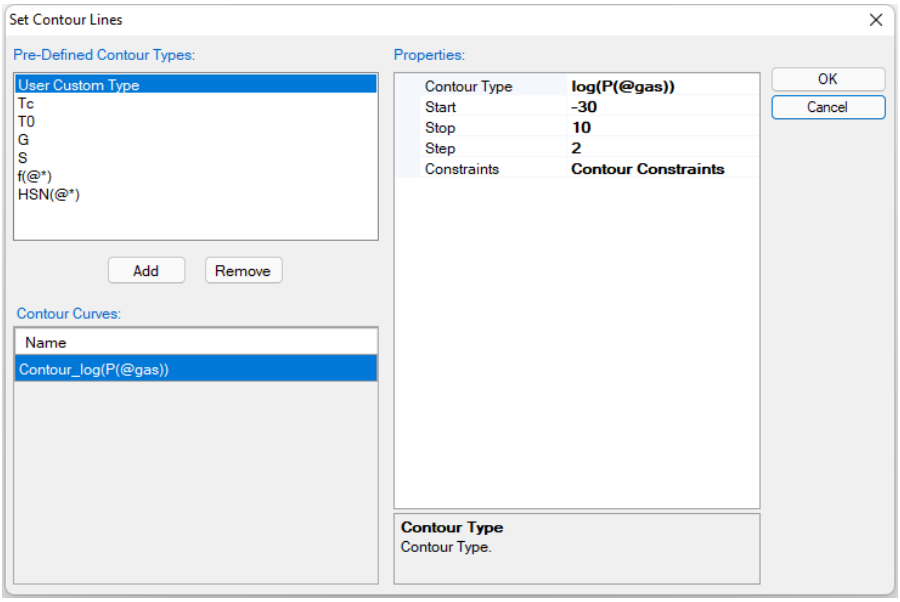


Figure 1.16.2: Type in “log(P(@gas))” for the Contour Type in the “Properties” window, it is to calculate the total pressure contour lines from logP = -30 to 10 with step 2

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User’s Guide 2.3.1;
- Label each line by putting the cursor on each line and wait for the tool tip to pop out, then press F2;

Information obtained from this calculation:

- Figure 1.16.3 shows the contour diagram of total pressure in Ti-N system;
- If we type in “log(P(N2@gas))” as the Contour Type in the “Properties” window in Figure 1.16.2, we will obtained the contour diagram for partial pressure logP(N2) as shown in Figure 1.16.4;

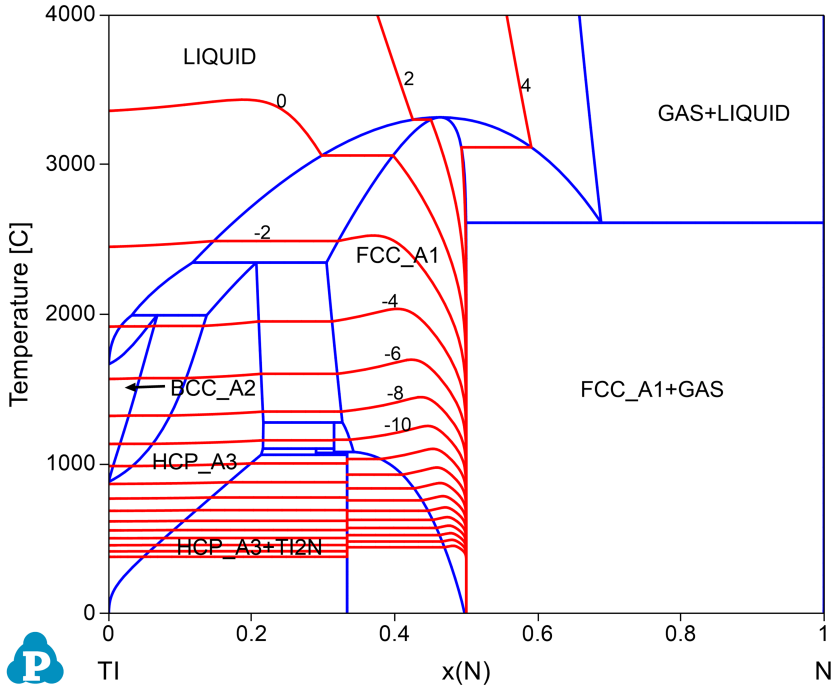


Figure 1.16.3: Calculated contour diagram of total pressure in the Ti-N system

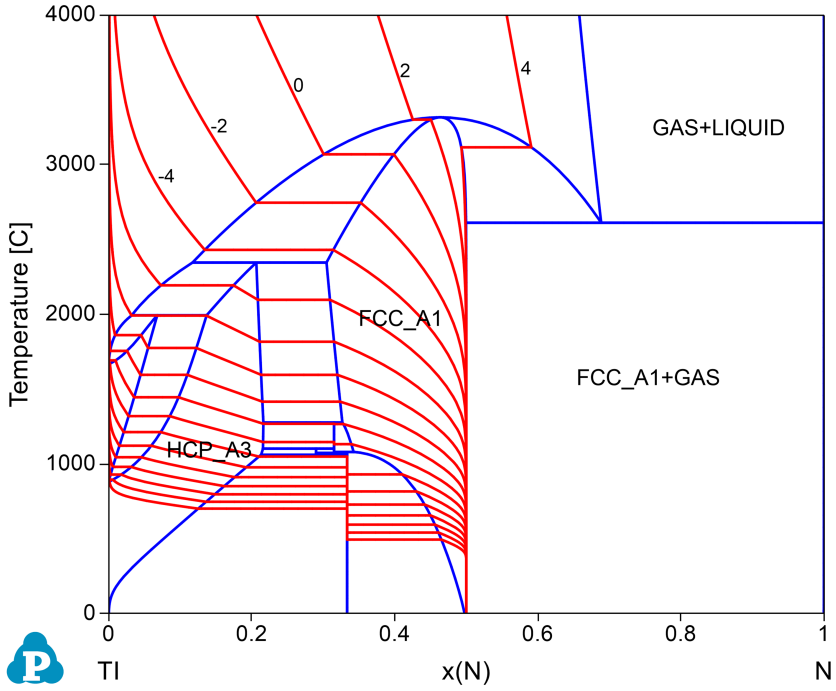


Figure 1.16.4: Calculated contour diagram of partial pressure of N_2 in the Ti-N system

Example 1.17 3D Diagram

Purpose: Learn to calculate a 3D diagram. In this example, 3D diagram is calculated for a hypothetical ternary system

Module: PanPhaseDiagram

Thermodynamic Database: `ABC.tdb`

Batch file: `Example_#1.17.pbfx`

Calculation Procedures:

- Load `ABC.tdb` following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Perform phase projection following the procedure in Pandat User's Guide 3.3.6;
- Set calculation condition as shown in Figure 1.17.1. From this setting, * is selected as Target Phase which means all the phases in the system are selected in the calculation.

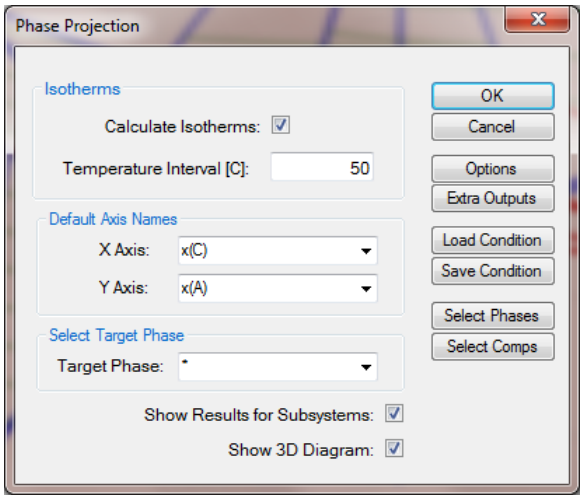


Figure 1.17.1: Setup calculation for a 3D diagram

Post Calculation Operation:

- In the Property window, under "**`4: Invariant Tieline Property`**", choose "**`True`**" for the "**`Show Invariant Tieline`**", the invariant reaction lines in the three binaries as well as in the ternary will be shown (Figure 1.17.2);

- Rotate the 3D diagram to a position you like;
- Add a new Table as shown in Figure 1.17.3 to get the phase boundary data just for the BCC phase. Select `x(C)` as x-axis by selecting this column first, then press **`Ctrl`** and select `x(A)` as y-axis, then press **`Ctrl`** and select `T` as z-axis, plot 3D diagram as shown in Figure 1.17.4;
- Add a new Table as shown in Figure 1.17.5 to get the isothermal lines just for the BCC phase, notice that the Table Type must be "**`isotherm`**";
- Double click to open the 3D diagram for BCC (Figure 1.17.4), single click the table name for the isothermal lines. From the **`Property`** window, drag in `x(C)` first, then press **`Ctrl`** and drag in `x(A)`, then press **`Shift`** and drag in `T`, the isothermal lines for the BCC phase will be plotted on it as shown in Figure 1.17.6;

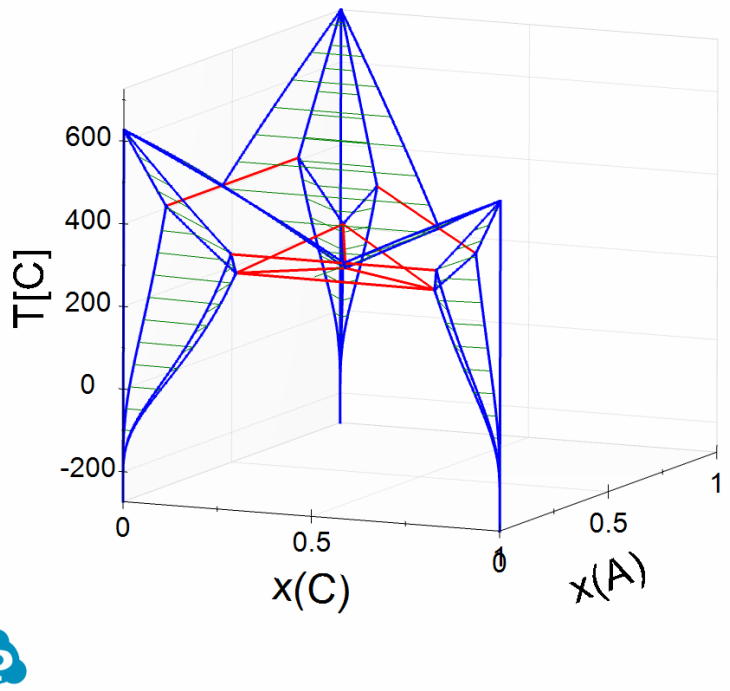


Figure 1.17.2: Calculated liquidus projection of the Al-Mg-Zn system

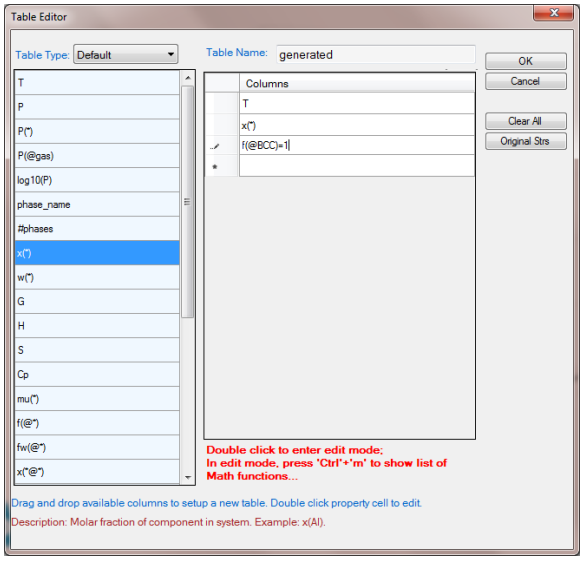


Figure 1.17.3: Add a new Table to get the phase boundary data just for the BCC phase

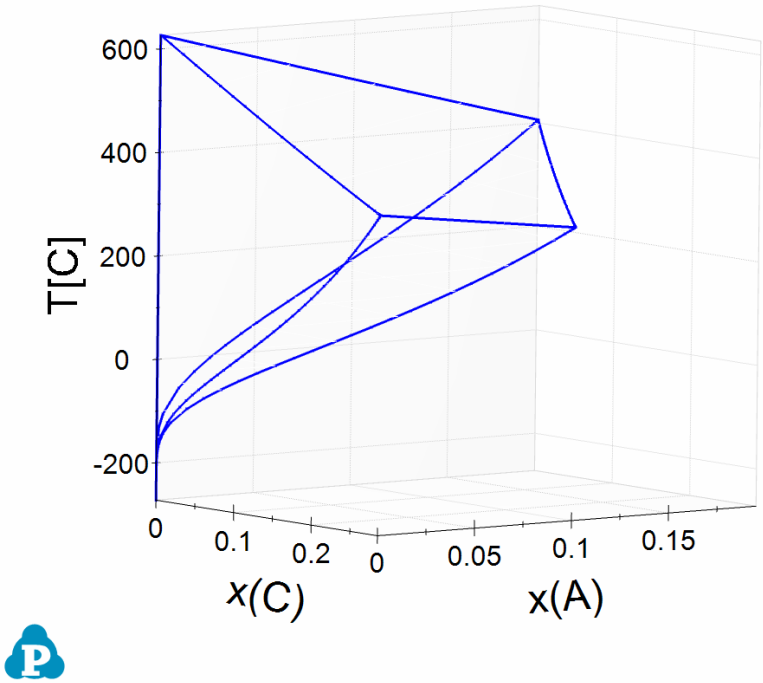


Figure 1.17.4: Plot 3D diagram for BCC phase only

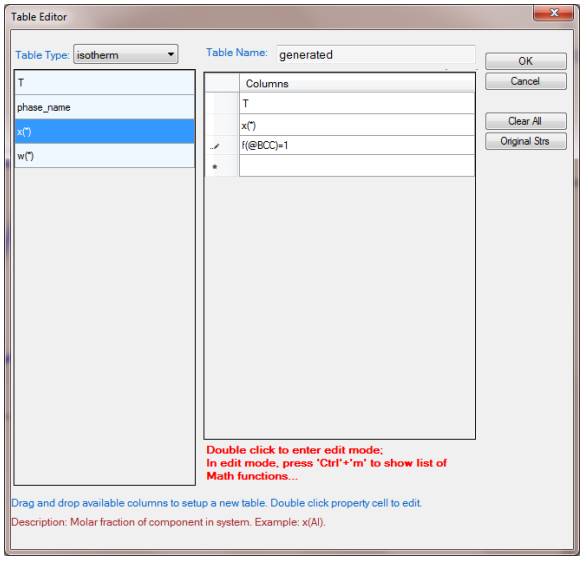


Figure 1.17.5: Add a new Table to get the isothermal lines just for the BCC phase

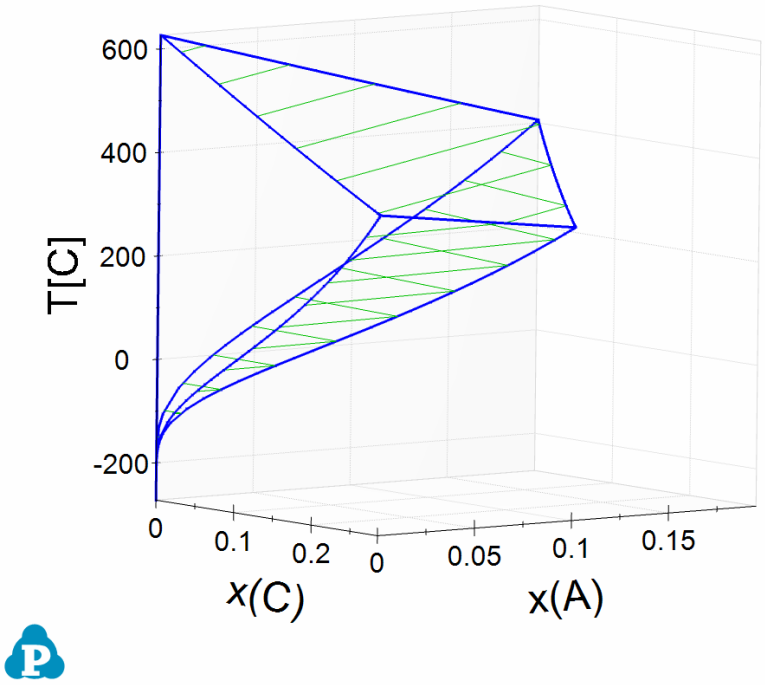


Figure 1.17.6: 3D diagram for the BCC phase with isothermal lines

Example 1.18 Temperature-Pressure Diagram

Purpose: Learn to calculate a Temperature-Pressure diagram. In this example, a Temperature-Pressure diagram is calculated for pure Fe component.

Module: PanPhaseDiagram

Thermodynamic Database: `Fe_Pressure.tdb`

Batch file: `Example_#1.18.pbfx`

Calculation Procedures:

- Load `Fe_Pressure.tdb` following the procedure in Pandat User's Guide 3.2.1;
- Perform a Section Calculation from PanPhaseDiagram, and set the calculation condition as shown in Figure 1.18.1;

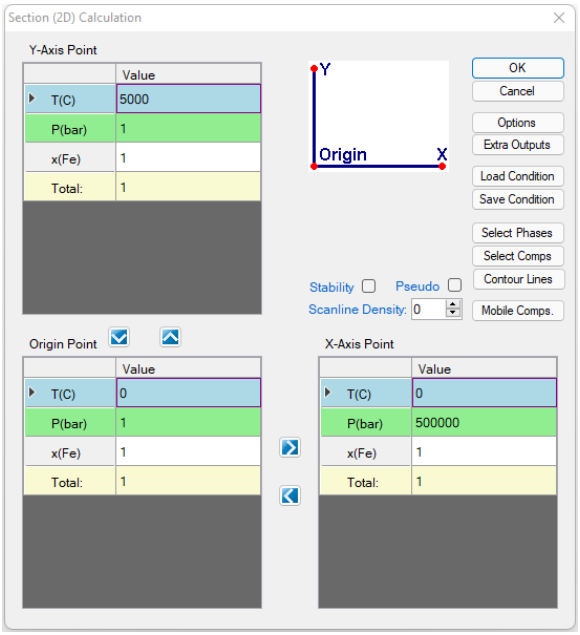


Figure 1.18.1: Setup calculation of T-P diagram for pure Fe, x-axis is P and y-axis is T

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Label the graph following the procedure in Pandat User's Guide 2.3.3;

Information obtained from this calculation:

- Figure 1.18.2 shows the default plot when calculation is finished, it is T-log10(P). It clearly demonstrates the stability of each phase at different temperature and pressure;
- Detailed information on the three-phase reactions, i.e., the temperatures and pressures at triple points can be found in the “invariant” table;
- From Default table, other plots, such as T-P diagram, can be plotted as shown in Figure 1.18.3;

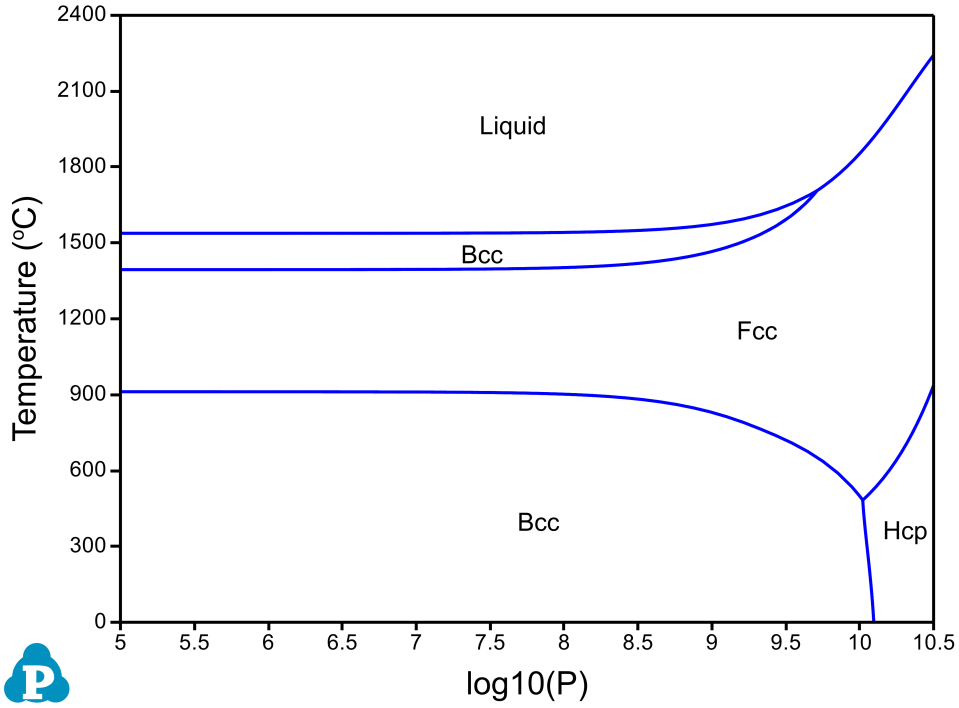


Figure 1.18.2: Temperature-log (Pressure) diagram for pure Fe component

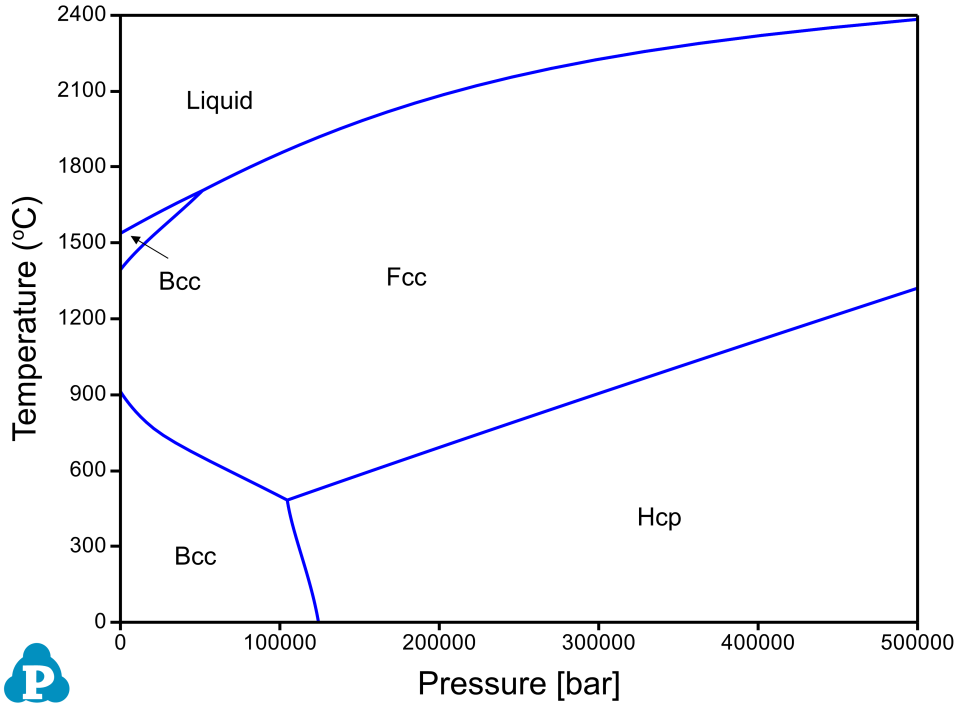


Figure 1.18.3: Temperature-Pressure diagram for pure Fe component

Example 1.19 Phase Fraction Contour Diagram for Ti64

Purpose: Learn to calculate and plot phase fraction contour diagram in a multi-component system. In this example, a contour diagram is calculated and plotted for an isopleth in the Ti-Al-V-N-O five components system.

Module: PanPhaseDiagram

Thermodynamic Database: `PanTi.pdb`(this database is a thermodynamic database for multi-component titanium alloys which is only available to users who have licensed it.)

Calculation Procedures:

- Load `PanTi.pdb` following the procedure in Pandat User's Guide 3.2.1;
- Perform a Section Calculation from PanPhaseDiagram, and set the calculation condition as shown in Figure 1.19.1;

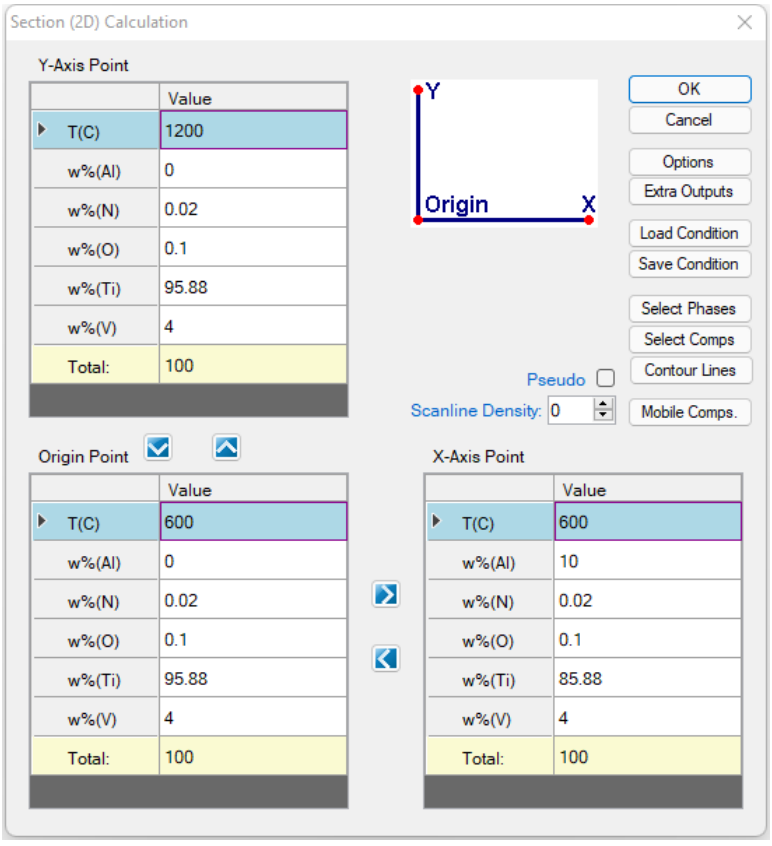


Figure 1.19.1: Setup a calculation for an isopleth along Ti-Al side with fixed V, O, and N compositions

- Click “Contour Lines” in the dialog shown in Figure 1.19.1, then set the Contour Type as shown in Figure Figure 1.19.2;

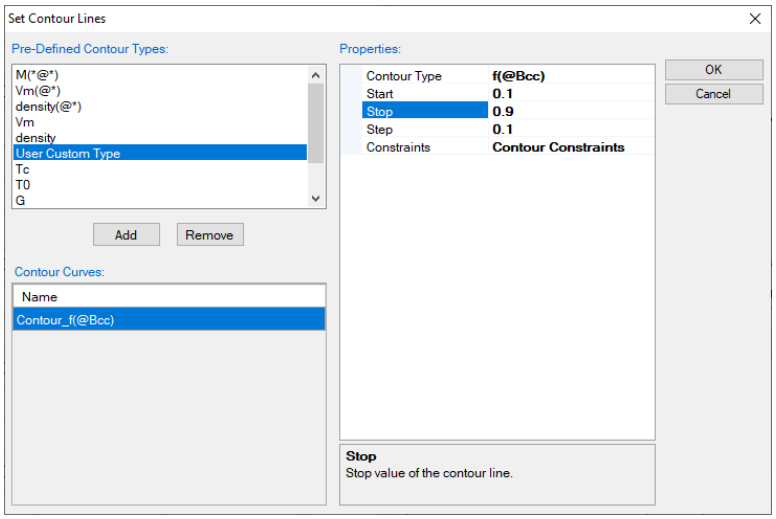


Figure 1.19.2: Setup contour lines as the fraction of Bcc (β) phase

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User’s Guide 2.3.1;
- Label the graph following the procedure in Pandat User’s Guide 2.3.3;
- Label each line by putting the cursor on each line and wait for the tool tip to pop out, then press F2;

Information obtained from this calculation:

- Figure 1.19.3 shows the isopleth Ti-Al-4V-0.1O-0.02N (wt%) with contour lines of fractions of the β phase. It clearly shows how the fraction of the β phase varies with temperature and composition. This plot provides a guidance on the selection of alloy composition and heat treatment condition if certain fraction of β phase is needed in the microstructure;
- For Ti64 (6 wt% of Al as indicated by the black dash line), the fraction of β phase (and α phase) in the α+β two-phase structure can be read from the contour diagram directly given a heat treatment temperature;

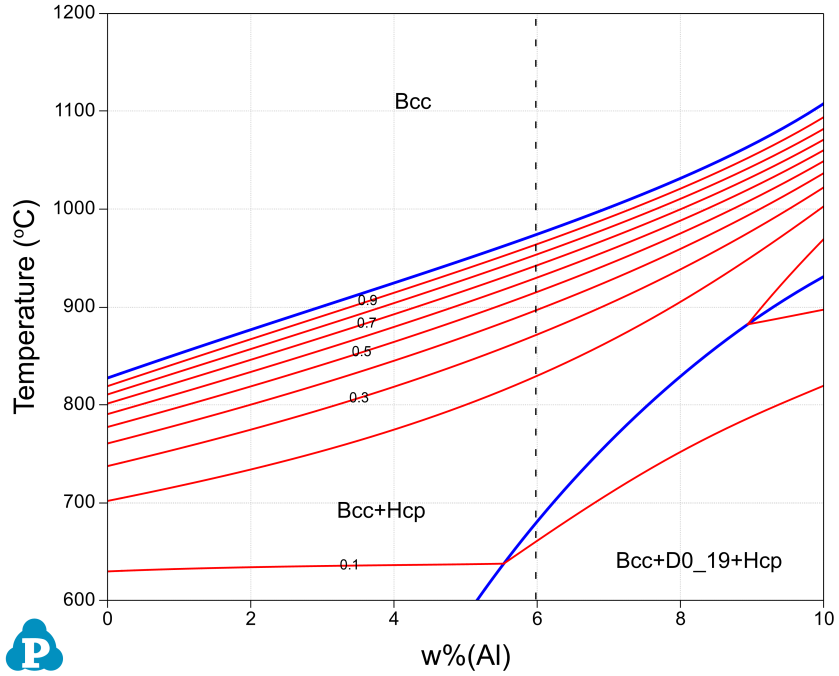


Figure 1.19.3: Contour diagram of the β phase fraction on the isopleth of Ti-Al-4V-0.1O-0.02N (wt%)

Example 1.20 Phase Forming Driving Force in High Entropy Alloys

Purpose: Learn to calculate and plot driving force contour lines on a multi-component phase diagram. Figure 1.20.1 shows an isopleth of CoCrFeNi – Al_xCoCrFeNi which indicates that addition of Al promotes the formation of Bcc and B2. However, it does not tell which phase has higher thermodynamic driving force at different temperature and composition. In this example, the driving force contour lines for B2 and Bcc are plotted on the Liquid+Fcc diagram in the Al-Co-Cr-Fe-Ni system to view the driving force of forming B2 and Bcc in this system.

Module: PanPhaseDiagram

Thermodynamic Database: `PanHEA.pdb`(this database is a thermodynamic database for high entropy alloys which is only available to users who have licensed it.)

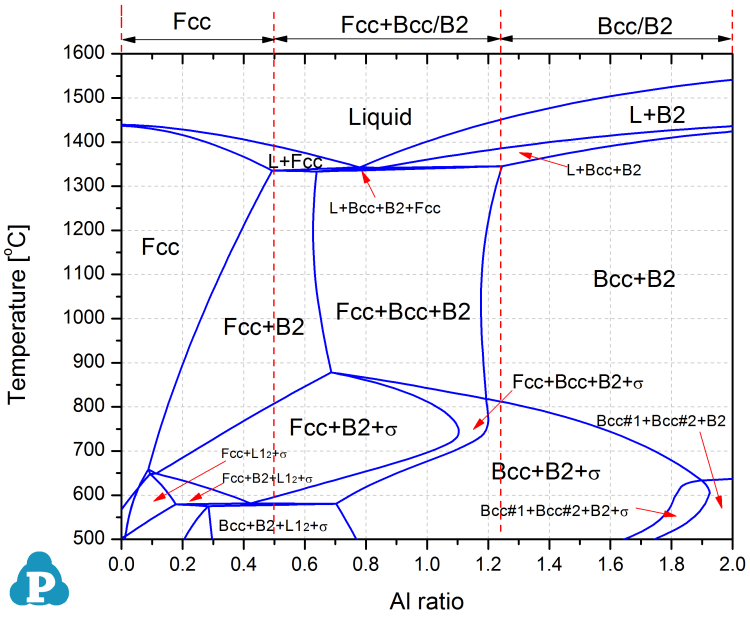


Figure 1.20.1: Calculated isopleth of the CoCrFeNi–Al_xCoCrFeNi with x=0~2

Calculation Procedures:

- Load `PanHEA.pdb` following the procedure in Pandat User's Guide 3.2.1;
- Perform a Section Calculation from PanPhaseDiagram, and set the calculation condition as shown in Figure 1.20.2;
- Click "**`Select Phases`**" and set status of each phase as shown in Figure 1.20.3;

- Click "**Contour Lines**" and then set the Contour Type as shown in Figure 1.20.4 to calculate the driving force contour lines for B2 phase, click OK;
- Click "**Contour Lines**" and then set the Contour Type as shown in Figure 1.20.5 to calculate the driving force contour lines for Bcc phase, click OK;

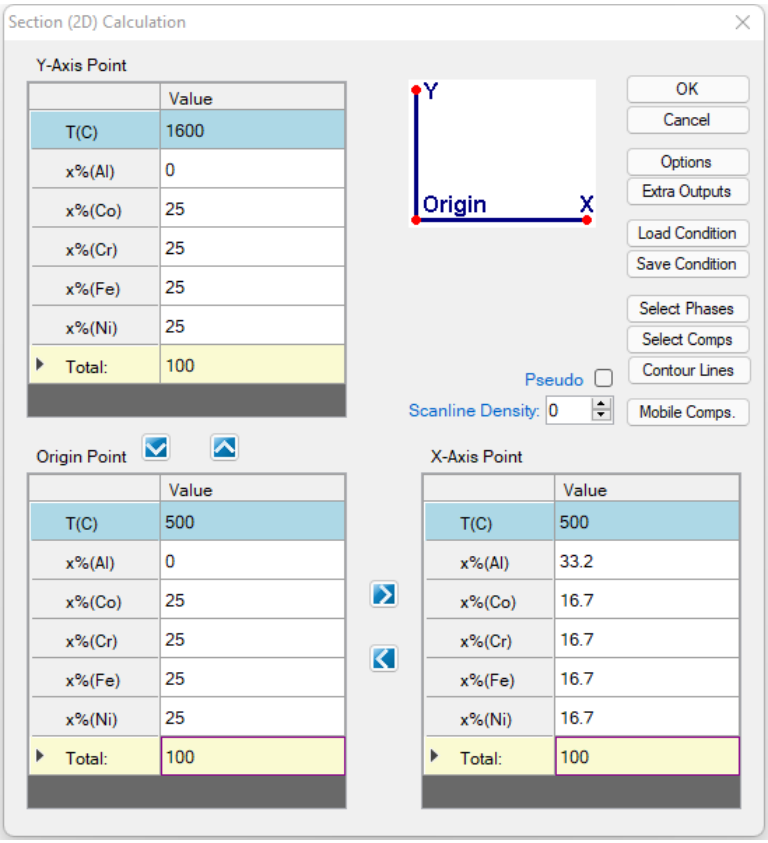


Figure 1.20.2: Setup calculation for the isopleth CoCrFeNi–Al_xCoCrFeNi

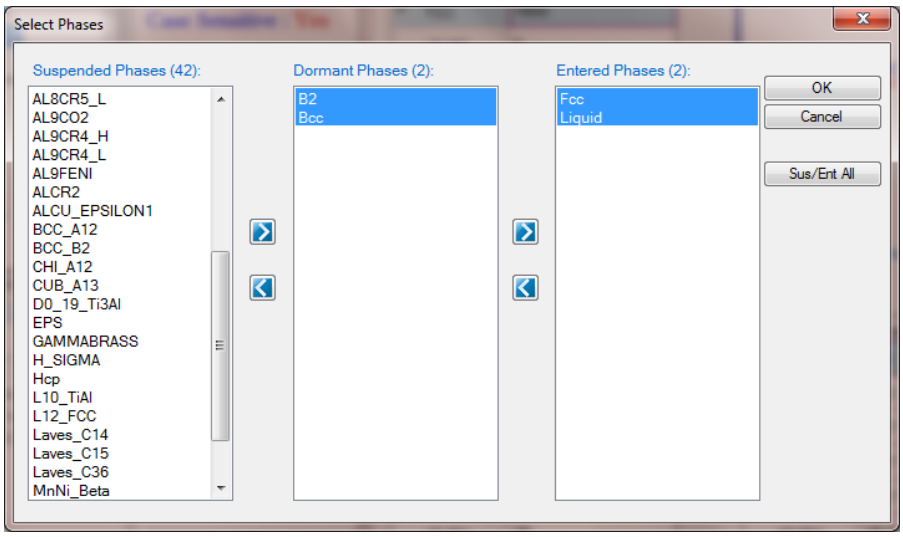


Figure 1.20.3: Fcc and Liquid are selected to enter the calculation, B2 and Bcc are dormant in the calculation, but their driving force to become stable phases can be calculated

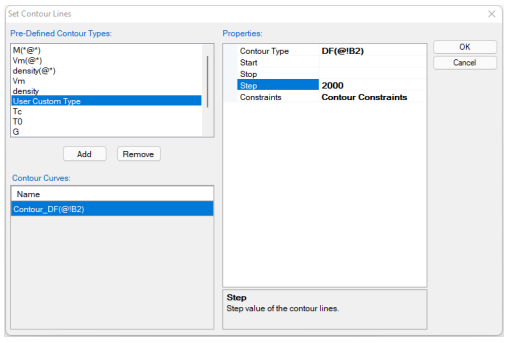


Figure 1.20.4: Setup calculation of driving force contour lines for B2 phase

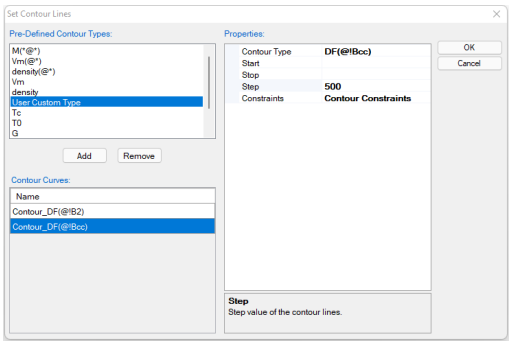


Figure 1.20.5: Setup calculation of driving force contour lines for Bcc phase

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Label the graph following the procedure in Pandat User's Guide 2.3.3;
- Label each line by putting the cursor on each line and wait for the tool tip to pop out, then press **F2**;

Information obtained from this calculation:

- After operation of Figure 1.20.4, a diagram with driving force contour lines of B2 will be plotted, and after operation of Figure 1.20.5, a diagram with driving force contour lines of Bcc will be plotted;
- To merge the two plots together by choose one of the diagram, say the one with Bcc contour lines, to be shown in the main display window, then single click **`Table->Contour_DF(@!B2)`** table, drag `x%(Al)` to the main display window, then press **`Ctrl`** and drag `T` to the main display window;
- The merged diagram is shown in Figure 1.20.6. From this figure it is seen that at low Al composition, neither B2 or Bcc has the driving force to form (negative driving force); with high Al composition, both phases have the driving force to form, and B2 has higher driving force than that of the Bcc phase;

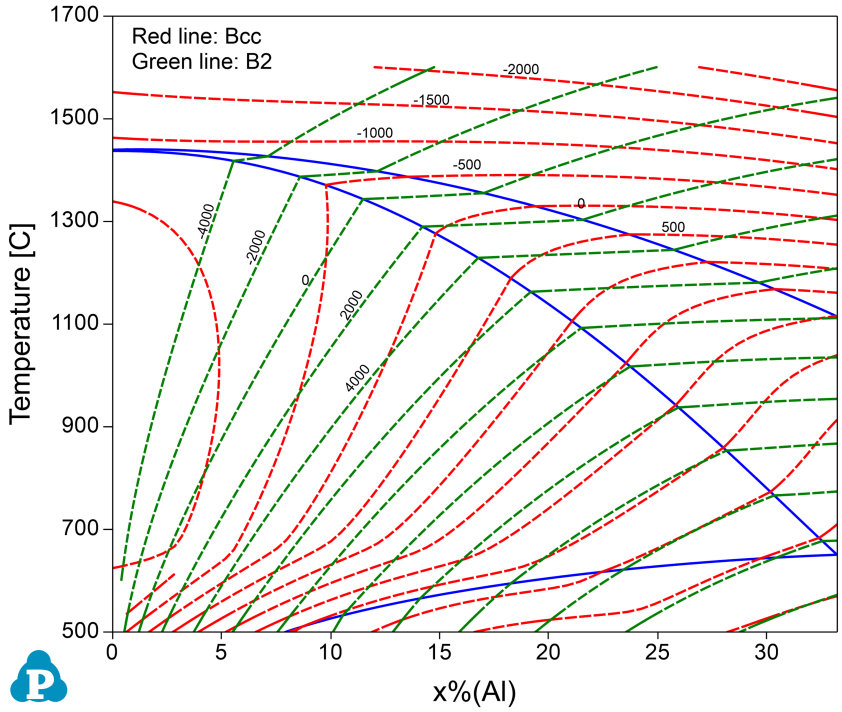


Figure 1.20.6: Driving force contour diagram for both Bcc and B2 phases

Example 1.21 User-defined Property

Purpose: Learn to define any property in a database in a format similar to that of the Gibbs energy and plot the contour lines of the defined property on a multi-component phase diagram.

Module: PanPhaseDiagram

Thermodynamic and property Database: `AlNi_U.tdb`

Batch file: `Example_#1.21.pbfx`

The molar volume of Al-Ni binary system is taken as an example here. Instead of using the specific variable V_m for molar volume, we define a property of *U* to represent the molar volume. In the database file (`.tdb`), first define the property *U* with the keyword "`USER_PROPERTY`" as

```
Type_Definition a USER_PROPERTY U 1 !
```

Then, define the property *U* as a function of *x*, the mole fraction, with the keyword "`VARIABLE X`":

```
Type_Definition b GES AMEND_PHASE_DESCRIPTION * VARIABLE_X U !
```

For any phase with such a property U, include "`ab`" in the phase definition such as in "`Liquid`" phase,

```
Phase Liquid %ab 1 1 !
```

The parameters for the property are defined in the format similar to that of the Gibbs energy. An example file "`AlNi.tdb`" is included in the Pandat example folder. A batch file "`Example_#1.21.pbfx`" is also included in the same folder, which produces an identical contour diagram as shown in Figure 1.21.1 except that the property name is *U* instead of V_m. It should emphasize again that *U* can be any property.

Calculation Procedures:

- Load `AlNi_U.tdb` following the procedure in Pandat User's Guide 3.2.1, and select both components;
- Pop out dialog for Section (2D) Calculation, then click "**`Contour Lines`**" to open the contour line dialog as shown in Figure 1.21.2;

- Choose "**User Custom Type**" and click **Add**Type in "*U*" for the Contour Type in the "**Properties**" window as shown in Figure 1.21.2.
- Click OK and perform calculation. The obtain diagram with labeling is shown as Figure 1.21.1.

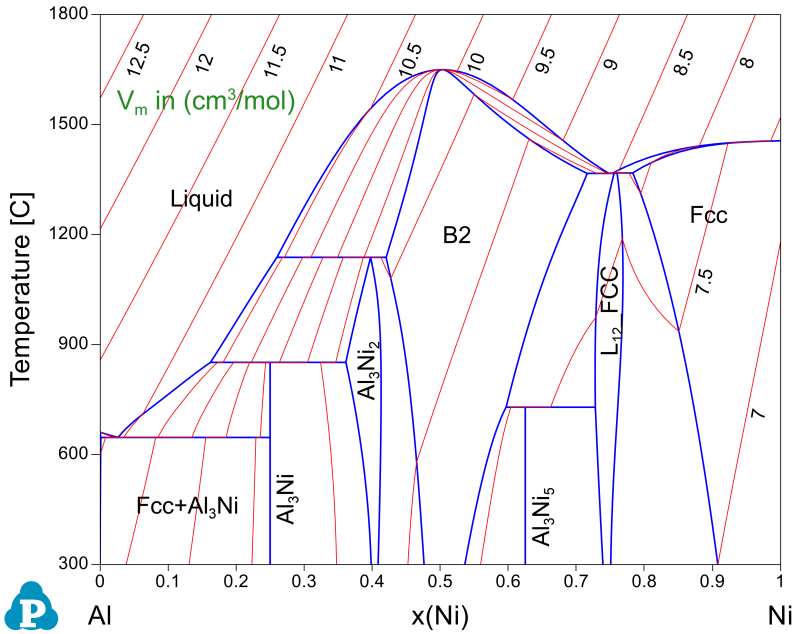


Figure 1.21.1: Al-Ni binary phase diagram with the calculated contour lines of molar volume (cm^3/mol)

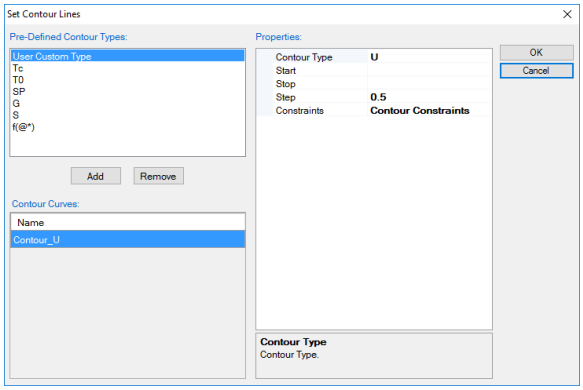


Figure 1.21.2: Setup contour lines for Property *U* from interface

Example 1.22 Run Pandat in Console Mode

Purpose: Learn to run Pandat in the console mode for the calculation of Al-Mg binary phase diagram.

Module: PanPhaseDiagram

Thermodynamic Database: `AlMgZn.tdb`

Batch file: `Example_#1.22.pbfx`

Calculation Procedures:

- Run through a windows (`.bat`) file, double click the `Example_#1.22.bat`;

  The content of an example (`.bat`) file is shown below:

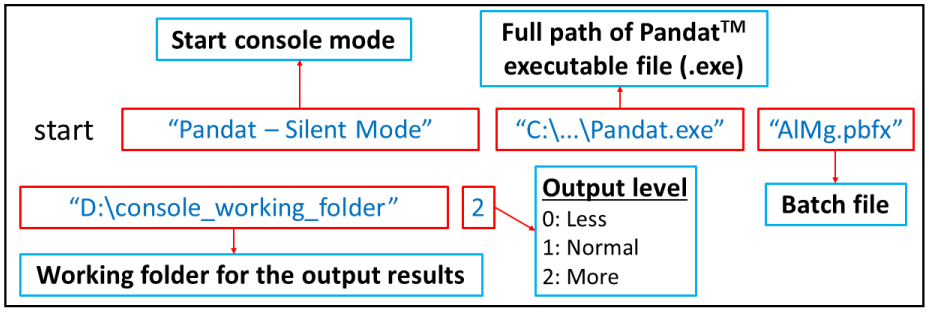


Figure 1.22.1: Example of the (.bat) file for console mode

Note that above figure shows an example windows (`.bat`) file. There are a few things that user needs to make sure before running this example:

- The full path of "`Pandat.exe`". The default path for Pandat 2025 is: "`C:\Program Files\CompuTherm LLC\Pandat 2025\bin\Pandat.exe`
- If the batch file (`.pbfx`) is not in the same folder of the windows (`.bat`) file, the full path of the batch file (`.pbfx`) needs to be given.
- The working folder for the console mode must have been created before running the windows (`.bat`) file. Then a Pandat workspace will be created in this folder and all simulation results are saved under this workspace. This argument is optional and no

graph files are generated if the working folder is not given. This will save many computer resources. In general, the user may not pass this argument so that only data (`.dat`) files are generated after each simulation. In "`Example_#1.22.pbfx`":

```
<table name="AlMg_PhaseDiagram.dat" source="default">
```

- A table name "`AlMg_PhaseDiagram.dat`" is given with an extension "`.dat`" and then a data file (`.dat`) will be created in the same folder as the batch file. User may give a full path for the data file in order to save it into a specified folder.
- 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.

Example 1.23 High Throughput Calculation (HTC): Pattern Compositions

Purpose: Learn to run high throughput calculation by setting pattern composition range and steps.

Module: PanPhaseDiagram

Thermodynamic Database: `AlMgZn.tdb`

Calculation Procedures:

- Load `AlMgZn.tdb` following the procedure in Pandat User's Guide3.2.1, and select all three components;
- Choose the HTC function from the menu "**`Batch Calc → High Throughput Calculation (HTC)`**" (as shown in Example 1.23).

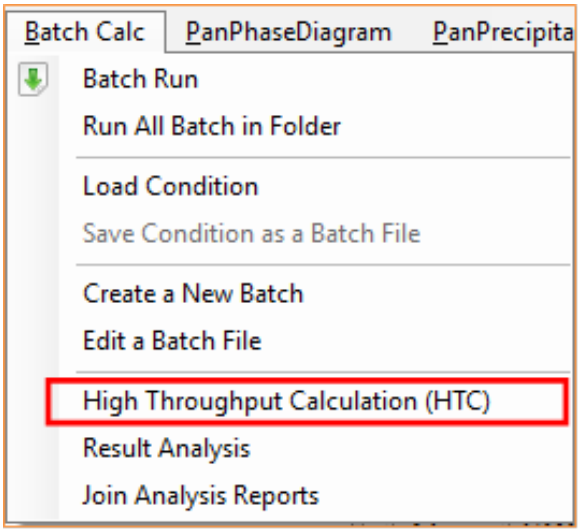


Figure 1.23.1: HTC function under the "Batch Calc" menu

- Choose the calculation type from the drop-down list of HTC pop-up window and select "Solidification".

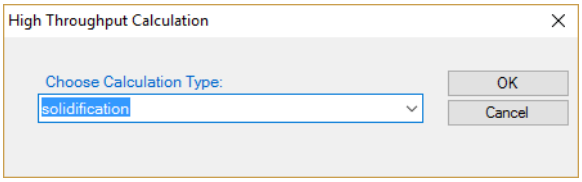


Figure 1.23.2: Dialog to choose calculation type of HTC

- Define the compositional space for HTC simulation;

  After choosing the calculation type, a window pops out as shown in Figure 1.23.3. 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 30x30=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 setting the composition pattern, user can also export these HTC alloy composition to a file by clicking the small icon marked with red square in Figure 1.23.3 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.

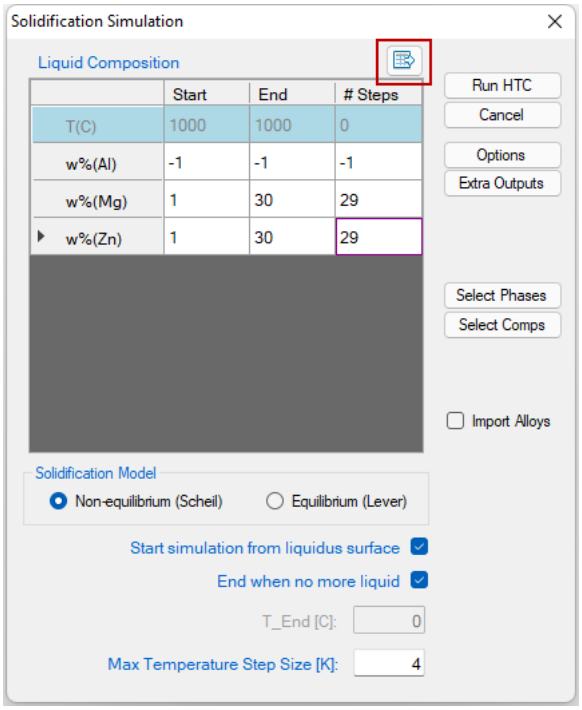


Figure 1.23.3: Dialog to setup compositional space for HTC

- 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.

- Choose "**`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.

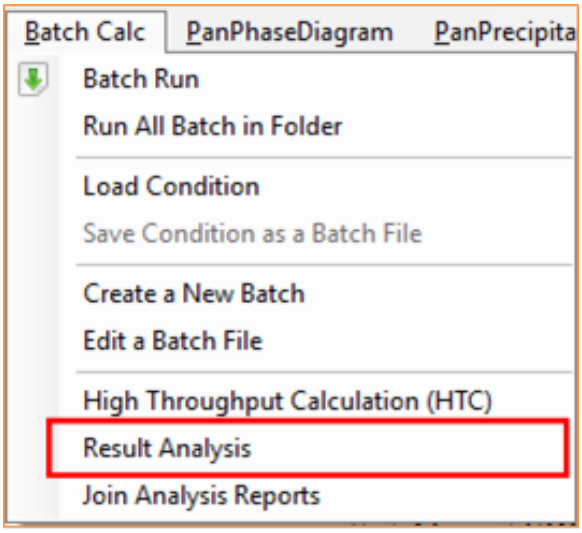


Figure 1.23.4: "Result Analysis" function under the "Batch Calc" menu

- 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 1.23.5.

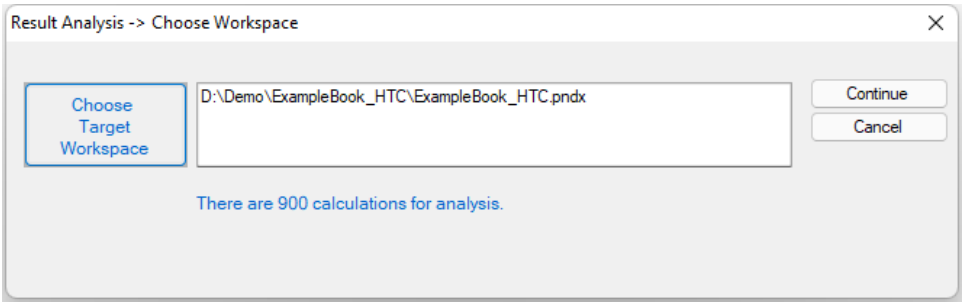


Figure 1.23.5: "Result Analysis" popup dialog to choose target workspace

- Define the criteria of the properties as filters for result analysis

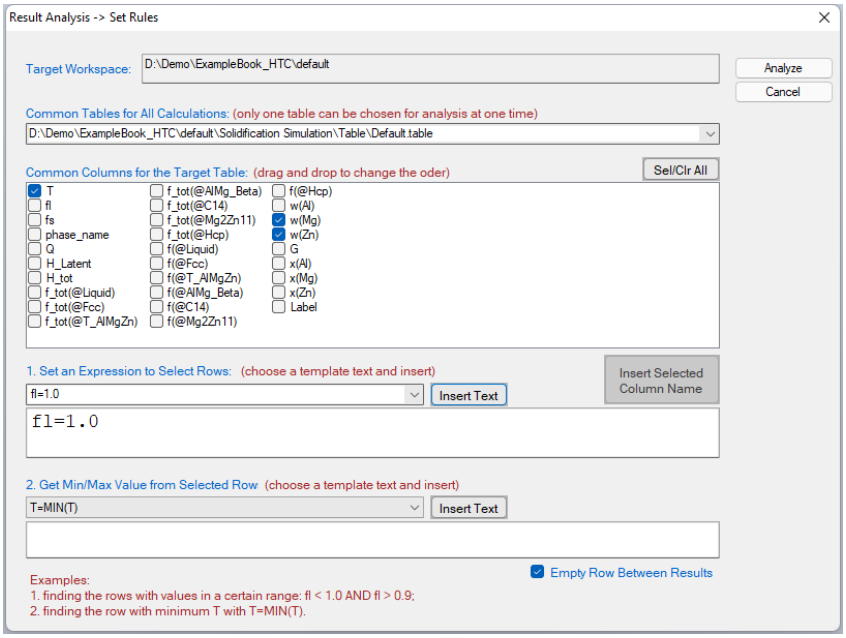


Figure 1.23.6: "Result Analysis" popup dialog to define the criteria of the properties

In Figure 1.23.6, 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 1.23.6, 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 Figure 1.23.6, 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 1.23.7. 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 1.23.8.

TL.report

	CalculationName	AlloyChemistry	T	w(MG@LIQUID)	w(ZN@LIQUID)
			C	%	%
1	solidification_default	98AL+1MG+1ZN in w%	653.5360	1.000000	1.000000
2					
3	solidification_default_1	97AL+1MG+2ZN in w%	651.6410	1.000000	2.000000
4					
5	solidification_default_2	96AL+1MG+3ZN in w%	649.7380	1.000000	3.000000
6					
7	solidification_default_3	95AL+1MG+4ZN in w%	647.8280	1.000000	4.000000
8					
9	solidification_default_4	94AL+1MG+5ZN in w%	645.9110	1.000000	5.000000
10					
11	solidification_default_5	93AL+1MG+6ZN in w%	643.9860	1.000000	6.000000
12					
13	solidification_default_6	92AL+1MG+7ZN in w%	642.0550	1.000000	7.000000
14					
15	solidification_default_7	91AL+1MG+8ZN in w%	640.1160	1.000000	8.000000
16					
17	solidification_default_8	90AL+1MG+9ZN in w%	638.1690	1.000000	9.000000
18					
19	solidification_default_9	89AL+1MG+10ZN in w%	636.2160	1.000000	10.000000
20					
21	solidification_default_10	97AL+2MG+1ZN in w%	648.4620	2.000000	1.000000
22					
23	solidification_default_11	96AL+2MG+2ZN in w%	646.5690	2.000000	2.000000
24					
25	solidification_default_12	95AL+2MG+3ZN in w%	644.6700	2.000000	3.000000
26					
27	solidification_default_13	94AL+2MG+4ZN in w%	642.7640	2.000000	4.000000
28					
29	solidification_default_14	93AL+2MG+5ZN in w%	640.8510	2.000000	5.000000
30					
31	solidification_default_15	92AL+2MG+6ZN in w%	638.9320	2.000000	6.000000

Figure 1.23.7: Analysis report file of T_L

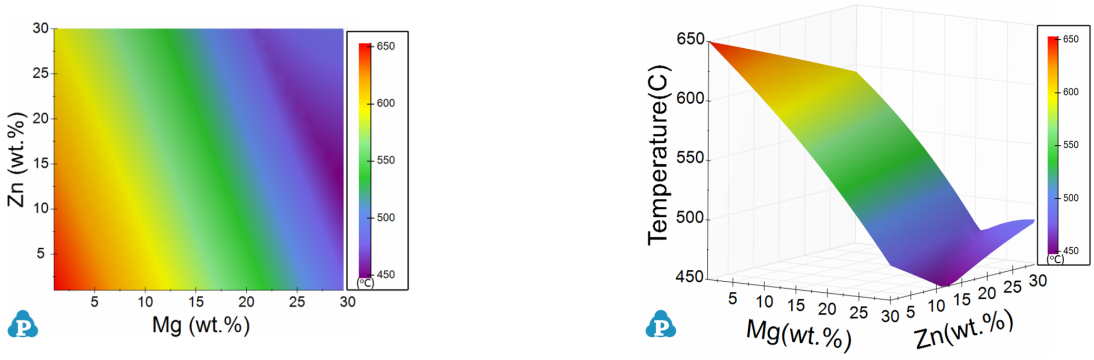


Figure 1.23.8: 3D diagrams of the liquidus temperatures: colormap (left) and 3D surface (right)

Example 1.24 High Throughput Calculation (HTC): Random Compositions

Purpose: Learn to run high throughput calculation by importing alloy Compositions.

Module: PanPhaseDiagram

Thermodynamic Database: `AlMgZn.tdb`

Calculation Procedures:

- Load `AlMgZn.tdb` following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Start the HTC function from the menu "**Batch Calc → High Throughput Calculation (HTC)**" Then choose "**solidification**" as calculation type.
- Check the "**Import Alloys**" box at the solidification simulation popup window, and then click the "**Import**" button to import the pre-prepared alloy composition file (`Example_#1.24_alloys.txt`).
- Click the "**Run HTC**" button perform HTC simulations
- Save the workspace of the HTC results for further analysis as mentioned in Example 1.23 : High Throughput Calculation (HTC): Pattern Compositions

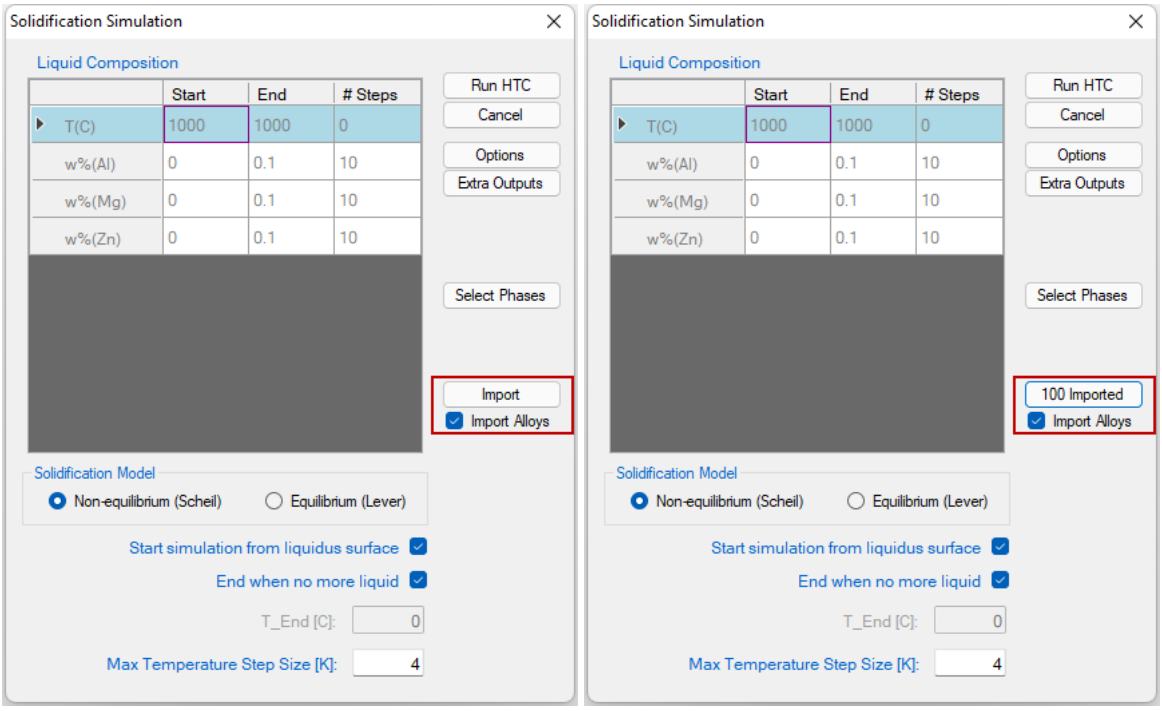


Figure 1.24.1: HTC solidification dialogs before (left) and after (right) import alloy composition file

Please refer to the Pandat User's Guide 1.1 10.1 for detail information of preparing the alloy composition file.

Example 1.25 Friction-stir welding between AA5454 Al alloy and AZ91 Mg alloy

Purpose: Learn to perform complicated multi-component vertical section calculations and understand the application of zero phase fraction (ZPF) line of the liquid phase. Commercial Mg database is required to perform the calculation of this example.

Module: PanPhaseDiagram

Thermodynamic Database: `PanMg.pdb`(this database is a thermodynamic database for multi-component magnesium alloys which is only available to users who have licensed it.)

Due to the formation of brittle intermetallic phases in the fusion zone, joining Mg alloys with Al alloys through fusion welding is not very suitable. Friction stir welding (FSW) provides a potential method for joining Mg alloys and Al alloys. In this example, an AZ91 cast Mg alloy and rolled AA5454 Al alloy are assumed to be jointed through FSW. A vertical section from the composition of AZ91 to AA5454 shows the possible intermetallic phases could be formed in the welding interface. In addition, the zero phase fraction (ZPF) line of the liquid phase indicates the maximum temperature that can be tolerated during the welding process to avoid the melting zone in the interface. In Pandat , The ZPF line the liquid phase can be output through function "f (@Liquid) = 0" in the table.

Calculation Procedures:

- Load `PanMg.pdb` following the procedure in Pandat User's Guide 3.2.1, and select components: Al, Fe, Mg, Mn, Zn;
- Perform 2D calculation following the procedure in Pandat User's Guide 3.3.3;
- Set Calculation Condition as shown in Figure 1.25.1;

Post Calculation Operation:

- Add a new Table as shown in Figure 1.25.2 to get the ZPF line data of the liquid phase (**f(@Liquid)=0**);
- Plot the ZPF line data in the added table into the default graph following the procedure in Pandat User's Guide 2.4.3;
- Label phase field following the procedure in Pandat User's Guide 2.3.3;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;

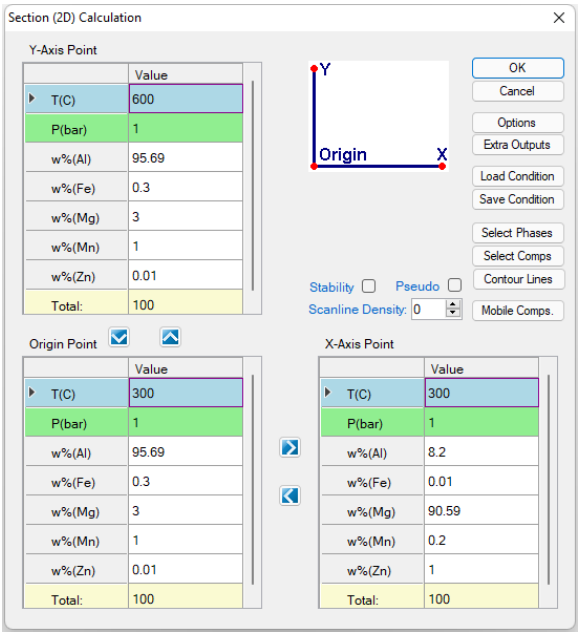


Figure 1.25.1: Set vertical section calculation conditions: Composition from AA5454: Al-3Mg-1Mn-0.3Fe-0.01Zn(wt.%) at left edge to AZ91: Mg-8.2Al-1Zn-0.2Mn-0.01Fe (wt.%) at right edge; Temperature range from 300 °C to 500 °C

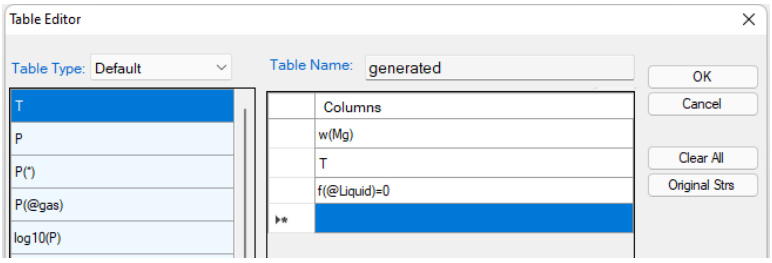


Figure 1.25.2: Output the ZPF line data of the liquid phase

Information obtained from this calculation:

- The obtained phase diagram is shown in Figure 1.25.3. To prevent partial melting during the friction-stir welding process, the local temperatures in the welding zone must be maintained below the threshold indicated by the red line. In this case, the minimum temperature to avoid such melting is 435.7 °C.
- Different intermetallic phases may form in the joining zone: The Al_3Mg_2 phase with some Al_6Mn precipitate near the Al alloy side, and $Mg_{17}Al_{12}$ phase with minor precipitation of Al_4Mn near the Mg alloy side.
- A similar approach can also be applied to analyze interactions between other materials, such as coating/substrate reactions.

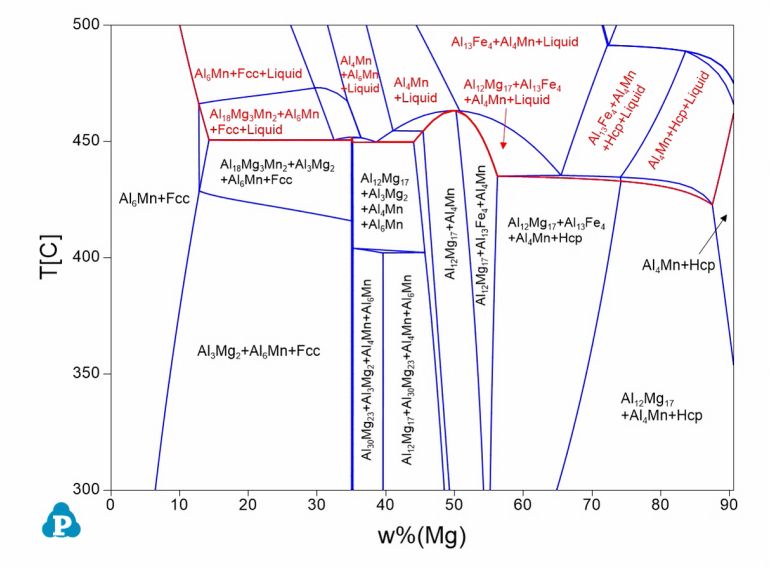


Figure 1.25.3: The vertical phase diagram from AA5454 to AZ91 with phase field labels (The phase fields including Liquid phase are labeled as red)

Example 1.26 Calculation of Open Circuit Voltage (OCV) under Equilibrium Condition

Purpose: Learn to perform equilibrium calculation, use extra output table and extra output graph to output chemical potential and voltage value to simulate the open circuit voltage curve of an alloy system for battery application.

Module: PanPhaseDiagram

Thermodynamic Database: `LiSn.tdb`

Batch file: `Example_#1.26.pbfx`

Background: Carbon based anode material is widely used in Li-ion batteries. But its low charge density motivates the search for next generation of anode materials. Sn based alloy is one of potential anode candidates. The calculation of open circuit voltage curve of the Li-Sn system sheds a light on the potential capacity of the alloy system. This example shows how to calculate the open circuit voltage curves directly from PanPhaseDiagram module and compare with experimental data. In an alloy system, the equilibrium open-circuit voltage E is associated with chemical potential through the Nernst equation: $\mu_{Li} - \mu_{Li}^{o,ref} = -nFE$. *F* is Faraday's constant, 94685 C/volt. In this example of Li-Sn system, *n* = 1, then $E = -(\mu_{Li} - \mu_{Li}^{o,ref})/F$. At 688 K, Li and Sn are in liquid state, so the reference state is liquid Li.

Calculation Procedures:

- Load `LiSn.tdb` following the procedure in Pandat User's Guide 3.2.1;
- Perform line (1D) calculation following the procedure in Pandat User's Guide 3.3.2;
- Set the calculation conditions as shown in Figure 1.26.1. The temperature is set as 688 K, as experimental data are available at 688 K for comparison. The composition range is from pure Sn, i.e. `x(Sn) = 1`, to pure Li, i.e. `x(Li) = 1`. The Number of steps is set to be 100;

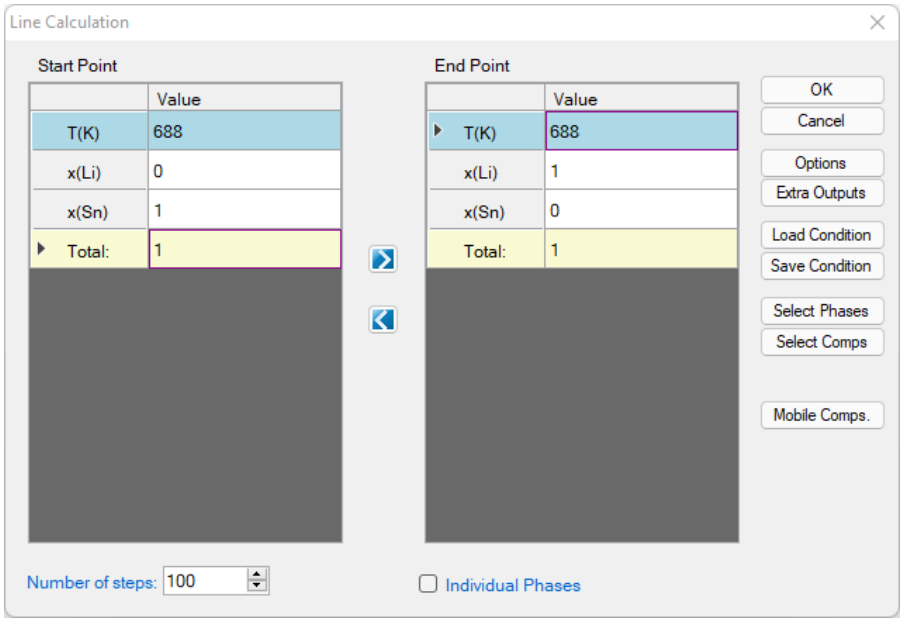


Figure 1.26.1: Line calculation conditions setting

- Set "**`Extra Outputs table`**": In order to output the open-circuit voltage value, some extra outputs are required. Click "**`Extra Outputs`**" in the interface shown in Figure 1.26.1, a new interface will appear as shown in Figure 1.26.2. Then click the blue "+" symbol to pop out the **`Table Editor`** as shown in Figure 1.26.3. From this **`Table Editor`**, one can select to output Extra properties which are not shown in the default table;

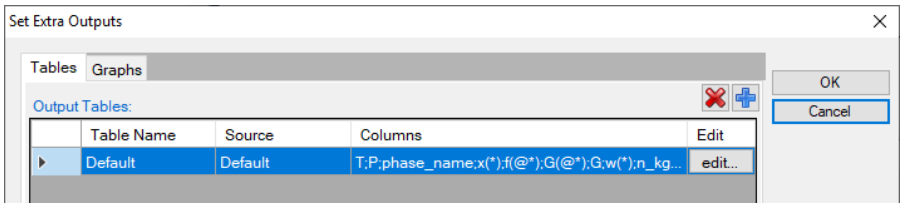


Figure 1.26.2: Dialog to set Extra Output

- In this example, we output `mu(Li:Liquid[Li])` as the chemical potential of Li in the system with reference to the liquid phase, i.e. . Then, we add another quantity `-mu(Li:Liquid[Li])/96485` which is equivalent to in this system. The quantity `x(Li)/x(Sn)` represents the y in Li_ySn system. The settings are shown in Figure 1.26.3. After setting the table editor, click **`OK`**;

Tips: The properties can be dragged from the left column to the right column, or directly type in the right column. When click a property in the left column, the description of this property is shown as description in the bottom of the interface. For example, in Figure 1.26.3, `a(*:Liquid[*])`; Description: Activity of component in system with given reference state. Some simple calculations are also applied in the table setting, such as – `mu(Li:Liquid[Li])/96485` and `x(Li)/x(Sn)` in this example.

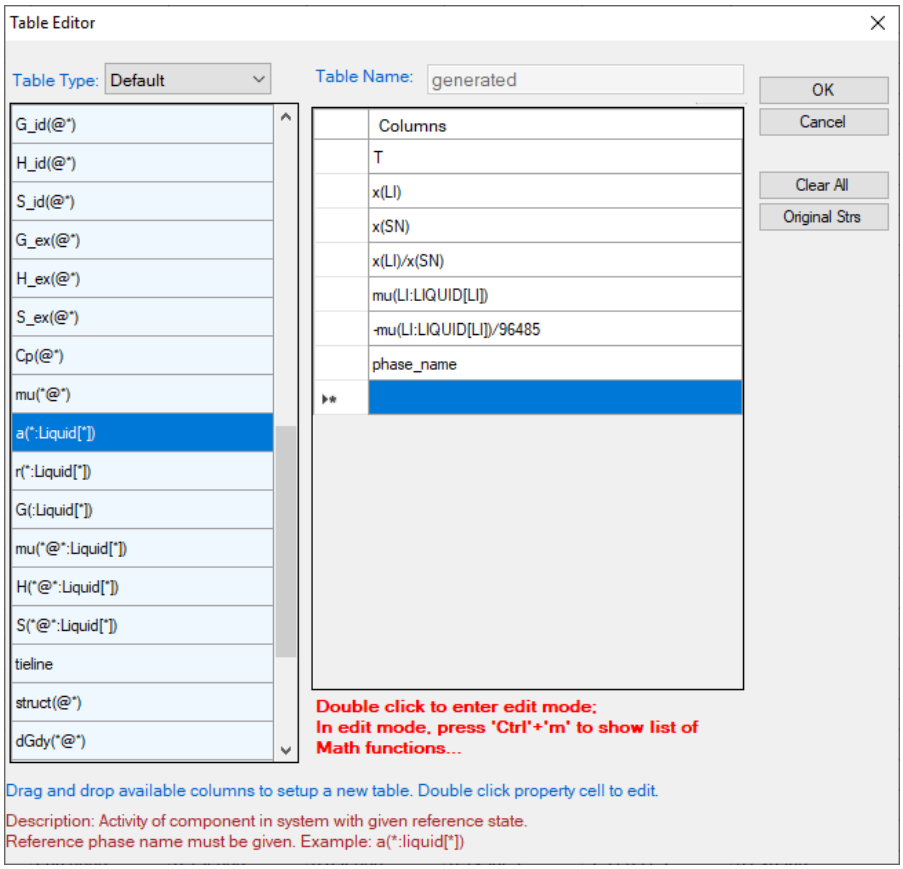


Figure 1.26.3: Define extra output table by drag properties from the left column to the right column or directly type in in the right column

- Set "**Extra Outputs graph**": Click the icon "**Graph**" in "**Set extra output**" interface as shown in Figure 1.26.4, then click the blue "+" symbol to add extra Graph. An interface as shown in Figure 1.26.5 will appear. Select the "**generated**" table set in previous step in the "**Table source**". Drag `x(Li)/x(Sn)` from the left column to X axis in the right column; drag `-mu(Li:Liquid[Li])/96485` from the left column to Y axis in the right column. Then click **OK**;
- When the interface goes back to Figure 1.26.1, click **OK**. Calculation starts.

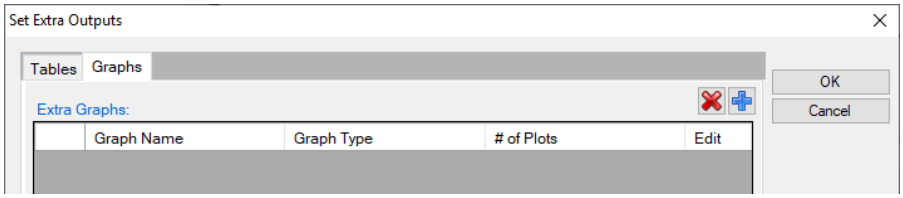


Figure 1.26.4: Dialog to set Extra Graph Output

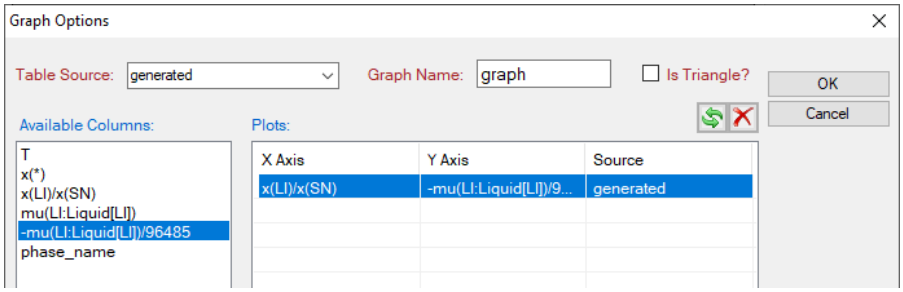


Figure 1.26.5: Output Graphs options interface

Post Calculation Operation:

- Rescale the axis, and edit the axis title.

  After the calculation, the calculated open circuit voltage curve of Li-Sn system is shown in Figure 1.26.6 with the default settings. Set the x-axis range from 0 to 6, and obtained as shown in Figure 1.26.7

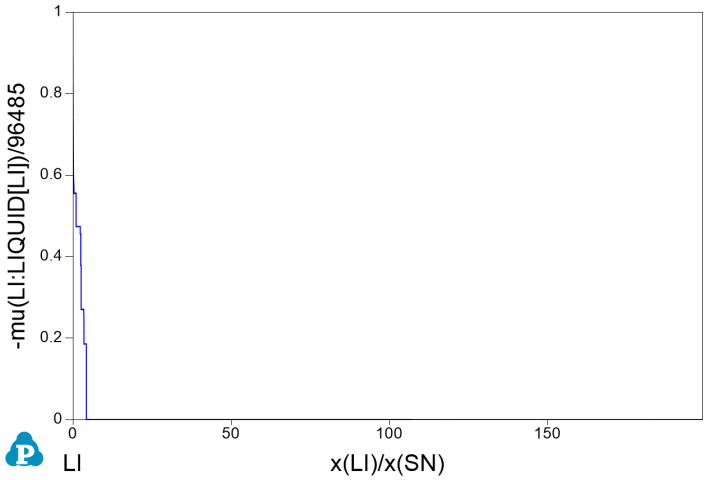


Figure 1.26.6: Calculated open circuit voltage curve of Li-Sn system

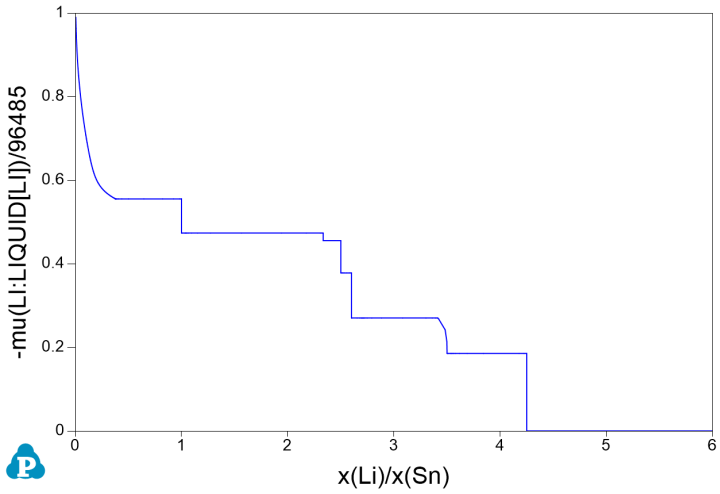


Figure 1.26.7: Calculated open circuit voltage curve of Li-Sn system: Rescale x-axis of x(Li)/x (Sn) to 0-6

- Import experimental data. From the menu, click **Table → Import Table From Files**, choose `LiSn.txt` file to import the experimental data table into the Pandat workspace;
- Compare calculated results with experimental data. From the menu, click **Graph → Edit Plots**, or click the button from the toolbar to open the setup Plot interface as shown in Figure 1.26.8. Select the imported `LiSn` table, choose `LixSn` as `X` axis, and `E_Li(V)` as `Y` axis. Then click **OK**;
- Then change "**Plot Type**" as "**Point**", "**Marker Color**" as "**Transparent**", "**Marker Style**" as "**Circle**"; Then experimental data are changed to red open symbol, added legend, change the Title of `Y` axis as `(E vs E`$_{Li}$` ) / V`. The final produced figure is shown in Figure 1.26.9.

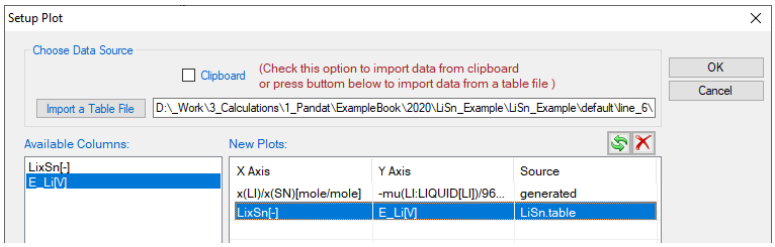


Figure 1.26.8: Setup Plot, add the experimental data into generated figure

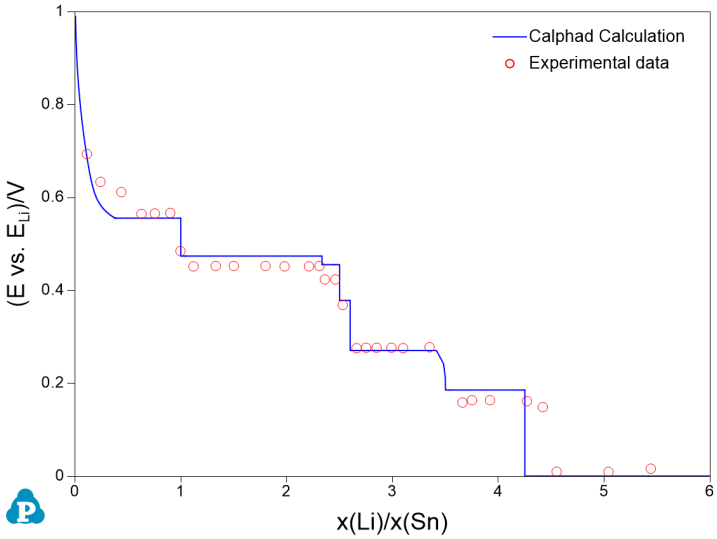


Figure 1.26.9: The calculated OCV curve of Li-Sn system at 688 K in comparison with experimental data

Example 1.27 Para-equilibrium Phase Diagram

Purpose: Learn to perform phase diagram calculations in para-equilibrium condition with fast diffusion elements.

Module: PanPhaseDiagram

Thermodynamic Database: `FeNiC.tdb`

Batch file: `Example_#1.27.pbfx`

Background: In certain systems, some interstitial elements, such as C and N, diffuse much faster than others. Therefore, those elements can be treated as "mobile" components, while the others are treated as immobile components. The common case is the austenite to ferrite reaction in steels by a rapid carbon-diffusion controlled process.

Calculation Procedures:

- Load `FeNiC.tdb` following the procedure in Pandat User's Guide 3.2.1;
- Perform a Section Calculation from PanPhaseDiagram, and set the calculation condition as shown in Figure 1.27.1;
- Click "**`Mobile Comps.`**", set "`C`" the mobile component as shown in Figure 1.27.2;
- After properly selected the C as mobile component, then click OK, it returns to the calculation condition window as shown in Figure 1.27.3. The mobile element highlighted with orange color.

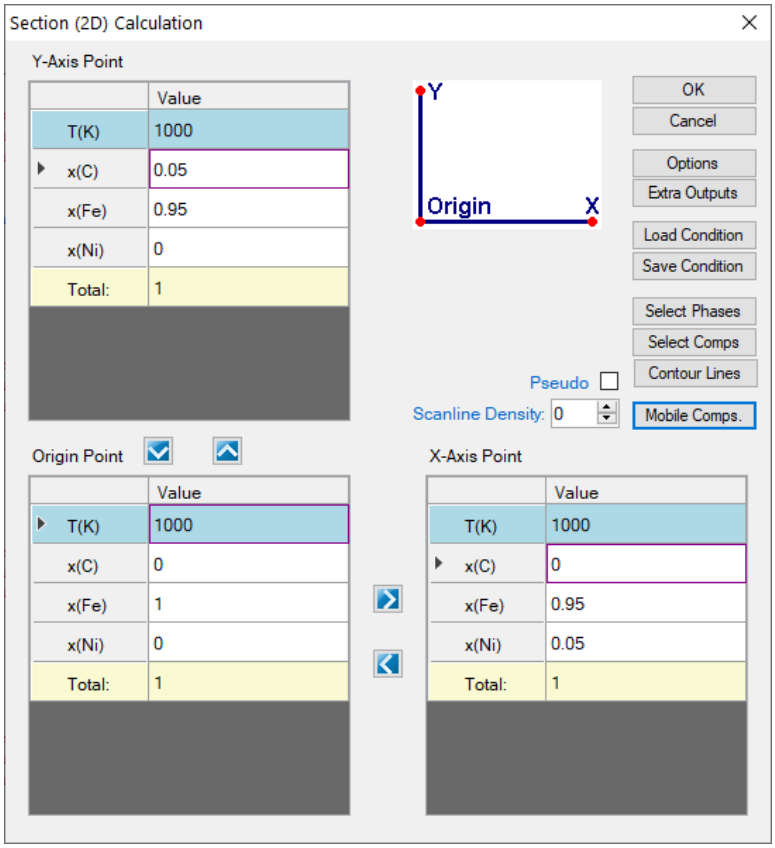


Figure 1.27.1: Normal 2D calculation of an isotherm of Fe-Ni-C at 1000 K

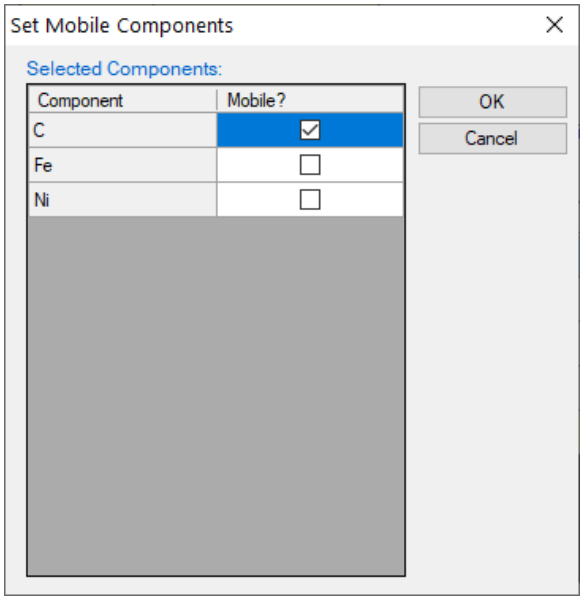


Figure 1.27.2: Set mobile components

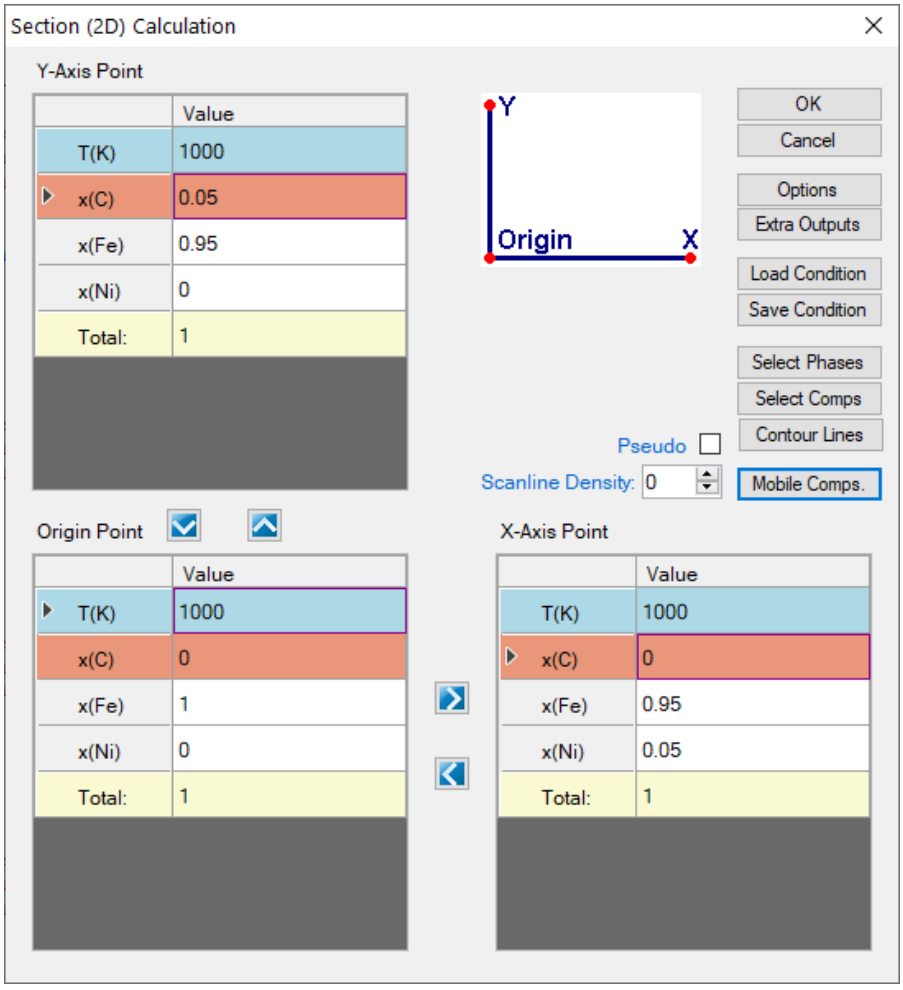


Figure 1.27.3: Calculation condition of para-equilibrium isothermal section of Fe-Ni-C at 1000 K

Post Calculation Operation:

- Add tie-lines and change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Label the graph following the procedure in Pandat User's Guide 2.3.3;
- The Para-equilibrium isothermal section is shown as Figure 1.27.4

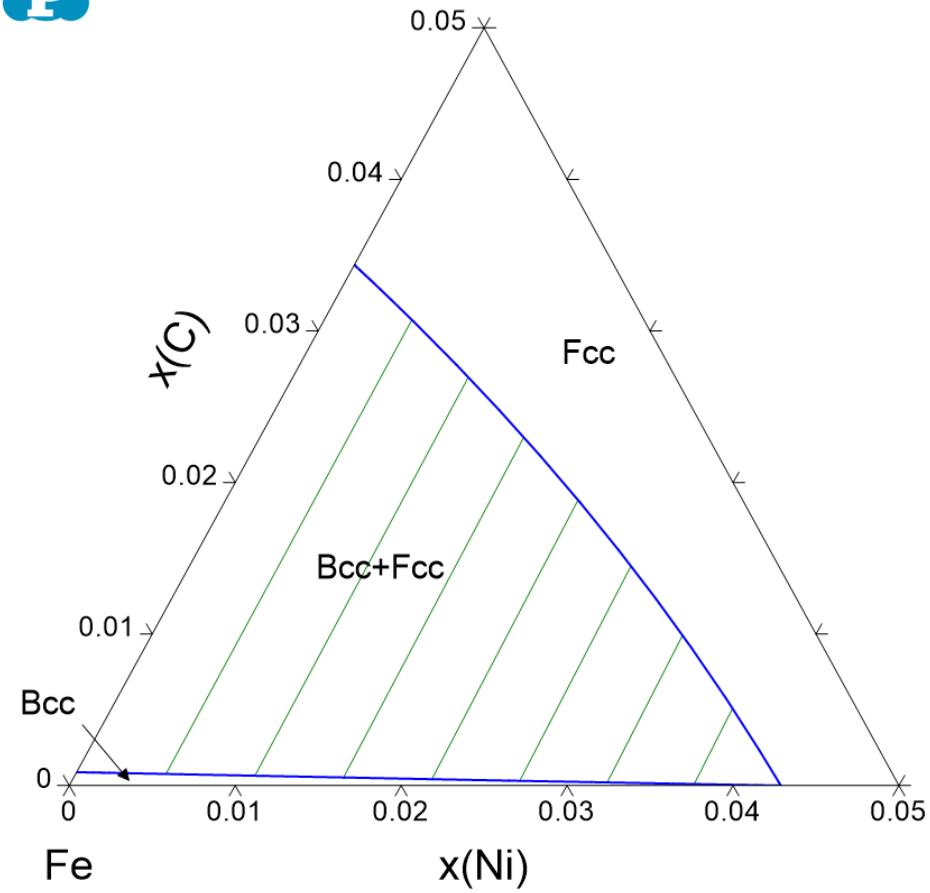


Figure 1.27.4: Calculated para-equilibrium isothermal section of Fe-Ni-C at 1000 K

Example 1.28 Calculation of T_0 curve

Purpose: Learn to calculate the T_0 curve between two phases.

Module: PanPhaseDiagram

Thermodynamic Database: `AlMgZn.tdb`

Batch file: `Example_#1.28.pbfx`

Background: 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. It is the limit of partitionless phase transition, such as martensite transformation. In this example, we will learn how to calculate the T_0 curve between two solution phases. The T_0 curves between Hcp/Liquid and Fcc/Liquid are used as example in this case.

Calculation Procedures:

- Load `AlMgZn.tdb` following the procedure in Pandat User's Guide 3.2.1;
- Perform section (2D) calculation following the procedure in Pandat User's Guide 3.3.3;
- Set the calculation condition as shown in Figure 1.28.1; This is a normal setting for phase diagram calculation as shown in Example 1.1 : Al-Mg Binary Phase Diagram
- The Contour Lines function is used to calculate the T_0 curve, click the "Contour Lines" icon, the "Set Contour Lines" window pop up as shown in Figure 1.28.2 . Add the T0 as the Contour Curves, select "Phase Name" as "Liquid", and the "Phase Name #2" as " * ", Pandat will calculate the T_0 curve between liquid and all solid solution phases. In this example, they are Fcc in Al side, and Hcp in Mg side .

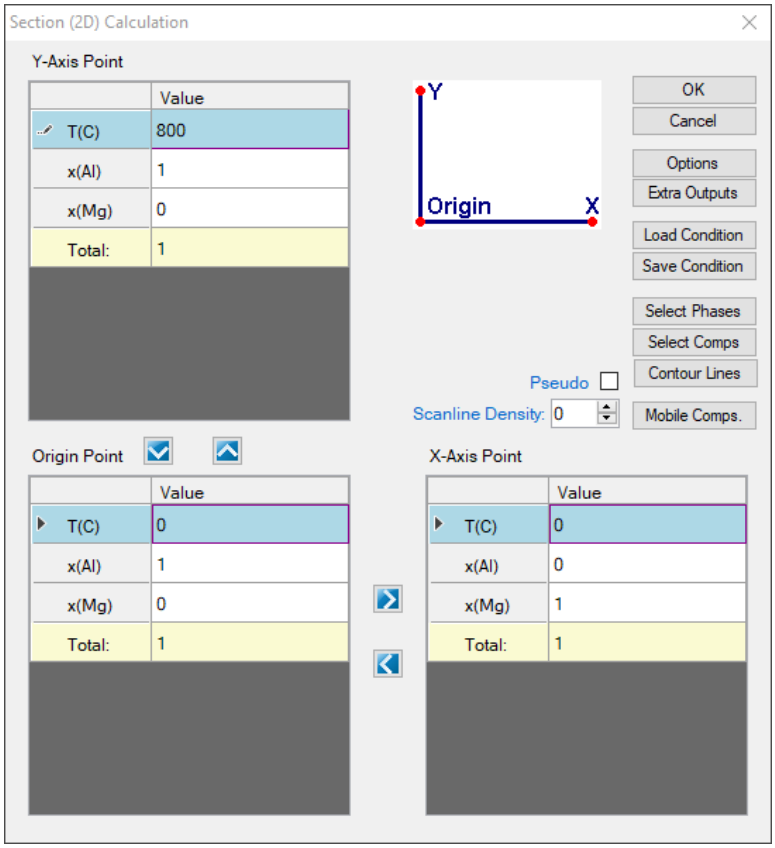


Figure 1.28.1: 2D calculation with composition from pure Al to pure Mg and temperature from 0°C to 800°C

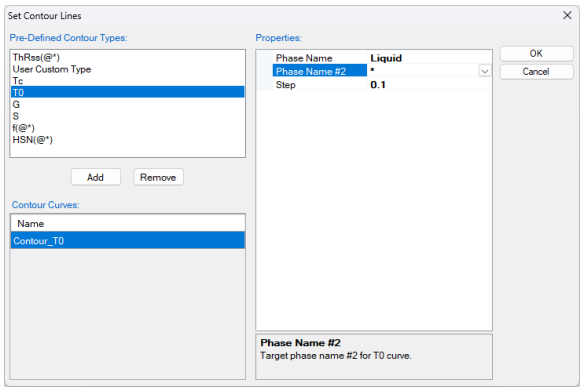


Figure 1.28.2: The Set Contour Lines window

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Add Label to the graph following the procedure in Pandat User's Guide 2.3.3;

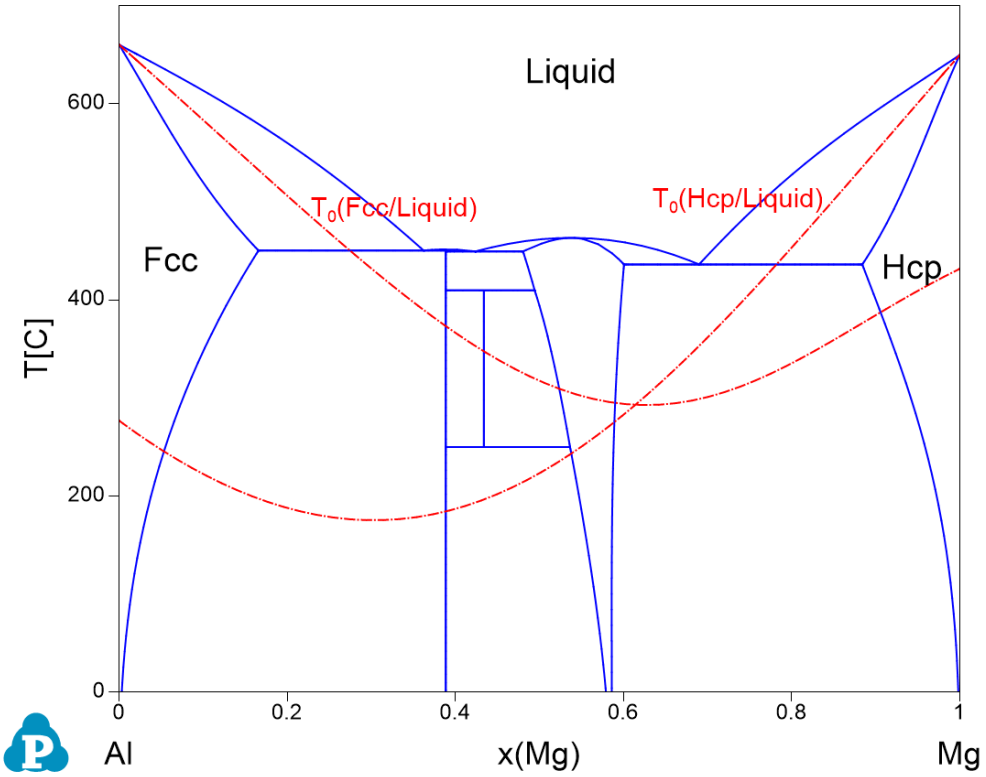


Figure 1.28.3: The calculated Al-Mg phase diagram together with T_0 curves of Fcc/Liquid and Hcp/Liquid

Information obtained from this calculation:

- The T0 curves in Al-Mg system between Fcc/Liquid and Hcp/liquid are obtained.

Example 1.29 Material to Material Calculation: Friction-stir welding between AA5454 Al alloy and AZ91 Mg alloy

Purpose: This example demonstrate the material to material function in Pandat software. The calculation conditions are the same as Example 1.25 .

Module: PanPhaseDiagram

Thermodynamic Database: `PanMg.pdb`(this database is a thermodynamic database for multi-component magnesium alloys which is only available to users who have licensed it.)

Calculation Procedures:

- Load `PanMg.pdb` following the procedure in Pandat User's Guide 3.2.1, and select components: Al, Fe, Mg, Mn, Zn;
- Perform Material to Material calculations through the menu bar "**`PanPhaseDiagram → Section Calculation: Material to Material`**";
- Set Calculation Condition as shown in Figure 1.29.1 The left edge material is defined as AA5454: Al-3Mg-1Mn-0.3Fe-0.01Zn(wt.%); the right edge material is AZ91: Mg-8.2Al-1Zn-0.2Mn-0.01Fe (wt.%). The temperature range is from 300 °C to 500 °C. Note that, instead of manually entering the composition, users can directly select the material from the Materials Chemistry Database (DB) if it has been saved, as described in Pandat User's Guide: Material-to-Material Calculation 3.3.6.

Post Calculation Operation:

- Add a new Table as shown in Figure 1.29.2 to get the ZPF line data of the liquid phase (**`f(@Liquid)=0`**);
- Plot the ZPF line data in the added table into the default graph following the procedure in Pandat User's Guide 2.4.3;
- Label phase field following the procedure in Pandat User's Guide 2.3.3;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;

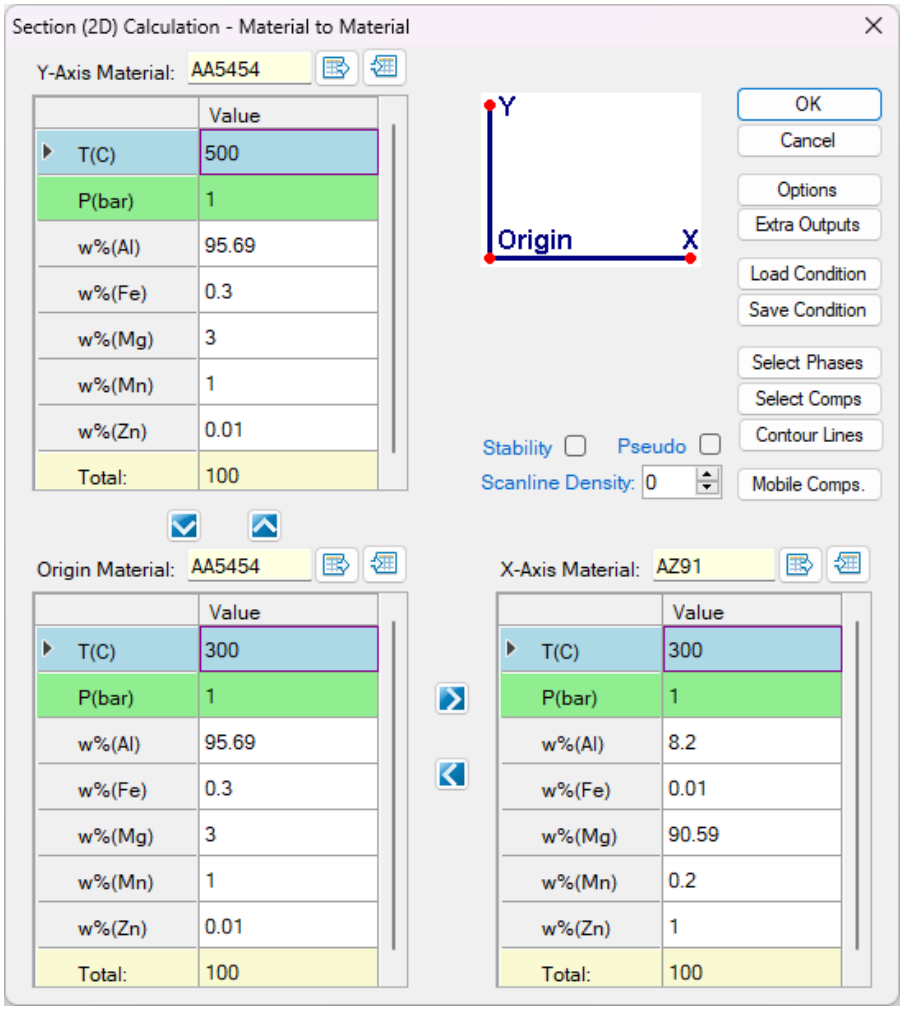


Figure 1.29.1: Set material to material section calculation conditions

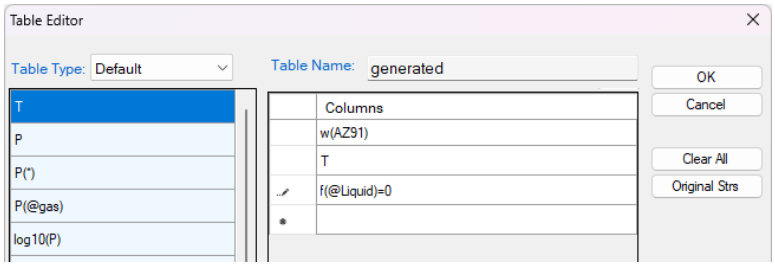


Figure 1.29.2: Output the ZPF line data of the liquid phase

Information obtained from this calculation:

- The obtained phase diagram is shown in Figure 1.29.3. The weight percent of the material AZ91 is used as X-axis. This figure is similar to the Figure 1.25.3 in Example 1.25 where the weight percent of element Mg is used as X-axis.

- To prevent partial melting during the friction-stir welding process, the local temperatures in the welding zone must be maintained below the threshold indicated by the red line. In this case, the minimum temperature to avoid such melting is 435.7 °C.
- Different intermetallic phases may form in the joining zone: The Al_3Mg_2 phase with some Al_6Mn precipitate near the Al alloy side, and $Mg_{17}Al_{12}$ phase with minor precipitation of Al_4Mn near the Mg alloy side.
- A similar approach can also be applied to analyze interactions between other materials, such as coating/substrate reactions.

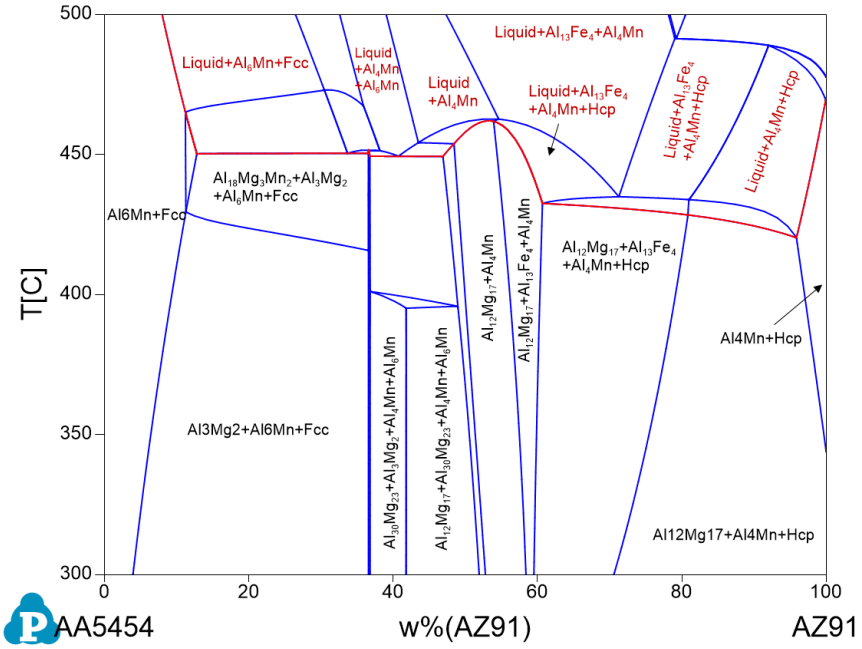


Figure 1.29.3: The vertical phase diagram from AA5454 to AZ91 with phase field labels (The phase fields including Liquid phase are labeled as red)

2 PanOptimizer Example

Example 2.1 Parameter Optimization for the Fe-Cr-Ni Ternary System

Purpose: Learn to optimize thermodynamic parameters for a ternary system.

Module: PanOptimizer

Database: `Fe-Cr-Ni_OPT.tdb`

pop file: `Fe-Cr-Ni_OPT.pop`

Figure 2.1.1 shows an experimentally determined isothermal section of the Fe-Cr-Ni ternary system at 900°C. Two solution phases, Bcc (α) and Fcc (γ), and one intermetallic compound (σ) are stable at this temperature. The experimental data includes tie-lines (equilibrium between two different phases) and tie-triangles (equilibrium of three different phases). This example shows how to optimize the thermodynamic parameters for this system using the given experimental data.

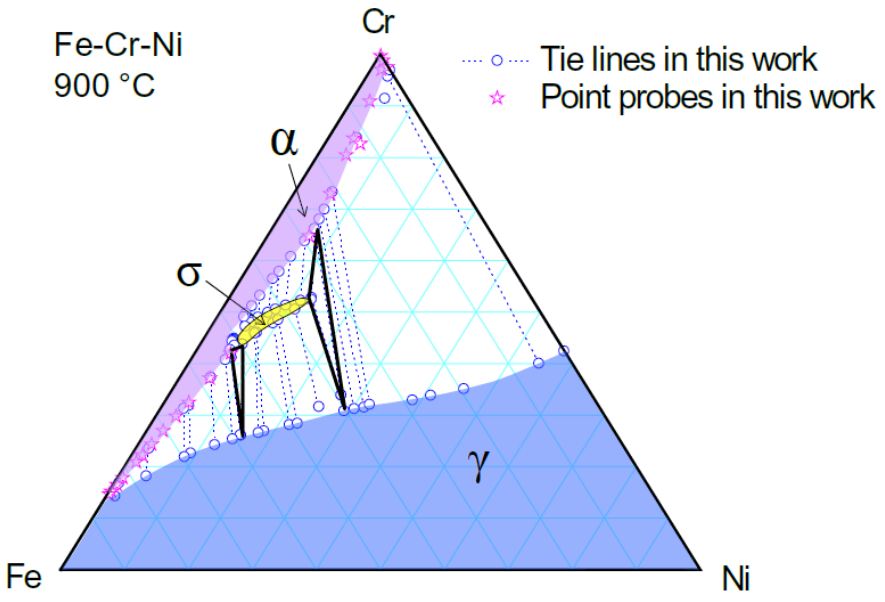


Figure 2.1.1: Experimentally determined Fe-Cr-Ni isothermal section at 900 °C

Prepare file:

- Prepare the database file and pop following the procedure in Pandat User's Guide: Step 1: Prepare Files 4.3.1;

The binary thermodynamic parameters are selected from literature, which are proven to describe the corresponding binary systems precisely. And the ternary interaction parameters are set for optimization. User may go through the database file (Fe-Cr-Ni_OPT.tdb) for more details.

The experimental data are input into the pop file (Fe-Cr-Ni_OPT.pop). The tie-lines are stored in table format by giving an overall alloy composition at themidpoint of the each tie-line. The tie-triangles are input by giving an overall alloy composition at centre point of each triangle. In both cases, the phases use "ENTER" status so that PanOptimizer can easily find the corresponding equilibrium.

Perform Optimization:

- Load the database and experimental files (tdb and pop files) following the procedure in Pandat User's Guide 4.3.1 ;

  User may check the parameters to be optimized by clicking the "Parameters" button on the optimization control panel, and check the difference between calculated equilibrium and experiments by clicking the "Experimental Data" button as shown in the red box in Figure 2.1.2;

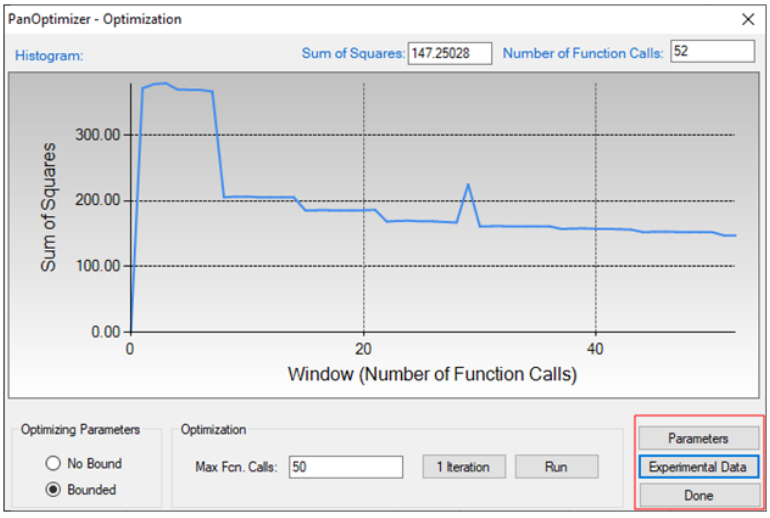


Figure 2.1.2: PanOptimizercontrol interface for optimization setting

After several runs of optimization, the sum of squares will reach a minimum and does not change, which means PanOptimizer has found an optimal result for the parameters. User may calculate an isothermal section at 900 °C and compare to the experimental data. As shown in Figure 2.1.3, the calculated phase boundaries are in good agreement with the experimental data. And user may also need to check the values of the parameters and make sure that they are reasonable as shown in Figure 2.1.4. If there is noticeable difference between calculated boundary and the experimental data, user need to figure out new ternary parameters that need to be included in optimization or using more complicated model to describe the corresponding phases.

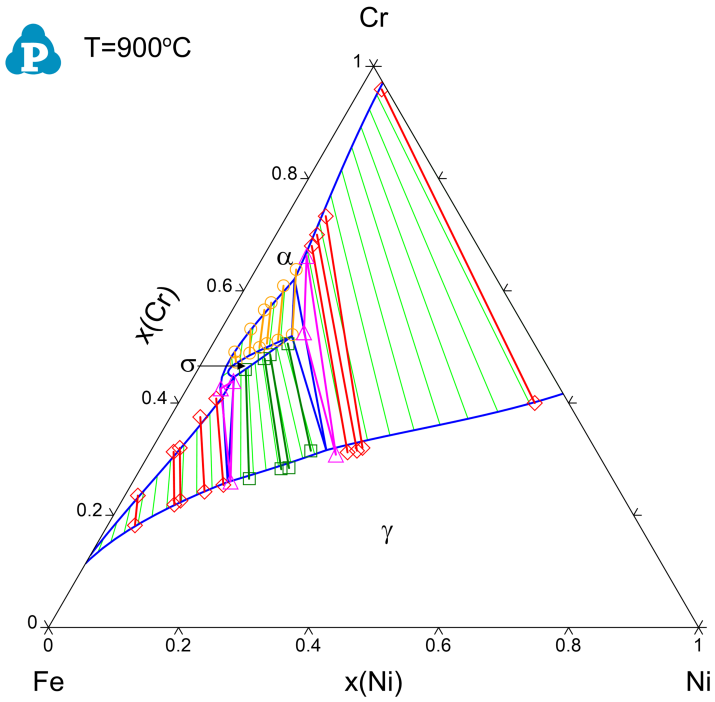


Figure 2.1.3: Comparison between calculated isothermal section at 900°C and experimental data

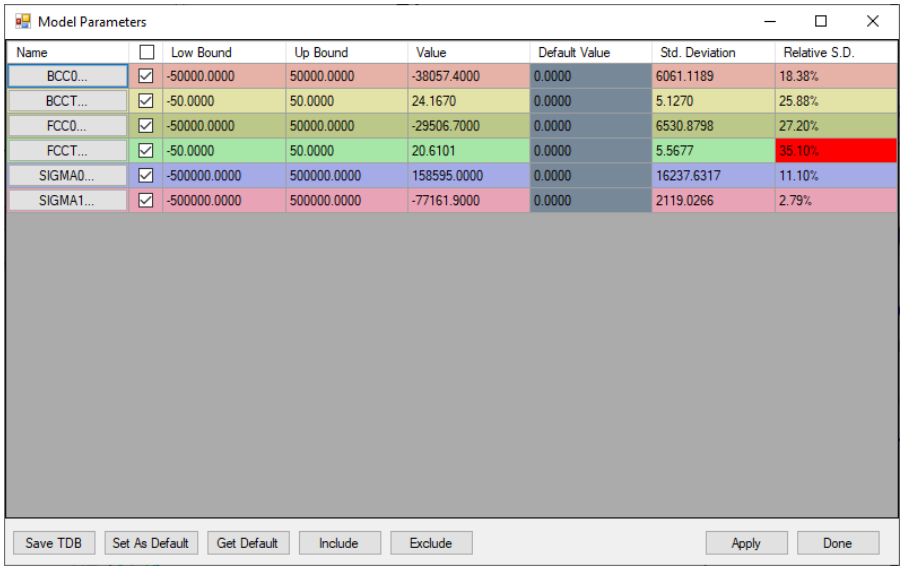


Figure 2.1.4: Optimization results

3 PanEvolution/PanPrecipitation Examples

Example 3.1 Precipitation Simulation of Ni-14Al (at%) Alloy

Purpose: Learn to perform a precipitation simulation of a binary alloy. In this example, precipitation simulation will be performed for Ni-14Al alloy during isothermal ageing at 550 °C, and experimental data will be added to the plots

Module: PanEvolution

Thermodynamic and Mobility Database: `AlNi_Prep.tdb`

Kinetic Parameters Database: `Ni-14Al_Precipitation.kdb`

Batch file: `Example_#3.1.pbfx`

Calculation Procedures:

- Create a workspace and select the PanEvolution module following Pandat User's Guide 2.1;
- Load `AlNi_Prep.tdb` following the procedure in Pandat User's Guide 3.2.1;
- Click on PanEvolution/PanPrecipitation on the menu bar and select "**Load KDB or EKDB**", then select the `Ni-14Al_Precipitation.kdb`, a dialog will pop out as shown in Figure 3.1.1. This dialog shows the key information stored in the `Ni-14Al_Precipitation.kdb`, i.e, the matrix phase is `Fcc`, and the precipitate phase is `L12_FCC`;
- Click menu "**File → Open File**" to open the `Ni-14Al_Precipitation.kdb`. As shown in Figure 3.1.2, in addition to the matrix phase and precipitate phase, other parameters, such as, molar volume and interfacial energy are also defined in this file. Details on these parameters can be found in Pandat User's guide Section 5.3.;
- Click on PanEvolution/PanPrecipitation on the menu bar and click "**Precipitation Simulation**". A dialog will pop out as shown in Figure 3.1.1, set up the alloy chemistry on the left and the heat treatment condition on the right. In this setting, an isothermal ageing is performed at 550 °C assuming the initial state is pure Fcc phase; Add Intermediate PSD outputs at 1 hour, 10 hours and 50 hours.

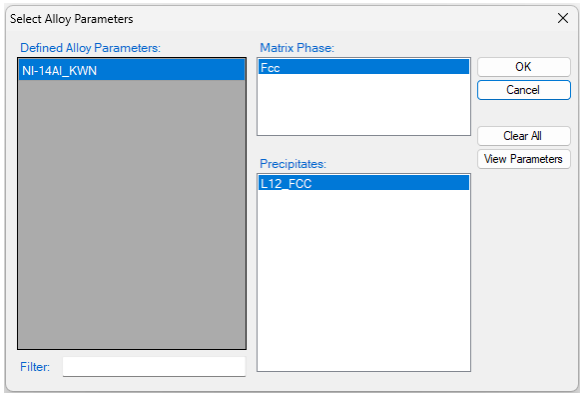


Figure 3.1.1: Loading the Ni-14Al_Precipitation.kdb

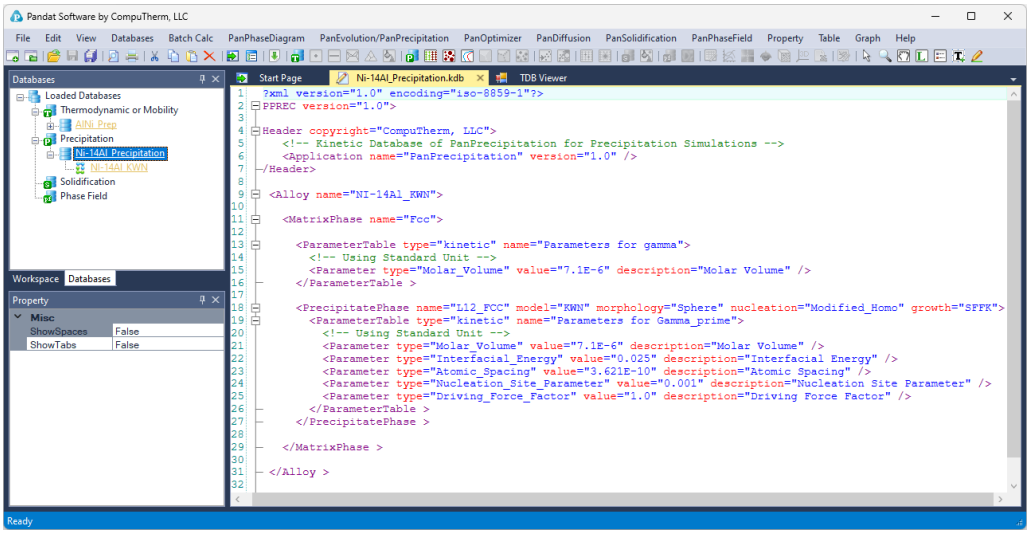


Figure 3.1.2: Parameters defined in the Ni-14Al_Precipitation.kdb

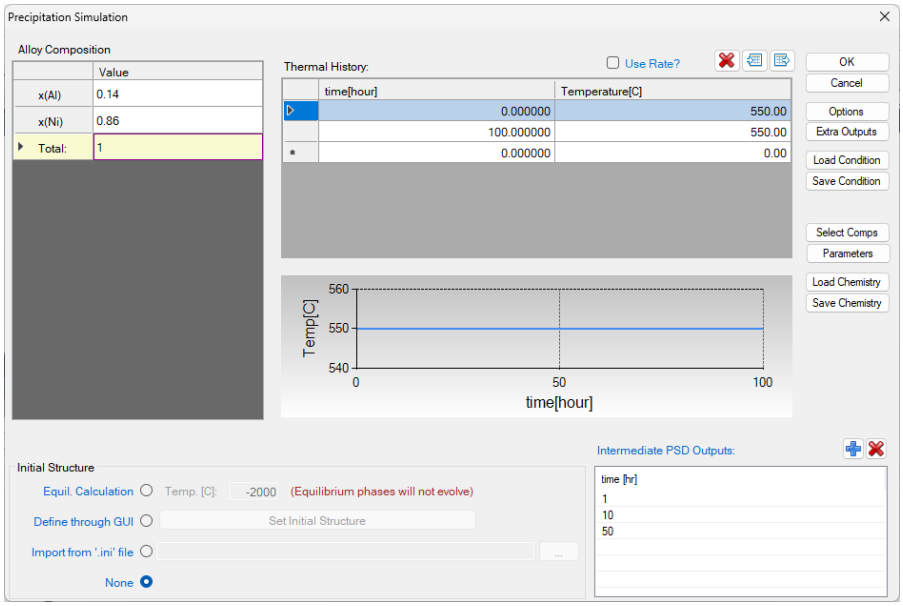


Figure 3.1.3: Setup the alloy chemistry (Ni-14 at%Al) and heat treatment condition (isothermal ageing at 550 °C) for the simulation

Post Calculation Operation:

- Right click the Default graph and rename it as **`Vf`**;
- Create a new table as shown in Figure 3.1.4. A new table with two columns will be created with the first time in hour and the second size of L12_FCC in nanometer. Create a plot from this table and rename it as **`Size`**;
- Create a new table as shown in Figure 3.1.5. A new table with two columns will be created with the first log(time in minute) and the second the number density of L12_FCC in cm^3. Create a plot from this table and rename it as **`nd`**;
- Import a table from a file as shown in Figure 3.1.6, and select `Ni-14Al_Exp.dat`;
- Open the Size graph, single click the `Ni-14Al_Exp` table and drag in the `t(hr)` as x-axis, press **`Ctrl`** and drag in the `radius(nm)` as y-axis. In the Property window set the "**`Plot Type`**" as `Point`, the plot with experimental data point is shown in Figure 3.1.7;
- Open the **`nd`** graph and add the experimental data on it as shown in Figure 3.1.8;

- Create a new table as shown in Figure Figure 3.1.9, select psd as the Table Type; select the `psd_s(L12_FCC)` and the `psd_nnd(L12_FCC)` two columns to create a new plot as shown in Figure 3.1.10;

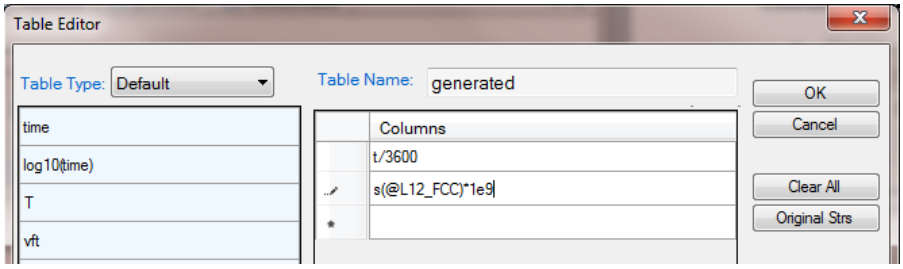


Figure 3.1.4: Create a new table with two columns with the first column time (hour) and the second column the precipitate size (nm)

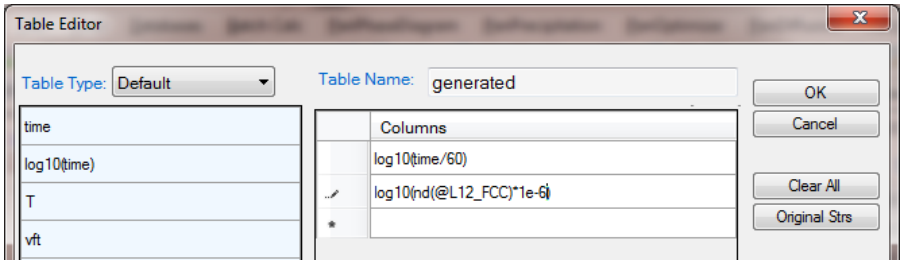


Figure 3.1.5: Create a new table with two columns with the first column log(time) and the second the number density of the precipitate per cm^3

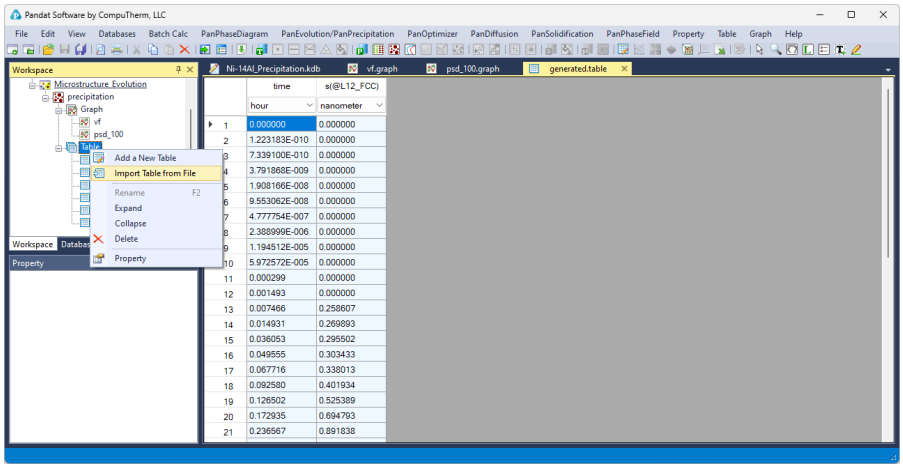


Figure 3.1.6: Import an experimental data table from a file

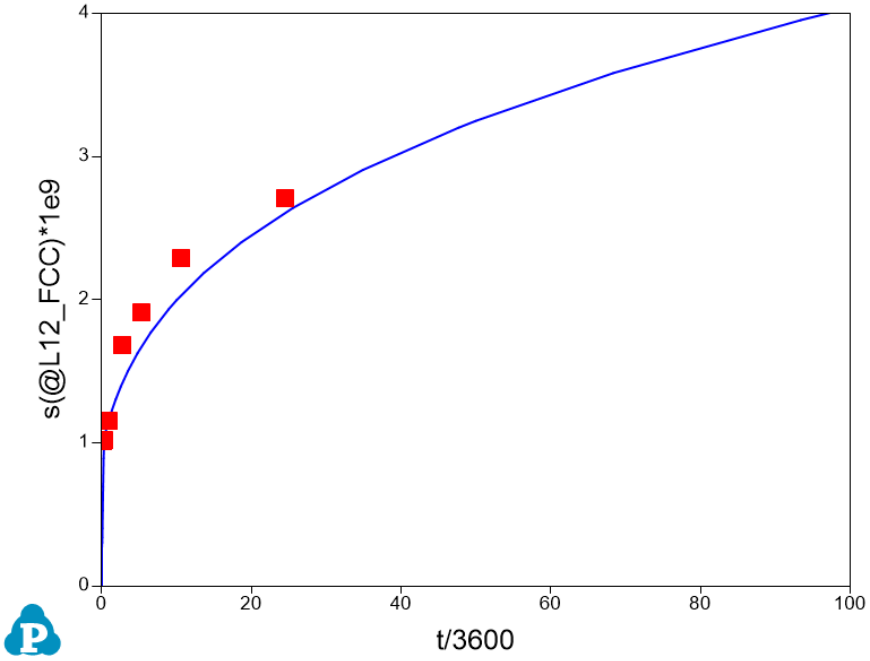


Figure 3.1.7: Plot of size evolution with experimental data

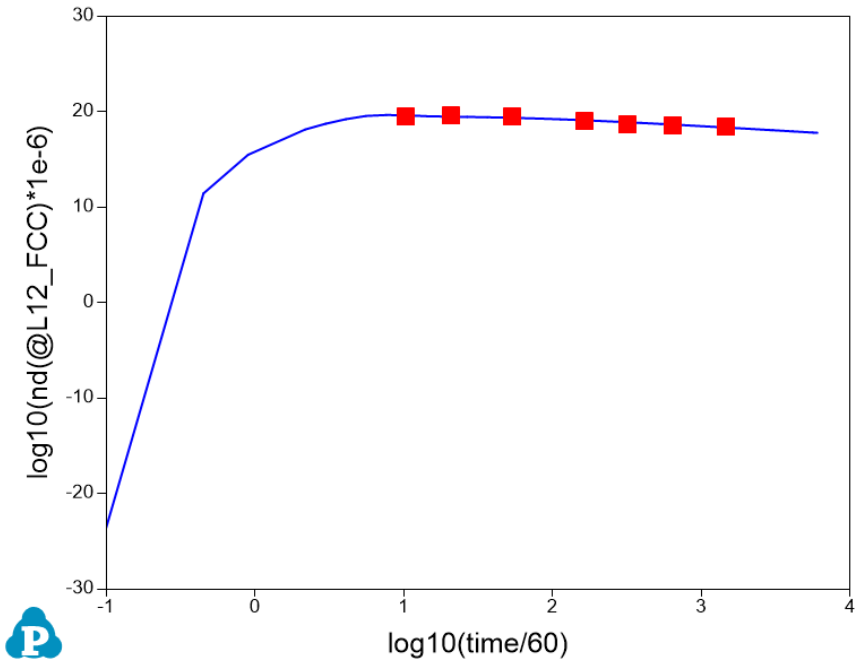


Figure 3.1.8: Plot of number density evolution with experimental data

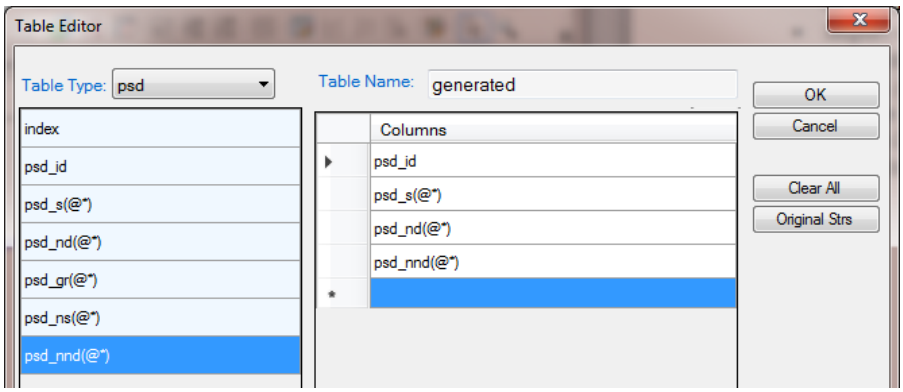


Figure 3.1.9: Create a new table for particle size distribution

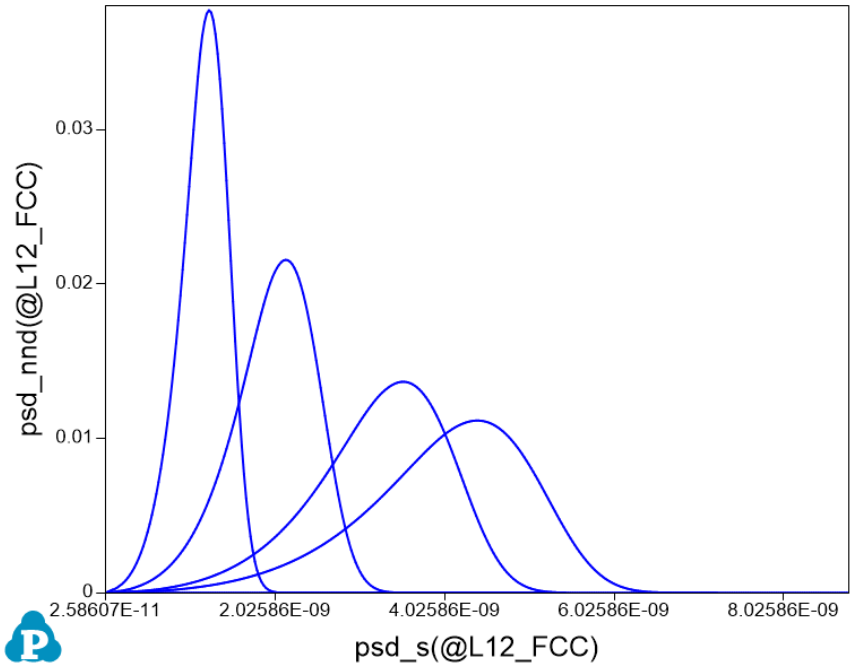


Figure 3.1.10: Plot of particle size distribution

Information obtained from this calculation:

- It is common practice to plot the experimental data on the calculated diagram. When doing so, it is important to make unit consistency between the experimental data and the calculated property. In Pandat calculation, international standard unit is used, i.e., second for time, meter for length and cube meter for volume, and so on;
- Particle number density counts the number of particles in a unit volume. Default output from Pandat is number per m^3, it was converted to number per cm^3 in Figure 3.1.8;

- The `psd_nnd(L12_FCC)` in Figure 3.1.10 is normalized number density, which equals to the particle numbers of each size class divided by the total particle numbers;
- Figure 3.1.10 shows four distribution curves at four different times. The sharp one is at early nucleation stage which shows small particle size and high number density, the flat one shows the particle size distribution as final time (100 hours in this simulation). The corresponding time of each distribution can be found in the table. When create the table, simply put this time information in the table as shown in Figure 3.1.11;
- To only plot the particle size distribution curve at one time, set the inde `x=1`, or `2` ... or `i`. inde`x=i` means the final distribution. Figure 3.1.12 shows the table created for the final size distribution and Figure 3.1.13 shows the distribution curve.

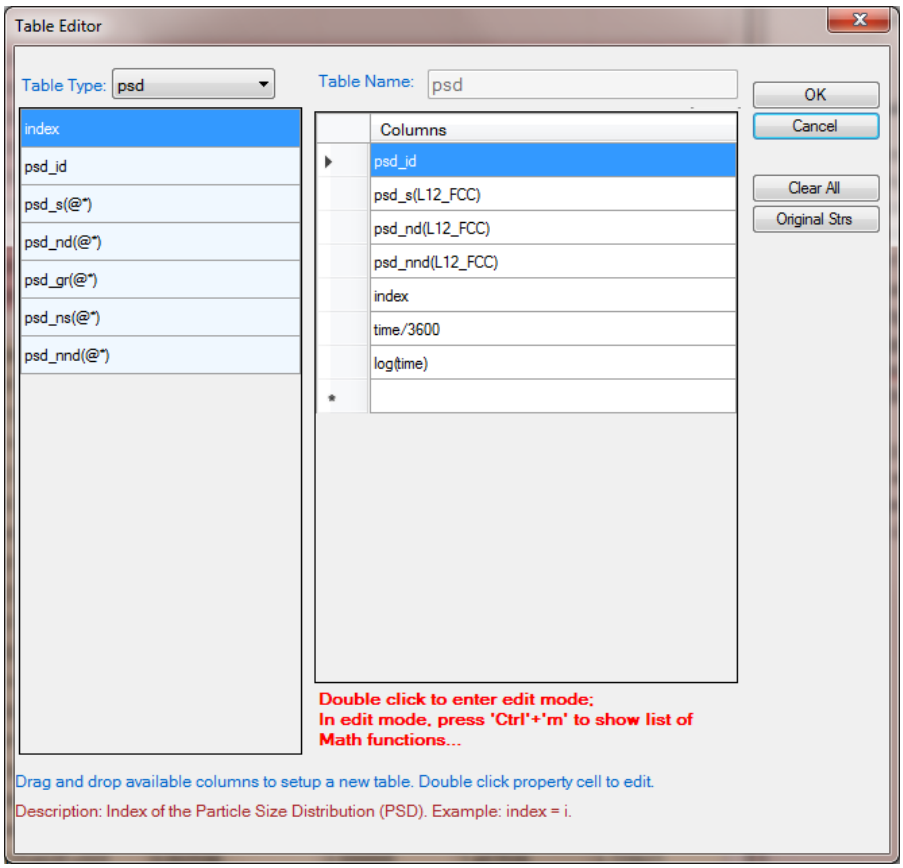


Figure 3.1.11: List the index and corresponding time for each size distribution curve

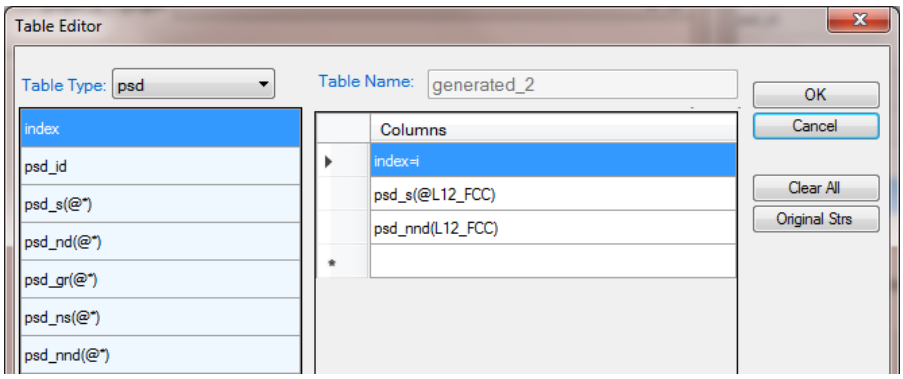


Figure 3.1.12: Create the table for final size distribution

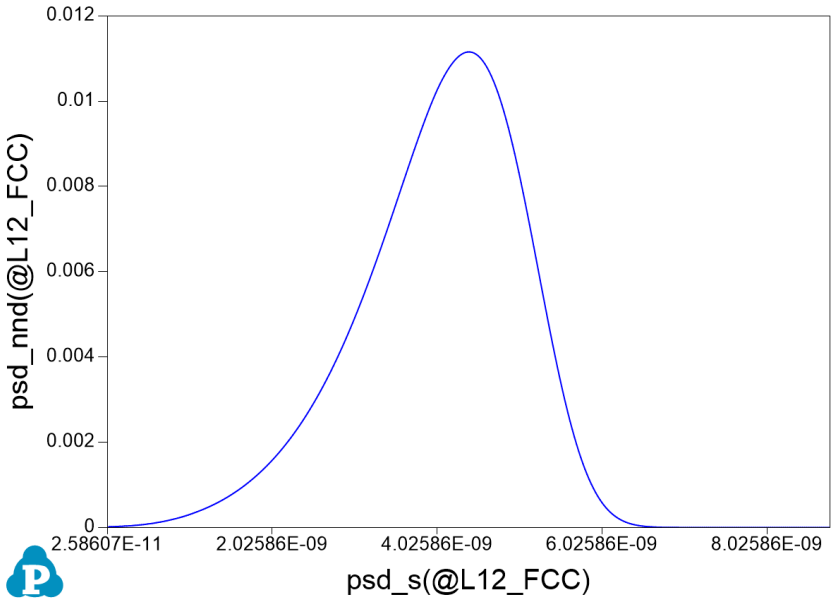


Figure 3.1.13: Plot for final size distribution and the plot

Example 3.2 TTT diagram of Ni-14Al (at%) Alloy

Purpose: Learn to calculate the TTT curve for a given alloy.

Module: PanEvolution

Thermodynamic and Mobility Database: `AlNi_Prep.tdb`

Kinetic Parameters Database: `Ni-14Al_Precipitation.kdb`

Batch file: `Example_#3.2.pbfx`

Calculation Procedures:

- Create a workspace and select the PanEvolution module following Pandat User's Guide 2.1;
- Load `AlNi_Prep.tdb` following the procedure in Pandat User's Guide 3.2.1;
- Click on PanEvolution/PanPrecipitation on the menu bar and select "**`Load KDB or EKDB`**", then select the `Ni-14Al_Precipitation.kdb`;
- Click on PanEvolution/PanPrecipitation on the menu bar and click "**`TTT Simulation`**". A dialog will pop out as shown in Figure 3.2.1, In this dialog, user needs to input the alloy chemistry (left), temperature range and step (bottom right) and the Target volume fraction (top right). If the "Relative Vol%" box is checked, it means the Target Vol% is relative to the equilibrium fraction of the precipitate phase at each temperature, otherwise it is the volume fraction of the precipitate phase.

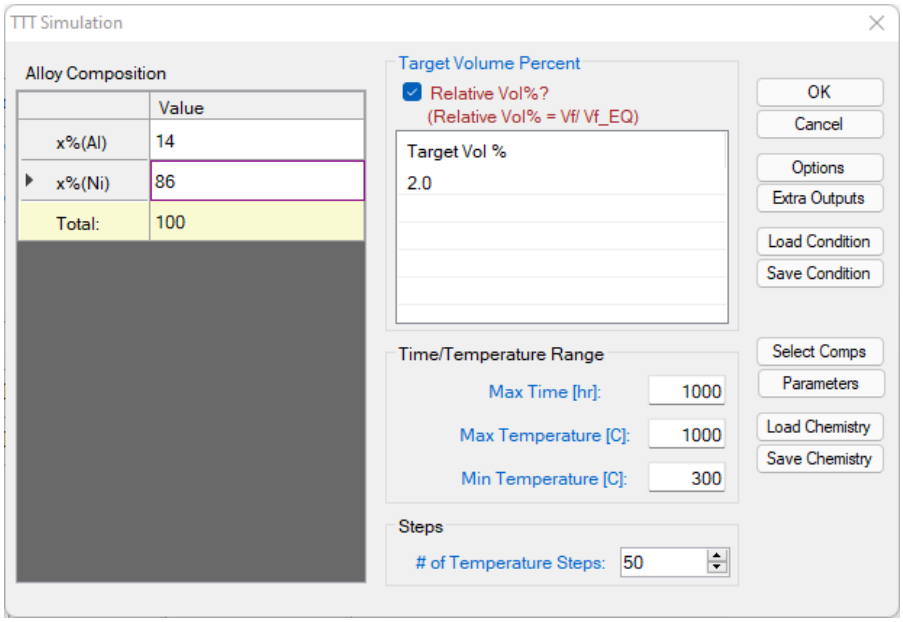


Figure 3.2.1: Setup a calculation of TTT curve for Ni-14Al (at%) alloy

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;

Information obtained from this calculation:

- Figure 3.2.2 shows the default plot from the calculation. It should point out that this TTT curve represents the time-Temperature curve when 2% of the equilibrium precipitate at each temperature comes out. For example, the equilibrium fraction of L12_FCC precipitate phase is 16.56% at 650°C, 2% of it is 0.33%. In other words, it takes 6.5 second to precipitate 0.33% of L12_FCC at this temperature.
- Perform another calculation for 10% and merge the two plots as shown in Figure 3.2.3;
- Details on the time, temperature and fraction of precipitate can be found in the Default table;

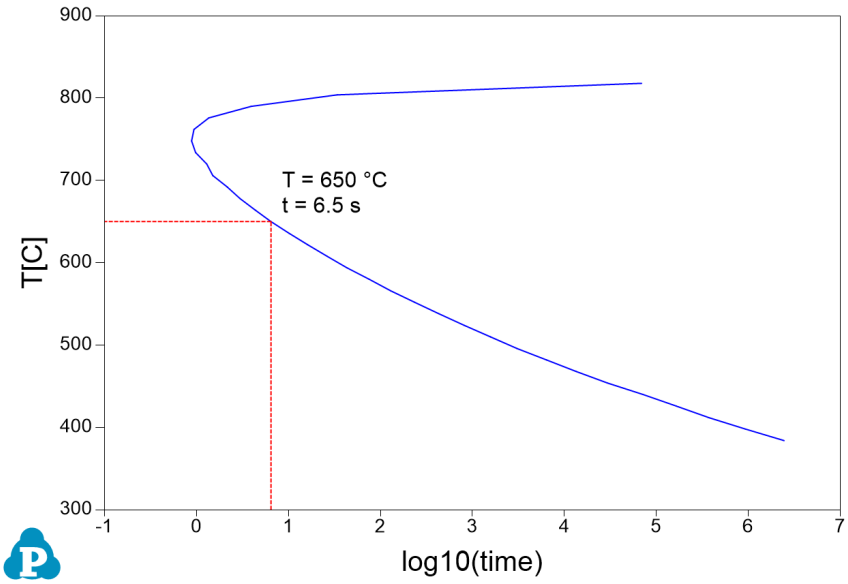


Figure 3.2.2: TTT curve for Ni-14Al (at%) when 2% of equilibrium L12_FCC formed

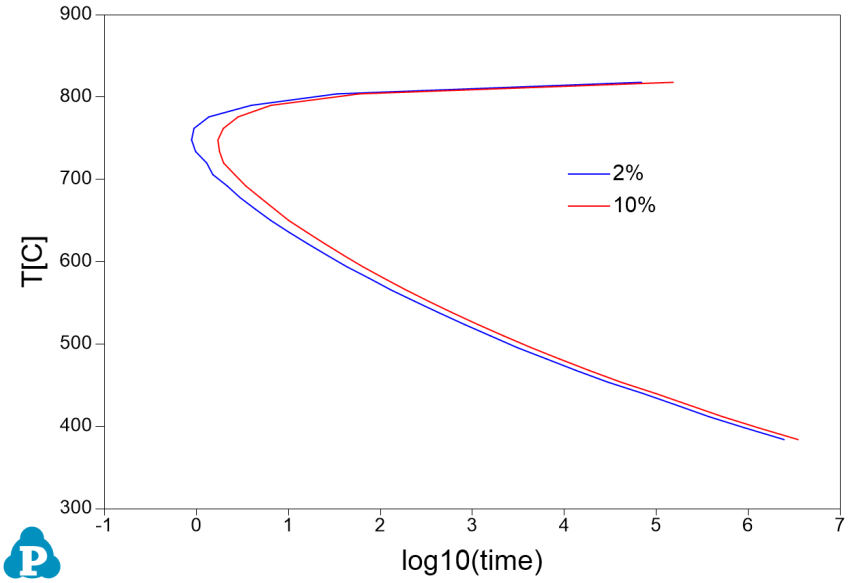


Figure 3.2.3: Comparison of TTT curves for Ni-14Al (at%) when 2% or 10% of equilibrium L12_FCC formed

Example 3.3 Co-precipitation of γ' and γ'' in Ni-Al-Nb Ternary

Purpose: Learn to calculate co-precipitation of γ' and γ'' for an alloy in a pseudo-ternary system.

Module: PanEvolution

Thermodynamic and Mobility Database: `NiAlNb_Pseudo.tdb`

Kinetic Parameters Database: `Ni-2.4Al-3.8Nb.kdb`

Batch file: `Example_#3.3.pbfx`

Calculation Procedures:

- Create a workspace and select the PanEvolution module following Pandat User's Guide 2.1;
- Load `NiAlNb_Pseudo.tdb` following the procedure in Pandat User's Guide 3.2.1;
- Click on PanEvolution/PanPrecipitation on the menu bar and select "**Load KDB or EKDB**", then select the `Ni-2.4Al-3.8Nb.kdb`; the pop-out window is shown in Figure 3.3.1 which include the alloy name, the matrix phase and the precipitates. Two precipitates are defined in this case. The phase name in the kdb file is L12_Fcc and gamma_double_prime for γ' and γ'', respectively;
- Open the `Ni-2.4Al-3.8Nb.kdb` from Pandat workspace through the menu "**File → Open File**", and view the kinetic parameters as shown in Figure 3.3.2;
- Click on the menu "**PanEvolution/PanPrecipitation → Precipitation Simulation**", and set up the calculation condition as shown in Figure 3.3.3.

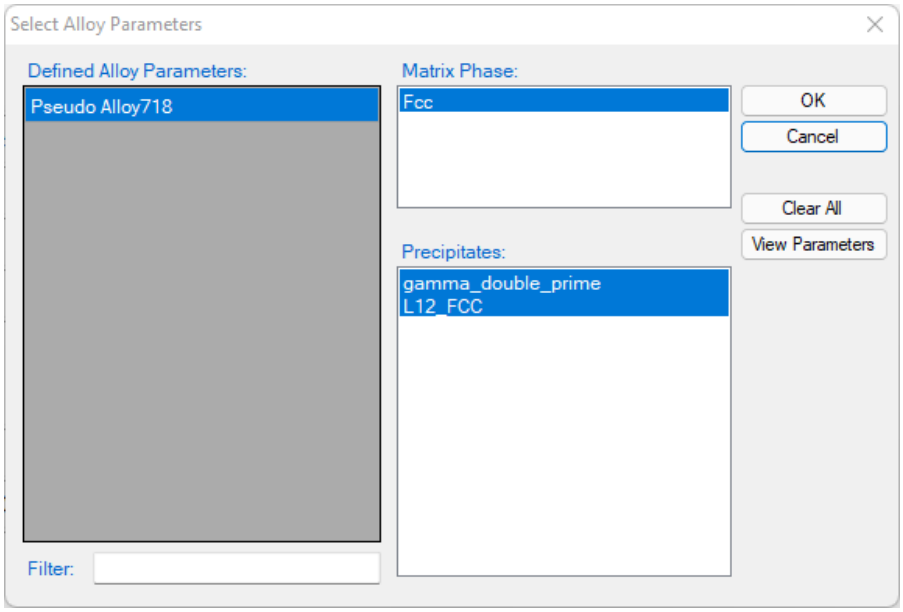


Figure 3.3.1: Pop-out window when loading the Ni-2.4Al-3.8Nb.kdb

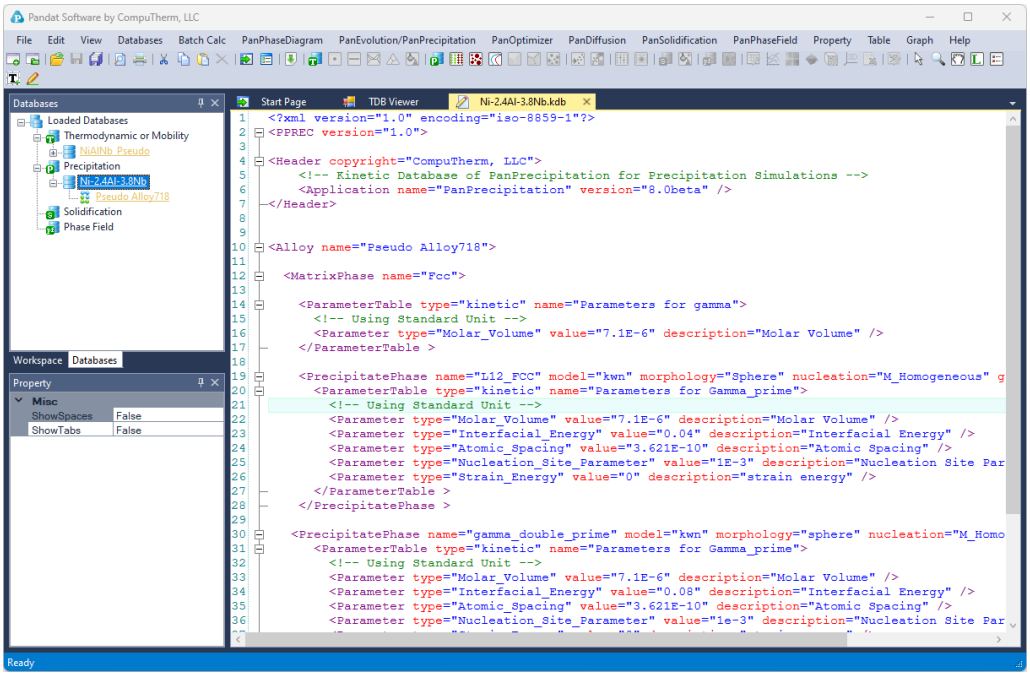


Figure 3.3.2: Open the Ni-2.4Al-3.8Nb.kdb in Pandat workspace to view the kinetic parameters of the two precipitate phases

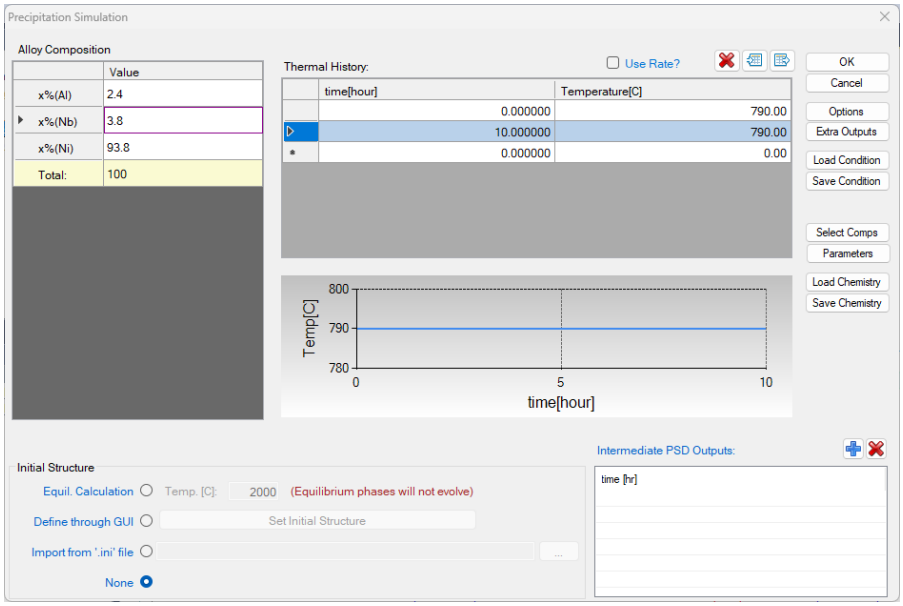


Figure 3.3.3: Precipitation simulation of alloy Ni-2.4Al-3.8Nb ageing at 790 °C for 10h

Post Calculation Operation:

- The default plot shows the total volume fraction of γ' (L12_Fcc) and γ'' as a function of time shown in Figure 3.3.4.
- Open the Default Table, create time vs sizes of γ' and γ'' phases plots as shown in Figure 3.3.5;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Add legend for graph following the procedure in Pandat User's Guide 2.3.3;

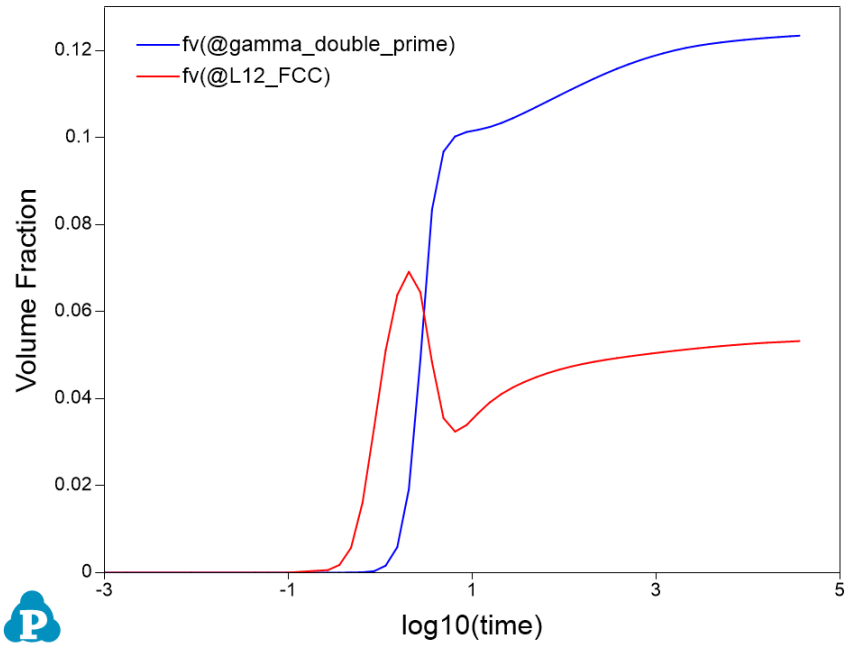


Figure 3.3.4: Default plot showing the volume fraction evolution of the two precipitate phases

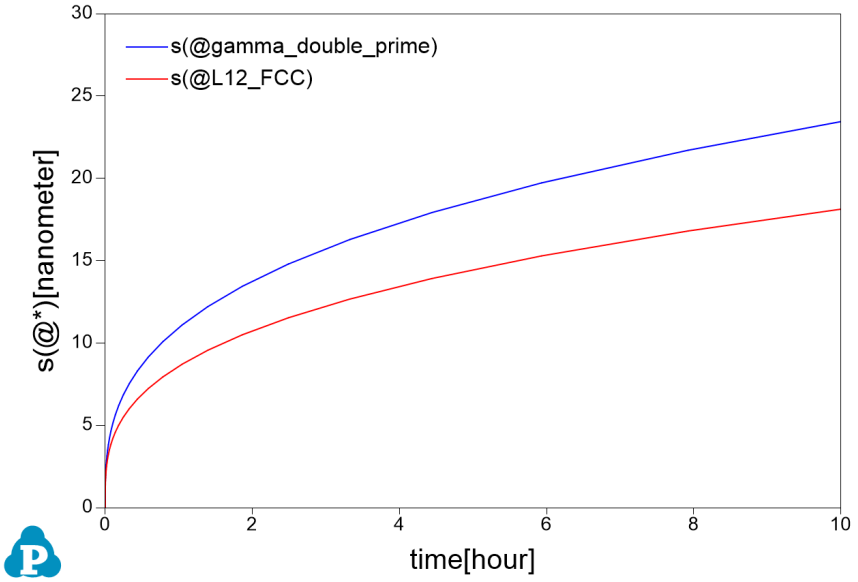


Figure 3.3.5: Calculated average size evolution of the two precipitate phases

Information obtained from this calculation:

- Figure 3.3.4 shows the calculated evolution of volume fraction of the two precipitate phases. It is seen that γ' precipitated quickly at very early stage, but gave way to γ'' at later time;
- Figure 3.3.5 shows the calculated evolution of the average size of the two precipitate phases. It is seen that γ'' is bigger than γ';
- Add a new table as shown in Figure 3.3.6 with the "**`Table Type`**" as **`psd`**. The Columns are particle sizes and number densities with (@*) means all precipitate phases. The default calculated size is in meter, which is converted to nm by multiplying the column by 1e+9. The default calculated number density is number/m^3, which is converted to mol/m_3 by multiplying 1/6.02e+23. The inde x = i means to populate the size and number density at the final state t=10 h;
- Plot particle size distribution from the new table by selecting the particle size as x-axis and number density as y-axis. Plot it for L12 (γ') phase first and then add the one for γ'' as shown in Figure 3.3.7.

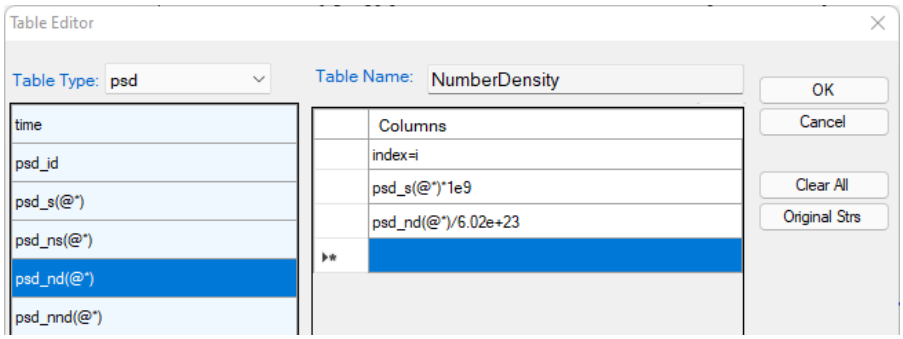


Figure 3.3.6: Create a new table with particle sizes and number densities at final stage

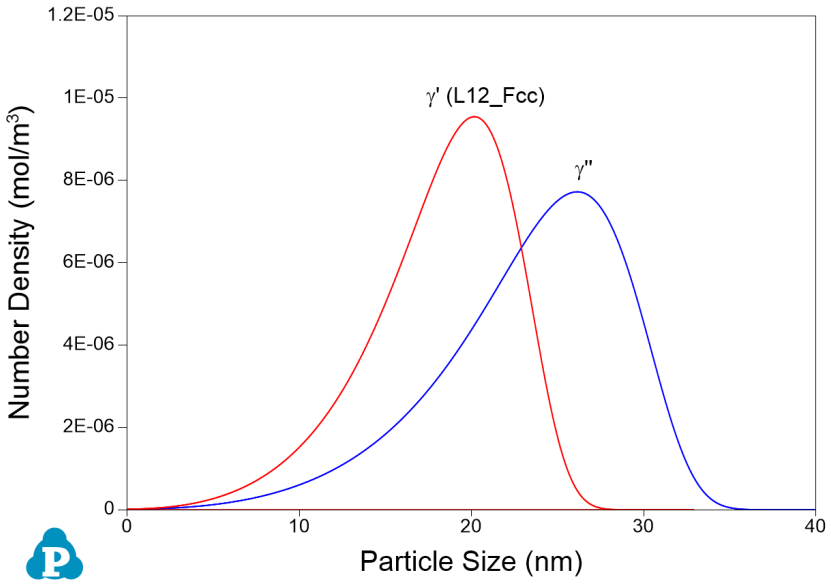


Figure 3.3.7: Particle number densities of γ' and γ'' at final stage

Example 3.4 Simulation of Hardness of Aluminum Alloy 6005

Purpose: Learn to calculate the particle size, number density and hardness of aluminum alloy 6005

Module: PanEvolution

Thermodynamic and Mobility Database: `AlMgSi.tdb`

Kinetic Parameters Database: `AA6xxx.kdb`

Batch file: `Example_#3.4.pbfx`

Calculation Procedures:

- Create a workspace and select the PanEvolution module following Pandat User's Guide 2.1;
- Load `AlMgSi.tdb` following the procedure in Pandat User's Guide 3.2.1;
- Click on PanEvolution/PanPrecipitation on the menu bar and select "**Load KDB or EKDB**", then select the `AA6xxx.kdb`; the pop-out window is shown in Figure 3.4.1 which include the alloy name, the matrix phase and the precipitate phase;
- Open the `AA6xxx.kdb` from Pandat workspace through the menu "**File → Open File**", and view the kinetic parameters;
- Click on the menu "**PanEvolution/PanPrecipitation → Precipitation Simulation**", and set up the calculation condition as shown in Figure 3.4.2. Note the alloy composition is wt% (click Option button to select the unit);

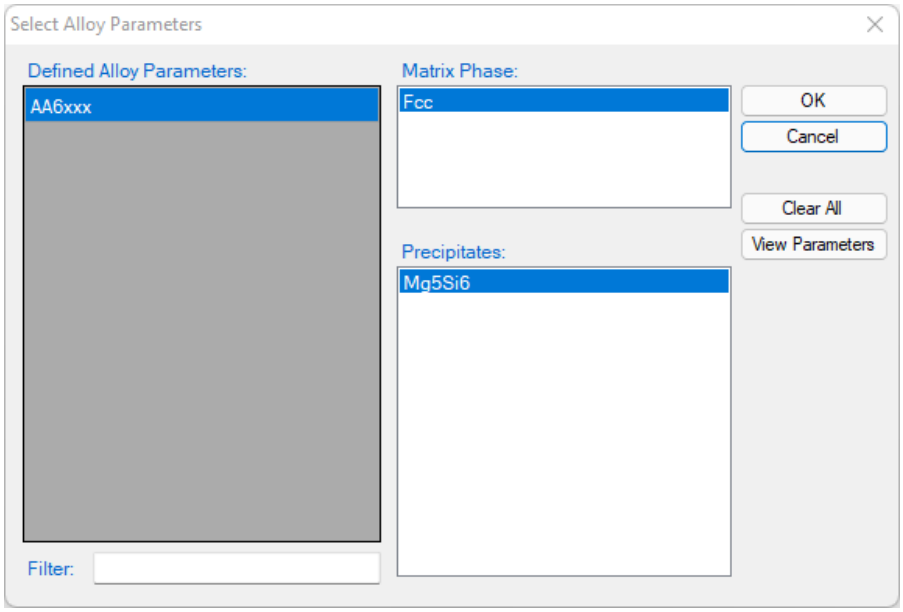


Figure 3.4.1: The matrix phase and the precipitate phase for AA6005

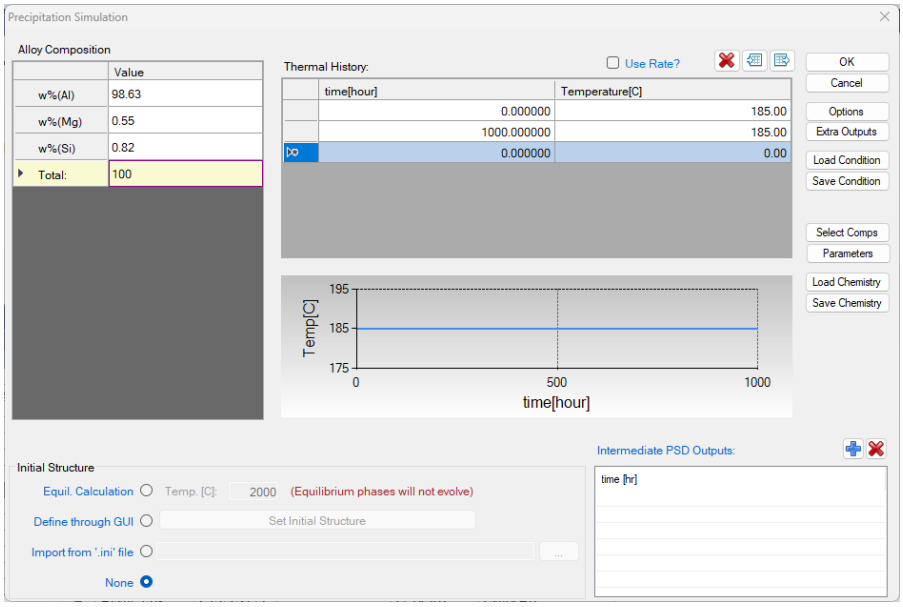


Figure 3.4.2: Setup alloy composition and heat treatment condition as ageing at 185°C for 1000 hours

Post Calculation Operation:

- The default plot shows the total volume fraction of the Mg_5Si_6 phase as a function of time shown in Figure 3.4.3.
- Create a new table as shown in Figure 3.4.4, and plot the log10(time) vs. log(nd), log10 (time) vs. log(size), and log10(time) vs. hv;
- Right Click on the **Table** node below the Graph and choose "**Import Table from File**", import three tables: `AA6005-nd_exp.dat`, `AA6005-size_exp.dat`, and `AA6005-hv_exp.dat` one by one;
- Plot the experimental data in the corresponding plot by drag in the x-axis and then press **Ctrl** and drag in the y-axis of the experimental data table;
- The default plot of the experimental data is a line instead of points. In the **Property Window**, change the **Plot Type** as **Point**;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Add legend for graph following the procedure in Pandat User's Guide 2.3.3;

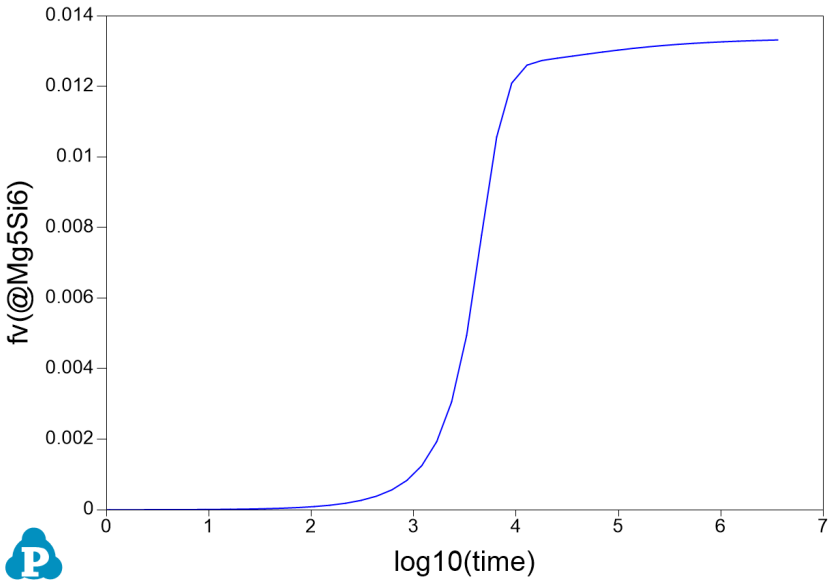


Figure 3.4.3: Default plot of volume fraction evolution of the precipitate

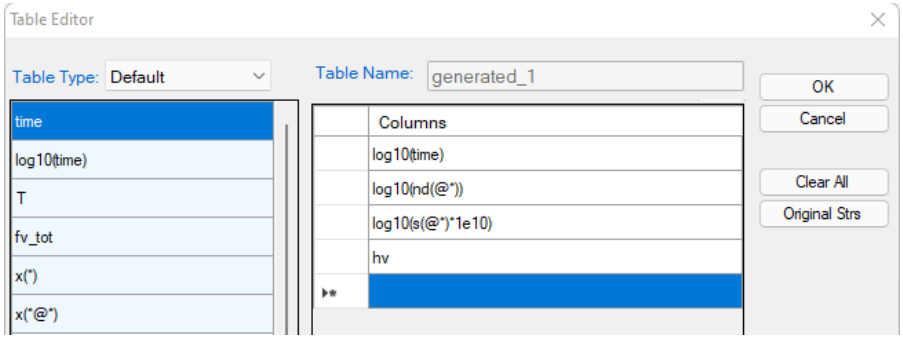


Figure 3.4.4: Create a new table

Information obtained from this calculation:

- Figure 3.4.3 shows the default plot of the simulation which is volume fraction evolution of the precipitate phase. The time is in second;
- Figure 3.4.5 shows the calculated number density evolution; Figure 3.4.6 shows the size evolution, and Figure 3.4.7 the hardness change with time. Experimental data are plotted on them for comparison;
- It is seen that the number density reaches the highest value at ~1000 s (~0.3 h), but the particle size is very small. The hardness reaches peak at ~10000 s (~2.8 h) when both the number density and the particle size are favorable.

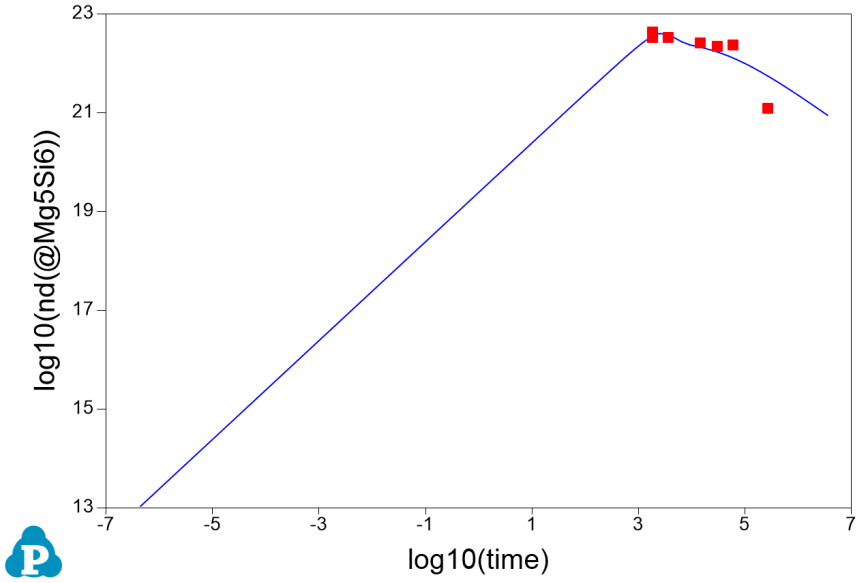


Figure 3.4.5: Calculated evolution of the particle number density with experimental data

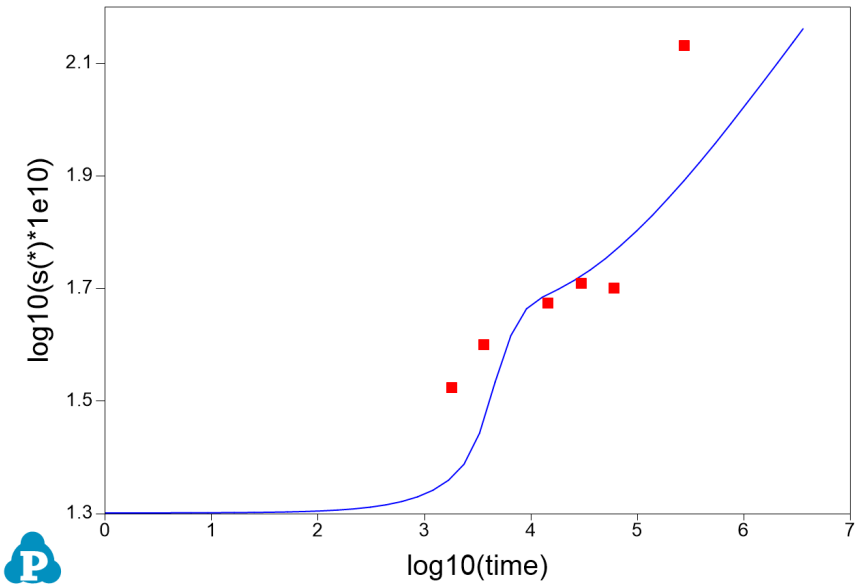


Figure 3.4.6: Calculated evolution of the particle size with experimental data

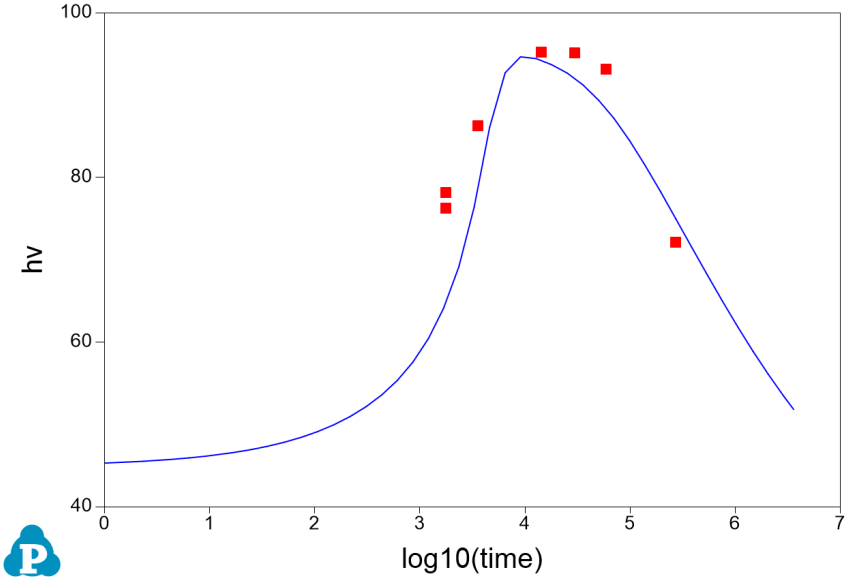


Figure 3.4.7: Calculated evolution of hardness with experimental data

Example 3.5 Simulation of Softening of Aluminum Alloy 6005

Purpose: Learn to calculate the particle size, number density and hardness of aluminum alloy 6005 during ageing and reheating

Module: PanEvolution

Thermodynamic and Mobility Database: `AlMgSi.tdb`

Kinetic Parameters Database: `AA6xxx.kdb`

Batch file: `Example_#3.5.pbfx`

Calculation Procedures:

- Create a workspace and select the PanEvolution module following Pandat User's Guide 2.1;
- Load `AlMgSi.tdb` following the procedure in Pandat User's Guide 3.2.1;
- Click on PanEvolution/PanPrecipitation on the menu bar and select "**Load KDB or EKDB**", then select the `AA6xxx.kdb`;
- Click on the menu "**PanEvolution/PanPrecipitation → Precipitation Simulation**", and set up the calculation condition as shown in Figure 3.5.1.

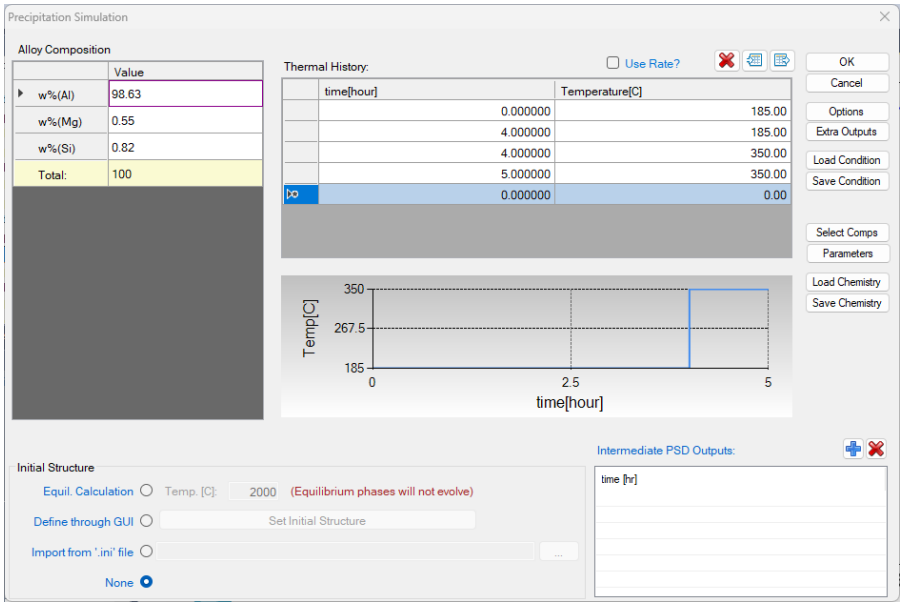


Figure 3.5.1: Setup heat treatment condition as ageing at 185°C for four hours and then quickly heat up to 350°C and hold for 1 hour

Post Calculation Operation:

- Create a new table as shown in Figure 3.5.2, and plot the `time vs. log10(nd)`, `time vs. log(size)`, and `time vs. hv`;
- Right Click on the **`Table`** node below the Graph and choose "**`Import Table from File`**", import table: `AA6005-reheat_exp.dat`;
- Plot the experimental data in the corresponding plot by drag in the x-axis and then press **`Ctrl`** and drag in the y-axis of the experimental data table;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Add legend for graph following the procedure in Pandat User's Guide 2.3.3;

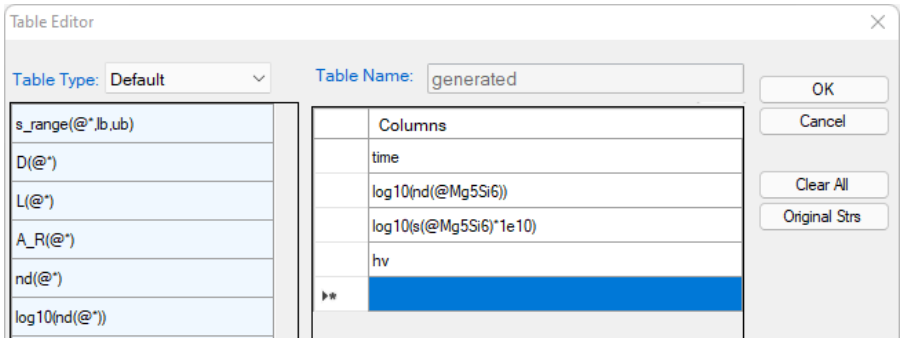


Figure 3.5.2: Create a new table

Information obtained from this calculation:

- Figure 3.5.3 shows the calculated evolution of particle number density with experimental data, time is in second. It is seen that the particle number density increases quickly within the first hour and then decreases slightly during ageing at 185 °C. It decreases drastically when heating up to 350 °C;
- Figure 3.5.4 shows the calculated evolution of particle size with experimental data. It is seen that the particle size increases gradually during ageing at 185 °C. It increases drastically when heating up to 350 °C;
- Figure 3.5.5 shows the calculated evolution of hardness with experimental data. It is seen that the hardness increases gradually during ageing at 185 °C. It drops quickly when heating up to 350 °C.

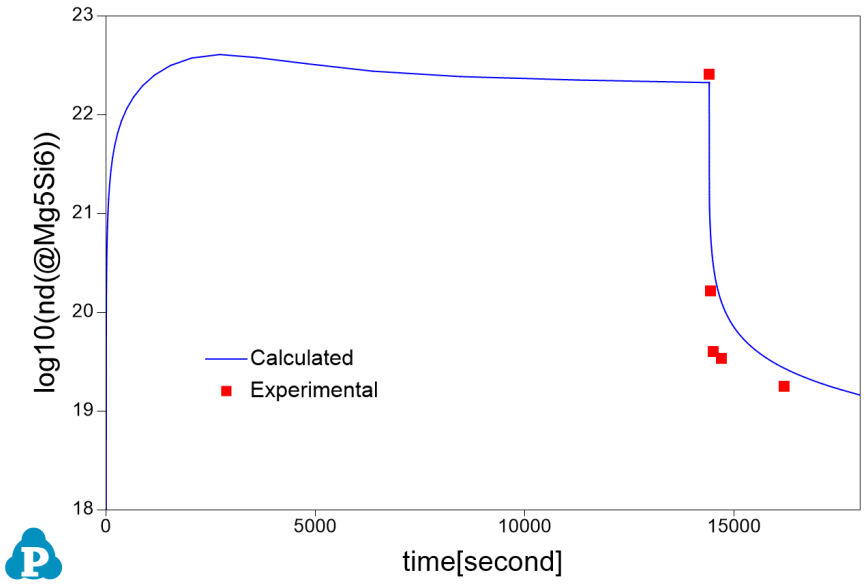


Figure 3.5.3: Calculated evolution of the particle number density with experimental data

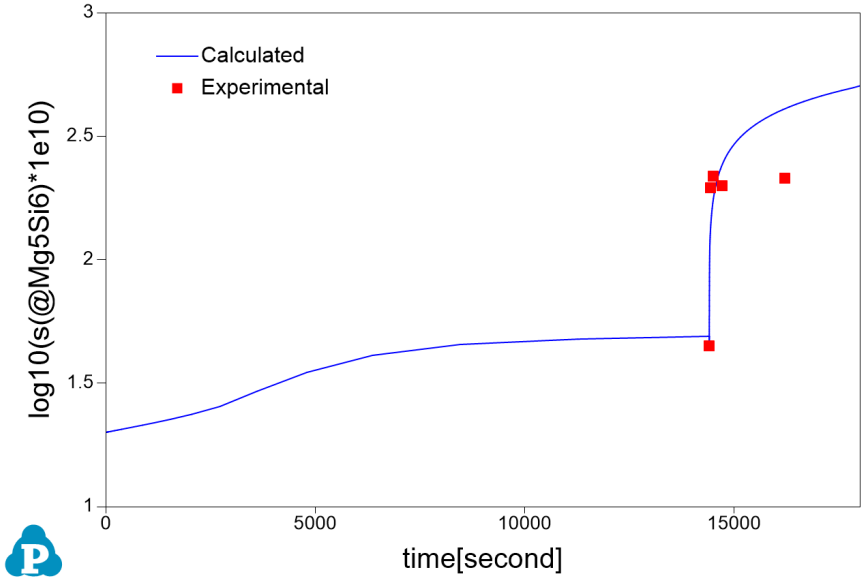


Figure 3.5.4: Calculated evolution of the particle size with experimental data

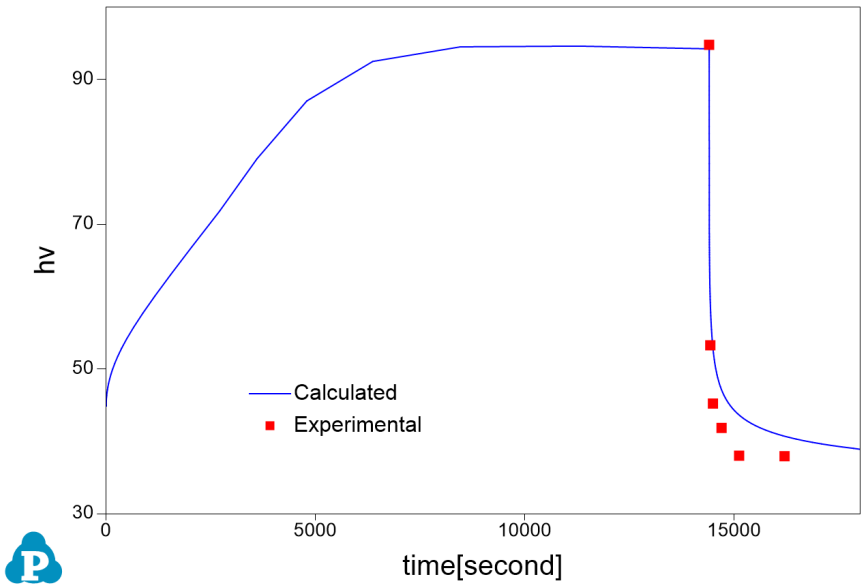


Figure 3.5.5: Calculated evolution of hardness with experimental data

Example 3.6 Simulation of Yield Strength of Aluminum Alloy 356

Purpose: Learn to calculate yield strength including intrinsic, solid solution, and precipitation strengthening of aluminum alloy 356 during the process of ageing

Module: PanEvolution

Thermodynamic and Mobility Database: `AlMgSi.tdb`

Kinetic Parameters Database: `AA3xx.kdb`

Batch file: `Example_#3.6.pbfx`

Calculation Procedures:

- Create a workspace and select the PanEvolution module following Pandat User's Guide 2.1;
- Load `AlMgSi.tdb` following the procedure in Pandat User's Guide 3.2.1;
- Click on PanEvolution/PanPrecipitation on the menu bar and select "**Load KDB or EKDB**", then select the `AA3xx.kdb`;
- Click on the menu "**PanEvolution/PanPrecipitation → Precipitation Simulation**", and set up the calculation condition as shown in Figure 3.6.1. Note that the "Equilibrium Calculation" button under Initial Structure (bottom) should be checked and the solution temperature (540 °C in this case) should be given;

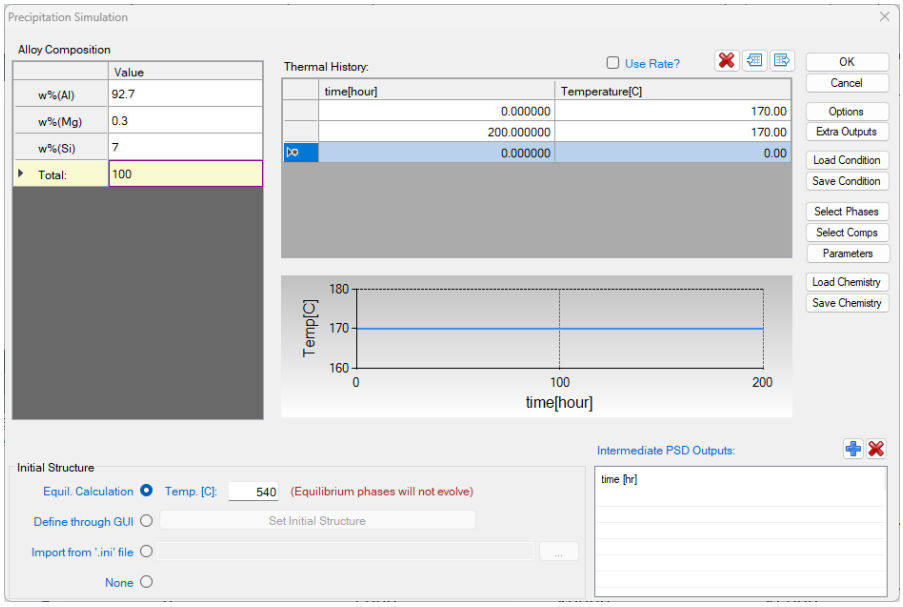


Figure 3.6.1: Setup calculation condition for aluminum alloy 356

Post Calculation Operation:

- Create a new table as shown in Figure 3.6.2, and select all the columns in the newly created table to create a plot;
- Right Click on the **`Table`** node below the Graph and choose "**`Import Table from File`**", import table: `AA356-ys_exp.txt`; Note that the extension of a data file can be either txt or dat;
- Plot the experimental data in the corresponding plot by drag in the `logt` as x-axis and then press **`Ctrl`** and drag in the experimental data `ys` as the y-axis, then repeat it to add experimental data of `ysp`, `ysi` and `yss`;
- Create a new table as shown in Figure 3.6.4, select log10(time/3600) as x-axis, and x%(Mg@_Fcc) and x%(Si@_Fcc) as y-axis to create a plot as shown in Figure 3.6.5;
- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;
- Add legend for graph following the procedure in Pandat User's Guide 2.3.3;

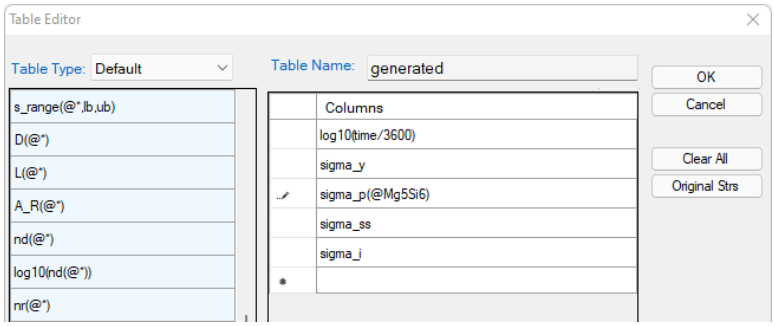


Figure 3.6.2: Create a new table for yield strength plot

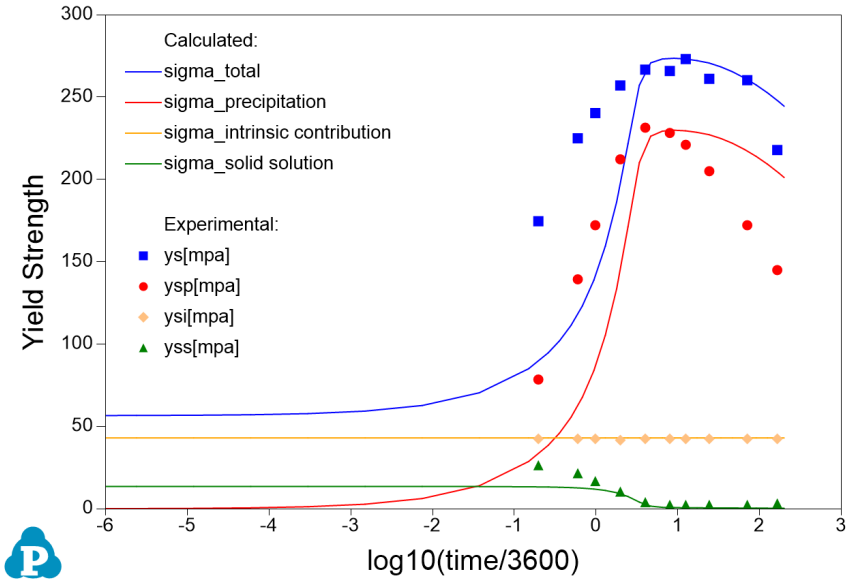


Figure 3.6.3: A comparison of the calculated yield strength (lines) with the experimental data (symbols)

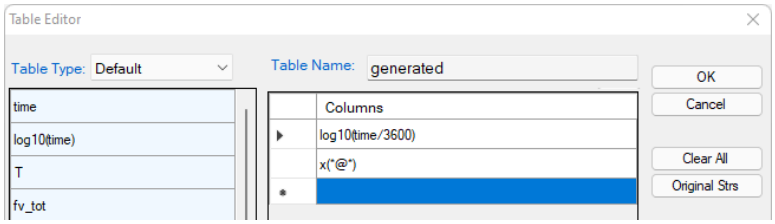


Figure 3.6.4: Create a new table to show the evolution of phase compositions

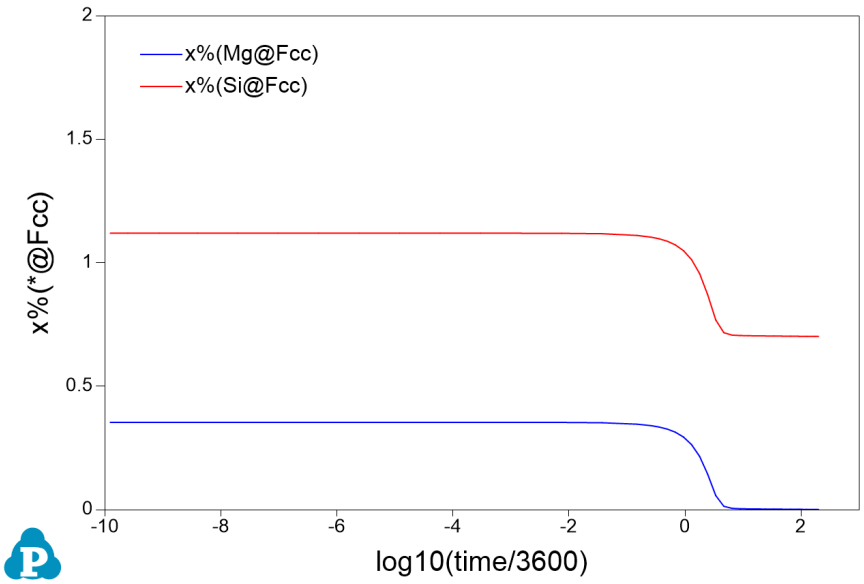


Figure 3.6.5: Evolution of elemental solubility in the matrix Fcc

Information obtained from this calculation:

- Example 3.6 shows a comparison of the calculated yield strength (lines) with the experimental data (symbols). The orange line (symbols) represents the intrinsic contribution; the green line (symbols) represents the solid solution strengthening; the red line (symbols) represents the precipitation strengthening; and the blue line (symbols) is the total from all three contributions;
- It is clearly seen from Figure 3.6.3 and Figure 3.6.5 that with the formation of Mg_5Si_6 precipitate, the solubility of Mg and Si in Fcc decreases and solution strengthening also decreases.

Example 3.7 CCT diagram of Ni-14Al (at%) Alloy

Purpose: Learn to calculate the CCT curve of a given alloy.

Module: PanEvolution

Thermodynamic and Mobility Database: `AlNi_Prep.tdb`

Kinetic Parameters Database: `Ni-14Al_Precipitation.kdb`

Batch file: `Example_#3.7.pbfx`

Calculation Procedures:

- Create a workspace and select the PanEvolution module following Pandat User's Guide 2.1;
- Load `AlNi_Prep.tdb` following the procedure in Pandat User's Guide 3.2.1;
- Click on PanEvolution/PanPrecipitation on the menu bar and select "**`Load KDB or EKDB`**", then select the `Ni-14Al_Precipitation.kdb`;
- Click on PanEvolution/PanPrecipitation on the menu bar and click "**`CCT Simulation`**". A dialog will pop out as shown in Figure 3.7.1, In this dialog, user needs to input the alloy chemistry (left), temperature range, cooling rate range and step (bottom right) and the Target volume fraction (top right).

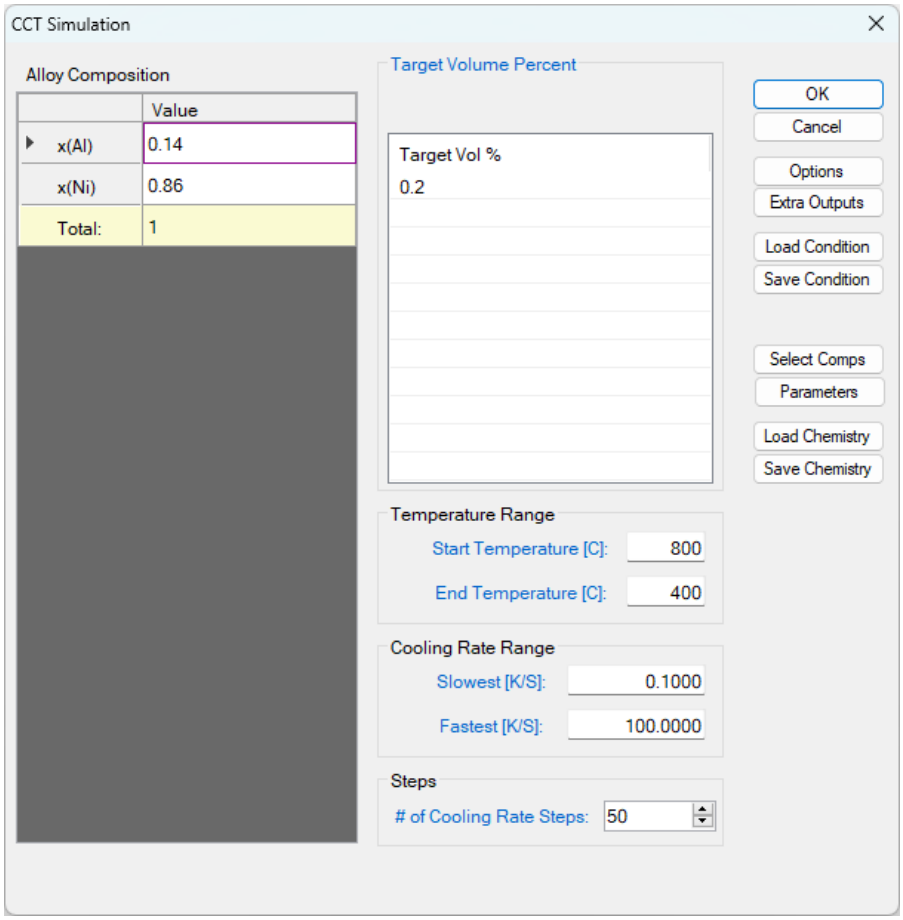


Figure 3.7.1: Setup a calculation of CCT curve for Ni-14Al (at%) alloy

Post Calculation Operation:

- Change graph appearance following the procedure in Pandat User's Guide 2.3.1;

Information obtained from this calculation:

- Figure 3.7.2 shows the default plot from the calculation. On this diagram, the green lines are the cooling curves with different cooling rate, the blue line is the CCT curve represents the temperature when 0.2 vol% of L12_Fcc phase is precipitated under different cooling rates.
- Perform another calculation for 1% and merge the two plots as shown in Figure 3.7.3;
- Details on the time, temperature and fraction of precipitate can be found in the Default table;

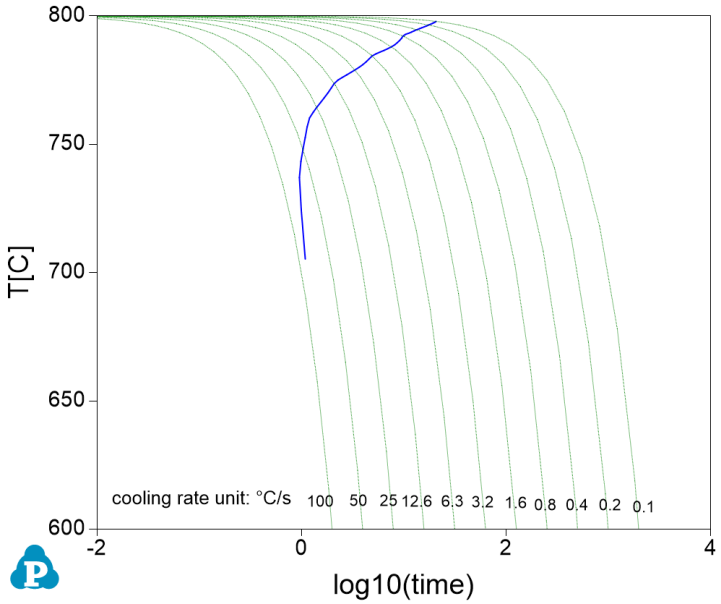


Figure 3.7.2: CCT curve for Ni-14Al (at%) when 0.2% of L12_FCC is precipitated under different cooling rates.

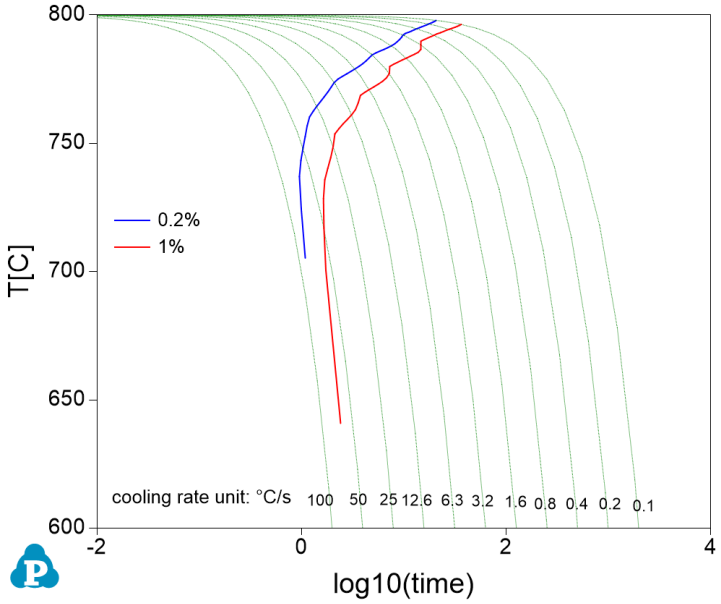


Figure 3.7.3: Comparison of CCT curves for Ni-14Al (at%) when 0.2% or 1% of L12_FCC precipitated under different cooling rates

4 PanDiffusion Examples

Example 4.1 Diffusion within a Single Phase: Uniform Initial Compositions

Purpose: Learn to perform diffusion simulation at constant temperature for a diffusion couple with both sides having the same single phase structure and uniform composition through each side before diffusion.

Module: PanDiffusion

Thermodynamic and Mobility Database: `FeCrNi.tdb`

Batch file: `Example_#4.1.pbfx`

Calculation Procedures:

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load `FeCrNi.tdb` following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Click on the menu "**PanDiffusion → Diffusion Simulation**" and set up the calculation condition as shown in Figure 4.1.1. First select "**Region Composition Distribution**" as **Uniform**, which means that composition in each region is uniform before diffusion. Click on **Region_1** and set the composition of the left side of the diffusion couple as `30Cr-10Fe-60Ni` (at%), then click on **Region_2** and set the composition of the right side of the diffusion couple as `10Cr-20Fe-70Ni` (at%) (which is not shown in Figure 4.1.1).
- The length of both **Region_1** and **Region_2** is set to be 100 μm, and the total number of grids (# of Grids) is 100.
- The Thermal History is holding the diffusion couple at 1000 °C for 1000 hours.
- The default output includes composition profiles of the initial and final stages. Composition profiles can also be plotted and listed in the table for intermediate times. By clicking the blue "+" next to the "**Moments for Profile Outputs**" composition profiles for number of intermediate stages can be outputted. As shown in Figure 4.1.1, those at 200 hour and 500 hour will be outputted. Click **OK** to start calculation.

- User can define the "**`Geometry`**" as "**`Planar`**, **`Cylindrical`**, and **`Spherical`**";
- User can also select "**`Interface Flux Model`**" and set "**`boundary conditions`**". Details on these options can be found in Pandat User's Guide sections 6.3.11 and 6.3.12.

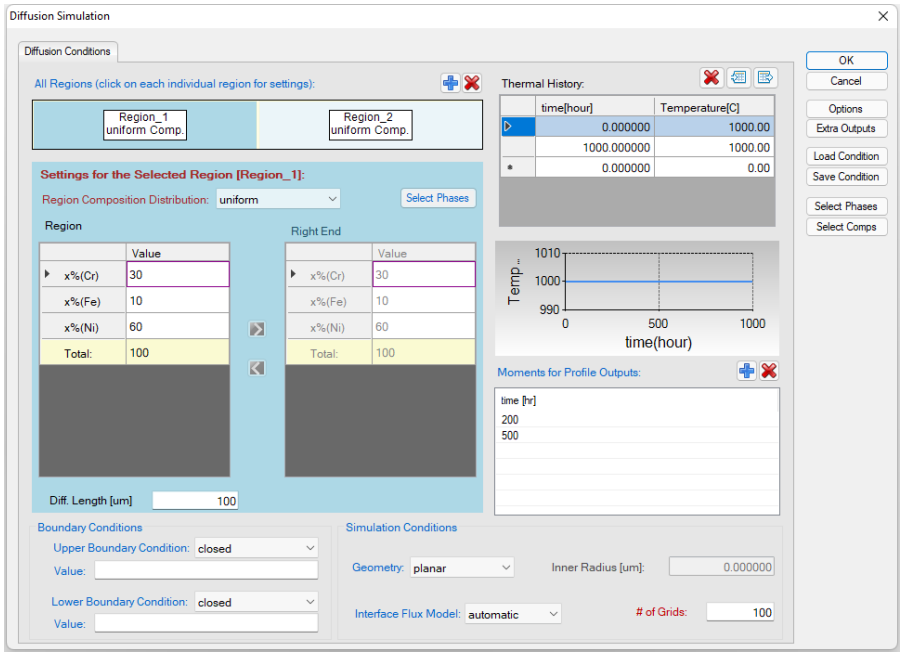


Figure 4.1.1: Setting of the simulation condition

Post Calculation Operation:

- Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3. The calculated plot is show in Figure 4.1.2
- In addition to Default table, composition profiles at selected times are given in separated tables under Table, which can be plotted separately as shown in Figure 4.1.3.

Information obtained from this calculation:

- In this example, the initial compositions of the two regions of the diffusion couple are both in the single Fcc phase field as shown in the isotherm of Fe-Cr-Ni at 1000°C in Figure 4.1.4;
- Composition profiles at selected times can be obtained.

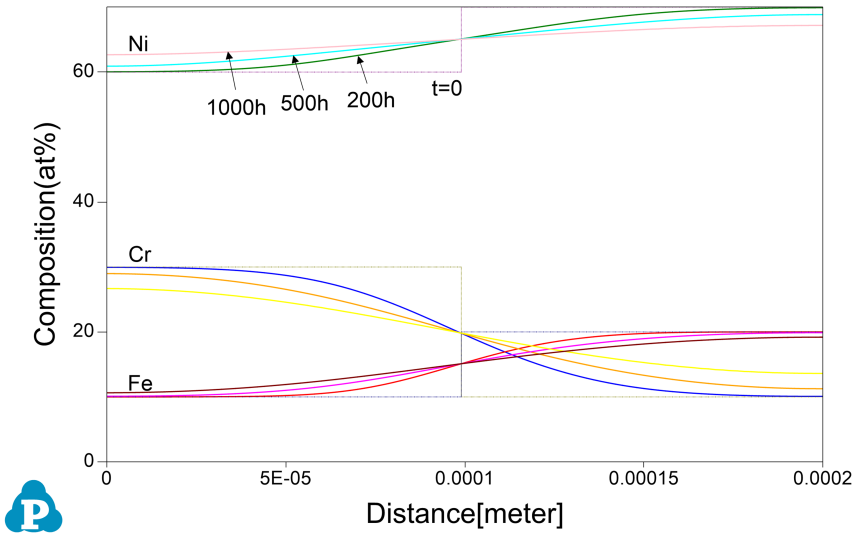


Figure 4.1.2: Calculated composition profiles after diffusion for 200, 500 and 1000 hours, respectively

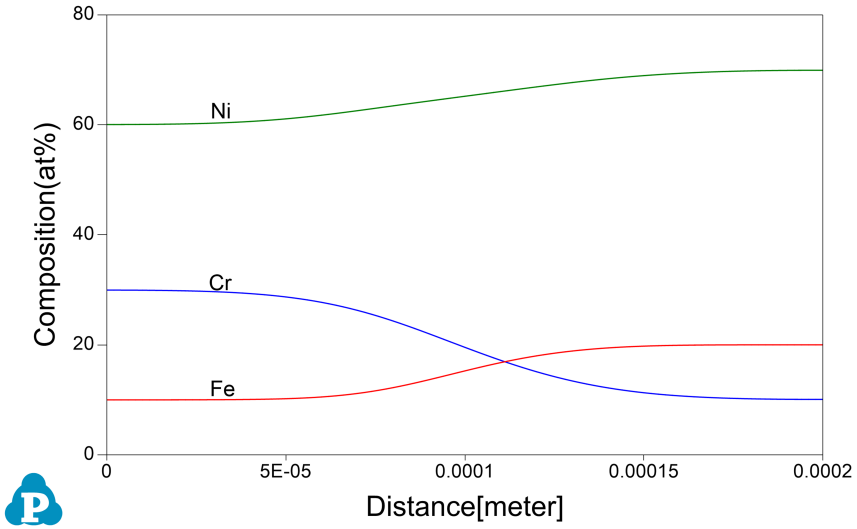


Figure 4.1.3: Calculated composition profiles after diffusion for 200 hours

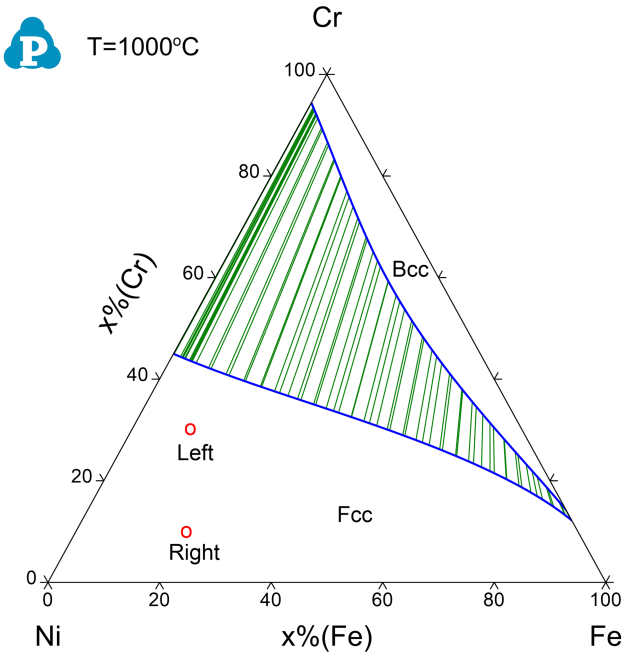


Figure 4.1.4: Isothermal section of Ni-Cr-Fe at 1000 °C, the initial compositions of both sides locate in the single Fcc phase field

Example 4.2 Diffusion within a Single Phase: Linear Initial Compositions

Purpose: Learn to perform diffusion simulation at constant temperature for a diffusion couple with both sides having the same single phase structure and composition varies linearly through each side before diffusion.

Module: PanDiffusion

Thermodynamic and Mobility Database: `FeCrNi.tdb`

Batch file: `Example_#4.2.pbfx`

Calculation Procedures:

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load `FeCrNi.tdb` following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Click on the menu "**PanDiffusion → Diffusion Simulation**" and set up the calculation condition as shown in Figure Figure 4.2.1. First select "**Region Composition Distribution**" as **Linear**, which means that composition in each region varies linearly from the left edge to the right edge. Click on **Region_1** and set the composition of the left side of the diffusion couple as `30Cr-10Fe-60Ni` (at%), then click on **Region_2** and set the composition of the left edge of the diffusion couple as `10Cr-20Fe-70Ni` (at%), and that of the right edge as `30Cr-10Fe-60Ni` (at%) (which is not shown in Figure 4.2.1).
- The length of both **Region_1** and **Region_2** is set to be 100 μm, and the total number of grids (# of Grids) is 100.
- The Thermal History is holding the diffusion couple at 1000 °C for 1000 hours.
- The output composition profiles include the initial and final stages and one intermediate stage at 100 hours. Click **OK**

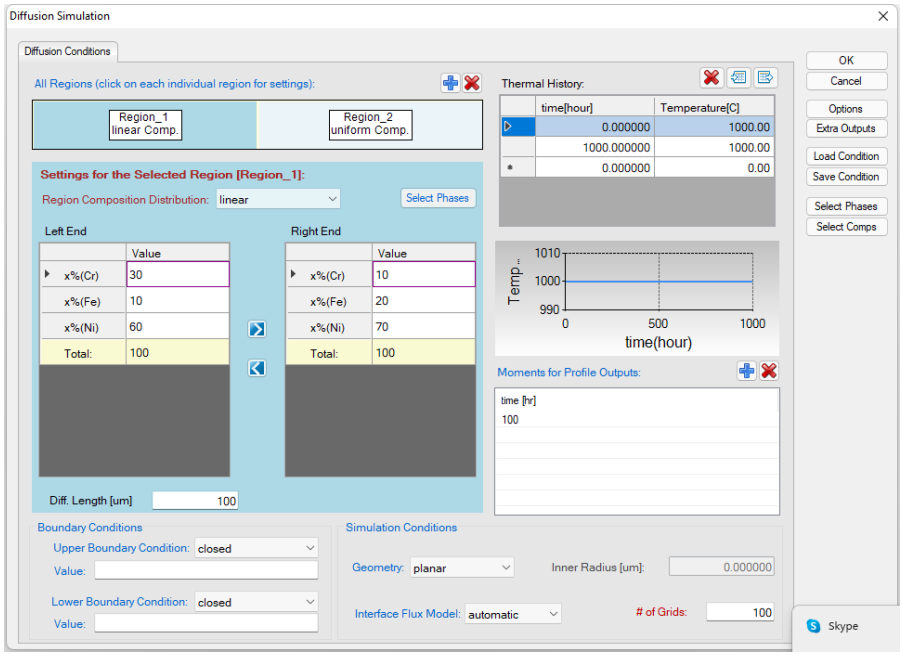


Figure 4.2.1: Setting of the simulation condition

Post Calculation Operation:

- Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3. The calculated plot is show in Figure 4.2.2

Information obtained from this calculation:

- Composition shows linear distribution in both regions at the beginning;
- After holding the diffusion couple at 1000 °C for 1000 hours, the diffusion couple becomes nearly homogenized.

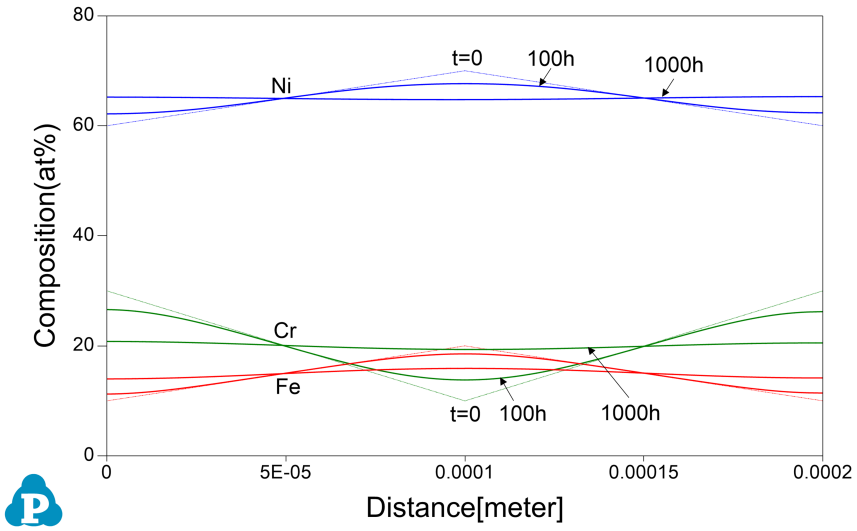


Figure 4.2.2: Calculated composition profiles at 100 hour and 1000 hour

Example 4.3 Diffusion between Two Phases: Uniform Initial Compositions

Purpose: Learn to perform diffusion simulation at constant temperature for a diffusion couple with the two sides having different phase structure and uniform composition through each side before diffusion.

Module: PanDiffusion

Thermodynamic and Mobility Database: `FeCrNi.tdb`

Batch file: `Example_#4.3.pbfx`

Calculation Procedures:

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load `FeCrNi.tdb` following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Click on the menu "**PanDiffusion → Diffusion Simulation**" and set up the calculation condition as shown in Figure 4.3.1. First select "**Region Composition Distribution**" as **Uniform**, which means that composition in each region is uniform before diffusion. Click on **Region_1** and set the composition of the left side of the diffusion couple as `30Cr-10Fe-60Ni` (at%), then click on **Region_2** and set the composition of the right side of the diffusion couple as `55Cr-40Fe-5Ni` (at%) (which is not shown in Figure 4.3.1).
- The length of both **Region_1** and **Region_2** is set to be 100 μm, and the total number of grids (# of Grids) is 100.
- The Thermal History is holding the diffusion couple at 1000 °C for 200 hours.
- In the settings shown in Figure 4.3.1, composition profiles only at the initial and final stages will be outputted. Click OK to perform calculations.

Post Calculation Operation:

- Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3. The calculated plot is show in Figure 4.3.2

Information obtained from this calculation:

- The two sides of the diffusion couple locate at different phase fields, one in Fcc and the other in Bcc as shown in the isotherm of Fr-Cr-Ni at 1000°C in Figure 4.3.3, therefore diffusion between them pass through the Fcc+Bcc two-phase field;
- After holding the diffusion couple at 1000 °C for 200 hours, boundary between the Fcc and Bcc moved.

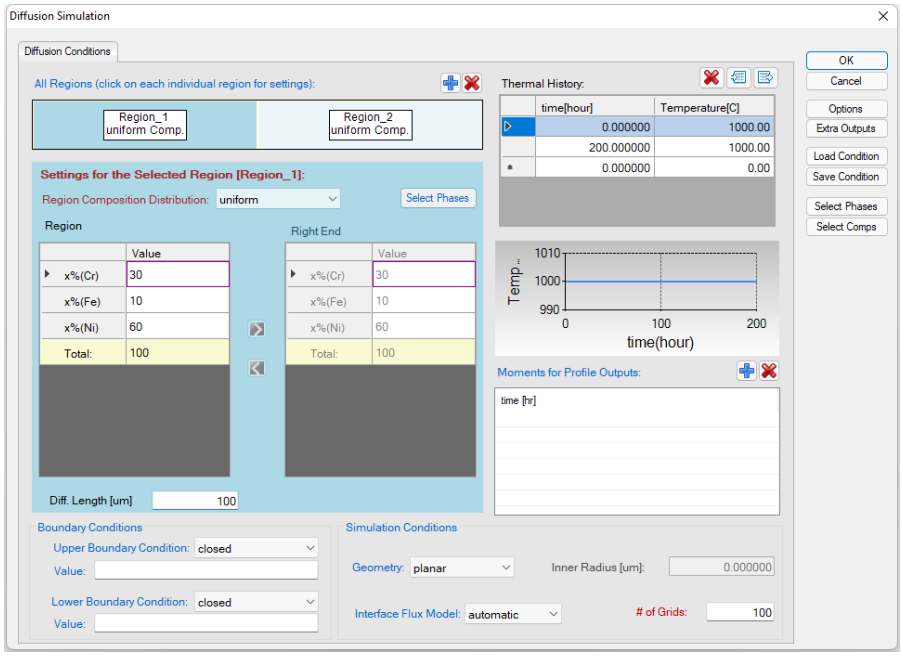


Figure 4.3.1: Setting of the simulation condition

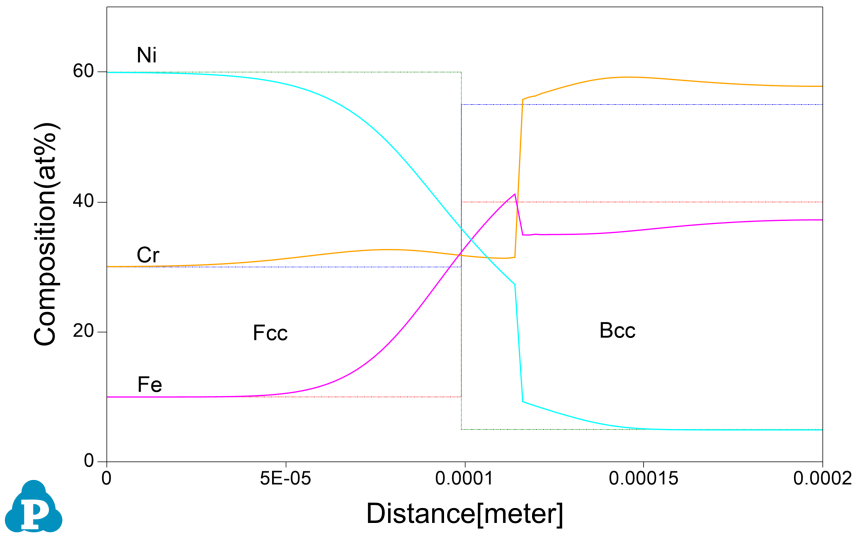


Figure 4.3.2: Calculated composition profiles after diffusion at 1000°C for 200 hours

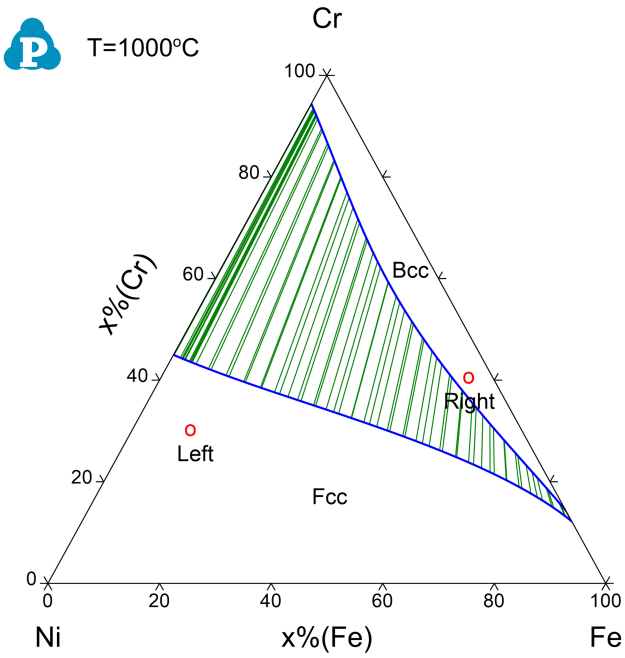


Figure 4.3.3: Isothermal section of Ni-Cr-Fe at 1000 °C, the initial compositions of the two sides locate in different phase fields, one in Fcc and the other in Bcc

Example 4.4 Diffusion between Two Phases at Varied Temperatures

Purpose: Learn to perform diffusion simulation at varied temperatures for a diffusion couple with the two sides having different phase structure and uniform composition through each side before diffusion.

Module: PanDiffusion

Thermodynamic and Mobility Database: `FeCrNi.tdb`

Batch file: `Example_#4.4.pbfx`

Calculation Procedures:

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load `FeCrNi.tdb` following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Click on the menu "**PanDiffusion → Diffusion Simulation**" and set up the calculation condition as shown in Figure 4.4.1. First select "**Region Composition Distribution**" as **Uniform**, which means that composition in each region is uniform before diffusion. Click on **Region_1** and set the composition of the left side of the diffusion couple as `30Cr-10Fe-60Ni` (at%), then click on **Region_2** and set the composition of the right side of the diffusion couple as `55Cr-40Fe-5Ni` (at%) (which is not shown in Figure 4.4.1).
- The length of both **Region_1** and **Region_2** is set to be 100 μm, and the total number of grids (# of Grids) is 100.
- The Thermal History is holding the diffusion couple at 1000°C for 200 hours, then the temperature decreases from 1000°C to 900°C linearly in the next 100 hours.
- Click "Select Phase" and set Fcc and Bcc as the entered phases.
- In the settings shown in Figure 4.4.1, composition profiles only at the initial and final stages will be outputted. Click OK to perform calculations.

Post Calculation Operation:

- Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3. The calculated plot is show in Figure 4.4.2

Information obtained from this calculation:

- After holding the diffusion couple at 1000 °C for 200 hours, the temperature decreases gradually in the next 100 hours to 900 °C. Composition profiles after the entire thermal history can be obtained;
- Learn to set up multi-step thermal history for a diffusion simulation.

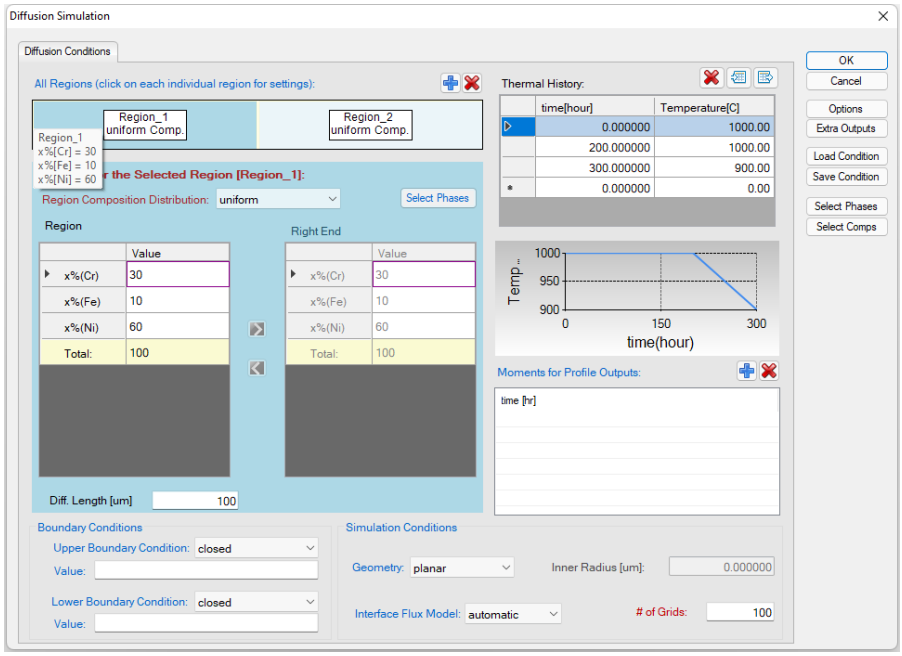


Figure 4.4.1: Setting of the simulation condition

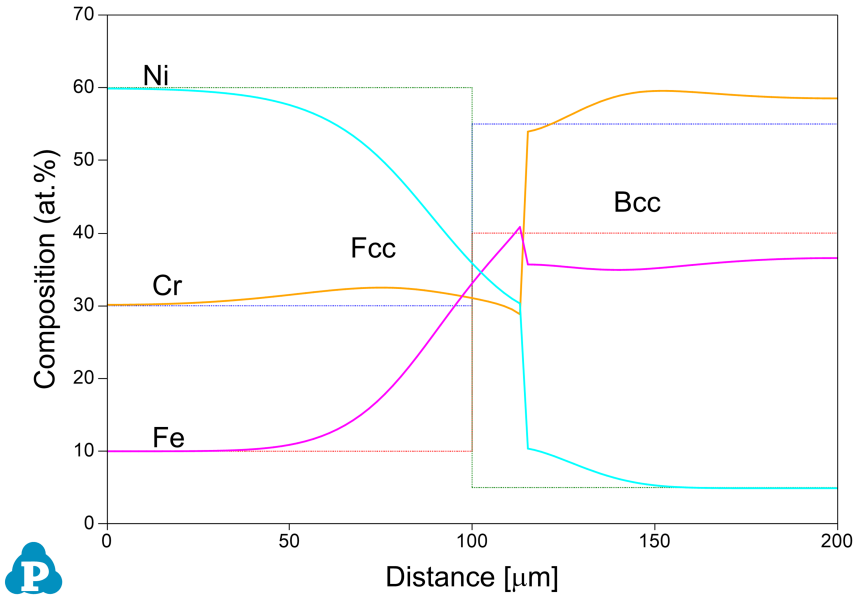


Figure 4.4.2: Calculated composition profiles at 300 hours

Example 4.5 Diffusion among Multiple Regions

Purpose: Learn to perform diffusion simulation at constant temperature for a diffusion sandwich with different phase structure but uniform composition through each region before diffusion.

Module: PanDiffusion

Thermodynamic and Mobility Database: `FeCrNi.tdb`

Batch file: `Example_#4.5.pbfx`

Calculation Procedures:

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load `FeCrNi.tdb` following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Click on the menu "**PanDiffusion → Diffusion Simulation**" and set up the calculation condition as shown in Figure 4.5.1. First click the blue "**+**" above Regions to add another region, **Region_3**. Select "**Region Composition Distribution**" as **Uniform**.
- Click on **Region_1** and set the composition of the left region of the diffusion couple as `30Cr-10Fe-60Ni` (at%), Select Fcc as the entered phase in "**Select Phases**" of "**Settings for the Selected Region [Region_1]**".
- Click on **Region_2** and set the composition of the middle region of the diffusion couple as `55Cr-40Fe-5Ni` (at%). Select Bcc as the entered phase in "**Select Phases**" of "**Settings for the Selected Region [Region_2]**".
- Click on **Region_3** and set the composition of the right region of the diffusion couple as `10Cr-20Fe-70Ni` (at%). Select Fcc as the entered phase in "**Select Phases**" of "**Settings for the Selected Region [Region_3]**".
- The length of each region is set to be 100 μm, and the total number of grids (# of Grids) is 100.
- The Thermal History is holding the diffusion couple at 1000 °C for 500 hours.

- Click “Select Phase” and set Fcc and Bcc as the entered phases.
- In the settings shown in Figure 4.5.1, composition profiles at the initial and final stages, as well as that at 200 hour will be outputted. Click OK to perform calculations.

Post Calculation Operation:

- Change graph appearance and add text following the procedure in Pandat User’s Guide Sections 2.3.1 and 2.3.3. The calculated plot is show in Figure 4.5.2

Information obtained from this calculation:

- The three regions of the diffusion triple locate at different phase fields, the one in Bcc is sandwiched between two regions in the Fcc as shown in Figure 4.5.3;
- After holding the diffusion couple at 1000°C for 500 hours, composition profiles can be viewed at final stage (500h) and intermediate stage (200h). The phase boundaries are moved;

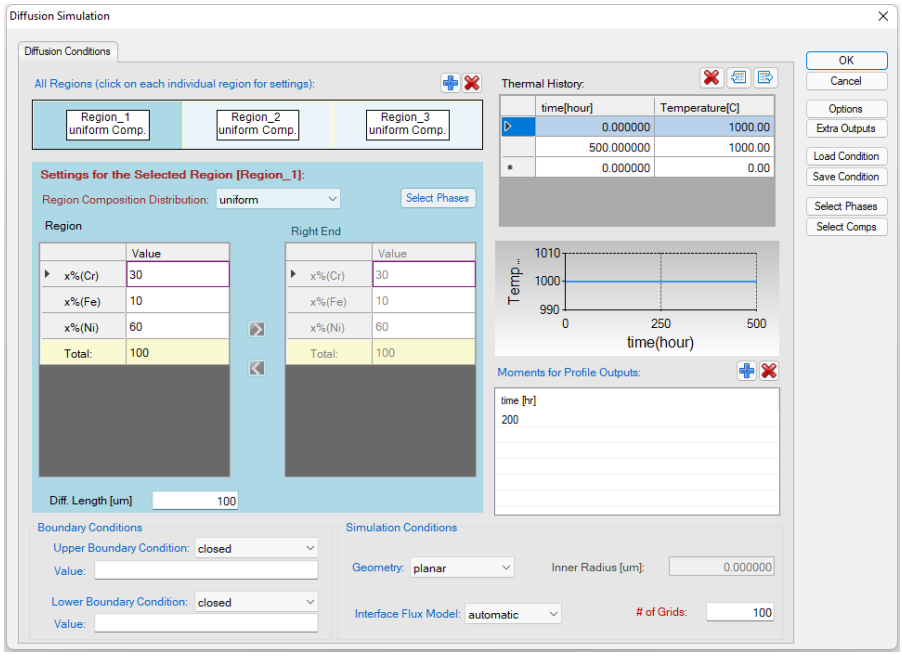


Figure 4.5.1: Setting of the simulation condition

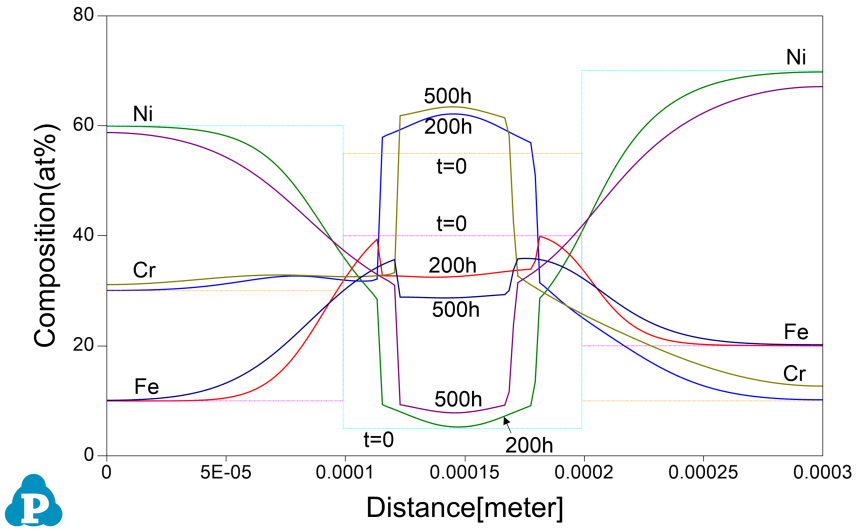


Figure 4.5.2: Calculated composition profiles for the diffusion sandwich at 1000°C for 200h and 500h

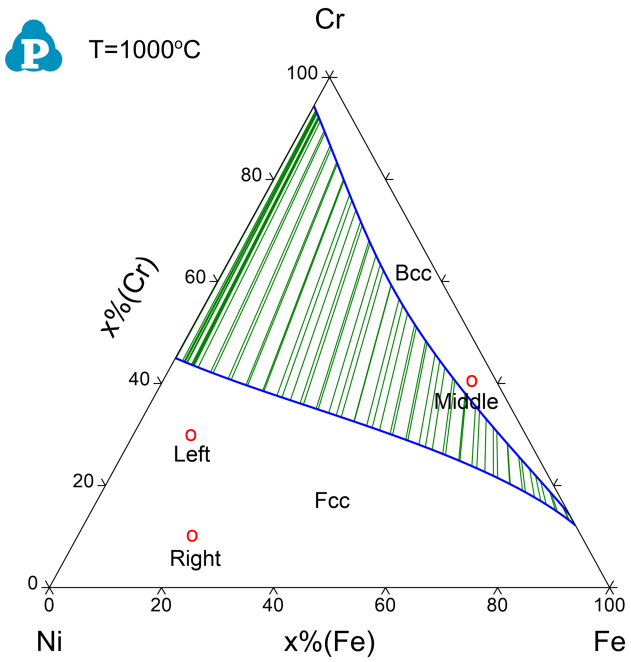


Figure 4.5.3: Isothermal section of Ni-Cr-Fe at 1000 °C, the initial compositions of the left and right regions locate in the single Fcc phase field, while the middle region locates in the Bcc phase field

Example 4.6 Carburization with Fixed Composition at Boundary

Purpose: Learn to perform diffusion simulation at constant temperature for a carburization process with a fixed chemical composition at boundary.

Module: PanDiffusion

Thermodynamic and Mobility Database: `Fe-Si-C.tdb`

Batch file: `Example_#4.6.pbfx`

Calculation Procedures:

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load `Fe-Si-C.tdb` following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Click on the menu "**PanDiffusion → Diffusion Simulation**" and set up the calculation condition as shown in Figure 4.6.1. First click the red "**X**" above Regions to delete **Region_2** and leave one Region only.
- Click on **Region_1** and set the composition as `0.5C-99.5Fe` (at%), the Diff. Length as 100 μm, and the # of Grids as 100.
- The Thermal History is set as 1200 K for 25 seconds;
- Click on **Lower Boundary Condition** (left edge of Region_1) and select "`fixed_composition`", and set the Value as "`x%(C)=3.0`";
- In the settings shown in Figure 4.6.1, composition profiles at the initial and final stages will be outputted. Click OK to perform calculations.

Post Calculation Operation:

- Enlarge the composition range between 0 and 4 (at%) to clearly display Carbon composition. The calculated plot is show in Figure 4.6.2Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3.

Information obtained from this calculation:

- Carbonization process in Fcc phase in the Fe-C system. Lower boundary condition is a fixed carbon composition;
- After holding the material at 1200K for 25 seconds, composition profiles can be viewed at final stage (25 s). The carbon gradually diffused into the Fcc phase from the boundary;

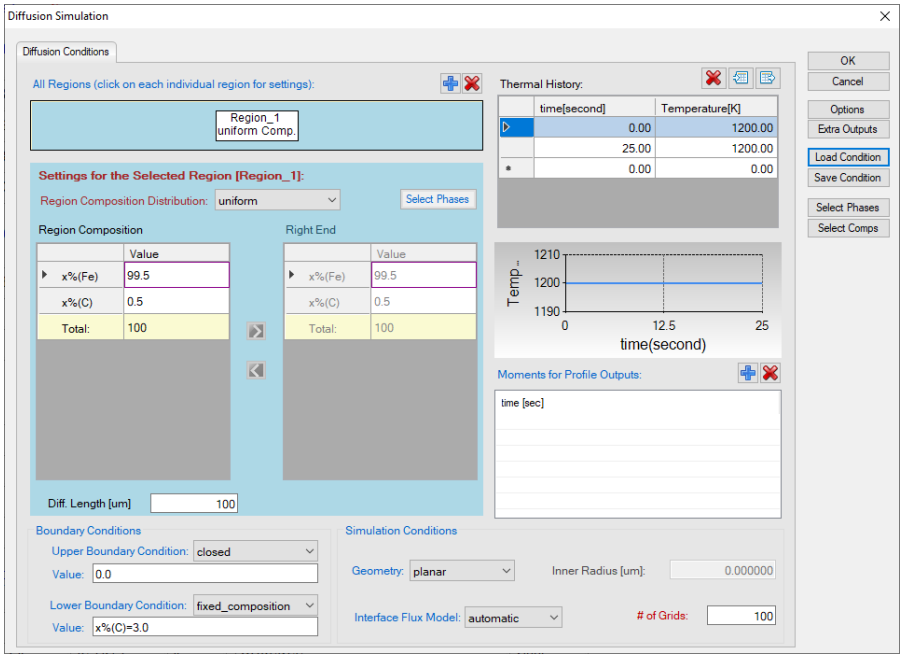


Figure 4.6.1: Setting of the simulation condition

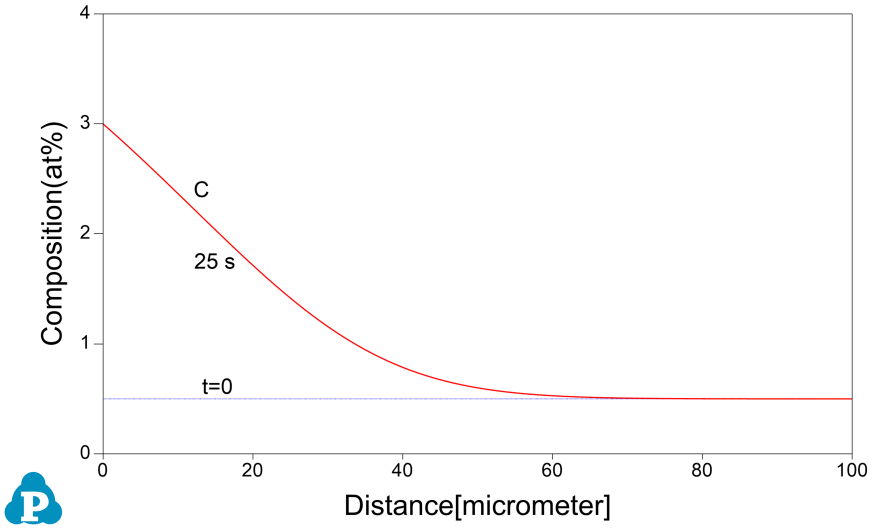


Figure 4.6.2: Calculated C composition profile for diffusion at 1200K for 25s

Example 4.7 Carburization with Input Flux

Purpose: Learn to perform diffusion simulation at constant temperature for a carburization process with an input flux as boundary condition.

Module: PanDiffusion

Thermodynamic and Mobility Database: `Fe-Si-C.tdb`

Batch file: `Example_#4.7.pbfx`

Calculation Procedures:

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load `Fe-Si-C.tdb` following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Click on the menu "**PanDiffusion → Diffusion Simulation**" and set up the calculation condition as shown in Figure 4.7.1. First click the red "**X**" above Regions to delete **Region_2** and leave one Region only;
- Click on **Region_1** and set the composition as `0.15C-99.85Fe` (wt%), the Diff. Length as 3 mm, and the # of Grids as 200;
- The Thermal History is at 1173 K for 18000 seconds;
- Click on **Lower Boundary Condition** (left edge of Region_1) and select "`flux`", and set the Value as "`J(C)=-8.25E-9*(a(C:Graphite[*])-0.64)/7e-006`";
- In the settings shown in Figure 4.7.1, composition profiles at the initial and final stages, as well as at 100s, 1000s and 5000s, will be outputted. Click OK to perform calculations.

Post Calculation Operation:

- Enlarge the composition range between 0 and 1 (wt%) to clearly display Carbon composition. The calculated plot is show in Figure 4.7.2Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3.

Information obtained from this calculation:

- Carbonization process in Fcc of the Fe-C system. Lower boundary condition is an input flux. This setting provides user an option when the flux of C is known in the environment;
- After holding the material at 1173K for 18000 seconds, composition profiles can be viewed at selected stages. The carbon composition gradually diffused from the boundary to the body;

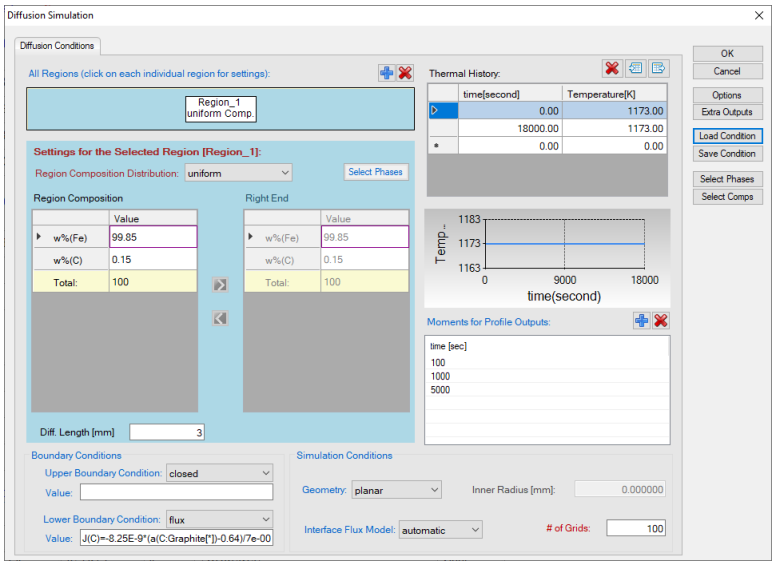


Figure 4.7.1: Setting of the simulation condition

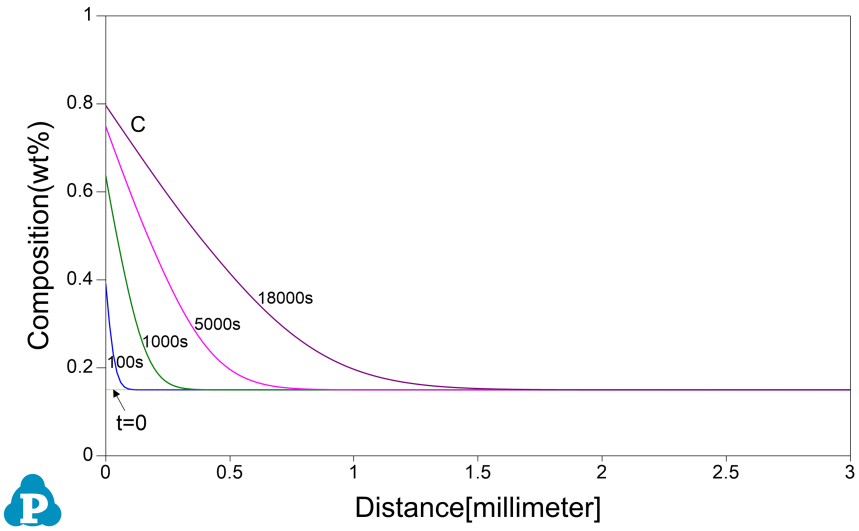


Figure 4.7.2: Calculated C composition profiles for diffusion at 1173 K for 100s, 1000s, 5000s, and 18000s

Example 4.8 Carburization of a Tube with Fixed Environmental Activity

Purpose: Learn to perform diffusion simulation at constant temperature for a carburization process with an input flux as boundary condition.

Module: PanDiffusion

Thermodynamic and Mobility Database: `Fe-Si-C.tdb`

Batch file: `Example_#4.8.pbfx`

Calculation Procedures:

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load `Fe-Si-C.tdb` following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Click on the menu "**PanDiffusion → Diffusion Simulation**" and set up the calculation condition as shown in Figure 4.8.1. First click the red "**X**" above Regions to delete **Region_2** and leave one Region only;
- Click on **Region_1** and set the composition as `0.05C-98.65Fe-1.3Si` (wt%), the Diff. Length as 10 mm, and the # of Grids as 200;
- Click "Select Phase" and set Fcc as the entered phase;
- The Thermal History is at 1273 K for 2E5 seconds;
- Click on **Upper Boundary Condition** and select "`activity`", and set the activity value at the right edge of Region_1 as "`a(C:graphite[*])=1E-5`". Click on **Lower Boundary Condition** and select "`activity`", then set the activity value at the left edge of Region_1 as "`a(C:graphite[*])=0.9`";
- In order to set a tube geometry, select "`cylindrical`" in "**Geometry**", and apply `20 mm` to "**Inner Radius**";
- In the settings shown in Figure 4.8.1, composition profiles at the initial and final stages, as well as at 1E4 s, will be outputted. Click OK to perform calculations.

Post Calculation Operation:

- Enlarge the composition range between 0 and 1.4 (wt%) to clearly display Carbon composition. The calculated plot is show in Figure 4.8.2Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3.

Information obtained from this calculation:

- Learn to set up Boundary conditions for a tube geometry, and fixed activities at both inner and outer surfaces;
- Observe carbon diffusion from inner surface (high activity) into the tube;

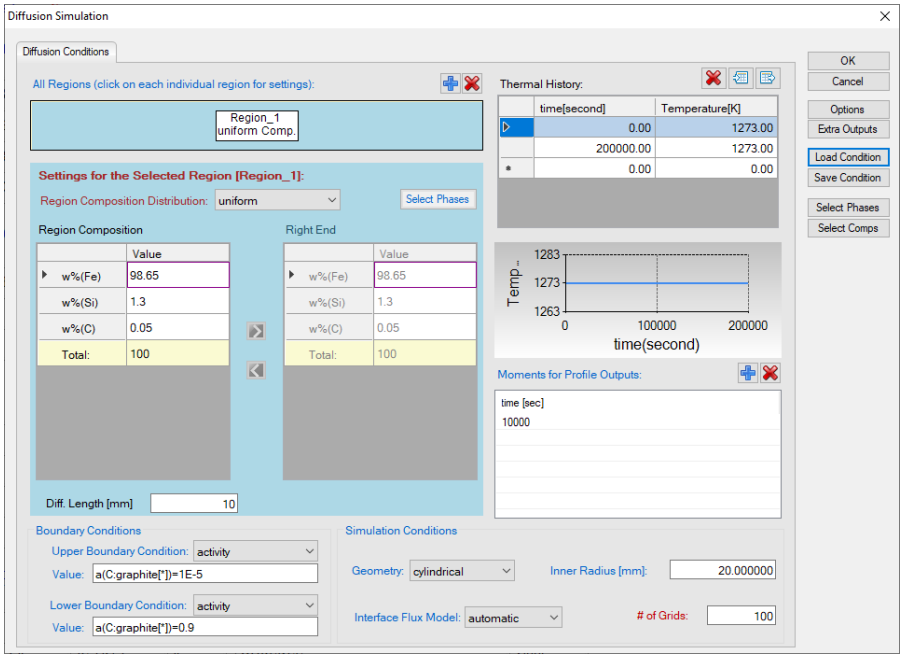


Figure 4.8.1: Setting of the simulation condition

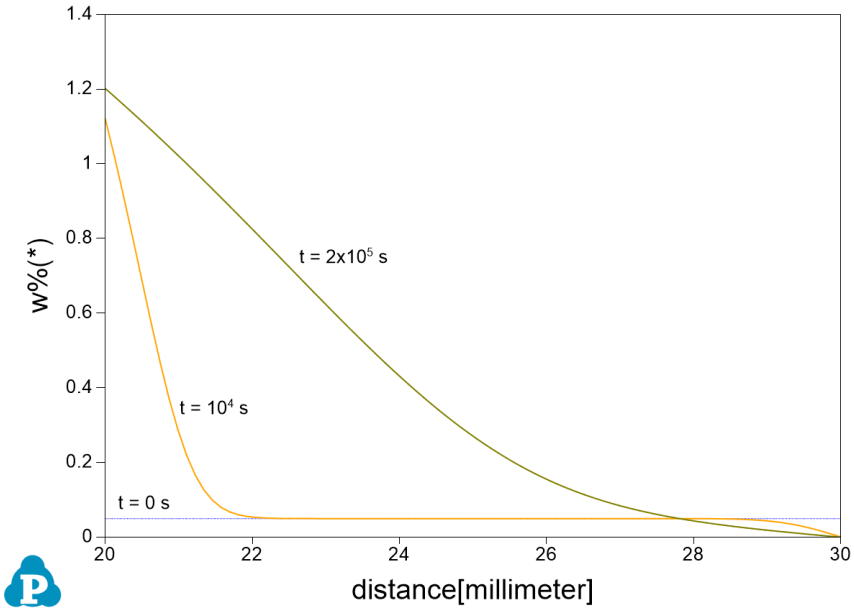


Figure 4.8.2: Calculated composition profiles at 1273 K for 1E4s, and 2E5s

Example 4.9 Dissolution of γ' Particle in γ Matrix

Purpose: Learn to perform diffusion simulation at constant temperature where a γ' particle (L12, Ni3Al) dissolve into γ matrix (Fcc, Ni-Al). Learn to select entered phase(s) in each region.

Module: PanDiffusion

Thermodynamic and Mobility Database: `AlNi_Diff.tdb`

Batch file: `Example_#4.9.pbfx`

Calculation Procedures:

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load `AlNi_Diff.tdb` following the procedure in Pandat User's Guide 3.2.1;
- Click on the menu "**PanDiffusion → Diffusion Simulation**" and set up the calculation condition as shown in Figure 4.9.1;
- Click on **Region_1** and set the composition as `25Al-75Ni` (at%), and select L12_FCC as the entered phase in "**Select Phases**" of "**Settings for the Selected Region [Region_1]**". In **Region_1**, set the Diff. Length as 5 um. Click on **Region_2** and set the composition as `15Al-85Ni` (at%) and select Fcc as the entered phase in "**Select Phases**" of "**Settings for the Selected Region [Region_2]**". In **Region_2**, set the Diff. Length as 10 um.
- The Thermal History is at 1473 K for 100 seconds;
- In order to set a tube geometry, select "`spherical`" in "**Geometry**", The total number of grids (# of Grids) is 100;
- In the settings shown in Figure 4.9.1, composition profiles at the initial and final stages, as well as at 10s, 30s, 50s and 70s, will be outputted. Click OK to perform calculations.

Post Calculation Operation:

- The calculated plot is show in Figure 4.9.2Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3.

Information obtained from this calculation:

- Learn to set up simulation for dissolution of spherical particles;
- After holding the material at 1473K for 100s, composition profiles can be viewed at selected stages. The interface moving from γ phase to γ' indicates the dissolution of γ' particles.

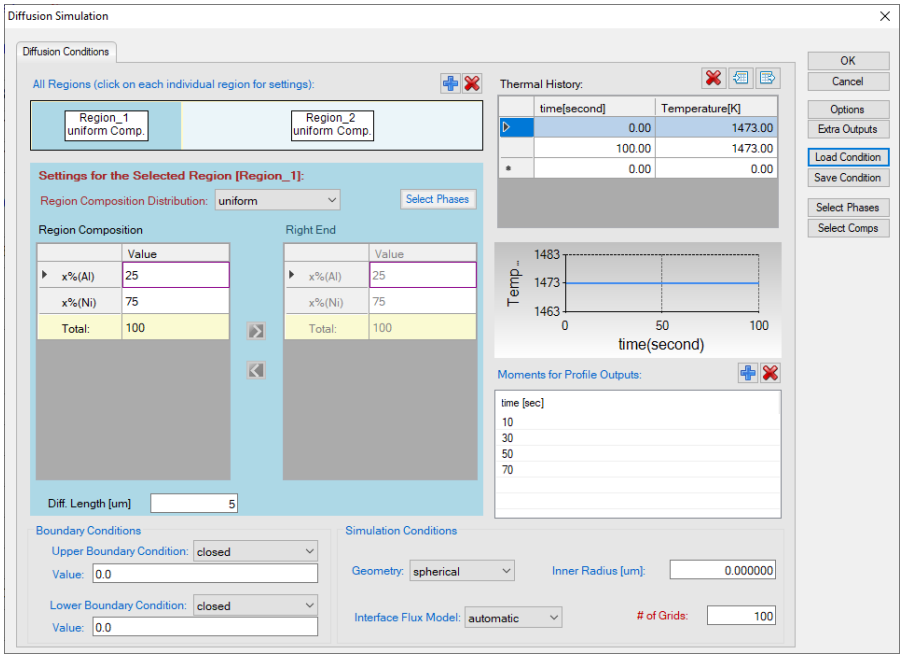


Figure 4.9.1: Setting of the simulation condition

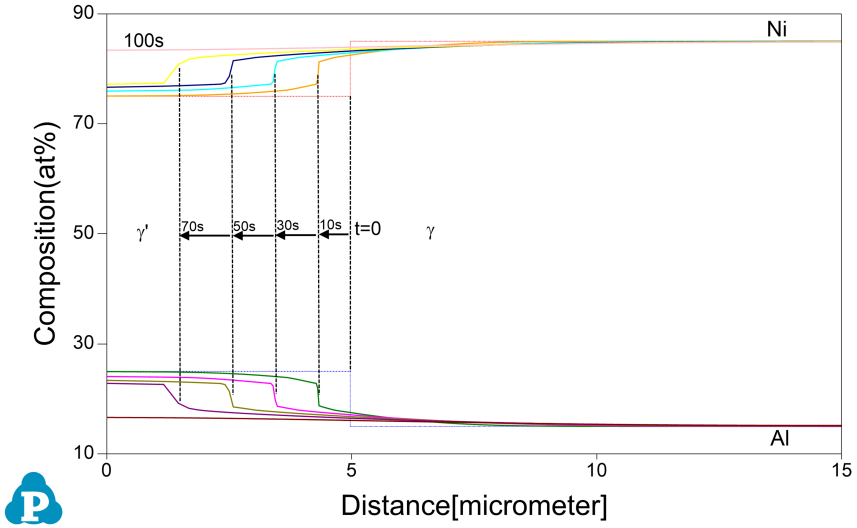


Figure 4.9.2: Calculated composition profiles at 1473 K for 10s, 30s, 50s, 70s and 100s

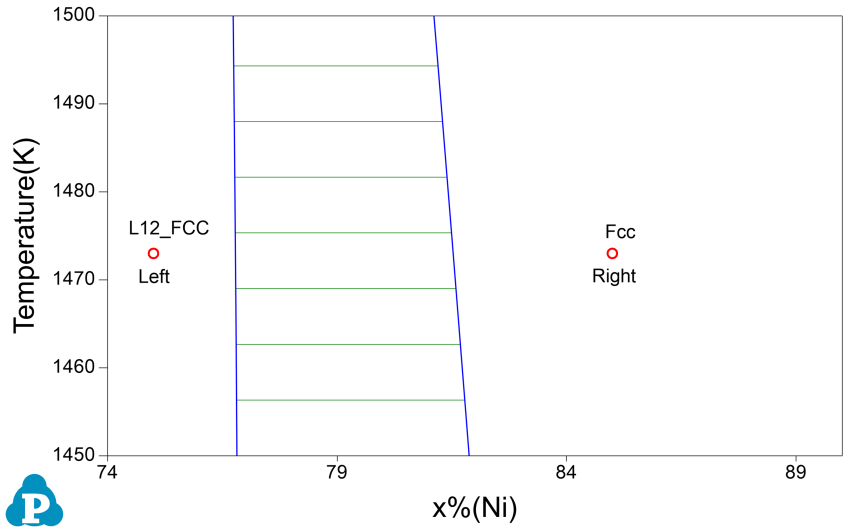


Figure 4.9.3: Ni-Al phase diagram. The initial composition of left-hand side locates in the single L12-FCC phase field. The initial composition of right-hand side locates in the single Fcc phase field

Example 4.10 Transformation from γ to α

Purpose: Learn to perform diffusion simulation at constant temperature where a γ → α transformation happens in Fe-C alloy. Learn to select entered phase(s) in each region.

Module: PanDiffusion

Thermodynamic and Mobility Database: `Fe-Si-C.tdb`

Batch file: `Example_#4.10.pbfx`

Calculation Procedures:

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load `Fe-Si-C.tdb` following the procedure in Pandat User's Guide 3.2.1 and select elements `Fe` and `C`.
- Click on the menu "**PanDiffusion → Diffusion Simulation**" and set up the calculation condition as shown in Figure 4.10.1;
- Click on **Region_1** and set the composition as `100Fe-0C` (wt%), and select Bcc as the entered phase in "**Select Phases**" of "**Settings for the Selected Region [Region_1]**". In **Region_1**, set the Diff. Length as 1E-5 mm. Click on **Region_2** and set the composition as `99.85Fe-0.15C` (wt%) and select Fcc as the entered phase in "**Select Phases**" of "**Settings for the Selected Region [Region_2]**". In **Region_2**, set the Diff. Length as 2 mm;
- The Thermal History is at 1050 K for 1E6 seconds;
- The total number of grids (# of Grids) is 100;
- In the settings shown in Figure 4.10.1, composition profiles at the initial and final stages, as well as at 1E3 seconds and 1E5 seconds, will be outputted. Click OK to perform calculations.

Post Calculation Operation:

- Enlarge the composition range between 0 and 0.5 (wt%) to clearly display Carbon composition.The calculated plot is show in Figure 4.10.2Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3.

Information obtained from this calculation:

- Observe composition profiles of C and interface movement from α to γ which indicates the γ → α phase transformation.

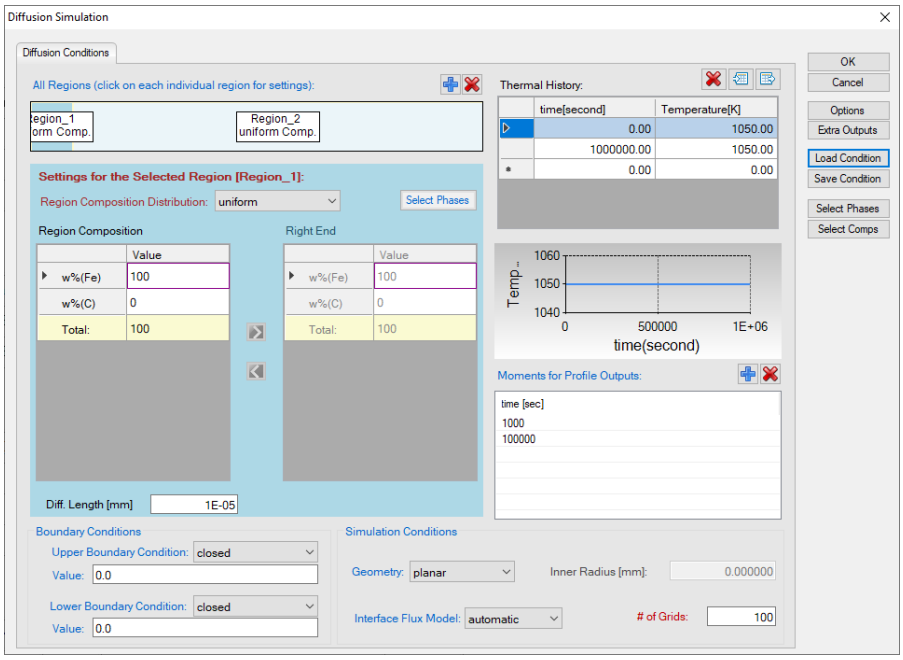


Figure 4.10.1: Setting of the simulation condition

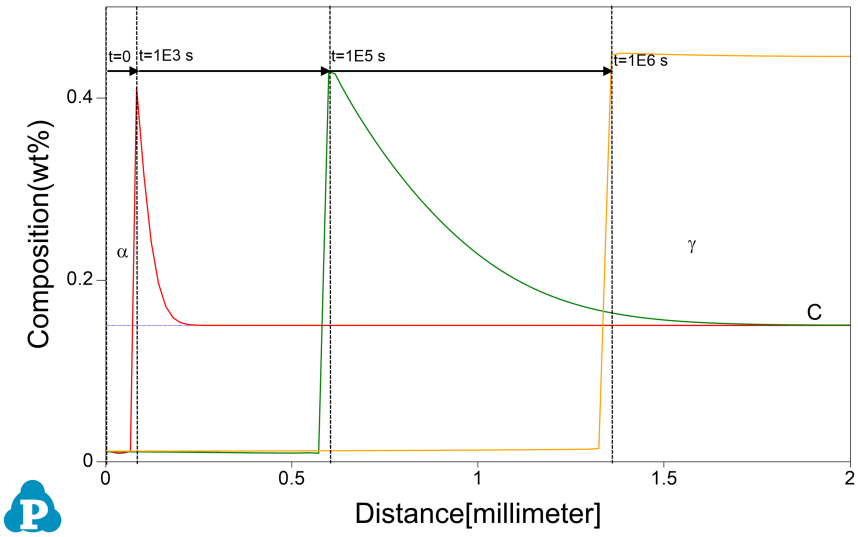


Figure 4.10.2: Calculated composition profiles at 1050 K for 1E3 seconds, 1E5 seconds and 1E6 seconds

Example 4.11 Fe-Si-C Uphill Diffusion

Purpose: Learn to perform uphill diffusion simulation in a Fcc matrix at a constant temperature.

Module: PanDiffusion

Thermodynamic and Mobility Database: `Fe-Si-C.tdb`

Batch file: `Example_#4.11.pbfx`

Calculation Procedures:

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load `Fe-Si-C.tdb` following the procedure in Pandat User's Guide 3.2.1 and select all three elements;
- Click on the menu "**PanDiffusion → Diffusion Simulation**" or click the icon  and set up the calculation condition as shown in Figure 4.11.1;
- Click on "Select Phases" and make Fcc the entered phase, while other phases are suspended;
- Click on **Region_1** and set the composition as `Fe-3.8Si-0.49C` (wt%). In **Region_1**, set the length (Diff. Length) as 25 mm.
- Click on **Region_2** and set the composition as `Fe-0.05Si-0.45C` (wt%). In **Region_2**, set the length (Diff. Length) as 25 mm;
- The **Thermal History** is a period of 312 hours (13 days) with a constant temperature at 1050 °C;
- The total number of grids (# of Grids) is 100;
- In the settings shown in Figure 4.11.1, composition profiles at the initial and final stages, as well as 100 and 200 hours, will be outputted. Click OK to perform calculations;
- Details on these options can be found in Pandat User's Guide sections 6.3.11 and 6.3.12.

Post Calculation Operation:

- Set the scale of the Y axis to be 0.3-0.6 (wt%); Remove composition profiles of Fe and Si; Add grid to the graph by setting “Show Major Grid” as "True" in the property window; The calculated plot is show in Figure 4.11.2Change graph appearance and add text following the procedure in Pandat User’s Guide Sections 2.3.1 and 2.3.3.

Information obtained from this calculation:

- Composition profile of carbon in Fcc Matrix after an uphill diffusion.

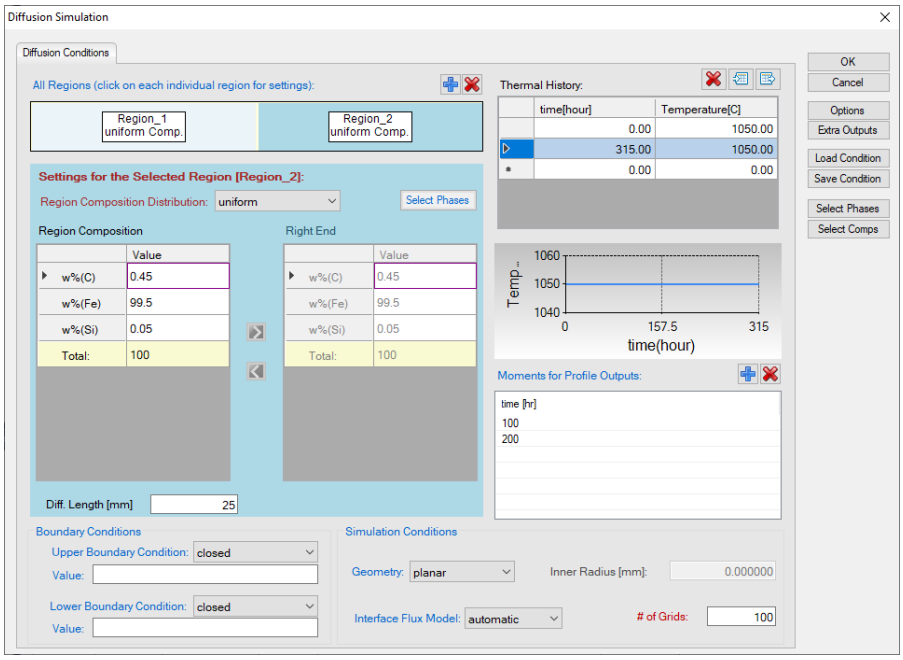


Figure 4.11.1: Setting of the simulation condition

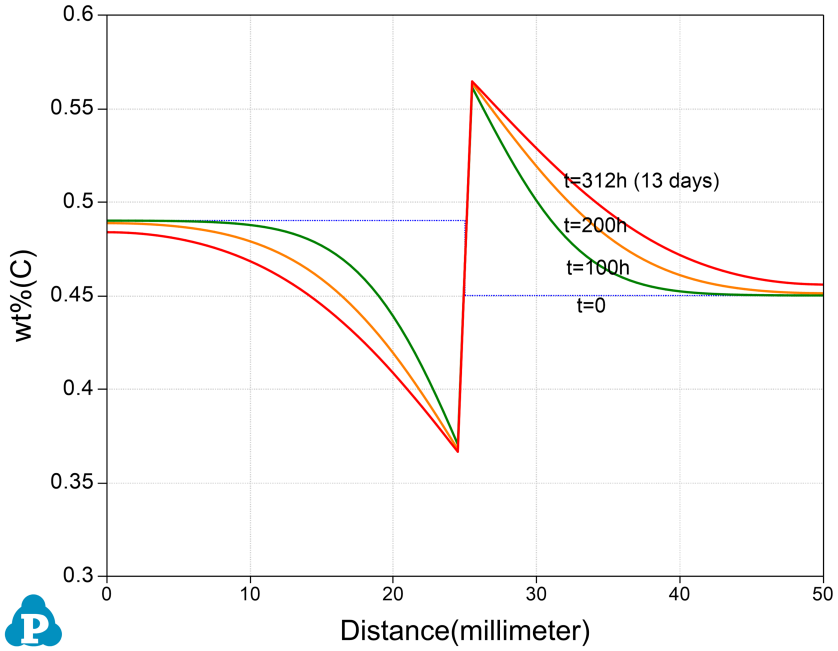


Figure 4.11.2: Composition profile of Carbon

Example 4.12 Dissolution of a Single θ-Al2Cu Particle in FCC Matrix

Purpose: Learn to perform single-particle dissolution simulation.

Module: PanDiffusion

Thermodynamic and Mobility Database: `AlCu_MB.tdb`

Batch file: `Example_#4.12.pbfx`

Calculation Procedures:

- Create a workspace and select the PanDiffusion module following Pandat User's Guide section 2.1;
- Load `AlCu_MB.tdb` following the procedure in Pandat User's Guide section 3.2.1 and select both two elements;
- Click on the menu "**`PanDiffusion → Dissolution Simulation`**" or click the icon  and set up the calculation condition as shown in Figure 4.12.1;
- Click on "**`Select Phases`**" and make `Fcc` and `AlCu_Theta` the entered phases, while other phases are suspended;
- In Alloy Composition set a composition of `Al-1.55Cu` (at%);
- The total number of grids (# of Grids) is 100;
- The Geometry of particles is set to "`Spherical`";
- In "**`Phase Information`**", select `Fcc` as "`Matrix Phase`".
- To add a particle, click the blue "**+**" button in the "**`Particle`**" field, then select `AlCu_Theta` in "`Phase Name`". "`Particle Size`" is set to 3.0 μm. "`Vol. Fraction`" is set to 0.008;
- The "**`Thermal History`**" is a period of 35 minutes at 550°C;
- Click OK to start calculation;

- By default, dissolution simulation gives time-evolution of particle size as output. In order to display composition profile at desired moments, click the blue "**+**" button next to the "**Moments for Profile Outputs**" and input a time value. As shown in Figure 4.12.1, profiles at 10 minutes and 15 minutes will be outputted. Click OK to start calculation;
- Details on these options can be found in Pandat User's Guide section 6.4.

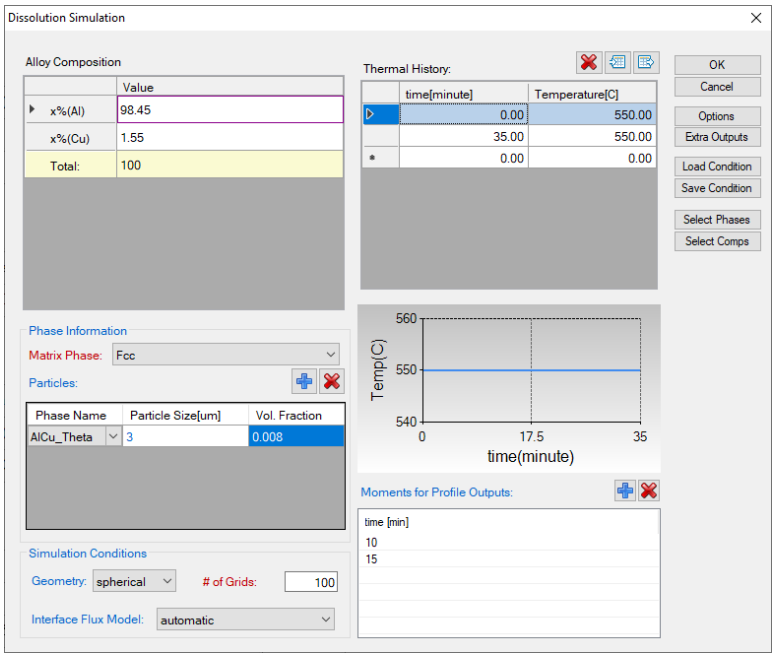


Figure 4.12.1: Setting of the simulation condition

Post Calculation Operation:

- The calculated particle dissolution with time is shown in Figure 4.12.2 User can modify it by changing the title, the scale and so on from the **Property** Window. User can also add experimental data by clicking menu "**Table → Import Table From Files**", and select `Example_#4.12.txt`, and then follow Example 3.1 : Precipitation Simulation of Ni-14Al (at%) Alloy to add the experimental data on the plot. More information about change graph appearance can be found in Pandat User's Guide Section 2.3.1.
- Click and open the **Default** table and select "`distance`", "`x%(Al)`" and "`x%(Cu)`" to plot the composition profiles at starting, ending and the two selected intermediate times as shown in Figure 4.12.3.

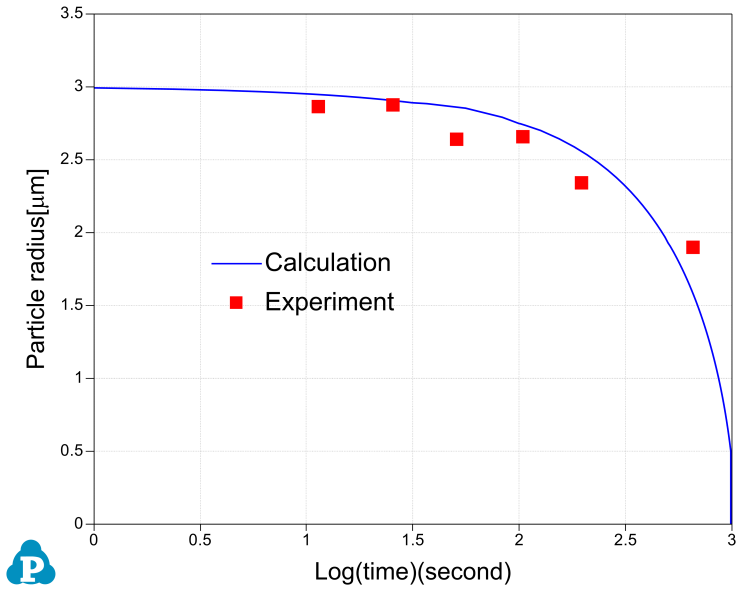


Figure 4.12.2: The simulation result of particle-size evolution

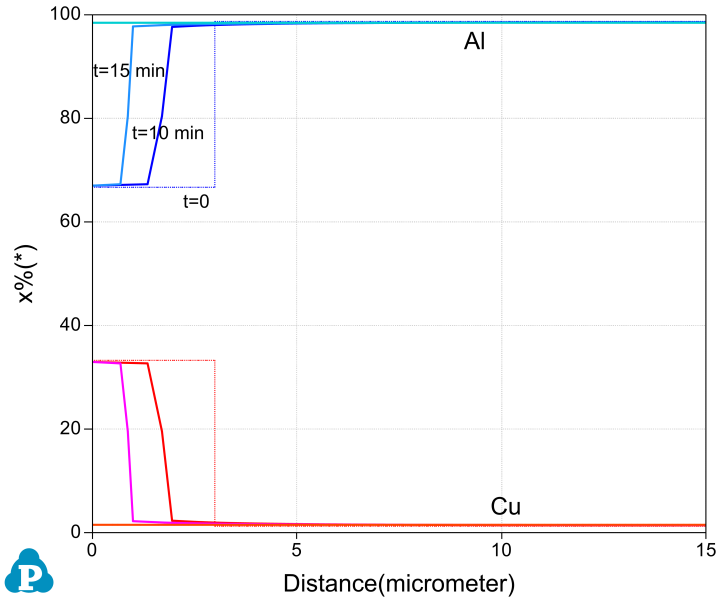


Figure 4.12.3: The simulation result of composition-profile evolution

Example 4.13 Dissolution of Multiple Particles

Purpose: Learn to perform multi-particle dissolution simulation. Two Al2Cu particles, with different sizes and volume fractions, dissolve into the Fcc matrix.

Module: PanDiffusion

Thermodynamic and Mobility Database: `AlCu_MB.tdb`

Batch file: `Example_#4.13.pbfx`

Calculation Procedures:

- Create a workspace and select the PanDiffusion module following Pandat User's Guide section 2.1;
- Load `AlCu_MB.tdb` following the procedure in Pandat User's Guide section 3.2.1 and select both two elements;
- Click on the menu "**`PanDiffusion → Dissolution Simulation`**" or click the icon and set up the calculation condition as shown in Figure 4.13.1;
- Click on "**`Select Phases`**" and make `Fcc` and `AlCu_Theta` the entered phases, while other phases are suspended;
- In Alloy Composition set a composition of `Al-1.55Cu` (at%);
- The total number of grids (# of Grids) is 75;
- The Geometry of particles is set to "`Spherical`";
- In "**`Phase Information`**", select `Fcc` as "`Matrix Phase`".
- To add the first particle, click the blue "**+**" button in the "**`Particle`**" field, then select `AlCu_Theta` in "`Phase Name`". "`Particle Size`" is set to 3.0 μm. "`Vol. Fraction`" is set to 0.008;
- To add the second particle, click the blue "**+**" button in the "**`Particle`**" field, then select `AlCu_Theta` in "`Phase Name`". "`Particle Size`" is set to 1.0 μm. "`Vol. Fraction`" is set to 0.001;
- The "**`Thermal History`**" is a period of 35 minutes at 550 °C;

- Click OK to start calculation;
- Details on these options can be found in Pandat User's Guide section 6.4.

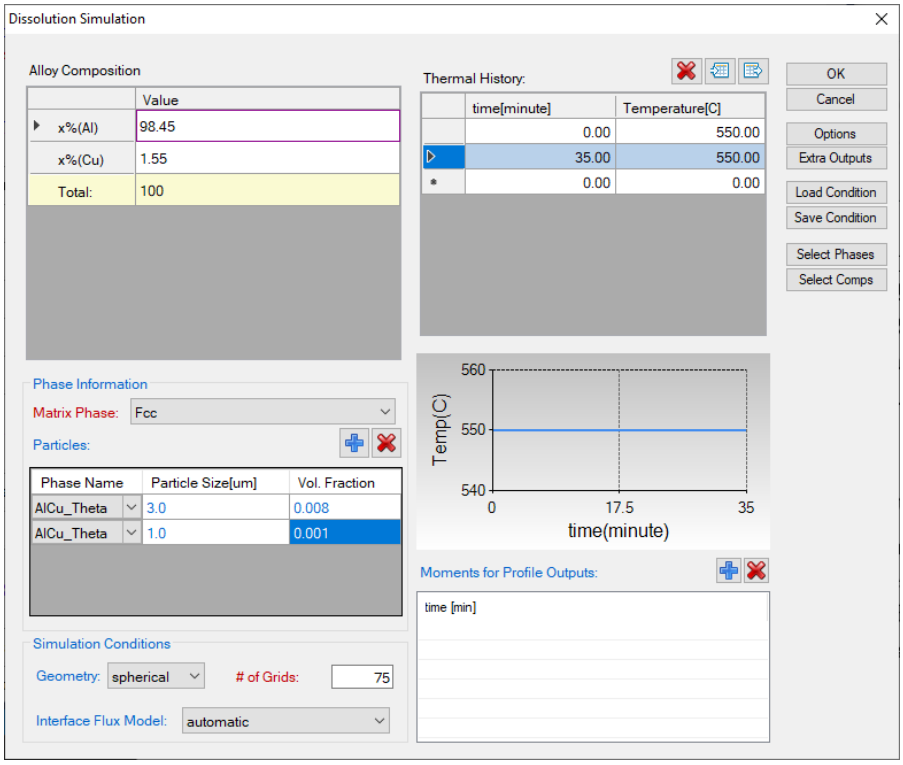


Figure 4.13.1: Setting of the simulation condition

Post Calculation Operation:

- The calculated particle dissolution with time is shown in Figure 4.13.2 User can modify it by changing the title, the scale, and add grid to the graph by setting "Show Major Grid" True in the **`Property`** Window.More information about change graph appearance can be found in Pandat User's Guide Section 2.3.1.

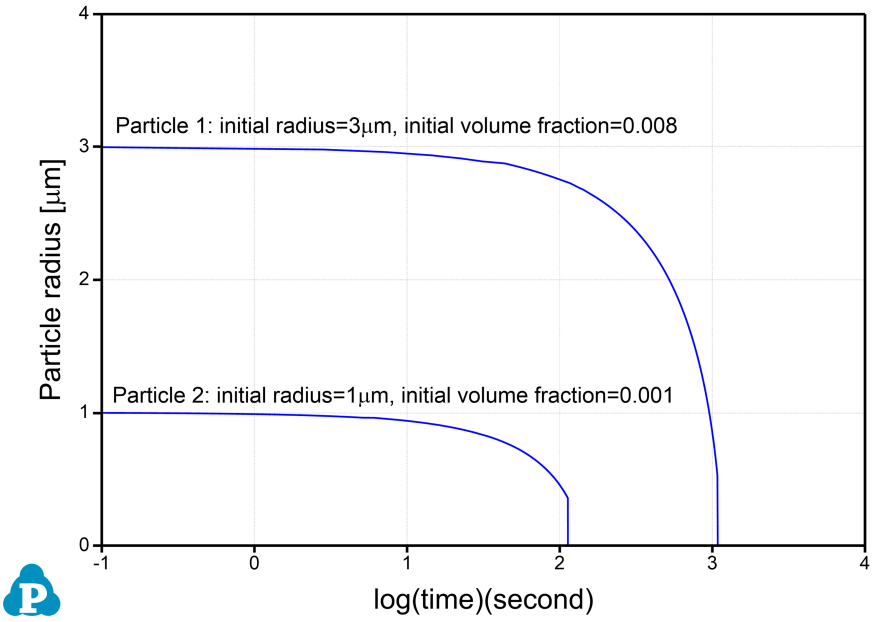


Figure 4.13.2: The simulation result of particle-size evolution

Example 4.14 Decarburization of Fe-C Matrix

Purpose: Learn to perform decarburization simulation at constant temperature with a fixed activity at boundary.

Module: PanDiffusion

Thermodynamic and Mobility Database: `Fe-Si-C.tdb`

Batch file: `Example_#4.14.pbfx`

Calculation Procedures:

- Create a workspace and select the PanDiffusion module following Pandat User's Guide 2.1;
- Load `Fe-Si-C.tdb` following the procedure in Pandat User's Guide 3.2.1, and select all three components;
- Click on the menu "**PanDiffusion → Diffusion Simulation**" or click the icon and set up the calculation condition as shown in Figure 4.14.1.
- First click the red "**X**" above Regions to delete **Region_2** and leave one Region only.
- Click on **Region_1** and set the composition as `0.5C-99.5Fe` (at%), The length (Diff. Length) as 100 μm, and the # of Grids as 100.
- The Thermal History is a period of 10 seconds with a constant temperature at 1000 °C;
- Click on **Lower Boundary Condition** (left edge of Region_1) and select fixed "`activity`", and set the Value as "`a(C:graphite[*])=0.01`";
- In the settings shown in Figure 4.14.1, composition profiles at the initial and final stages will be outputted. Click OK to perform calculations.
- By default, dissolution simulation gives time-evolution of particle size as output. In order to display composition profile at desired moments, click the blue "**+**" button next to the "**Moments for Profile Outputs**" and input a time value. As shown in Figure 4.14.1, profiles at 1 second and 5 second will be outputted. Click OK to start calculation;
- Details on these options can be found in Pandat User's Guide section 6.4.

Post Calculation Operation:

- Set the scale of the Y axis to be 0.1-0.6 (at%). Remove composition profile of Fe. The calculated composition profiles are displayed in Figure 4.14.2Change graph appearance and add text following the procedure in Pandat User's Guide Sections 2.3.1 and 2.3.3.

Information obtained from this calculation:

- Decarburization process in Fcc phase in the Fe-C system. Lower boundary condition is a fixed carbon activity (0.01, Graphite as the reference state).

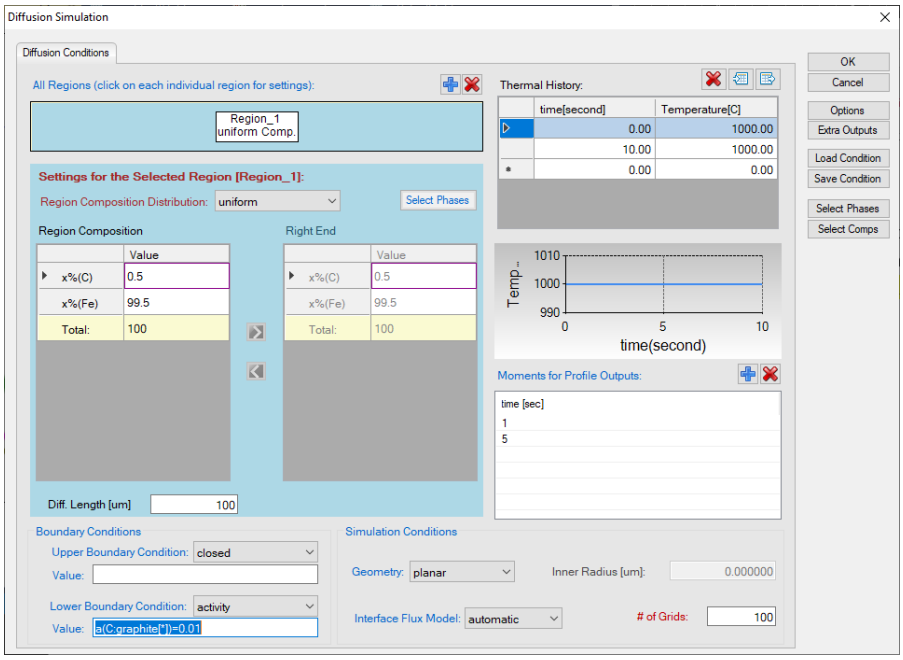


Figure 4.14.1: Setting of the simulation condition

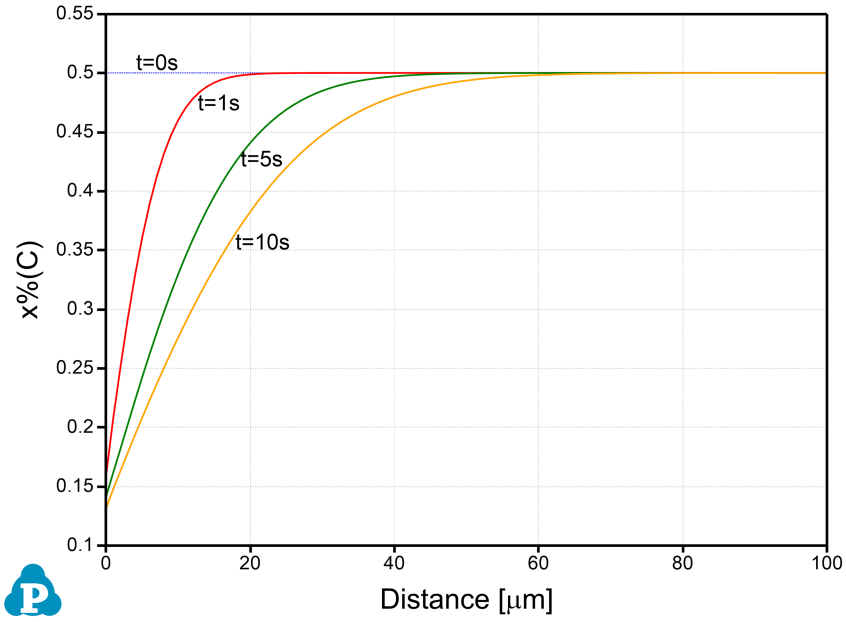


Figure 4.14.2: Simulation result of carbon composition profile

5 PanSolidification Examples

Example 5.1 Solidification Simulation of a Mg-Al alloy under a Given Cooling Rate

Purpose: Learn to perform solidification simulation of a Mg-Al binary alloy under specified solidification conditions using PanSolidification Module. Learn to use the features in PanSolidification Module.

Module: PanSolidification

Thermodynamic and Mobility Database: `AlMg_MB.tdb`

Kinetic Parameters Database: `Mg_Alloys.sdb`

Batch file: `Example_#5.1.pbfx`

Calculation Procedures:

- Create a workspace and select the PanSolidification module following Pandat User's Guide section 2.1;
- Load `AlMg_MB.tdb` through menu "**`Database → Load TDB or PDB`**" or by click icon , and then select `Al` and `Mg` two components;
- Load SDB file Mg_Alloys.sdb through menu "**`PanSolidification → Load SDB`**" or by click icon , select the available alloys: `Mg alloys`, as shown in Figure 5.1.1;
- Set Solidification simulation conditions as shown in Figure 5.1.2. The alloy composition is Mg-9wt.% Al. The cooling rate is 0.38 K/s is setting in Thermal History solidifying from 680 °C to 300 °C with 1000 second. Solidification rate is set as 50 μm/s. Please pay attention to the units of the time and length when set conditions;
- Then Click OK to perform Solidification simulation. (Detailed description also in Pandat User's Guide 1.1 7.4).

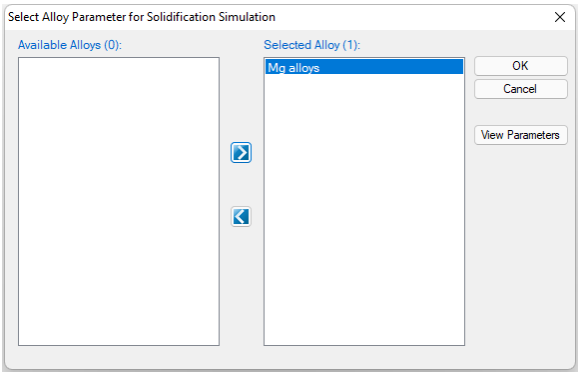


Figure 5.1.1: Load the Mg_Alloys.sdb file and select alloy

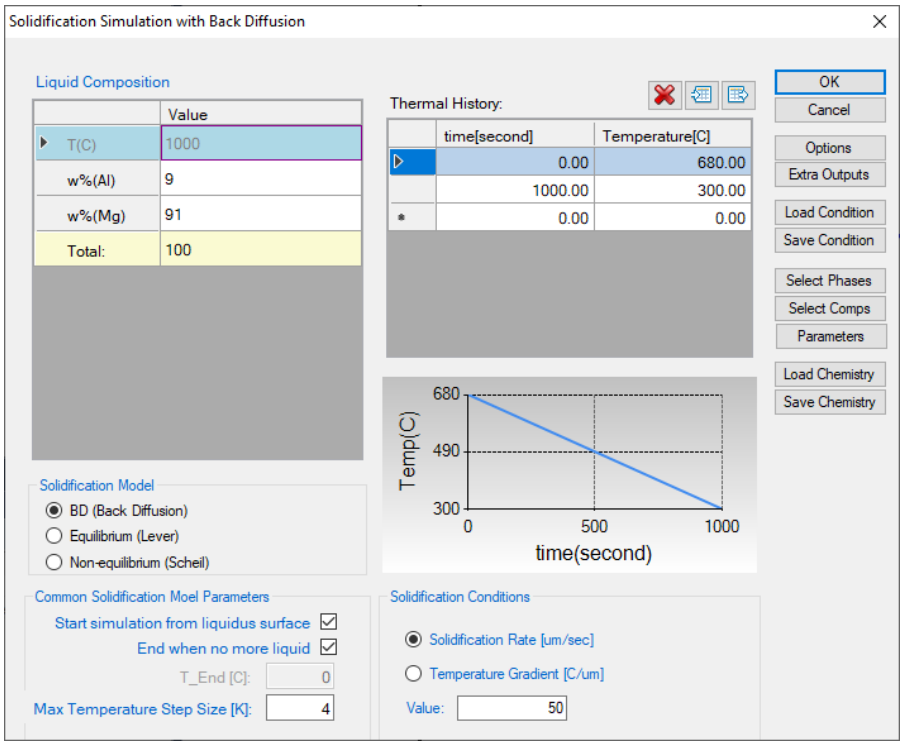


Figure 5.1.2: Set up conditions for solidification simulation

Post Calculation Operation:

- The default plot presents the relationship between fraction of solid (fs) and temperature during solidification as shown in Figure 5.1.3.
- The Default table contains many more calculated results as different columns: such as the secondary dendrite arm spacing (`arm_space`), the amount of $Al_{12}Mg_{17}$ phase (`f_tot(@Al12Mg17)`) column, and the composition of Al in the solid phase (`w_S(Al)`). Users

can create other plots from these data.

- The evolution of secondary dendrite arm spacing during solidification is shown in Figure 5.1.4.
- Experimental data can be imported through menu "**`Table → Import table from File`**". The comparison of the calculated and experimentally measured Al composition in solid is shown in Figure 5.1.5.

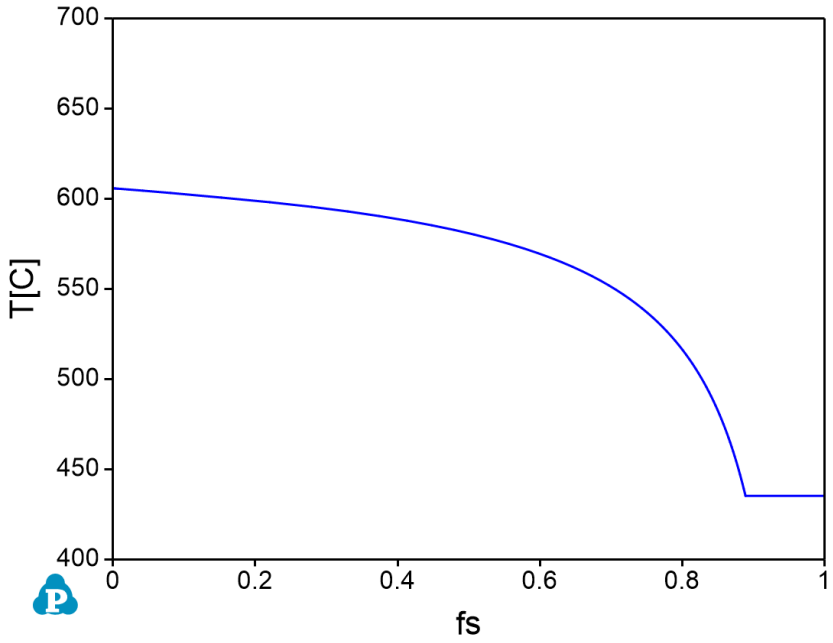


Figure 5.1.3: Default plot showing fraction of solid as a function of Temperature

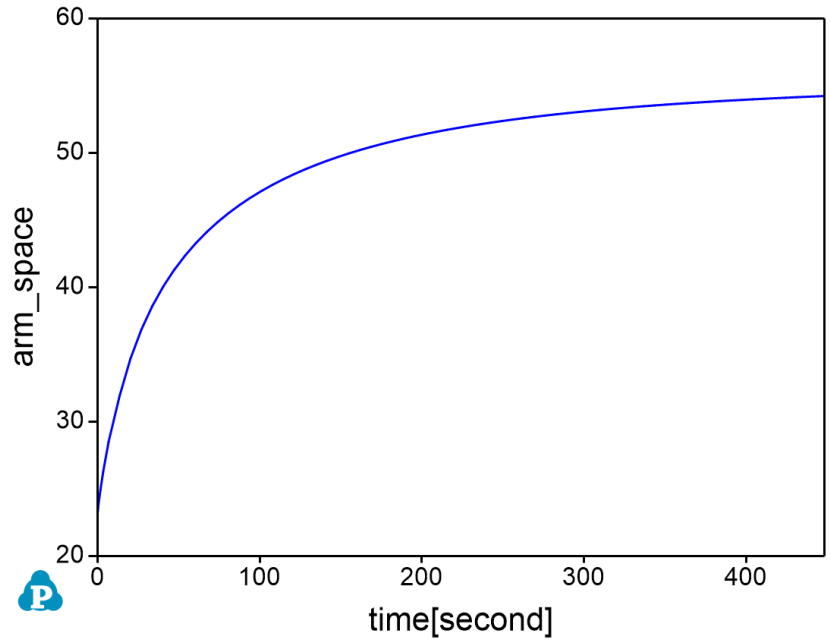


Figure 5.1.4: The evolution of secondary dendrite arm spacing

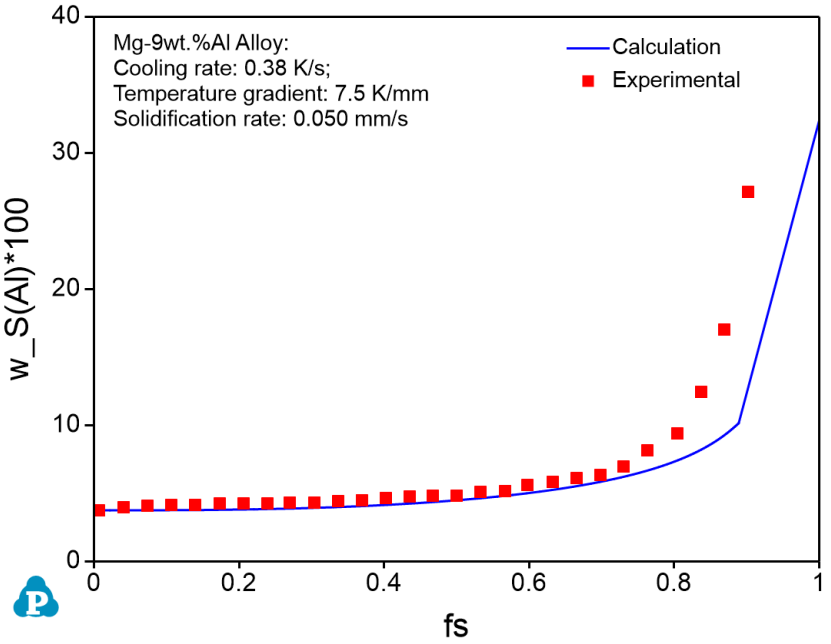


Figure 5.1.5: Comparison of the calculated and experimentally measured Al composition profile vs. fs in the primary (Mg) dendrites

Example 5.2 Prediction of Hot Cracking Susceptibility of an Al-Cu-Mg Alloy

Purpose: Learn to perform solidification simulation to predict the hot cracking susceptibility index of an alloy in PanSolidification Module.

Module: PanSolidification

Thermodynamic and Mobility Database: `PanAl_TH+MB.pdb`

Kinetic Parameters Database: `Al_Alloys.sdb`

Note: In Pandat 2022 version, the property **CSI** is defined as "`-T//sqrt(fs)`". In the "**Table editor**" window, users can directly select `CSI` or simply type in `CSI` rather than using the math operation of "`-T//sqrt(fs)`".

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 in several Al alloy systems. In this example, users will learn how to perform solidification simulation of an Al-Cu-Mg alloy and output the relationship of $|dT/d(f_s)^{1/2}|$ vs $(f_s)^{1/2}$ directly from Pandat, and thus determine the CSI value of the alloy. Users will also learn to set extra output tables with some specified properties and extra output plots from this example. Commercial database of `PanAl_TH+MB.pdb` including the thermodynamic and mobility data is required to perform the calculation of this example.

Calculation Procedures:

- Create a workspace and select the PanSolidification module following Pandat User's Guide 1.1 section 2.1;
- Load `PanAl_TH+MB.pdb` through menu "**Database → Load TDB or PDB**" or by click icon , and then select `Al`, `Cu` and `Mg` three components;
- Load SDB file `Al_Alloys.sdb` through menu "**PanSolidification → Load SDB**" or by click icon , select the available alloys: Al alloys.

- Set Solidification simulation conditions as shown in Figure 5.2.1. The alloy composition is Al-5wt.%Cu-2wt.%Mg. The cooling rate is 20 K/s is setting in Thermal History solidifying from 680 °C to 380 °C with 15 second. Temperature gradient is set as 10^{-3} °C/μm. Please pay attention to the units of the time and length when set conditions.
- Set "**Extra Outputs table**". Click the "**Extra Outputs**" in Figure 5.2.1, a new interface as shown in Figure 5.2.2 will appear. Click the blue "**+**" symbol in Figure 5.2.2 to pop out the **Table Editor** as shown in Figure 5.2.3. From this **Table Editor**, users can specify and type in properties to output, such as `sqrt(fs), -T//sqrt(fs)` in this example. `-T//sqrt(fs)` refers to $-dT/d(f_s)^{1/2}$, as the syntax // means derivative in Pandat software. Note that with this setting, a "`generated`" table will be created in addition to the Default table (In Pandat 2022, the `CSI` property is introduced to replace the "`-T//sqrt(fs)`".)
- Set "**Extra Outputs graph**". Click the icon "**Graph**" in "**Set extra output**" interface as shown in Figure 5.2.2, then click the blue "**+**" symbol to add extra Graph. An interface as shown in Figure 5.2.4 will appear. Select the "`generated`" table generated by the previous step. Drag sqrt(fs) from the left column to X axis in the right column; drag `-T//sqrt(fs)` from the left column to Y axis in the right column. Then click OK. Note that with this setting, a "graph" of `-T//sqrt(fs)` vs. `sqrt(fs)` will be plotted automatically in addition to the Default graph.
- Then Click OK to perform Solidification simulation. (Detailed description also in Pandat User's Guide 7.4).

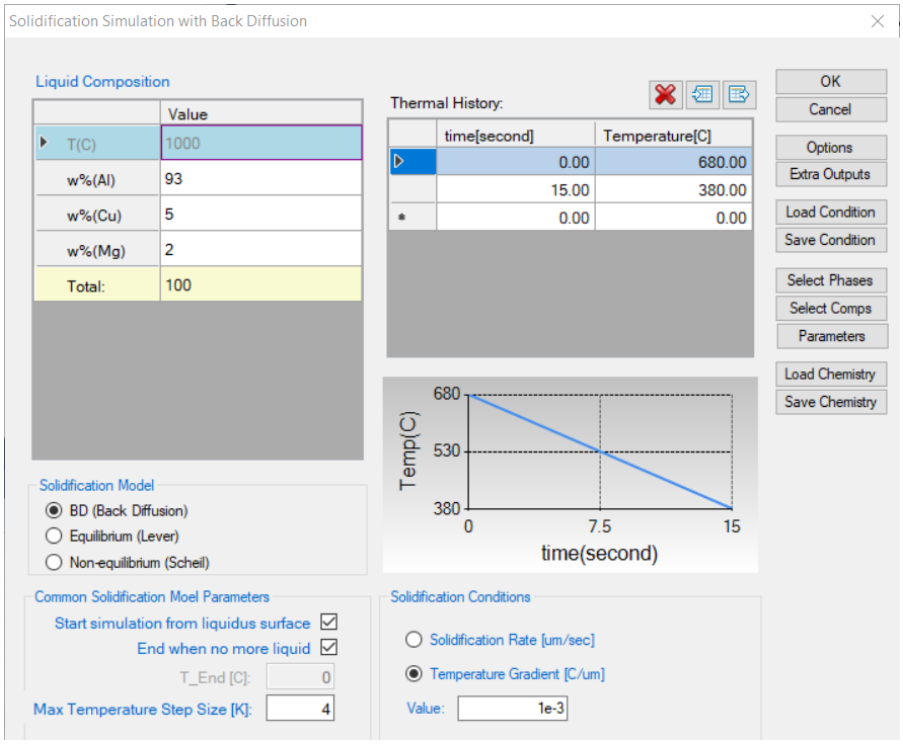


Figure 5.2.1: Set up conditions for solidification simulation

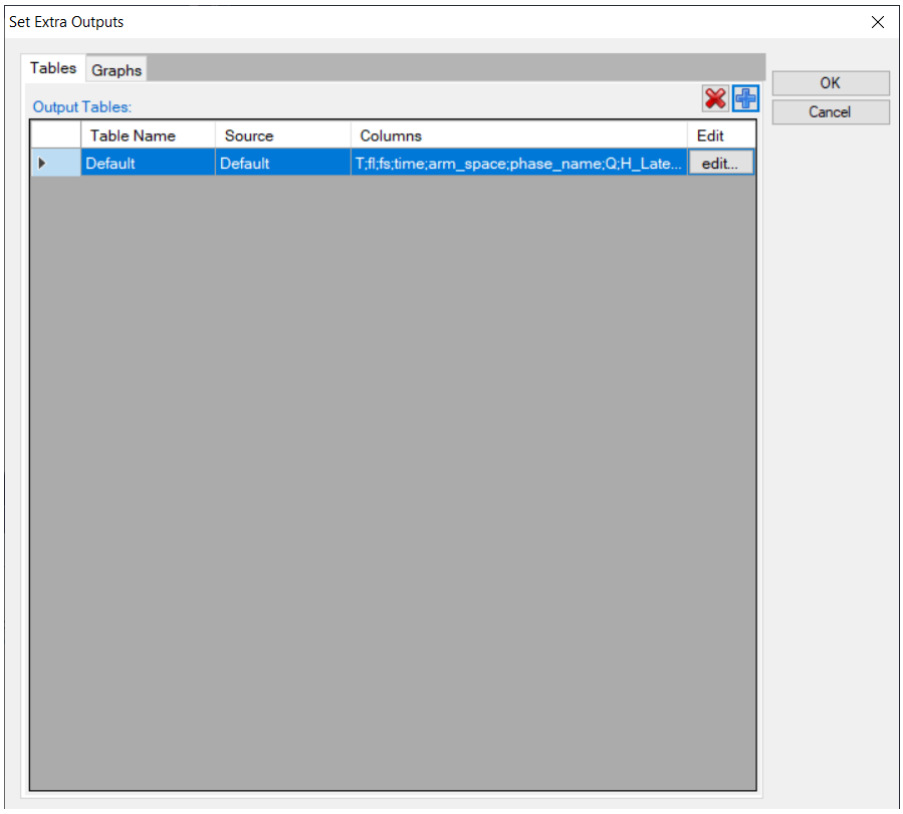


Figure 5.2.2: Extra Output interface

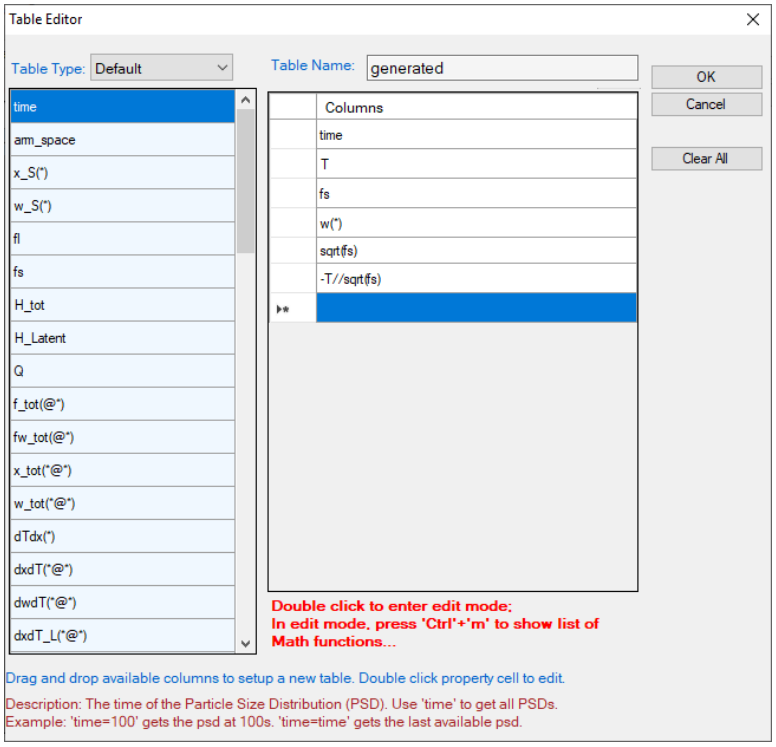


Figure 5.2.3: Define properties in the extra output table

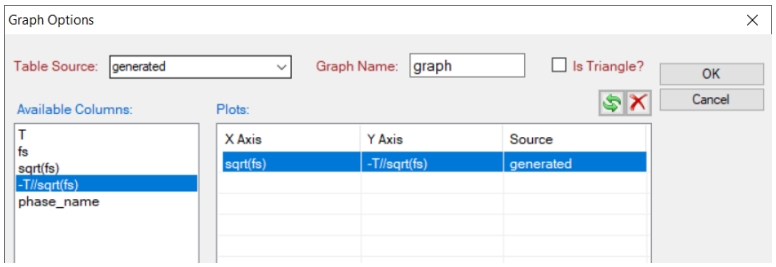


Figure 5.2.4: Define the axes of the extra graph

Post Calculation Operation:

- The default plot presents the relationship between fraction of solid (fs) and temperature during solidification as shown in Figure 5.2.5.
- The extra graph specified is plotted automatically as shown in Figure 5.2.6.
- Rescale Figure 5.2.6. as shown in Figure 5.2.7. The hot cracking susceptibility index (CSI) is defined as the maximum value of $-dT/d(f_s)^{1/2}$ with $(f_s)^{1/2} < 0.99$.

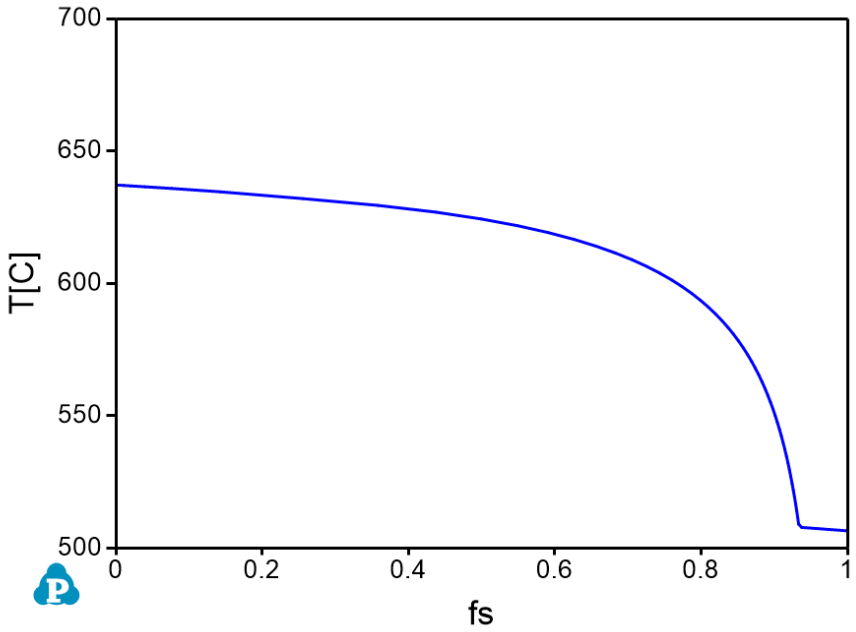


Figure 5.2.5: : Default plot showing the relation between temperature and fraction of solid

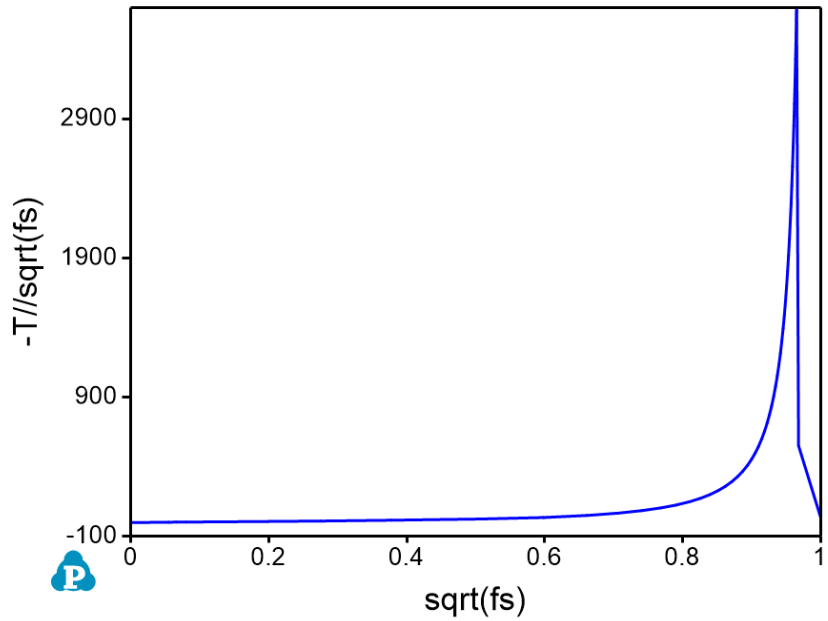


Figure 5.2.6: Extra plot specified by Extra Graph setting

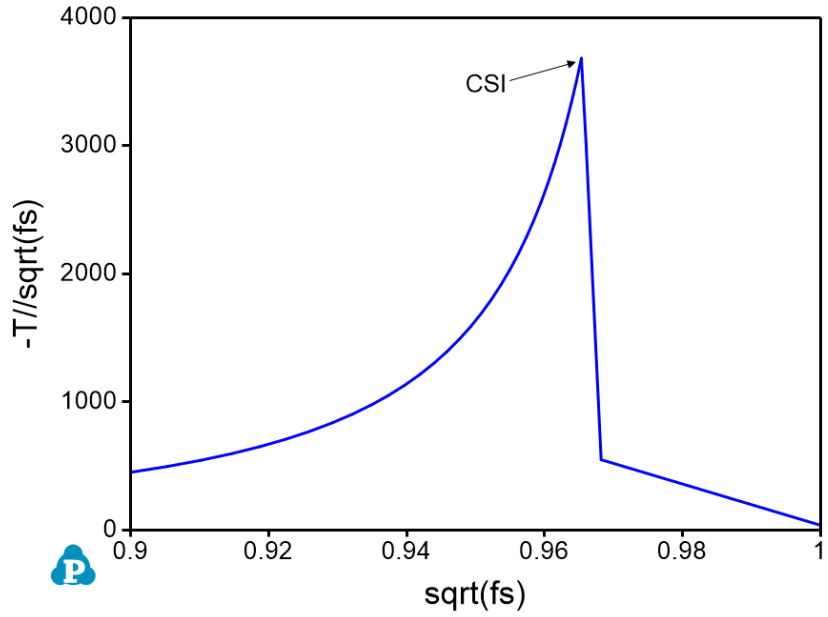


Figure 5.2.7: Rescale of Figure 5.2.6 showing the maximum point of -T//sqrt(fs) with sqrt(fs) < 0.99.

Example 5.3 Hot Cracking Susceptibility Map of Al-Cu-Mg at Al-Corner

Purpose: In the Example 5.2 : Prediction of Hot Cracking Susceptibility of an Al-Cu-Mg Alloy, Users have learned how to obtain the crack susceptibility index (CSI) value of a single alloy under certain solidification conditions. In this example, users will learn to use High Throughput Calculation (HTC) calculations to obtain a susceptibility index map in Al-Cu-Mg ternary system.

Module: PanSolidification

Thermodynamic and Mobility Database: `PanAl_TH+MB.pdb`

Kinetic Parameters Database: `Al_Alloys.sdb`

Note: In Pandat 2022 version, the property **CSI** is defined as "`-T//sqrt(fs)`". In the "**Table editor**" window, users can directly select `CSI` or simply type in `CSI` rather than using the math operation of "`-T//sqrt(fs)`".

Calculation Procedures:

- Create a workspace and select the PanSolidification module. Before calculation, save the workspace in a user assigned folder different from the default workspace. The HTC calculation results will be saved automatically under this folder. (Detailed description also in the Pandat User's Guide section 2.1;
- Load `PanAl_TH+MB.pdb` through menu "**Database → Load TDB or PDB**" or by click icon , and then select `Al`, `Cu` and `Mg` three components;
- Load SDB file `Al_Alloys.sdb` through menu "**PanSolidification → Load SDB**" or by click icon , select the available alloys: Al alloys;
- Start HTC function through menu "**Batch Calc → High Throughput Calculation (HTC)**";
- Choose calculation type from the drop-down list of HTC pop-up window and select "**pan_solidification**" as shown in Figure 5.3.1;

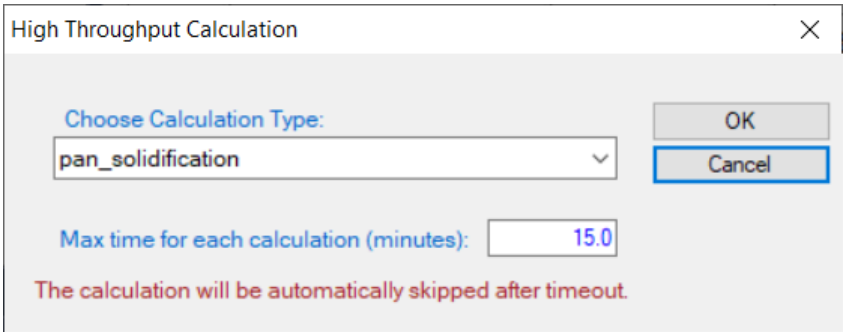


Figure 5.3.1: Dialog to choose calculation type of HTC in PanSolidification

- Define the compositional space for HTC simulation. The composition range is set to 0-5 wt.% Cu and 0-5 wt.% Mg, and mouse right click on the composition field of Al to set as the remaining composition, which is shown as -1 in all the composition field of Al, as shown in Figure 5.3.2.;
- Define the solidification conditions for HTC simulation. The solidification conditions with cooling rate of 20 K/s and Temperature gradient is set as 10^{-3} °C/μm, as shown in Figure 5.3.2;
- Set "**`Extra Outputs table`**". Click the "**`Extra Outputs`**" in Figure 5.3.2, a new interface as shown in Figure 5.3.3 will appear. Click the blue "**+**" symbol in Figure 5.3.3 to pop out the **`Table Editor`** as shown in Figure 5.3.4. From this **`Table Editor`**, users can specify and type in properties to output, such as `sqrt(fs), -T//sqrt(fs)` in this example. `-T//sqrt(fs)` refers to $-dT/d(f_s)^{1/2}$, as the syntax // means derivative in Pandat software. Note that with this setting, a "`generated`" table will be created in addition to the Default table;
- Set "**`Extra Outputs graph`**". Using the procedure described in Example 5.2, click the icon "**`Graph`**" in "**`Set extra output`**", set `sqrt(fs)` as X axis and `-T//sqrt(fs)` as Y axis. Then click OK;
- Click "Run HTC" button to perform HTC simulations.(Detailed description also in Pandat User's Guide section 10.2.3).

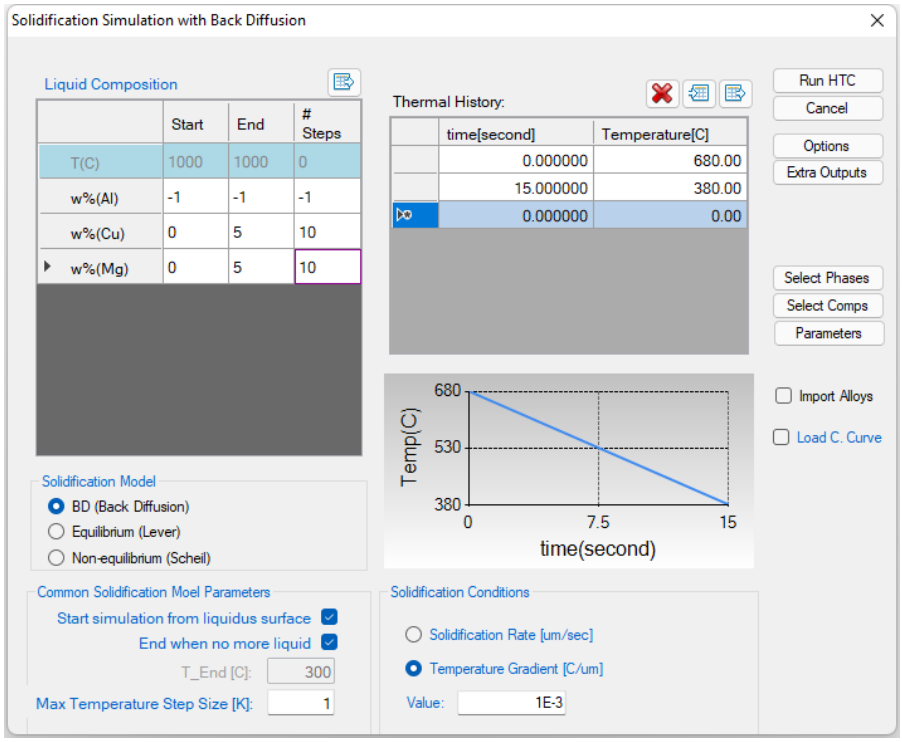


Figure 5.3.2: Dialog to setup compositional space and solidification conditions for PanSolidification HTC

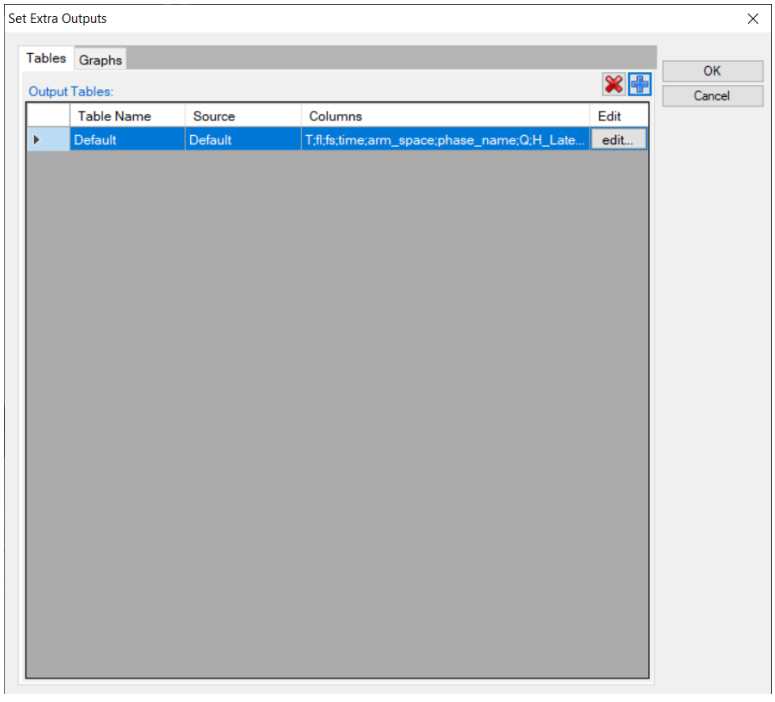


Figure 5.3.3: Extra Output interface

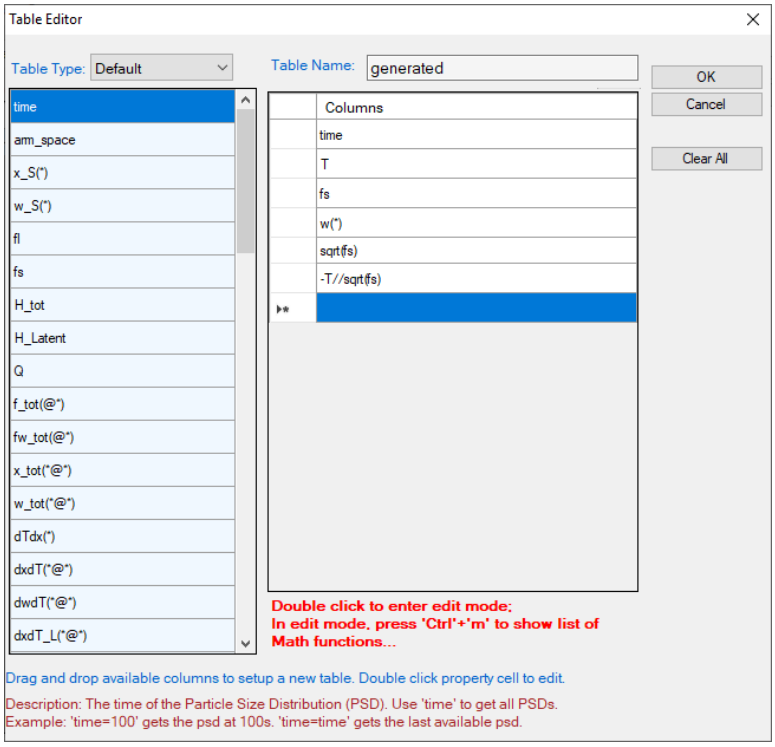


Figure 5.3.4: Define properties in the extra output table

Post Calculation Operation: Result Analysis

- After all calculations have been finished, analyze the results through menu "**`Batch Calc → Result Analysis`**". User can then analyze the results of the selected HTC calculation by opening the corresponding workspace as shown in Figure 5.3.5.

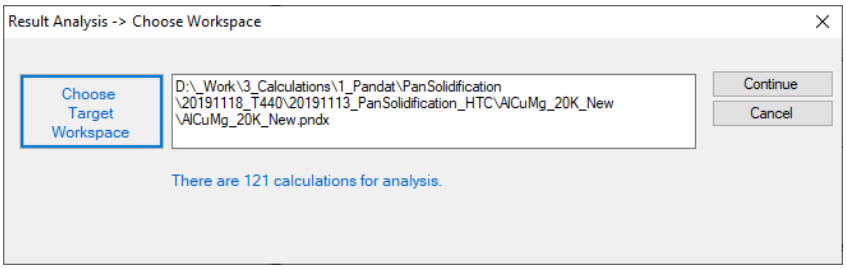


Figure 5.3.5: : “Result Analysis” popup dialog to choose target workspace

- Define the criteria of the properties as filters for result analysis. As shown in the following Figure 5.3.6, analysis the “**`generated table`**”, set the condition to find the CSI for each alloy composition, i.e., CSI = MAX(-T//sqrt(fs)) at sqrt(fs)< 0.99;

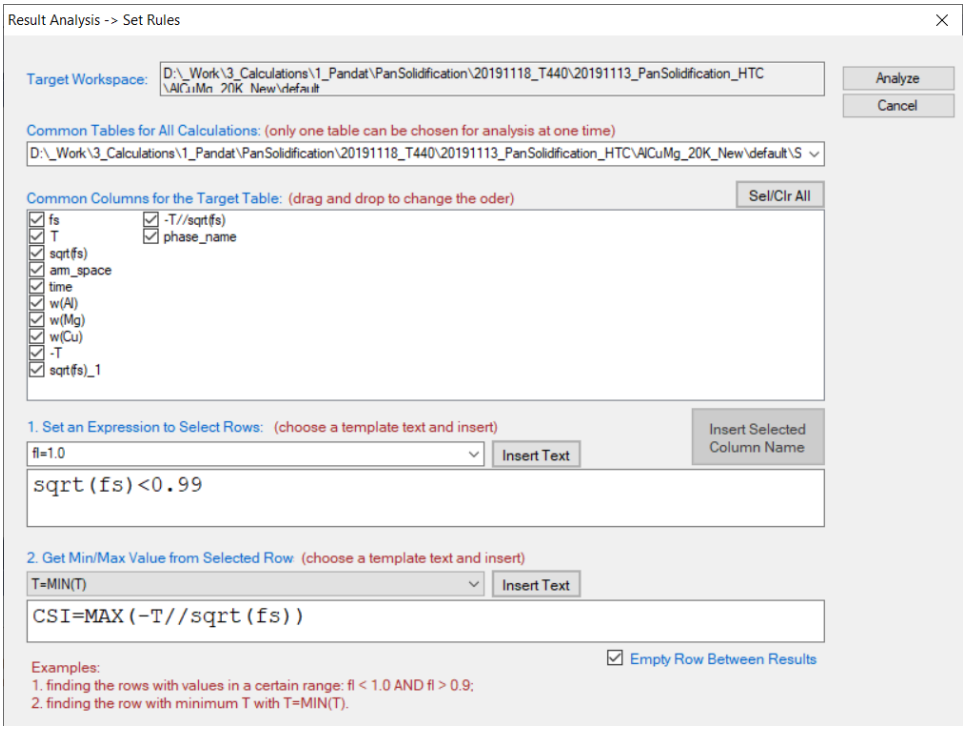


Figure 5.3.6: Criteria for Cracking Susceptibility Index setting from solidification results analysis

- After results analysis, a table which list CSI = MAX(-T//sqrt(fs)) for each alloy composition is generated as shown in Figure 5.3.7;
- Select w%(Cu) as X-axis, press Ctrl then select w%(Mg) and (-T//sqrt(fs)) as Y-axis and Z-axis, respectively, click on the tool bar to generate Figure 5.3.8 which shows the crack susceptibility map for Al-Cu-Mg alloys with cooling rate of 20 K/s;
- The simulated result is comparable with the experimental results shown in Figure 5.3.9.

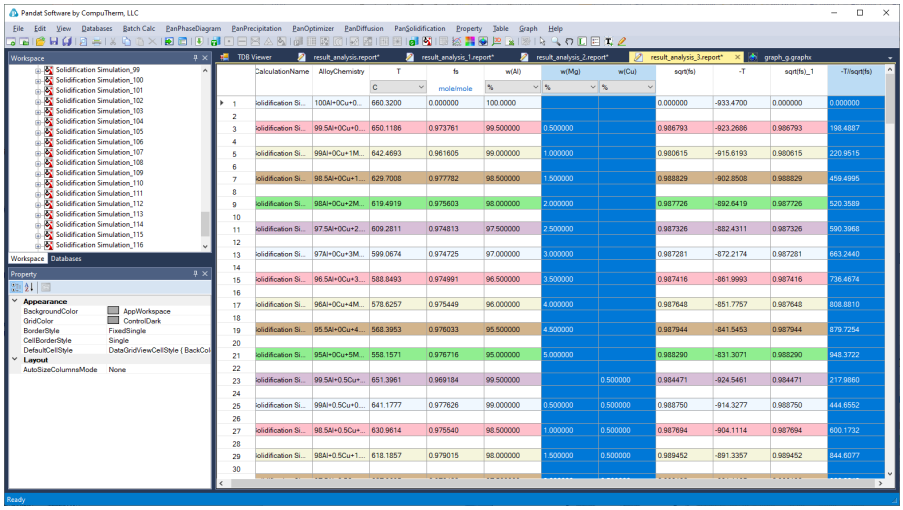


Figure 5.3.7: A table which lists the CSI = MAX(-T//sqrt(fs)) for each alloy composition is generated after the results analysis

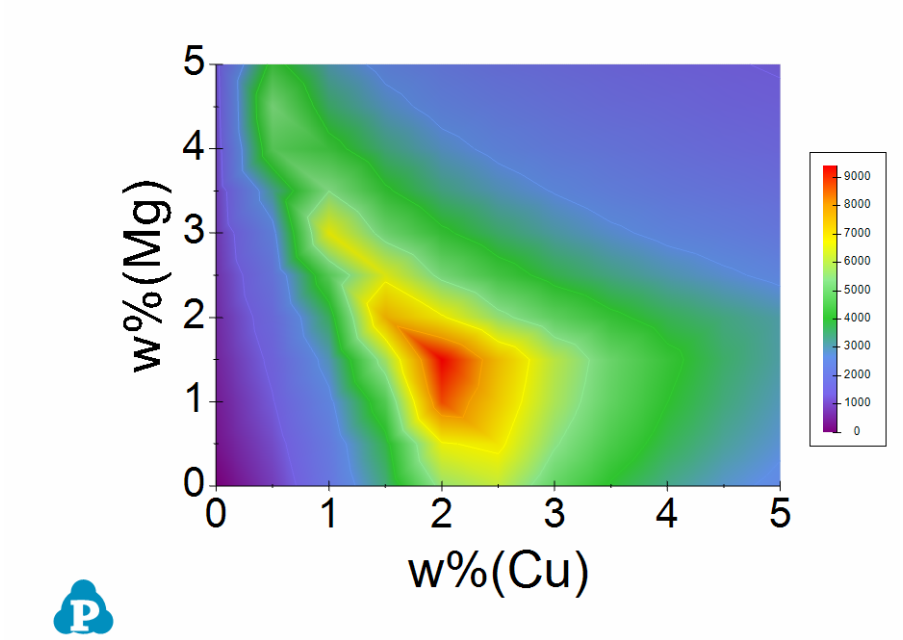


Figure 5.3.8: Al-Cu-Mg crack susceptibility map with cooling rate of 20 K/s

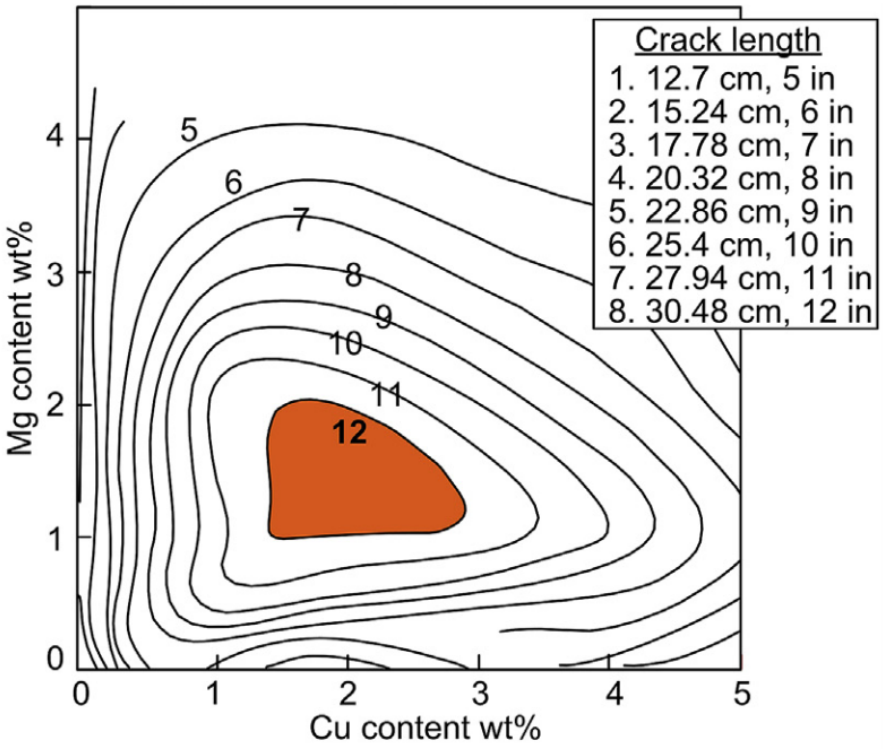


Figure 5.3.9: Experimental crack susceptibility test results