

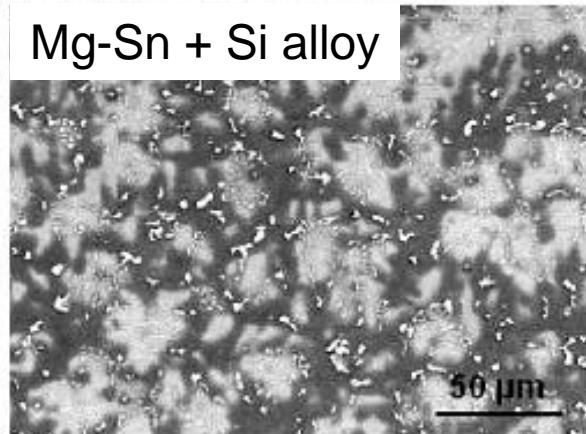
Alloy Design

Basics and Advanced

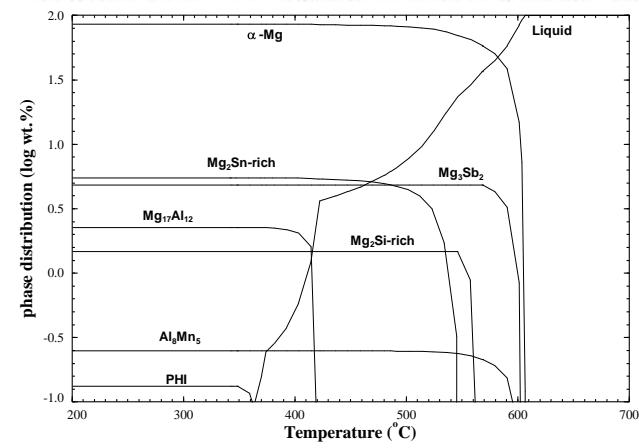
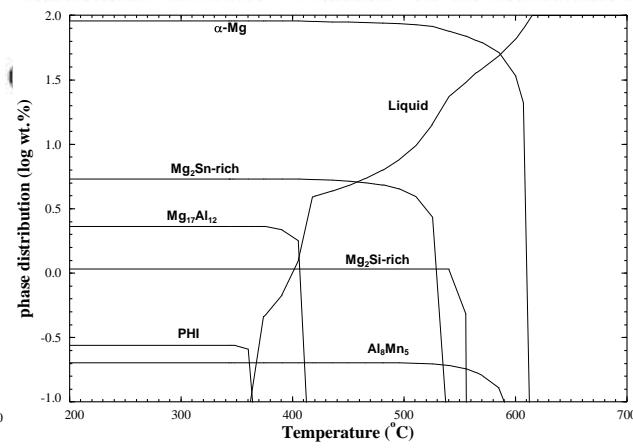
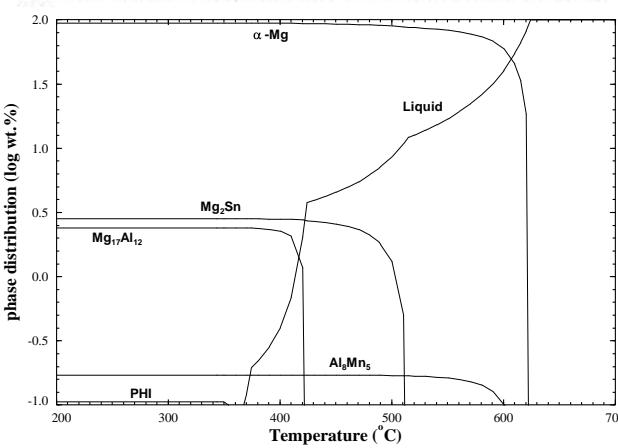
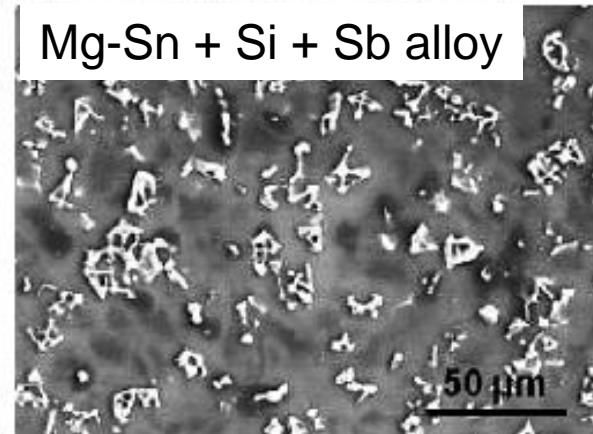
Mg-Sn alloy



Mg-Sn + Si alloy



Mg-Sn + Si + Sb alloy



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All materials processes involve
“Thermodynamics” and “Kinetics”.

Thermodynamics (Equilibrium) tells where we go.
Kinetics tells how fast we can go.

FactSage can provide Thermodynamic calculations for:

- Multicomponent (< 48 elements) Chemical reaction equilibria
- Phase diagrams up to 8 component systems (*FactSage 70: even more than 8 components are allowed*)
- Thermodynamic properties such as heat balance, G, H, S, etc.

Alloy Design Concept using FactSage Calculations

Gas, Oxide, Salt and Alloy databases



Scheil Cooling Calculation

as cast microstructure

Equilibrium Calculation

Data mining program
(FactOptimal)

Equilibrium reactions
as annealed microstructure

Phase diagram

Multicomponent
phase diagram section

Alloy design

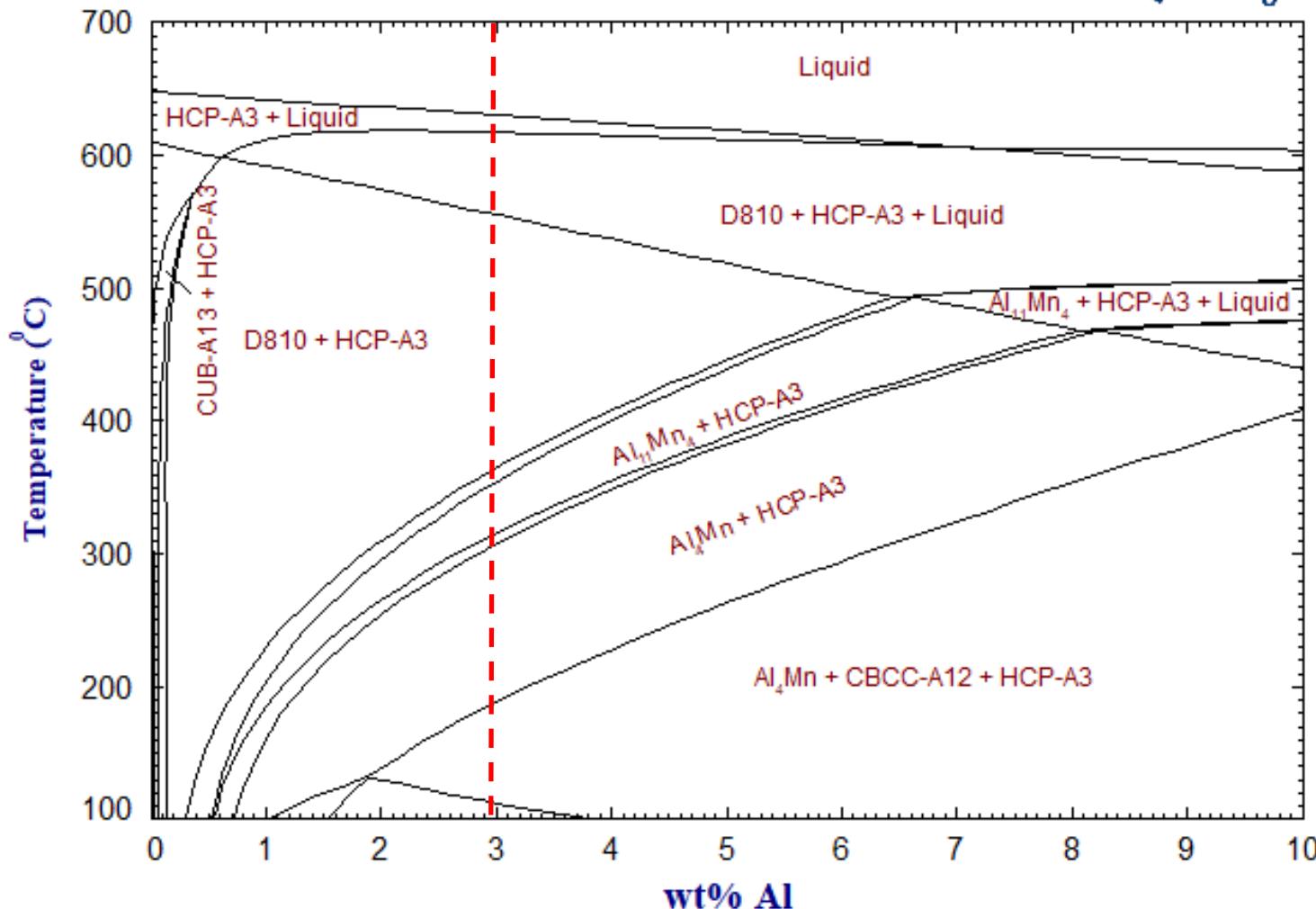
Material Processing and FactSage

Process	What can we do with FactSage
Extraction / Refining / Recycling	Gas/Slag/Matte/Salt/Metal/Refractory reactions
Casting	Scheil cooling calculation (as-cast microstructure) Solidification software
Annealing / Homogenization	Multicomponent equilibrium calculations Secondary phase precipitation Solidification software
TMP / Forming	
Final treatment: Oxidation / Corrosion / Surface treatment	Oxidation phase diagram, E-pH diagram, Gas corrosion reactions
Thermodynamic properties	All kinds of thermodynamic properties: Heat balance, G, H, S, activity, partial pressure of gases, etc..

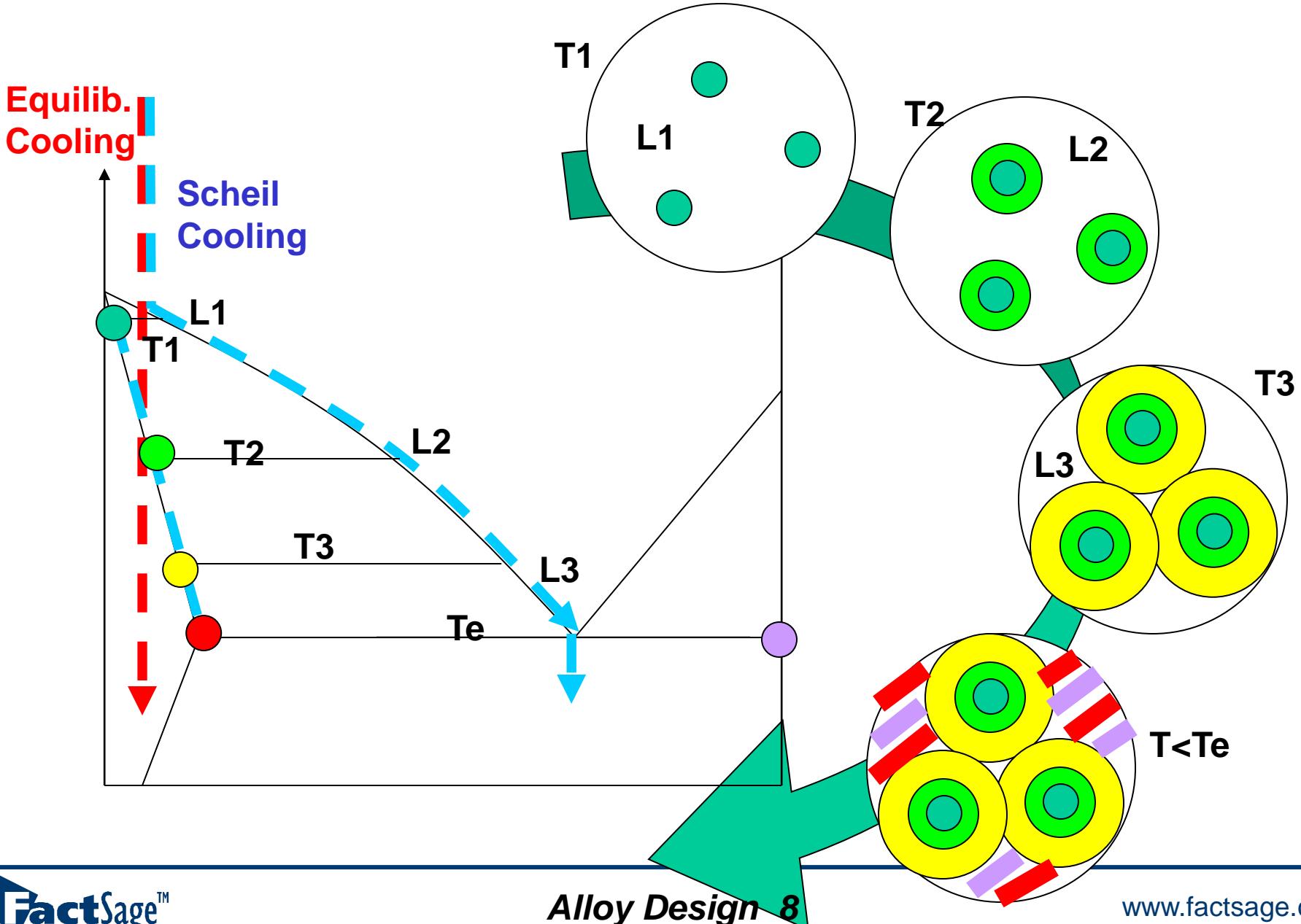
Alloy design (I): Phase diagram calculation to find out final target composition

Mg - Al - 1%Zn - 0.3%Mn

FactSage™

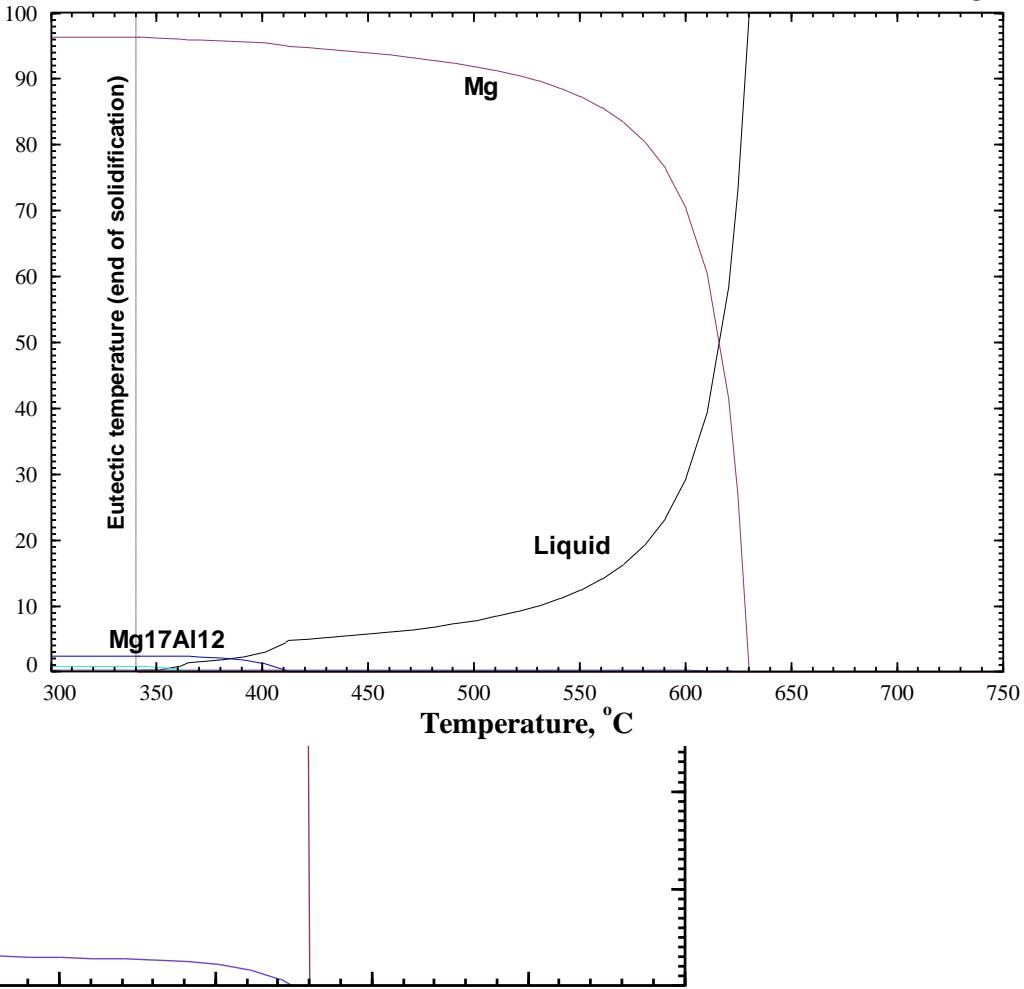
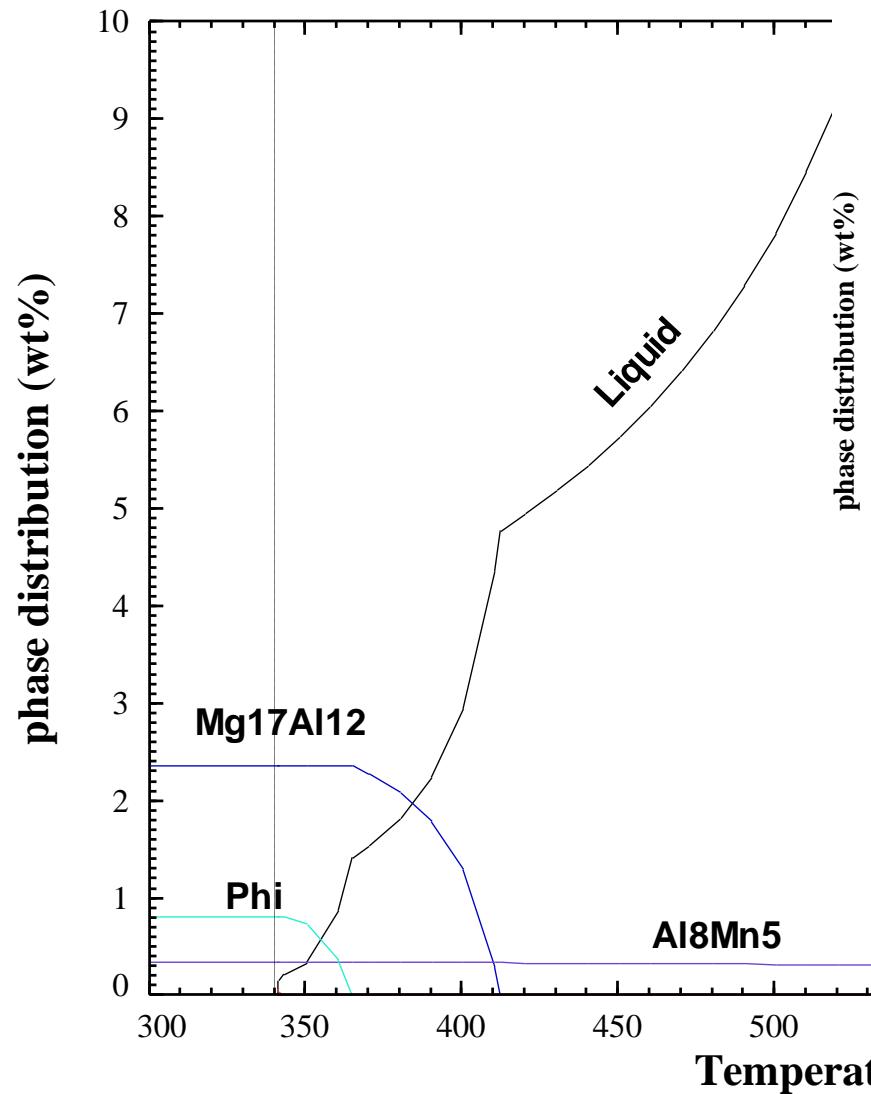


Alloy design (II): Estimating of as-cast microstructure to find out whether solidification can be reasonable.



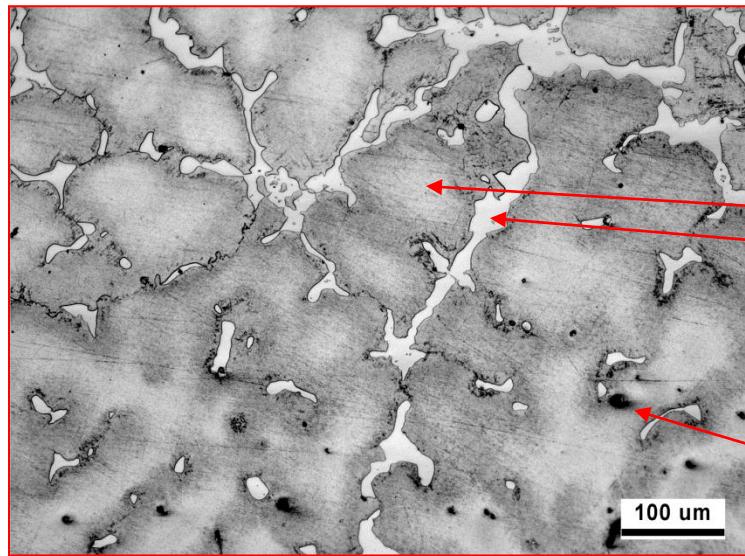
Scheil cooling calculation of AZ31 alloy

FactSage™

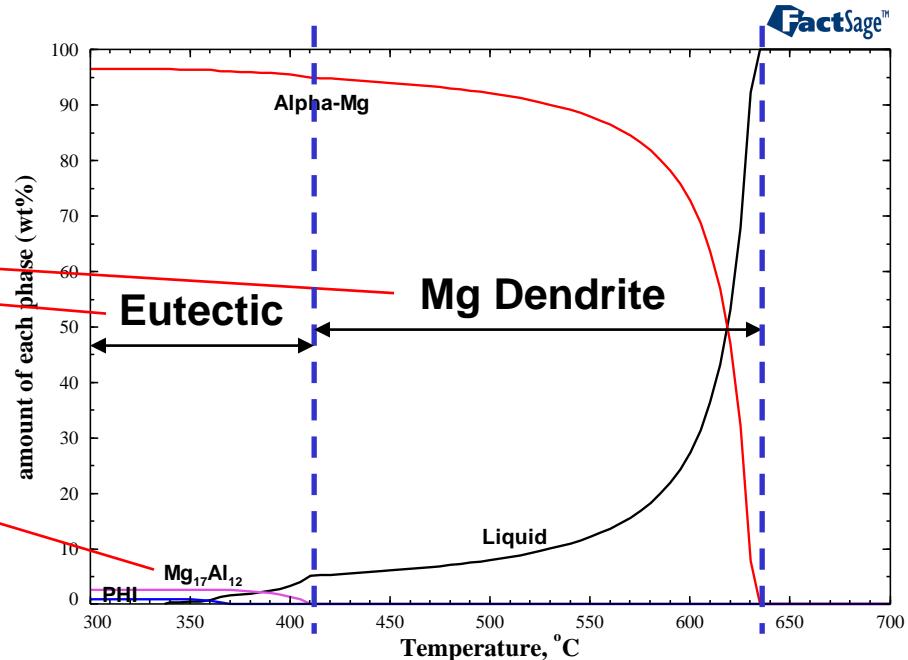


Scheil cooling calculation: as cast microstructure

Solidification path calculation: AZ31



Microstructure of as-cast AZ31



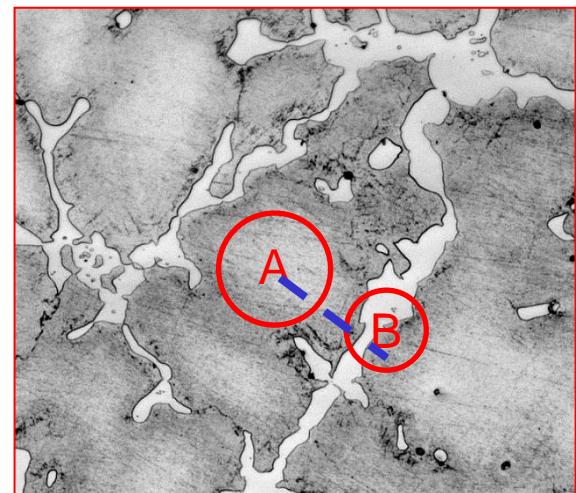
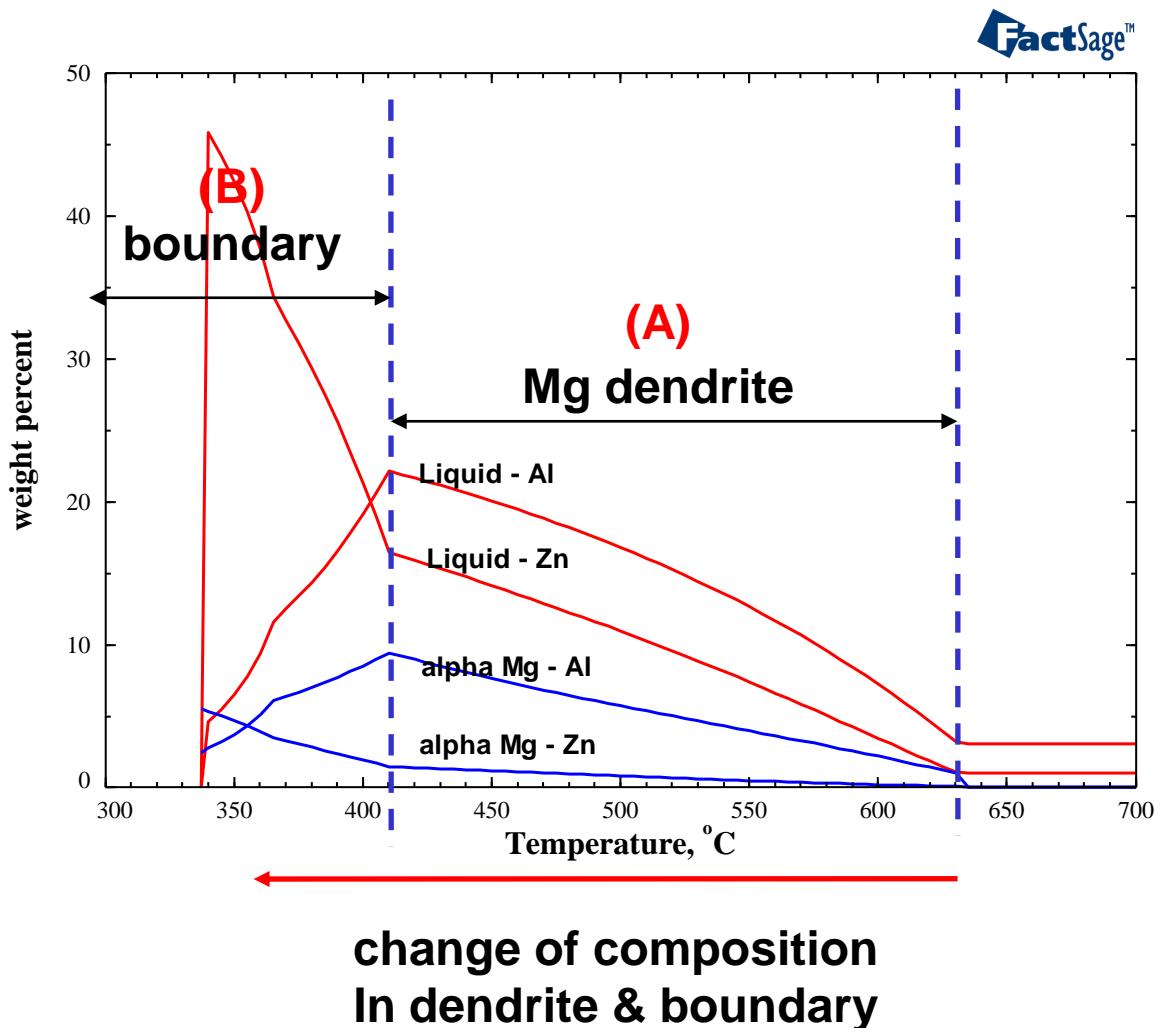
Scheil Cooling calculation

Scheil cooling calculations tell us the solidification path

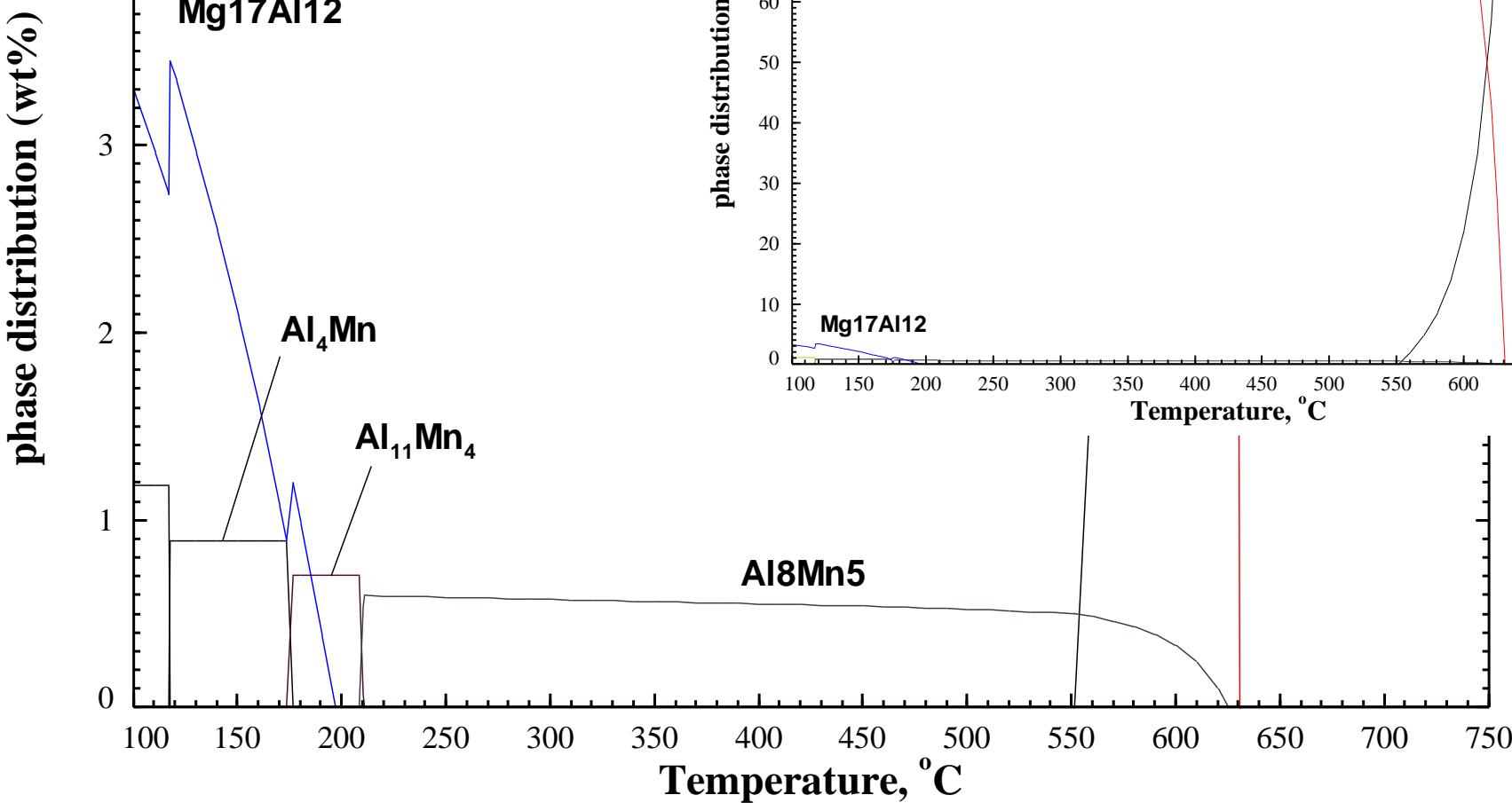
- Primary phase, precipitation, and eutectic reaction.
 - Dendrite boundary (eutectics, segregation)
- > Estimation of as-cast microstructure

Scheil cooling calculation: as cast microstructure

Corning effect of Mg dendrite: AZ31



Alloy design (III): Calculate the final target microstructure AZ31



FTlite database

FTlite Database for FactSage 8.3

The FTLite Database is designed for thermodynamic and phase equilibrium calculations involving **Al** alloys, **Mg** alloys and **Ti** alloys using the FactSage 8.0 Thermochemical Software Package (and later versions). The FTLite Database can also be used to perform calculations involving mixtures of **Li-Na-K-Mg-Ca-Sr-Ba** with several other elements.

Al Alloys
Ag, Al, As, Au, B, Ba, Be, Bi, C, Ca, Ce, Co, Cr, Cu, Dy, Er, Eu, Fe, Ga, Gd, Ge, H, Ho, In, K, La, Li, Lu, Mg, Mn, Mo, N, Na, Nb, Nd, Ni, O, P, Pb, Pr, Pt, Sb, Sc, Si, Sm, Sn, Sr, Ta, Tb, Ti, Tm, V, W, Y, Yb, Zn, Zr
Mg Alloys
Ag, Al, B, Ba, Be, Bi, C, Ca, Ce, Co, Cr, Cu, Dy, Er, Eu, Fe, Ga, Gd, Ge, H, Ho, In, K, La, Li, Lu, Mg, Mn, Na, Nb, Nd, Ni, O, Pb, Pr, Pt, Sb, Sc, Si, Sm, Sn, Sr, Tb, Ti, Tm, V, Y, Yb, Zn, Zr
Ti Alloys
Ag, Al, B, Ba, C, Ca, Ce, Co, Cr, Cu, Dy, Er, Eu, Fe, Ga, Gd, H, Ho, K, La, Li, Lu, Mg, Mn, Mo, N, Na, Nb, Nd, Ni, O, Pr, Sc, Si, Sm, Sn, Sr, Ta, Tb, Ti, Tm, V, W, Y, Yb, Zn, Zr
Color codes
Red : Al or Mg Blue : Major alloying elements (full optimisations of binary systems with Al, Mg and Ti and with several minor alloying elements, Al-Mg-Xx ternary systems evaluated (good for Al+Mg-rich regions), several quaternary systems included); Green : Minor alloying elements (full optimisation of binary systems with Al, Mg, Ti and with several minor alloying elements, Al-Mg-Xx ternary systems evaluated (good for Al+Mg-rich regions), several quaternary systems included); Black : Optimized for the M-Zz system and

Please look at “Documentation” to check new updates of FTLite database in FactSage 83.

FSStel database

The elements included in the FactSage FSStel steel database are:

**Al, B, Bi, C, Ca, Co, Cr, Cu, Fe, H, Hf, Mg, Mn, Mo, N, O, Nb, Ni, P, Pb, S, Sb, Si, Sn, Ta, Ti, V, W, Zn, Zr, RE
(Sc, Y, La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu)**

The FactSage FSStel steel database is based on relevant steel sub-systems from the old SGTE Solution database, but now incorporates updates of those systems as well as new published assessments. “Tramp elements” have also been included to allow calculations relating to recycling and removal of unwanted impurities to be performed.

The database contains **379** completely assessed **61** partially assessed binary alloy systems, together with approximately **158** ternary and **28** quaternary systems for which assessed parameters are available for phases of practical relevance. It contains **186** solution phases and **1014** stoichiometric compounds.

The liquid phase is described by the **Modified Quasichemical Model (MQM)** since FSStel 7.3 version. With this model, many previous optimizations with the random mixing model and new optimizations with the MQM can be combined to give a more accurate description of the liquid solution in binary, ternary and higher-order systems. The thermodynamic behaviors of O, N, S, and P in liquid steel are well described by this model. For the accurate description of the deoxidation of Fe-Ca and Fe-Mg liquid solutions, CaO and MgO associate species as proposed by Jung, Degterov and Pelton [1], have been incorporated in the liquid phase.

Updates in FactSage 8.3 version

In this update, numerous binary **Cr-RE** (RE = Rare Earth elements) system were newly added as part of our continue effort to put RE in steel database. Many **binary systems containing Ca, Mg, Nb and Zn** were newly added or updated for more accurate chemical reaction calculations in the refining process of super alloys and Zn galvanizing process of high alloyed steels. **Binary systems containing Sc** were also largely updated. These include 47 new binary systems, and several new ternary systems. 2 new solution phases and 57 new compounds are included in 8.3 version.

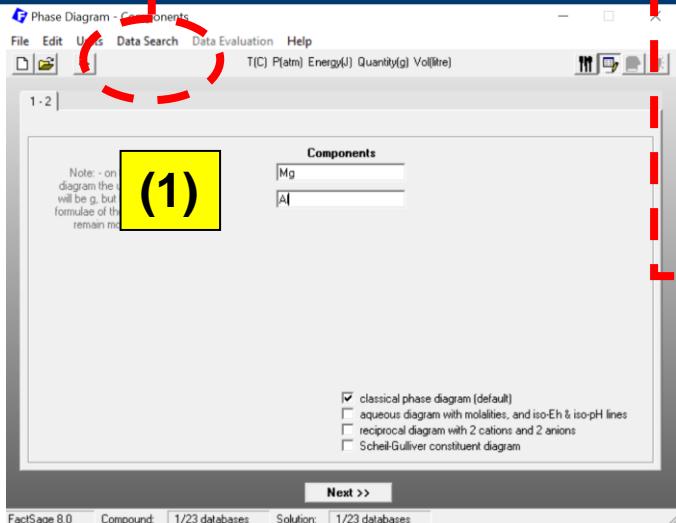
Please look at “Documentation” to check new updates of FSStel database in FactSage 83.

Alloy database: Others

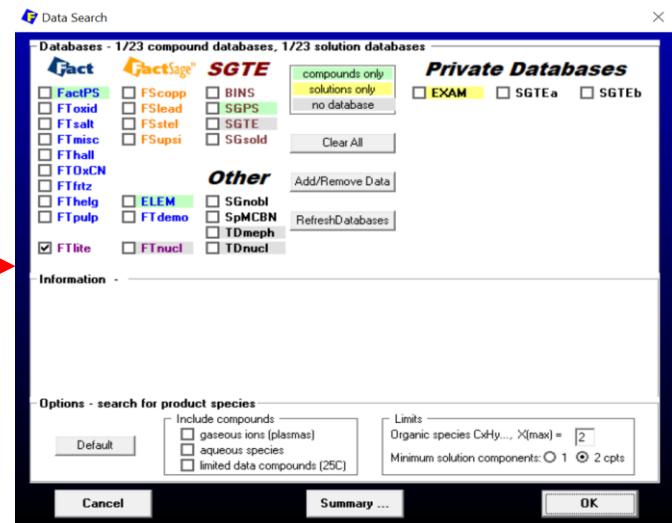
- **FSCopp**: Copper alloy development (all binary Cu-X systems)
- **FSupsi**: High purity Si database for solar cell grade Si production
- **FSnobl**: Noble alloy database for Ag, Au, Ir, Os, Pd, Pt, Rh, Ru refining
- **SGnobl**: Similar to FSnobl
- **SGsold**: Solder alloy database
- **SGTE 2014, 2017, 2020**: developed by SGTE (www.sgte.org): Applicable to all general alloy system. But less accurate than other dedicated databases for specific region.

APPLICATION EXAMPLES

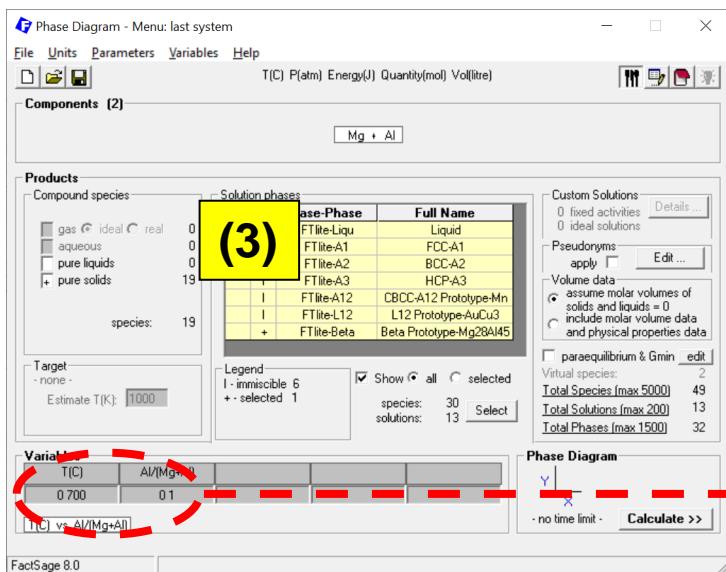
EX1 Binary phase diagram: Mg-Al binary system



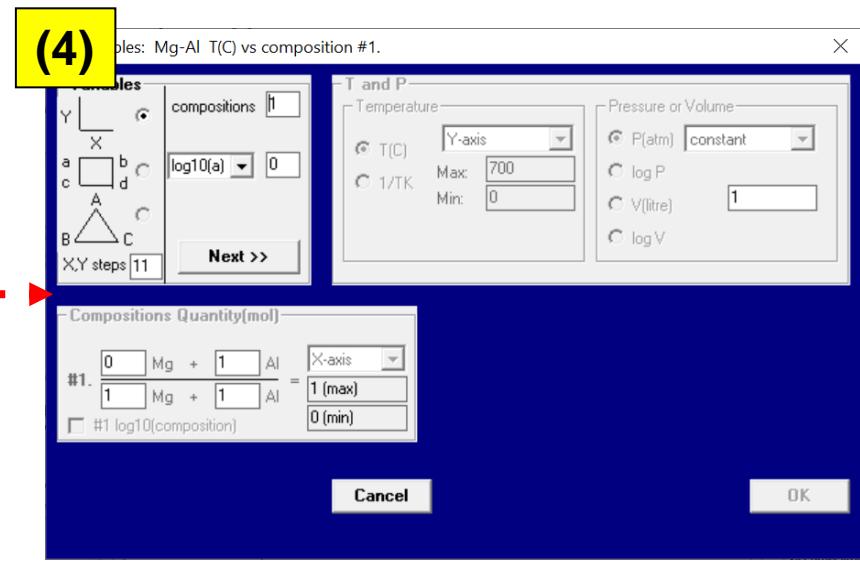
(1) Entering elements/components



(2) Database selection



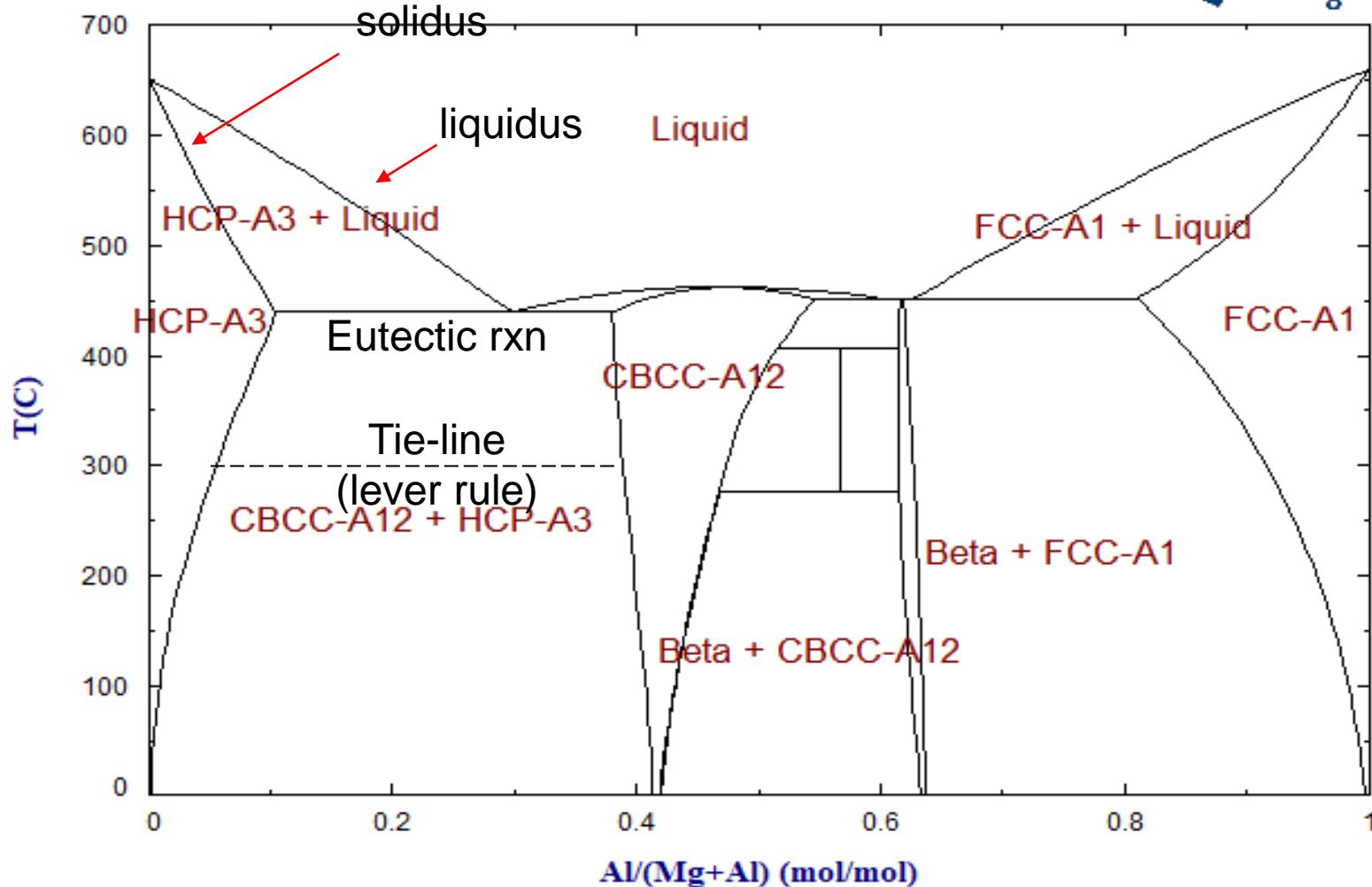
(3) Phases (compounds and solutions) selection



(4) Calculation conditions (T, X, P, etc.)

Mg - Al

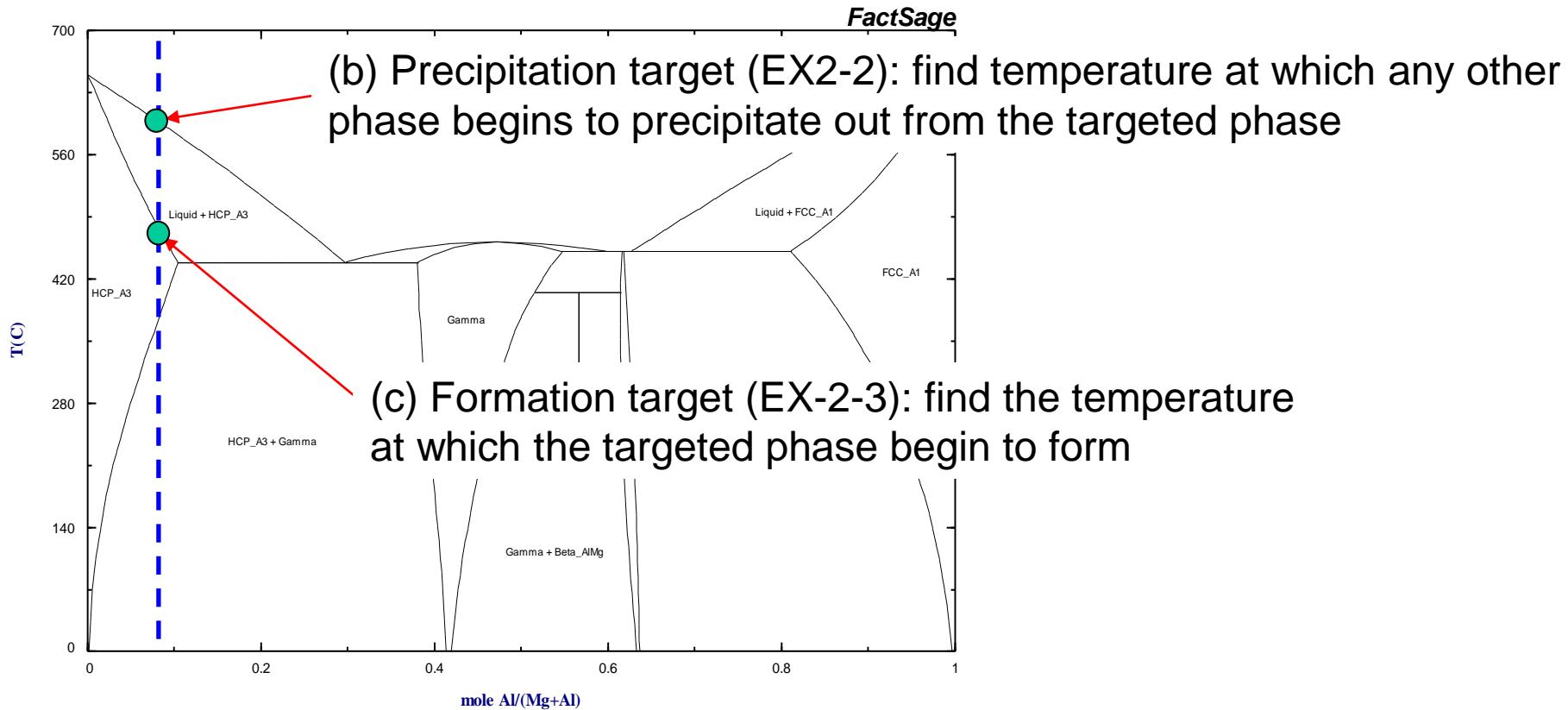
FactSage™



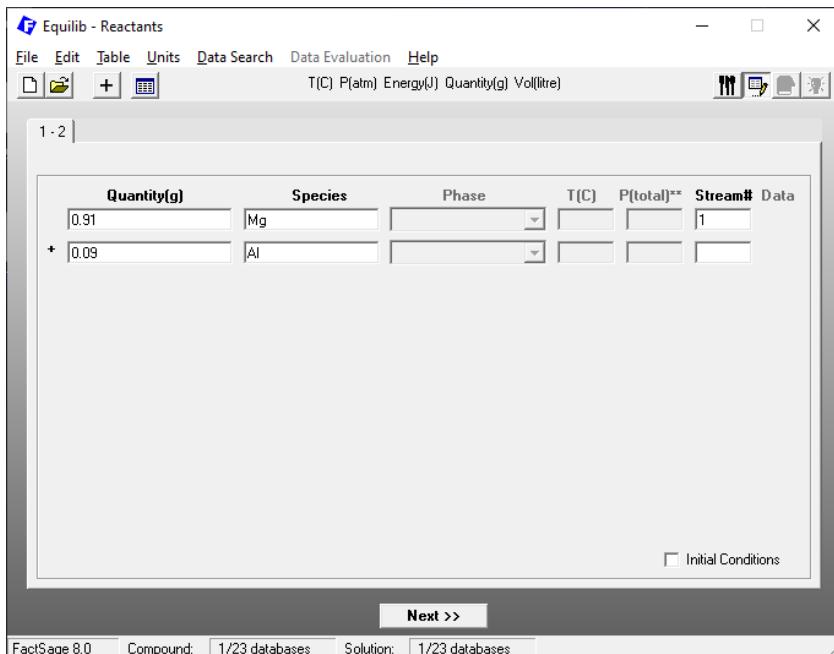
EX2. Target calculations

(a) Transitions (EX2-1):

do calculation between initial and final temperature and find all phase transition between them



EX2-1. Transition calculation



The screenshot shows the 'last system' window of FactSage 8.0. It displays the same composition as the previous window: (gram) 0.91 Mg + 0.09 Al. A 'Solution phases' table is shown, listing various crystal structures like Liquid, FCC-A1, BCC-A2, HCP-A3, etc. On the right side, there are several configuration options: 'Custom Solutions' (fixed activities, ideal solutions), 'Pseudonyms' (apply, edit), 'Volume data' (assume molar volumes of solids and liquids = 0, include molar volume data and physical properties data), and 'Equilibrium' settings (normal, normal + transitions, transitions only, open, no time limit, Calculate >>). Red dashed arrows point from the 'Final Conditions' section at the bottom left to the 'T(C)', 'P(atm)', and 'Product H(J)' fields, and from the 'Equilibrium' section to the 'Calculate >>' button.

Range of temperature: “initial final interval”
Calculate Initial (0 °C) to final (700°C) temperature with interval of 10 °C

Equilib - Results 300 C (page 31/74)

Output Edit Show Pages Final Conditions

	T(C)	P(atm)	Energy(J)	Quantity(g)	Vol(litre)					
460 C	470 C	476.56 C								
360 C	370 C	377.22 C	380 C	390 C	400 C	410 C	420 C	430 C	440 C	450 C
250 C	260 C	270 C	280 C	290 C	- 300 C -	310 C	320 C	330 C	340 C	350 C

(gram) 0.91 Mg + 0.09 Al = *input composition*

```

0.91744 gram HCP-A3#1
(0.91744 gram, 1.8759E-02 mol)
+ 0 gram HCP-A3#2
    (300 C, 1 atm, a=1.0000)
    ( 6.0939 wt.% Al2Va
    + 93.906 wt.% Mg2Va)

System component      Amount/mol      Amount/gram      Mole fraction      Mass fraction
Al                  2.0721E-03      5.5907E-02      5.5227E-02      6.0939E-02
Mg                  3.5447E-02      0.86153          0.94477          0.93906

+ 8.2560E-02 gram CBCC-Al12#1
(8.2560E-02 gram, 5.6167E-05 mol)
+ 0 gram CBCC-Al12#2
    (300 C, 1 atm, a=1.0000)
    ( 3.6736 wt.% Mg10Al24Al24
    + 0.39068 wt.% Mg10Al24Mg24
    + 86.552 wt.% Mg10Mg24Al24
    + 9.3755 wt.% Mg10Mg24Mg24)

Site fraction of sublattice constituents:
Mg_2a+8c           1.0000      Stoichiometry = 10
-----
Al_24g              3.9081E-02  Stoichiometry = 24
Mg_24g              0.96092
-----
Al_24g              0.09826     Stoichiometry = 24
Mg_24g              0.10174
-----
System component      Amount/mol      Amount/gram      Mole fraction      Mass fraction
Al                  1.2636E-03      3.4093E-02      0.38787      0.41294
Mg                  1.9941E-03      4.8468E-02      0.61213      0.58706

```

Final Conditions

<A>		T(C)	P(atm)	Product H(J)	71+ calculations
		070010	1		X
+ 0	+ 0				

Calculate >

Calculation results at every 10 °C intervals

What is this complex thing ?
-> model structure in database
-> output for modeling people

elemental composition of CBCC-Al12 (gamma Mg17Al12) phase

Phase transition happens at this temperature

(gram) 0.91 Mg + 0.09 Al =

1.0000 gram HCP-A3#1
(1.0000 gram, 2.0388E-02 mol)
+ 0 gram HCP-A3#2
(377.22 C, 1 atm, a=1.0000)
(9.0000 wt.% Al2Va
+ 91.000 wt.% Mg2Va)

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Al	3.3356E-03	9.0000E-02	8.1802E-02	9.0000E-02
Mg	3.7441E-02	0.91000	0.91820	0.91000

+ 0 gram CBCC-Al2#1
+ 0 gram CBCC-Al2#2
(377.22 C, 1 atm, a=1.0000)
(6.4107 wt.% Mg10Al24Al24
+ 1.0638 wt.% Mg10Al24Mg24
+ 79.379 wt.% Mg10Mg24Al24
+ 13.147 wt.% Mg10Mg24Mg24)

Site fraction of sublattice constituents:
Mg_2a+8c 1.0000 Stoichiometry = 10

Al_24g 7.1830E-02 Stoichiometry = 24
Mg_24g 0.92817

Al_24g 0.05239 Stoichiometry = 24
Mg_24g 0.14761

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Al	0	0	0.38244	0.40740
Mg	0	0	0.61756	0.59260

Final Conditions

<A>		T(C)	P(atm)	Product H(J)	71+ calculations	X
		070010	1			Calculate >

Although the amount of Gamma phase is zero, the activity (a = 1) tells Gamma phase begins to form at this temperature

If formed, this is composition

EX2-2. Precipitation target calculation

The screenshot shows the FactSage software interface. On the left, the 'Reactants' window displays input fields for quantity (0.91 Mg and 0.09 Al) and phase selection. The 'Products' window lists compound species (gas, ideal, real, aqueous, pure liquids, pure solids) and solution phases. A red dashed circle highlights the 'Precipitate Target' section, which includes a dropdown for 'Base-Phase' (set to 'FTlite-Liqu'), an 'Estimate T(C)' input field (set to 1000), and a 'Quantity(g)' input field (set to 0). Another red dashed circle highlights the 'Final Conditions' section, specifically the 'T(C)' input field (set to 1). A red box labeled 'automatic default estimated value' surrounds the 'Estimate T(C)' field.

For target calculation, this temperature should remain blank

automatic default estimated value

*	+ Base-Phase	Full Name
*	IP	FTlite-Liqu
+	T	FTlite-A1
I	FTlite-A2	FCC-A1
I	FTlite-A3	BCC-A2
I	FTlite-A12	HCP-A3
I	FTlite-L12	CBCC-A12 Prototype-Mn
+	FTlite-L12	L12 Prototype-AuCu3
+	FTlite-Beta	Beta Prototype-Mg28Al45

Legend:
I - immiscible 6
P - precipitate target
+ - selected 1

Show all selected
species: 30 solutions: 13 Select

Total Species (max 5000) 49
Total Solutions (max 200) 13
Total Phases (max 1500) 32

Equilibrium
 normal normal + transitions
 transitions only open
- no time limit - Calculate >

Liquid is selected as precipitation target phase (P). Then, FactSage will calculate **liquidus temperature** of a given composition

EX2-3. Formation target calculation

The screenshot shows two FactSage windows. The left window, 'Reactants - Equilib', displays mass inputs for Mg (0.91 g) and Al (0.09 g). The right window, 'Menu - Equilib: Target-Formation: Mg-Al', shows the resulting equilibrium phases: Liquid, FCC_A1, HCP_A3, BCC_A2, Laves_C14, Laves_C15, and Beta_AlMg. A red dashed circle highlights the 'Formation Target' section where 'FTlite-Liqu' is selected as the target phase, and a temperature of 1000°C is estimated. Another red dashed circle highlights the 'Conditions' section where the temperature input field is blank.

automatic default estimated value

For target calculation, this temperature should remain blank

Liquid is selected as formation target phase (F). Then, FactSage will calculate **solidus temperature** of a given composition

EX3. Variation of phase fraction with temperature (equilibrium)

Equilib - Reactants

File Edit Table Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

1 - 2

Quantity(g) Species Phase

0.91 Mg + 0.09 Al

Next >

FactSage 8.0 Compound: 1/23 databases Solution: 1/23 databases

Equilib - Menu: comments

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (2)

(gram) 0.91 Mg + 0.09 Al

Products

Compound species

gas	<input checked="" type="radio"/> ideal	<input type="radio"/> real	0
aqueous			0
pure liquids			0
+ pure solids			19
species: 19			

Transitions - temperature

Number of transitions: All

Solution phases

*	+	Base-Phase	Full Name
I		FTlite-Liqu	Liquid
I		FTlite-A1	FCC-A1
I		FTlite-A2	BCC-A2
I		FTlite-A3	HCP-A3
I		FTlite-A12	CBCC-A12 Prototype-Mn
I		FTlite-L12	L12 Prototype-AuCu3
+		FTlite-Beta	Beta Prototype-Mg28Al45

Legend
I - immiscible 6
+ - selected 1

Show all selected

species: 30 solutions: 13 Select

Custom Solutions

0 fixed activities
0 ideal solutions

Pseudonyms apply Edit ...

Volume data

assume molar volumes of solids and liquids = 0
 include molar volume data and physical properties data

paraequilibrium & Gmin edit

Total Species (max 5000) 49
Total Solutions (max 200) 13
Total Phases (max 1500) 32

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		700 200 10	1	
10 steps	<input type="checkbox"/> Table	51+ calculations		

Equilibrium

normal normal + transitions
 transitions only open
- no time limit - Calculate >

FactSage 8.0 C:\Workshop80\Workshop\ex3.equi

Transition calculation from 700°C to 200°C with 10°C interval

Equilib - Results 700 C (page 1/54)

Output Edit Show Pages Final Conditions

Save or Print As ... T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Plot Plot Results ... 120 C | 510 C | 500 C | 610 C | 600 C | FactSage 8.0

Equilib Results file Repeat Plot - ...

Stream File Format

Fact-XML

Fact-Optimal #1 mol

Fact-Function-Builder #2 a=1.0000 Al Mg

Refresh ... Swap loops ...

3.3356E-03 9.0000E-02 8.1802E-02 9.0000E-02

3.7441E-02 0.91000 0.91820 0.91000

+ 0 gram HCP-A3#1
+ 0 gram HCP-A3#2
(700 C, 1 atm, a=0.88858)
(3.0308 wt.% Al2Va
+ 96.969 wt.% Mg2Va)

+ 0 gram BCC-A2#1

Result Processor: C:\Workshop80\Workshop\Equi0.res

File Help

0.91 Mg + 0.09 Al

Axes	Variables	Minimum	Maximum
activity	0	1	
mole	0	4.0776E-02	
mole fract. soln. species	0	0.98918	
gram	0	1	
weight % soln. species	0	98.8	
Alpha	0	0	
T(C)	200	700	
P(atm)	1	1	
Cp(J/K)	1.1709	7.7022	
G(J)	-1929	-696.86	
Vol(litre)	0	0	
H(J)			
V(litre)			
S(J/K)			
- page -	1	54	

(2) Click to setup axes

(4) Select the phase to plot

(3) Click to select X, Y axes

(3) Click to select X, Y axes

Activity mole mole fract. soln. species

gram

Y-axis: gram vs T(C)

X-variable Y-variable Swap Axes

Y-axis: gram

maximum: 1
minimum: 0
tick every: .1

X-axis: T(C)

maximum: 700
minimum: 200
tick every: 50

Y log(Y) ln(Y) exp(Y) 1/Y phase distribution

**Selection of phases
(All stable phases option)**

(5) Selection of phases (All stable phases option)

Plot Species Selection - Equilib Results: gram vs T(C)

File Show Select

#	Species	Mole (min)	Mole (max)	Fraction (min)	Fraction (max)	Activity (min)	Activity (max)
50	GAS	0	0	0	0	0	0
51	LiqH1	0	4.0776E-02	0	0	0.486695	1
52	LiqH2	0	0	0	0	0.486695	1
53	A1#1	0	0	0	0	0.63085	0.806656
54	A1#2	0	0	0	0	0.63085	0.806656
55	A2#1	0	0	0	0	0.576269	0.832095
56	A2#2	0	0	0	0	0.576269	0.832095
57	A3#1	0	2.0388E-02	0	0	0.889578	1
58	A3#2	0	0	0	0	0.889578	1
59	A12#1	0	1.0467E-04	0	0	3.9219E-11	1
		0	0	0	0	0.146709	0.557871
		0	0	0	0	0.146709	0.557871
		0	0	0	0	1.1595E-20	1.3950E-04

Select all stable phases
Select stable pure liquids
Select stable pure solids
Select stable solution phases
Clear

Display: color, reactants, file name, offset
Labels: size 9, no: 4
Graph: full screen, viewer, figure
Plot >>

Display: source, phase, name, [page]
Mass: mole, gram
Order: integer #, mass (max), fraction (max), activity (max)
Select Top: 15, 3 species selected
Ignore species and phases with zero mass
Select... OK
54 pages

Click to setup axes

Select all stable phases
 Select stable pure liquids
 Select stable pure solids
 Select stable solution phases
 Clear

Special care is required for the phase selection

A simple way is click “Select all stable phases”
 Then, FactSage will select all phases having activity = 1

Plot Species Selection - Equilib Results: vs

File Show Select

+	#	Species	Mole (min)	Mole (max)	Fraction (min)	Fraction (max)	Activity (min)	Activity (max)
Pure Solids								
31	Mg	0	0	0	0	0.864403	0.977341	
32	Mg	0	0	0	0	0.856503	0.966681	
33	Mg	0	0	0	0	0.560324	0.760395	
34	Mg	0	0	0	0	0.57nnn1	0.819915	
35	Mg	0	0	0	0			
36	Mg	0	0	0	0			
37	Mg	0	0	0	0			
38	Al	0	0	0	0			
39	Al	0	0	0	0			
40	Al	0	0	0	0			
41	Al	0	0	0	0			
42	Al	0	0	0	0			
43	Al	0	0	0	0			
44	Al	0	0	0	0			
45	Al	0	0	0	0			
46	Al	0	0	0	0			
47	AlMg	0	0	0	0			
48	Al3Mg	0	0	0	0			
49	Al30Mg23	0	0	0	0			
SOLUTIONS								
50	GAS	0	0	0	0			
51	Liqu#1	0	4.0776E-02	0	0			
52	Liqu#2	0	0	0	0	0.486635	1	
53	A1#1	0	0	0	0	0.63085	0.806656	
54	A1#2	0	0	0	0	0.63085	0.806656	
55	A2#1	0	0	0	0	0.576269	0.832085	
56	A2#2	0	0	0	0	0.576269	0.832085	
57	A3#1	0	2.0388E-02	0	0	0.888578	1	

Display Mass Order
 source mole integer #
 phase gram mass (max)
 name fraction (max)
 [page] activity (max)
 54 pages Select Top 15 0 species selected
 ignore species and phases with zero mass
 Select ... OK
 Click on the '+' column to add or remove species.

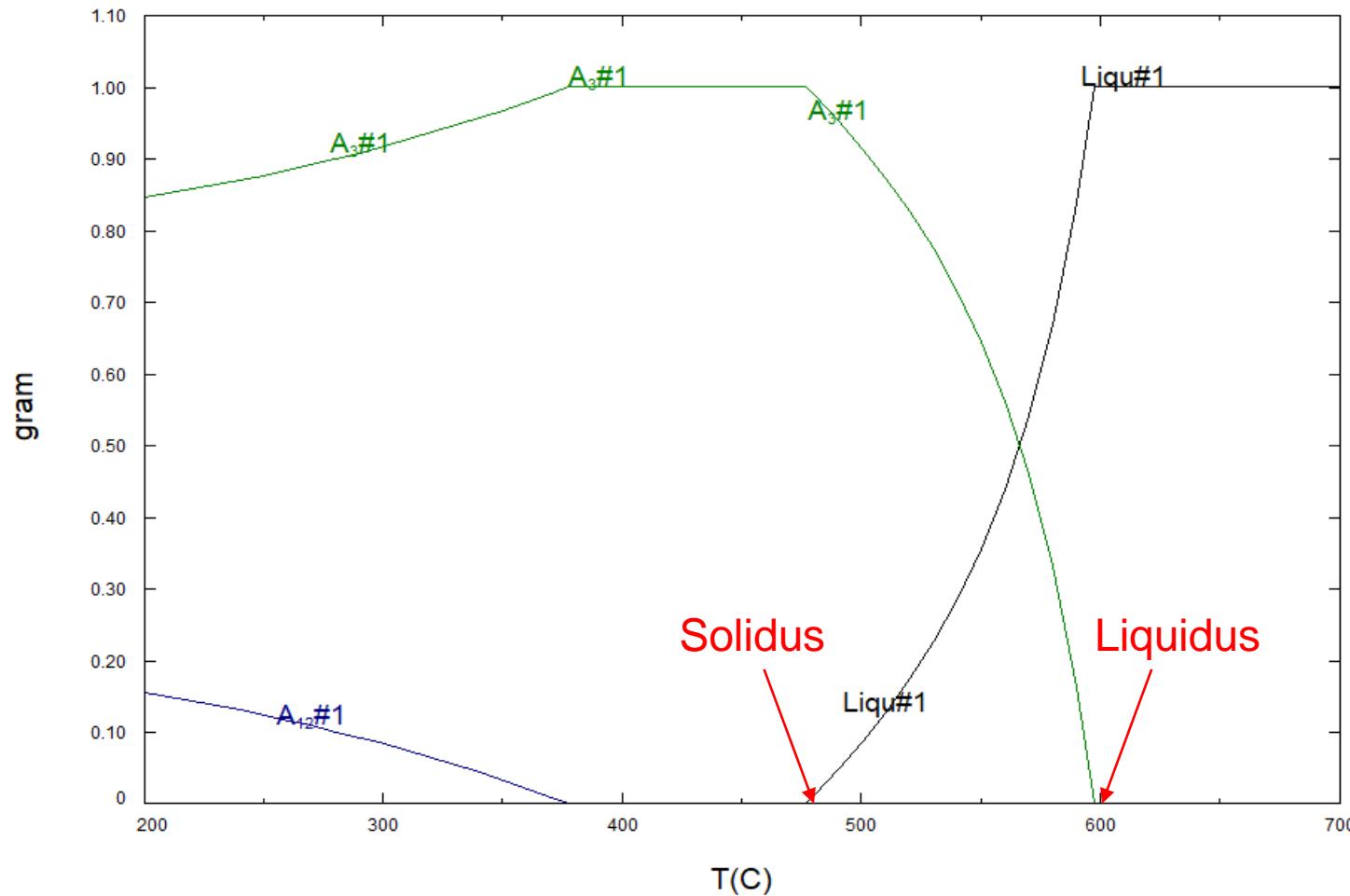
Manual selection

Tip for
 “phase fraction vs. temperature diagram”

All phases which have amount > 0 in “Pure Solids”
 and “SOLUTIONS” should be selected.

0.91 Mg + 0.09 Al

C:\Workshop80\Workshop\Equi0.res 19Dec19



Plot Species Selection - Equilib Results: gram vs T(C)

File Show Select

+	#	Species	Mole (min)	Mole (max)	Fraction (min)	Fraction (max)	Activity (min)	Activity (max)
ELEMENTS								
64		Al_GAS	0	0	0	0	0	0
65		Mg_GAS	0	0	0	0	0	0
66		Al_Liq#1	0	3.3356E-03	0	0.244638	0	0
67		Mg_Liq#1	0	3.7441E-02	0	0.918198	0	0
68		Al_Liq#2	0	0	0	0	0	0
69		Mg_Liq#2	0	0	0	0	0	0
70		Al_A1#1	0	0	0	0	0	0
71		Mg_A1#1	0	0	0	0	0	0
72		Al_A1#2	0	0	0	0	0	0
73		Mg_A1#2	0	0	0	0	0	0
74		Al_A2#1	0	0	0	0	0	0
75		Mg_A2#1	0	0	0	0	0	0
76		Al_A2#2	0	0	0	0	0	0
77		Mg_A2#2	0	0	0	0	0	0
78		Al_A3#1	0	3.3356E-03	0	8.1802E-02	0	0
79		Mg_A3#1	0	3.7441E-02	0	0.973952	0	0

Display **Mass** **Order** **Select Top** 15 **0 species selected**

source mole integer # mass (max)

phase name [page]

ignore species and

Clear

Click on the '+' column to add or remove species.

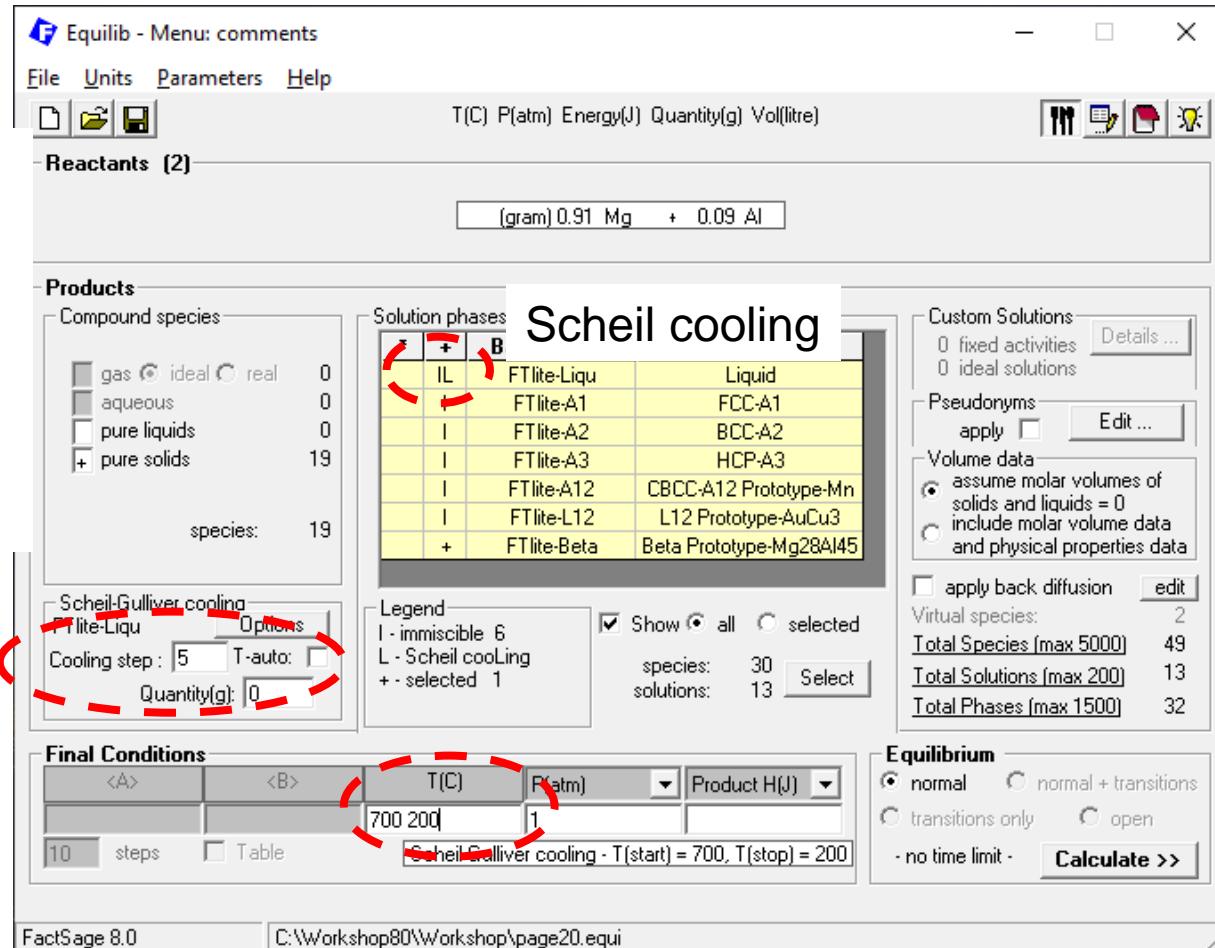
If we want to plot the compositional variation inside of solution phases, we have to select the elements in this “ELEMENTS” section.

For example, if we want to plot the variation of Al and Mg concentrations in liquid phase with temperature, we have to select Al_Liq#1 and Mg_Liq#1.

EX4. Variation of phase fraction with temperature (Scheil cooling)

Cooling step: In most of cases, 5 degree is enough to simulate solidification process

This cooling step is not directly related to solidification rate (cooling speed)

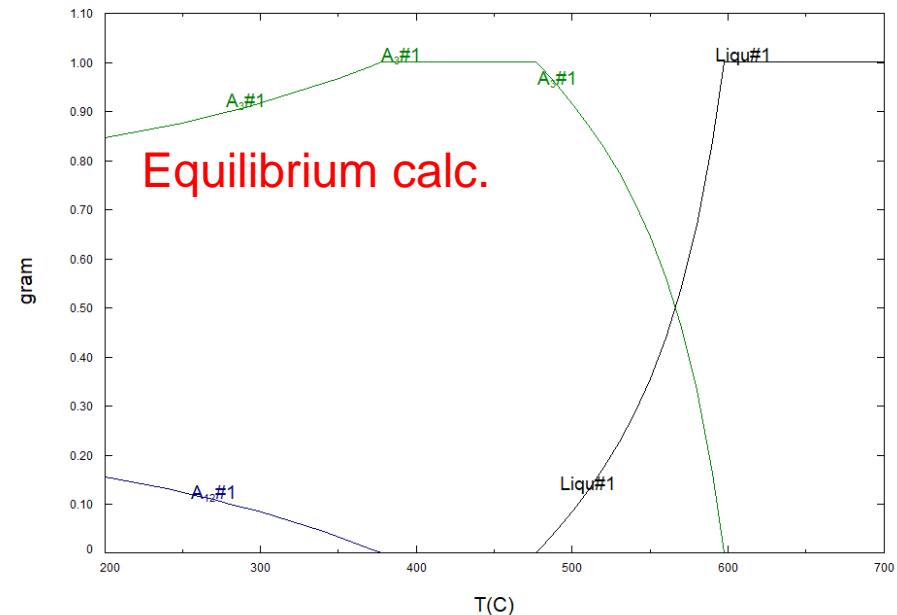


Temperature:

- starting temperature and final temperature
- starting temperature: program will automatically calculate the final solidification temperature

0.91 Mg + 0.09 Al

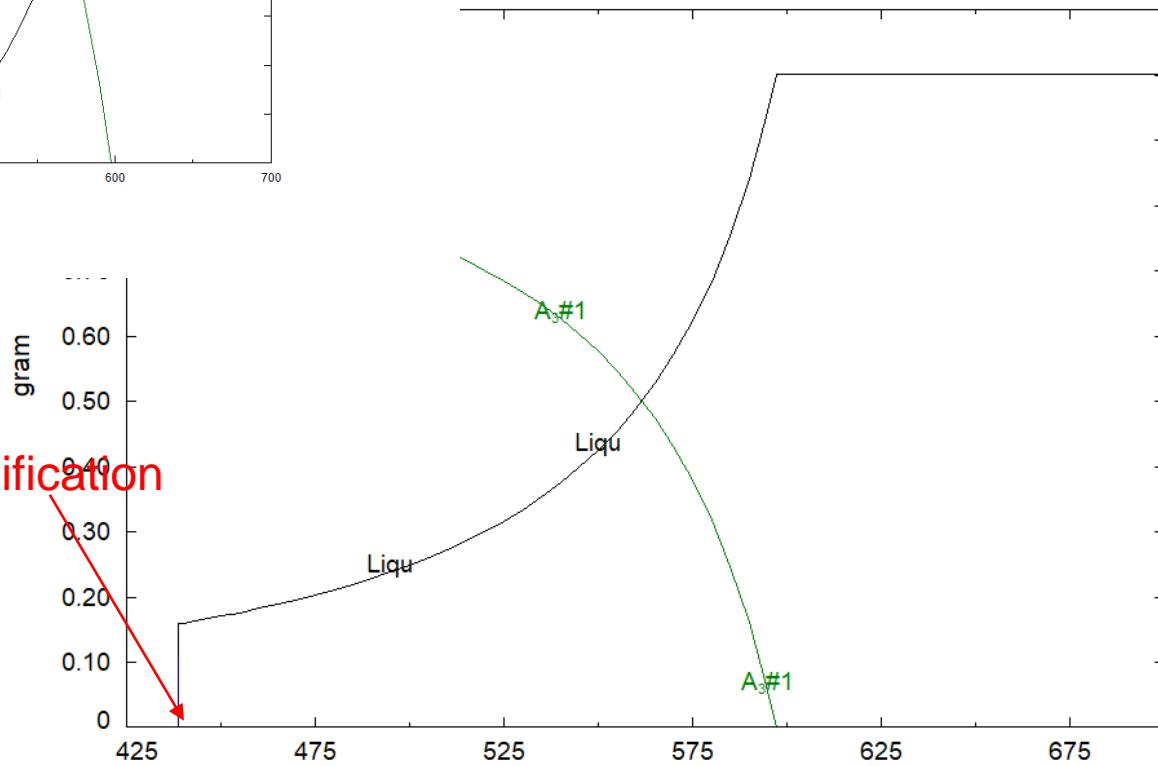
C:\Workshop80\Workshop\Equi0.res 19Dec19



Scheil cooling calc.

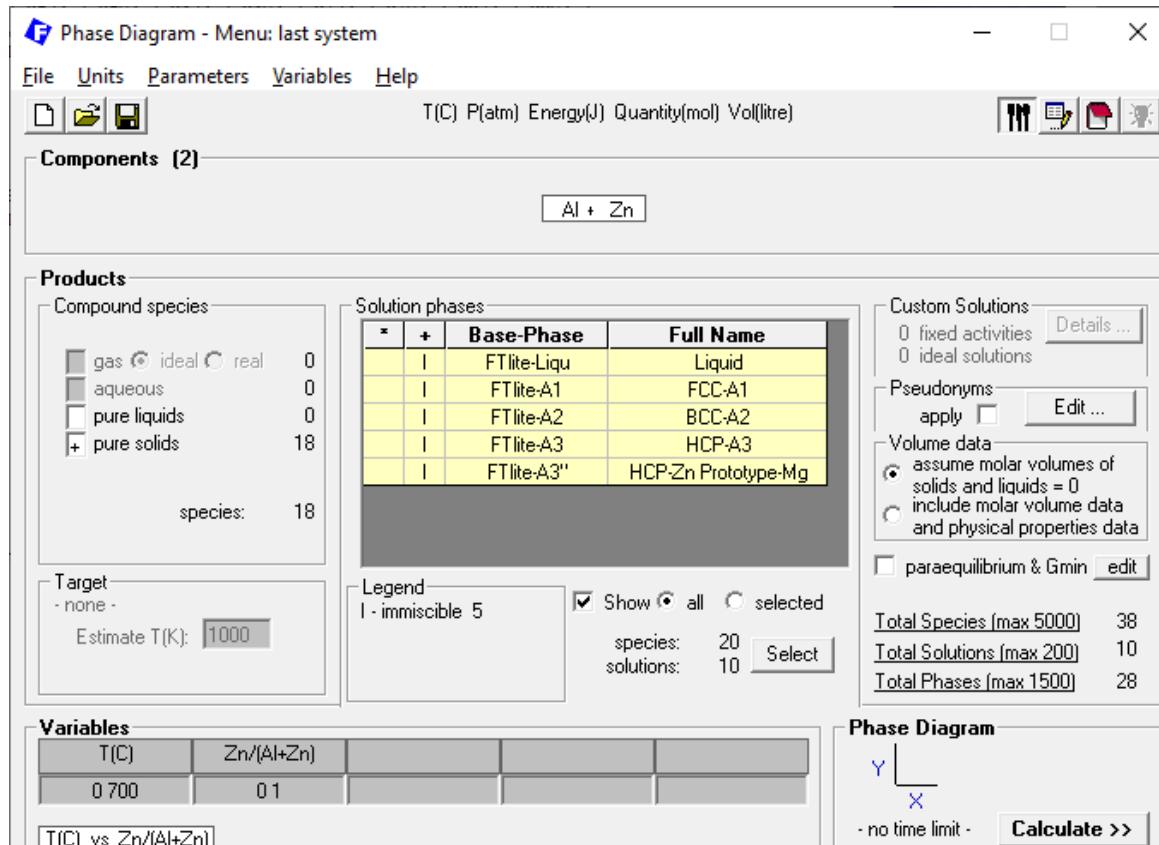
0.91 Mg + 0.09 Al

C:\Workshop80\Workshop\Equi0.res 19Dec19



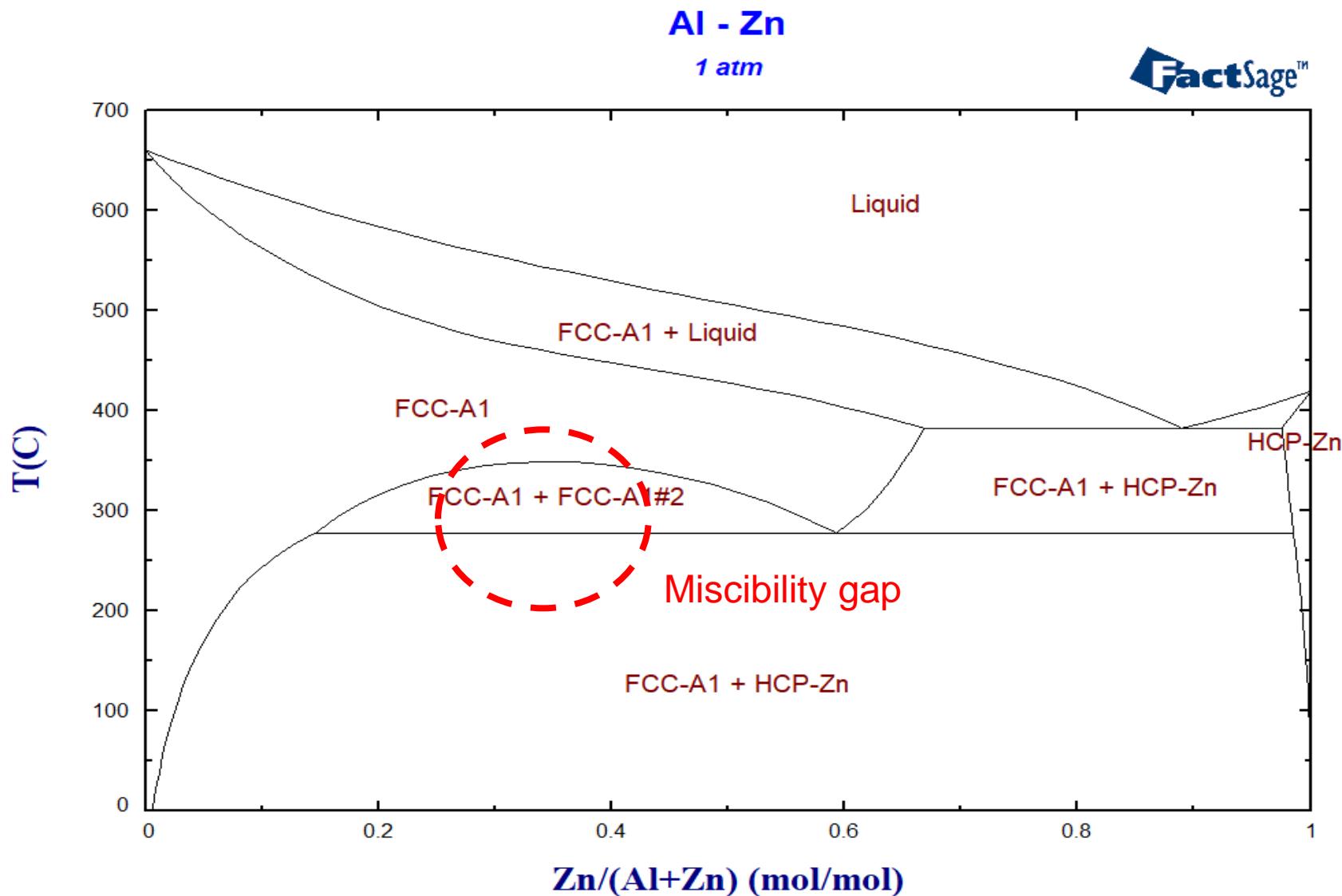
Scheil cooling calculation is terminated when liquid phase disappears

EX5. I option (miscibility gap)



"I" Option: when the phase has a miscibility gap (solid state or liquid state phase separation), I option should be selected to do more accurate calculations (most cases, I option will be automatically selected).

For example, fcc phase in Al-Zn system has a solid state miscibility gap as in this example. Liquid oxide slag has a miscibility gap in the high SiO₂ region.



EX6. Isothermal Ternary phase diagram: Mg-Al-Zn

Phase Diagram - Components

File Edit Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

1 - 3

Components

- Mg
- Al
- Zn

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Components (3)

(gram) Mg + Al + Zn

Products

Compound species	Base-Phase	Full Name
gas (ideal real	FTlite-Liqu	Liquid
aqueous	FTlite-A1	FCC-A1
pure liquids	FTlite-A2	BCC-A2
+ pure solids	FTlite-A3	HCP-A3
	FTlite-A3"	HCP-Zn Prototype-Mg
	FTlite-A12	CBC-A12 Prototype-Mn
	FTlite-C14	C14 Prototype-MgZn2
	FTlite-C36	C36 Prototype-MgNi2

species: 35

Target
- none -
Estimate T(K): 1000

Legend
I - immiscible 9
+ - selected 6

Show all selected

species: 118
solutions: 24 Select

Variables

Y	X	compositions
a	b	2
c	d	
A	C	
B		
X,Y steps	11	

T and P

Temperature: T(C) constant 400

Pressure or Volume: P(atm) constant 1

Compositions Quantity(g)

#1. $1 \text{ Mg} + 0 \text{ Al} + 0 \text{ Zn} = 1 \text{ (max)} \\ 1 \text{ Mg} + 1 \text{ Al} + 1 \text{ Zn} = 0 \text{ (min)}$

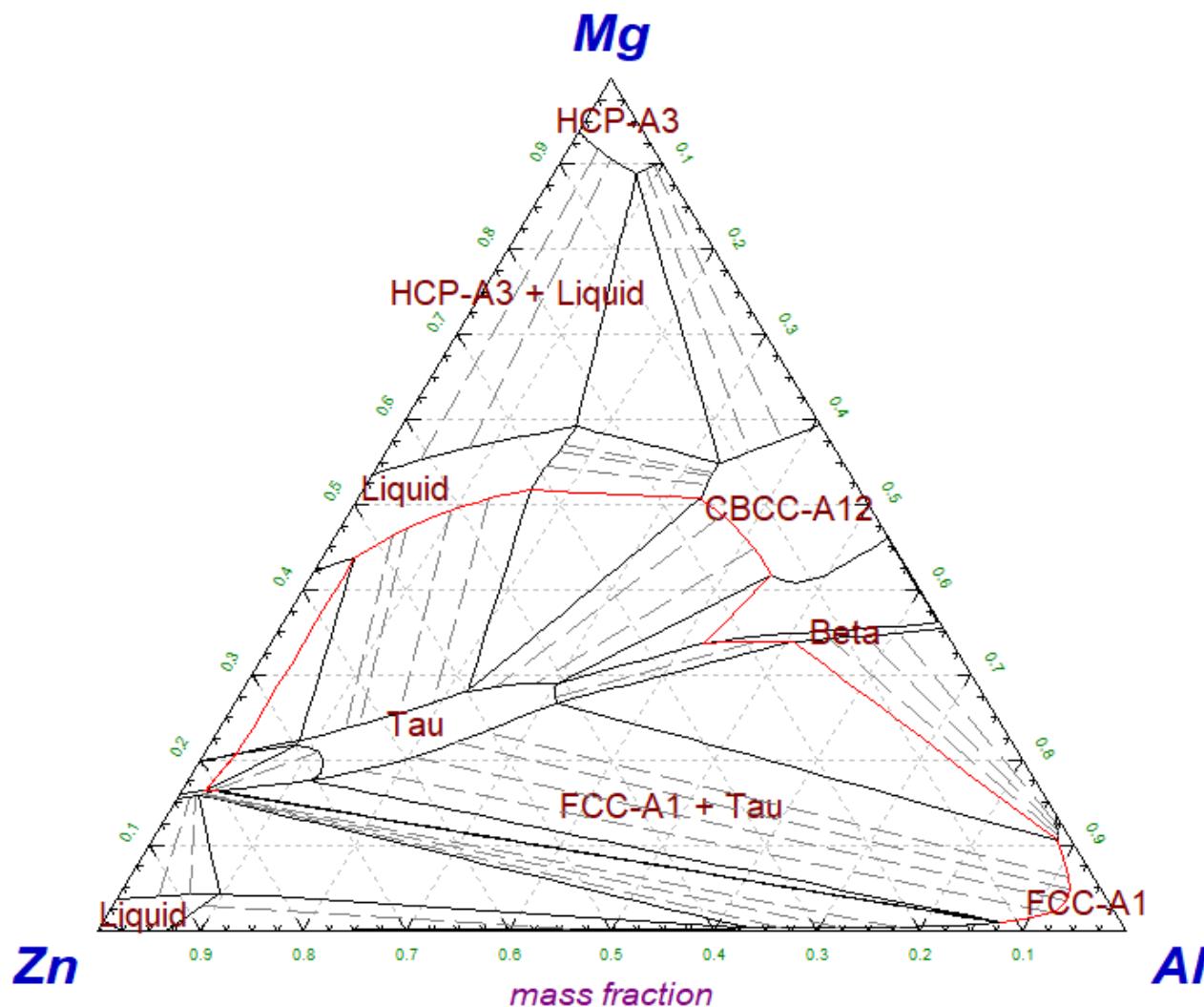
#2. $0 \text{ Mg} + 1 \text{ Al} + 0 \text{ Zn} = 1 \text{ (max)} \\ 1 \text{ Mg} + 1 \text{ Al} + 1 \text{ Zn} = 0 \text{ (min)}$

#3. $0 \text{ Mg} + 0 \text{ Al} + 1 \text{ Zn} = 1 \text{ (max)} \\ 1 \text{ Mg} + 1 \text{ Al} + 1 \text{ Zn} = 0 \text{ (min)}$

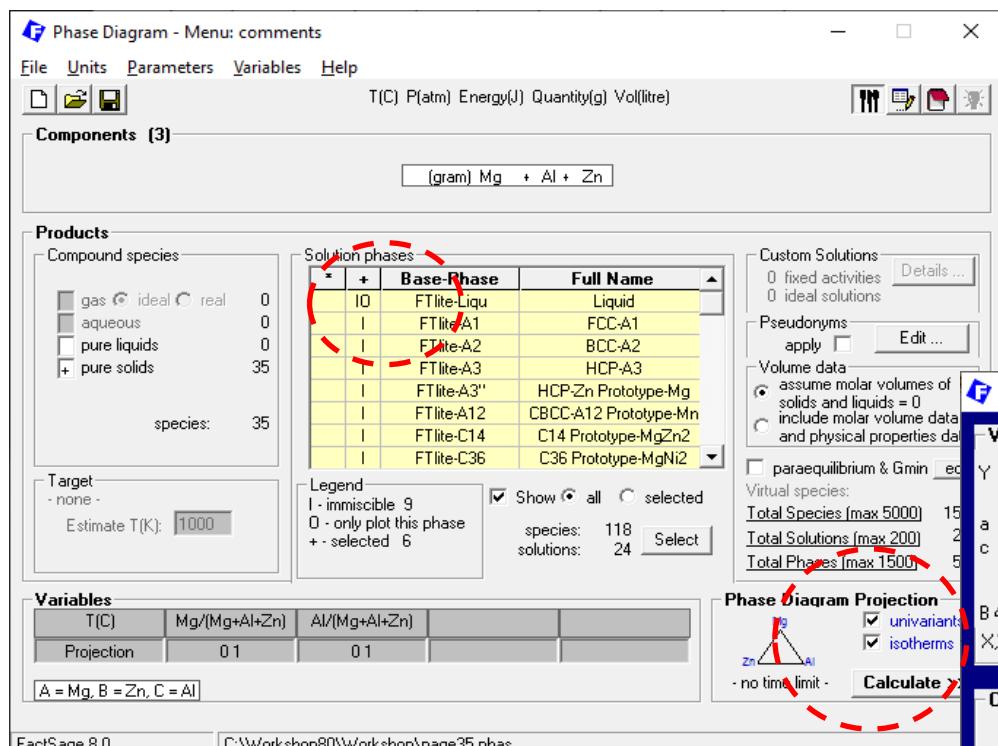
Cancel **OK**

Mg - Al - Zn

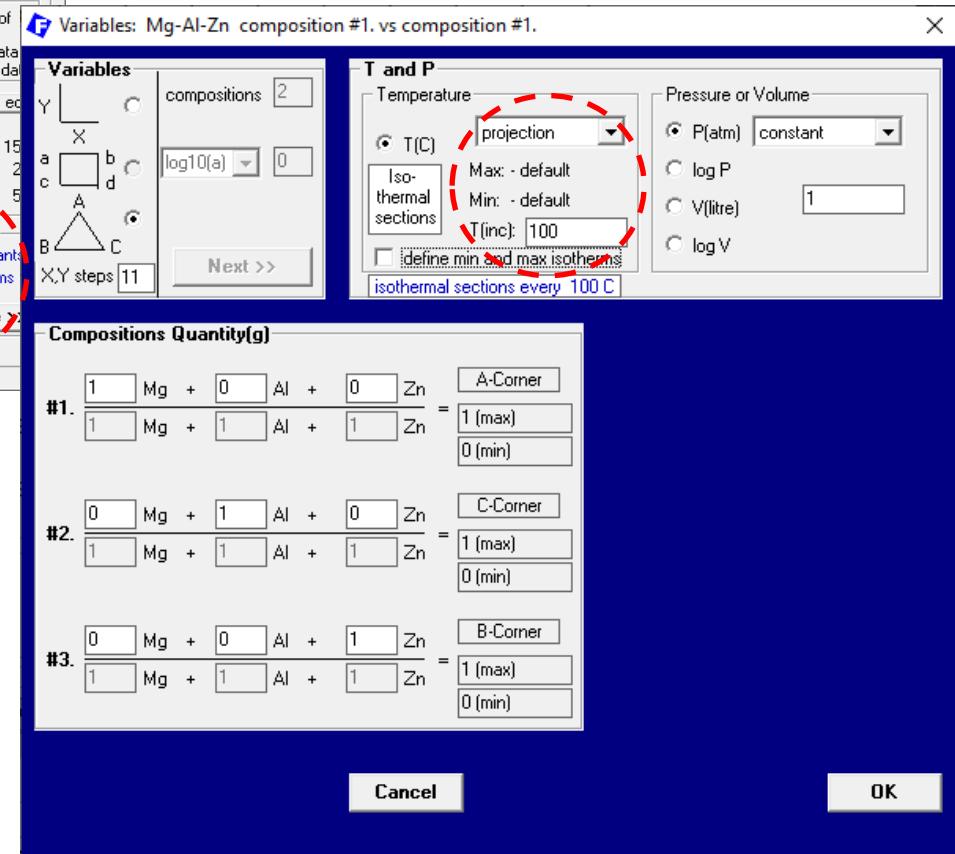
400°C, 1 atm



EX7. Projection calculation (Liquidus projection): Mg-Al-Zn



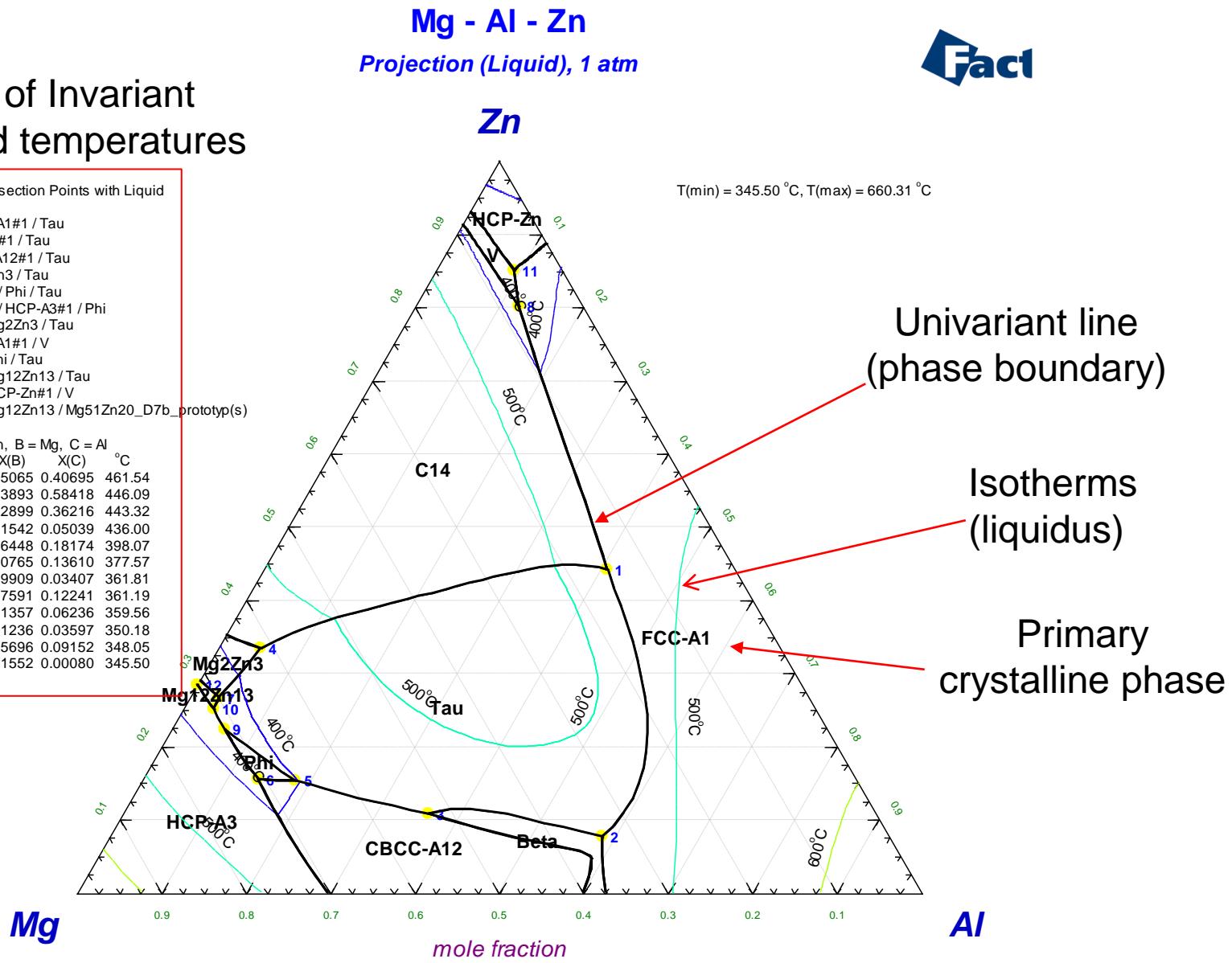
Step: interval of isothermal temperature liquidus lines



"O" option for the target projection phase
(Liquid in most of cases)

Summary of Invariant reactions and temperatures

Four-Phase Intersection Points with Liquid				
1:	C14#1 / FCC-A1#1 / Tau			
2:	Beta / FCC-A1#1 / Tau			
3:	Beta / CBCC-A12#1 / Tau			
4:	C14#1 / Mg2Zn3 / Tau			
5:	CBCC-A12#1 / Phi / Tau			
6:	CBCC-A12#1 / HCP-A3#1 / Phi			
7:	Mg12Zn13 / Mg2Zn3 / Tau			
8:	C14#1 / FCC-A1#1 / V			
9:	HCP-A3#1 / Phi / Tau			
10:	HCP-A3#1 / Mg12Zn13 / Tau			
11:	FCC-A1#1 / HCP-Zn#1 / V			
12:	HCP-A3#1 / Mg12Zn13 / Mg51Zn20_D7b_prototyp(s)			
A = Zn, B = Mg, C = Al				
X(A) X(B) X(C) °C				
1:	0.44240	0.15065	0.40695	461.54
2:	0.07688	0.33893	0.58418	446.09
3:	0.10884	0.52899	0.36216	443.32
4:	0.33419	0.61542	0.05039	436.00
5:	0.15378	0.66448	0.18174	398.07
6:	0.15625	0.70765	0.13610	377.57
7:	0.26684	0.69909	0.03407	361.81
8:	0.80168	0.07591	0.12241	361.19
9:	0.22407	0.71357	0.06236	359.56
10:	0.25166	0.71236	0.03597	350.18
11:	0.85152	0.05696	0.09152	348.05
12:	0.28368	0.71552	0.00080	345.50



EX8. Scheil cooling calculation for AZ31 alloy (Mg-3Al-1Zn-0.3Mn)

Equilib - Menu: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (4)

(gram) 95.7 Mg + 3 Al + Zn + 0.3 Mn

Products

Compound species:

- gas ideal real 0
- aqueous 0
- pure liquids 0
- + pure solids 49

species: 49

Scheil-Gulliver cooling

FTlite-Liqu Options

Cooling step: 25 T-auto:

Quantity(g): 0

Solution phases

-	+	Base-Phase	Full Name
IL	FTlite-Liqu	Liquid	
I	FTlite-A1	FCC-A1	
I	FTlite-A2	BCC-A2	
I	FTlite-A3	HCP-A3	
I	FTlite-A3"	HCP-Zn Prototype-Mg	
I	FTlite-A12	CBCC-A12 Prototype-Mn	
I	FTlite-A13	CUB-A13 Prototype-Mn	
I	FTlite-B2_d	BCC-B2d!BCC-A2	

Legend

- I - immiscible 12
- L - Scheil cooling
- + - selected 10

Show all selected

species: 258

solutions: 34 Select

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		700 100	1	

10 steps Table

Scheil-Gulliver cooling - T(start) = 700, T(stop) = 100

Custom Solutions

- 0 fixed activities
- 0 ideal solutions

Pseudonyms

- apply Edit

Volume data

- assume molar volume solids and liquids = 0
- include molar volume and physical properties

Equilibrium

- normal normal + transitions
- transitions only open
- no time limit -

Calculations

Equilib - Results 700 C (page 1/56)

Output Edit Show Pages Final Conditions

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

359.55 C | 357.05 C | 354.39 C |
 525 C | 500 C | 487.86 C | 475 C | 458.62 C | 450 C | 425 C | 415.28 C | 400 C | 377.56 C | 375 C |
 Summary | Transitions - 700 C - | 675 C | 650 C | 629.71 C | 625 C | 616.51 C | 600 C | 575 C | 550 C |

FactSage 8.0

(gram) 95.7 Mg + 3 Al + Zn + 0.3 Mn = [Accumulated Scheil]

100.00 gram Liquid#1
 (100.00 gram, 4.0694 mol)
 + 0 gram Liquid#2
 (700 C, 1 atm, a=1.0000)
 (3.0000 wt.% Al
 + 95.700 wt.% Mg
 + 0.30000 wt.% Mn
 + 1.0000 wt.% Zn)

System component Amount/mol Amount/gram Mole fraction Mass fraction
 Zn 1.5295E-02 1.0000 3.7586E-03 1.0000E-02
 Mn 5.4607E-03 0.30000 1.3419E-03 3.0000E-03
 Al 0.11119 3.0000 2.7323E-02 3.0000E-02
 Mg 3.9375 95.700 0.96758 0.95700

+ 0 gram HCP-A3#1
 + 0 gram HCP-A3#2
 (700 C, 1 atm, a=0.92264)
 (0.92266 wt.% Al2Va
 + 98.724 wt.% Mg2Va
 + 0.25767 wt.% Mn2Va
 + 9.5722E-02 wt.% Zn2Va)

+ 0 gram HCP-Zn#1
 + 0 gram HCP-Zn#2
 (700 C, 1 atm, a=0.90926)
 (0.78607 wt.% Al
 + 99.098 wt.% Mg
 + 0.11584 wt.% Zn)

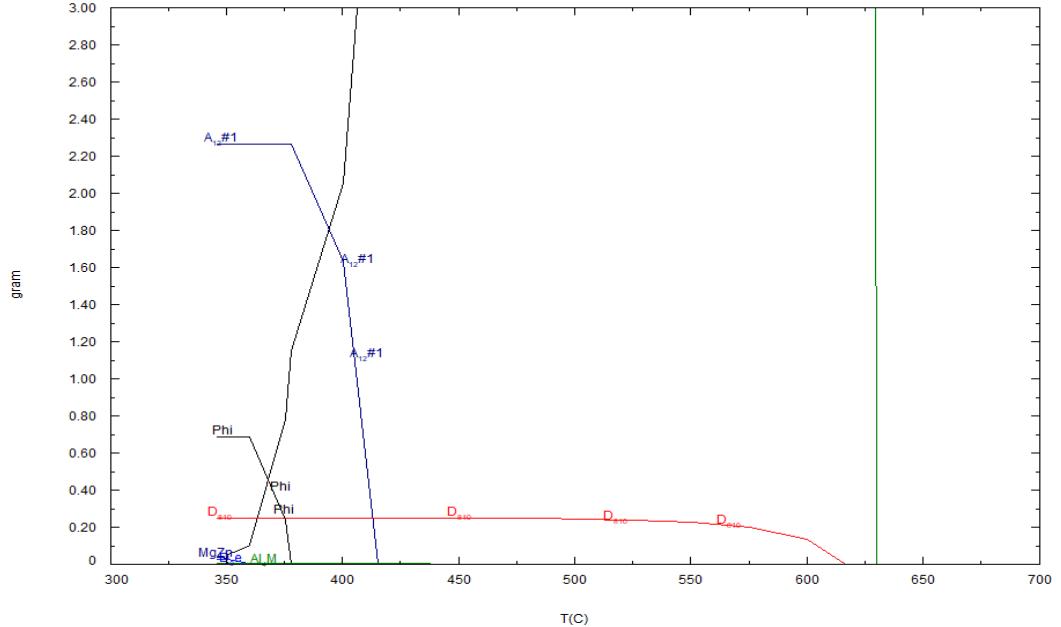
+ 0 gram BCC-A2#1
 (700 C, 1 atm, a=0.80869)

Final Conditions

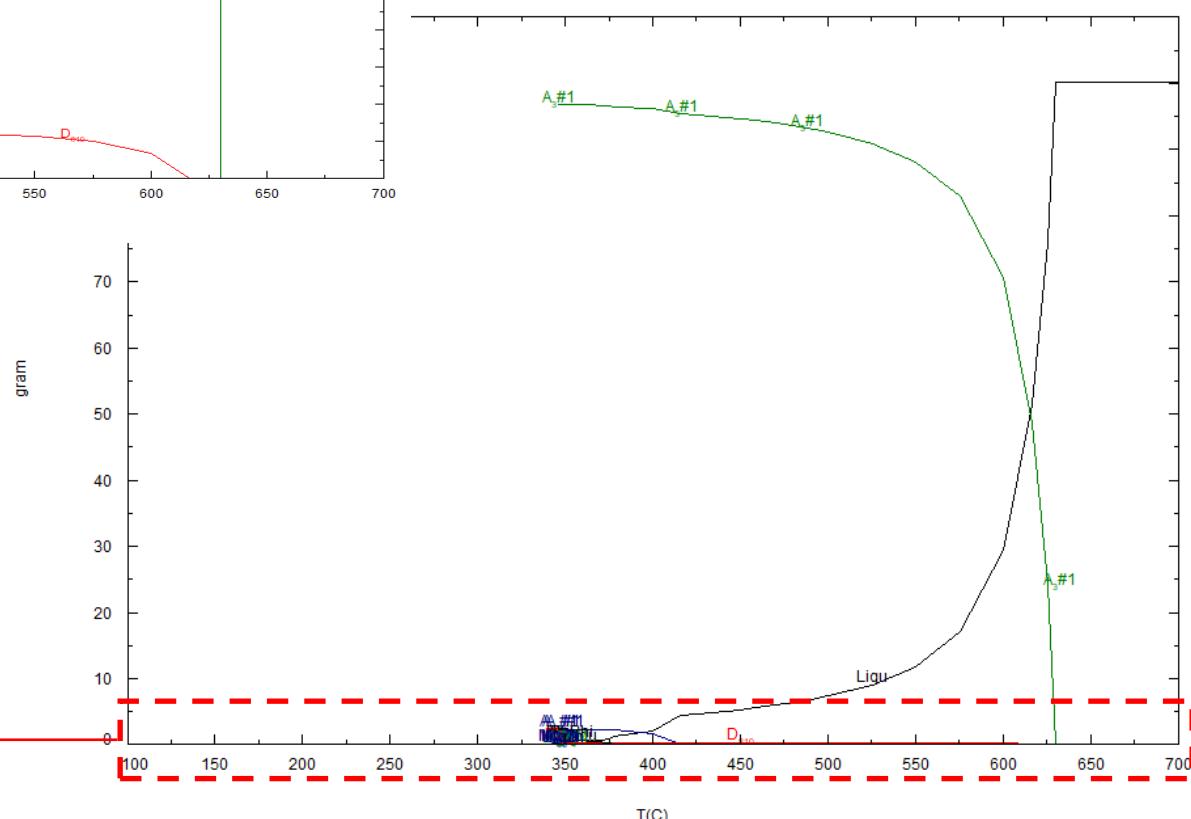
<A>		T(C)	P(atm)	Product H(J)
		700 100	1	

Deactivated for Scheil cooling

95.7 Mg + 3 Al + Zn + 0.3 Mn
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5.7 Mg + 3 Al + Zn + 0.3 Mn
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EX9. Equilibrium calculation for AZ31 alloy (Mg-3Al-1Zn-0.3Mn)

Equilib - Menu: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (4)

(gram) 95.7 Mg + 3 Al + Zn + 0.3 Mn

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- + pure solids 49

species: 49

Transitions - temperature

Number of transitions: All

Solution phases

*	+	Base-Phase	Full Name
		FTlite-Liqu	Liquid
		FTlite-A1	FCC-A1
		FTlite-A2	BCC-A2
		FTlite-A3	HCP-A3
		FTlite-A3"	HCP-Zn Prototype-Mg
		FTlite-A12	CBCC-A12 Prototype-Mn
		FTlite-A13	CUB-A13 Prototype-Mn
		FTlite-B2_d	BCC-B2d BCC-A2

Legend
I - immiscible 12
+ - selected 10

Show all selected

species: 258 solutions: 34 Select

Custom Solutions

- 0 fixed activities
- 0 ideal solutions

Pseudonyms

apply Edit ...

Volume data

- assume molar volumes of solids and liquids = 0
- include molar volume data and physical properties data

paraequilibrium & Gmin edit

Total Species (max 5000) 307
Total Solutions (max 200) 34
Total Phases (max 1500) 83

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		700 100 10	1	61+ calculations

10 steps Table

Equilibrium

normal normal + transitions
 transitions only open
 - no time limit - **Calculate >**

Equilib - Results Summary

Output Edit Show Pages Final Conditions

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

620 C | 616.76 C | 610 C | 600 C | 590 C | 580 C | 570 C | 560 C | 554.68 C |
- Summary - | Transitions | 700 C | 690 C | 680 C | 670 C | 660 C | 650 C | 640 C | 630 C | 629.71 C |

EQUILIBRIUM COOLING

COMPONENTS:

Mg	AMOUNT/gram = 9.5700E+01
Al	AMOUNT/gram = 3.0000E+00
Zn	AMOUNT/gram = 1.0000E+00
Mn	AMOUNT/gram = 3.0000E-01

CONSTITUENTS AND PHASES AT 554.68 C
(temperature of final disappearance of Liquid)

CONS. PHASE	TOTAL AMT/g.atom	TOTAL AMT/gram
1 1 HCP-A3	2.0452E+00	4.9878E+01
TOTAL:	2.0452E+00	4.9878E+01
2 1 HCP-A3	2.0137E+00	4.9703E+01
2 2 D810	1.0525E-02	4.1804E-01
TOTAL:	2.0242E+00	5.0122E+01

HCP-A3	TOTAL AMT/g.atom	TOTAL AMT/gram
D810	4.0589E+00	9.9582E+01
	1.0525E-02	4.1804E-01

('Double-Click' on any phase listed above to recycle it through EQUILIB)

SUMMARY OF REACTIONS

Cooling
700 to 629.71 C (DELTA H = -9.7757E+03 J)
Liquid cooling

Constituent 1
629.71 to 616.76 C (DELTA H = -1.8586E+04 J)
Liquid \rightarrow HCP-A3

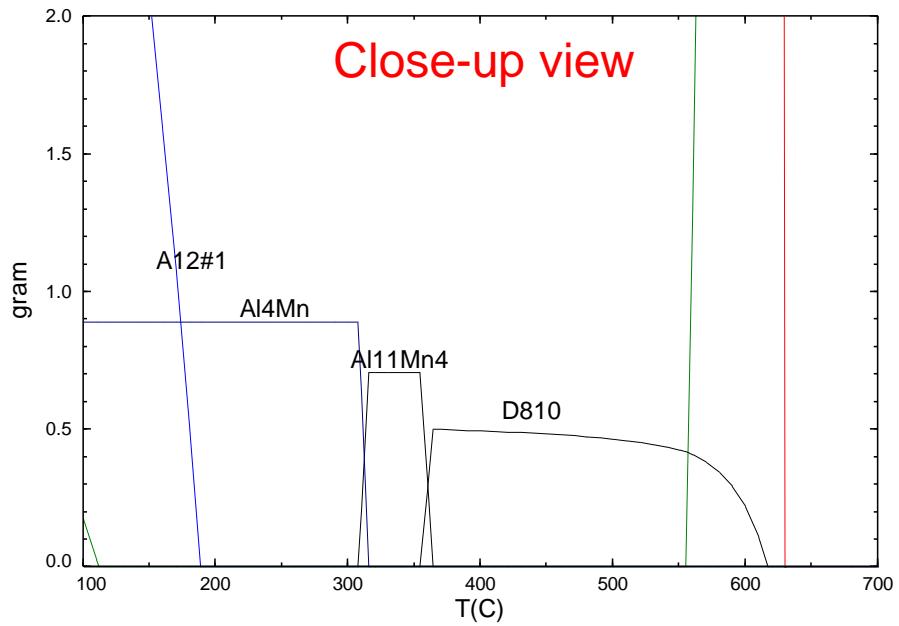
Final Conditions

Constitu	<A>		T(C)	P(atm)	Product H(J)
616.76 t			700 100	1	
Liquid					

Deactivated for Scheil cooling

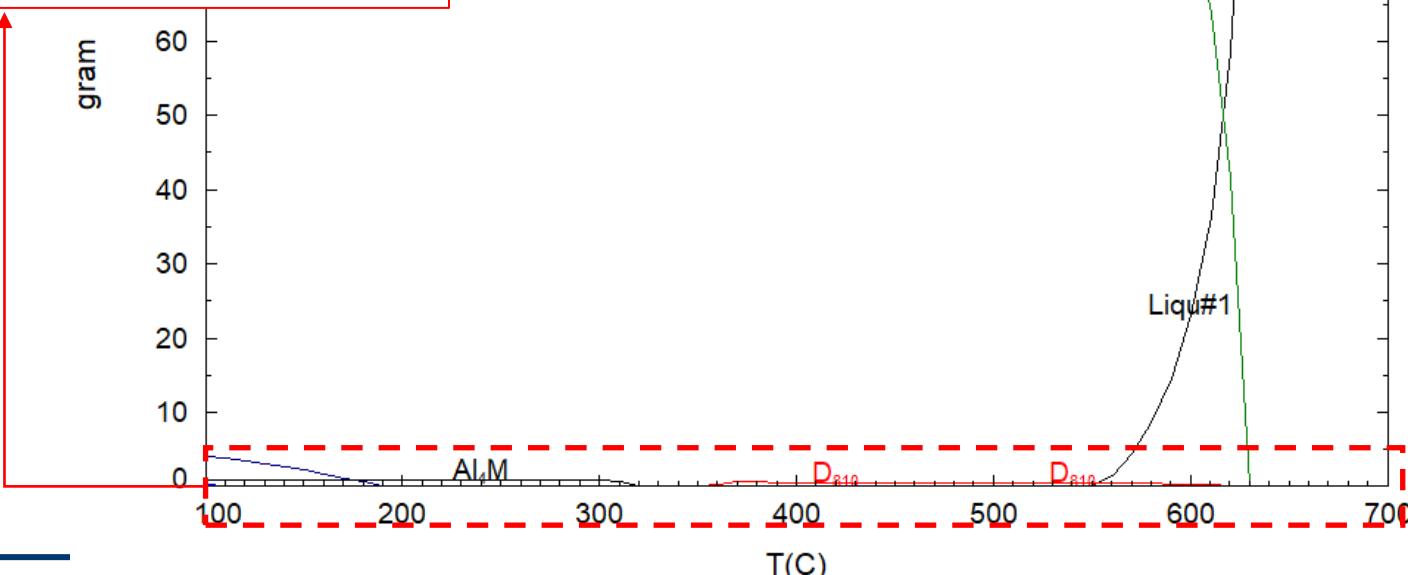
95.7 Mg + 3 Al + Zn + 0.3 Mn

Close-up view



95.7 Mg + 3 Al + Zn + 0.3 Mn

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EX10. Phase diagram : AZ31 – Sr phase diagram

The screenshot shows two windows of the FactSage software interface:

- Phase Diagram - Components** window (left):
 - Toolbar: File, Edit, Units, Data Search, Data Evaluation, Help.
 - Buttons: Open, Save, New, Print.
 - Text: T(C) P(atm) Energy(J) Quantity(g) Vol(litre).
 - Text area: Components: Mg0.96897Al0.027277Zn0.0037517 + Sr.
 - Note: Note: - on the phase diagram the units of mass will be g, but the chemical formulae of the components remain molar values.
 - Checkboxes for phase diagram types: classical phase diagram (default), aqueous diagram with molalities, and iso-Eh & iso-pH, reciprocal diagram with 2 cations and 2 anions, Scheil-Gulliver constituent diagram.
 - Buttons: Next >, Previous <.
 - Status bar: FactSage 8.0 Compound: 1/23 databases Solution: 1/23 databases.
- Phase Diagram - Menu: comments** window (right):
 - Toolbar: File, Units, Parameters, Variables, Help.
 - Text area: Components (2): (gram) Mg0.96897Al0.027277Zn0.0037517 + Sr.
 - Products** section:

Compound species	Solution phases
gas ideal real 0	I FTlite-Liqu Liquid
aqueous 0	I FTlite-A1 FCC-A1
pure liquids 0	I FTlite-A2 BCC-A2
+ pure solids 55	I FTlite-A3 HCP-A3
	I FTlite-A3" HCP-Zn Prototype-Mg
	I FTlite-A12 CBCC-A12 Prototype-Mn
	I FTlite-C14 C14 Prototype-Mg ₂ N ₂
	I FTlite-C36 C36 Prototype-MgNi ₂
 - Variables** section:

T(C)	Sr/(L+Sr)
0.700	0.005
 - Legend: I - immiscible 14, + - selected 8.
 - Custom Solutions, Pseudonyms, Volume data, paraequilibrium & Gmin, Virtual species, Total Species (max 5000), Total Solutions (max 200), Total Phases (max 1500).
 - Phase Diagram section: Y-axis, X-axis, Calculate button.
 - Status bar: FactSage 8.0 C:\Workshop80\Workshop\ex10.phas

In FactSage, all the input is in molar formula.

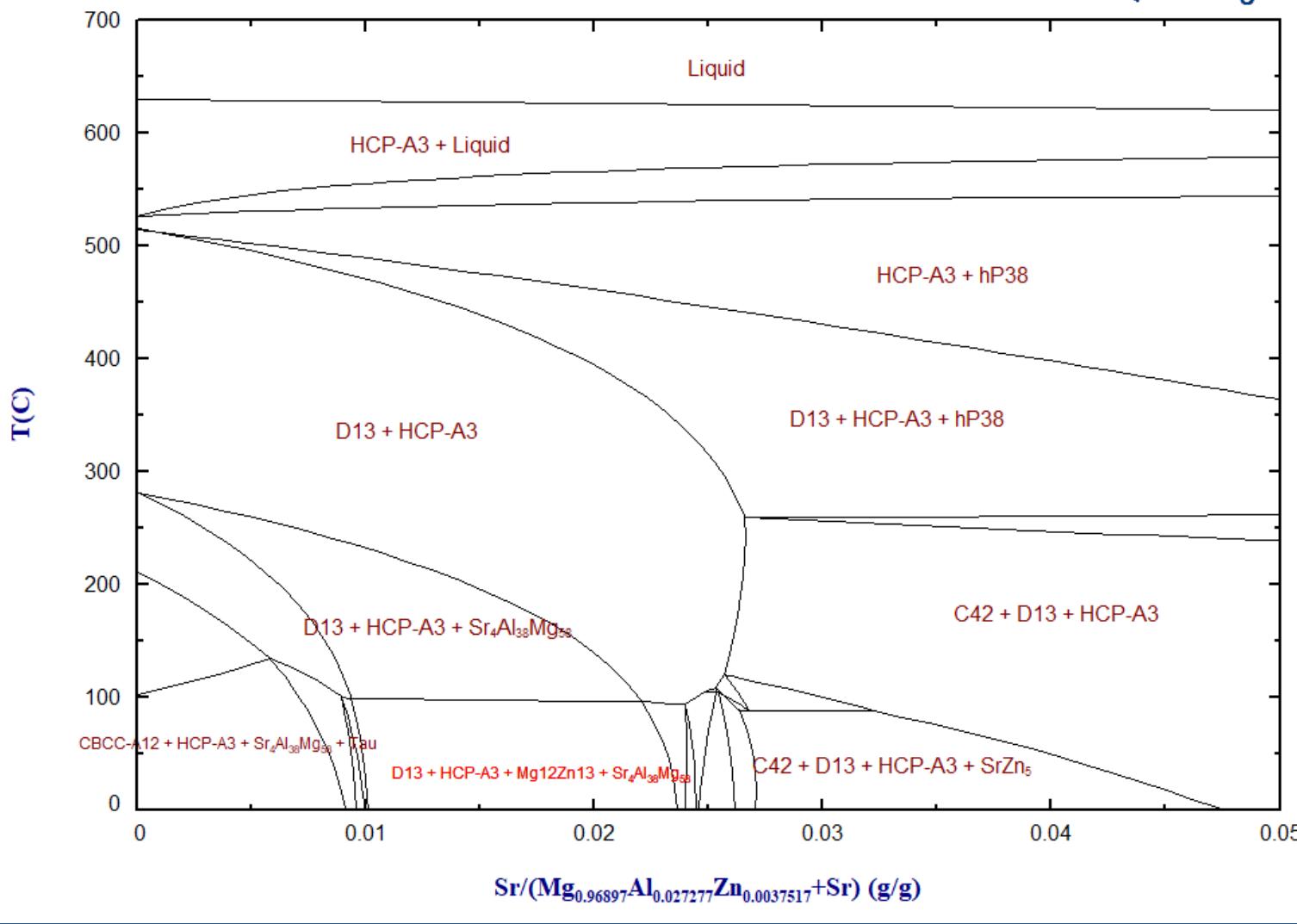
Thus, in order to add AZ31 (97wt%Mg-3wt%Al-1wt%Zn), we have to do conversion of the composition into molar fraction first. Then, add this molar formula as input

$$97\text{wt\%Mg}-3\text{wt\%Al}-1\text{wt\%Zn} \rightarrow 0.96897\text{Mg}-0.027277\text{Al}-0.0037517\text{Zn}$$

$Mg_{0.96897}Al_{0.027277}Zn_{0.0037517}$ - Sr

1 atm

FactSage™



EX11. Phase diagram: AZ31 – Sr – Ca isothermal section

Menu - Phase Diagram: Complex phase diagram calculation in multicomponent system : AZ3- ...

Components (3)

(gram) Mg0.96897Al0.027277Zn0.0037517 + Sr + Ca

Products

Compound species: 64

Solution species:

*	Base-Phase	Full Name
I	FTlite-Liqu	Liquid
I	FTlite-FCC	FCC_A1
I	FTlite-HCP	HCP_A3
I	FTlite-BCC	BCC_A2
I	FTlite-LC14	Laves_C14
I	FTlite-LC15	Laves_C15
I	FTlite-LC36A	ALaves_C36

Custom Solutions:

- fixed activities
- ideal solutions
- activity coefficients

Pseudon...

Variables: Mg0.96897Al0.027277Zn0.0037517-Sr-Ca composition #2. vs composition #1.

Variables:

compositions: 2

Temperature: T(C) constant 300

Pressure or Volume: P(atm) constant 1

Legend: I - immiscible 8
+ - selected 10

Show all selected species: 146

solutions: 26

Phase Diagram: A triangle with vertices A, B, C. X, Y, Z axes. XY steps: 11.

Next >>

Compositions Quantity(g):

#1. L = Mg0.96897Al0.027277Zn0.0037517

0 L + 1 Sr + 0 Ca = X-axis 0.03 (max)
1 L + 0 Sr + 1 Ca = 0 (min)

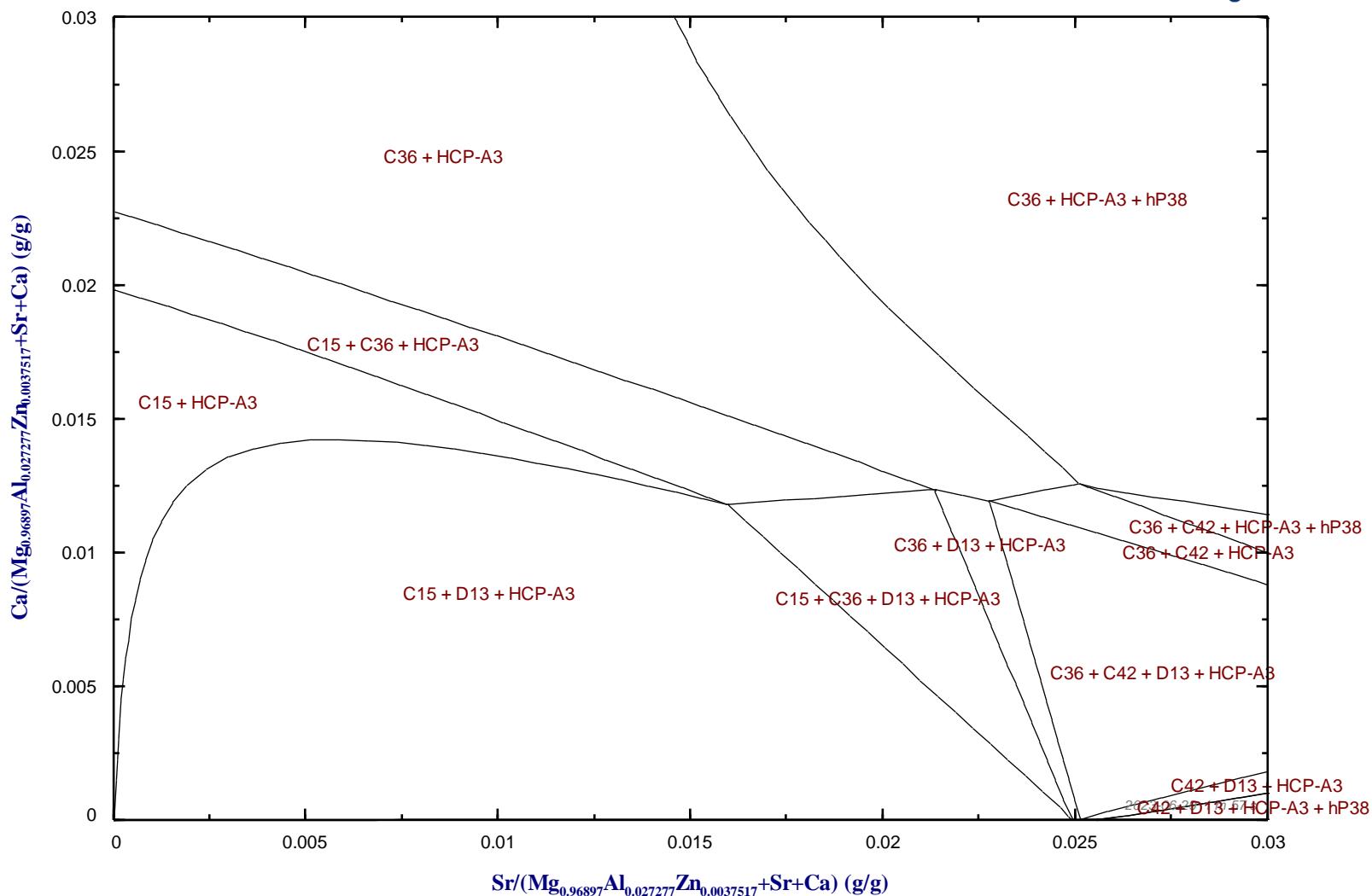
#2. L = Mg0.96897Al0.027277Zn0.0037517

0 L + 0 Sr + 1 Ca = Y-axis 0.03 (max)
1 L + 1 Sr + 0 Ca = 0 (min)

Cancel OK

$Mg_{0.96897}Al_{0.027277}Zn_{0.0037517}$ - Sr - Ca
300°C, 1 atm

FactSage™



EX12-1. Mg-Al-Zn + 1% Sr triangle /rectangular isothermal section

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Components (4)

(gram) Mg + Al + Zn + Sr

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- + pure solids 55

species: 55

Target - none -

Estimate T(K): 1000

Variables

	Base-Phase	Full Name
*	I	FTlite-Liqu
+	I	FCC-A1
	I	BCC-A2
	I	HCP-A3
	I	HCP-Zn Prototype-Mg
	I	CBCC-A12 Prototype-Mn
	I	C14 Prototype-MgZn2
	I	C36 Prototype-MgNi2

Legend
I - immiscible 14
+ - selected 8

Show all selected
species: 235
solutions: 36 Select

Solution phases

Variables: Mg-Al-Zn-Sr composition #2. vs composition #1.

Variables

compositions 3
 $\log_{10}(a)$ 0
 $\log_{10}(b)$ 0
 $\log_{10}(c)$ 0
 $\log_{10}(d)$ 0
A
B
C
X,Y steps 11
Next >

T and P

Temperature
 T(C)
constant 300

Pressure or Volume
 P(atm)
constant 1

Compositions Quantity(g)

#1. $1 \text{ Mg} + 0 \text{ Al} + 0 \text{ Zn} + 0 \text{ Sr} = \text{A-Corner}$
 $1 \text{ Mg} + 1 \text{ Al} + 1 \text{ Zn} + 0 \text{ Sr} = 1 \text{ (max)}$
 $0 \text{ Mg} + 1 \text{ Al} + 1 \text{ Zn} + 1 \text{ Sr} = 0 \text{ (min)}$

Composition #
#1 max = 4

Cancel **OK**

Compositions Quantity(g)

#4. $0 \text{ Mg} + 0 \text{ Al} + 0 \text{ Zn} + 1 \text{ Sr} = \text{Constant}$
 $1 \text{ Mg} + 1 \text{ Al} + 1 \text{ Zn} + 1 \text{ Sr} = 0.01$

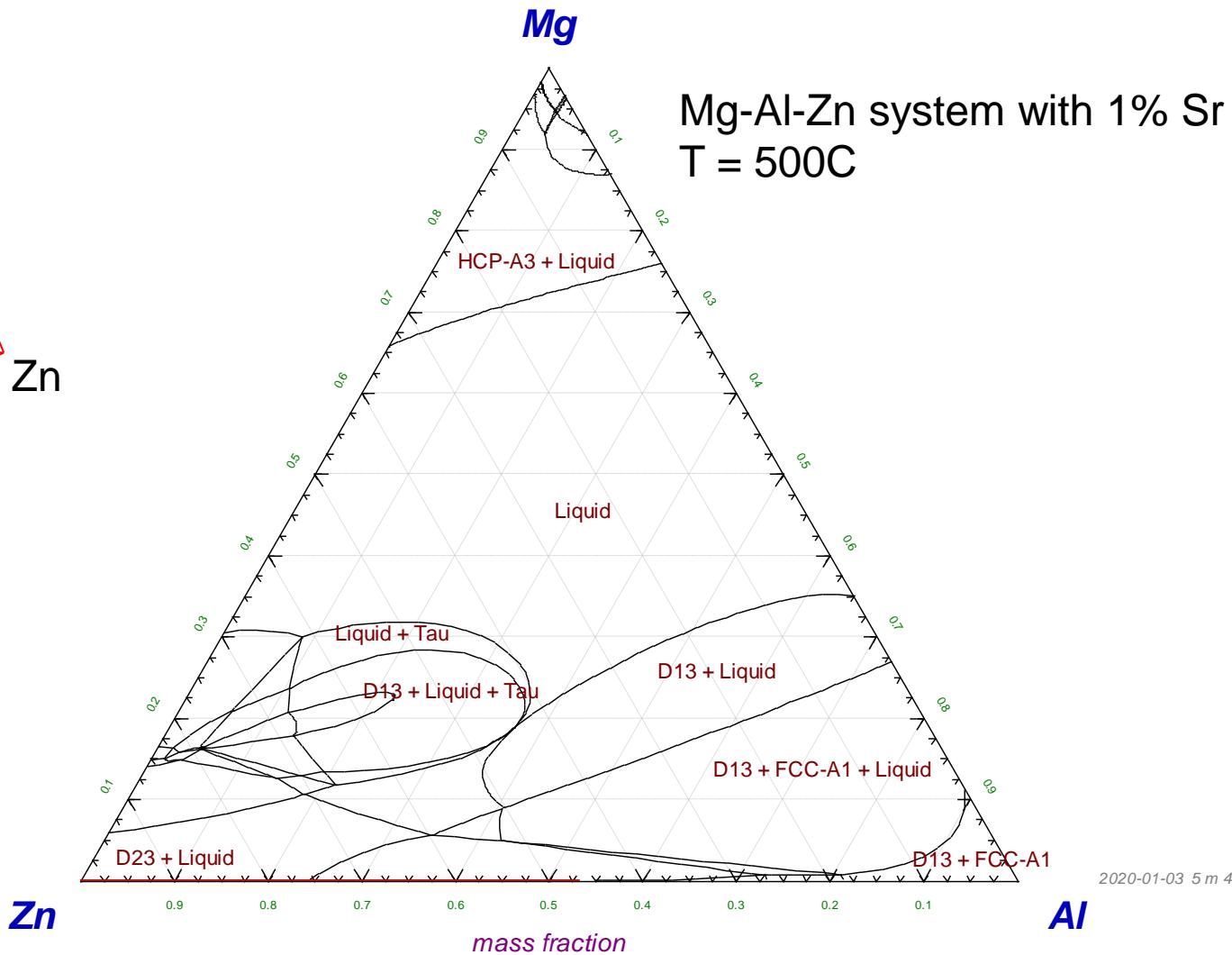
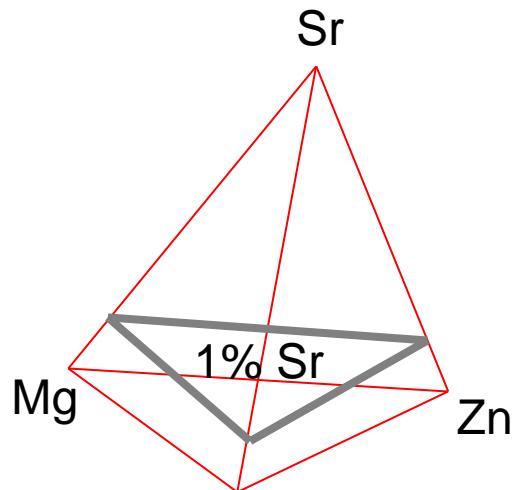
#4 $\log_{10}(\text{composition})$

Composition #
#4 max = 4

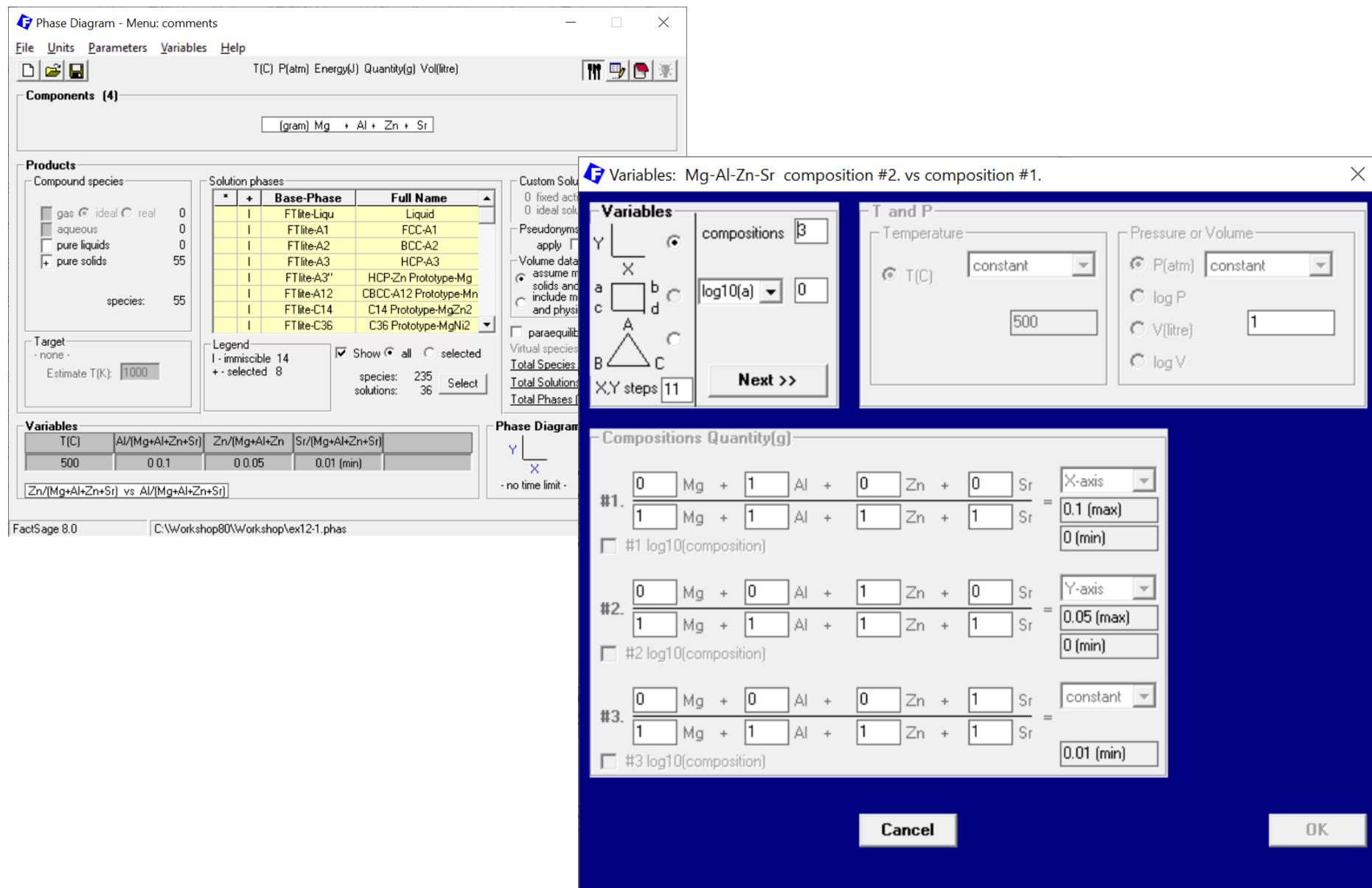
In the triangle diagram, the composition of 4th element is constant.

Mg - Al - Zn - Sr

$Sr/(Mg+Al+Zn+Sr) \text{ (g/g)} = 0.01, 500^\circ\text{C}, 1 \text{ atm}$

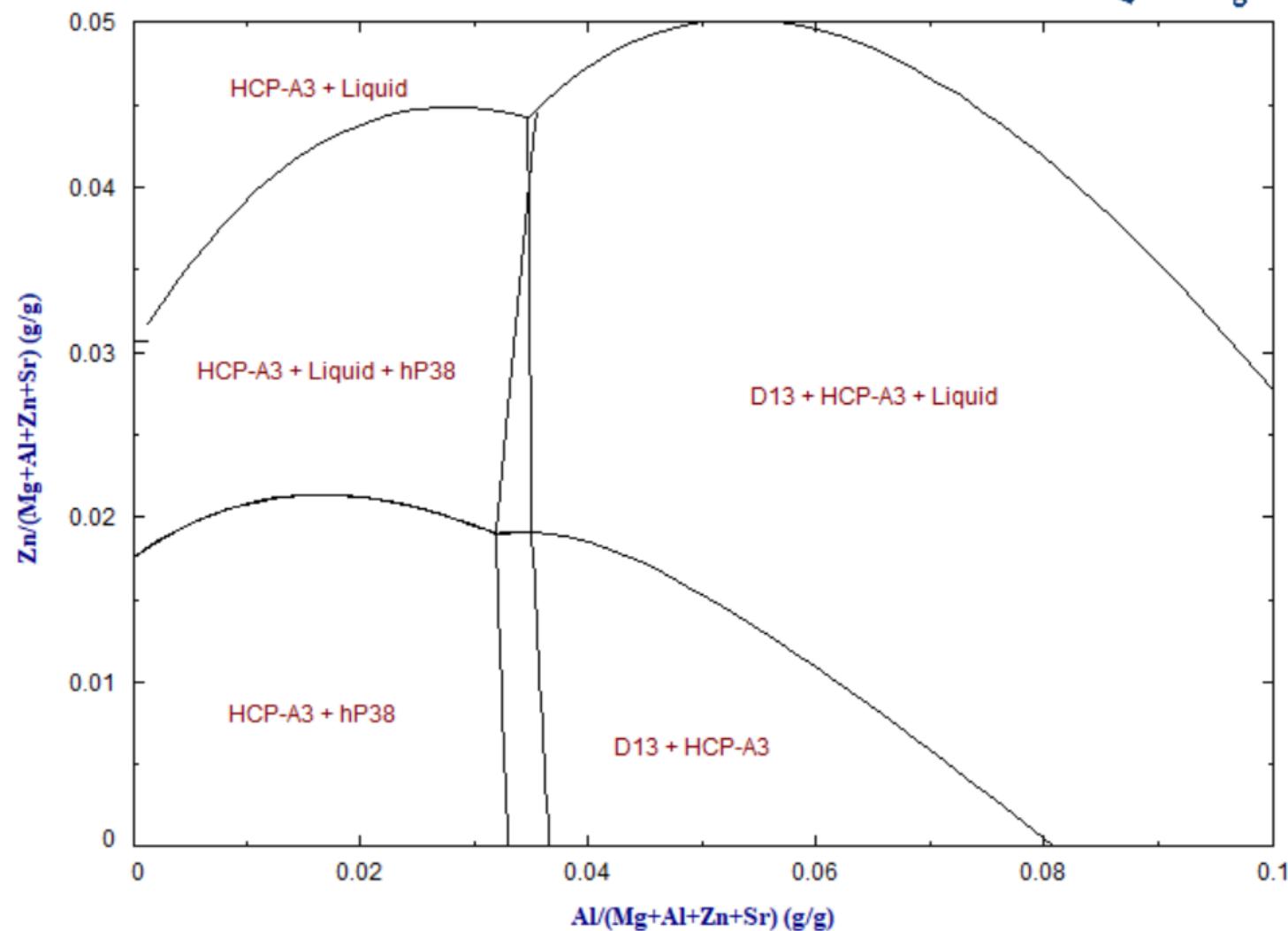


EX12-2. Mg-Al-Zn + 1% Sr triangle /rectangular isothermal section



Mg - Al - Zn - Sr

$Sr/(Mg+Al+Zn+Sr) (g/g) = 0.01, 500^\circ C, 1 \text{ atm}$



EX13. Metastable phase: Fe-C binary system w/wo C (Fe3C)

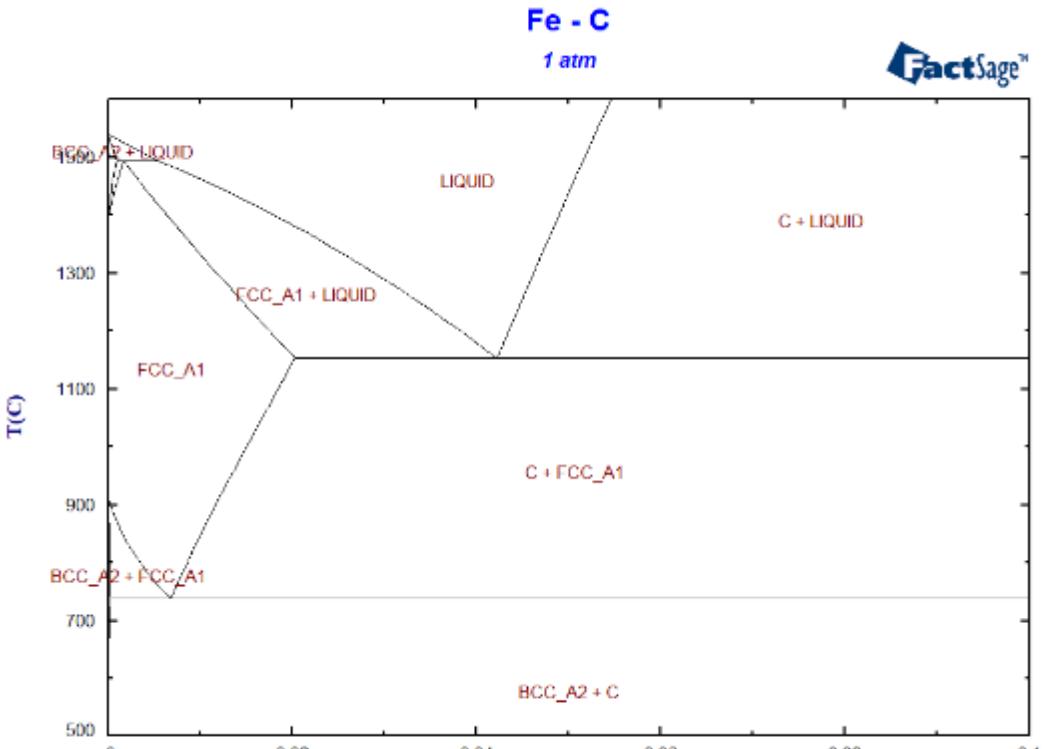
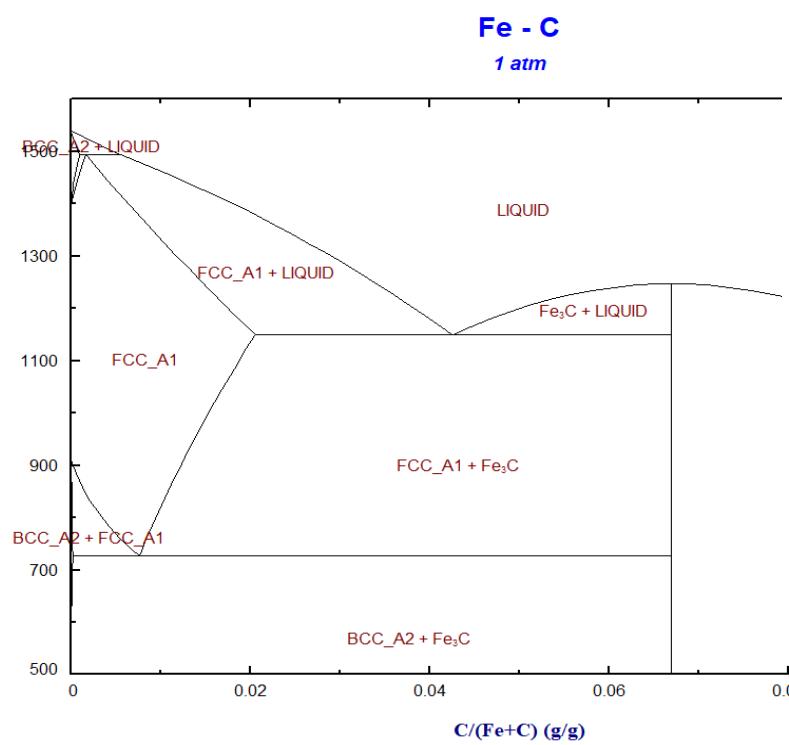
The screenshot shows two windows from the FactSage software:

- Phase Diagram - Menu: last system**: This window displays a phase diagram for the Fe-C system. It includes sections for Components (2), Products, Solution phases, Variables, and a Phase Diagram plot.
- Selection - Phase Diagram - no results -**: This window shows a table of selected species. The table has columns: +, Code, Species, Data, Phase, T, V, Activity, and M. The rows listed are:

+	3	C(s)	FSstel	graphite	V			
+	4	C(s2)	FSstel	diamond	V			
+	5	Fe(s)	FSstel	BCC_A2	o			
+	6	Fe(s2)	FSstel	FCC_A1	o			
+	7	Fe3C(s)	FSstel	CEMENTITE	o			
+	8	Fe3C(s2)	FSstel	KSI_CARBIDE	o			

Although C (carbon) is thermodynamically stable phase than Fe3C, C is not appearing in most of low carbon steel. Thus, in order to do proper calculations, C should be removed from above compound list in particular in steel.

In the same way, if a certain phase is not readily formed (sluggish to form), we can unselect the phase to simulate the system more realistically.

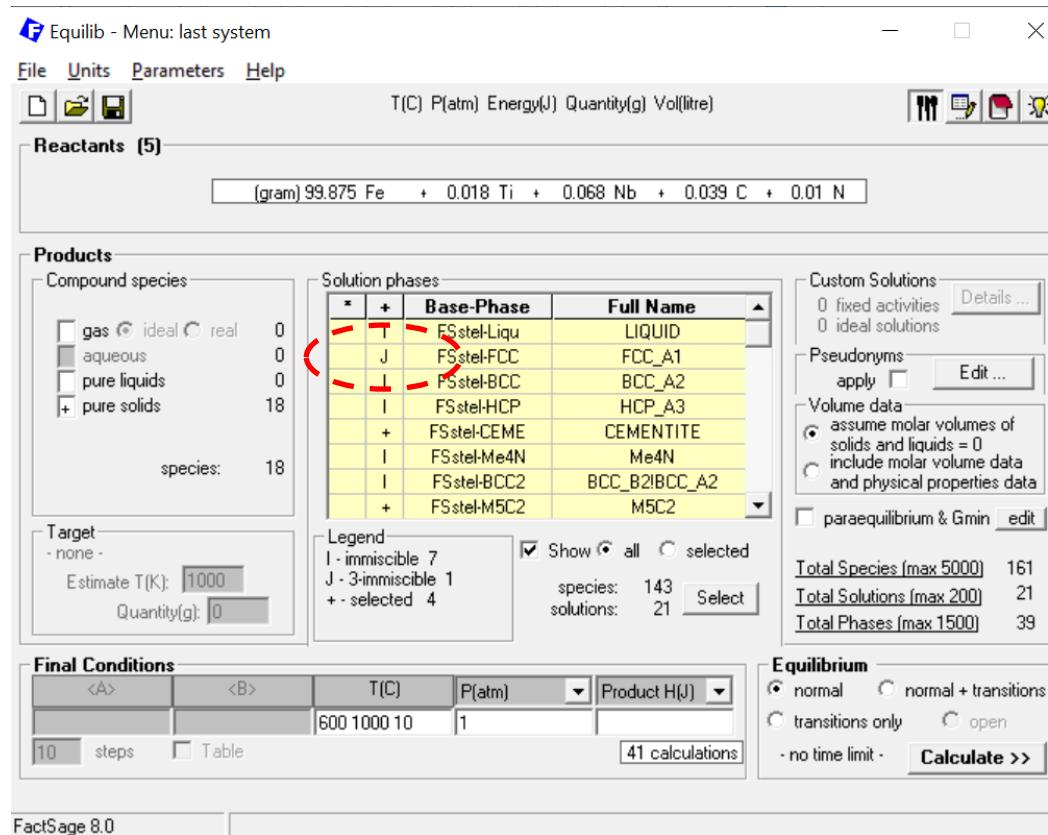


Stable phase diagram with C

Metastable phase diagram without C

EX14-1. J option (3 possible miscibility gaps): Fe-Nb-Ti-C-N system

Unselect “C(s)”



“J” option (default) is needed for a phase which has more than 2 possible miscibility gaps. Most well known example is Fe FCC phase in steel with (Ti,Nb)(C,N) phase formation. Since Ti(C,N) and Nb(C,N) have FCC crystal structure, we describe both FCC metallic phase and carbonitride phase using the same FCC phase model. Thus, in order to do proper calculations, J option should be applied to FCC phase in this case.



T(C) P(atm) Energy(J) Quantity(g) Vol(litres)

[980 C](#) | [990 C](#) | [1000 C](#) |
[850 C](#) | [860 C](#) | [870 C](#) | [880 C](#) | [890 C](#) | [- 900 C -](#) | [910 C](#) | [920 C](#) | [930 C](#) | [940 C](#) | [950 C](#) | [960 C](#) | [970 C](#)

(gram) 99.865 Fe + 0.018 Ti + 0.068 Nb + 0.039 C

(gram) 0.01 N =  99.905 gram FCC Al#1

99.905 gram FCC_Al#1
(99.905 gram, 1.7883 mol)
(900 C, 1 atm, a=1.0000)

(99.797 wt.% Fe
+ 5.3332E-03 wt.% Nb
+ 4.8704E-06 wt.% Ti
+ 0.19369 wt.% FeC

+ 9 + 9.2296E-02 gram FCC_Al#2
+ 9 (9.2296E-02 gram, 1.614E-03 mol)
+ 3

+ 1 (900 C, 1 atm,
+ 1 (4.2141E-05 wt.% F
+ 0.11450 wt.% N

Sit	+ 2.9825E-02	wt.% Ti
Fe	+ 1.1763E-02	wt.% Fe
Nb	+ 29.706	wt.% Nb

Ti	+ 8.5709	wt.% Ti
---	+ 1.9048E-02	wt.% Fe
Va	+ 47.616	wt.% Nb
C	+ 13.931	wt.% Ti

Site fraction of sub-

Site fraction of sub

Va
S

— N

Va	Fe	0.18033	Stoichiometry = 1
C	Nb	2.1307E-02	
N	Ti	0.79836	

Site fraction of sublattice constituents

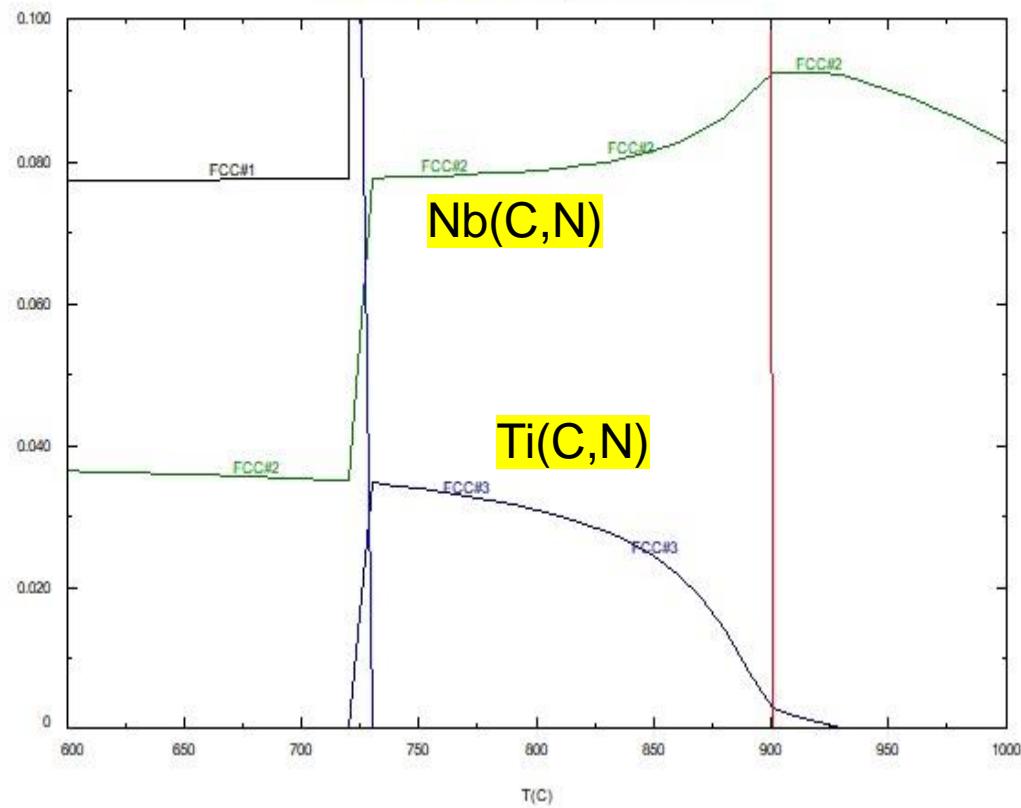
Fe 0.18033 Stoichiometry = 1

Nb 2.1307E-0

Ti 0.7983

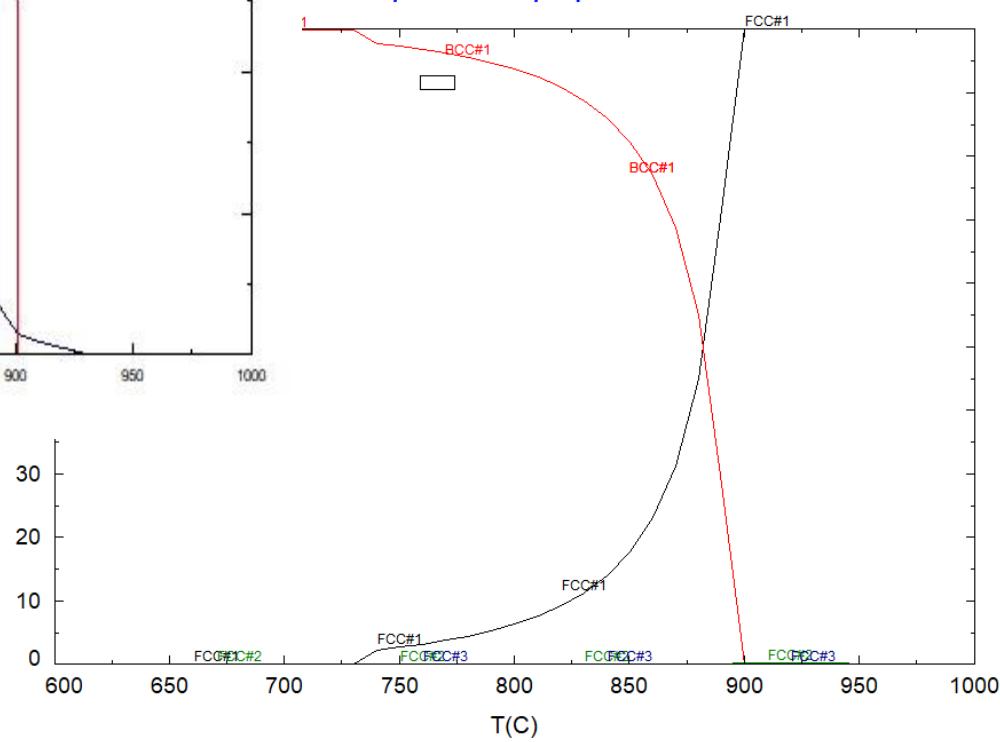
99.865 Fe + 0.018 Ti + 0.068 Nb + 0.039 C +

C:\FACTSAGEWS\Equi0.res 03Jul23



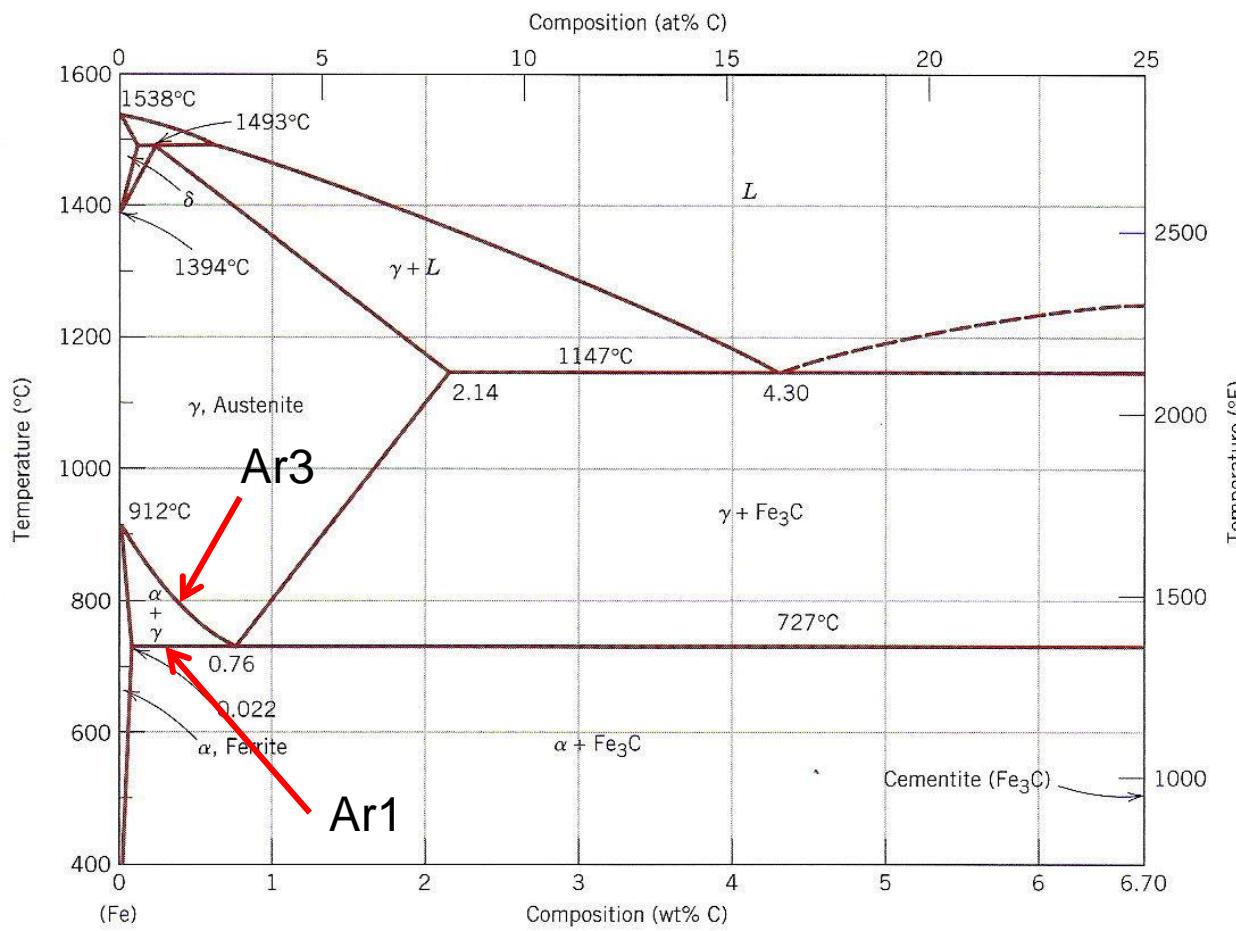
99.865 Fe + 0.018 Ti + 0.068 Nb + 0.039 C +

Workshop80\Workshop\Equi0.res 19Dec19



EX14-2. Carbide and Nitride precipitation in microalloyed steels

Microalloyed steels are used for special high-strength applications such as pipelines. In order for the steel to acquire good mechanical properties, it needs to be thermo-mechanically treated. FactSage can help in finding the correct temperatures for treating these steels.



The steel is annealed in the austenite region and then cooled through the temperatures Ar3 and Ar1 temperatures (continuous cooling austenite to ferrite transformation start and finish).

The goal of this study is to find the ideal annealing temperatures to avoid precipitation of Nb carbonitrides and promote precipitation of NbC.

EX14-2. Carbide and Nitride precipitation in microalloyed steels

1. A typical microalloyed steel composition is entered (For more information, refer to J. Calvo et al. / Materials Science and Engineering A 520 (2009) 90–96)

The screenshot shows two windows from the FactSage software interface.

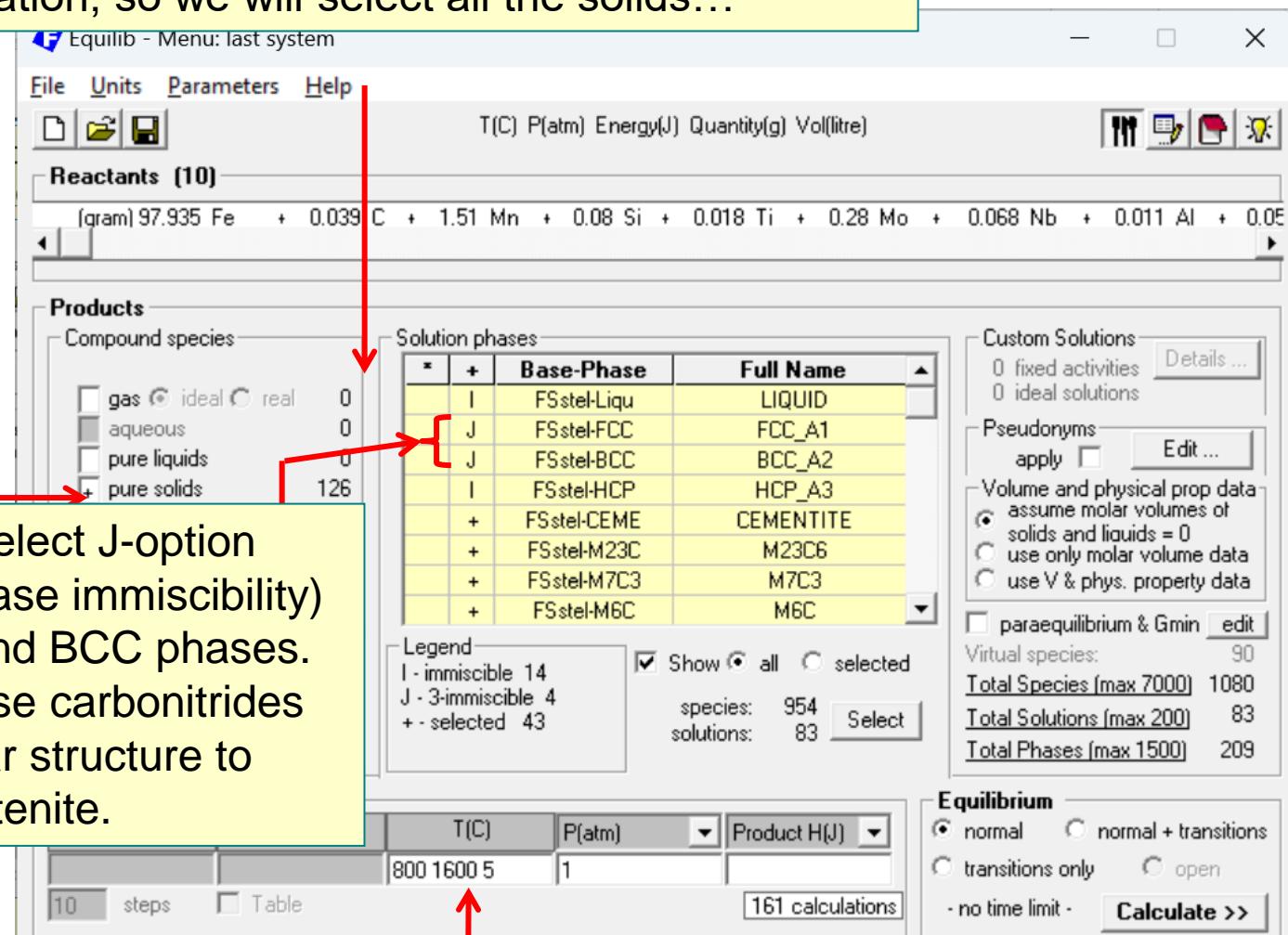
Equilib - Reactants window (left): This window displays a composition table with 'Quantity(g)' and 'Species' columns. The composition is as follows:

Species	Quantity(g)
Fe	97.935
C	0.039
Mn	1.51
Si	0.08
Ti	0.018
Mo	0.28
Nb	0.068
Al	0.011
V	0.05
N	0.0095

Data Search window (right): This window lists various databases under three main categories: Fact, FactSage, and SGTE. The 'Fact' category includes FactPS, FToxid, FTsalt, FTmisc, FThall, FTOxCN, FTfrtz, FThelg, FTpulp, FTlite, and FTpul. The 'FactSage' category includes FSropp, FSlead, FSstel (which is checked), and FSpsi. The 'SGTE' category includes BINS, SGPS, SGTE, and SGsold. To the right, there is a section for 'Private Databases' with checkboxes for EXAM, SGTEa, and SGTEb. Below the databases are sections for 'Other' (SGnobl, SpMCBN, TDmeph, TDnucl) and 'Information'. At the bottom, there are 'Options - search for product species' settings for 'Include compounds' (gaseous ions, aqueous species, limited data compounds) and 'Limits' (Organic species CxHy..., X(max) = 2, Minimum solution components: 1 or 2 cpts). Buttons for 'Cancel', 'Summary...', and 'OK' are at the bottom right.

Task: 2. Select only the FSstel database.

1. We are interested in carbide, nitride and carbonitride precipitation, so we will select all the solids...



2. ... and select J-option (possible 3-phase immiscibility) for the FCC and BCC phases. This is because carbonitrides have similar structure to austenite.

3. We will select a range of temperature encompassing the whole austenite phase.

1. Plot g vs T(C) for all stable solids and solutions
 (by click “select All stable phases”)

Plot Species Selection - Equilib Results: gram vs T(C)

File Show Select

#	Species	Mole (min)	Mole (max)	Fraction (min)	Fraction (max)	Activity (min)	Activity (max)
1080	MoNbN	0	0	0	0	1.8371E-05	4.0479E-03
SOLUTIONS							
1081	GAS	0	0	0	0	0	0
+ 1082	Liqu#1	0	1.7934	0	0	0.578831	1
+ 1083	Liqu#2	0	0	0	0	0.578831	1
+ 1084	FCC#1	0	1.7892	0	0	0.954964	1
+ 1085	FCC#2	0	1.1401E-03	0	0	0.954964	1
+ 1086	FCC#3	0	6.7841E-04	0	0	0.13109	1
+ 1087	BCC#1	0	1.7892	0	0	0.962916	1
+ 1088	BCC#2	0	0	0	0	1.4406E-02	1
+ 1089	BCC#3	0	0	0	0	9.7787E-04	1
1090	HCP#1	0	0	0	0	0.670344	0.76236
1091	HCP#2	0	0	0	0	0.18217	0.719492
1092	CEME	0	0	0	0	1.6061E-03	8.8501E-02
1093	M23C	0	0	0	0	7.2122E-18	2.2417E-07
1094	M7C3	0	0	0	0	2.2489E-09	8.7626E-05
1095	M6C	0	0	0	0	6.1026E-06	4.5564E-03

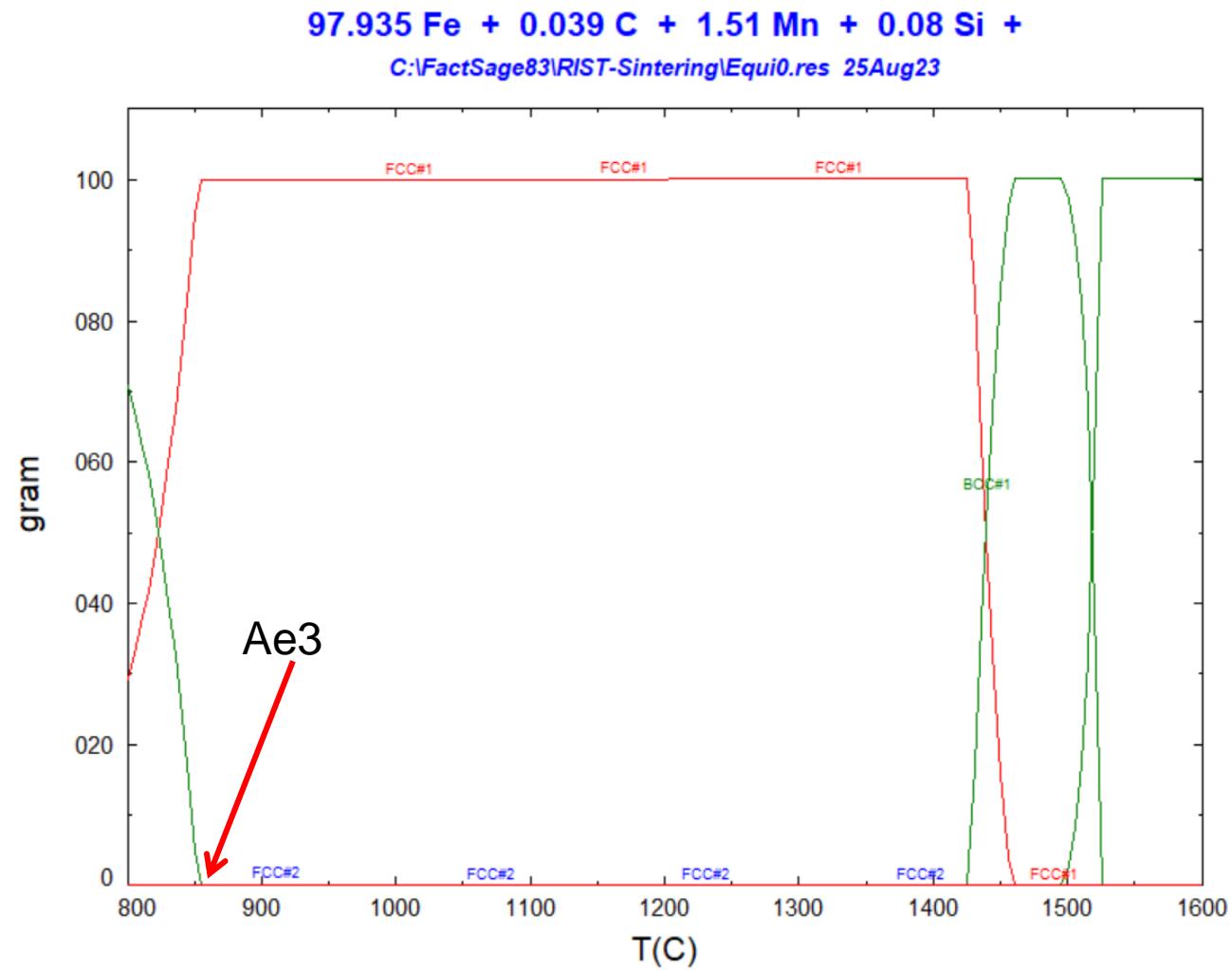
Display source phase name [page] **Mass** mole mass (max) gram **Order** integer # mass (max) fraction (max) activity (max)

Select Top 15 9 species selected ignore species and phases with zero mass **Select ...** **Select all stable phases** **Select stable pure liquids** **Select stable pure solids** **Select stable solution phases**

Click on the '+' column to add or remove species. 161 pages Clear

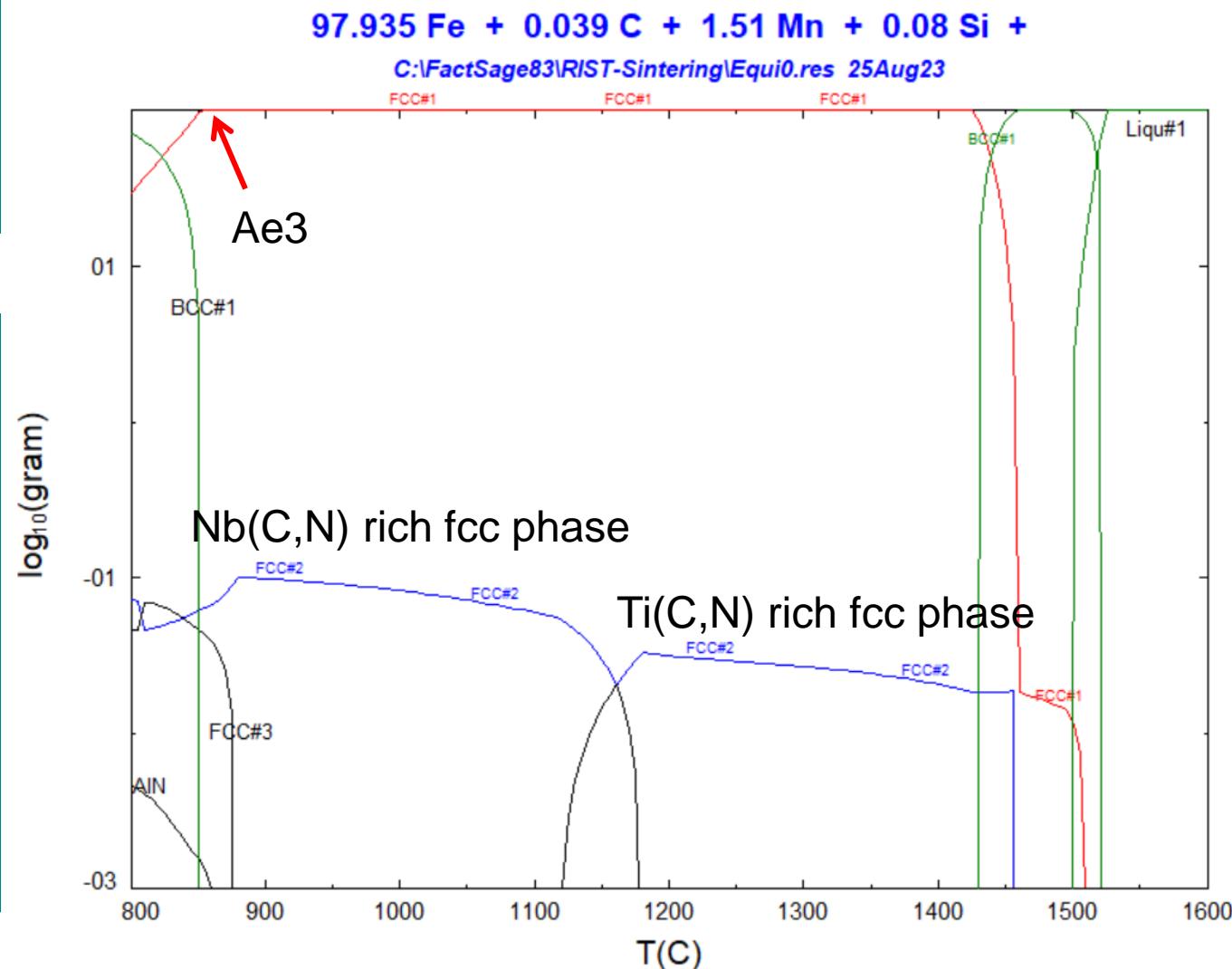
1. From the graph, we can deduce equilibrium transformation temperatures from austenite to ferrite.

2. We should also look at the very low compositions, since all the microalloyed elements will be present in very small quantities.



1. Using a log scale is very convenient for looking at the microalloyed elements.

2. It is clearly seen that the FCC#1, #2 and #3 phases are forming. In this case, they are probably carbides and nitrides.
We can check this by plotting their composition with temperature



1. We will first select all the species in FCC#1 and see how they are distributed.

Plot Species Selection - Equilib Results: log10(gram) vs T(C)

File Show Select

+	#	Species	Mole (min)	Mole (max)	Fraction (min)	Fraction (max)	Activity (min)	Activity (max)
		FCC#1		FCC A1				
+	21	Al	0	4.0708E-04	4.7860E-18	2.4867E-04	4.1356E-12	3.0119E-06
+	22	Fe	0	1.7511	2.0399E-06	0.985055	0.772987	0.979446
+	23	Mn	0	2.7444E-02	1.8261E-07	6.6014E-02	1.0493E-02	5.9879E-02
+	24	Mo	0	2.9133E-03	1.0253E-07	6.2586E-03	8.1993E-04	4.0316E-03
+	25	Nb	0	7.2576E-04	5.6861E-08	2.0250E-02	7.4692E-11	2.3562E-04
+	26	Si	0	2.8442E-03	4.8736E-15	1.5906E-03	2.1637E-13	1.0937E-06
+	27	Ti	0	1.3524E-04	1.4386E-09	1.5861E-02	1.0348E-13	1.5213E-05
+	28	V	0	9.7821E-04	2.1452E-05	1.8696E-02	5.9493E-08	1.1250E-04
+	29	AlC	0	7.3519E-07	1.3737E-16	7.2734E-07	4.1651E-17	1.4266E-10
+	30	FeC	0	3.1624E-03	5.8551E-05	2.5067E-02	2.0009E-05	3.2646E-04
+	31	MnC	0	5.7900E-05	5.4987E-07	9.9594E-03	1.7967E-06	9.1140E-03
+	32	MoC	0	2.1415E-04	2.8467E-07	0.1283	1.0672E-05	0.112674
+	33	NbC	0	7.0559E-04	1.5744E-09	0.543254	8.8343E-04	0.722589
+	34	SiC	0	5.1367E-06	1.3989E-13	2.6215E-05	1.3645E-13	9.9780E-09
+	35	TiC	0	3.4792E-05	3.9832E-11	7.0975E-02	1.9573E-04	4.3605E-03
+	36	VC	0	6.3969E-04	1.6128E-07	0.383256	3.6960E-05	0.350844
+	37	AlN	0	9.5017E-08	1.3034E-19	1.0813E-07	2.7165E-14	5.1200E-07
+	38	FeN	0	4.0871E-04	5.5554E-08	0.141664	7.8240E-10	3.5146E-05
+	39	MnN	0	6.4059E-06	1.2525E-07	3.9924E-05	2.8494E-07	2.2803E-05
+	40	MoN	0	1.2349E-06	1.7090E-09	7.3986E-04	4.9738E-08	1.8085E-05
+	41	NbN	0	3.9955E-06	1.2831E-13	1.4116E-02	1.2724E-04	0.19341
+	42	SiN	0	6.6387E-07	1.3273E-16	5.6314E-07	4.5708E-20	3.1051E-09
+	43	TiN	0	2.0838E-04	3.2462E-15	0.778242	4.3162E-02	0.604403
+	44	VN	0	3.6889E-06	4.8408E-11	4.4002E-03	1.0995E-03	0.302572
		FCC#2		FCC A1				
	45	Al	0	3.2904E-13	5.1067E-21	2.4867E-04	4.1356E-12	3.0119E-06
	46	Fe	0	5.9360E-07	3.1055E-07	0.985055	0.772987	0.979446
	47	Mn	0	5.3043E-07	8.0779E-13	1.6157E-02	1.0493E-02	5.9879E-02

Display source mole integer # phase name gram fraction (max) activity (max)

Order mole mass (max) fraction (max) activity (max)

Select Top 15 ignore species and phases with zero mass 24 species selected

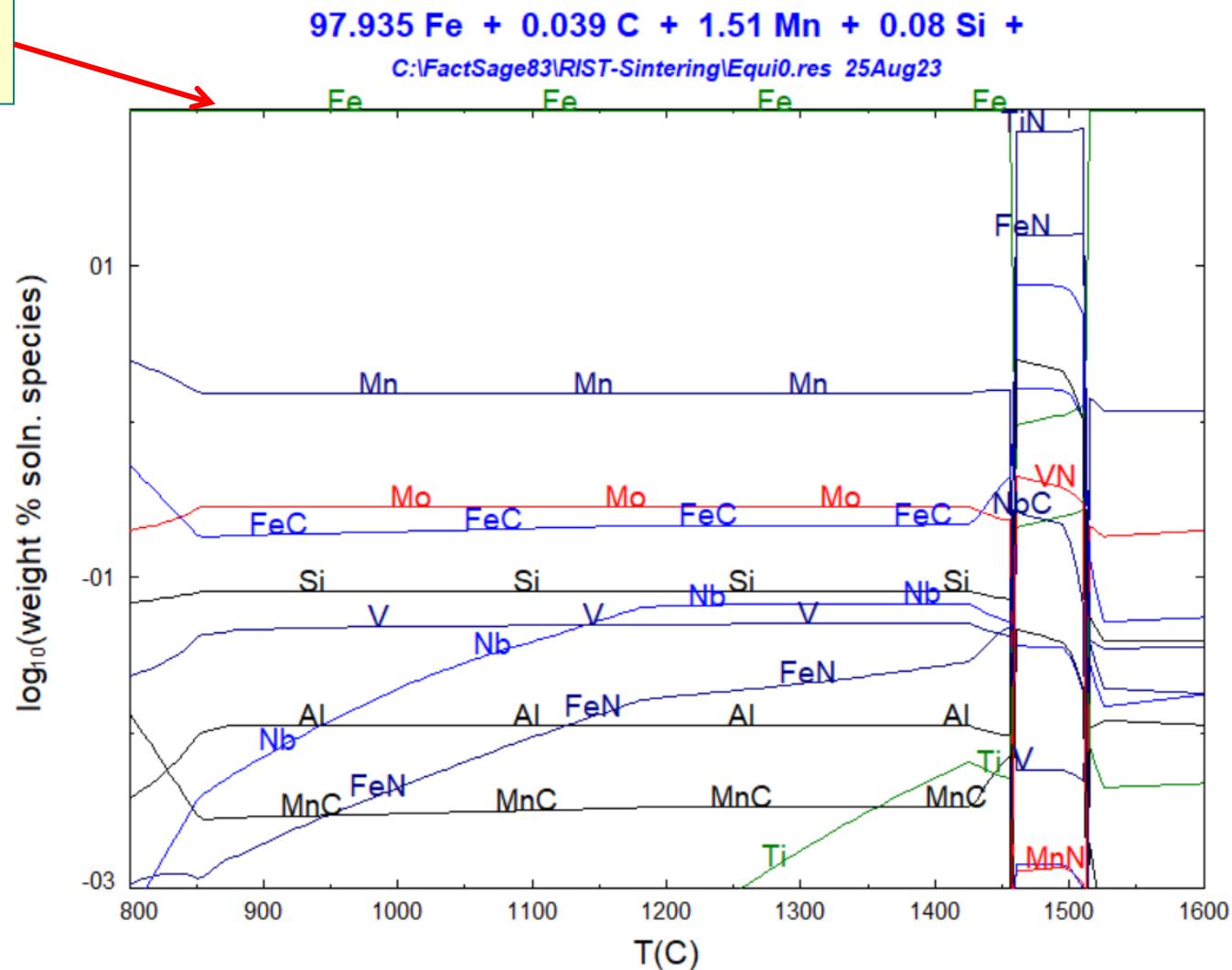
OK

Clear

Click on the '+' column to add or remove species.

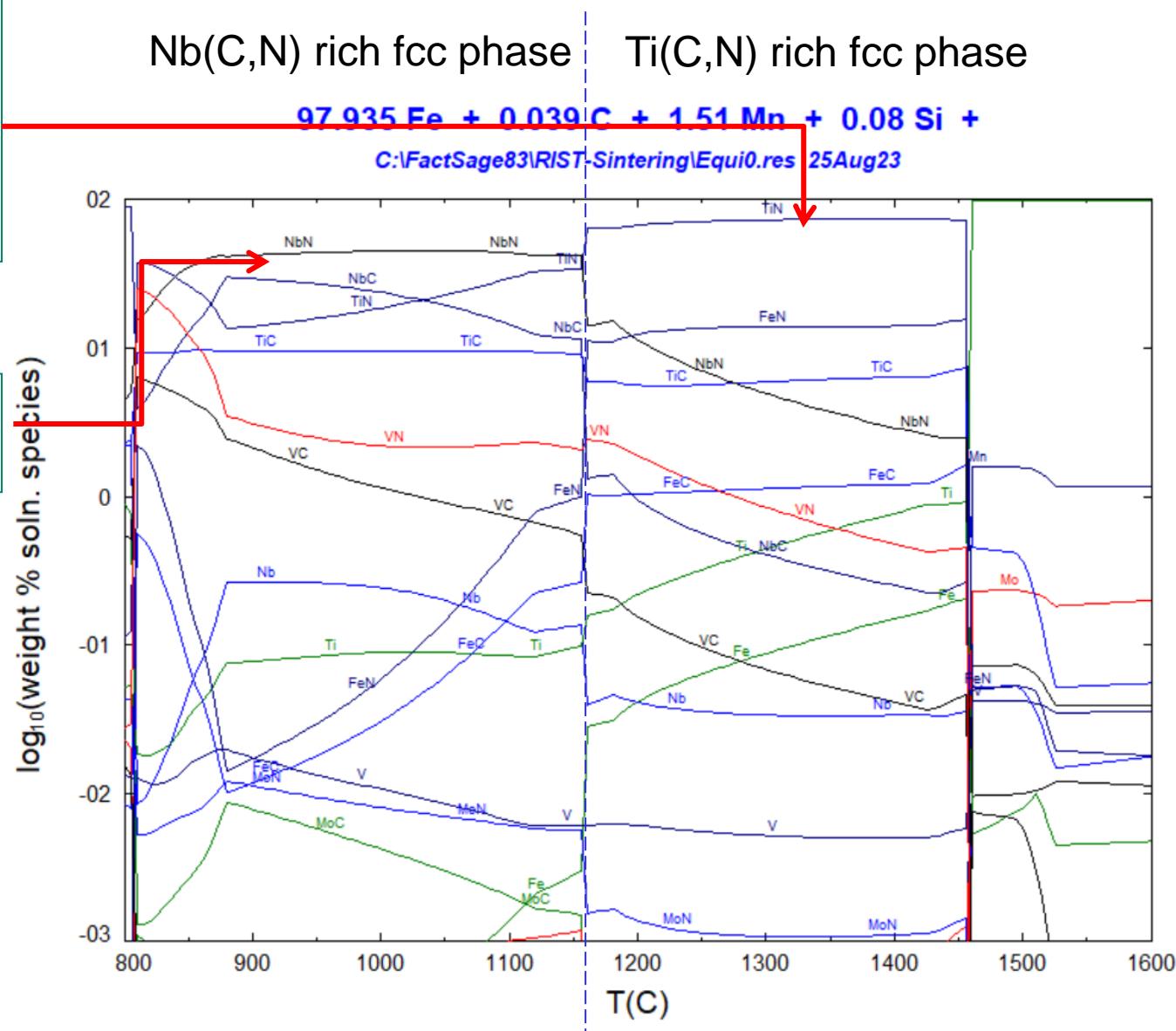
221 pages

1. In the austenite region, the FCC#1 phase is composed mostly of iron (FeVa)



1. The FCC#2 phase is composed mainly of TiN and TiC at austenite temperatures...

2. Mainly composed of NbN and NbC



EX15-1. Phase diagram PO₂ – T: Oxidation of pure Fe

Phase Diagram - Components

File Edit Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Components: O₂, Fe

Note: - on the phase diagram the units of mass will be g, but the chemical formulae of the components remain valid.

Data Search

Databases - 3/23 compound databases, 2/23 solution databases

Fact **FactSage™** **SGTE**

FactPS FScepp BINS EXA
 FToxid FSlead SGPS
 FTsalt FSstel SGTE
 FTmisc FSpost SGsold

FThall ELEM SGnobl TDmeph
 FTOxCN FTdemo SpMCBN TDnucl
 FTfritz FTpulp FTnucl TDnucl

Other

FTlite

compounds only solutions only no database

Clear All Add/Remove Data RefreshDatabases

Information

Options - search for product species

Include compounds: gaseous ions (plasmas) aqueous species limited data compounds (25C)

Limits: Organic species Minimum solu

Default Cancel Summary ...

Oxidation of steel requires multiple databases

- (a) FSStel: steel phases
- (b) FToxic: oxide phases
- (c) FactPS: gases and others

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Components (2): (gram) O₂ + Fe

Products

Compound species:

- gas (ideal) 0
- aqueous 0
- pure liquids 0
- pure solids 6
- * - custom selection species: 6

Solution phases:

*	+	Base-Phase	Full Name
I	+	FSstel-Liqu	LIQUID
J		FSstel-FCC	FCC_A1
I		FSstel-BCC	BCC_A2
I	+	FToxid-SLAGA	A-Slag-liq all oxides + S
+		FToxid-SPINA	A-Spinel
+	+	FToxid-MeO_A	A-Monoxide

Custom Solutions: 0 fixed activities, 0 ideal solutions

Pseudonyms: apply Edit ...

Volume data: assume molar volumes of solids and liquids = 0 include molar volume data and physical properties data

paraequilibrium & Gmin edit

Total Species (max 5000) 32
Total Solutions (max 200) 11
Total Phases (max 1500) 17

Variables

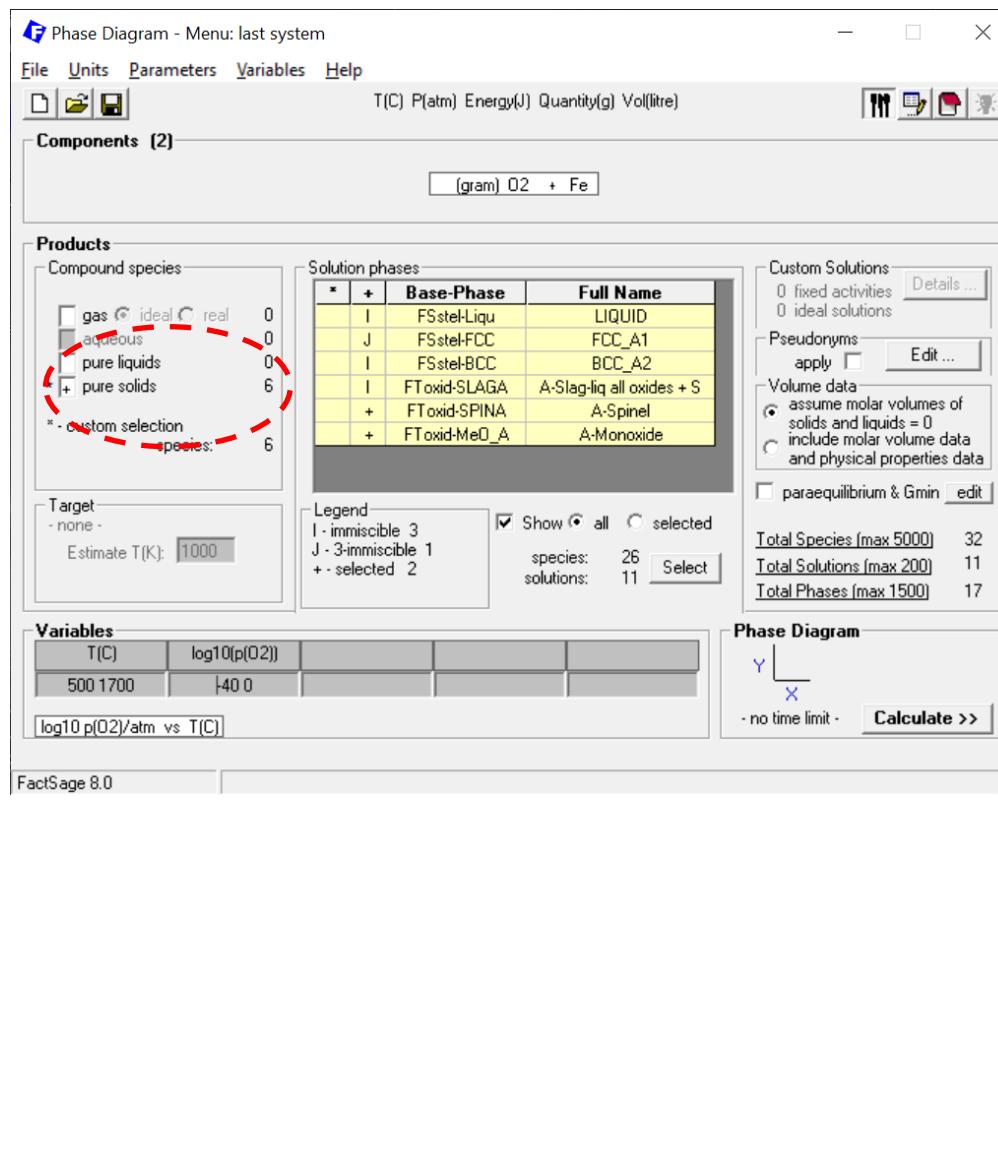
T(C)	log10(p(O ₂))			
500 1700	-40 0			

log10 p(O₂)/atm vs T(C)

Phase Diagram

Y X

- no time limit - Calculate >



Selection - Phase Diagram - no results -

File Edit Show Sort

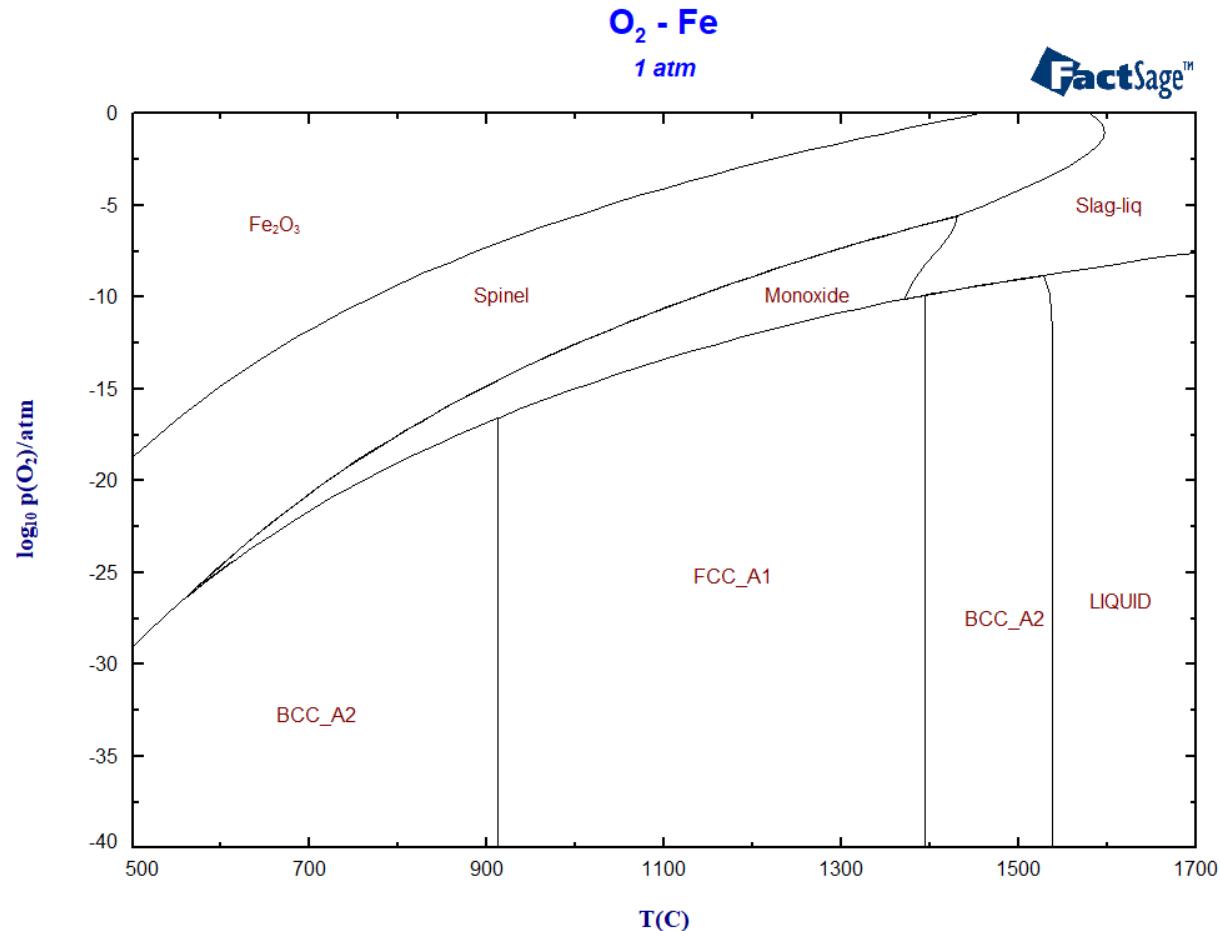
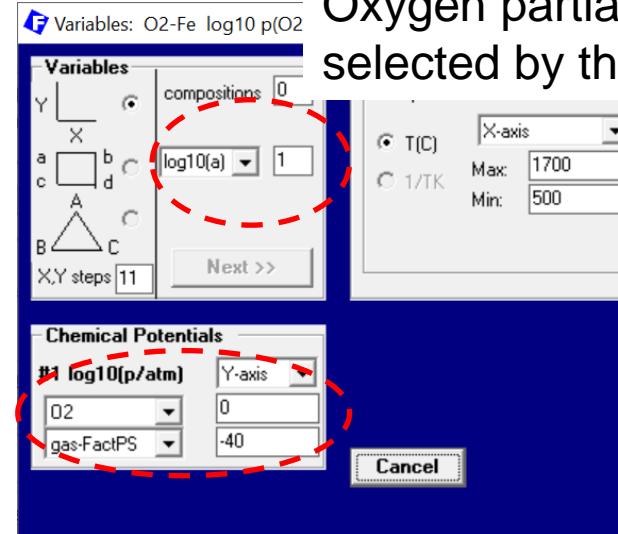
Selected: 6/23 SOLID Duplicates selected X denotes species excluded by default - no results -

+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
X	16	FeO(s)	FactPS	Wustite		V			
X	17	Fe2O3(s)	FactPS	hematite		V			
X	18	Fe2O3(s2)	FactPS	High-Pressure-H		V			
X	19	Fe2O3(s3)	FactPS	High-Pressure-H		V			
X	20	Fe3O4(s)	FactPS	Magnetite		V			
X	21	Fe3O4(s2)	FactPS	Magnetite		V			
X	22	Fe3O4(s3)	FactPS	High-Pressure-m		V			
X	23	Fe3O4(s4)	FactPS	High-Pressure-m		V			
+	24	Fe(s)	FSstel	BCC_A2	0				
+	25	Fe(s2)	FSstel	FCC_A1	0				
+	26	FeO(s)	FSstel	Wustite		V			
X	27	Fe2O3(s)	FSstel	hematite		V			
X	28	Fe2O3(s2)	FSstel	High-Pressure-H		V			
X	29	Fe2O3(s3)	FSstel	High-Pressure-H		V			
X	30	Fe3O4(s)	FSstel	Magnetite		V			
X	31	Fe3O4(s2)	FSstel	Magnetite		V			
X	32	Fe3O4(s3)	FSstel	High-Pressure-m		V			
X	33	Fe3O4(s4)	FSstel	High-Pressure-m		V			
+	34	Fe2O3(s)	FToxid	hematite		V			
+	35	Fe2O3(s2)	FToxid	High-Pressure-H		V			
+	36	Fe2O3(s3)	FToxid	High-Pressure-H		V			

permit selection of 'X' species [Help](#) [Suppress Duplicates](#) [Edit priority list](#):

Show Selected Select All Select/Clear... Clear OK

Oxygen partial pressure can be selected by this option



EX15-2. phase diagram PO₂ – X: Oxidation of Fe-Cr

If we want to use oxygen as one of axes, O₂ should be added as input component

Databases - 3/23 compound databases, 2/23 solution databases

FactSGE Private Databases

FactPS FSopp BINS compounds only
 FToxid FSlead SGPS solutions only
 FTsalt FSstel SGTE no database
 FTmisc FSups SGsold
Other EXAM SGTEa SGTEI
 ELEM SGnobl SpMCBN Add/Remove Data
 FTdemo TDmeph RefreshDatabases
 FTlite FTnucl TDnucl

Information

Options - search for product species

Include compounds
- gaseous ions (plasmas)
- aqueous species
- limited data compounds (25C)

Default Cancel Summary ...

Phase Diagram - Menu: comments

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Components (3)

(gram) O₂ + Fe + Cr

Products

Compound species

<input type="checkbox"/> gas	<input checked="" type="radio"/> ideal	<input type="radio"/> real	0
<input type="checkbox"/> aqueous			0
<input type="checkbox"/> pure liquids			0
<input checked="" type="checkbox"/> pure solids			17
* - custom selection		species:	17

* - custom selection species: 17

Target
- none -
Estimate T(K): 1000

Solution phases

*	+	Base-Phase	Full Name
*	+	FSstel-Liqu	LIQUID
J		FSstel-FCC	FCC_A1
I		FSstel-BCC	BCC_A2
+		FSstel-SIGM	SIGMA
I		FToxid-SLAGA	A-Slag-liq all oxides + S
+		FToxid-SPINA	A-Spinel
+		FToxid-MeO_A	A-Monoxide
+		FToxid-CORU	M2O ₃ (Corundum)

Legend
I - immiscible 3
J - 3-immiscible 1
+ - selected 4

Show all selected
species: 52 Select
solutions: 13 Select

Variables

T(C)	log10(p(O ₂))	Cr/(Fe+Cr)		
1200	-20.0	0.1		

log10 p(O₂)/atm vs Cr/(Fe+Cr)

Custom Solutions
0 fixed activities Details ...
0 ideal solutions

Pseudonyms
apply Edit ...

Volume data
 assume molar volumes of solids and liquids = 0
 include molar volume data and physical properties data

paraequilibrium & Gmin edit

Total Species (max 5000) 69
Total Solutions (max 200) 13
Total Phases (max 1500) 30

Phase Diagram

Y
X
- no time limit - Calculate >

Variables: O2-Fe-Cr log10 p(O₂)/atm vs composition #1.

Variables

- Y
- X
- a b
- c d
- A C
- B D
- X,Y steps [11]

compositions [1]

T and P

Temperature: T(°C) constant 1200

Pressure or Volume: P(atm) constant 1

log P

V(litre)

log V

Chemical Potentials

#1 log10(p/atm) Y-axis

O₂ 0 gas-FactPS -20

Compositions Quantity(g)

#1. 0 Fe + 1 Cr X-axis

1 Fe + 1 Cr = 1 (max)
0 (min)

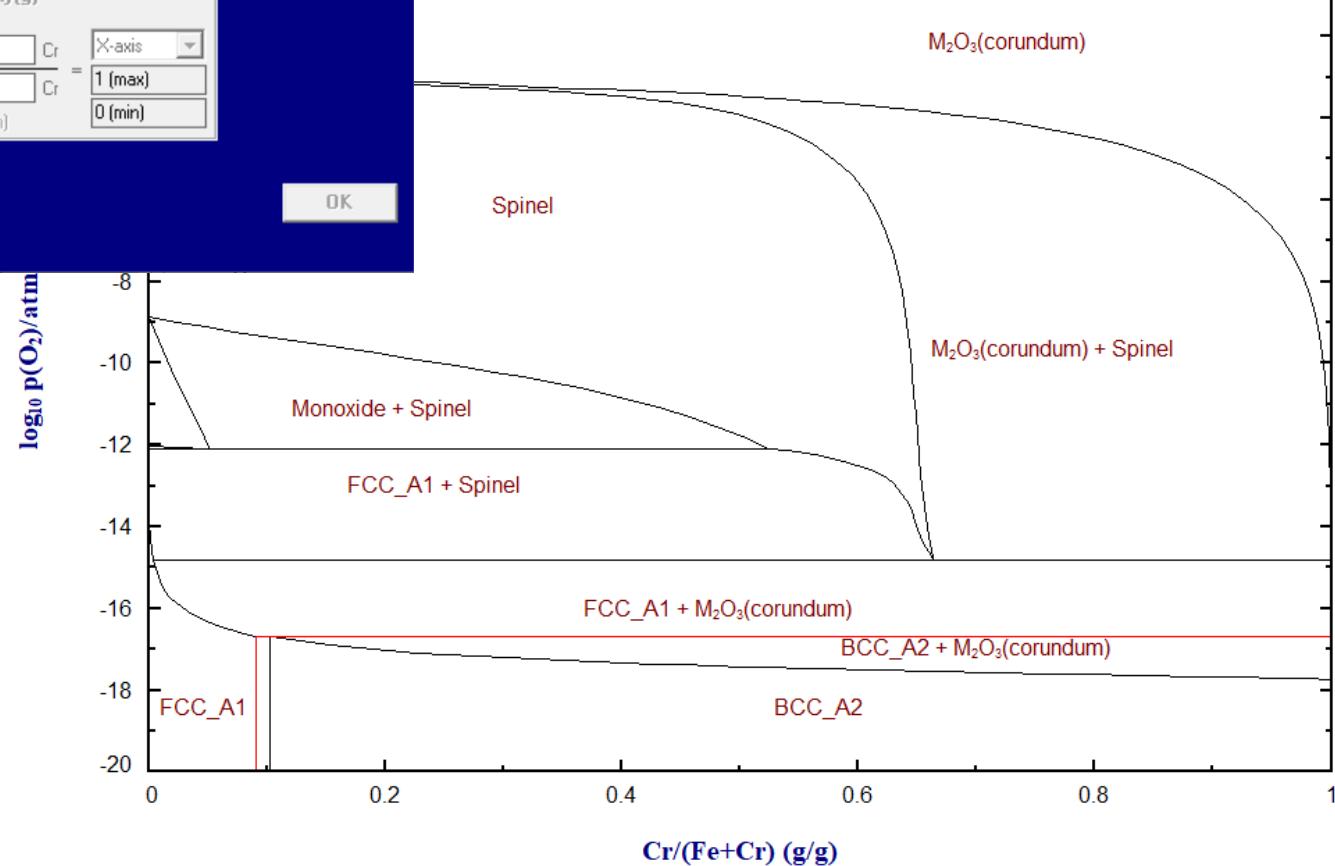
#1 log10(composition)

OK

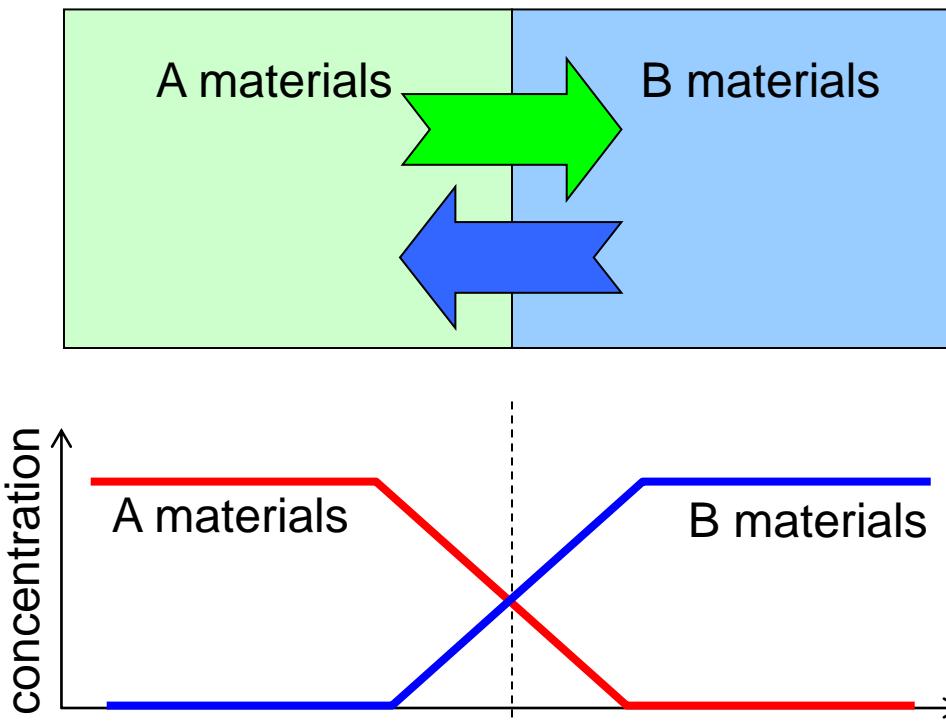
Cancel

O₂ - Fe - Cr
1200°C, 1 atm

FactSage™



EX16. <A> option: Simple counter-cross inter-diffusion calc.



Any kind of counter-cross inter-diffusion reaction at interface can be simulated with <A> option in Equilib. This assume the diffusivity of all components in both materials are the same.

Joining of <A>Al-Mg // <1-A>AZ31

Equilib - Reactants

File Edit Table Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

1 - 2 |

Quantity(g)	Species	Phase
<A>	Al0.97Mg0.03	
+ <1-A>	Mg0.965Al0.03Zn0.005	

T(C) P(total)** Stream# Data

Equilib - Menu: last system

File Units Parameters Help

로그인 사용자: Kim Taehyoung (hhkим1@naver.com)

Reactants (2)

(gram) <A> Al0.97Mg0.03 + <1-A> Mg0.965Al0.03Zn0.005

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- + pure solids 35

species: 35

Solution phases

*	+	Base-Phase	Full Name
		FTlite-Liqu	Liquid
		FTlite-A1	FCC-A1
		FTlite-A2	BCC-A2
		FTlite-A3	HCP-A3
		FTlite-A3"	HCP-Zn Prototype-Mg
		FTlite-A12	CBCC-A12 Prototype-Mn
		FTlite-C14	C14 Prototype-MgZn2
		FTlite-C36	C36 Prototype-MgNi2

Custom Solutions
 fixed activities
 ideal solutions

Pseudonyms
 apply

Volume data
 assume molar volumes of solids and liquids = 0
 include molar volume data and physical properties data

paraequilibrium & Gmin

Total Species (max 5000) 153
Total Solutions (max 200) 24
Total Phases (max 1500) 59

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
0 1 0.01		450	1	
10 steps	<input type="checkbox"/> Table	101 calculations		

FactSage 8.0 Equilibrium

normal normal + transitions
 transitions only open
- no time limit -

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

A=0.13	A=0.14	A=0.15	A=0.16	A=0.17	A=0.18	A=0.19	A=0.2	A=0.21	A=0.22	A=0.23	A=0.24	
A=0	A=0.01	A=0.02	A=0.03	A=0.04	A=0.05	A=0.06	A=0.07	A=0.08	A=0.09	A=0.1	A=0.11	A=0.12

(gram) <A> Al0.97Mg0.03 + <1-A> Mg0.965Al0.03Zn0.005 =

1.0000 gram HCP-A3#1
 (1.0000 gram, 2.0333E-02 mol)
 (450 C, 1 atm, a=1.0000)
 (3.2517 wt.% Al2Va
 + 95.379 wt.% Mg2Va
 + 1.3294 wt.% Zn2Va)

System component Amount/mol Amount/gram Mole fraction Mass fraction

Zn	2.0333E-04	1.3294E-02	5.0000E-03	1.3294E-02
Al	1.2200E-03	3.2917E		
Mg	3.9243E-02	0.95379		

+ 0 gram HCP-Zn#2

+ 0 gram HCP-Zn#1
 (450 C, 1 atm, a=0.98090)
 (2.9544 wt.% Al
 + 95.161 wt.% Mg
 + 1.8845 wt.% Zn)

+ 0 gram HCP-Zn#2

+ 0 gram Liquid#1
 (450 C, 1 atm, a=0.90212)
 (10.086 wt.% Al
 + 73.995 wt.% Mg
 + 15.829 wt.% Zn)

+ 0 gram Liquid#2

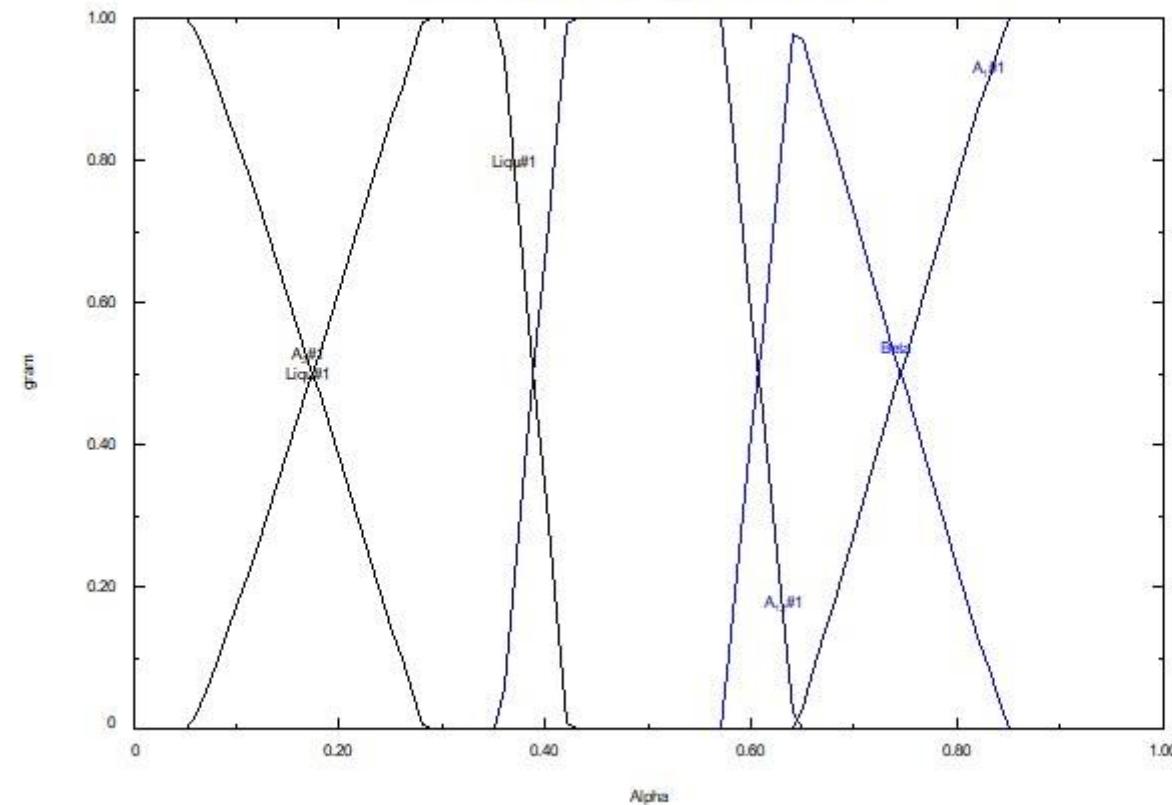
+ 0 gram BCC-A2#1
 (450 C, 1 atm, a=0.79240)
 (1.4444 wt.% Al
 + 87.489 wt.% Mg)

Final Conditions

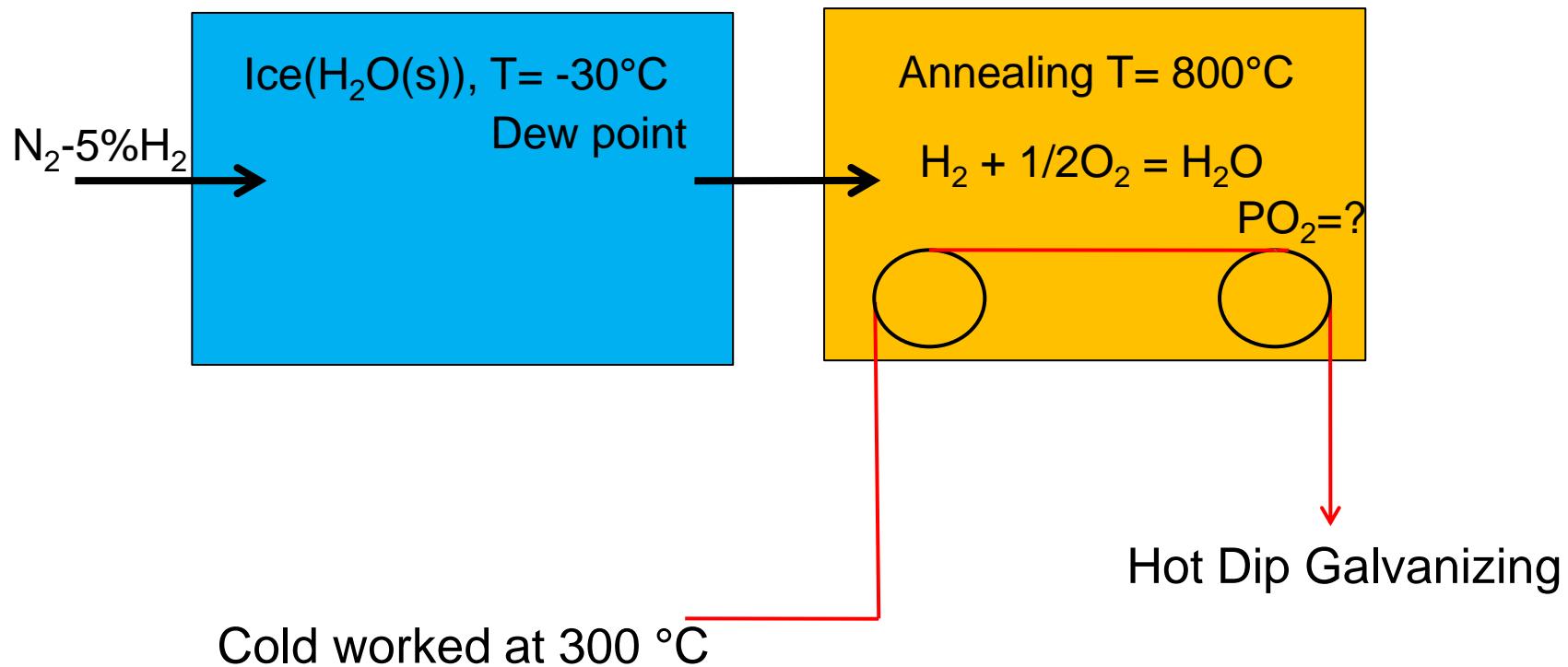
<A>		T(C)	P(atm)
010.01		450	1

<A> Al0.97Mg0.03 + <1-A> Mg0.965Al0.03Zn0.005

C:\FACTSAGEWS\Equi0.res 29Jun23



EX17. Oxygen partial pressure control for oxidation of metals



EX17-1. Oxygen partial pressure control using Dew-point concept

We should select real gas to obtain accurate Gibbs energy and volume fraction of gas at low temperature and high pressure.

The screenshot shows the FactSage 8.3 software interface. On the left, a 'Reactants' window displays the initial composition: 95 mol N₂, 5 mol H₂, and 1 mol H₂O. On the right, a 'Menu: last system' window shows the reaction equation: 95 N₂ + 5 H₂ + H₂O. Below these are sections for 'Products', 'Solution phases', and 'Final Conditions'. In the 'Products' section, there is a dropdown menu with options: 'gas', 'ideal', and 'real'. A red arrow points from the text in the top right towards this dropdown. The 'Solution phases' section includes a table for 'Base-Phase' and a 'Legend' section. The 'Final Conditions' section allows setting conditions for species <A>, , T(C), P(atm), and Product H(J). The bottom right contains 'Equilibrium' settings and a 'Calculate' button. The bottom of the screen shows the FactSage 8.3 logo and the page number 73.

F Equilib - Results -30 C

Output Edit Show Pages Final Conditions

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

FactSage 8.3

T = -30.00 C
P = 1 atm
V = 1927.2 dm³

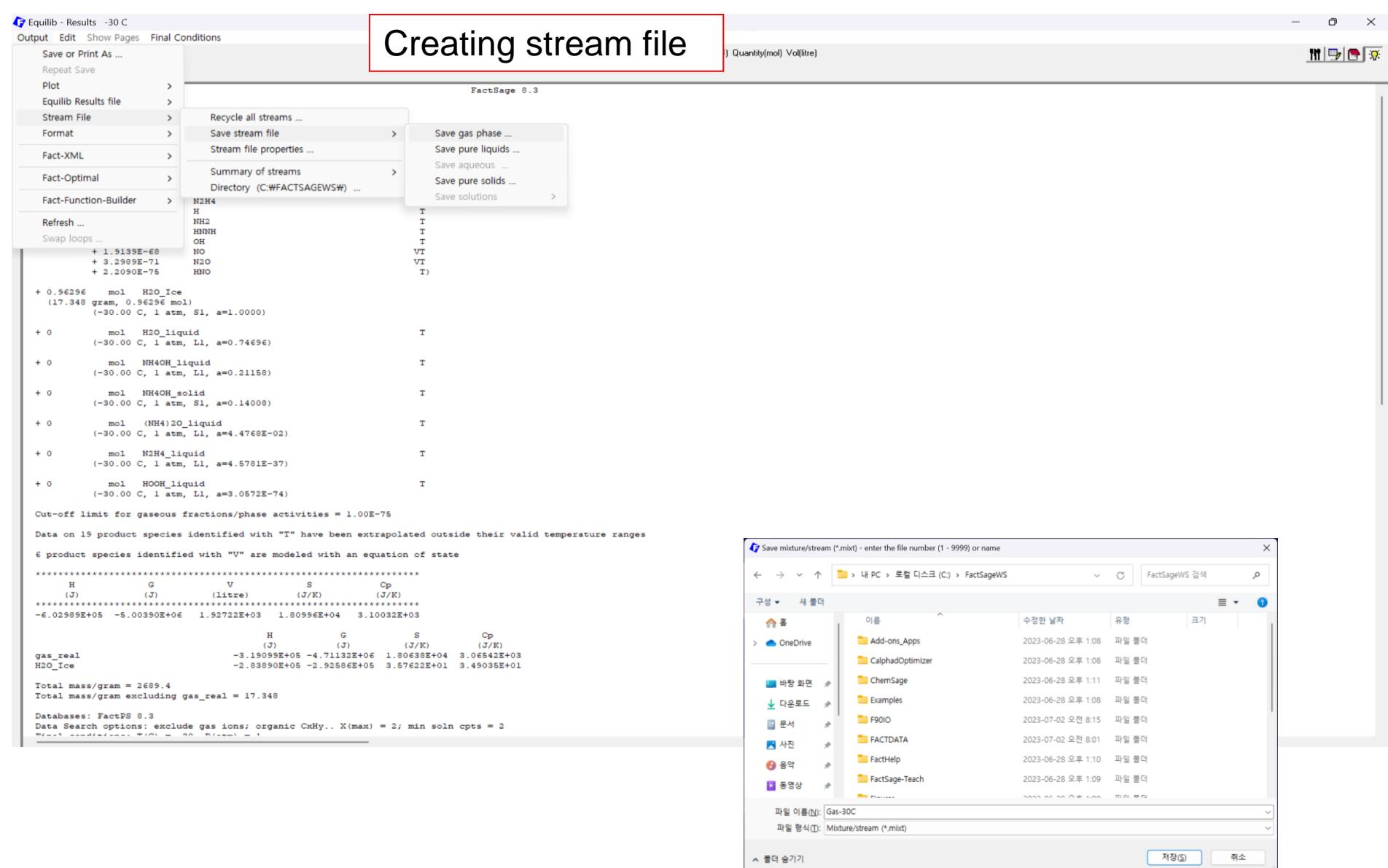
STREAM CONSTITUENTS

	AMOUNT/mol
N ₂	9.5000E+01
H ₂	5.0000E+00
H ₂ O	1.0000E+00

PHASE: gas_real

	EQUIL AMOUNT mol	MOLE FRACTION	FUGACITY atm	
N ₂	9.3336E+01	9.6512E-01	9.6421E-01	
NH ₃	3.3280E+00	3.4413E-02	3.4117E-02	
H ₂ O	3.7039E-02	3.8299E-04	3.7730E-04	
H ₂	7.9665E-03	8.2376E-05	8.2554E-05	
N ₂ H ₅ OH	4.9431E-38	5.1114E-40	5.1010E-40	
N ₂ H ₄	1.2503E-38	1.2928E-40	1.2902E-40	
H	4.9894E-45	5.1592E-47	5.1487E-47	
NH ₂	2.1431E-45	2.2160E-47	2.2115E-47	
HNNH	5.0399E-54	5.2114E-56	5.2008E-56	
OH	2.7152E-57	2.8076E-59	2.8019E-59	
NO	1.8509E-66	1.9139E-68	1.9111E-68	
N ₂ O	3.1904E-69	3.2989E-71	3.2770E-71	
HNO	2.1363E-73	2.2090E-75	2.2045E-75	
TOTAL:	9.6709E+01	1.0000E+00	1.0000E+00	
System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
O	3.7039E-02	0.59260	1.8509E-04	2.2178E-04
N	190.00	2661.3	0.94947	0.99598
H	10.074	10.154	5.0342E-02	3.8001E-03
			ACTIVITY	
H ₂ O_Ice(s)	9.6296E-01		1.0000E+00	
H ₂ O_liquid(liq)	T	0.0000E+00	7.4696E-01	
NH4OH_liquid(liq)	T	0.0000E+00	2.1158E-01	
NH4OH_solid(s)	T	0.0000E+00	1.4008E-01	
(NH4) ₂ O_liquid(liq)	T	0.0000E+00	4.4768E-02	
N ₂ H ₄ _liquid(liq)	T	0.0000E+00	4.5781E-37	
HOOH_liquid(liq)	T	0.0000E+00	3.0572E-74	

We will heat this gas at 800°C using stream file.



Importing stream file

File Edit Run Macro Table Units Data Search Data Evaluation Help

Add a new Reactant Ctrl+R

J) Quantity(mol) Vol(litre)



1
Add a new Reactant Ctrl+R
Insert new reactant before N2 ...
Delete reactant N2 ...
Delete all blank reactants

Mixtures and Streams >

Gas-30C GAS stream

Re-order

Export list of reactants

Import list of reactants

Clear

Example

Import a mixture >

Import a stream (or single-line mixture) >

Edit a mixture or stream >

Directory (C:\FACTSAGEWS\)...

 Initial Conditions

Next >>

Equilib - Reactants

File Edit Run Macro Table Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

1-1

Quantity(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
100%	[Gas-30C]					

Equilib - Menu: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Reactants (1)

100% [Gas-30C]

Products

Compound species

- gas ideal real 29
- aqueous 0
- pure liquids 8
- pure solids 8

species: 45

Target
- none -
Estimate T(K): 1000
Quantity(mol): 0

Solution phases

*	+	Base-Phase	Full Name

Legend Show all selected
species: 0 solutions: 0

Custom Solutions
0 fixed activities
0 ideal solutions

Pseudonyms
 apply

Volume and physical prop data
 assume molar volumes of solids and liquids = 0
 use only molar volume data
 use V & phys. property data

paraequilibrium & Gmin

Virtual species: 10
 Total Species (max 7000) 45
 Total Solutions (max 200) 0
 Total Phases (max 1500) 17

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		800	1	

10 steps Table

Equilibrium
 normal normal + transitions
 transitions only open
 - no time limit -

FactSage 8.3

Equilib - Results 800 C

Output Edit Show Pages Final Conditions

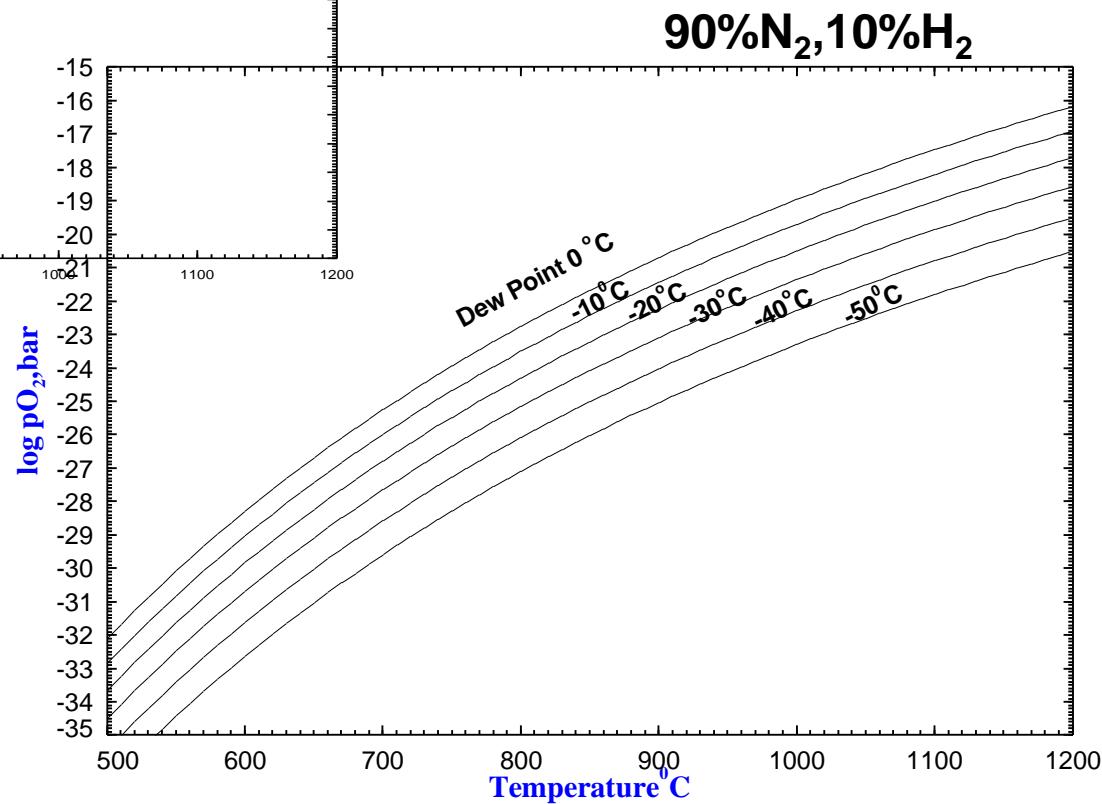
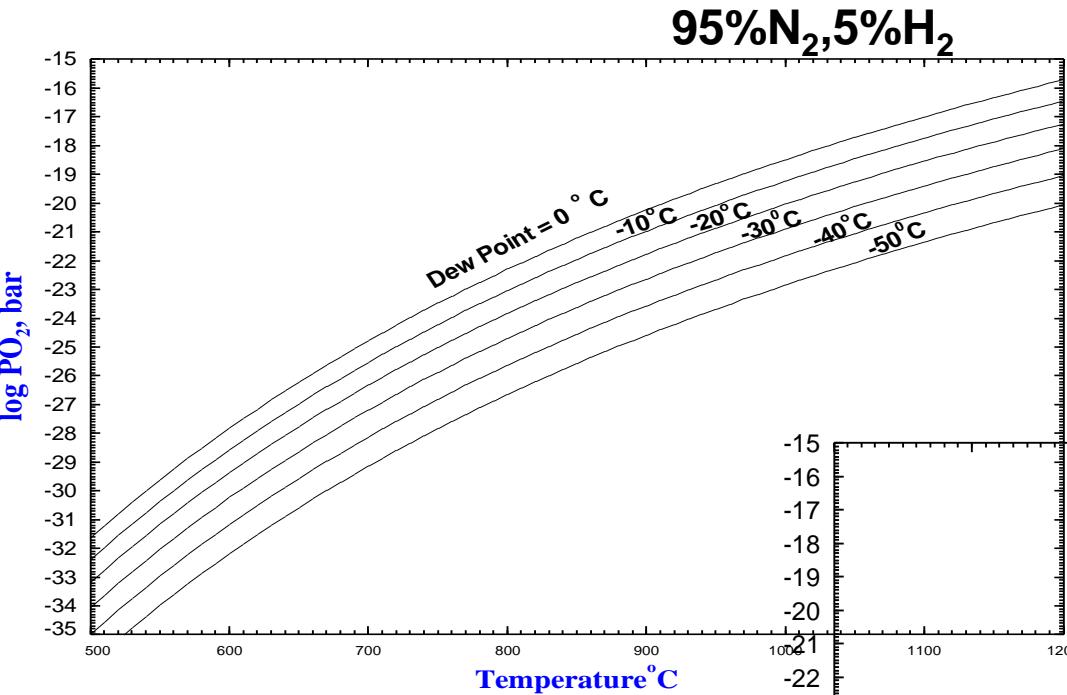
T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Final partial pressure of oxygen

when the temperature of ice is
-20°C

PHASE: gas_real	EQUIL AMOUNT	MOLE FRACTION	FUGACITY
	mol		atm
N2	V 9.5000E+01	9.4965E-01	9.5001E-01
H2	V 4.9994E+00	4.9976E-02	4.9991E-02
H2O	V 3.7039E-02	3.7025E-04	3.7026E-04
NH3	V 4.0986E-04	4.0971E-06	4.0979E-06
H	V 3.1242E-07	3.1231E-09	3.1242E-09
NH2		3.3130E-11	3.3118E-13
OH		8.9872E-12	8.9840E-14
NO	V 8.6783E-14	8.6751E-16	8.6781E-16
HNNH		3.1114E-16	3.1102E-18
NH		1.1411E-16	1.1407E-18
N2H4		9.4883E-18	9.4849E-20
N2O	V 6.2157E-18	6.2135E-20	6.2152E-20
HNO		5.7522E-18	5.7501E-20
N		1.4265E-18	1.4265E-20
O		6.0821E-19	6.0798E-21
O2	V 2.3991E-21	2.3982E-23	2.3989E-23
HOOH		1.1951E-21	1.1947E-23
N3		4.9610E-22	4.9592E-24
HONO(g2)		1.9949E-24	1.9941E-26
HOO		1.9209E-24	1.9202E-26
HONO(g)		1.5478E-24	1.5472E-26
NO2	V 3.0404E-26	3.0393E-28	3.0404E-28
N2H5OH	T 7.3321E-27	7.3294E-29	7.3321E-29
HONO2		1.4598E-37	1.4593E-39
O3	V 3.3353E-43	3.3340E-45	3.3357E-45
NO3		4.8740E-44	4.8722E-46
N2O3		1.1927E-46	1.1923E-48
N2O4		7.1335E-60	7.1308E-62
TOTAL:		1.00004E+02	1.00000E+00
System component	Amount/mol	Amount/gram	Mole fraction Mass fraction
O	3.7039E-02	0.59260	1.8509E-04 2.2178E-04
N	190.0	2661.3	0.94947 0.99598
H	10.074	10.154	5.0342E-02 3.8001E-03
N2H4			V 9.4763E-18 9.4669E-20 9.4703E-20
O			V 1.6505E-18 1.6488E-20 1.6494E-20
N			V 1.4269E-18 1.4255E-20 1.4260E-20
O2			V 1.7656E-20 1.7638E-22 1.7643E-22
HOOH			V 8.7896E-21 8.7808E-23 8.7840E-23
N3			V 4.9595E-22 4.9545E-24 4.9563E-24
HONO(g2)			V 1.4672E-23 1.4657E-25 1.4662E-25

Dew points – PO₂/T Relationship



EX17-2. phase diagram PO_2 – T: Oxidation of Fe-1%Mn-1%Si

Data Search - Equilib 8.3

Databases - 4/21 compound databases, 3/18 solution databases

FactSage™

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Components (4)

(gram) $\text{O}_2 + \text{Fe} + \text{Mn} + \text{Si}$

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- * pure solids 100
- * - custom selection species: 100

Solution phases

*	+	Base-Phase	Full Name
I		FSstel-Liqu	LIQUID
J		FSstel-FCC	FCC_A1
I		FSstel-BCC	BCC_A2
I		FSstel-HCP	HCP_A3
+		FSstel-CBCC	CBCC_A12
+		FSstel-CUB	CUB_A13
+		FSstel-M3Si1	Me3Si1
+		FSstel-M1Si1	Me1Si1

Custom Solutions

- 0 fixed activities
- 0 ideal solutions

Pseudonyms

- apply Edit ...

Volume and physical prop data

- assume molar volumes of solids and liquids = 0
- use only molar volume data
- use V & phys. property data

paraequilibrium & Gmin edit

Virtual species: 44

Total Species (max 7000) 406

Total Solutions (max 200) 59

Total Phases (max 1500) 159

Information

You have selected more than FTlite FSstel FSscopp FSlead SGTE

Since these databases may contain com it is strongly recommended that you

Options - search for product spe

Include co gaseo aquo limited

Default

Cancel

Variables

T(C)	$\log_{10}(p(\text{O}_2))$	$\text{Mn}/(\text{Fe}+\text{Mn}+\text{Si})$	$\text{Si}/(\text{Fe}+\text{Mn}+\text{Si})$
500 1000	-40 -20	0.01	0.01

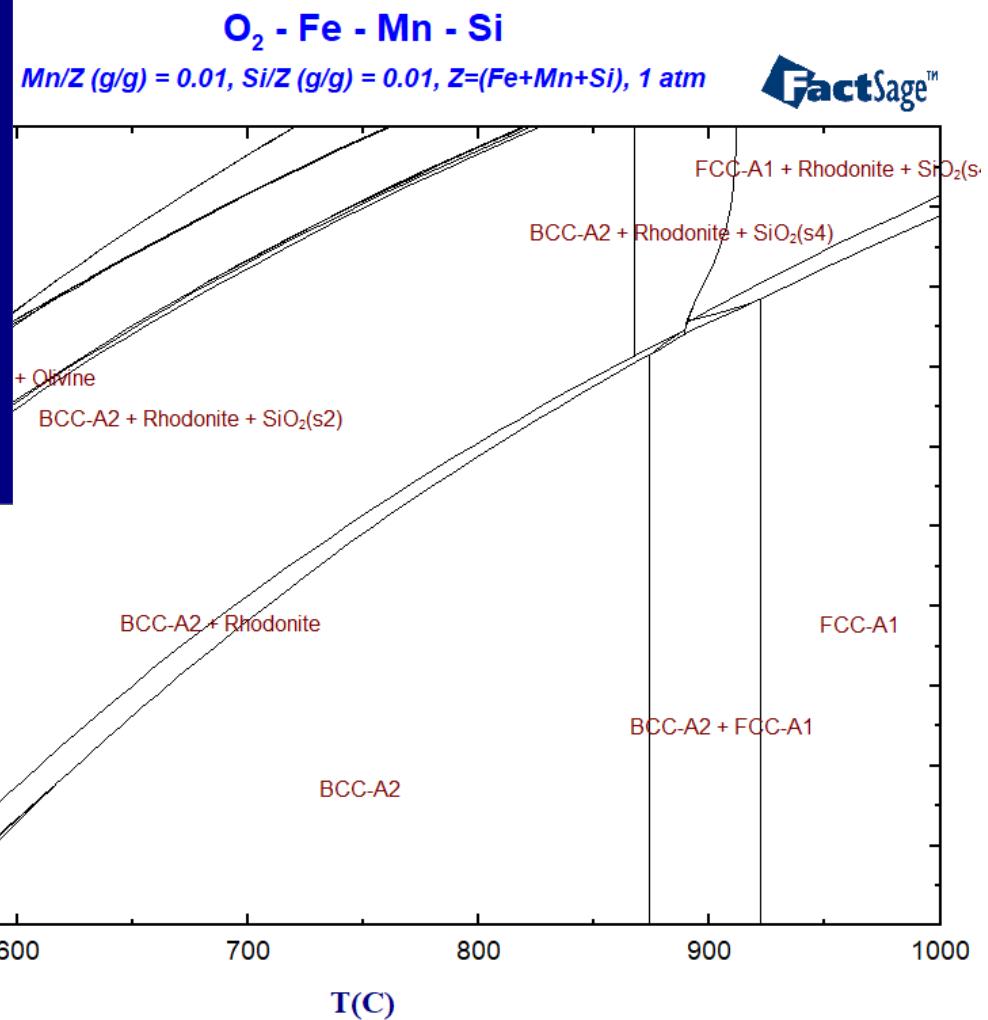
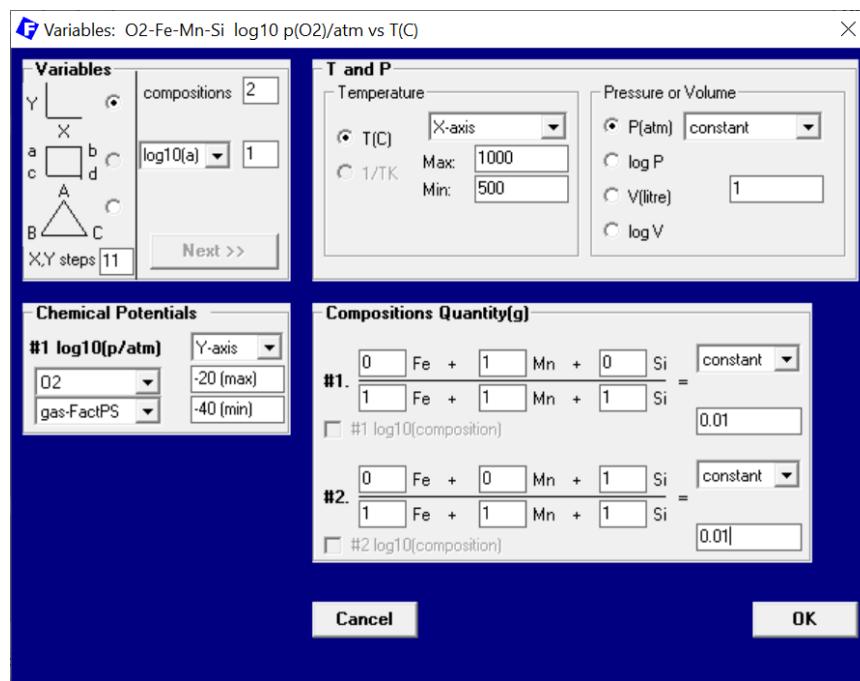
$\log_{10} p(\text{O}_2)$ vs T(C)

Phase Diagram

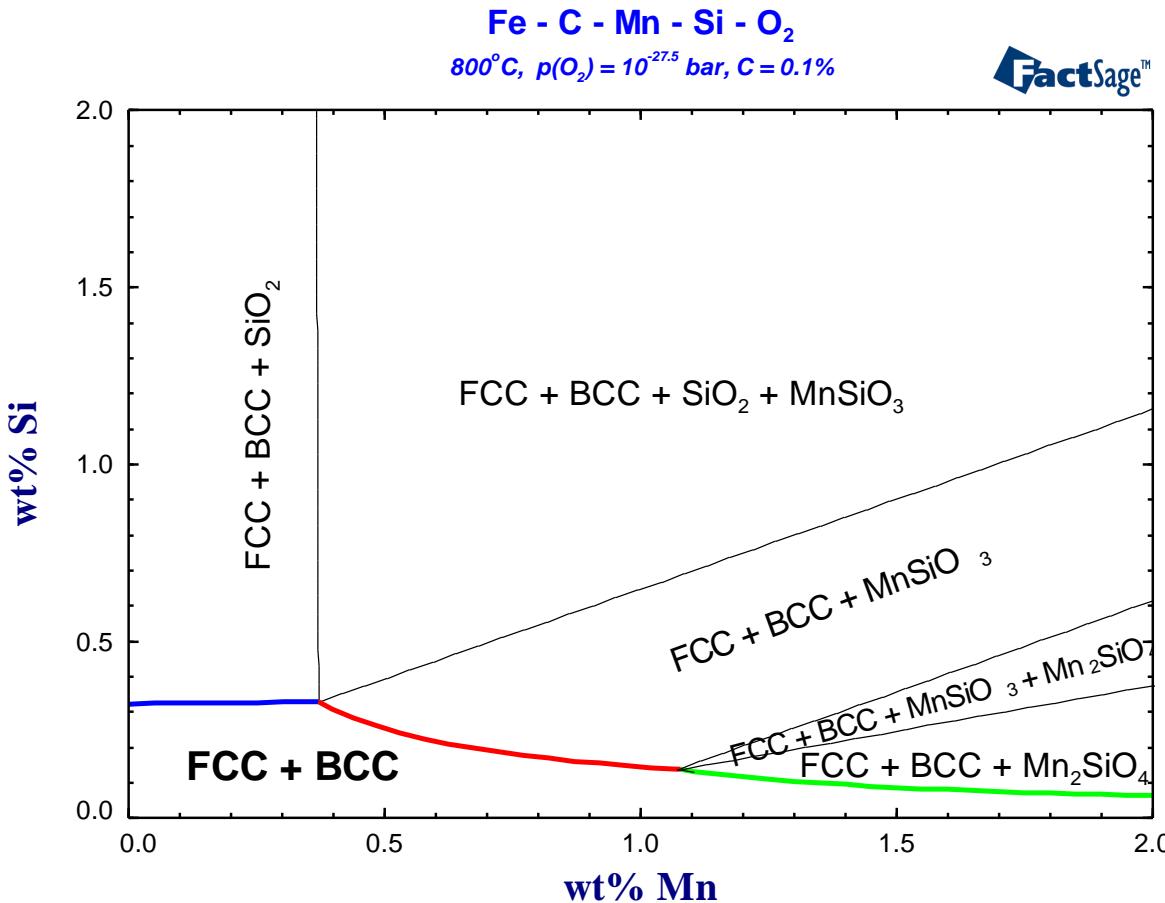
Y X

- no time limit - Calculate >

FactSage 8.3



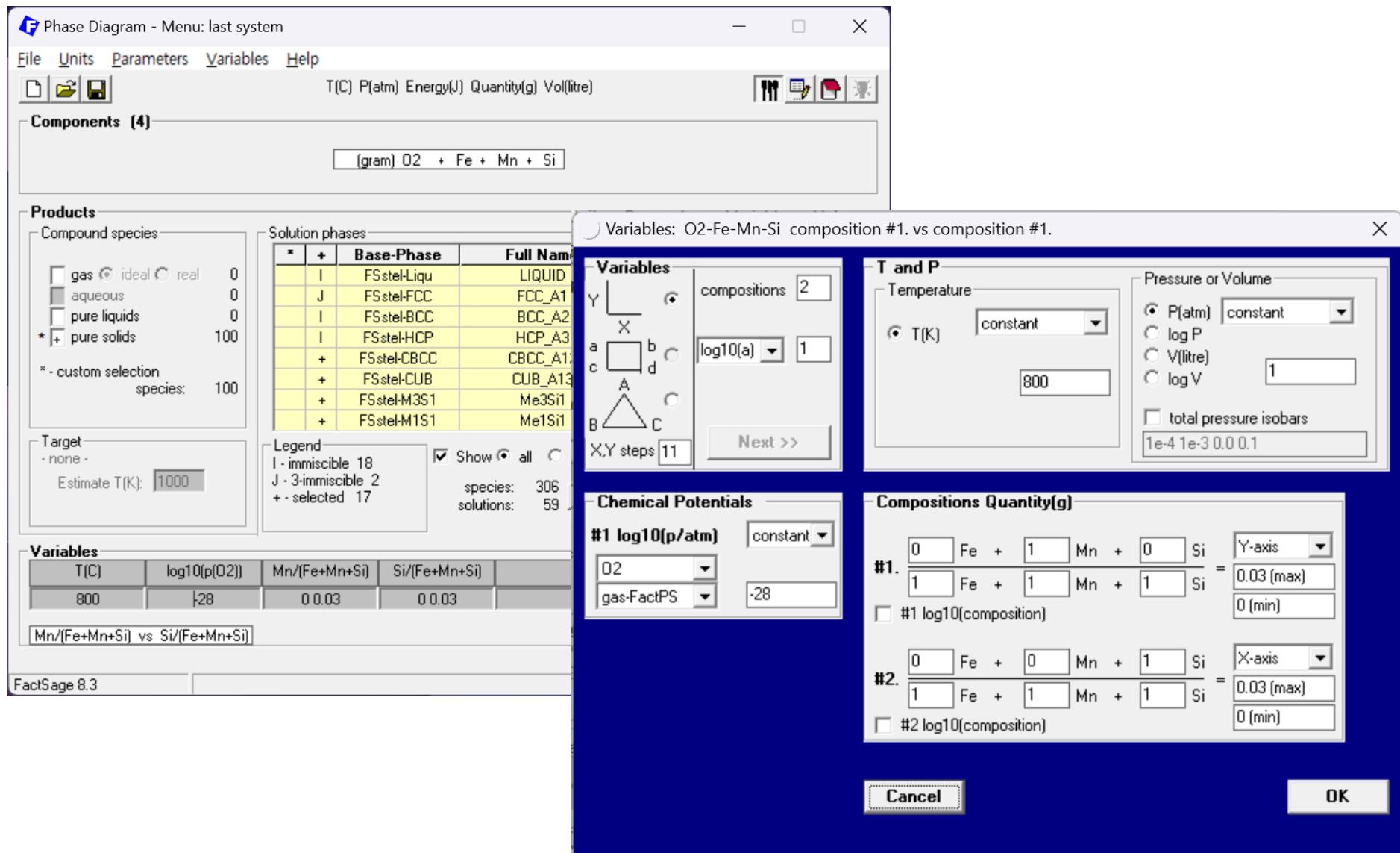
EX17-3. Primary oxide formation diagram



Drawing of the diagram:

- 1) Collect all blue/red/green lines at different PO₂ and superimpose them in one diagram.
- 2) The boundary of each color line (different phase) is the phase boundary of the primary oxide phase in the diagram.

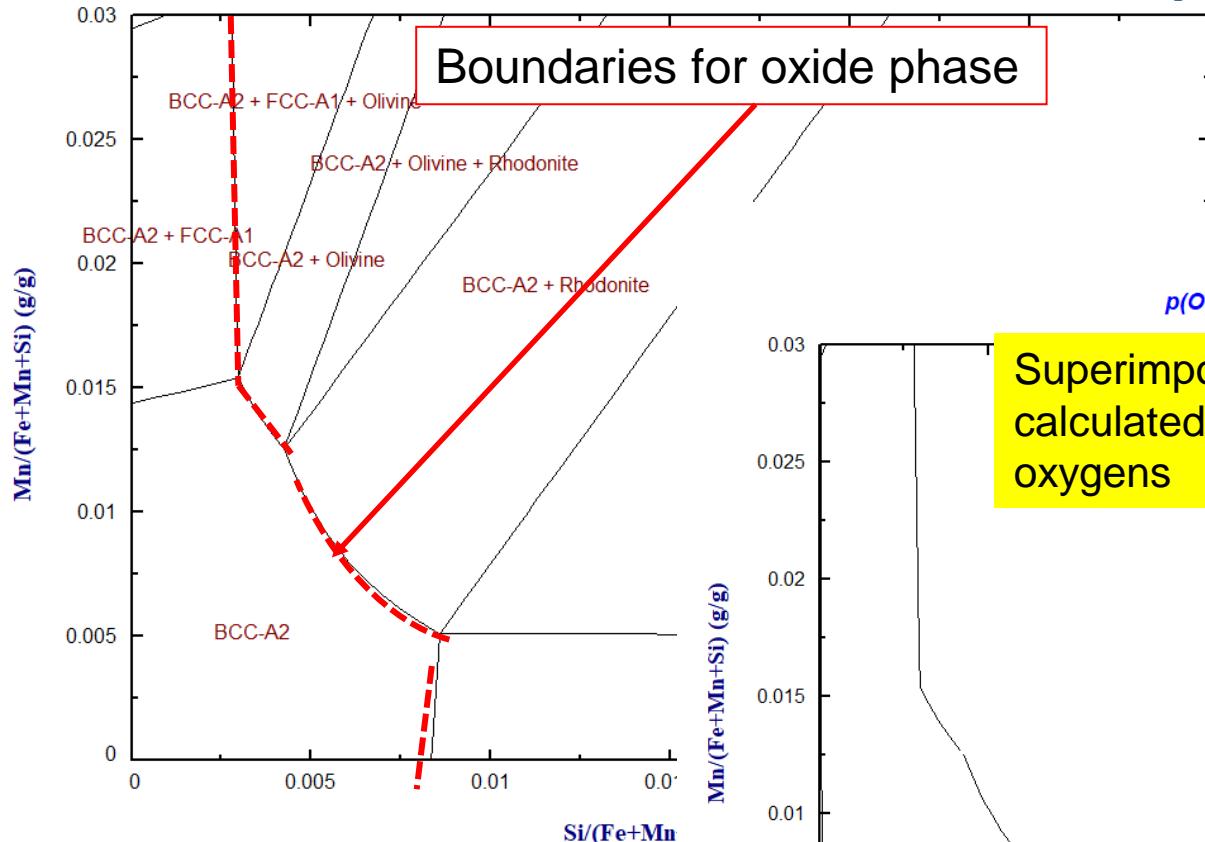
Fe-Mn-Si at $\text{PO}_2=10^{-28}\text{atm}$, T=800°C



EX17-3. Primary oxide formation diagram

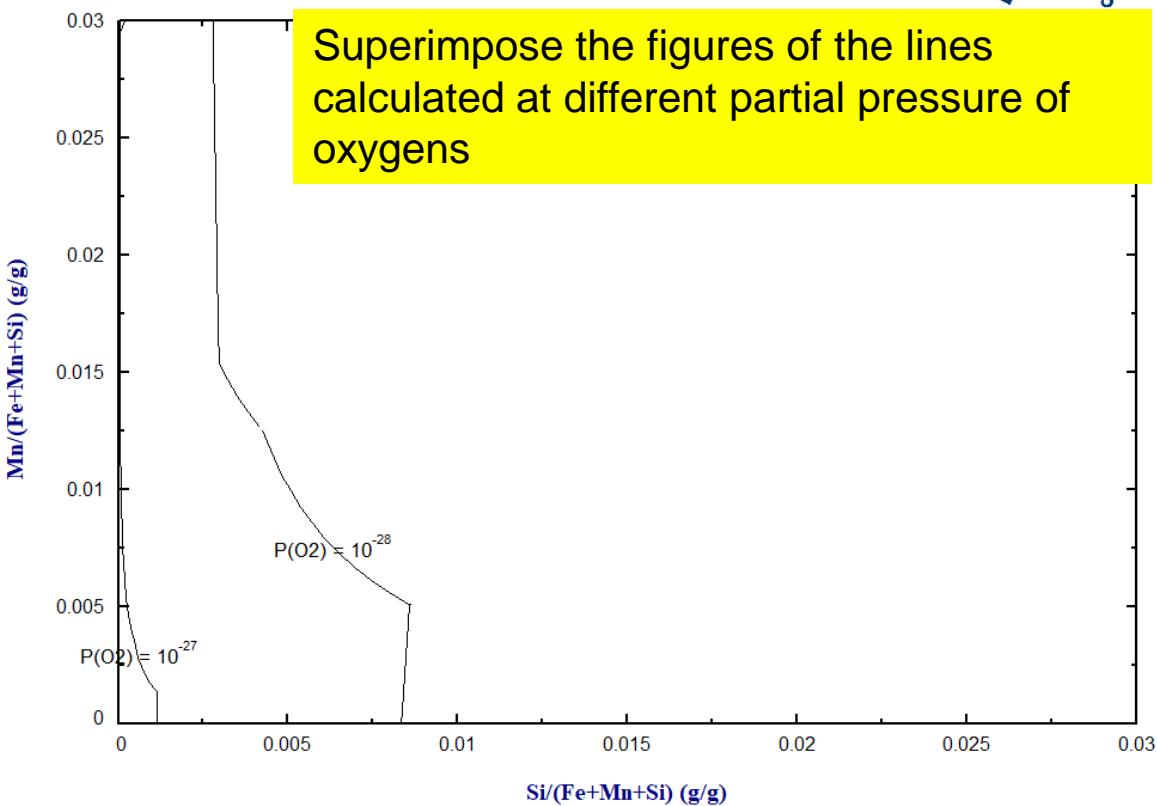
$O_2 - Fe - Mn - Si$
 $p(O_2) = 10^{-28} \text{ atm}, 800^\circ\text{C}, 1 \text{ atm}$

FactSage™

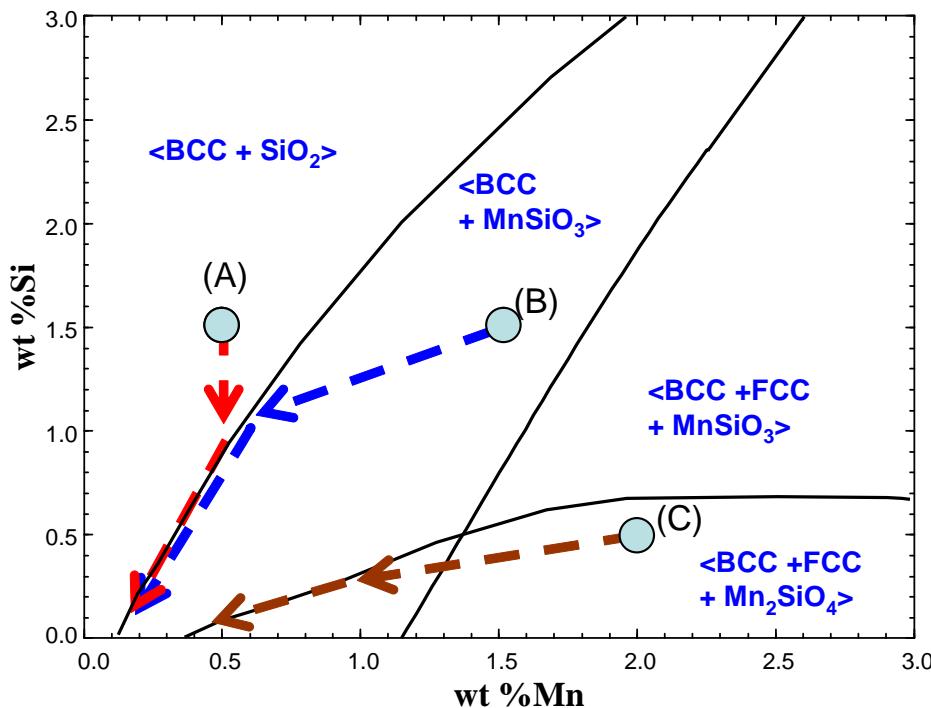


$O_2 - Fe - Mn - Si$
 $p(O_2) = 10^{-27} \text{ atm}, 800^\circ\text{C}, 1 \text{ atm}$

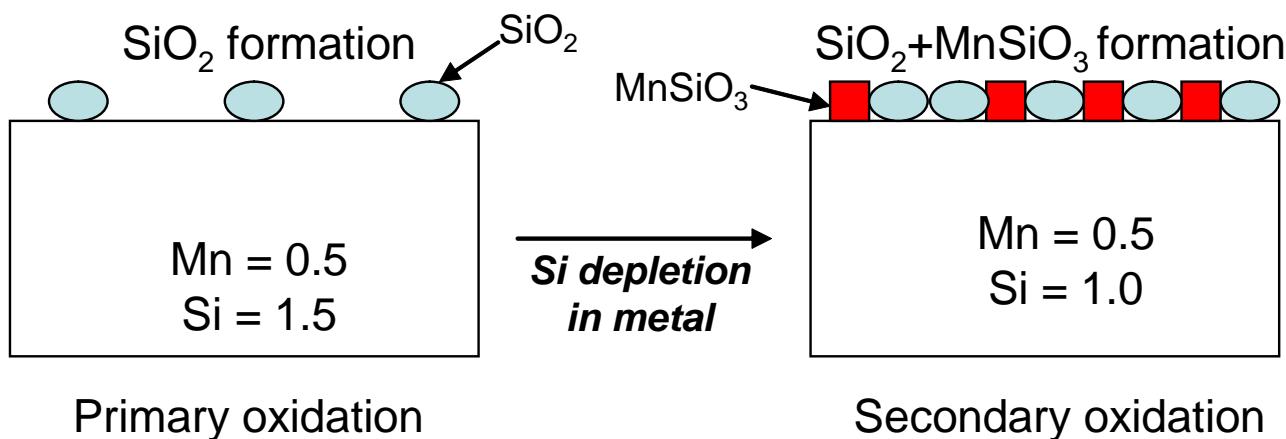
FactSage™



EX17-4. Primary and Secondary Oxidations

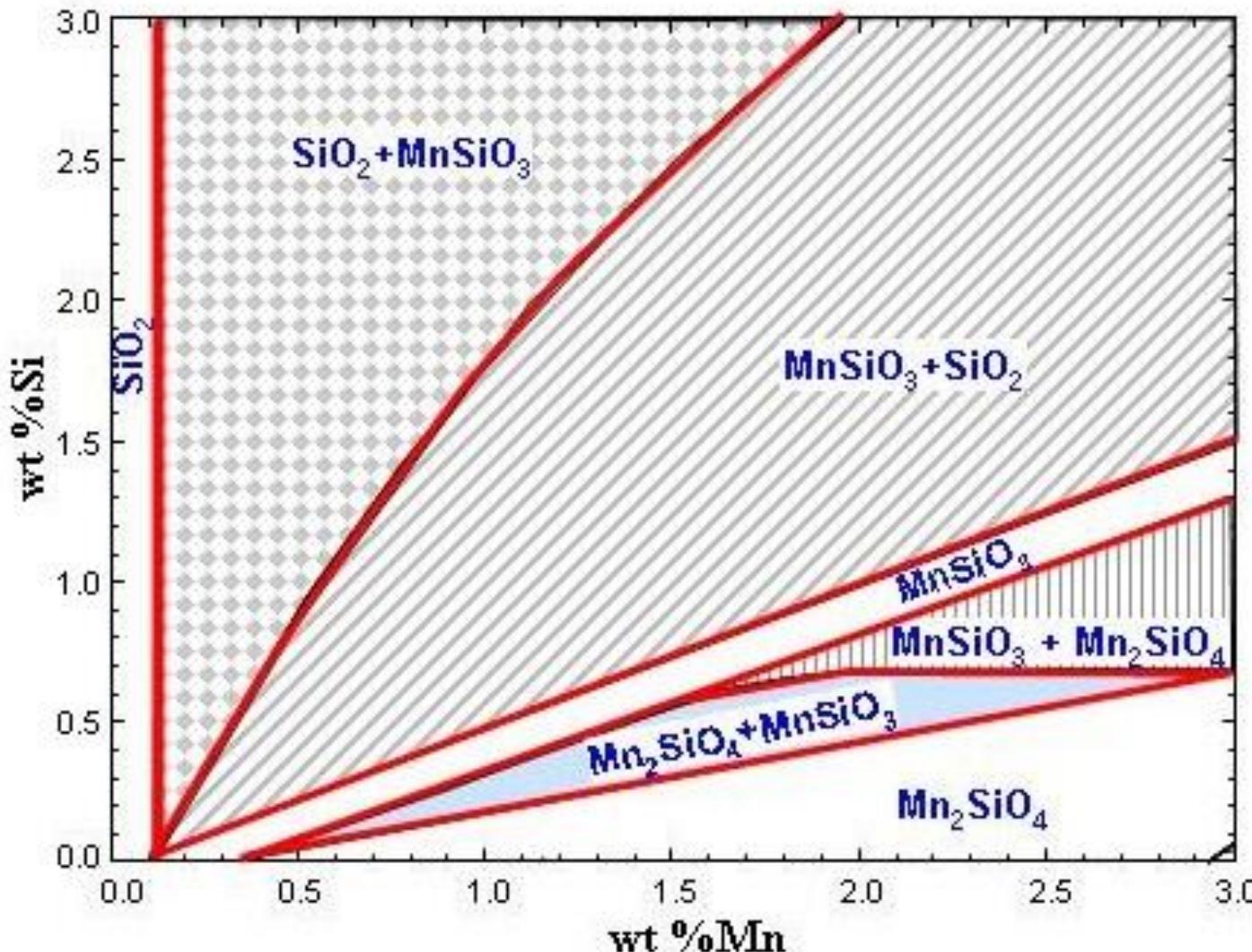


Concept of primary and secondary oxidations

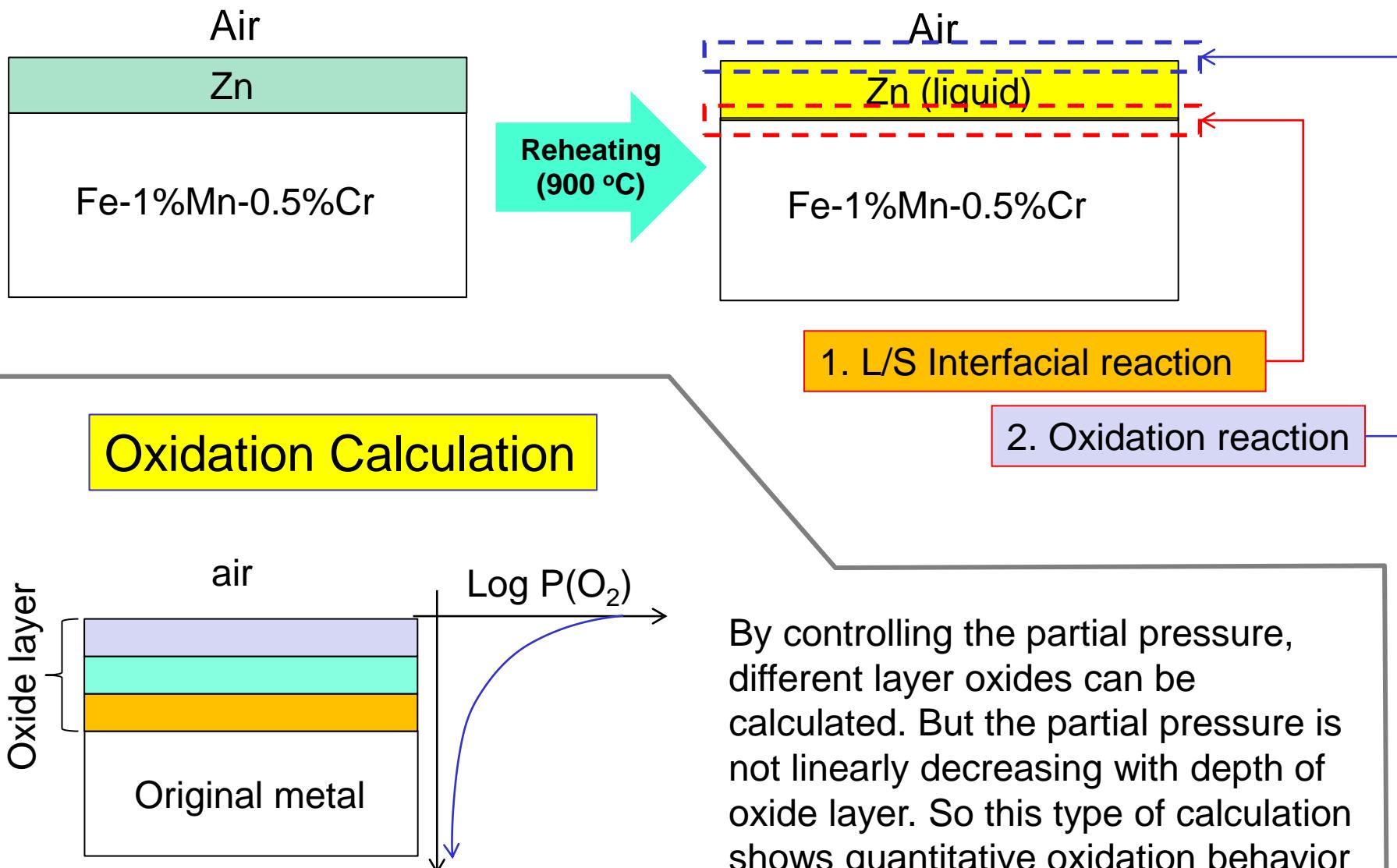


Oxidation phase diagram

Oxidation phase diagram of the Fe-0.002%C-Mn-Si steel at 800°C



EX18. Remelting and oxidation of Zn galvanized steel



EX18-1. Interface reaction between liquid Zn and steel

Data Search - Equilib 8.3

Databases - 1/21 compound databases, 1/18 solution databases

Fact **FactSage™ SGTE**

- FactIPS
- FTtoxic
- FTsulf
- FTsalt
- FTmisc
- FTHall
- FTOxCN
- FTfrtz
- FThelg
- FTpulp
- FTdemo
- FTlite
- FScoff
- FSlead
- FSstel
- FSups
- BINS
- SGPS
- SGTE
- SGold
- SGTEa

Private Databases

Other

- ELEM
- SGnobl
- SpMCBN
- FTlite
- TDmeph
- TDnucl

Information

Click on a box to include (or exclude) a database in the data search compound and solution database (when available) will be selected. (note, this is NOT recommended).

If database is stored on your PC but not listed here then you must 'a'

Options - search for product species

Include compounds

- gaseous ions (plasmas)
- aqueous species
- limited data compounds (25C)

Cancel **Summary**

Equilib - Menu: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (4)

(gram) 100 Zn + 99.5 Fe + 0.5 Cr + Mn

Products

Compound species

gas	<input type="radio"/> ideal	<input checked="" type="radio"/> real	0
aqueous	0		
pure liquids	0		
+ pure solids	32		
	species: 32		

Solution phases

*	+	Base-Phase	Full Name
I		FTlite-Liqu	Liquid
J		FTlite-A1	FCC-A1
I		FTlite-A2	BCC-A2
I		FTlite-A3	HCP-A3
I		FTlite-A3"	HCP-Zn Prototype-Mg
I		FTlite-A12	CBCC-A12 Prototype-Mn
I		FTlite-A13	CUB-A13 Prototype-Mn
I		FTlite-C14	C14 Prototype-MgZn2

Custom Solutions

- 0 fixed activities
- 0 ideal solutions

Pseudonyms

- apply
- Edit ...

Volume and physical prop data

- assume molar volumes of solids and liquids = 0
- use only molar volume data
- use V & phys. property data

Target

- none -

Estimate T(K): 1000

Quantity(g): 0

Legend

- I - immiscible 11
- J - 3-immiscible 1
- + - selected 2

Show all selected

species: 214

solutions: 27

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		900	1	

10 steps Table

1 calculation

Total Species (max 7000) 246

Total Solutions (max 200) 27

Total Phases (max 1500) 59

Equilibrium

- normal
- normal + transitions
- transitions only
- open

- no time limit -

Calculate >>

FactSage 8.3

FTlite database contains reasonable Zn bath data for Zn-galvanizing. So, this is chosen instead of FSStel.

EX18-1. Interface reaction between liquid Zn and steel

Equilib - Results 900 C

Output Edit Show Pages Final Conditions

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

(gram) 100 Zn + 99.5 Fe + 0.5 Cr + Mn =

148.90 gram BCC-A2#1
(148.90 gram, 2.5245 mol)
(900 C, 1 atm, a=1.0000)
(0.18332 wt.% Cr
+ 62.684 wt.% Fe-alpha
+ 0.50769 wt.% Mn
+ 36.625 wt.% Zn)

System component Amount/mol Amount/gram Mole fraction Mass fraction

Zn 0.83412 54.535 0.33041 0.36625
Fe 1.6713 93.336 0.66206 0.62684
Mn 1.3760E-02 0.75595 5.4506E-03 5.0769E-03
Cr 5.2495E-03 0.27296 2.0795E-03 1.8332E-03

+ 0 gram BCC-A2#2

+ 52.100 gram Liquid#1
(52.100 gram, 0.81458 mol)
(900 C, 1 atm, a=1.0000)
(0.43578 wt.% Cr
+ 11.830 wt.% Fe
+ 0.46843 wt.% Mn
+ 87.266 wt.% Zn)

System component Amount/mol Amount/gram Mole fraction Mass fraction

Zn 0.69540 45.465 0.85369 0.07266
Fe 0.11037 6.1635 0.13549 0.11830
Mn 4.4424E-03 0.24405 5.4536E-03 4.6843E-03
Cr 4.3666E-03 0.022704 5.3605E-03 4.3578E-03

+ 0 gram Liquid#2

+ 0 gram FCC-Al#1
(900 C, 1 atm, a=0.98256)
(3.5407 wt.% Cr
+ 70.241 wt.% Fe-gamma
+ 0.60866 wt.% Mn
+ 25.610 wt.% Zn)

+ 0 gram FCC-Al#2

We need this liquid Zn for the oxidation reaction
→ Save it as stream

Reaction products:
Zn-rich Liquid

Reaction products:
BCC + FCC

Original steel:
Fe-1%Mn-0.5%Cr

EX18-2. Oxidation reaction of liquid Zn

Data Search - Equilib 8.3

Databases - 2/21 compound databases, 1/18 solution databases

- FactPS
- FToxid
- FTsalt
- FTmisc
- FThall
- FTOxCN
- FTfritz
- FThelg
- FTlite
- FTpulp
- FTdemo

Information

Options - search for product species

- Include compounds
- gaseous
- aqueous
- limited

Default

Cancel

(1) Setting oxygen partial pressure: activity or log activity can be fixed

Equilib - Menu: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (2)

(1)

[gram] 100% [Zn-liquid] + 0 02

Products

Compound species

+ gas	<input type="radio"/> ideal	<input checked="" type="radio"/> real	11
aqueous	0		
pure liquids	0		
* pure solids	54		

* - custom selection species: 65

Target

- none -

Estimate T(K): 1000

Quantity(g): 0

Solution phases

*	+	Base-Phase	Full Name
*	+	I	FTlite-Liqu
J		J	FCC-A1
I		I	BCC-A2
I		I	HCP-A3
I		I	HCP-Zn Prototype
I		I	CBCC-A12 Prototype
I		I	CUB-A13 Prototype
I		I	C14 Prototype

Custom Solutions

0 fixed activities Details ...
0 ideal solutions

(1)-b

Enter the value of $\log_{10}(p)$
(or for a range of values enter 'first last step') for
2 O₂(g).

Press [Cancel] if the partial pressure is no longer fixed.

(1)-a

-30 0 0.5

Final Conditions

<A>		T(C)	P(atm)	Product
		900	1	

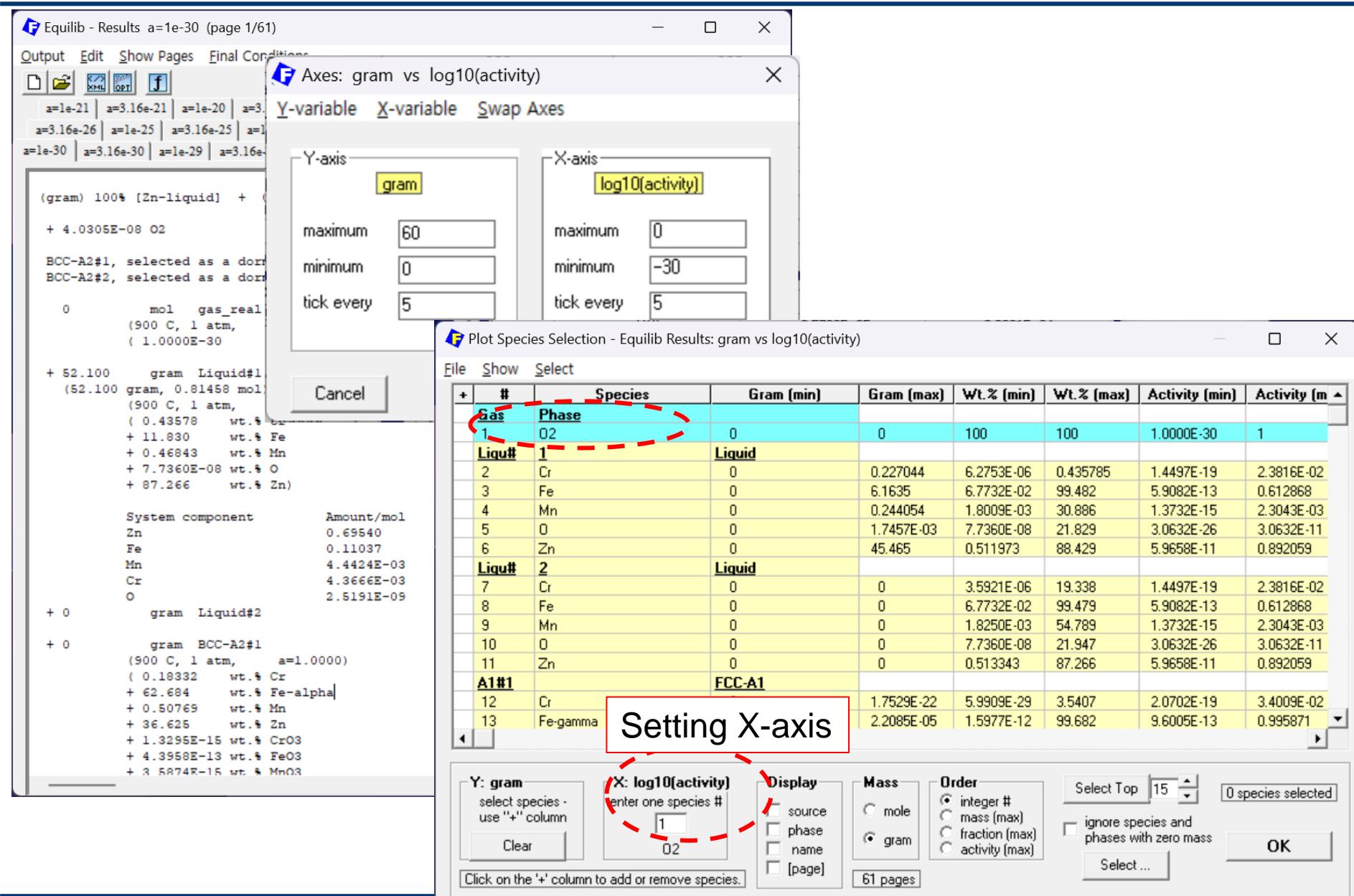
10 steps Table

FactSage 8.3

permit selection of * species Help Suppress Duplicates Edit priority list

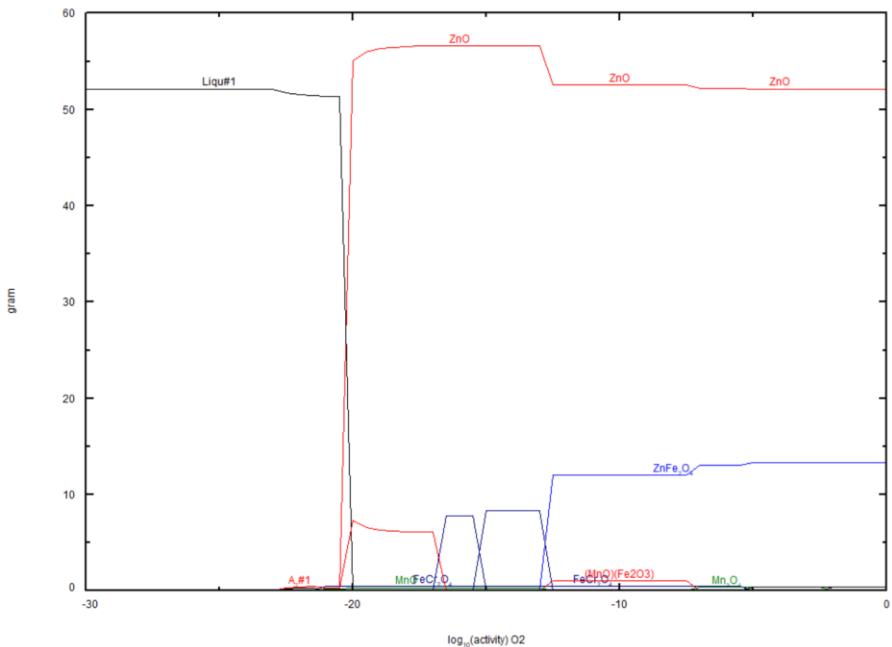
Show Selected Select All Select/Clear... Clear OK

EX18-2. Oxidation reaction of liquid Zn

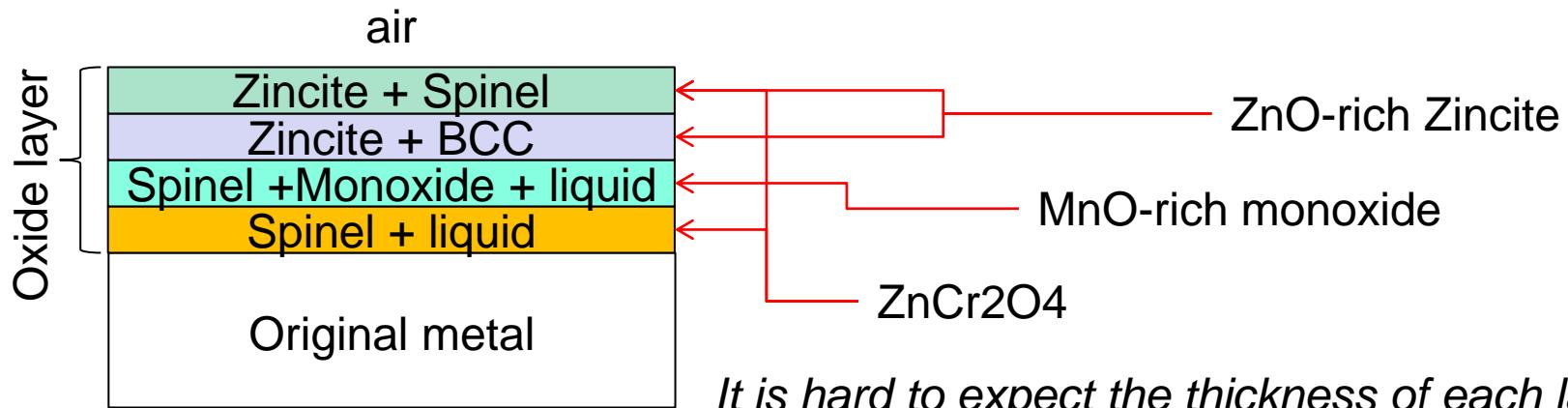
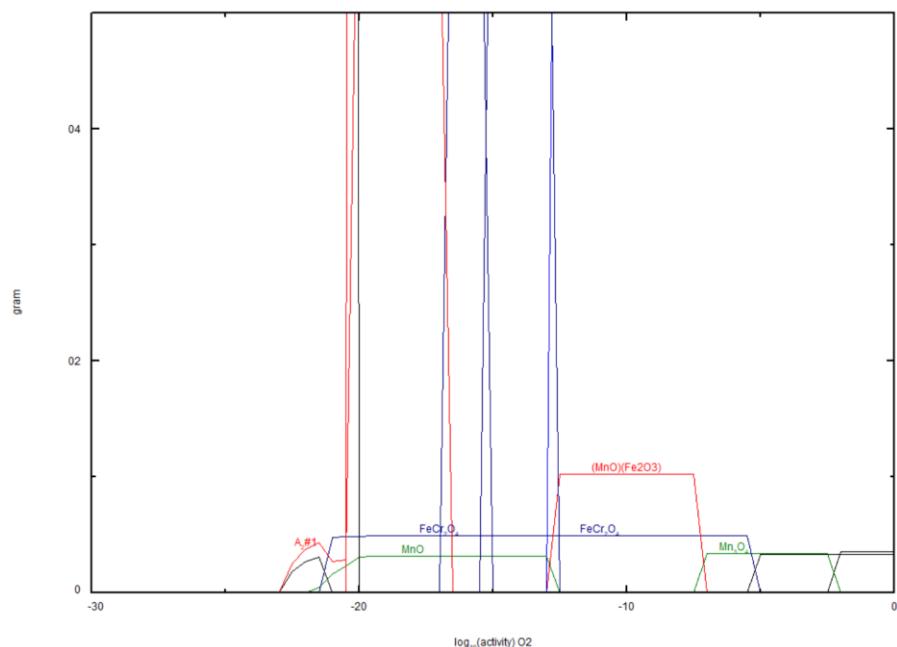


EX18-2. Oxidation reaction of liquid Zn

100% [Zn-liquid] + 0 O₂
C:\FACTSAGEWS\Equi0.res 02Jul23



100% [Zn-liquid] + 0 O₂
C:\FACTSAGEWS\Equi0.res 02Jul23



It is hard to expect the thickness of each layer

EX19. Carburization and Decarburization of Steel

Equilib - Reactants

File Edit Run Macro Table Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

1 - 6 |

Quantity(g)	Species	Phase
99.62	Fe	
+ 0.08	C	
+ 0.2	Mn	
+ 0.1	Si	
+ <1-A> mol	CO	
+ <A> mol	CO ₂	

Next >

FactSage 8.3 Compound: 2/21 databases Solution: 1/18 databases

CO / CO₂ is variable

Equilib - Menu: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (6)

(gram) 99.62 Fe + 0.08 C + 0.2 Mn + 0.1 Si + <1-A> mol CO + <A> mol CO₂

Products

Compound species

- * gas ideal real 24
- aqueous 0
- pure liquids 0
- pure solids 0

* - custom selection species: 24

Target - none - Estimate T(K): 1000 Quantity(g): 0

Solution phases

*	+	Base-Phase	Full Name
*	+	FSstel-Liqu	LIQUID
+	+	FSstel-FCC	FCC_A1
+	+	FSstel-BCC	BCC_A2
		FSstel-HCP	HCP_A3
		FSstel-CEME	CEMENTITE
		FSstel-M23C	M23C6
		FSstel-M7C3	M7C3
		FSstel-CBCC	CBCC_A12

Legend + - selected 2 Show all selected species: 16 solutions: 2 Select

Custom Solutions 0 fixed activities 0 ideal solutions Details ...

Pseudonyms apply Edit ...

Volume and physical prop data assume molar volumes of solids and liquids = 0 use only molar volume data use V & phys. property data paraequilibrium & Gmin edit

Total Species (max 7000) 40 Total Solutions (max 200) 2 Total Phases (max 1500) 3

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
0 1 0.01		1200	1	101 calculations
10 steps	Table			

FactSage 8.3 Equilibrium

normal normal + transitions
transitions only open
no time limit - Calculate >

EX19. Carburization and Decarburization of Steel

Equilib - Results A=0 (page 1/101)

Output Edit Show Pages Final Conditions

Save or Print As ...

Repeat Save

Plot >

Equilib Results file >

Stream File >

Format >

Fact-XML >

Fact-Optimal >

Fact-Function-Builder >

Refresh ...

Swap loops ...

+ 9.7324E-13
+ 1.2613E-13
+ 2.6199E-14
+ 3.8455E-15
+ 2.0591E-15
+ 3.6224E-19
+ 2.0001E-20
+ 1.6474E-22
+ 9.5268E-23
+ 5.7591E-23
+ 1.0751E-23
+ 7.8361E-24
+ 7.2598E-24
+ 3.5764E-29
+ 3.2144E-30
+ 2.1737E-30
+ 2.1296E-31

+ 100.17 gram FCC_A1
(100.17 gram, 1.7911 mol
(1200 C, 1 atm,

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

A=0.17 | A=0.18 | A=0.19 | A=0.2 | A=0.21 | A=0.22 | A=0.23 | A=0.24 | A=0.11 | A=0.12 | FactSage 8.3

Plot: gram vs Alpha

Plot Species Selection - Equilib Results: gram vs log10(Alpha)

#	Species	Gram (min)	Gram (max)	Wt.% (min)	Wt.% (max)	Activity (min)	Activity (max)
41	GAS	27.843	44.166	0	0	1	1
42	FCC	99.843	100.17	0	0	1	1
43	BCC	0	0	0	0	0.985282	0.994324
44	Fe_GAS	5.0991E-06	7.7525E-06	1.3133E-05	1.8321E-05	0	0
45	Mn_GAS	6.2074E-05	6.7131E-05	1.5200E-04	2.2691E-04	0	0
46	Si_GAS	7.5835E-05	7.7281E-02	2.7236E-04	0.174978	0	0
47	O_GAS	15.999	31.998	57.463	72.45	0	0
48	C_GAS	11.844	12.091	27.375	42.537	0	0
49	Fe_FCC	99.62	99.62	99.454	99.777	0	0
50	Mn_FCC	0.199933	0.199938	0.199605	0.200247	0	0
51	Si_FCC	2.2719E-02	9.9924E-02	2.2754E-02	9.9809E-02	0	0
52	O_FCC	1.0943E-07	4.6652E-04	1.0924E-07	4.6726E-04	0	0
53	C_FCC	1.0768E-06	0.247126	1.0785E-06	0.246714	0	0
54	Fe_BCC	0	0	0	0	0	0
55	Mn_BCC	0	0	0	0	0	0
56	Si_BCC	0	0	0	0	0	0

Plot: gram vs Alpha

Plot Species Selection - Equilib Results: gram vs log10(Alpha)

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46	Si_GAS	7.5835E-05	7.7281E-02	2.7236E-04	0.174978	0	0
47	O_GAS	15.999	31.998	57.463	72.45	0	0
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52	O_FCC	1.0943E-07	4.6652E-04	1.0924E-07	4.6726E-04	0	0
53	C_FCC	1.0768E-06	0.247126	1.0785E-06	0.246714	0	0
54	Fe_BCC	0	0	0	0	0	0
55	Mn_BCC	0	0	0	0	0	0
56	Si_BCC	0	0	0	0	0	0

Plot: gram vs Alpha

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52	O_FCC	1.0943E-07	4.6652E-04	1.0924E-07	4.6726E-04	0	0
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54	Fe_BCC	0	0	0	0	0	0
55	Mn_BCC	0	0	0	0	0	0
56	Si_BCC	0	0	0	0	0	0

Plot: gram vs Alpha

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53	C_FCC	1.0768E-06	0.247126	1.0785E-06	0.246714	0	0
54	Fe_BCC	0	0	0	0	0	0
55	Mn_BCC	0	0	0	0	0	0
56	Si_BCC	0	0	0	0	0	0

Plot: gram vs Alpha

Plot Species Selection - Equilib Results: gram vs log10(Alpha)

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49	Fe_FCC	99.62	99.62	99.454	99.777	0	0
50	Mn_FCC	0.199933	0.199938	0.199605	0.200247	0	0
51	Si_FCC	2.2719E-02	9.9924E-02	2.2754E-02	9.9809E-02	0	0
52	O_FCC	1.0943E-07	4.6652E-04	1.0924E-07	4.6726E-04	0	0
53	C_FCC	1.0768E-06	0.247126	1.0785E-06	0.246714	0	0
54	Fe_BCC	0	0	0	0	0	0
55	Mn_BCC	0	0	0	0	0	0
56	Si_BCC	0	0	0	0	0	0

Plot: gram vs Alpha

Plot Species Selection - Equilib Results: gram vs log10(Alpha)

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45	Mn_GAS	6.2074E-05	6.7131E-05	1.5200E-04	2.2691E-04	0	0
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52	O_FCC	1.0943E-07	4.6652E-04	1.0924E-07	4.6726E-04	0	0
53	C_FCC	1.0768E-06	0.247126	1.0785E-06	0.246714	0	0
54	Fe_BCC	0	0	0	0	0	0
55	Mn_BCC	0	0	0	0	0	0
56	Si_BCC	0	0	0	0	0	0

Plot: gram vs Alpha

Plot Species Selection - Equilib Results: gram vs log10(Alpha)

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51	Si_FCC	2.2719E-02	9.9924E-02	2.2754E-02	9.9809E-02	0	0
52	O_FCC	1.0943E-07	4.6652E-04	1.0924E-07	4.6726E-04	0	0
53	C_FCC	1.0768E-06	0.247126	1.0785E-06	0.246714	0	0
54	Fe_BCC	0	0	0	0	0	0
55	Mn_BCC	0	0	0	0	0	0
56	Si_BCC	0	0	0	0	0	0

Plot: gram vs Alpha

Plot Species Selection - Equilib Results: gram vs log10(Alpha)

#	Species	Gram (min)	Gram (max)	Wt.% (min)	Wt.% (max)	Activity (min)	Activity (max)
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42	FCC	99.843	100.17	0	0	1	1
43	BCC	0	0	0	0	0.985282	0.994324
44	Fe_GAS	5.0991E-06	7.7525E-06	1.3133E-05	1.8321E-05	0	0
45	Mn_GAS	6.2074E-05	6.7131E-05	1.5200E-04	2.2691E-04	0	0
46	Si_GAS	7.5835E-05	7.7281E-02	2.7236E-04	0.174978	0	0
47	O_GAS	15.999	31.998	57.463	72.45	0	0
48	C_GAS	11.844	12.091	27.375	42.537	0	0
49	Fe_FCC	99.62	99.62	99.454	99.777	0	0
50	Mn_FCC	0.199933	0.199938	0.199605	0.200247	0	0
51	Si_FCC	2.2719E-02	9.9924E-02	2.2754E-02	9.9809E-02	0	0
52	O_FCC	1.0943E-07	4.6652E-04	1.0924E-07	4.6726E-04	0	0
53	C_FCC	1.0768E-06	0.247126	1.0785E-06	0.246714	0	0
54	Fe_BCC	0	0	0	0	0	0
55	Mn_BCC	0	0	0	0	0	0
56	Si_BCC	0	0	0	0	0	0

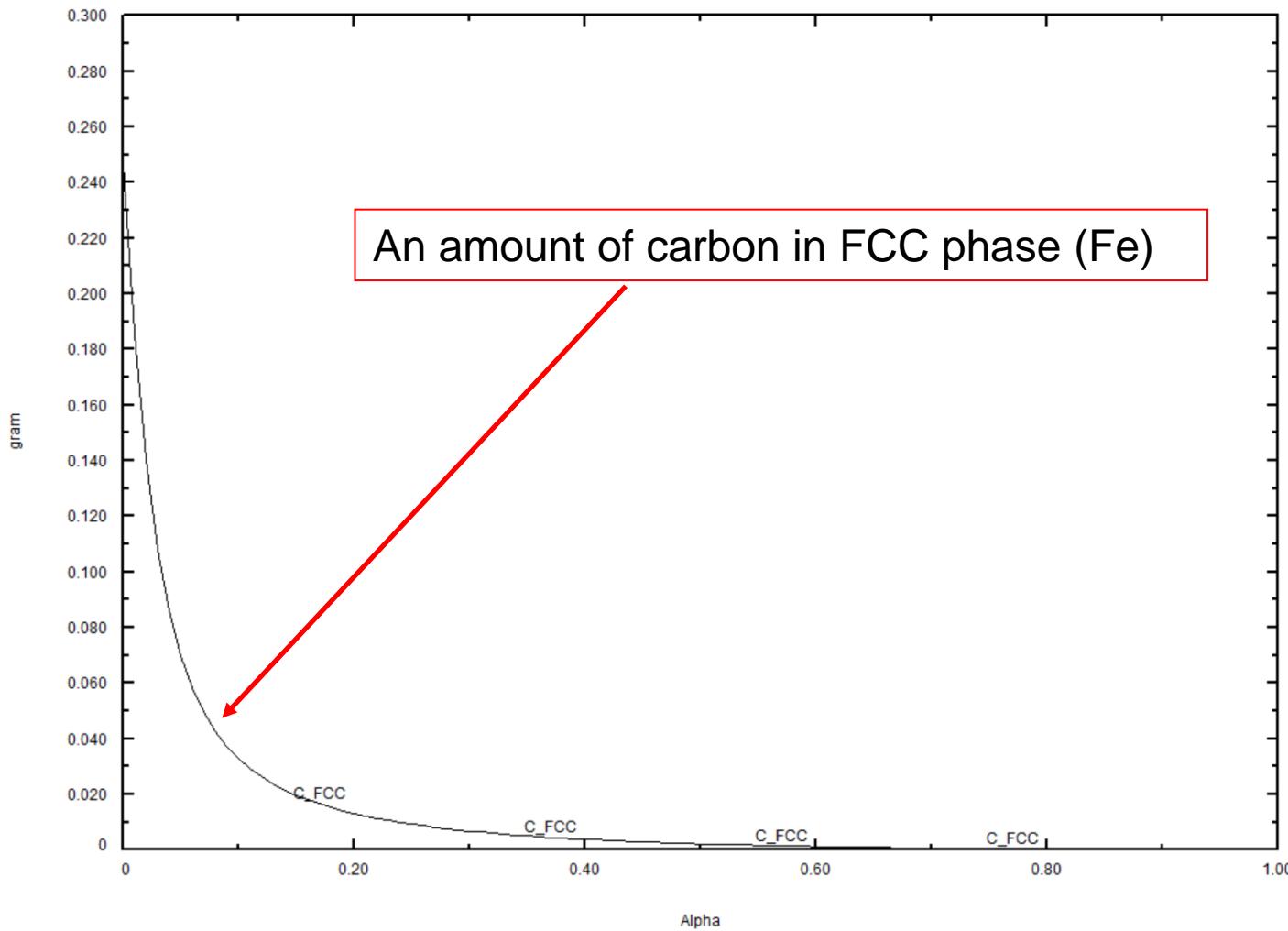
Plot: gram vs Alpha

Plot Species Selection - Equilib Results: gram vs log10(Alpha)

#	Species	Gram (min)	Gram (max)	Wt.% (min)	Wt.% (max)	Activity (min)	Activity (max)
41	GAS	27.843	44.166	0	0	1	1
42	FCC	99.843	100.17	0	0	1	1
43	BCC	0	0	0	0	0.985282	0.994324
44	Fe_GAS	5.0991E-06	7.7525E-06	1.3133E-05	1.8321E-05	0	0
45	Mn_GAS	6.2074E-05	6.7131E-05	1.5200E-04	2.2691E-04	0	0
46	Si_GAS	7.5835E-05	7.7281E-02	2.7236E-04	0.174978	0	0
47	O_GAS	15.999	31.998	57.463	72.45	0	0
48	C_GAS	11.844	12.091	27.375	42.537	0	0
49	Fe_FCC	99.62	99.62	99.454	99.777	0	0
50	Mn_FCC	0.199933	0.199938	0.199605	0.200247	0	0
51	Si_FCC	2.27					

99.62 Fe + 0.08 C + 0.2 Mn + 0.1 Si +

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EX19. Carburization and Decarburization: Composition target

Equilib - Menu: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (6)

(gram) 99.62 Fe + 0.08 C + 0.2 Mn + 0.1 Si + <1-A> mol CO + <A> mol CO₂

Products

Compound species

- * gas ideal 24
- aqueous 0
- pure liquids 0
- pure solids 0

* - custom selection species: 24

Target

- none -

Estimate T(K): 1000

Quantity(g): 0

Solution phases

*	+	Base Phase	Full Name
		FSstel-Liqu	LIQUID
C		FSstel-FCC	FCC_A1
	+	FSstel-BCC	BCC_A2
		FSstel-HCP	HCP_A3
		FSstel-CEME	CEMENTITE
		FSstel-M23C	M23C6
		FSstel-M7C3	M7C3
		FSstel-CBCC	CBCC_A12

Legend

- C - composition target
- element: C
- + - selected 1

Show all selected

species: 16 solutions: 2 Select

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
0 1 0.01		1200	1	

10 steps Table

101 calculations

FactSage 8.3

Composition Target:

" How to calculate optimum amount of CO₂ to reduce C in steel to a targeted composition"

Composition Target

Solution ST53-FCC

Variable

- species composition
- log10 (species composition)
- element composition
- log10 (element composition)
- species activity
- log10(species activity)
- none (removes targets) -

Species

Code numbers (169-176)
Fe, Mn, O, ...

169 Fe

Element

Elements C O Si Mn Fe

Element: C

Values

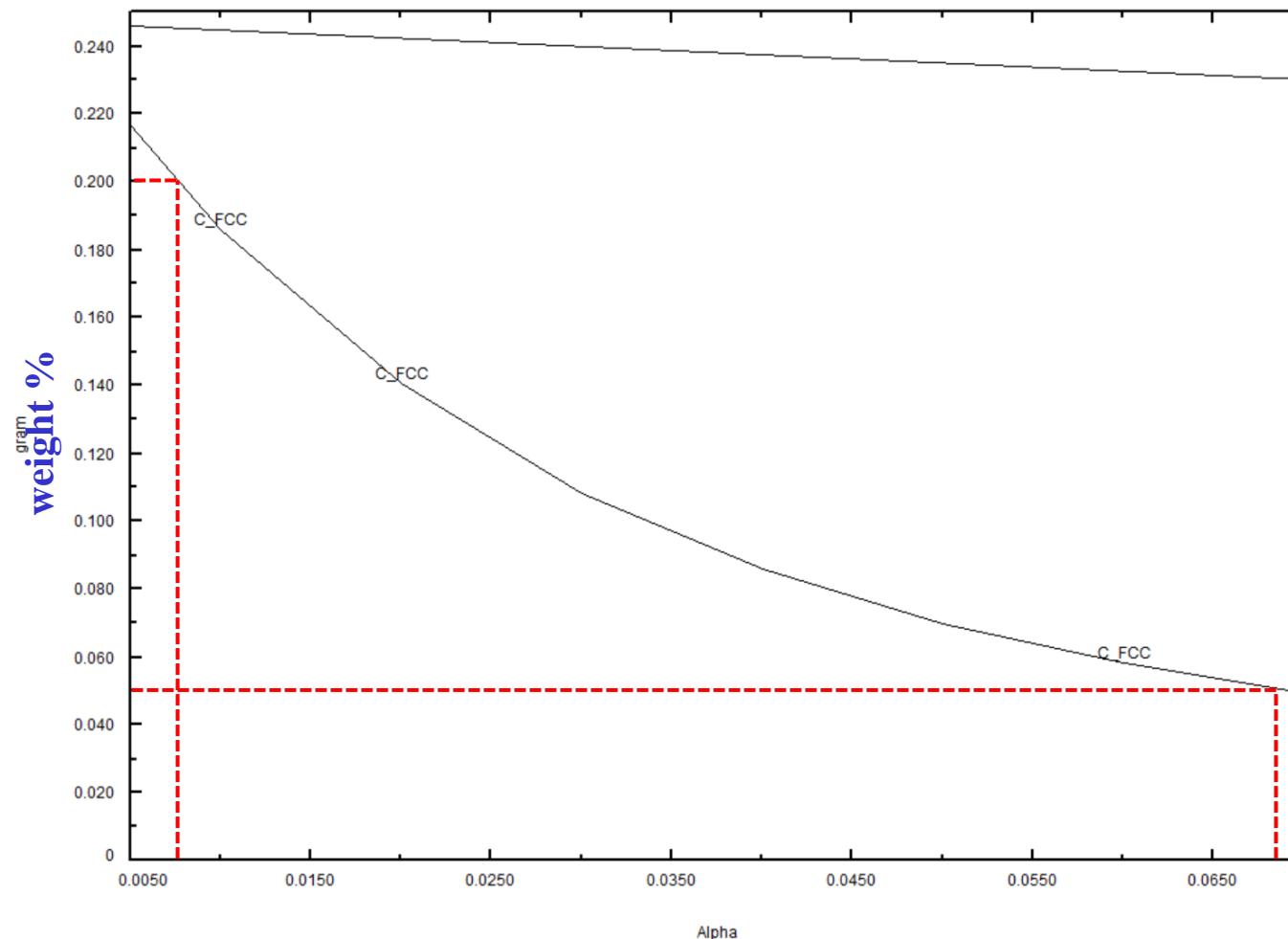
Enter a single value - or enter a range of values 'first last step'

Element C 0,0005 0,002 0,0001

mass fraction: (0.05%) (0.2%)

Cancel Help OK

99.62 Fe + 0.08 C + 0.2 Mn + 0.1 Si +
C:\FACTSAGEWS\Equi0.res 02Jul23



EX20-1. P reduction in high purity Si using vacuum

FactSage ultrapure silicon database
This is special database for high purity Si production

The screenshot shows the FactSage software interface. On the left, under 'Databases', 'FactPS' is selected (indicated by a red dashed box). Other databases listed include Fact, FactToxic, FactSalt, FactMisc, FactHall, FTOxCN, FTfritz, FThelg, FTpulp, FTlite, FactSage, SGTE, FSopp, FSlead, FSstel, FSups, BINS, SGPS, SGTE, SGnobl, SpMCBN, TDmeph, TDnucl, ELEM, FTdemo, and FTnucl. Under 'Information', there are options for 'Options - search for product species' and 'Include compounds' (checkboxes for gaseous ions, aqueous species, and limited data compounds). Buttons for 'Default', 'Cancel', and 'Summary ...' are at the bottom. On the right, the 'Equilib - Reactants' window is open, showing a table for inputting reactant information. The table has columns for 'Quantity(g)', 'Species', 'Phase', 'T(C)', 'P(total)**', 'Stream#', and 'Data'. The first row has values: 98, Si, (empty), (empty), (empty), 1. Subsequent rows have values: +1, B, (empty), (empty), (empty), 1; +1, P, (empty), (empty), (empty), 1; +1, Ar, (empty), (empty), (empty), 1. A checkbox for 'Initial Conditions' is at the bottom right. At the very bottom, status bars show 'FactSage 8.0', 'Compound: 2/26 databases', and 'Solution: 1/26 databases'.

Equilib - Menu: last system

File Units Parameters Help

T(C) P(bar) Energy(J) Quantity(g) Vol(litre)

Reactants (4)

(gram) 98 Si + B + P + Ar

Products

Compound species

- + gas ideal real 9
- aqueous 0
- pure liquids 0
- pure solids 0

species: 9

Target
- none -
Estimate T(K): 1000
Quantity(g): 0

Solution phases

*	+	Base-Phase	Full Name
	I	FSupsi-Liqu	Liquid
	I	FSupsi-Diam	Diamond_A4

Custom Solutions
0 fixed activities
0 ideal solutions

Pseudonyms
 apply

Volume data
 assume molar volumes of solids and liquids = 0
 include molar volume data and physical properties data

paraequilibrium & Gmin

Virtual species: 12
Total Species (max 5000) 23
Total Solutions (max 200) 4
Total Phases (max 1500) 5

Final Conditions

<A>		T(C)	log10(P(bar))	Product H(J)
		1600	-5.00.1	

10 steps Table

Equilibrium
 normal normal + transitions
 transitions only open
- no time limit -

Vacuum level (highlighted with a red box and arrow pointing to the log10(P(bar)) input field)

FactSage 8.0

06 litre, 1.9836E-09 gram.cm⁻³
a=1.0000)

a=1.0000)

+ 98.841 wt.% Si)

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Ar	4.8836E-12	1.9509E-10	1.5353E-12	2.2234E-12
P	5.8496E-04	1.8118E-02	1.8390E-04	2.0649E-04
Si	3.0879	86.726	0.97077	0.98841
B	9.2398E-02	0.99892	2.9048E-02	1.1385E-02

+ 0 gram Diamond_A4#1

e to search

F Axes: weight % soln. species vs log10(P(bar))

X

Y-variable X-variable Swap Axes

Y-axis
weight % soln. species

X-axis
log10(P(bar))

maximum 1

minimum 0

tick every 0.2

maximum 0

minimum -5

tick every 0.5

Plot Species Selection - Equilib Results: weight % soln. species vs log10(P(bar))

File Show Select

Cancel

+	#	Species	Gram (min)	Gram (max)	Wt.% (min)	Wt.% (max)	Activity (min)	A
Gas	Phase							
1	B	5.6622E-10	1.0850E-03	5.6573E-08	8.1840E-03	2.0913E-09	2	
2	B2	6.0258E-16	1.2912E-09	6.0206E-14	9.7398E-09	1.1128E-15	1.	
3	Si	6.1005E-06	10.516	6.0952E-04	79.322	8.6735E-06	8.	
4	Si2	2.7702E-07	0.480367	2.7678E-05	3.6235	1.9693E-07	2.	
5	Si3	1.5938E-07	0.278018	1.5924E-05	2.0971	7.5531E-08	7.	
6	P	3.3285E-06	0.115586	3.3257E-04	1.2504	8.6962E-08	4.	
7	P2	1.2310E-03	0.901149	0.122991	41.4	3.2588E-07	7.	
8	P4	2.0184E-08	8.3445E-06	1.5225E-07	6.3706E-04	3.7965E-15	2.	
9	Ar	0.999625	1	7.5431	99.876	5.8335E-07	0.	
Liquid	1	Liquid						
10	Ar	1.9509E-10	3.7460E-04	2.2234E-10	3.7460E-04	1.4794E-12	2	
11	B	0.999815	1	1	1.1385	7.8986E-02	8.	
+ 12	P	1.8118E-02	0.998766	2.0649E-02	0.998774	5.6219E-05	2	
13	Si	66.726	38	38.001	98.918	0.96692	0.	
Liquid	2	Liquid						
14	Ar	0	0	2.2234E-10	3.7460E-04	1.4794E-12	2	
15	B	0	0	1	1.1385	7.8986E-02	8.	

Display
 source
 phase
 name
 [page]

Mass
 mole
 gram
 fraction (max)
 activity (max)

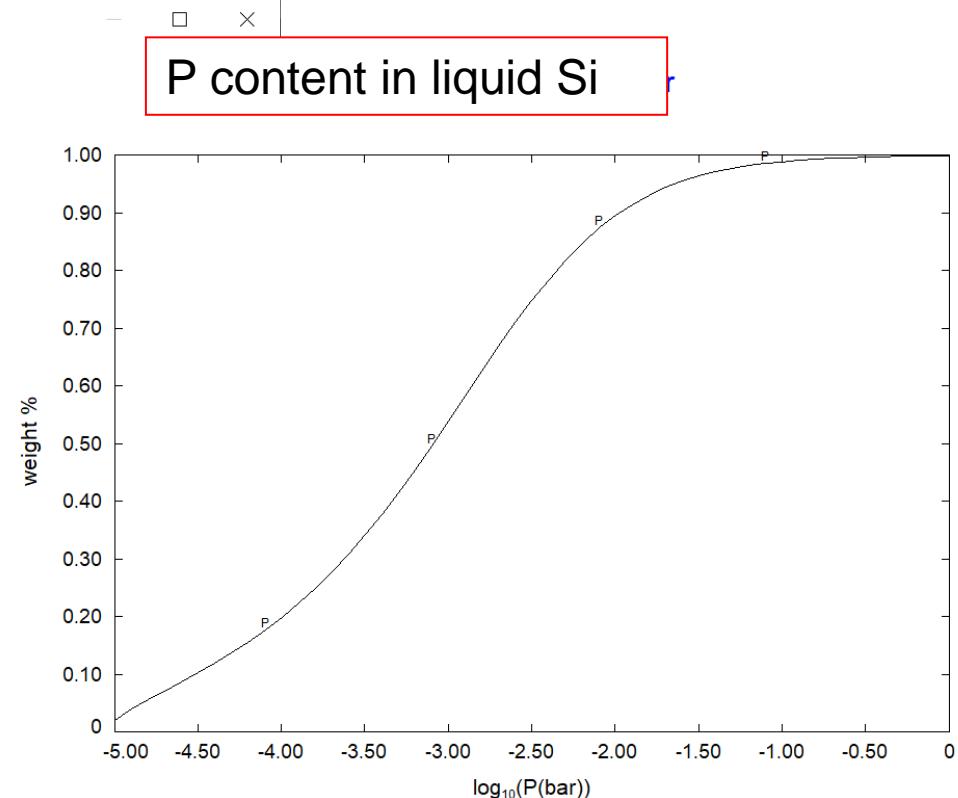
Order
 integer #
 mass (max)
 fraction (max)
 activity (max)

Select T
 ignore phase

Clear

Click on the '+' column to add or remove species.

51 pages



EX20-2. B reduction in high purity Si using H₂-H₂O mixture

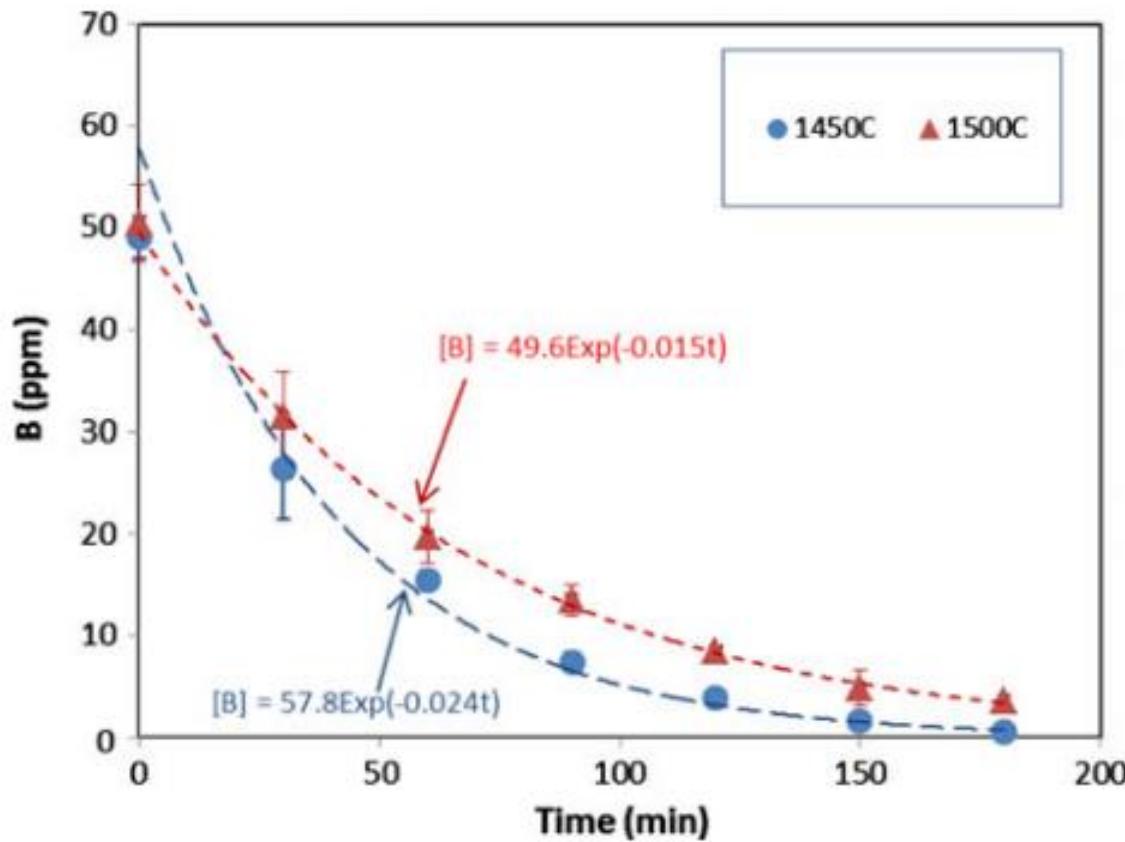


Fig. 1. B concentration changes in H₂-H₂O blowing determined by the resistivity meter

JOM, JOURNAL OF THE MINERALS, METALS AND MATERIALS SOCIETY
Volume 64, Number 8 (2012), 952-956

Open calculations:
Simple reactor module
with off-gas removal

The screenshot shows the FactSage software interface for a chemical equilibrium calculation. The main window displays a table of reactants and their quantities (98 g Si, 1 g B, 1 g P, <0.1A> H₂, <0.9A> H₂O) and a table of products (48 g FSups-Liqu, 0 g FSups-Diam). The bottom right panel shows the 'Equilibrium' section with 'open' selected and a 'Calculate >>' button.

Reactants (5)

Quantity(g)	Species	Phase
98	Si	
+ 1	B	
+ 1	P	
+ <0.1A>	H ₂	
+ <0.9A>	H ₂ O	

Products

Compound species	Base-Phase	Full Name
gas (ideal)	I	FSups-Liqu
aqueous	I	Liquid
		FSups-Diam
		Diamond_A4

Final Conditions

<A>		T(C)	P(bar)	Product H(J)
1		1420	1	
10 steps				Table

FactSage 8.0 | C:\Workshop80\Workshop\ex20-1.equi

“Open” menu
Addition of <A> amount of gas and make chemical reaction
→ Remove the gas as off gas
→ Add another <A> gas for chemical reaction
→ Remove the gas as off gas
→ Do this iteration until reaching “10” step

Equilib - Results Step 10 (page 10/10)

Output Edit Show Pages Final Conditions



T(C) P(bar) Energy(J) Quantity(g) Vol(litre)

Step 1 | Step 2 | Step 3 | Step 4 | Step 5 | Step 6 | Step 7 | Step 8 | Step 9 | Step 10 | - Step 10 -

(gram) 98 Si + B + P + <0.1A> H2 + Total <A> = 10.000

(gram) <0.9A> H2O =

```

0.14742 mol gas ideal
(2.3399 gram, 0.14742 mol, 20.753 litre, 1.1275E-04 gram.cm-3)
(1420 C, 1 bar, a=1.0000)
( 0.66859 H2
+ 0.31621 SiO
+ 8.3347E-03 HBO2
+ 3.3653B-03 B2O2
+ 1.7076B-03 B2O3
+ 4.9079B-04 (BO)2
+ 4.2382B-04 H2O
+ 3.5349B-04 P2
+ 3.3958B-04 B3H3O3
+ 1.2177B-04 R
+ 2.8460B-05 BO
+ 5.1185B-06 PH2
+ 3.6980B-06 TH3
+ 1.6029B-06 BH2
+ 1.5546B-06 PH
+ 7.8526B-07 SiR
+ 7.7129B-07 PO
+ 6.0586B-07 Si1
+ 5.6849B-07 Si1H4
+ 5.2530B-07 P
+ 4.4557B-07 SiO2
+ 3.1466B-07 BH3
+ 1.0561B-07 H3BO3
+ 8.7963B-08 (HBO2)3
+ 3.5081B-08 BO2
+ 1.9722B-08 P4
+ 8.6752B-09 Si2
+ 6.7747B-09 B2O
+ 5.7335B-09 B(OH)2
+ 3.7240B-09 OH
+ 3.6984B-09 Si3
+ 1.5193B-09 PO2
+ 9.2378B-11 BH
+ 1.3006B-11 B
+ 5.2195B-13 Si2H6
+ 4.9195B-13 O
+ 1.1455B-13 (P2O3)2
+ 4.8950B-14 B2(OH)4
+ 1.4285B-15 B2H6
+ 1.4010B-16 O2
+ 2.8333B-18 HOOH
+ 3.7332B-19 HOO
+ 3.2001B-19 B2
+ 5.0841B-23 T2O5
+ 5.6810B-31 B5H9
+ 1.7471B-32 O3
+ 1.7443B-42 (P2O5)2
+ 6.5858B-53 B10H14)

+ 87.859 gram Liquid#1
(87.859 gram, 3.1341 mol)
+ 0 gram Liquid#2
( 0.4260C, 1 bar, a=1.0000)
( 0.15378 wt.% B
+ 1.08803 wt.% Si
+ 3.0879E-07 wt.% O
+ 1.1057 wt.% P
+ 98.739 wt.% Si1

```

B product in gas phase

B reduction in liquid Si

Plot: gram vs - page -

File Help

98 Si + B + P + <0.1A> H2 +

Axes	Variables	Minimum	Maximum
	activity	0	1
	mole	0	3.5689
	soln. species	0	0.998994
	am	0	98.978
	oln. species	0	99.939
	Alpha	0	0
	T(C)	1420	1420
	P(bar)	1	1
	Cp(J/K)	96.898	150.36
	G(J)	-3.0366E+05	-2.7380E+05
	Vol(litre)	18.721	20.753
	H(J)	2.7022E+05	3.0511E+05
	V(litre)	18.721	20.753
	S(J/K)	321.31	359.55
X-axis	- page -	1	10

species selected

Graph

Labels size: 9 no: 4

Display color full screen colors ...

chemical integer # none

reactants file name offset

Plot >

FactSage 8.0 C:\W\

Axes: gram vs - page -

Y-variable X-variable Swap Axes

Y-axis gram

maximum 1

minimum 0

tick every 0.1

X-axis - page -

maximum 10

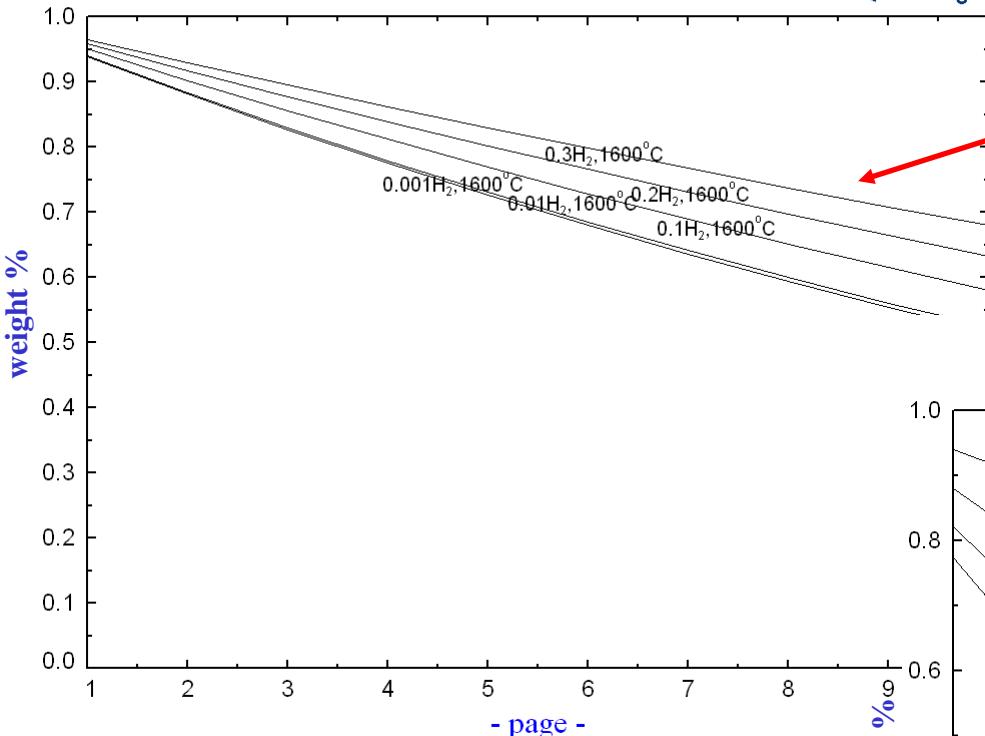
minimum 1

tick every 0.5

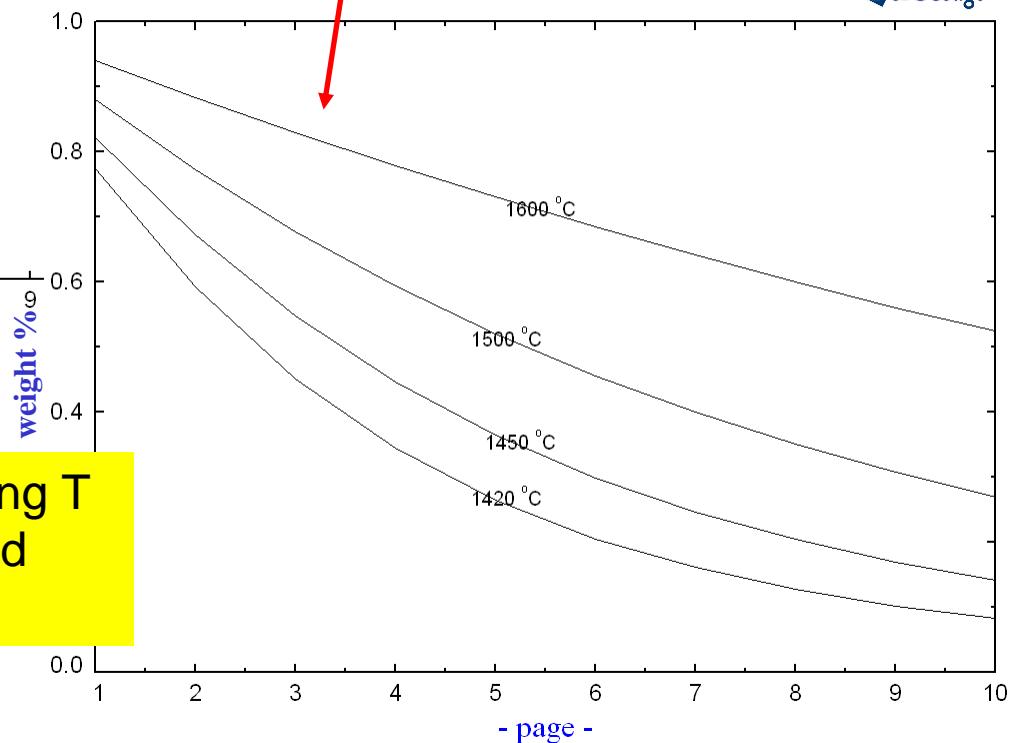
Cancel Refresh OK



1600 °C

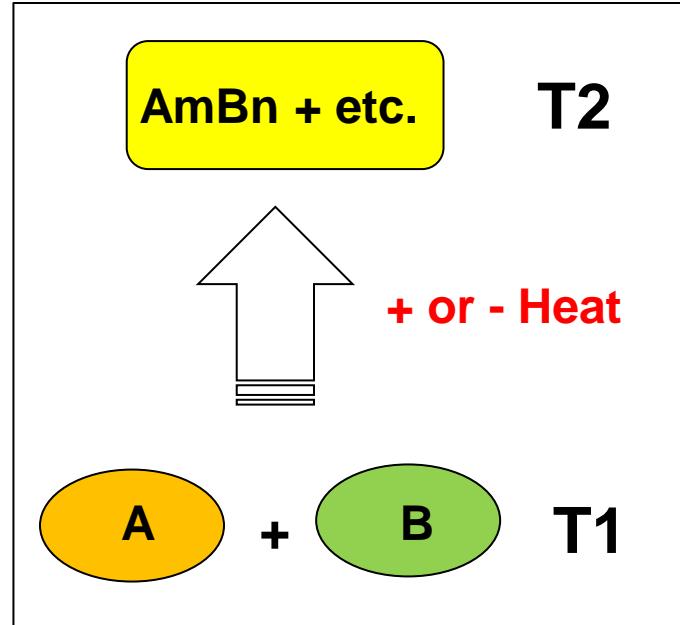


B content in liquid Si

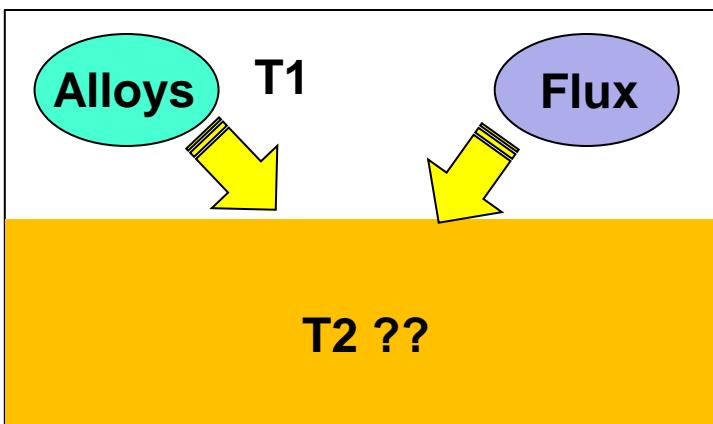


B content can be reduced with decreasing T
“page” in x-axis is amount of gas injected
(or considered as the degassing time)

EX21. Heat balance: very important for industrial process



Heat of formation + T increase



Heat of Dissolution

- 1) How much heat is required to increase temperature from T1 to T2 ?
- 2) If we add or remove a certain amount of H from mixtures of materials, what would be final temperature ?

→ Good for

- a) Furnace capacity design
- b) Heat balance calculation for alloying or fluxing of materials to melt bath
- c) Calculate exothermic or endothermic heat generated during explosion
- d) Process simulation for temperature change

2.

65%Mn-35%Fe
25°C

Final
Temperature ?

1.

1600 °C, Liquid

Fe-1wt.%Al-0.8wt.%C

1.

Use two stream

1.

```
(gram) 98.2 Fe + Al + 0.8 C =  
0 mol gas_ideal  
(1600 C, 1 atm, a=7.0931E-05)  
( 7.7712E-05 Fe  
+ 1.2185E-06 Al  
+ 8.6147E-13 Al2  
+ 5.4992E-14 C  
+ 4.1563E-15 AlC  
+ 3.6956E-15 Al2C2  
+ 3.2392E-15 AlC2  
+ 6.0846E-17 C3  
+ 6.0810E-17 C2  
+ 6.6732E-23 C4  
+ 3.8824E-24 C5)  
  
+ 100.00 gram LIQUID#1  
(100.00 gram, 1.8621 mol)  
(1600 C, 1 atm, a=1.0000)  
( 1.0000 wt.% Al  
+ 0.80000 wt.% C  
+ 98.200 wt.% Fe)
```

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	1.7584	98.200	0.94433	0.98200
Al	3.7062E-02	1.0000	1.9903E-02	1.0000E-02
C	6.6607E-02	0.80000	3.5770E-02	8.0000E-03

2.

```
(gram) 65 Mn + 35 Fe =  
0 mol gas_ideal  
(25 C, 1 atm, a=4.1207E-43)  
( 4.1207E-43 Mn  
+ 2.7767E-64 Fe)  
  
+ 79.544 gram CBCC_Al2  
(79.544 gram, 1.4438E mol)  
(25 C, 1 atm, a=1.0000)  
( 18.407 wt.% FeVa  
+ 81.593 wt.% MnVa)
```

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	0.26219	14.642	0.18163	0.18407
Mn	1.1814	64.902	0.81837	0.81593

```
+ 20.456 gram BCC_A2#1  
(20.456 gram, 0.36633 mol)  
(25 C, 1 atm, a=1.0000)  
( 99.521 wt.% Fe  
+ 0.47861 wt.% Mn)
```

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	0.36454	20.358	0.99514	0.99521
Mn	1.7821E-03	9.7905E-02	4.9848E-03	4.7861E-03

Adiabatic condition ($dH = 0$)

Equilib - Reactants

File Edit Run Macro Table Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

1 - 2 |

Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
100%	[FeLq-1600C]	[Stream]	1600	1	1	
+ <A>	[FEMN-25]	[Stream]	25	1	2	

** P(total) is the hydrostatic pressure above the phase.
For a gaseous stream this is the sum of the partial pressures of the species in that stream.

Reactants (2)

(gram) 100% [FeLq-1600C] + <A> [FEMN-25]
(1600C1600C),#1 (25C25),#2

Products

Compound species

* + gas	<input checked="" type="radio"/> ideal	<input type="radio"/> real	12
aqueous	0		
pure liquids	0		
* + pure solids	39		

* - custom selection species: 51

Solution phases

Base-Phase	Full Name
FSstel-Liqu	LQUID
FSstel-FCC	FCC_A1
FSstel-BCC	BCC_A2
FSstel-HCP	HCP_A3
FSstel-CEME	CEMENTITE
FSstel-M23C	M23C6
FSstel-M7C3	M7C3
FSstel-CBCC	CBCC_A12

Legend
+ - selected 3 Show all selected
species: 16 solutions: 3 Select

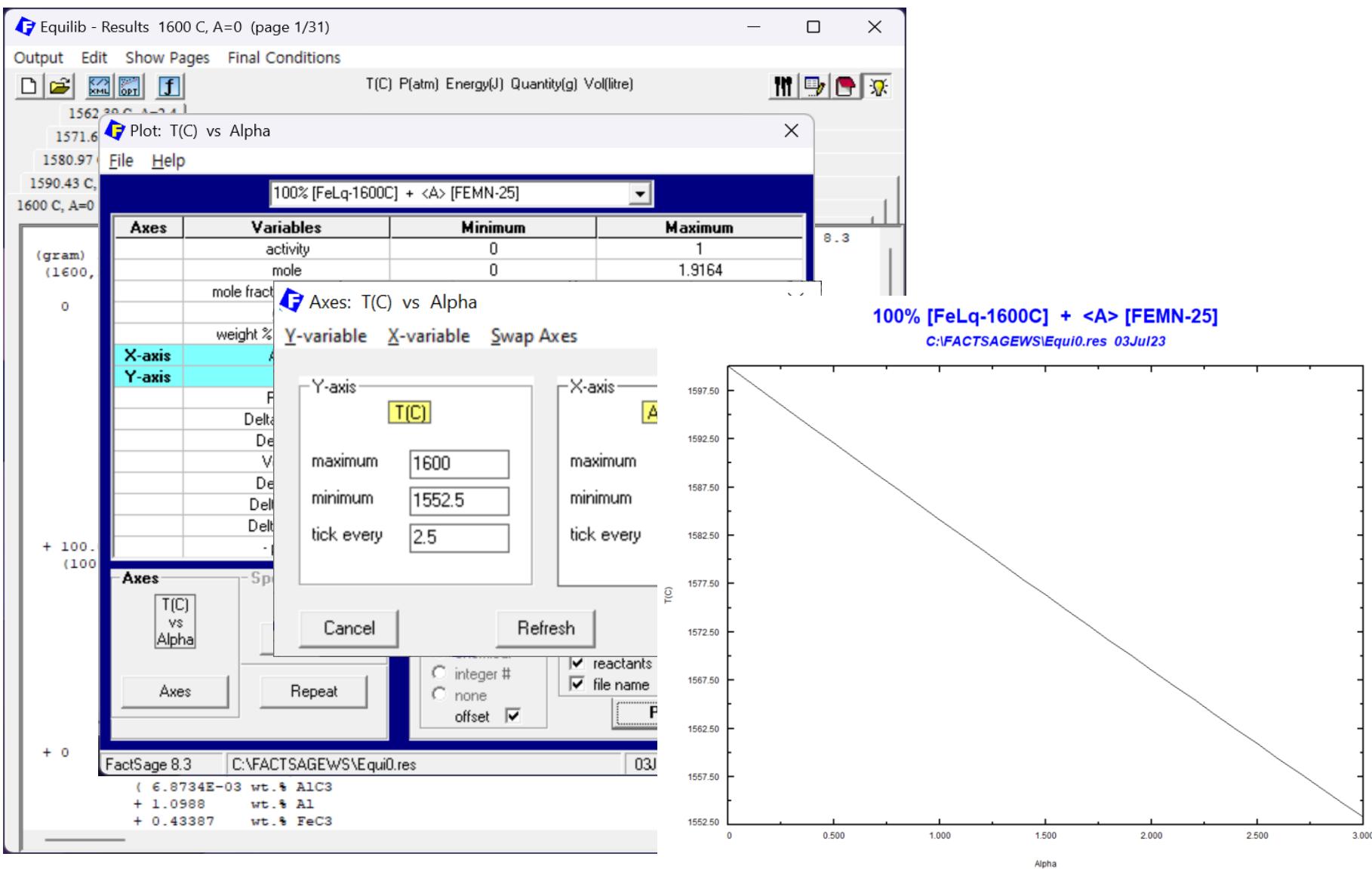
Final Conditions

<A>		T(C)	P(atm)	Delta H(J)
0.30.1		1	1	0
10 steps	<input type="checkbox"/> Table	<input type="button" value="31 calculations"/>		

Equilibrium

normal normal + transitions
 transitions only open
- no time limit -

If we know the heat loss of the ladle we can setup this here for the final Temperature prediction



EX21-2. Heat balance: Cooling of AZ91 from 600 to 300°C

Equilib - Reactants

File Edit Run Macro Table Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

1 - 3

Quantity(g)	Species
90	Mg
+ 9	Al
+ 1	Zn

Equilib - Menu: last system

File Units Parameters Help

T(C) P(bar) Energy(J) Quantity(g) Vol(litre)

Reactants (3)

(gram) 90 Mg + 9 Al + Zn

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- * pure solids 35
- * - custom selection species: 35

Solution phases

*	+	Base-Phase	Full Name
I		FTlite-Liqu	Liquid
J		FTlite-A1	FCC-A1
I		FTlite-A2	BCC-A2
I		FTlite-A3	HCP-A3
I		FTlite-A3"	HCP-Zn Prototype-Mg
I		FTlite-A12	CBCC-A12 Prototype-Mn
I		FTlite-C14	C14 Prototype-MgZn2
I		FTlite-C15	C15 Prototype-MgCu2

Custom Solutions
0 fixed activities
0 ideal solutions

Pseudonyms
 apply

Volume and physical prop data
 assume molar volumes of solids and liquids = 0
 use only molar volume data
 use V & phys. property data
 paraequilibrium & Gmin

Total Species (max 7000) 178
Total Solutions (max 200) 29
Total Phases (max 1500) 64

Final Conditions

<A>		T(C)	P(bar)	Product H(J)
		600	1	
10	steps	<input type="checkbox"/> Table		

1 calculation

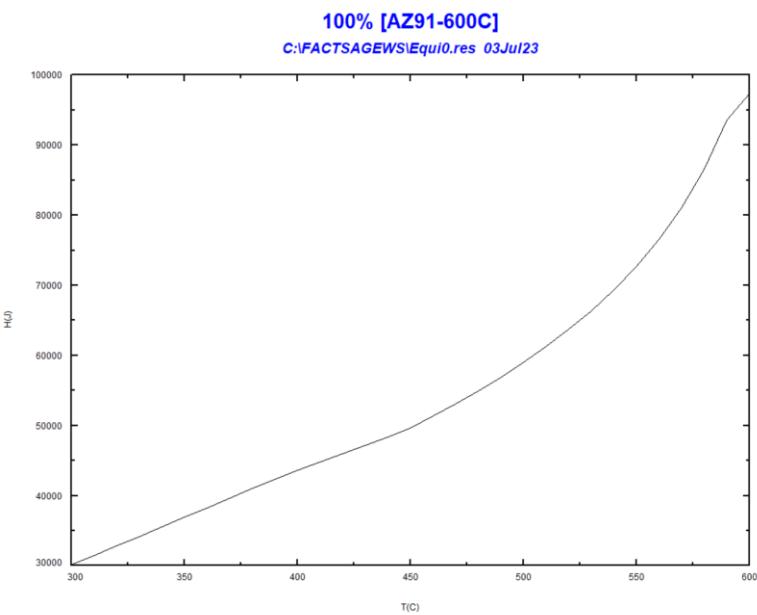
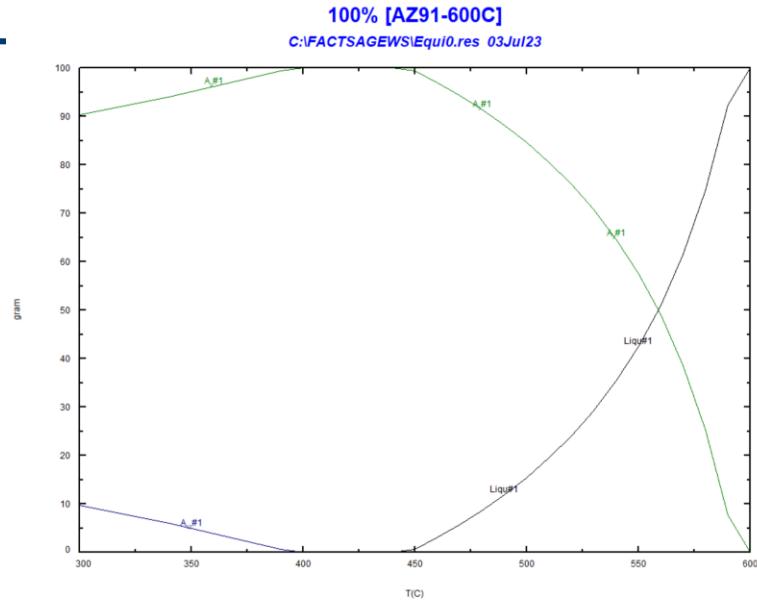
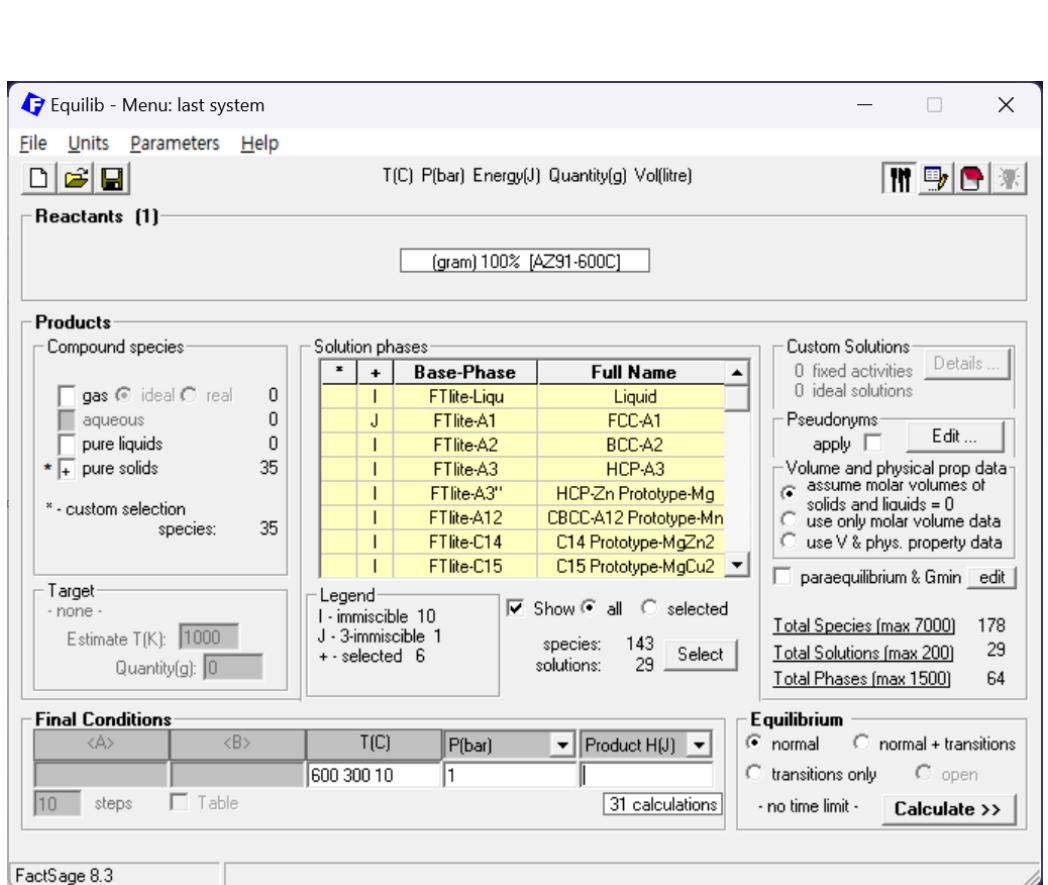
Equilibrium

normal normal + transitions
 transitions only open
- no time limit -

FactSage 8.3 Compound: 2/21 databases Solution:

FactSage 8.3

Stream : AZ31 alloy at 600 °C



EX22-1. Thermodynamic properties: Activity, ΔG, ΔH, ΔS etc.

Equilib - Reactants

File Edit Run Macro Table Units Data Search Data Evaluation Help

T(C) P(bar) Energy(J) Quantity(g) Vol(litre)

1 - 2 |

Quantity(g)	Species	Phase
<1-A>	Mg	liquid
+ <A>	Si	liquid

** P(total) is the hydrostatic pressure above the p
For a gaseous stream this is the sum of the partial pressures of the species in that stream

Equilib - Menu: last system

File Units Parameters Help

T(C) P(bar) Energy(J) Quantity(g) Vol(litre)

Reactants (2)

(gram) <1-A> Mg + <A> Si
(1600C,liq,#1) (1600C,liq,#1)

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- + pure solids 23

species: 23

Solution phases

-	+	Base-Phase	Full Name
-	+	I	FTlite-Liqu
-	+	J	FCC-A1
-	+	I	FCC-A2
-	+	I	HCP-A3
-	+	J	aC1 Prototype-CaF2
-	+	I	C14 Prototype-MgZn2
-	+	I	C15 Prototype-MgCu2

Custom Solutions

- 0 fixed activities
- 0 ideal solutions

Pseudonyms

apply Edit ...

Volume and physical prop data

- assume molar volumes of solids and liquids = 0
- use only molar volume data
- use V & phys. property data

paraequilibrium & Gmin edit

Total Species (max 7000) 70
Total Solutions (max 200) 16
Total Phases (max 1500) 39

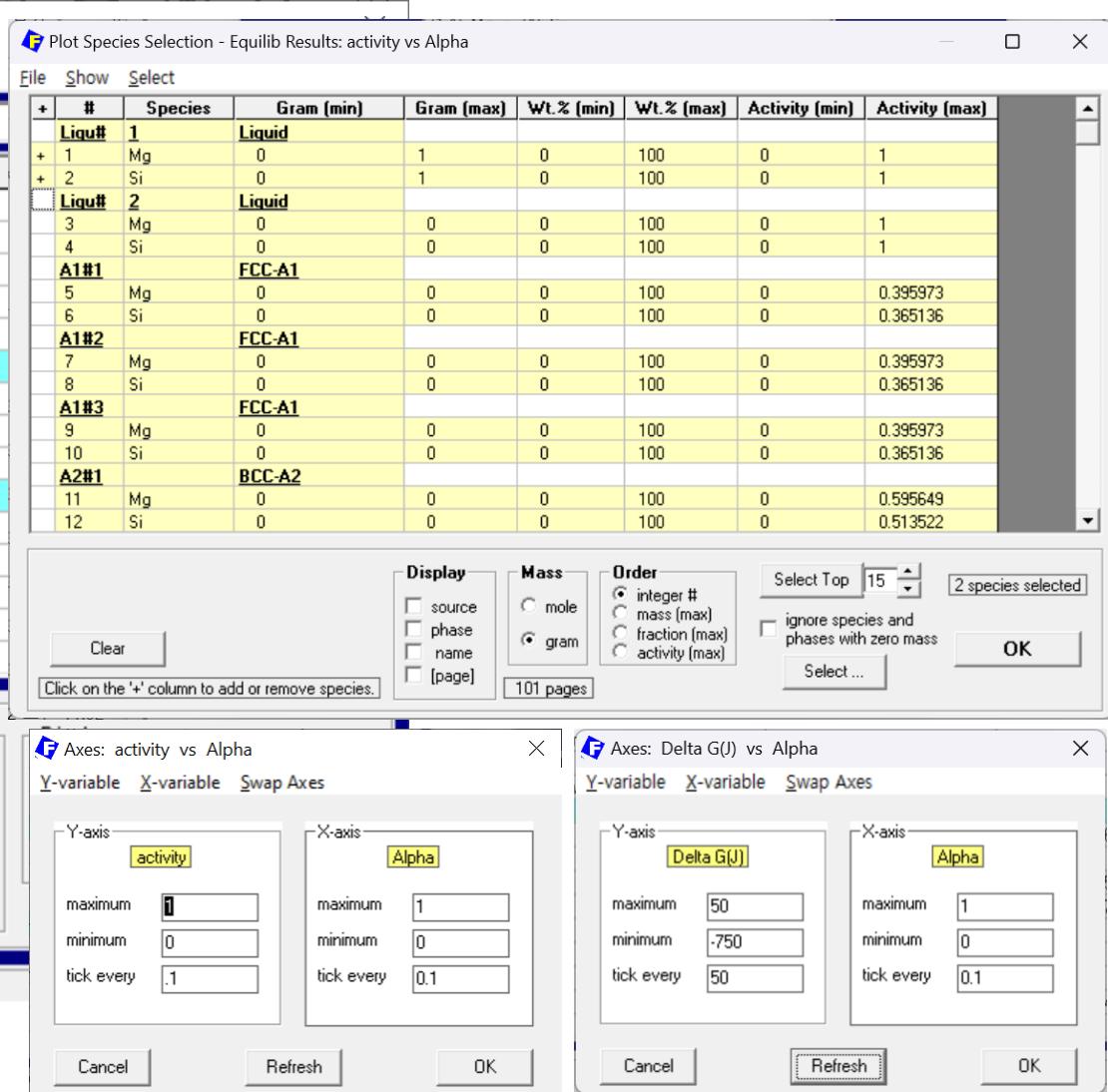
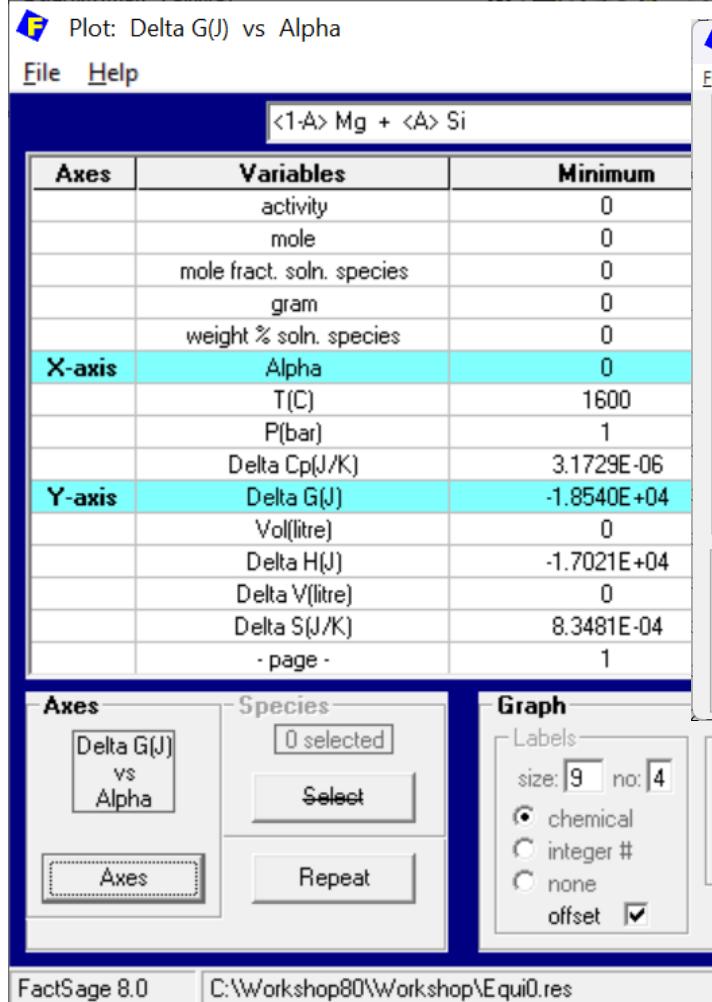
Final Conditions

<A>		T(C)	P(bar)	Delta H(J)
0 1 0.01		1600	1	
10 steps	Table			101 calculations

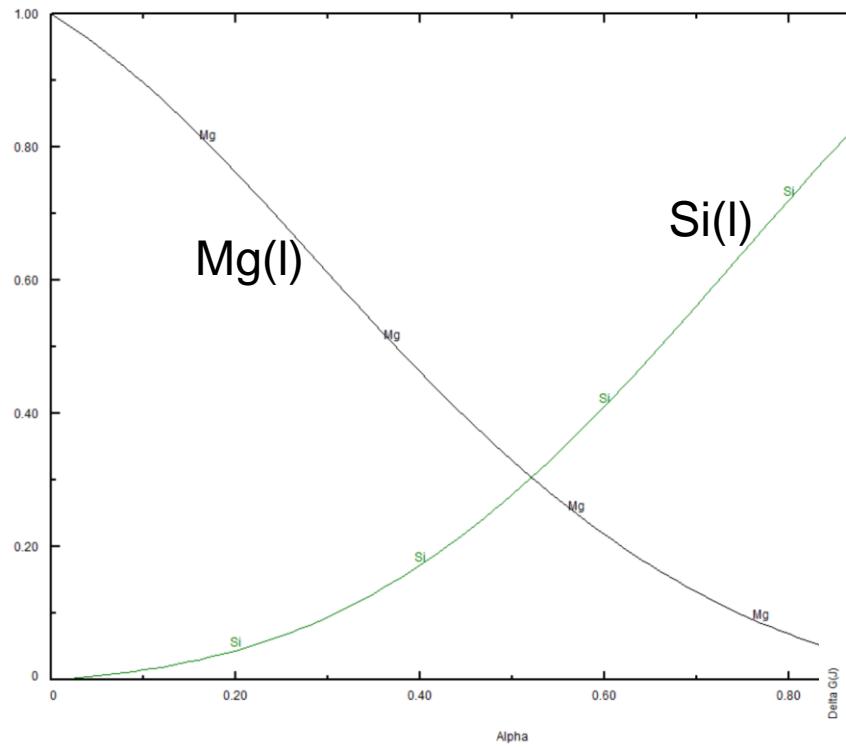
Equilibrium

- normal normal + transitions
- transitions only open
- no time limit - Calculate >

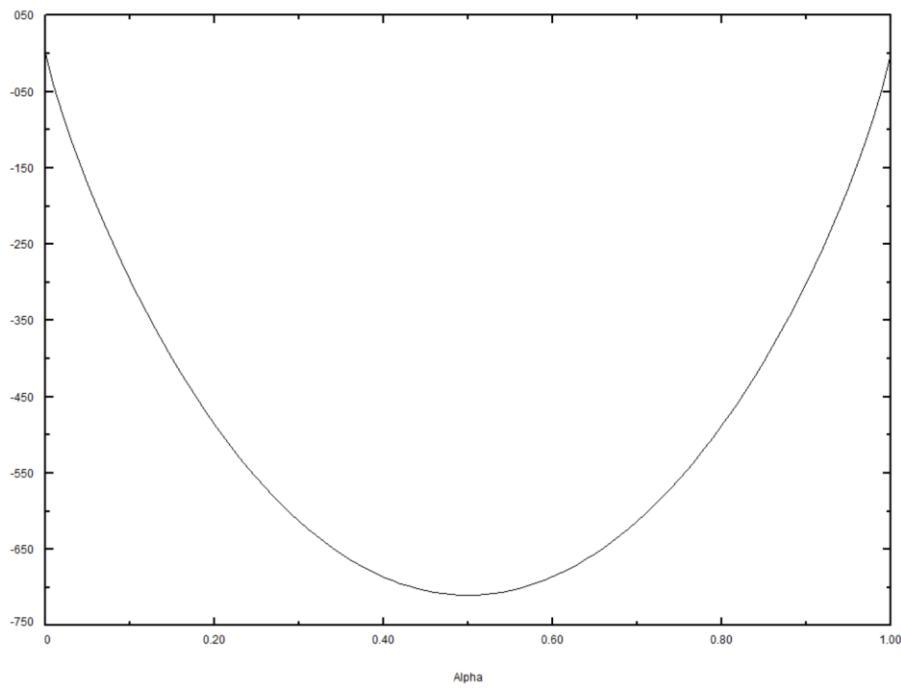
FactSage 8.3



<1-A> Mg + <A> Si
C:\FACTSAGEWS\Equi0.res 03Jul23

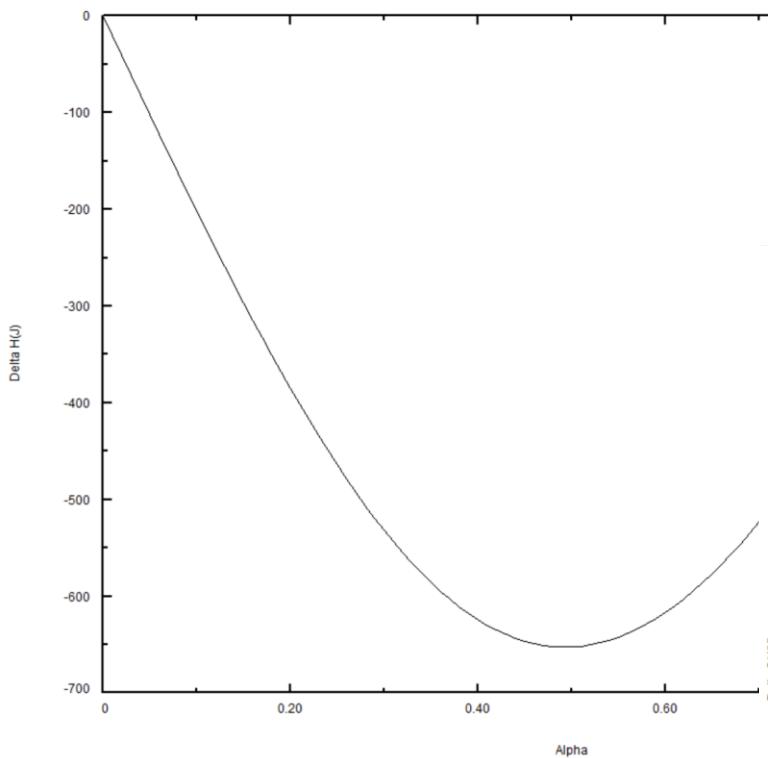


<1-A> Mg + <A> Si
C:\FACTSAGEWS\Equi0.res 03Jul23



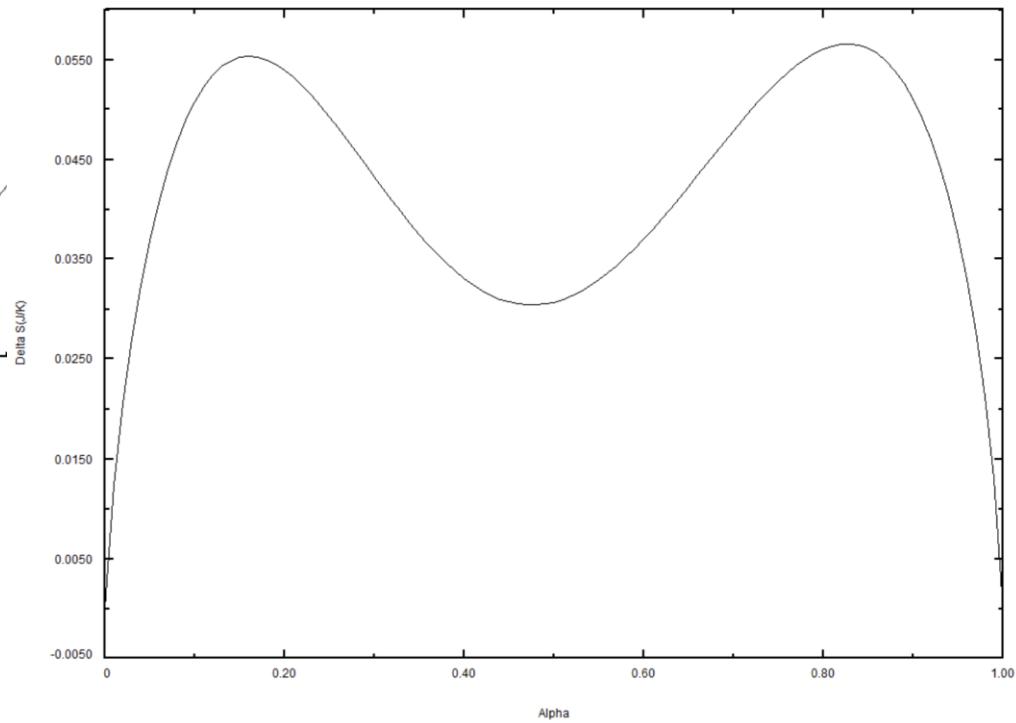
<1-A> Mg + <A> Si

C:\FACTSAGEWS\Equi0.res 03Jul23

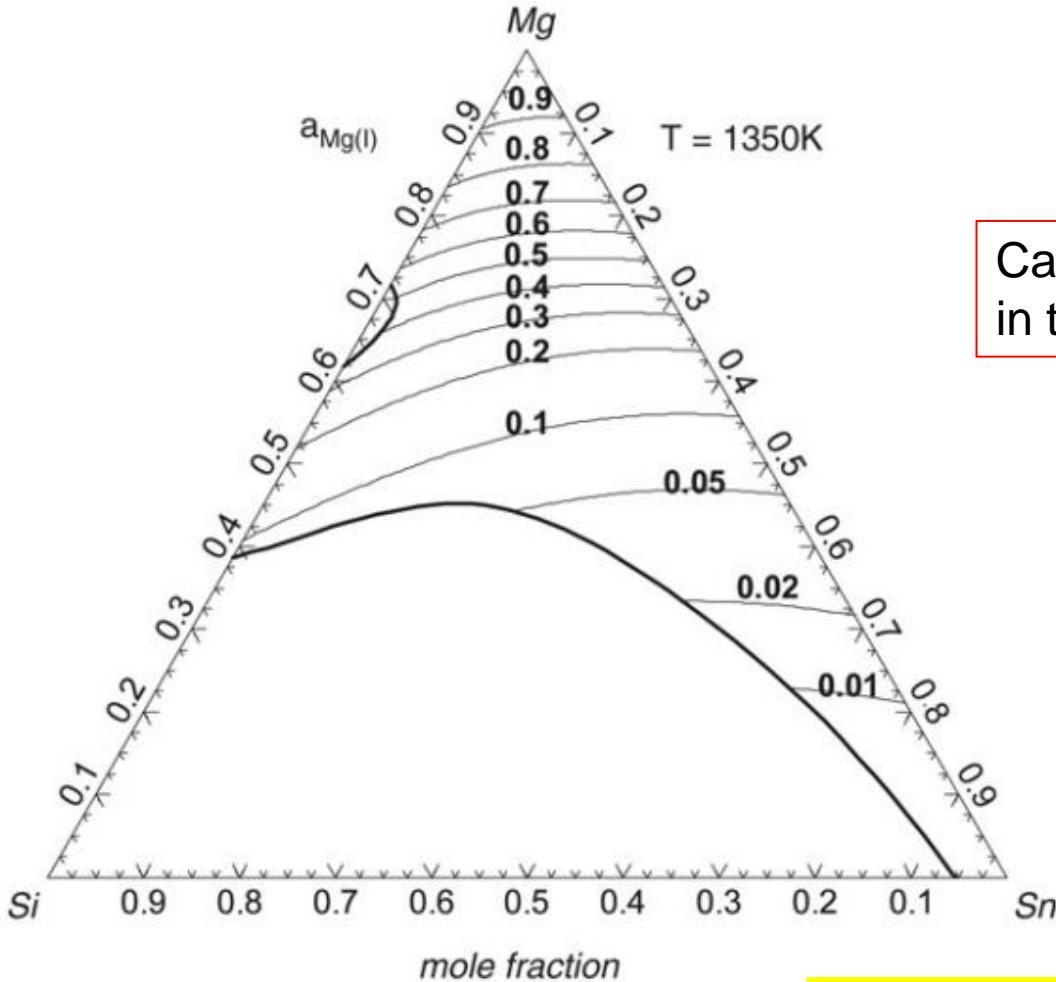


<1-A> Mg + <A> Si

C:\FACTSAGEWS\Equi0.res 03Jul23



EX22-2. Iso-activity line in ternary system



Calculation of iso-activity line of $\text{Mg}(\text{I})$ in the $\text{Mg}-\text{Si}-\text{Sn}$ system at $T=1350\text{ K}$

Now you can easily calculate iso-activity lines in "Phase Diagram" module (FactSage70)

Equilib - Reactants

File Edit Run Macro Table Units Data Search Data Evaluation Help
T(K) P(atm) Energy(J) Quantity(mol) Vol(litre)

Reactants (1)

Quantity(mol)	Species	Phase	T(K)	P[total]**	Stream#	Data
0.3	Mg				1	
<A>	Si				1	
<0.7-A>	Sn				1	

Equilib - Menu: last system

File Units Parameters Help
T(K) P(atm) Energy(J) Quantity(mol) Vol(litre)

Reactants (3)

0.3 Mg + <A> Si + <0.7-A> Sn

Product (2)

Components

gas	ideal	real
0	0	0
+ aqueous	0	0
+ pure liquids	3	3
+ pure solids	29	29

species: 32

Target - none -
Estimate T(K): 1000
Quantity(mol): 0

Solution phases

	Base-Phase	Full Name
I	FTlite-Liqu	Liquid
J	FTlite-A1	FCC-A1
I	FTlite-A2	BCC-A2
I	FTlite-A3	HCP-A3
I	FTlite-A4	DIAM-A4 Prototype-C
+	FTlite-A5	BCT-A5 Prototype-Sn
J	FTlite-C1a	aC1 Prototype-CaF2
I	FTlite-C14	C14 Prototype-MgZn2

Legend
I - immiscible 6
J - immiscible 2
+ - selected 1

Show all selected
species: 71
solutions: 19
Select

Custom Solutions
0 fixed activities
0 ideal solutions

Pseudonyms
apply
Volume and phys.
 assume molar v.
solids and liquids
 use only molar v.
 use V & phys. p.

paraequilibrium
- clear
+ - select

Total Species (max) ✓
Total Solutions (max) ✓
Total Phases (max) ✓

Equilibrium
 normal
 norm
 transitions only
- no time limit -
Ca

(1)

(2)

(3)

scan $X_{Mg} = 0.3$ from left to right of this triangle and ask FactSage to find out composition for activity of Mg(l) = 0.1

Selection - Equilib Page 1/71 : T(K) = 1350, P(atm) = 1

File Edit Show Sort
Selected: 3/3 LIQUID
Page 1/71 : T(K) = 1350, P(atm) = 1
1 Pages: 1 - [71] [page]

Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
1	Mg(liq)	FTlite	liquid	V	3.0801E-02	2.1436E-02 [23]	8.1343E-02 [71]	
2	Si(liq)	FTlite	liquid	V	0 [1]	0.4074 [71]		
3	Sn(liq)	FTlite	liquid	V	0.6110	0 [71]	0.6110 [1]	

Fixed Activity

Enter the activity
(or for a range of values enter 'first last step') for
1 Mg(liq)
Press [Cancel] if the activity is no longer fixed.

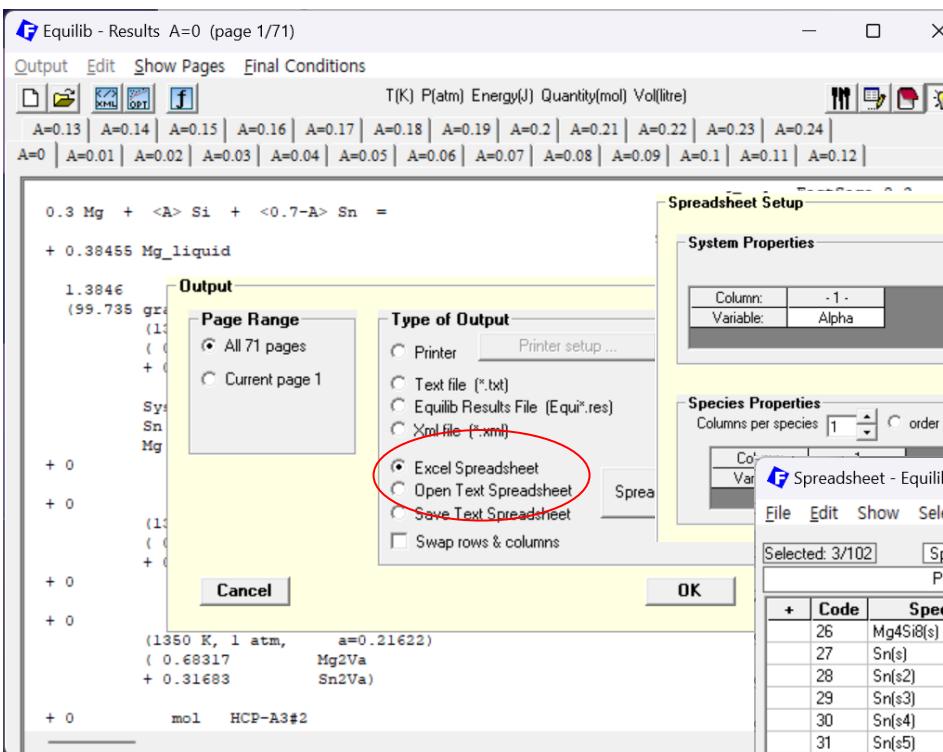
0.1

OK Cancel

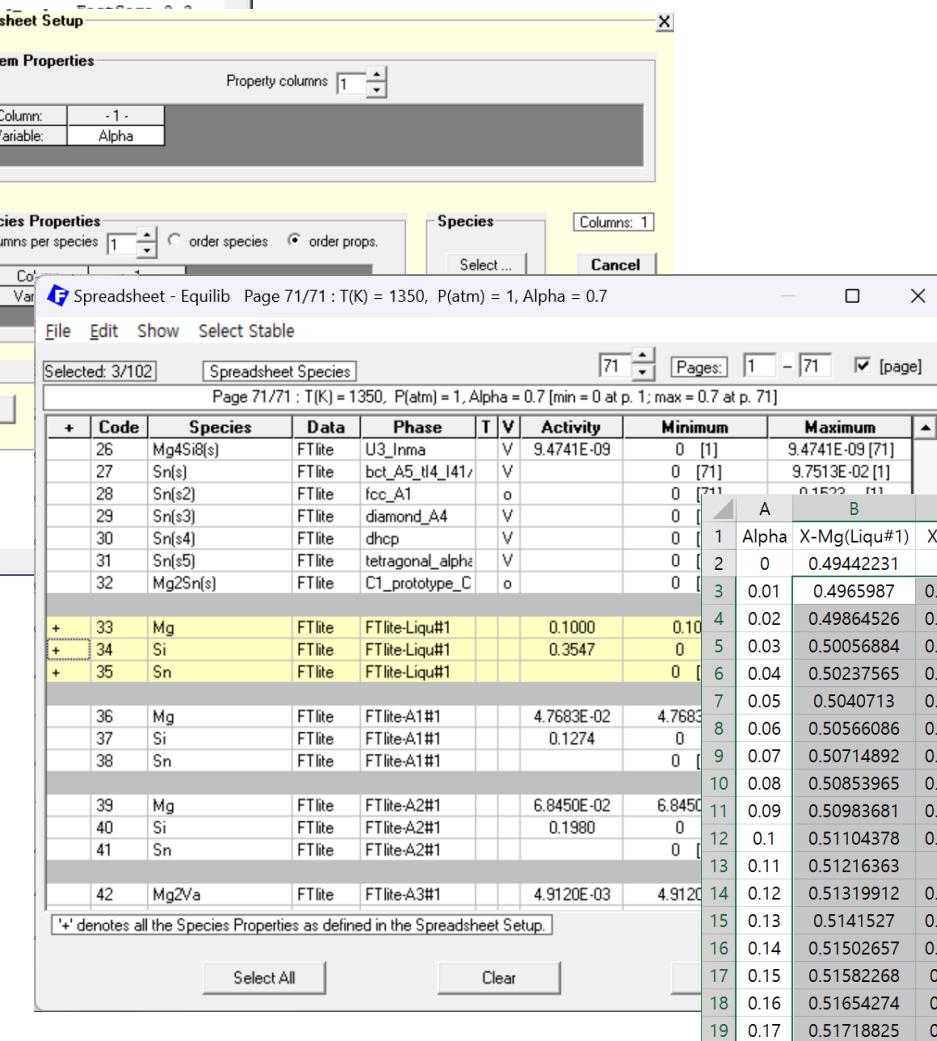
(3)

(1) Click mouth right button on “pure liquids” →

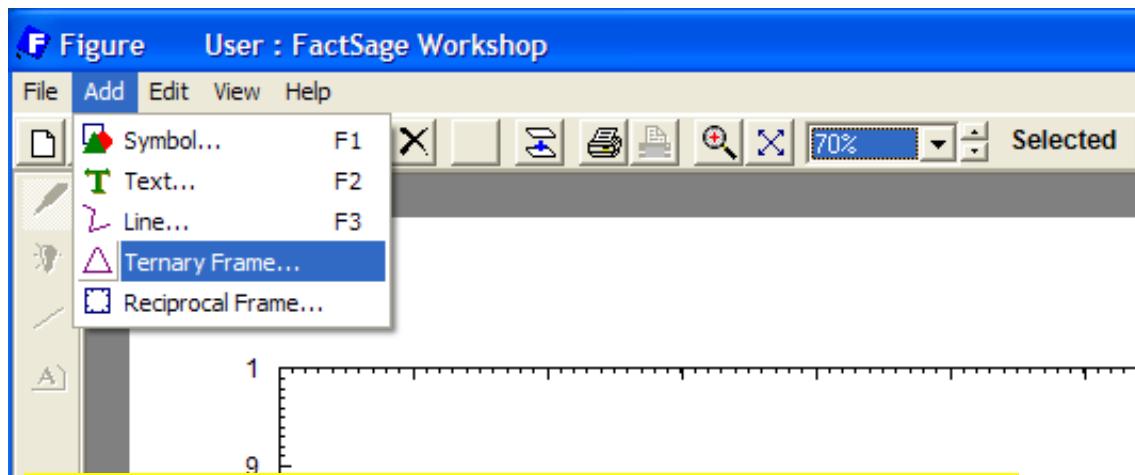
(2) Click “+” button to (3) setup activity of element (this case is for Mg)



Save results in excel
or spread sheet form



Selected: 3/102		Spreadsheet Species		71		Pages: 1 - 71		[page]				
Page 71/71 : T(K) = 1350, P(atm) = 1, Alpha = 0.7 [min = 0 at p. 1; max = 0.7 at p. 71]												
+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum	▲		
	26	Mg4Si8(s)	FTlite	U3_Inma	V	9.4741E-09		0 [1]	9.4741E-09 [71]			
	27	Sn(s)	FTlite	bct_A5_I4_I41/	V			0 [71]	9.7513E-02 [1]			
	28	Sn(s2)	FTlite	fcc_A1	o			0 [71]	0.1522 [1]			
	29	Sn(s3)	FTlite	diamond_A4	V			0 [71]	A	B	C	D
	30	Sn(s4)	FTlite	dhcp	V			0 [1]	Alpha	X-Mg(Liqu#1)	X-Si(Liqu#1)	X-Sn(Liqu#1)
	31	Sn(s5)	FTlite	tetragonal_alpha:	V			0 [2]	0	0.4944231	0	0.50557769
	32	Mg2Sn(s)	FTlite	C1_prototype_C	o			0 [3]	0.01	0.4965987	0.007191447	0.49620985
+	33	Mg	FTlite	FTlite-Liqu#1		0.1000		0.10 [4]	0.02	0.49864526	0.014324421	0.48703032
+	34	Si	FTlite	FTlite-Liqu#1		0.3547		0 [5]	0.03	0.50056884	0.021404192	0.47802696
+	35	Sn	FTlite	FTlite-Liqu#1				0 [6]	0.04	0.50237565	0.028435677	0.46918867
	36	Mg	FTlite	FTlite-A1#1		4.7683E-02		4.7683 [7]	0.05	0.5040713	0.035423479	0.46050522
	37	Si	FTlite	FTlite-A1#1		0.1274		0 [8]	0.06	0.50566086	0.042371927	0.45196722
	38	Sn	FTlite	FTlite-A1#1				0 [9]	0.07	0.50714892	0.049285108	0.44356597
	39	Mg	FTlite	FTlite-A2#1		6.8450E-02		6.8450 [10]	0.08	0.50983681	0.056166897	0.43529345
	40	Si	FTlite	FTlite-A2#1		0.1980		0 [12]	0.1	0.51104378	0.069850889	0.41910533
	41	Sn	FTlite	FTlite-A2#1				0 [13]	0.11	0.51216363	0.07666	0.41117637
	42	Mg2Va	FTlite	FTlite-A3#1		4.9120E-03		4.9120 [14]	0.12	0.51319912	0.083451579	0.4033493
'+' denotes all the Species Properties as defined in the Spreadsheet Setup.												
<input type="button" value="Select All"/>					<input type="button" value="Clear"/>							
								15	0.13	0.5141527	0.090228784	0.39561852
								16	0.14	0.51502657	0.096994686	0.38797874
								17	0.15	0.51582268	0.10375228	0.38042504
								18	0.16	0.51654274	0.11050452	0.37295274
								19	0.17	0.51718825	0.11725428	0.36555747



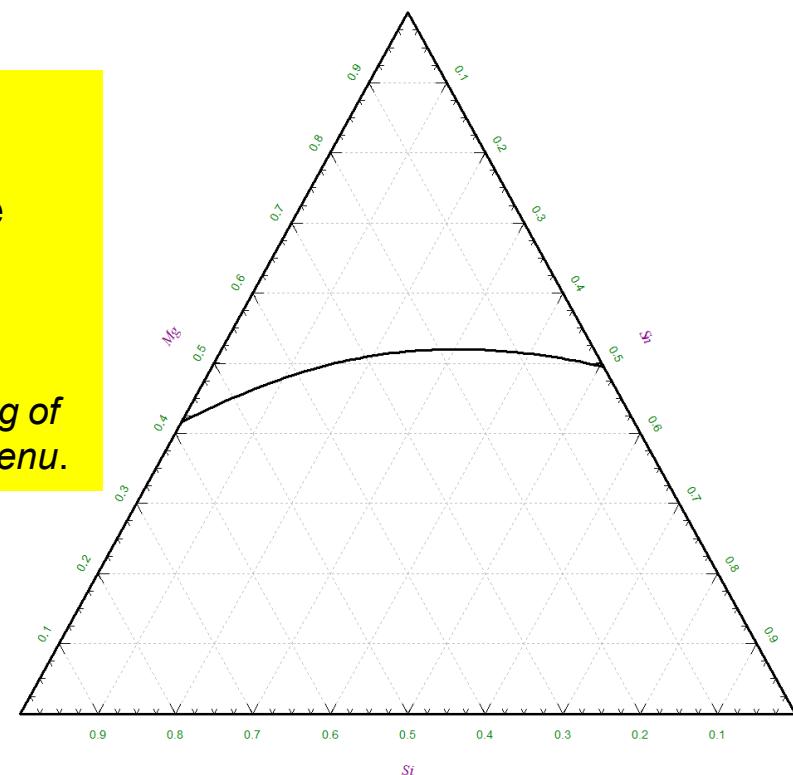
Plot the results in triangle diagram

- Prepare the triangle frame
- Plot the A,B,C coordinate numbers in triangle diagram

“Cont+C” → “Cont+V” or “copy” and “paste”.

Sometimes, “Cont+V” is not working due to the setting of values in Excel software, then use “paste” in “Edit” menu.

Mg - Si - Sn
1350 K, 1 atm



EX23. Calculation for Solidus lines (Solidus projection)

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J)

Components (3) Mg + Al + Zn

Calculating a polythermal projection – the first melting surface

(1) Solution phases

	Base-Phase	Full Name
0	IF	FTlite-Liqu
0	J	FTlite-A1
0	I	FTlite-A2
35	I	FTlite-A3
	I	HCP-Zn Prototype-Mg
	I	FTlite-A12
	I	CBCC-A12 Prototype-Mn
	I	FTlite-C14
	I	C14 Prototype-MgZn2
	I	FTlite-C15
	I	C15 Prototype-MgCu2

Compound species: 35

Target: - none -

Estimate T(K): 1000

Legend: I - immiscible 10
J - 3-immiscible 1
F - formation target
+ - selected 6

Show: all

Total Species (max 7000): 178

Species: 143

Solutions: 29

(2) Variables

compositions: 2

log10(a): 0

X, Y steps: 11

(3) Phase Diagram Projection

Y-axis: 0.3 (max)
X-axis: 0 (min)

#1. 0 Mg + 1 Al + 0 Zn = 0.3 (max)
#1 log10(composition)

#2. 0 Mg + 0 Al + 1 Zn = 0.3 (max)
#2 log10(composition)

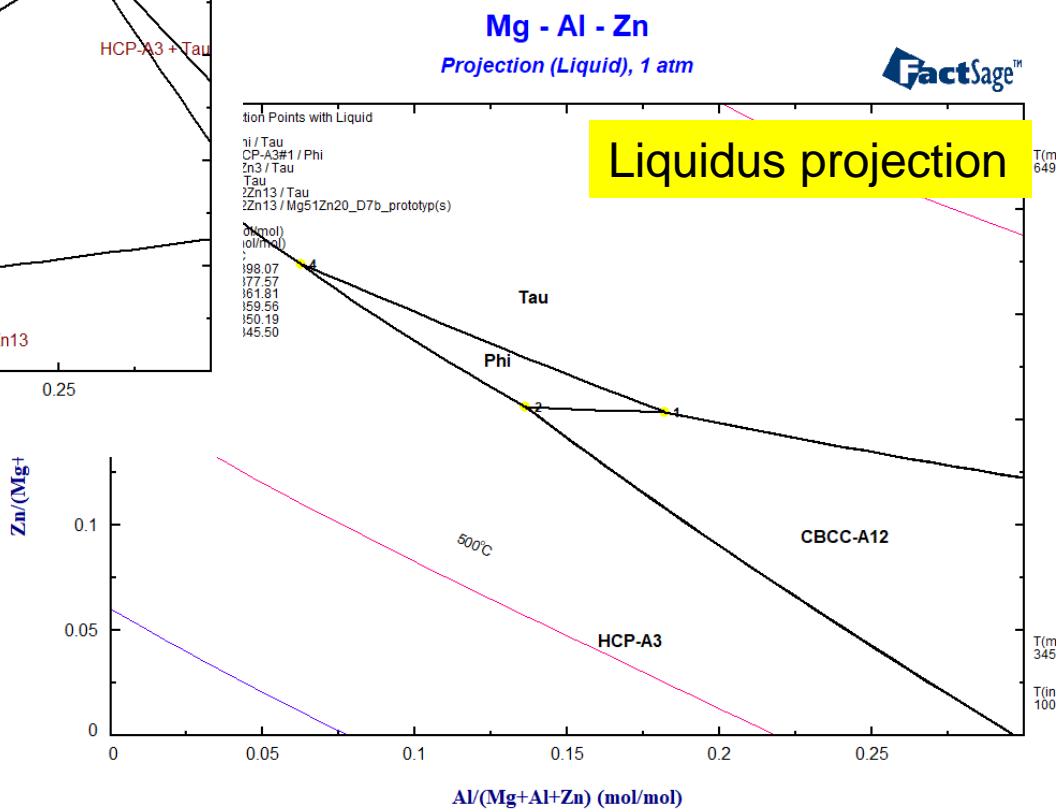
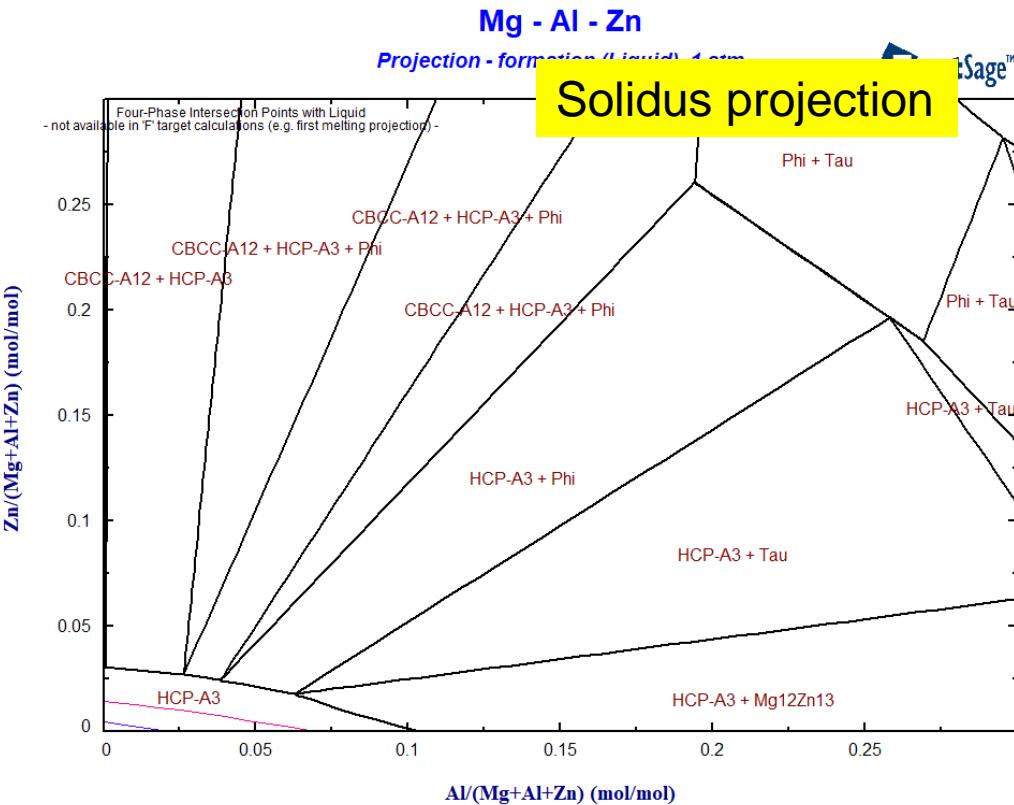
Temperature: T(C) projection
Max: 1000
Min: 500
T(inc): 100
6 isotherms

Pressure or Volume: P(atm) constant
C log P
C V(litre)
C log V
total pressure isobars
1e-4 1e-3 0.001

This is new feature in Phase diagram.

- Liquidus projection: plotting Liquidus in the temperature range with a certain interval (“O” option should be required for Liquid phase)
- Solidus projection: plotting Solidus in the same way as liquidus projection (“F” option should be required for Liquid phase)

EX23. Calculation for Solidus lines (Solidus projection)



EX24. Non-metallic Inclusion formation during metal solidification

Table 3 — Chemical Test Summary

Weld	C	S	P	Mn	Si	Al	Ni	Ti	O	N
High-aluminum E70T-4	0.234	<0.003	0.011	0.50	0.28	1.70	0.02	0.003	0.006	0.064
Low-aluminum E71T-8	0.149	<0.003	0.005	0.64	0.30	0.53	0.01	0.058	0.030	0.033

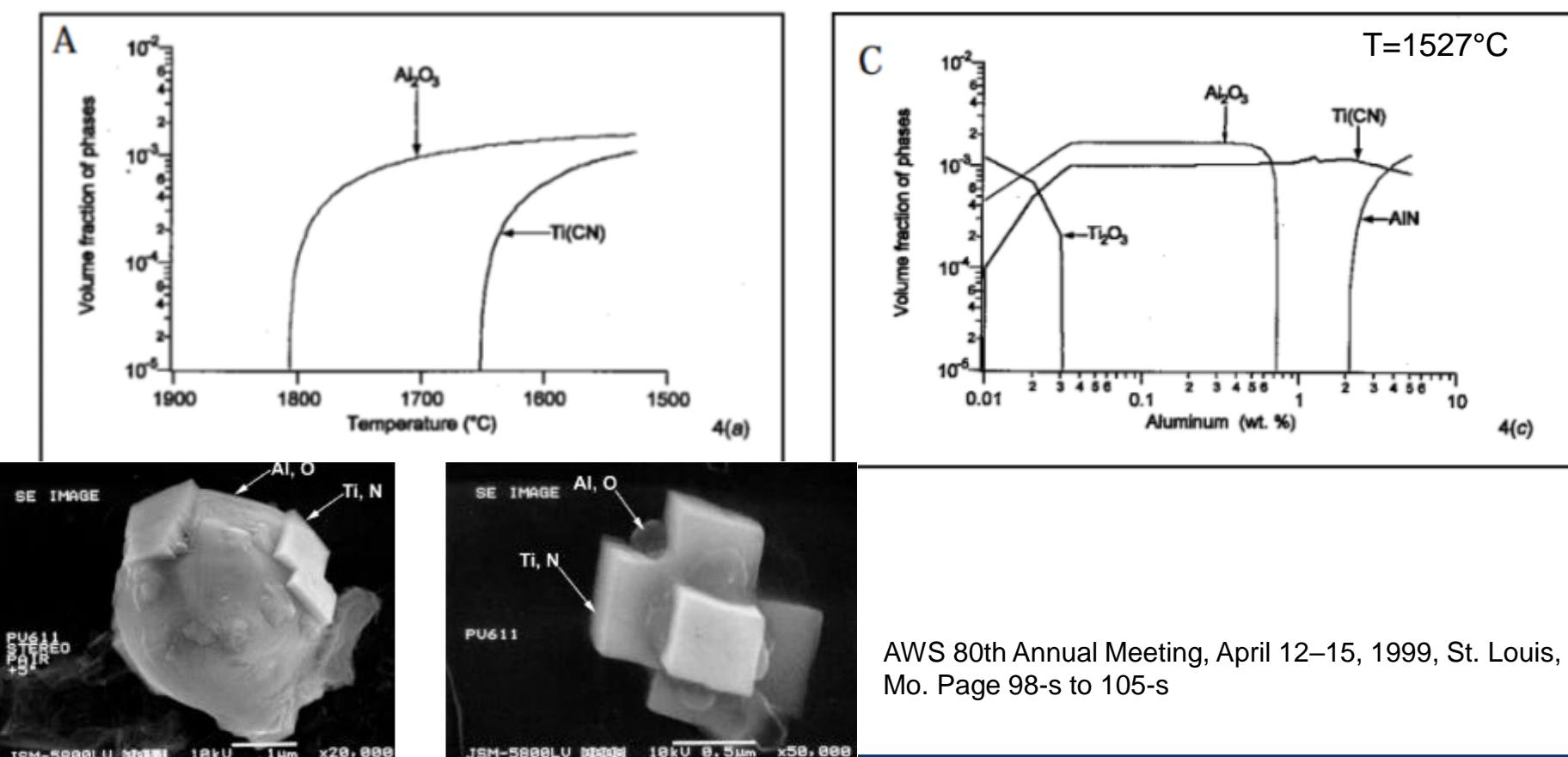


Table 3 — Chemical Test Summary

Weld	C	S	P	Mn	Si	Al	Ni	Ti	O	N
High-aluminum E70T-4	0.234	<0.003	0.011	0.50	0.28	1.70	0.02	0.003	0.006	0.064
Low-aluminum E71T-8	0.149	<0.003	0.005	0.64	0.30	0.53	0.01	0.058	0.030	0.033

Data Search - Equilib 8.3

Databases - 3/21 compound databases, 2/18 :

<input checked="" type="checkbox"/> FactPS	<input type="checkbox"/> FSscopp	<input type="checkbox"/> BINS	<input type="checkbox"/> SGPS
<input checked="" type="checkbox"/> FToxic	<input type="checkbox"/> FSlead	<input type="checkbox"/> SGTE	<input type="checkbox"/> SGold
<input type="checkbox"/> FTsulf	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGnobl	<input type="checkbox"/> SpMCBN
<input type="checkbox"/> FTsalt	<input type="checkbox"/> FSups	<input type="checkbox"/> ELEM	<input type="checkbox"/> TDmeph
<input type="checkbox"/> FTmisc	<input type="checkbox"/> FTHall	<input type="checkbox"/> FTfritz	<input type="checkbox"/> FTlite
<input type="checkbox"/> FTOxCN	<input type="checkbox"/> FThelg	<input type="checkbox"/> FTpulp	<input type="checkbox"/> FTnucl
<input type="checkbox"/> FTdemo		<input type="checkbox"/> FTnucl	

Private SGTEa

compounds only solutions only no database

Other Add/Remove Data RefreshDatabases

Information Click on a box to include (or exclude) a database in the data search. Normally databases compound and solution database (when available) will be selected. To 'uncouple' a database (note, this is NOT recommended).

If database is stored on your PC but not listed here then you must 'add the database to the system'.

Options - search for product species

Include compounds — gaseous ions (plasmas) aqueous species limited data compounds (25C)

Limits Organic species Minimum solution

Default Cancel Summary ...

Equilib - Menu: last system

File Units Parameters Help

T(C) P(bar) Energy(J) Quantity(g) Vol(litre)

Reactants (11)

(gram) 98.255 Fe + 0.149 C + 0.02 S + 0.005 P + 0.64 Mn + 0.30 Si + 0.53 Al + 0.01 Ni + 0.058 Ti

Products

*	+ Base-Phase	Full Name
I	FSstel-Liqu	LIQUID
J	FSstel-FCC	FCC_A1
I	FSstel-BCC	BCC_A2
	FSstel-HCP	HCP_A3
+	FSstel-CEME	CEMENTITE
+	FSstel-M23C	M23C6
	FSstel-M7C3	M7C3
	FSstel-CBCC	CBCC_A12

Transitions - temperature

Number of transitions: All

Legend

I - immiscible 2
J - 3-immiscible 1
+ - selected 2

Show all selected
species: 172
solutions: 9 Select

Final Conditions

<A>		T(C)	P(bar)	Product H(J)
		2500 1000 100	1	
10	steps	<input type="checkbox"/> Table		16+ calculations

Custom Solutions
0 fixed activities Details ...
0 ideal solutions

Pseudonyms apply Edit ...

Volume and physical prop data
 assume molar volumes of solids and liquids = 0
 use only molar volume data
 use V & phys. property data

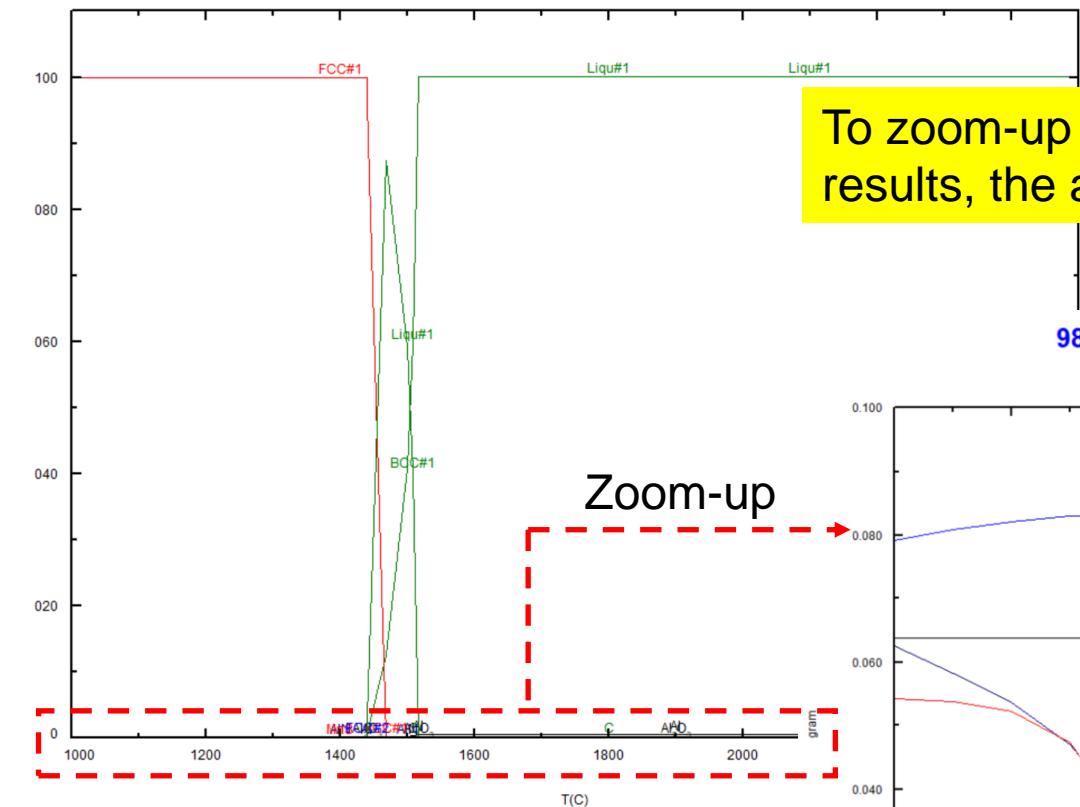
paraequilibrium & Gmin edit

Total Species (max 7000) 469
Total Solutions (max 200) 9
Total Phases (max 1500) 306

Equilibrium
 normal normal + transitions
 transitions only open
- no time limit - Calculate >>

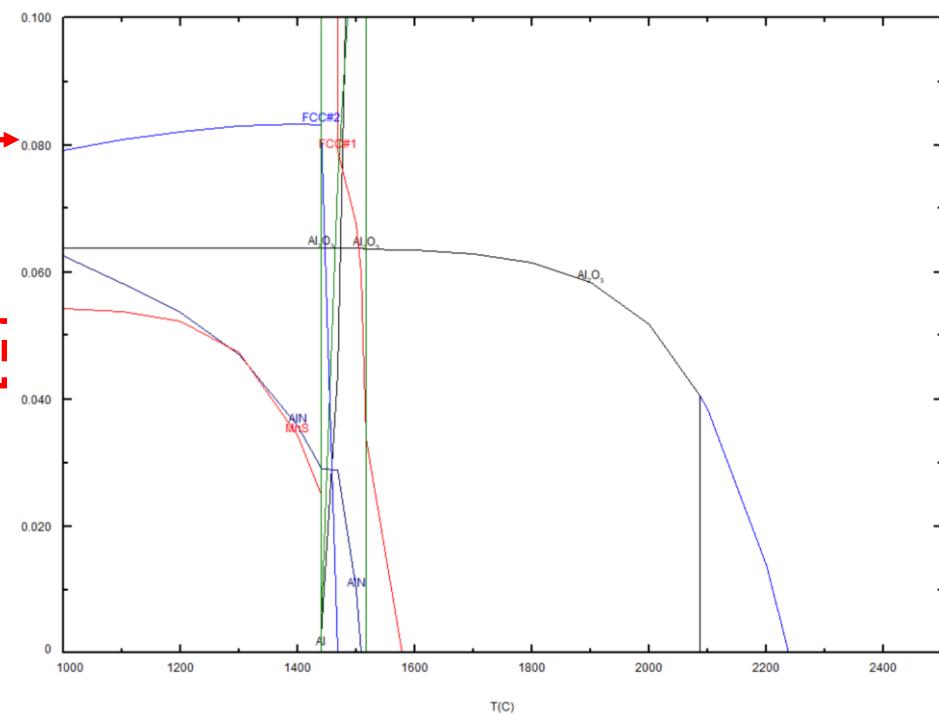
98.255 Fe + 0.149 C + 0.02 S + 0.005 P +

C:\FACTSAGEWS\Equi0.res 03Jul23



To zoom-up the small part of the calculated results, the axis of the figure should be changed

98.255 Fe + 0.149 C + 0.02 S + 0.005 P +
C:\FACTSAGEWS\Equi0.res 03Jul23



EX24. Non-metallic Inclusion formation during metal solidification

C	Si	Mn	Al	Ni	S	Ti	O	N
0.06	0.30	1.31	0.006	1.82	0.006	0.023	351ppm	115ppm

Data Search - Equilib 8.3

Databases - 3/21 compound databases, 2/18 solution databases

Fact **FactSage™ SGTE**

- FactPS
- FToxid
- FTsalt
- FTmisc
- FThall
- FToxCN
- FTfitz
- FThelg
- FTPulp
- FTdemo
- FSopp
- FSlead
- SGPS
- SGTE
- SGold
- FSust
- ELEM
- SGnobl
- SpMCBN
- FTlite
- FTmeph
- FTnucl

compounds only solutions only no database

Clear All Add/Remove Data RefreshDatabases

Information: Click on a box to include (or exclude) a database in the data search. Normally compound and solution database (when available) will be selected. To 'uncouple' (note, this is NOT recommended).

If database is stored on your PC but not listed here then you must 'add the data'.

Options - search for product species

Include compounds: gaseous ions (plasmas) aqueous species limited data compounds (25C)

Default Summary ...

Target: - none -

Estimate T(K): 1000 Quantity(g): 0

Final Conditions: <A> T(C) P(bar) Product H(J)

10 steps Table 2300 1000 10 1 131 calculations

FactSage 8.3

Equilib - Menu: last system

File Units Parameters Help

T(C) P(bar) Energy(J) Quantity(g) Vol(litre)

Reactants (10)

(gram) 96.109 Fe + 0.06 C + 0.006 S + 1.31 Mn + 0.3 Si + 0.006 Al + 1.82 Ni + 0.023 Ti + 351E-4 O

Products

Compound species

<input type="checkbox"/> gas	<input checked="" type="radio"/> ideal	<input type="radio"/> real	0
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	0
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	0
<input checked="" type="checkbox"/> pure solids	<input type="checkbox"/>	<input type="checkbox"/>	234
* - custom selection			
species: 234			

Solution phases

*	+	Base-Phase	Full Name
*	I	FSstel-Liqu	LIQUID
J	FSstel-FCC	FCC_A1	
I	FSstel-BCC	BCC_A2	
I	FSstel-HCP	HCP_A3	
+	FSstel-CEME	CEMENTITE	
+	FSstel-M23C	M23C6	
+	FSstel-M7C3	M7C3	
+	FSstel-CBCC	CBCC_A12	

Custom Solutions

0 fixed activities Details ...

0 ideal solutions

Pseudonyms

apply Edit ...

Volume and physical prop data

assume molar volumes of solids and liquids = 0

use only molar volume data

use V & phys. property data

paraequilibrium & Gmin edit

Total Species (max 7000) 1357
Total Solutions (max 200) 108
Total Phases (max 1500) 342

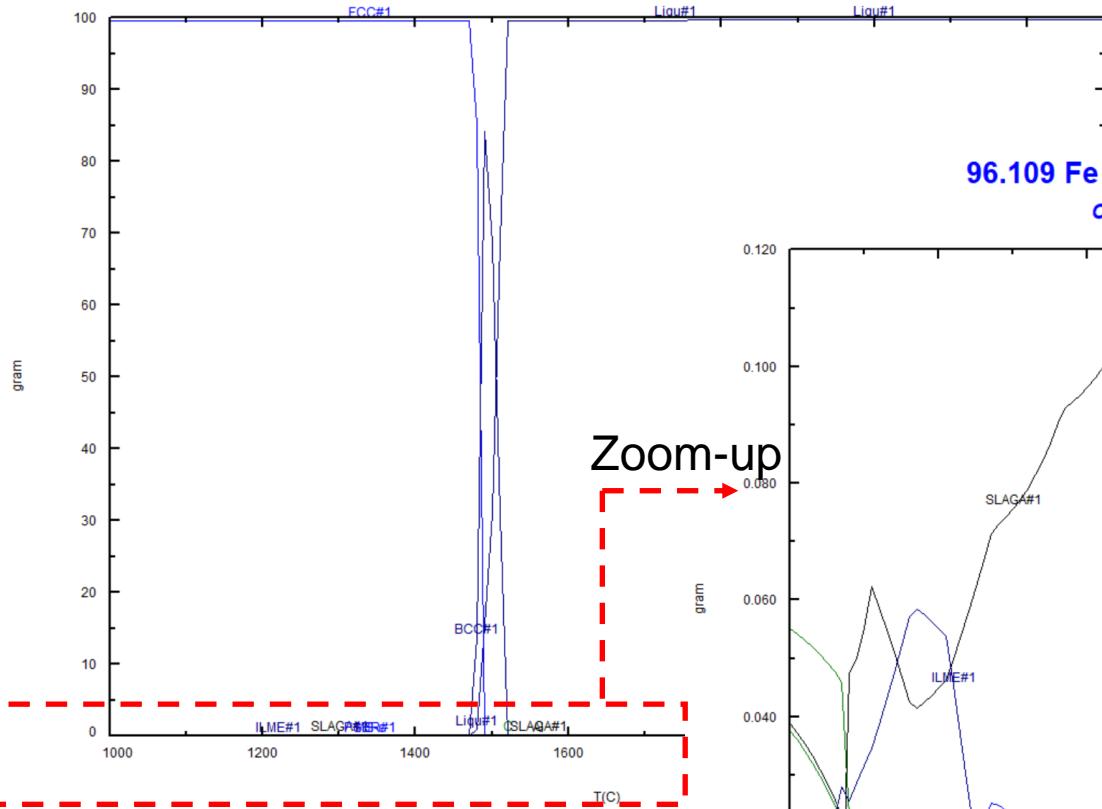
Legend: I - immiscible 23
J - 3-immiscible 2
+ - selected 56

Show all selected
species: 1123 Select
solutions: 108

Calculate >

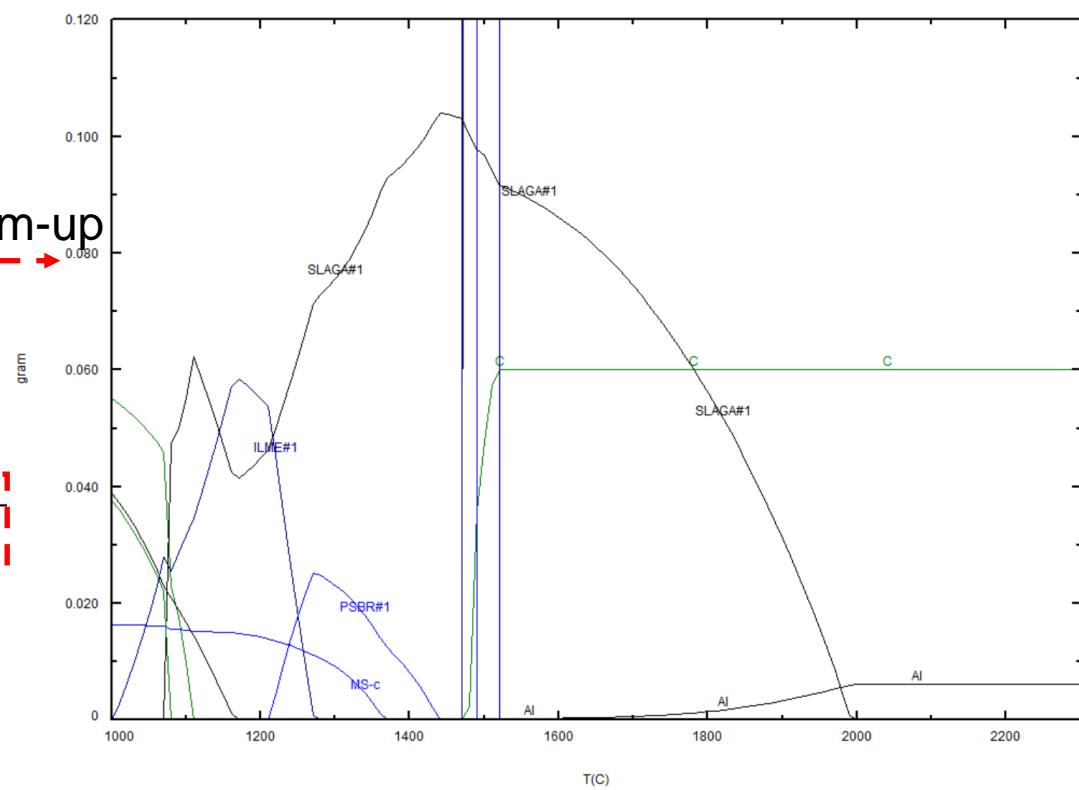
96.109 Fe + 0.06 C + 0.006 S + 1.31 Mn +

C:\FACTSAGEWS\Equi0.res 03Jul23



96.109 Fe + 0.06 C + 0.006 S + 1.31 Mn +

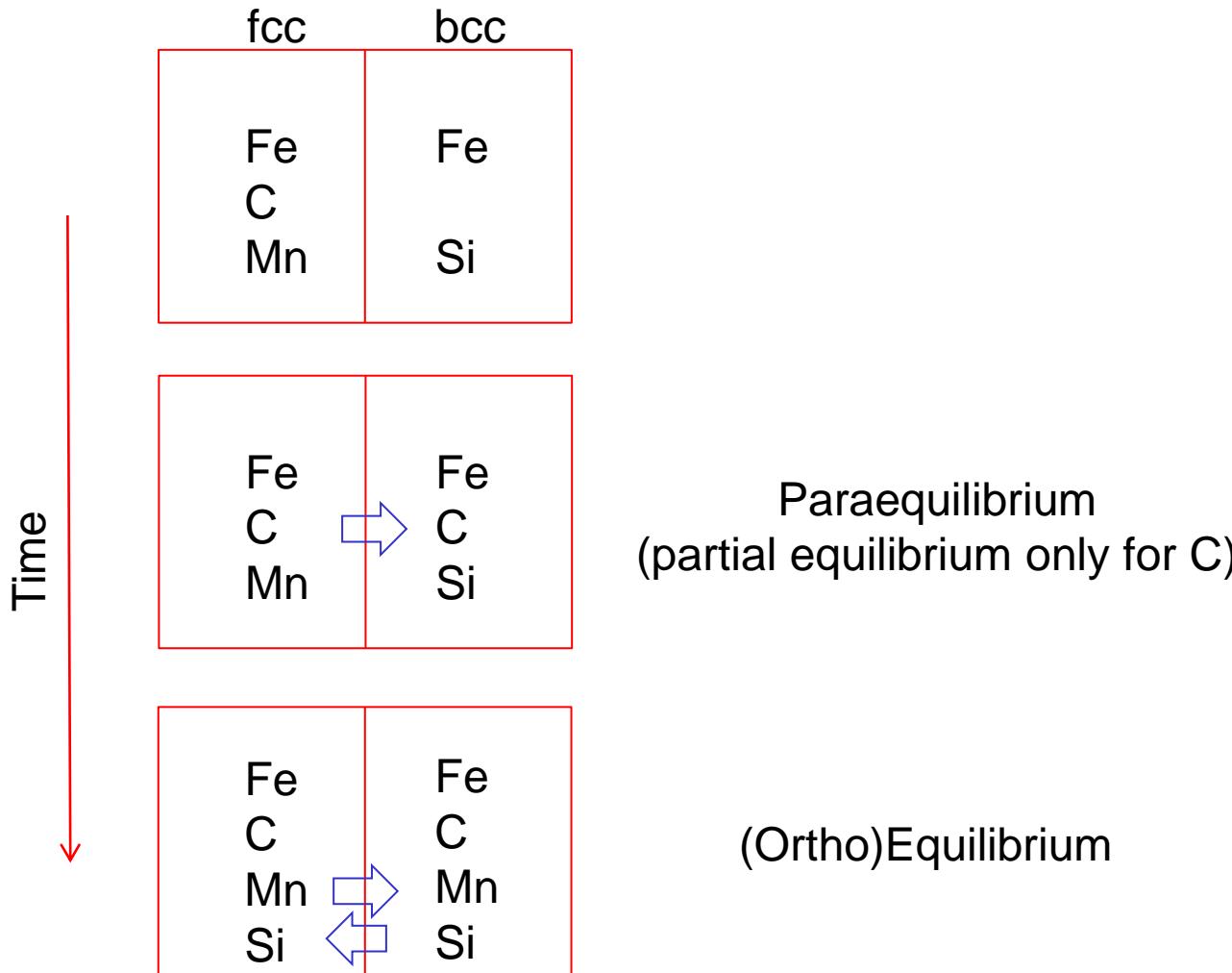
C:\FACTSAGEWS\Equi0.res 03Jul23



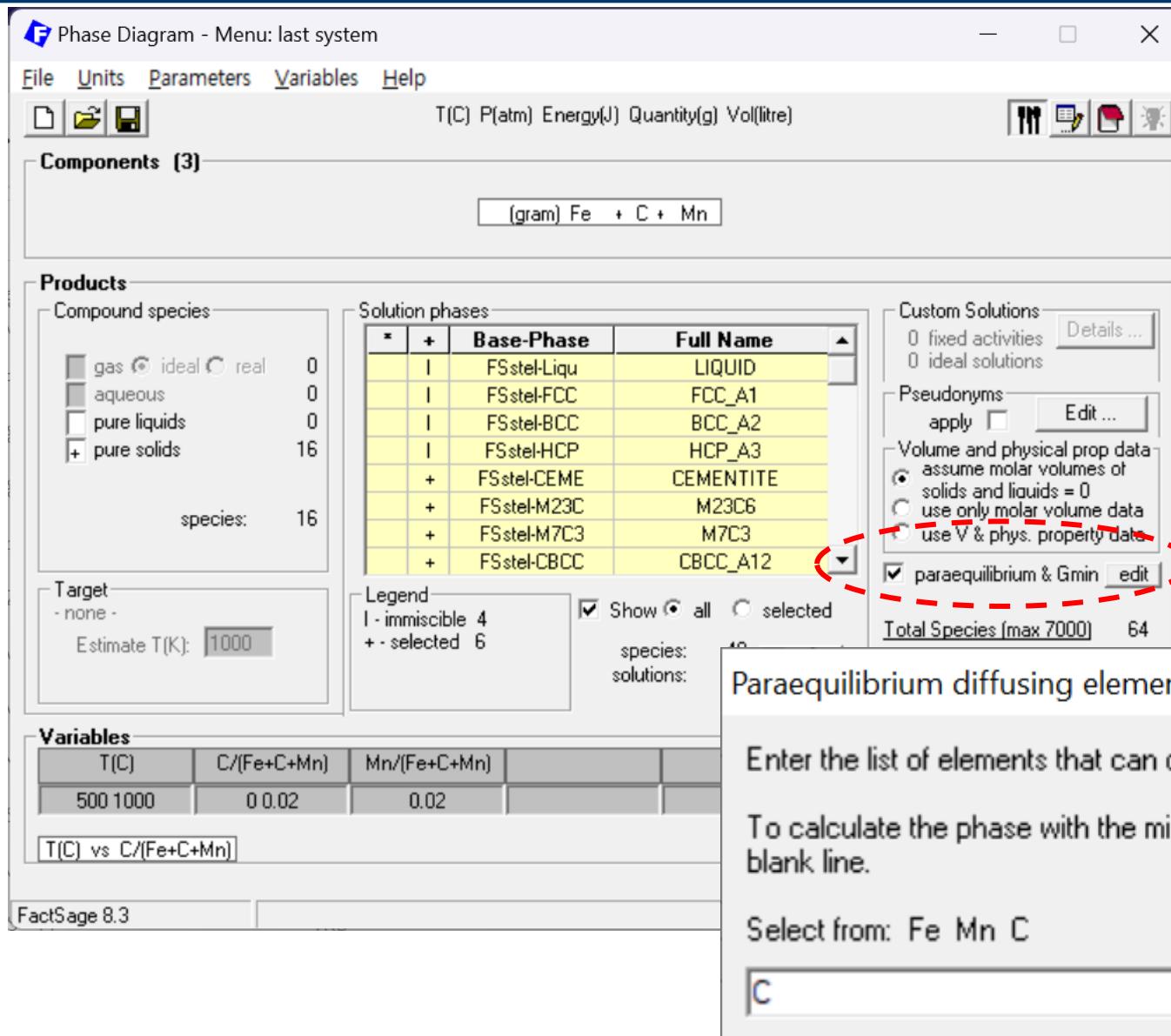
EX25. Paraequilibrium

Paraequilibrium (Partial equilibrium) vs Orthoequilibrium (Fully equilibrium)

Diffusion of C is much faster than Mn or Si



EX25-1. Paraequilibrium: Steel A3 temperature



Paraequilibrium diffusing elements

Enter the list of elements that can diffuse.

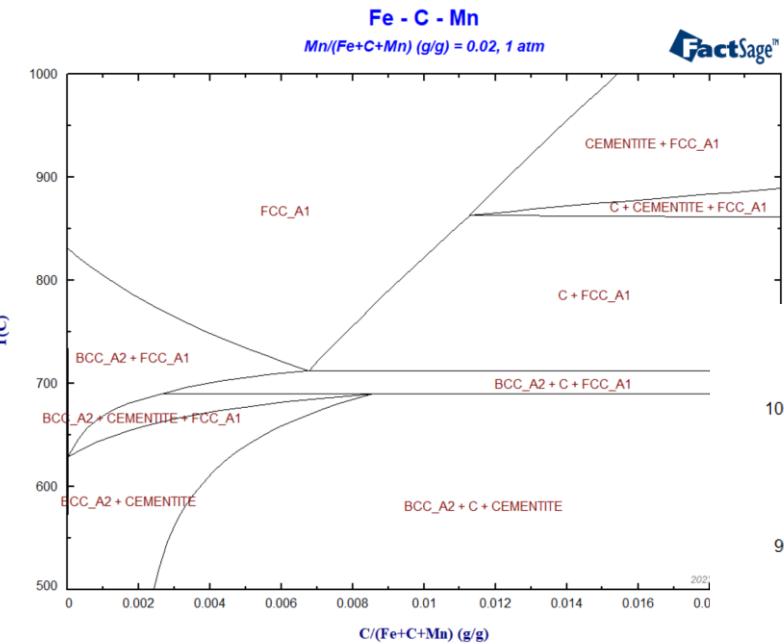
To calculate the phase with the minimum G, enter a blank line.

Select from: Fe Mn C

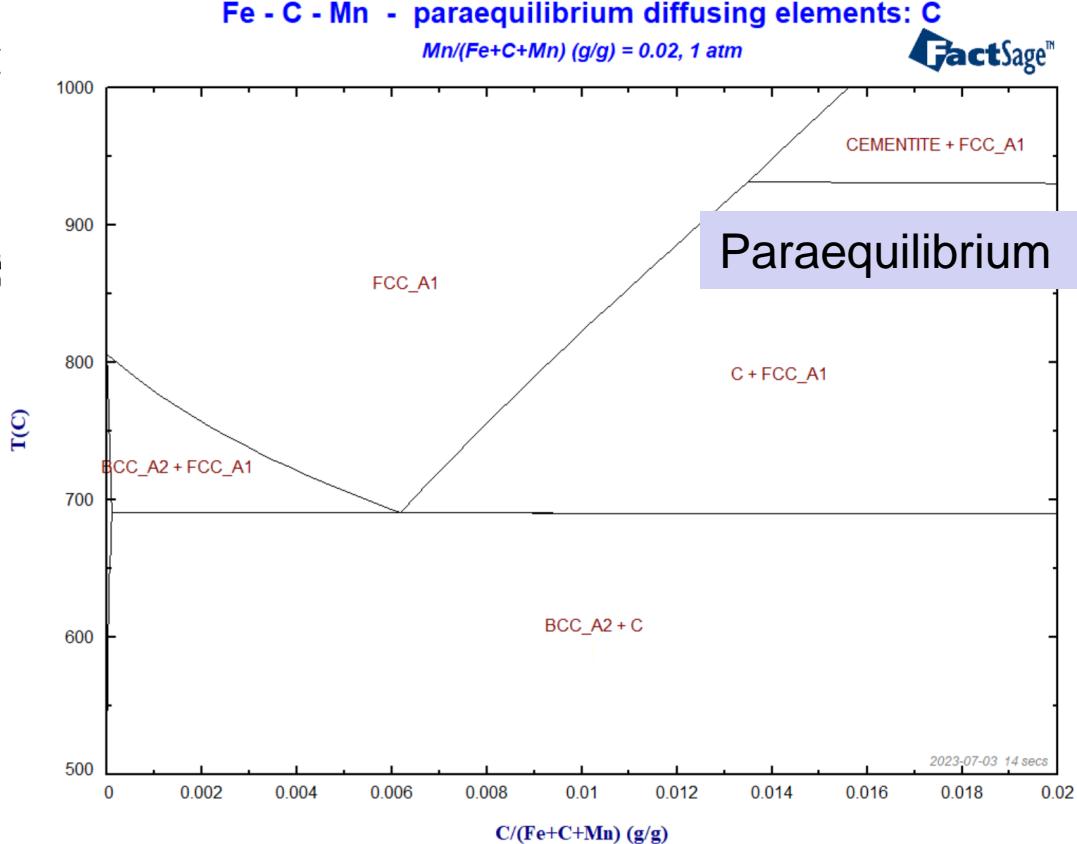
C

OK

Cancel



Full equilibrium



Paraequilibrium

EX25-2. Paraequilibrium: Rapid solidification for amorphous metal

Phase Diagram - Menu: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Quantity(mol) Vol(litre)

Components (2) Cu + Zr

Products

Compound species

- gas (radio button selected) ideal real
- aqueous
- pure liquids
- + pure solids

species: 20

Target: - none -

Estimate T(K): 1000

Solution phases

*	+	Base-Phase	Full Name
*	+	FTlite-Liqu	Liquid
*	+	FTlite-A1	FCC-A1

Paraequilibrium diffusing elements

Enter the list of elements that can diffuse.

To calculate the phase with the minimum G, enter a blank line.

Select from: Zr Cu

solutions: 4

Custom Solutions

- 0 fixed activities
- 0 ideal solutions

Pseudonyms

Apply Edit ...

ne and physical prop data
sume molar volumes of
lids and liquids = 0
e only molar volume data
e V & phys. property data

paraequilibrium & Gmin edit

species: 1

pecies (max 7000) 28

olutions (max 200) 4

Total Phases (max 1500) 24

Variables

T(C)	Zr/(Cu+Zr)
0 2000	0 1

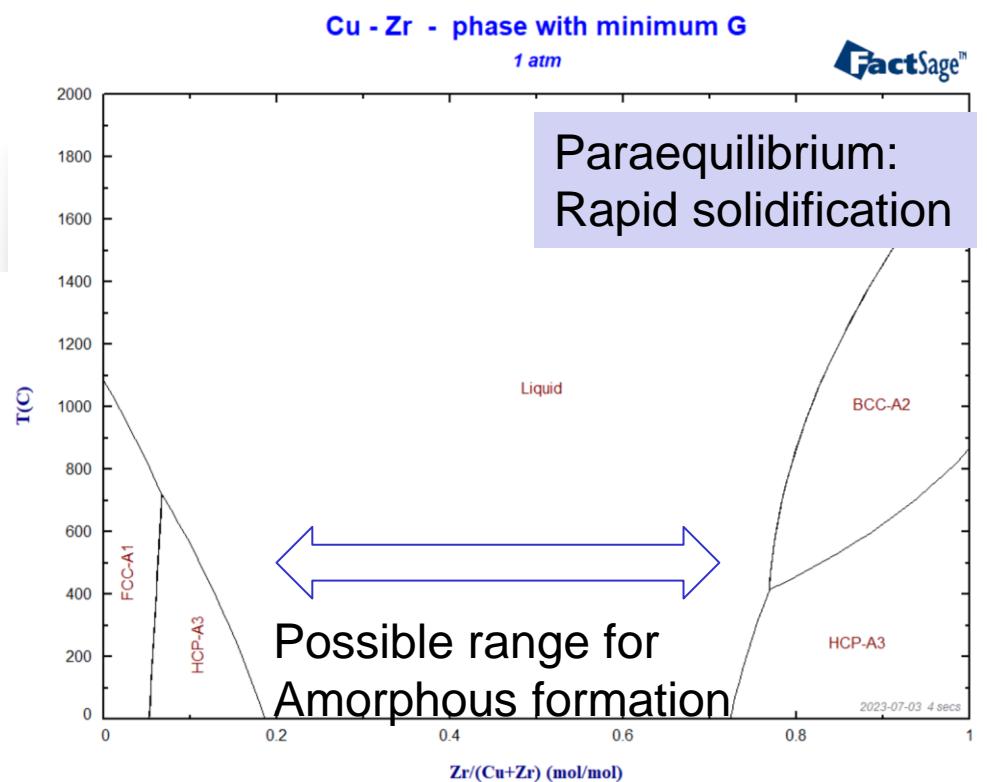
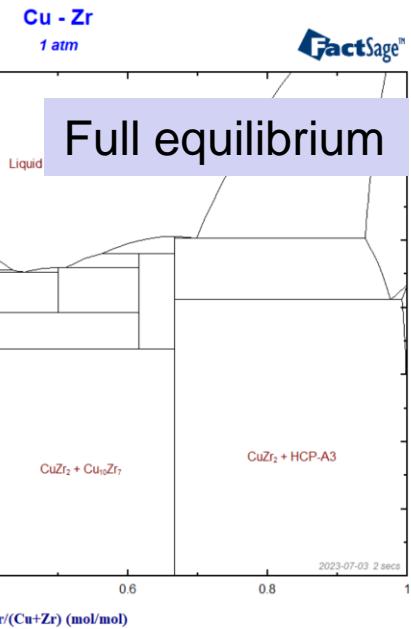
T(C) vs Zr/(Cu+Zr)

Phase Diagram

- no time limit - Calculate >

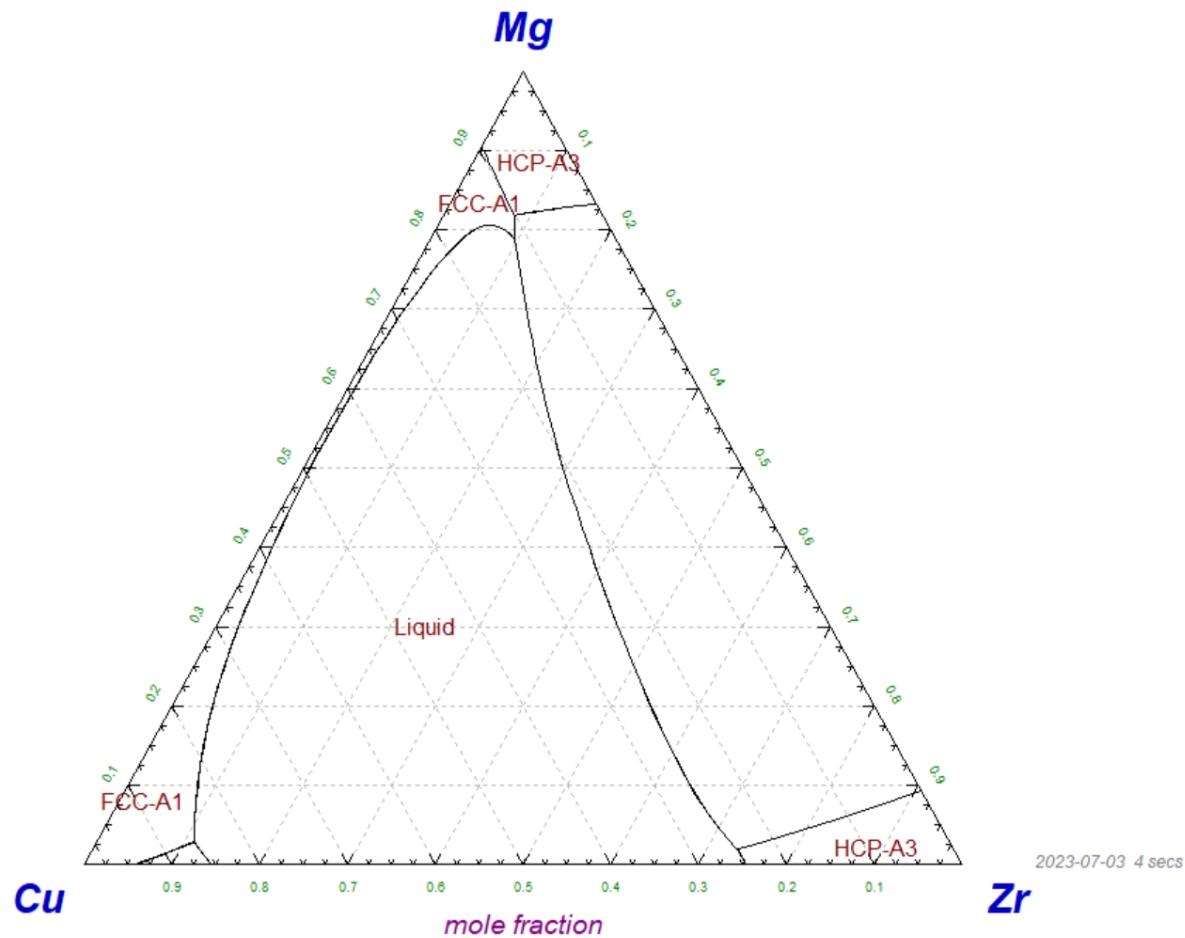
FactSage 8.3

Blank → no diffusion of any element: this is what happens during rapid solidification



Cu - Zr - Mg - phase with minimum G

300°C, 1 atm



2023-07-03 4 secs