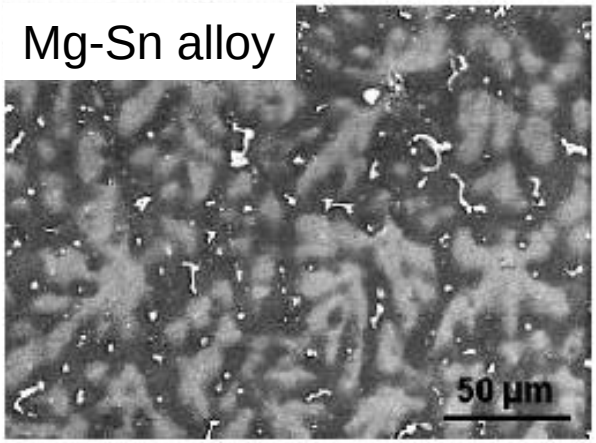
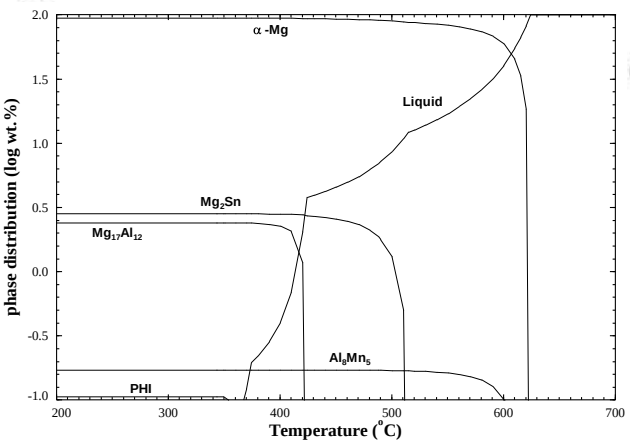
Alloy Design

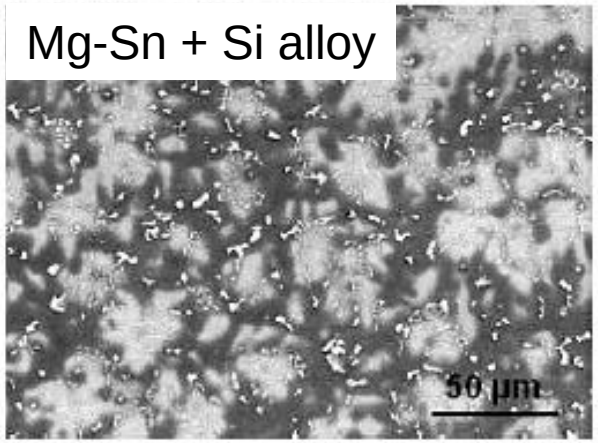
Basics and Advanced

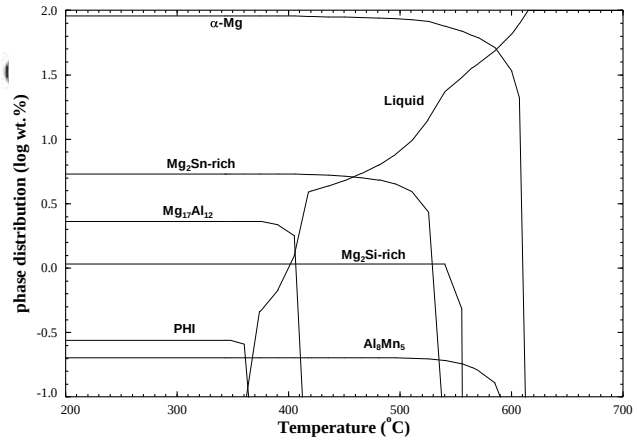
Mg-Sn alloy



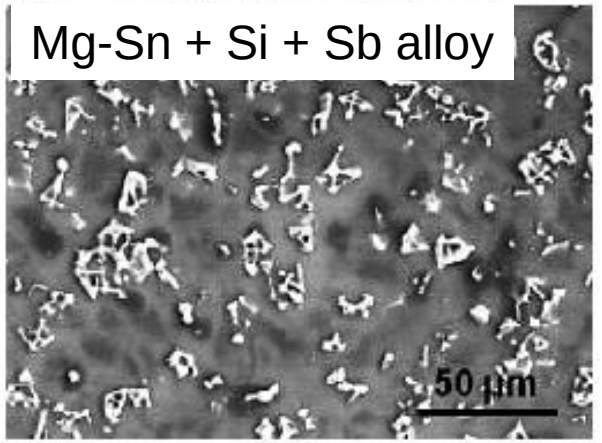


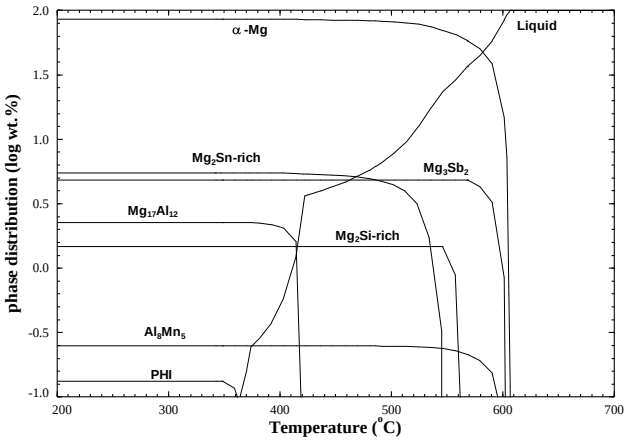
Mg-Sn + Si alloy





Mg-Sn + Si + Sb alloy





Contents

Contents

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

Equilibrium reactions as annealed microstructure

Data mining program (FactOptimal)

Phase diagram

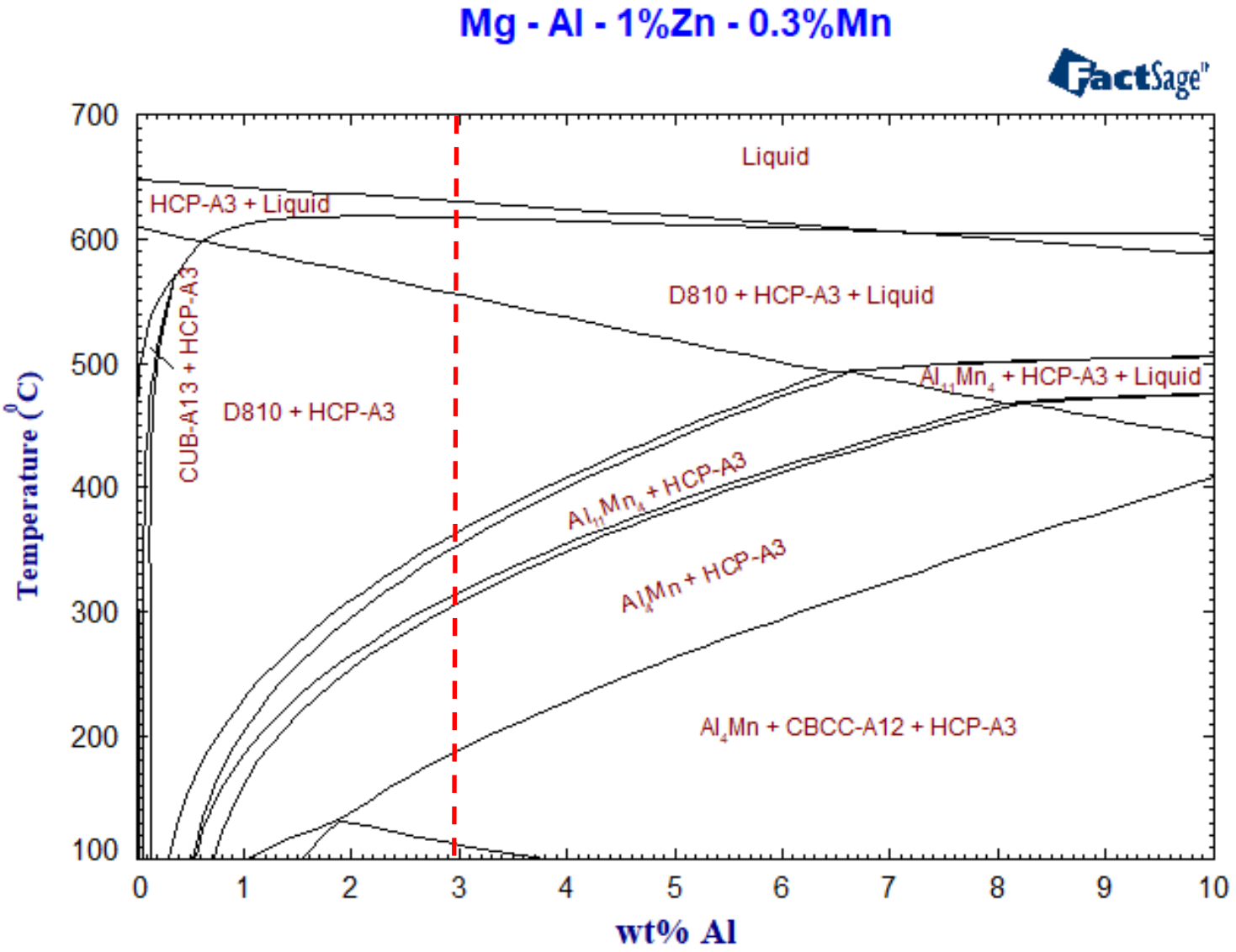
Multicomponent phase diagram section

Alloy design

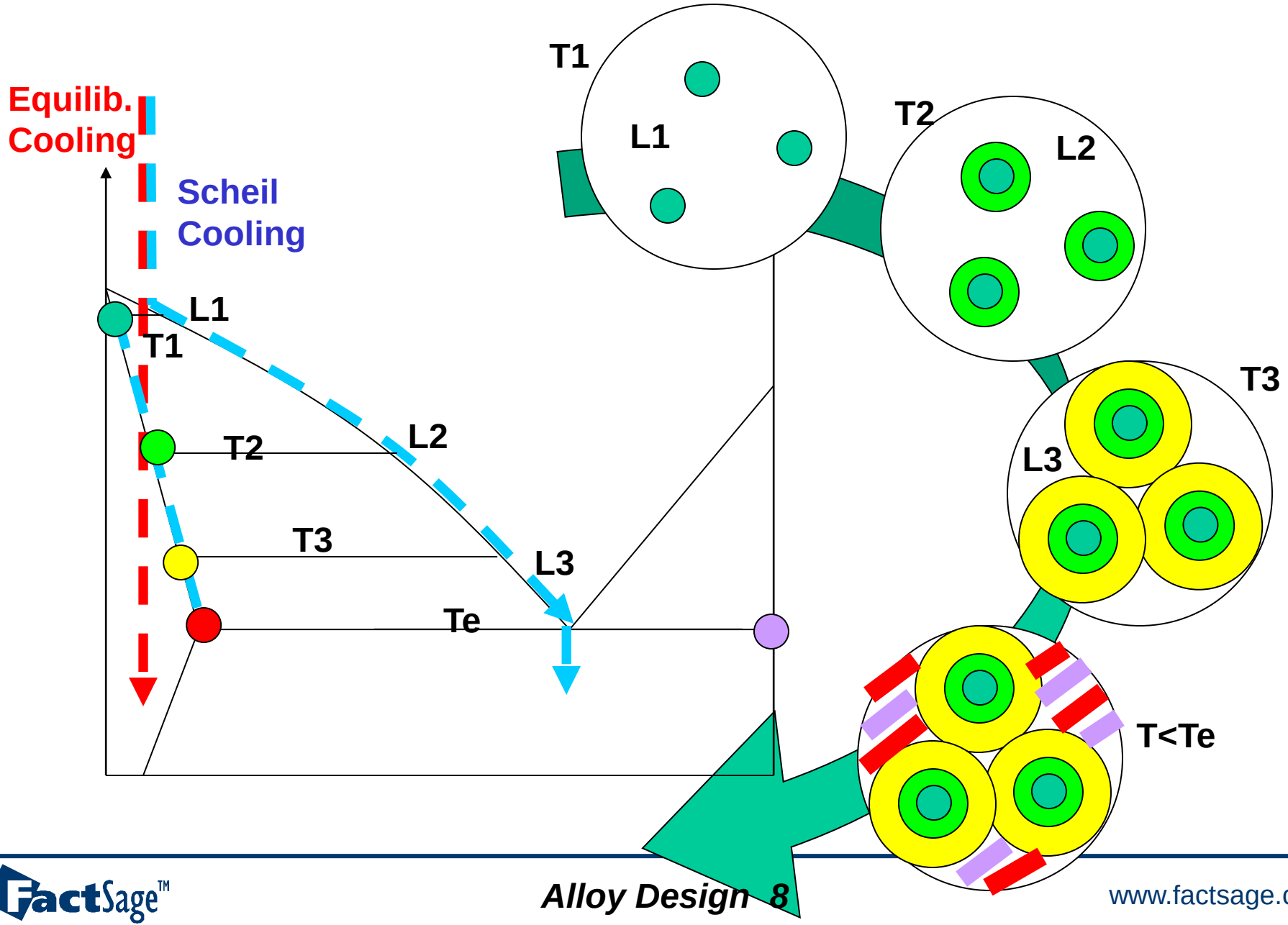
Material Processing and FactSage

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..

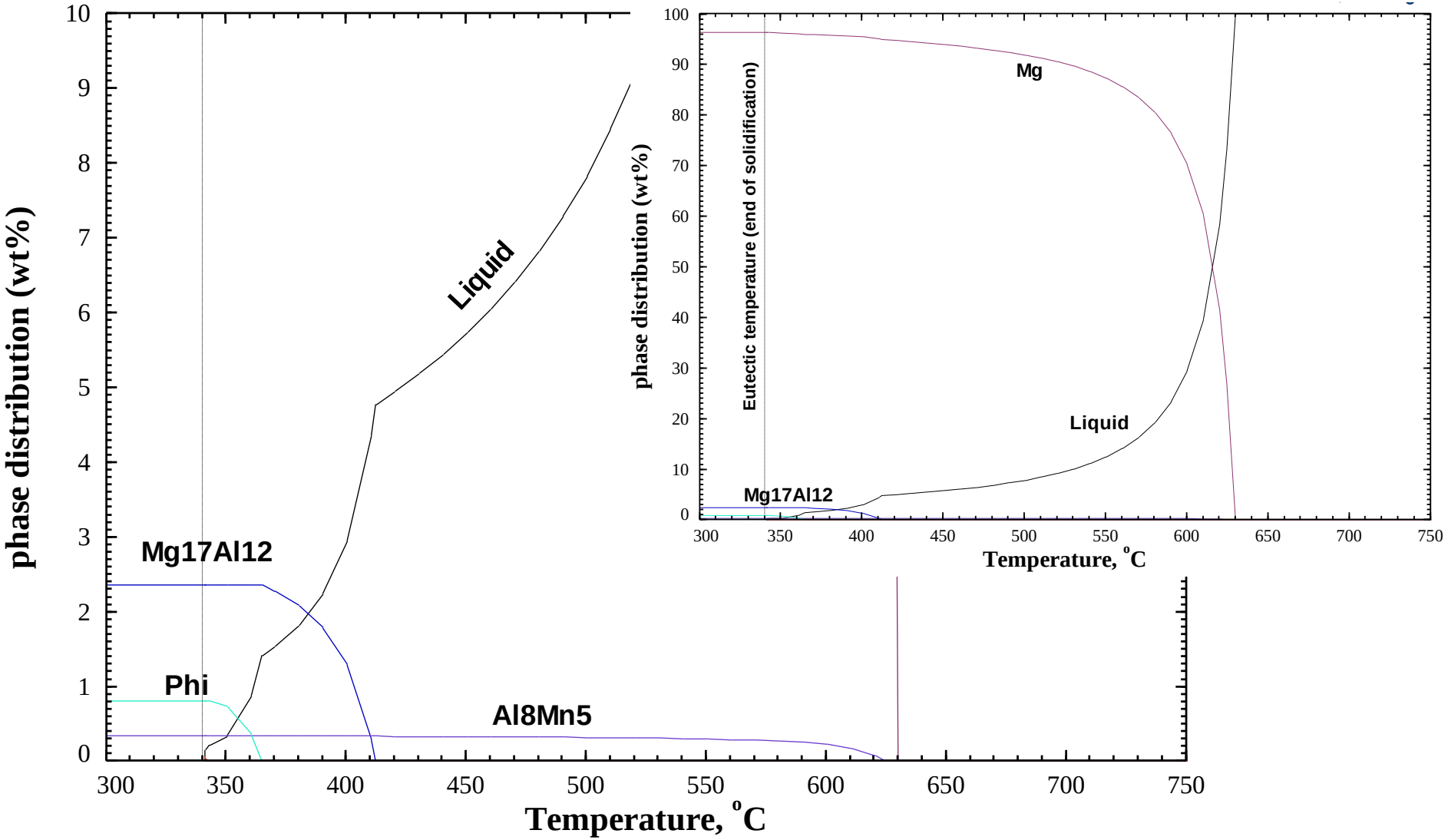
Alloy design (I): Phase diagram calculation to find out final target composition



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

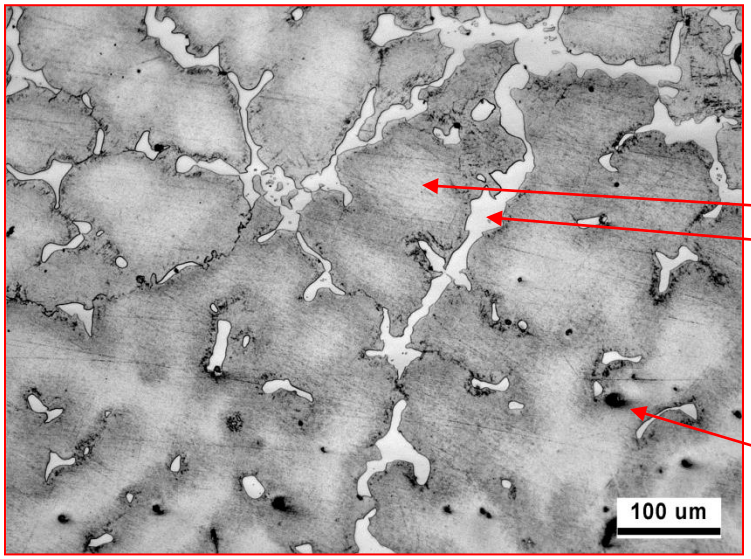


Scheil cooling calculation of AZ31 alloy

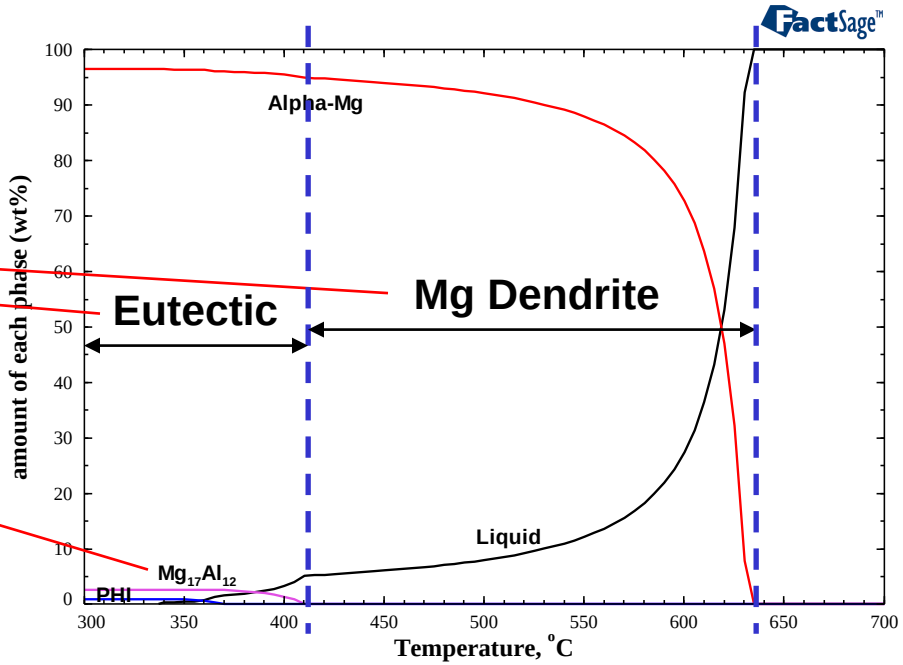


Scheil cooling calculation: as cast microstructure

Solidification path calculation: AZ31



Microstructure of as-cast AZ31



Scheil Cooling calculation

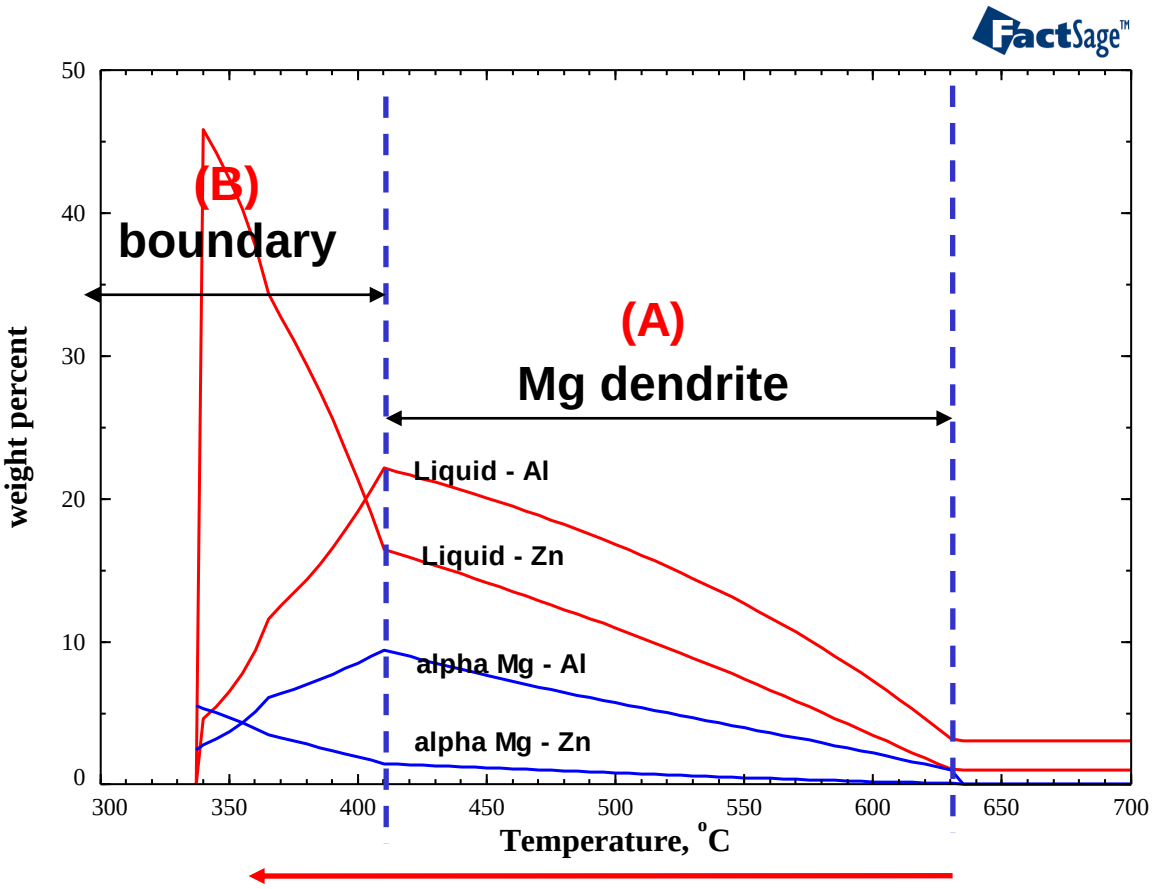
Scheil cooling calculations tell us the solidification path

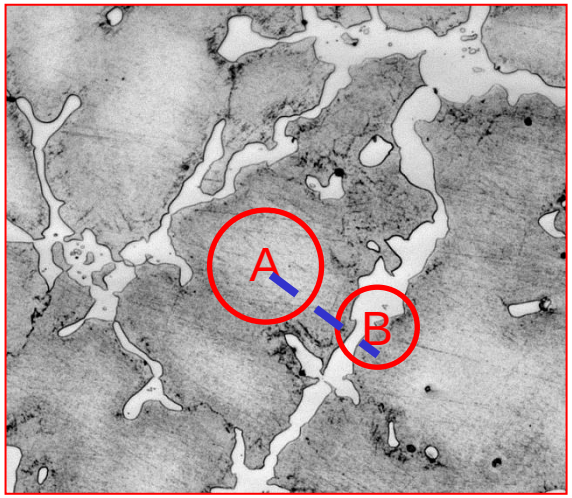
- **Primary phase, precipitation, and eutectic reaction.**
- **Dendrite boundary (eutectics, segregation)**

-> Estimation of as-cast microstructure

Scheil cooling calculation: as cast microstructure

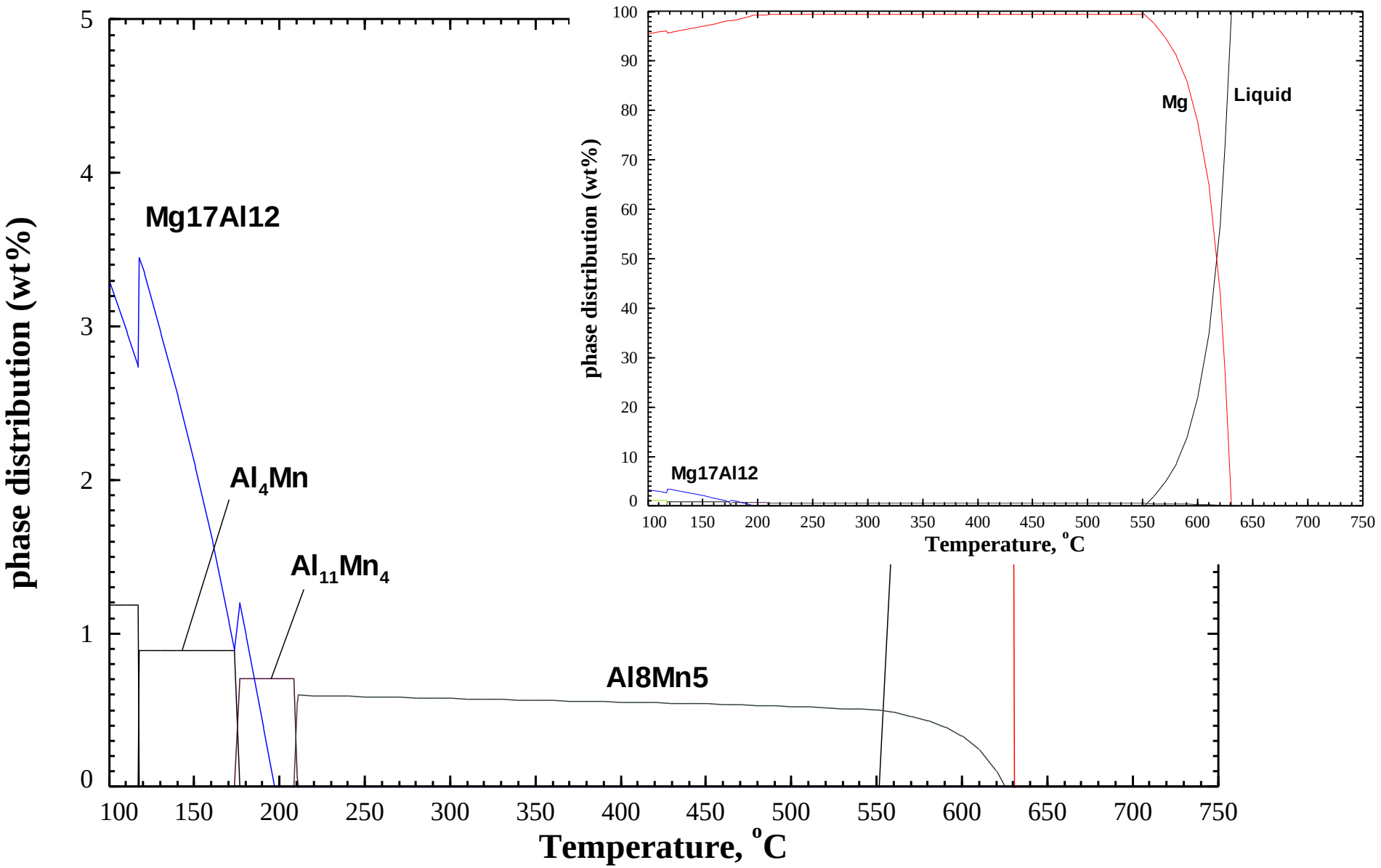
Corning effect of Mg dendrite: AZ31





change of composition
In dendrite & boundary

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, Hf, 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 optim 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.

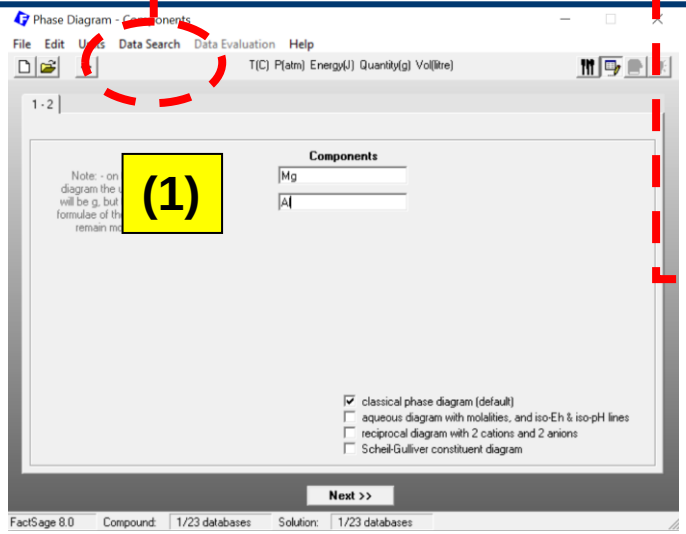
Please look at “Documentation” to check new updates of FSStel database in FactSage 83.

Alloy database: Others

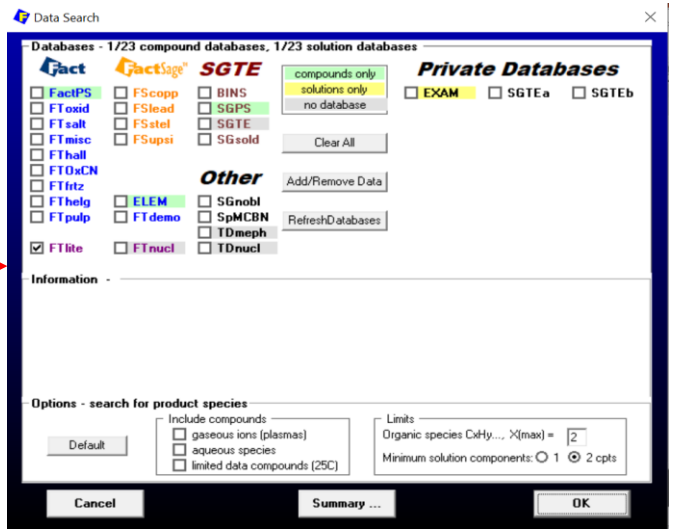
- **FSCopp**: Copper alloy development (all binary Cu-X systems
- **FSupsi**: High purity Si database for solar cell grade Si production
- **FSnobl**: Noble alloy database for Ag, Au, Ir, Os, Pd, Pt, Rh, Ru refining
- **SGnobl**: Similar to FSnobl
- **SGsold**: Solder alloy database
- **SGTE 2014, 2017, 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

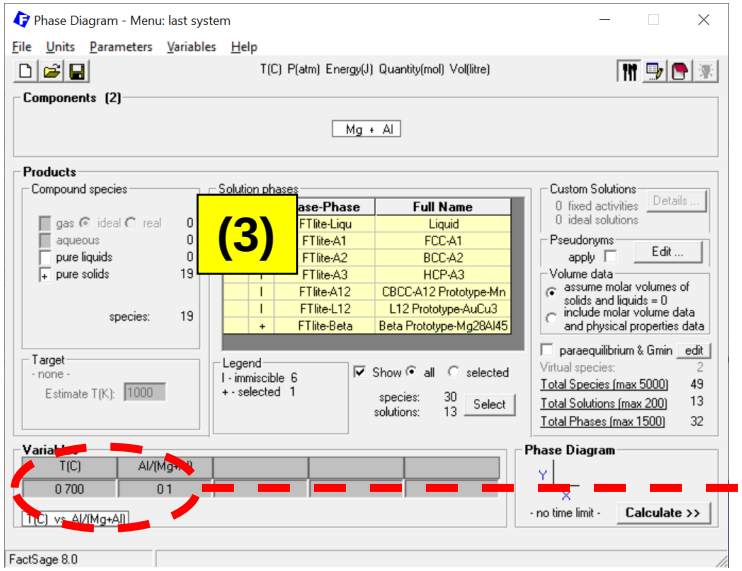
EX1. Binary phase diagram: Mg-Al binary system



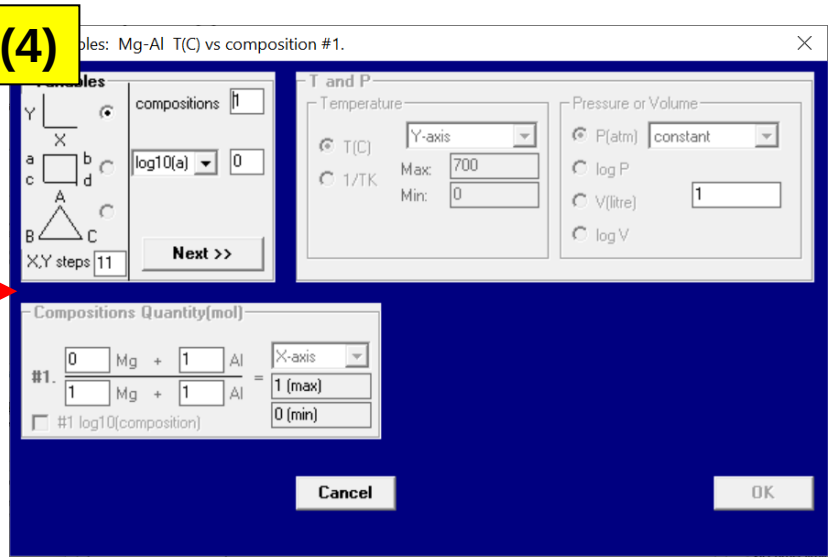
(1) Entering elements/components



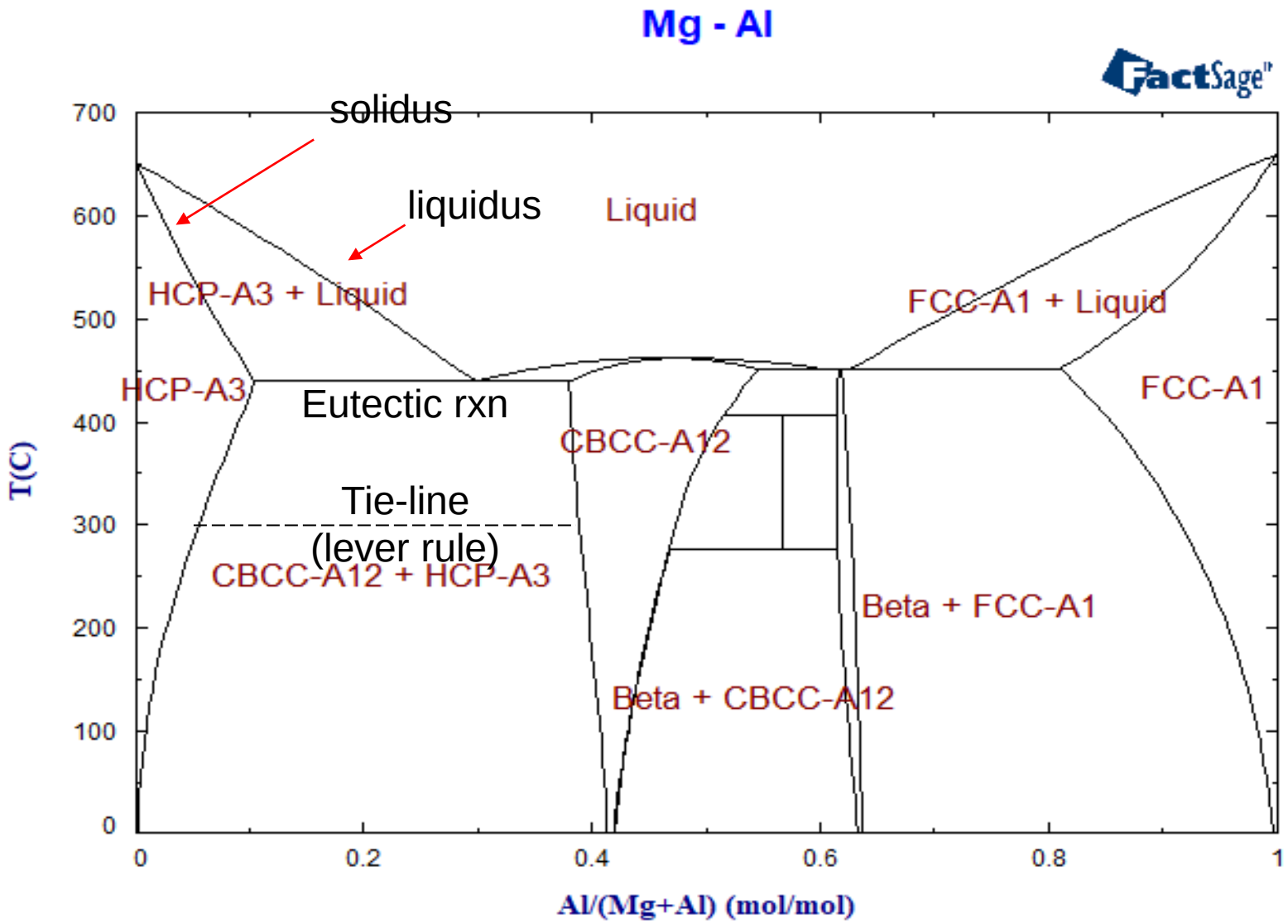
(2) Database selection



(3) Phases (compounds and solutions) selection



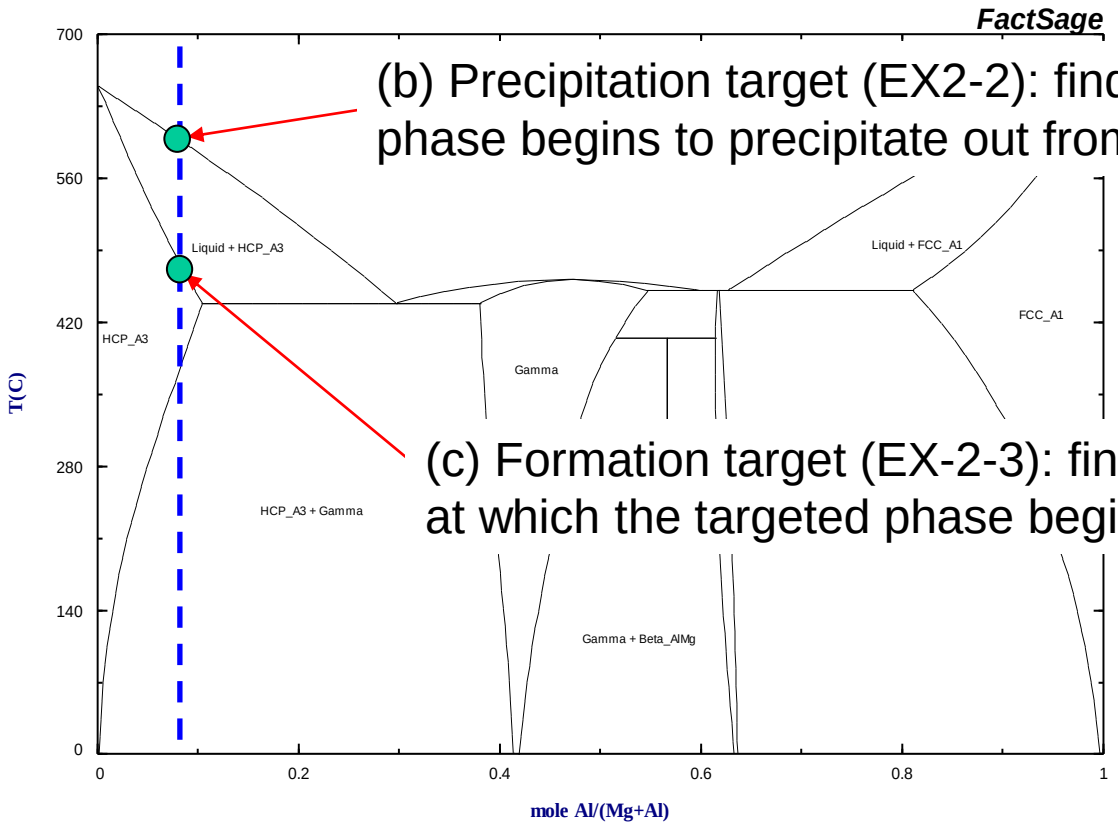
(4) Calculation conditions (T, X, P, etc.)


Mg - Al
FactSage
solidus
liquidus
Liquid
HCP-A3 + Liquid
FCC-A1 + Liquid
HCP-A3
Eutectic rxn
FCC-A1
CBCC-A12
Tie-line
(lever rule)
CBCC-A12 + HCP-A3
Beta + FCC-A1
Beta + CBCC-A12
T(C)
Al/(Mg+Al) (mol/mol)
700
600
500
400
300
200
100
0
0
0.2
0.4
0.6
0.8
1

EX2. Target calculations

(a)Transitions (EX2-1):

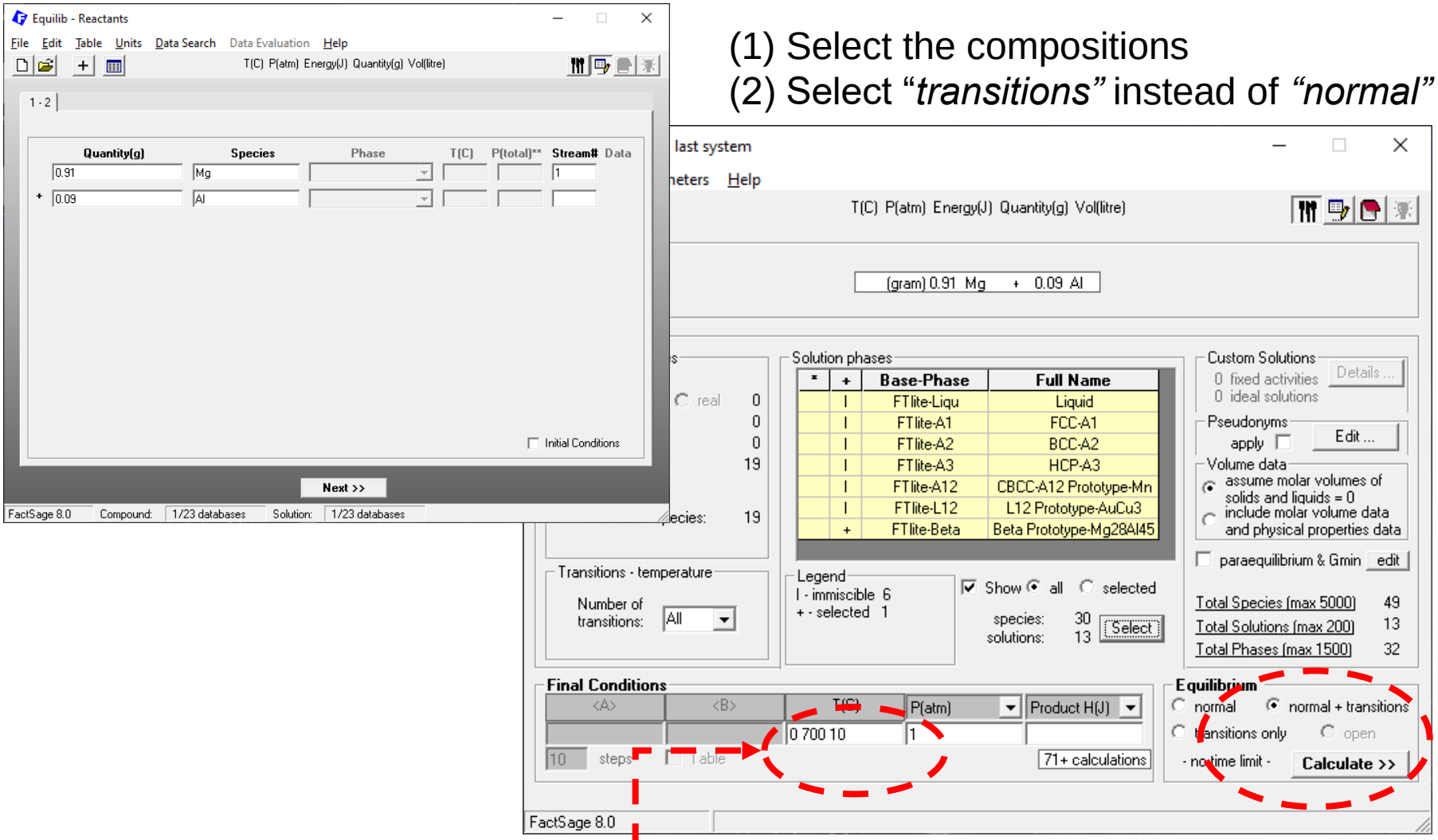
do calculation between initial and final temperature and find all phase transition between them



(b) Precipitation target (EX2-2): find temperature at which any other phase begins to precipitate out from the targeted phase

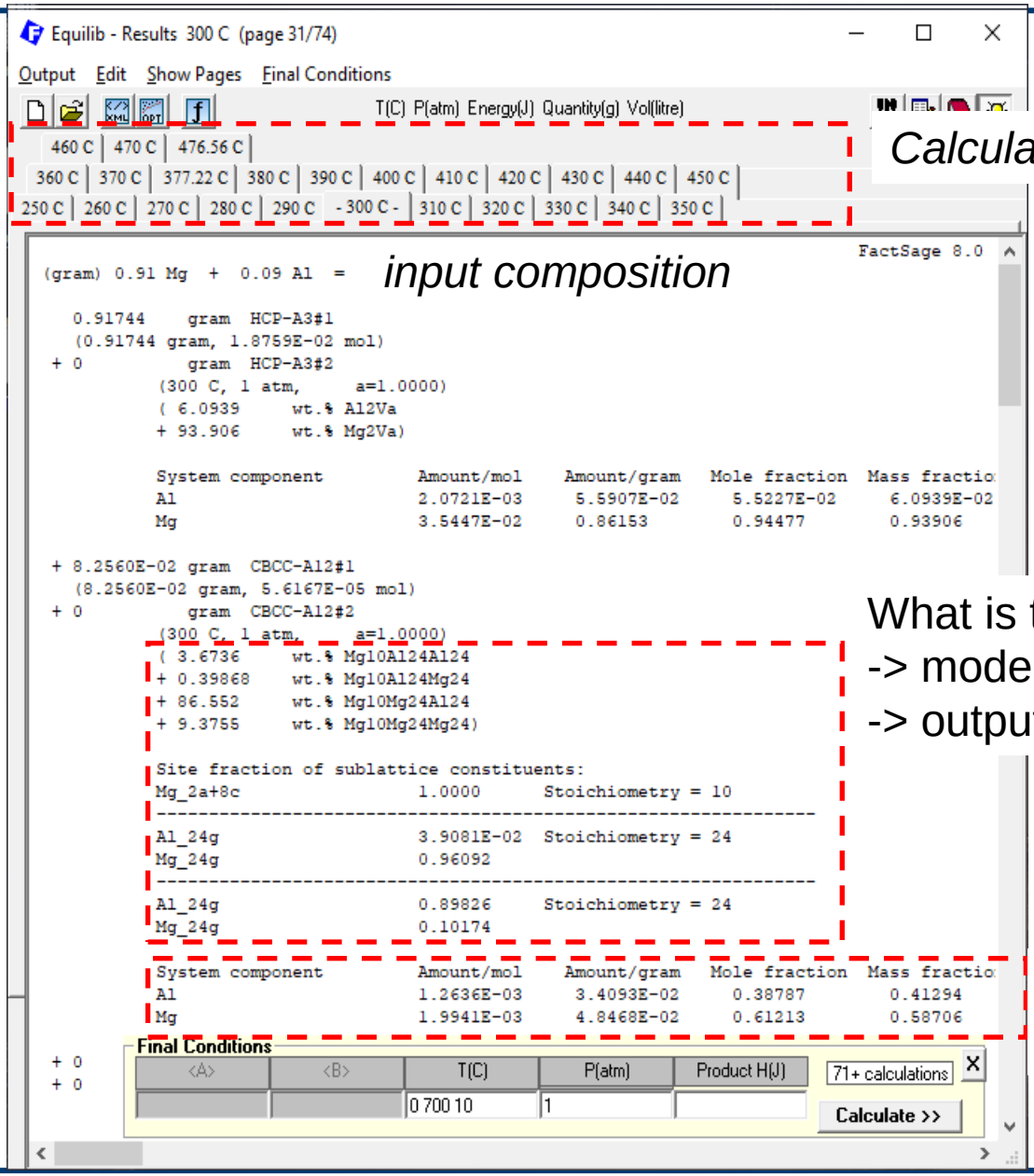
(c) Formation target (EX-2-3): find the temperature at which the targeted phase begin to form

EX2-1. Transition calculation



(1) Select the compositions
(2) Select "*transitions*" instead of *"normal"*

Range of temperature: "*initial final interval*"
Calculate Initial (0 ºC) to final (700ºC) temperature with interval of 10 ºC

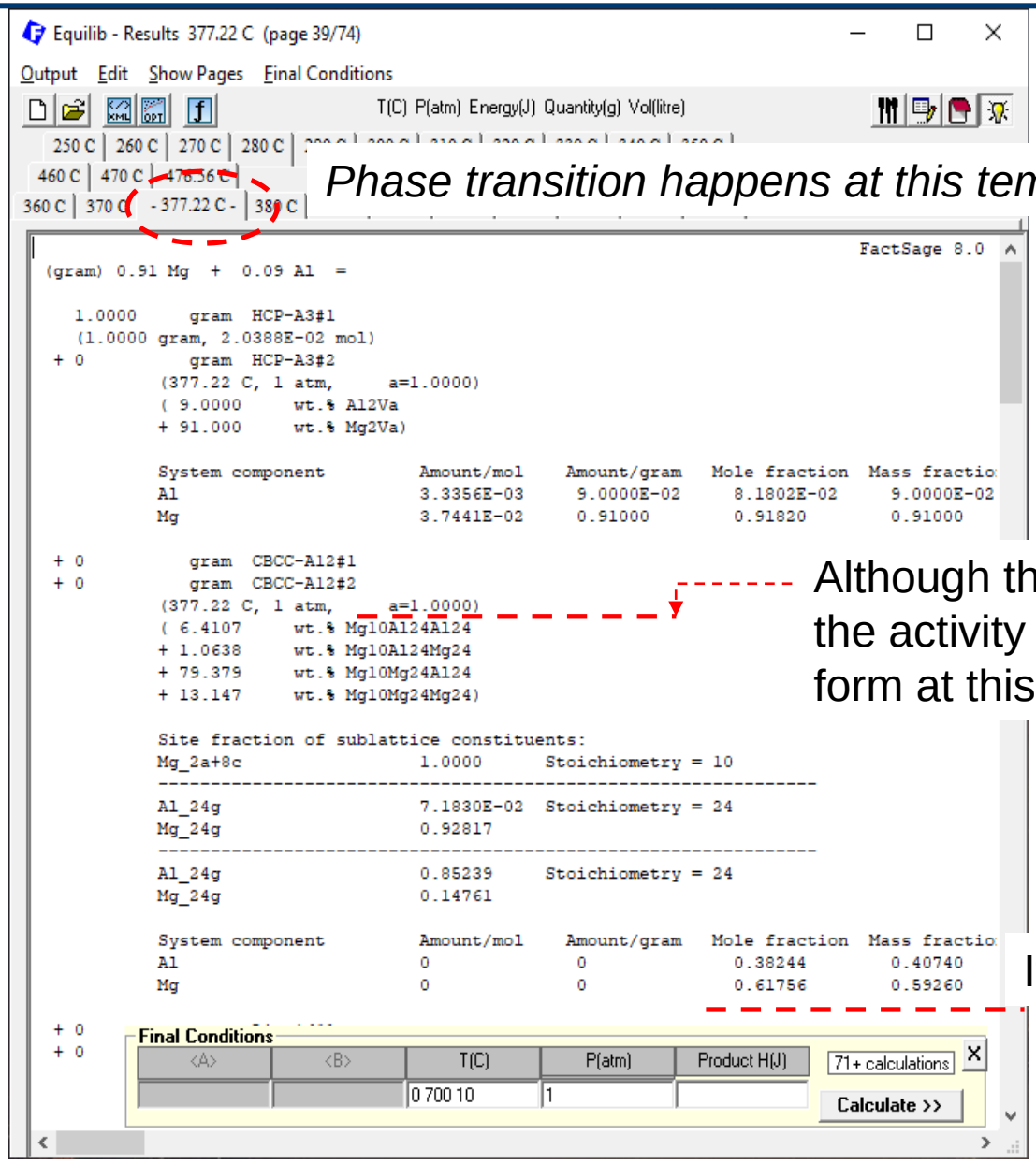


input composition

Calculation results at every 10 ^{o}C intervals

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

elemental composition of CBCC-A12 (gamma Mg17Al12) phase

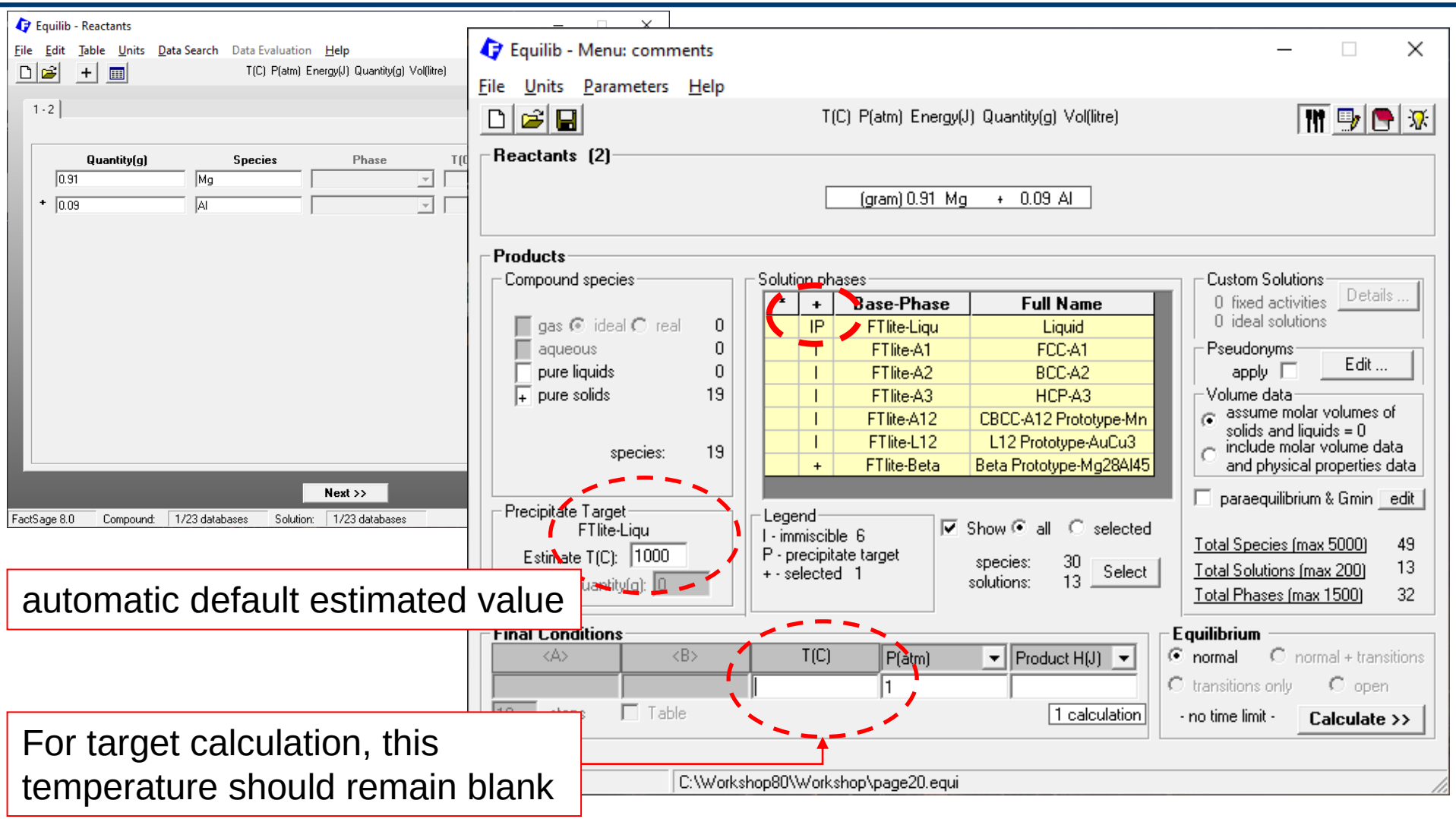


Phase transition happens at this temperature

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

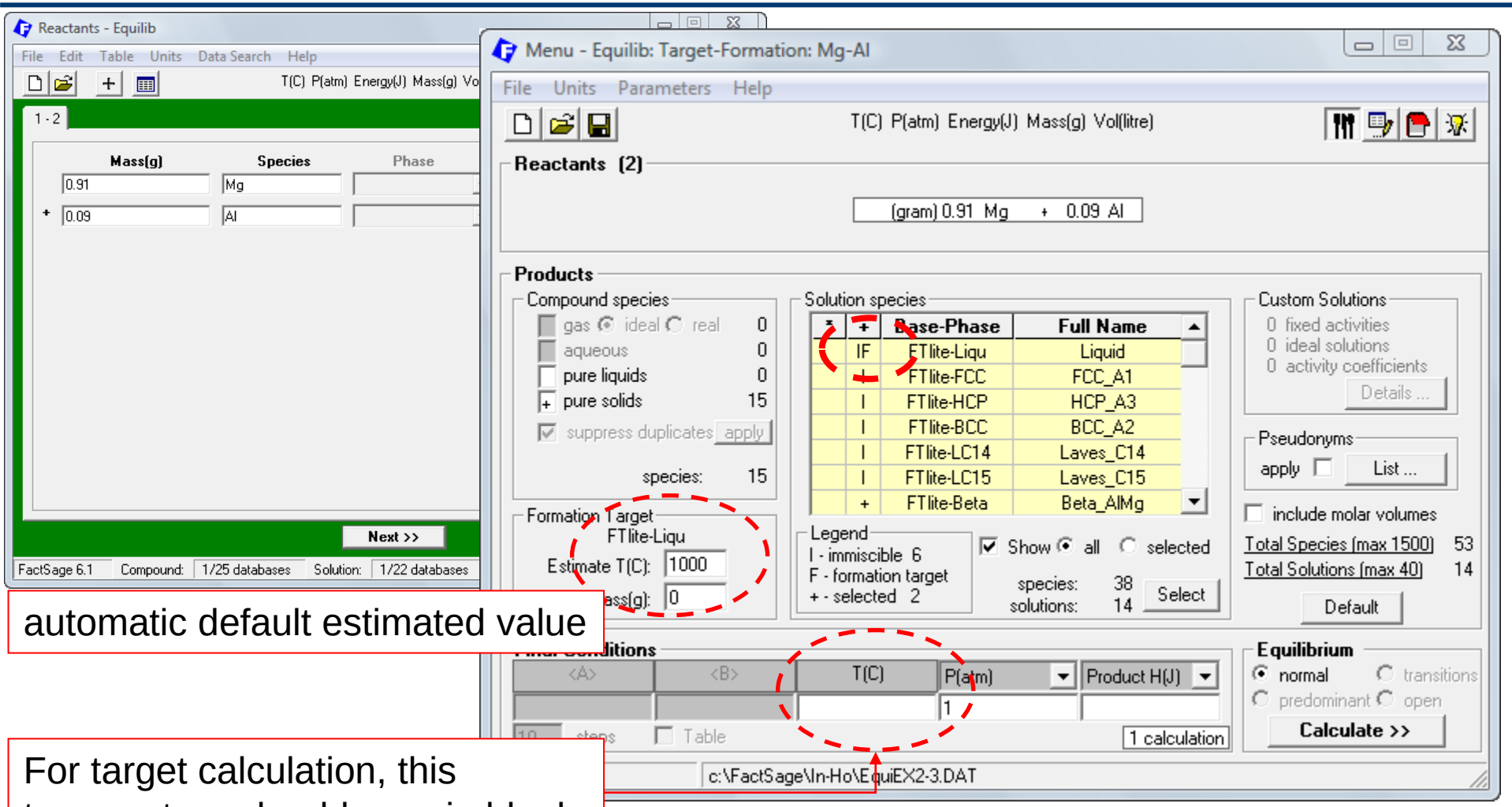


automatic default estimated value

For target calculation, this temperature should remain blank

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

EX2-3. Formation target calculation

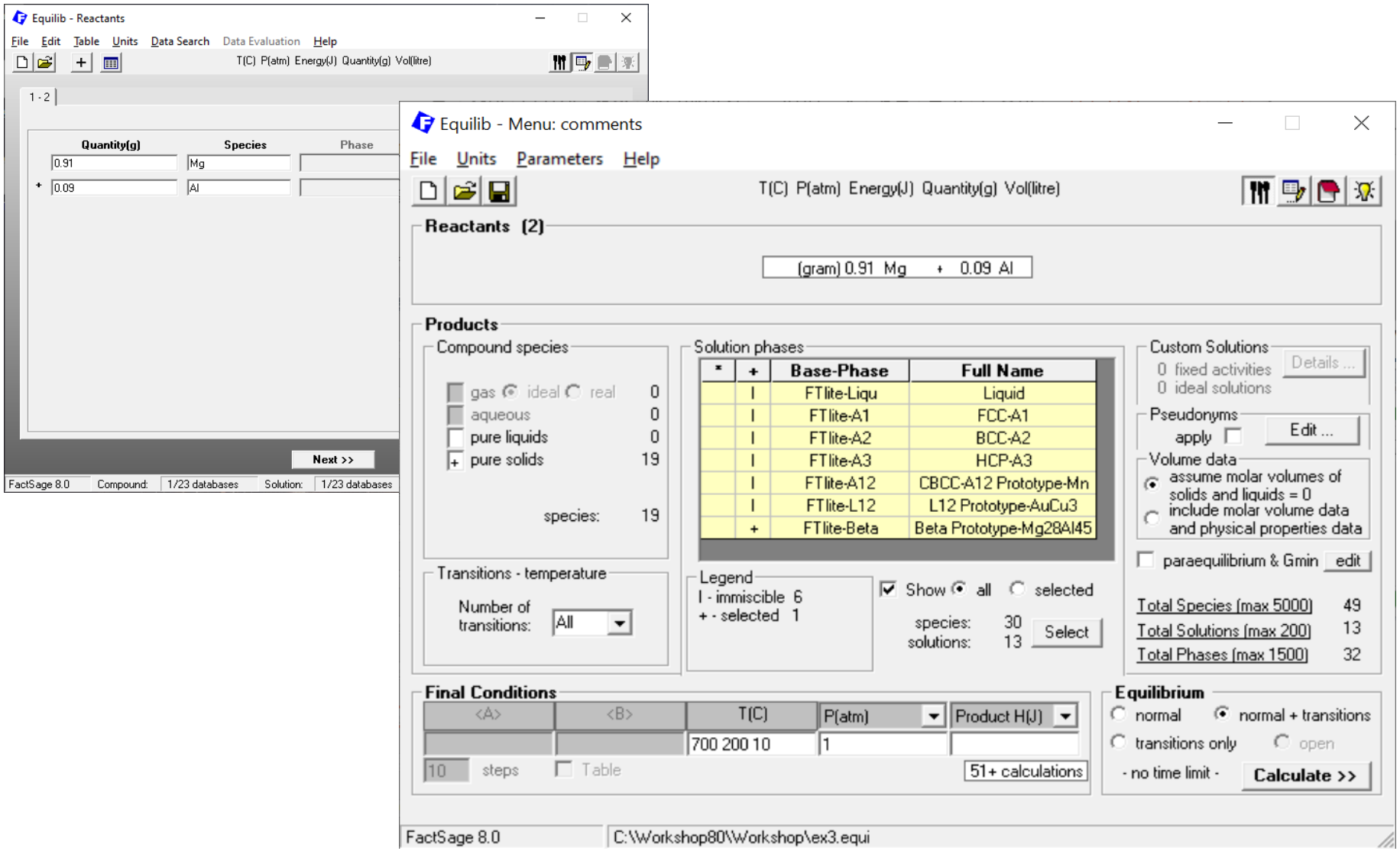


automatic default estimated value

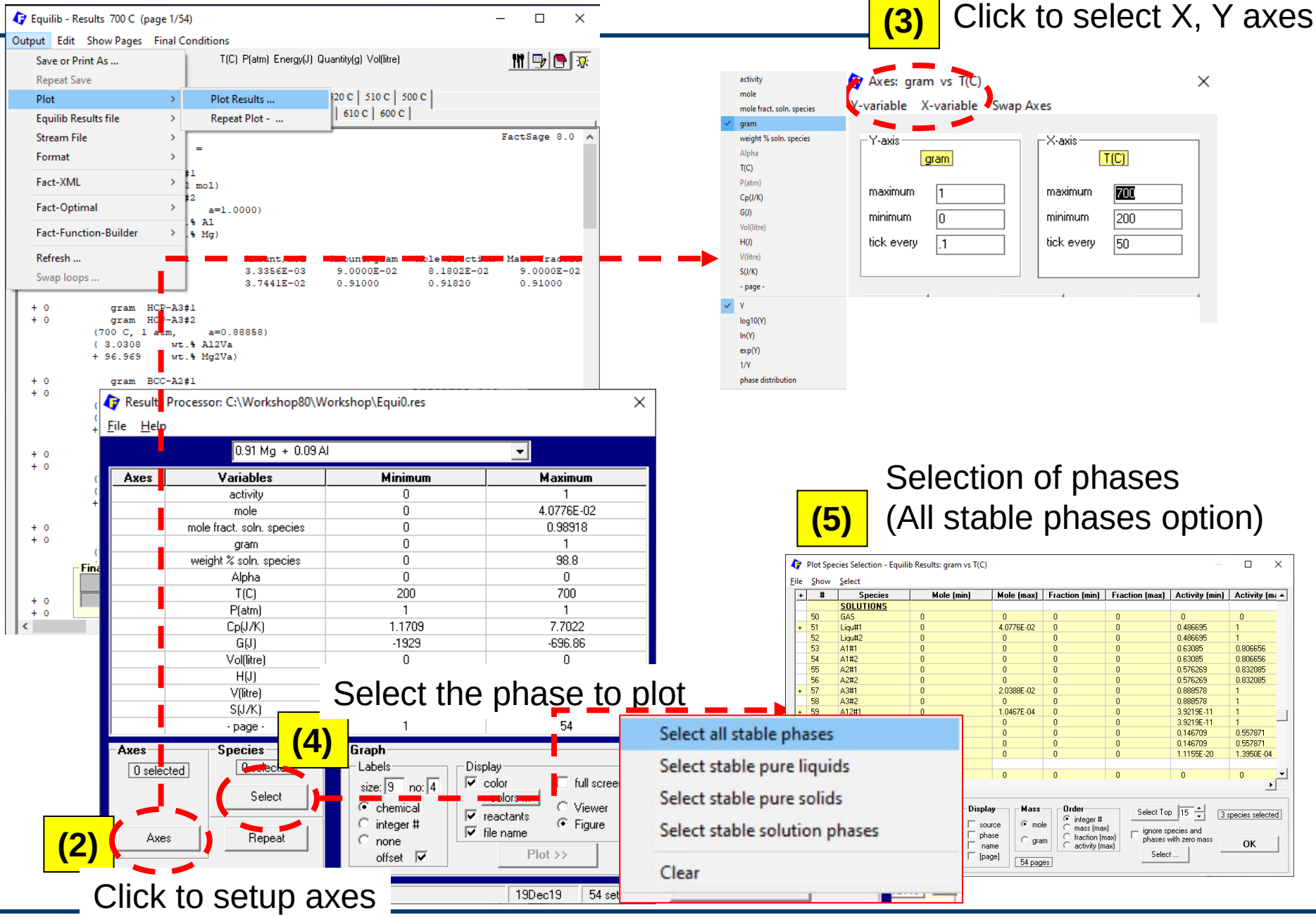
For target calculation, this temperature should remain blank

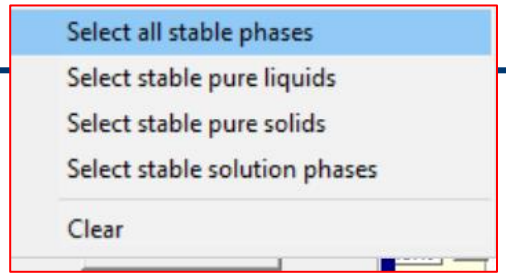
Liquid is selected as formation target phase (F). Then, FactSage will calculate solidus temperature of a given composition

EX3. Variation of phase fraction with temperature (equilibrium)



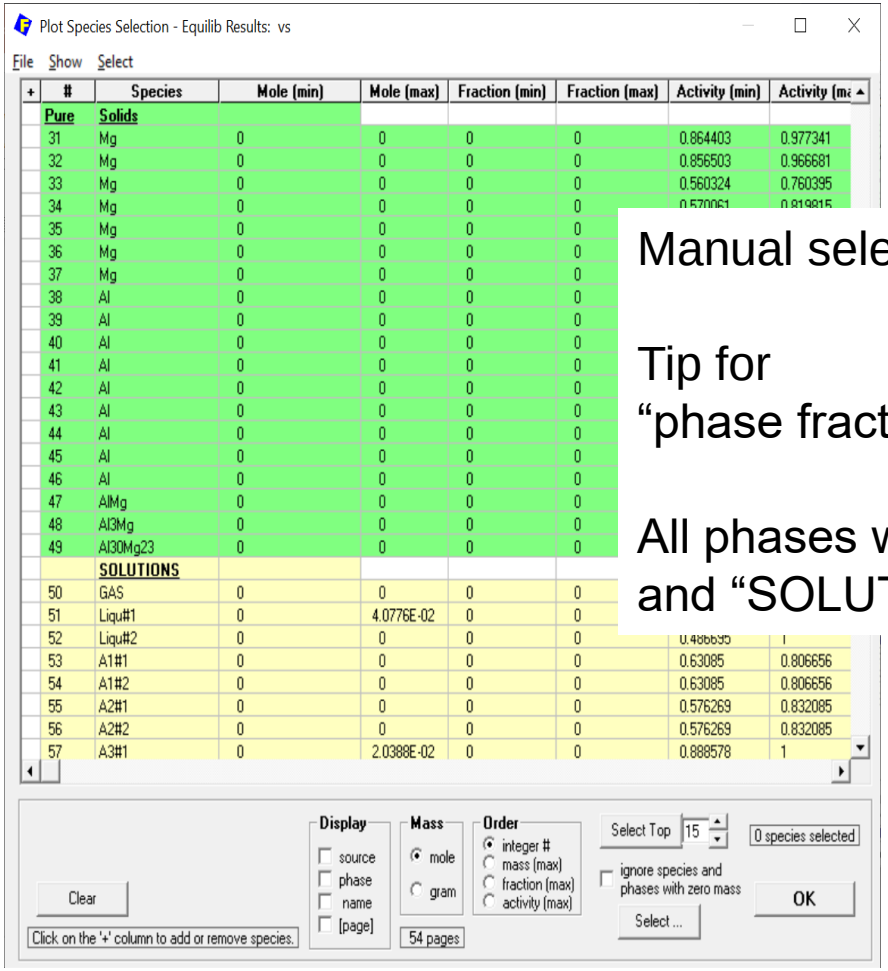
Transition calculation from 700°C to 200°C with 10°C interval


(3)
Click to select X, Y axes
Equilib - Results 700 C (page 1/54)
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 ...
Plot Results ...
Repeat Plot - ...
T(C) P(atm) Energy(J) Quantity(g) Vol(litre)
FactSage 8.0
Axes: gram vs T(C)
Y-variable X-variable Swap Axes
Y-axis
gram
maximum 1
minimum 0
tick every .1
X-axis
T(C)
maximum 700
minimum 200
tick every 50
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
(5)
Selection of phases
(All stable phases option)
Plot Species Selection - Equilib Results: gram vs T(C)
Select all stable phases
Select stable pure liquids
Select stable pure solids
Select stable solution phases
Clear
Select the phase to plot
(4)
Axes
0 selected
Species
Select
Repeat
Graph
Labels
Display
Plot >>
(2)
Axes
Click to setup axes



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

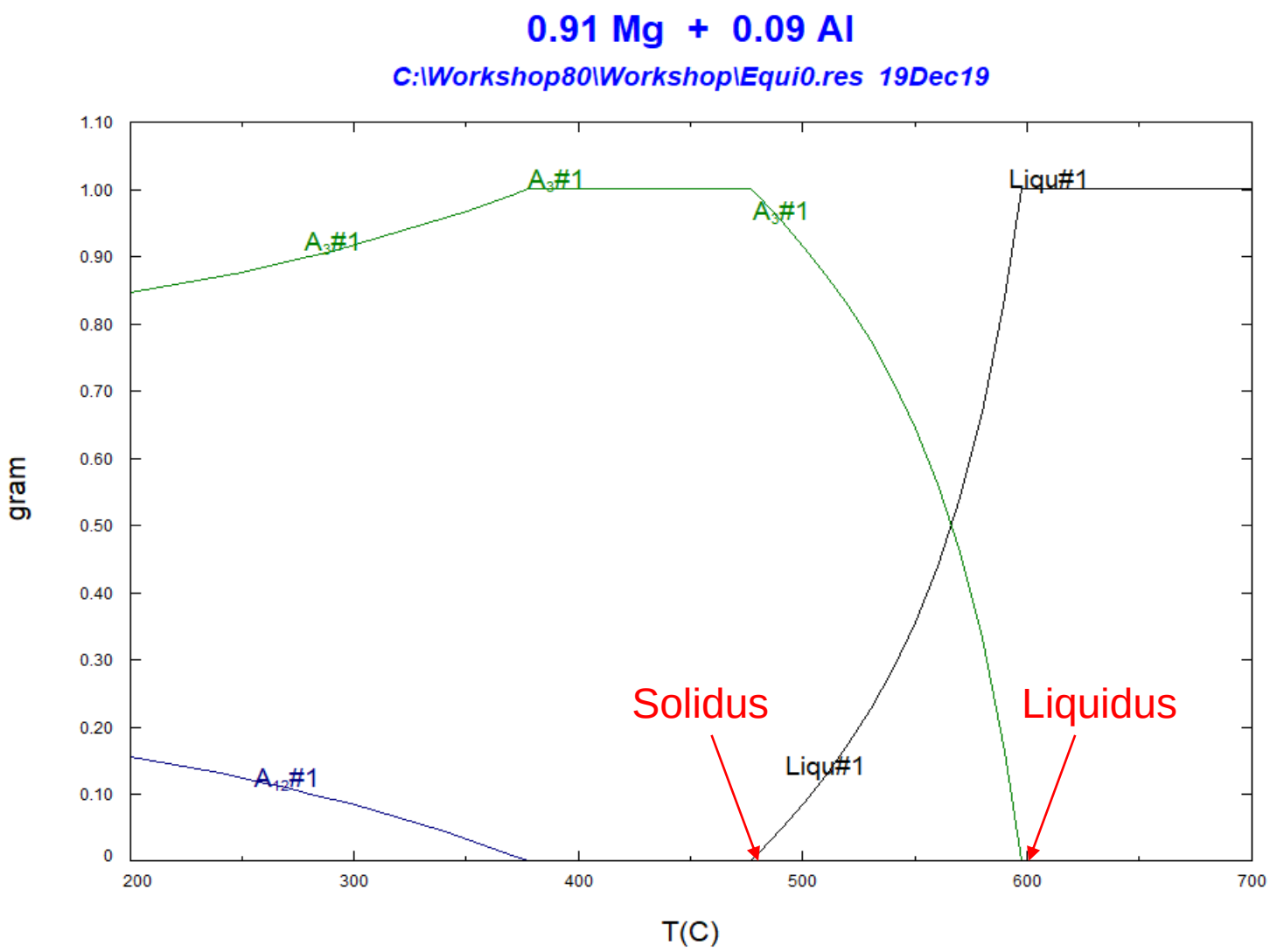


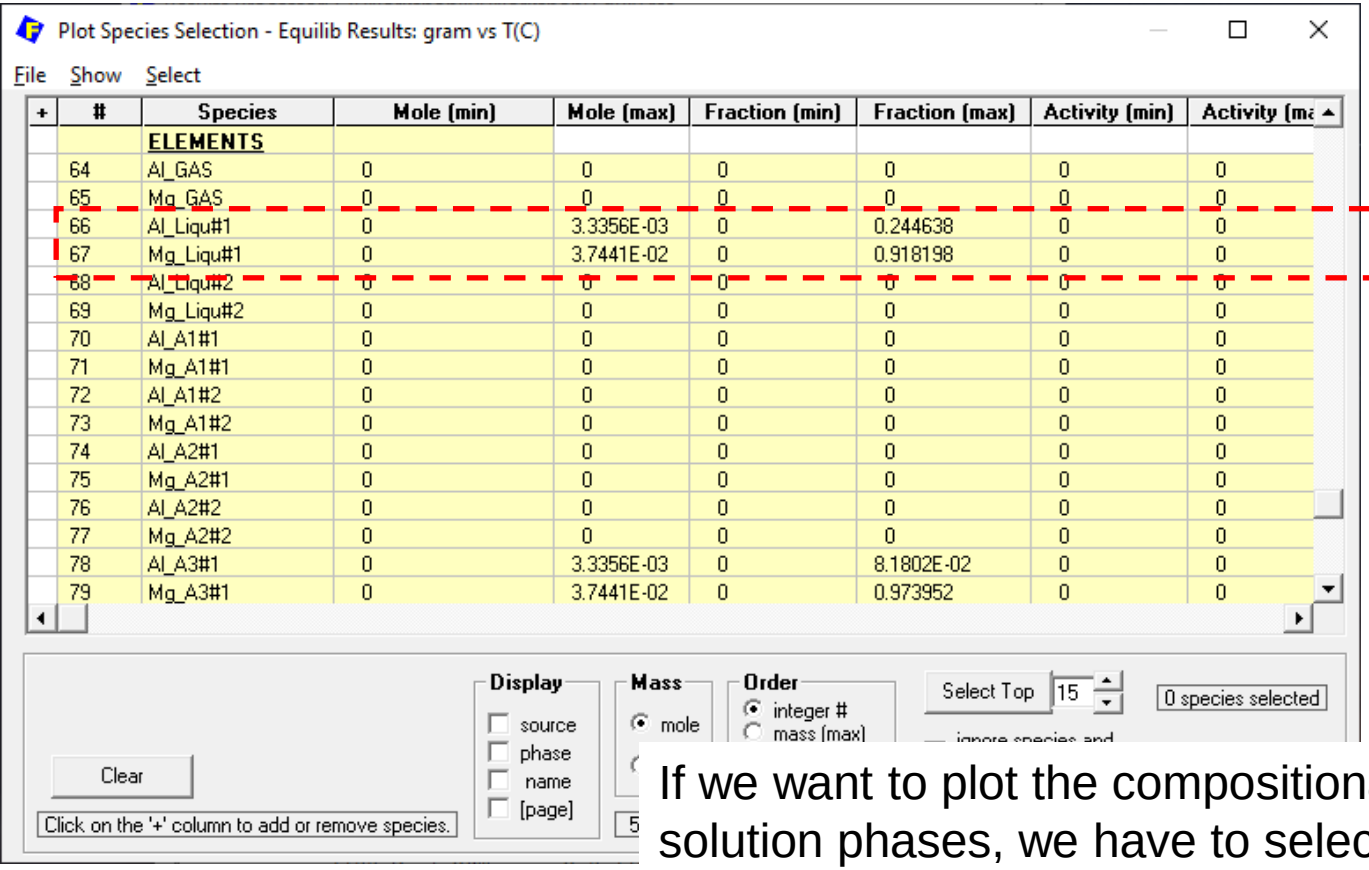
+	#	Species	Mole (min)	Mole (max)	Fraction (min)	Fraction (max)	Activity (min)	Activity (ma
	Pure	Solids						
	31	Mg	0	0	0	0	0.864403	0.977341
	32	Mg	0	0	0	0	0.856503	0.966681
	33	Mg	0	0	0	0	0.560324	0.760395
	34	Mg	0	0	0	0	0.570061	0.819815
	35	Mg	0	0	0	0		
	36	Mg	0	0	0	0		
	37	Mg	0	0	0	0		
	38	Al	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

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
gram
T(C)
A3#1
A3#1
A3#1
Liqu#1
A12#1
Liqu#1
Solidus
Liquidus
1.10
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0
200
300
400
500
600
700



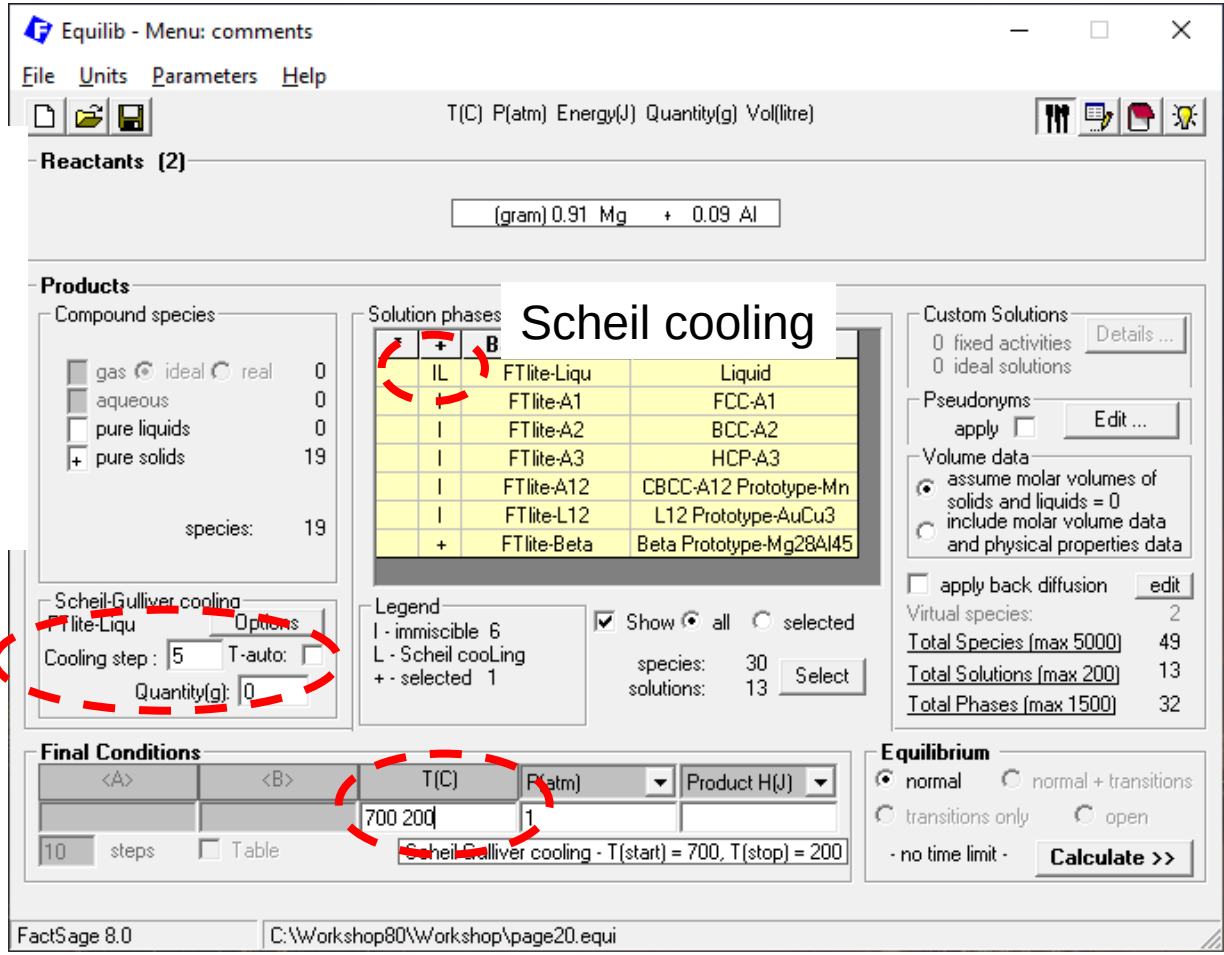
If we want to plot the compositional variation inside of solution phases, we have to select the elements in this "ELEMENTS" section.

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

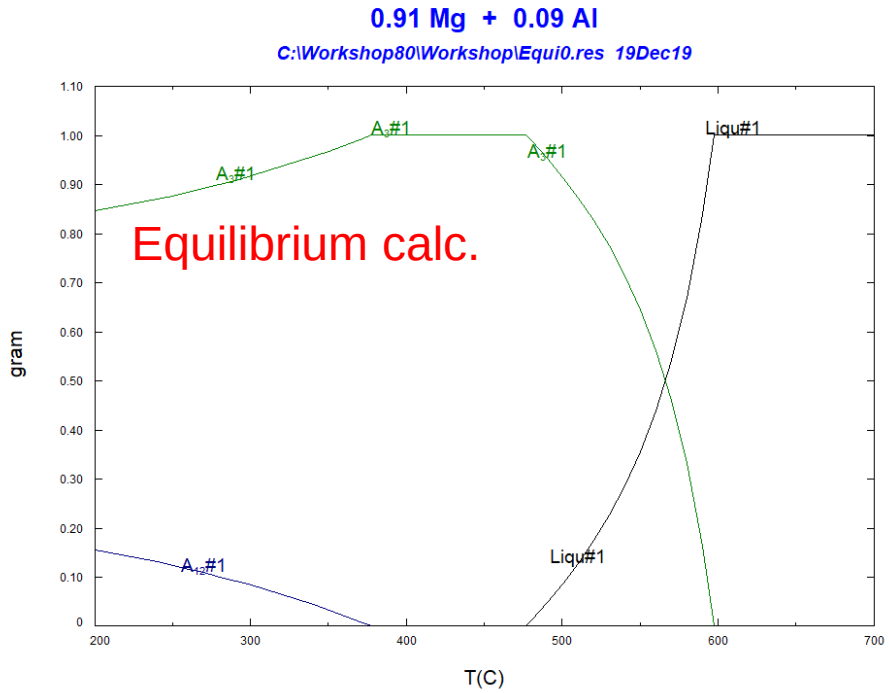
This cooling step is not directly related to solidification rate (cooling speed)



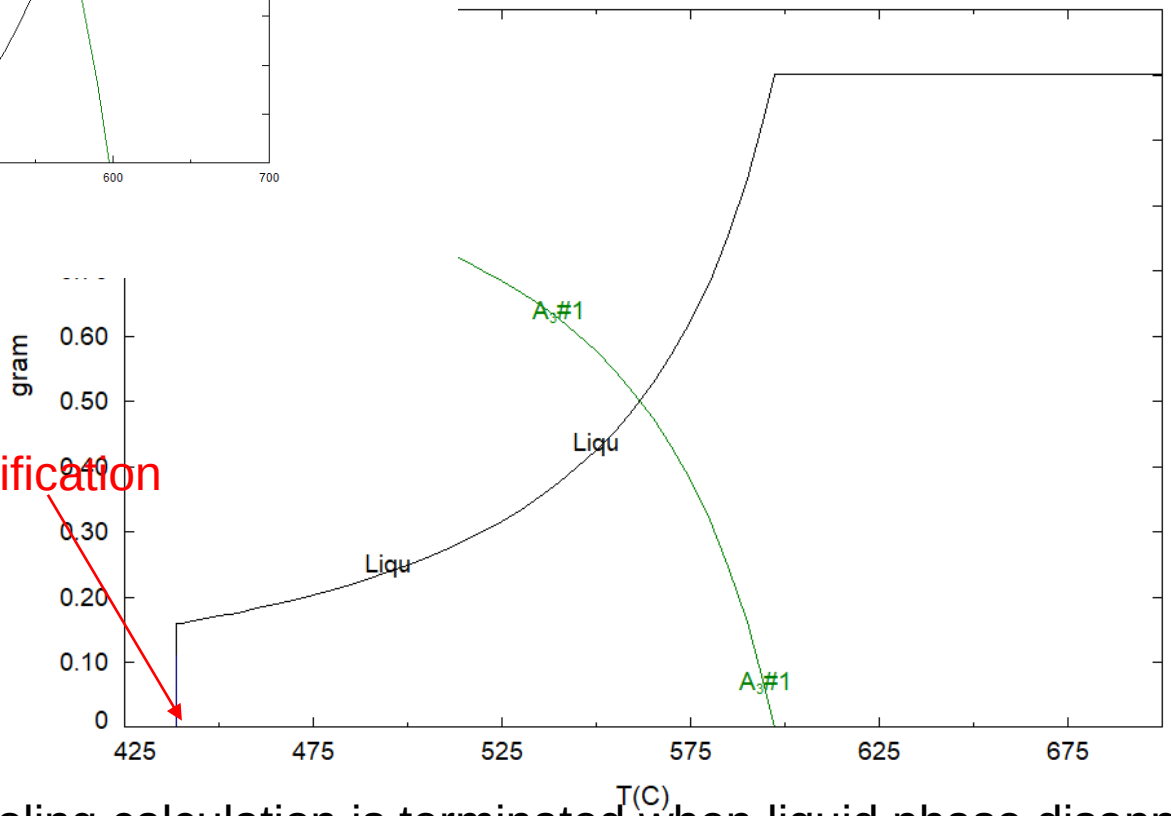
Temperature:

(i) starting temperature and final temperature

(ii) starting temperature: program will automatically calculate the final solidification temperature



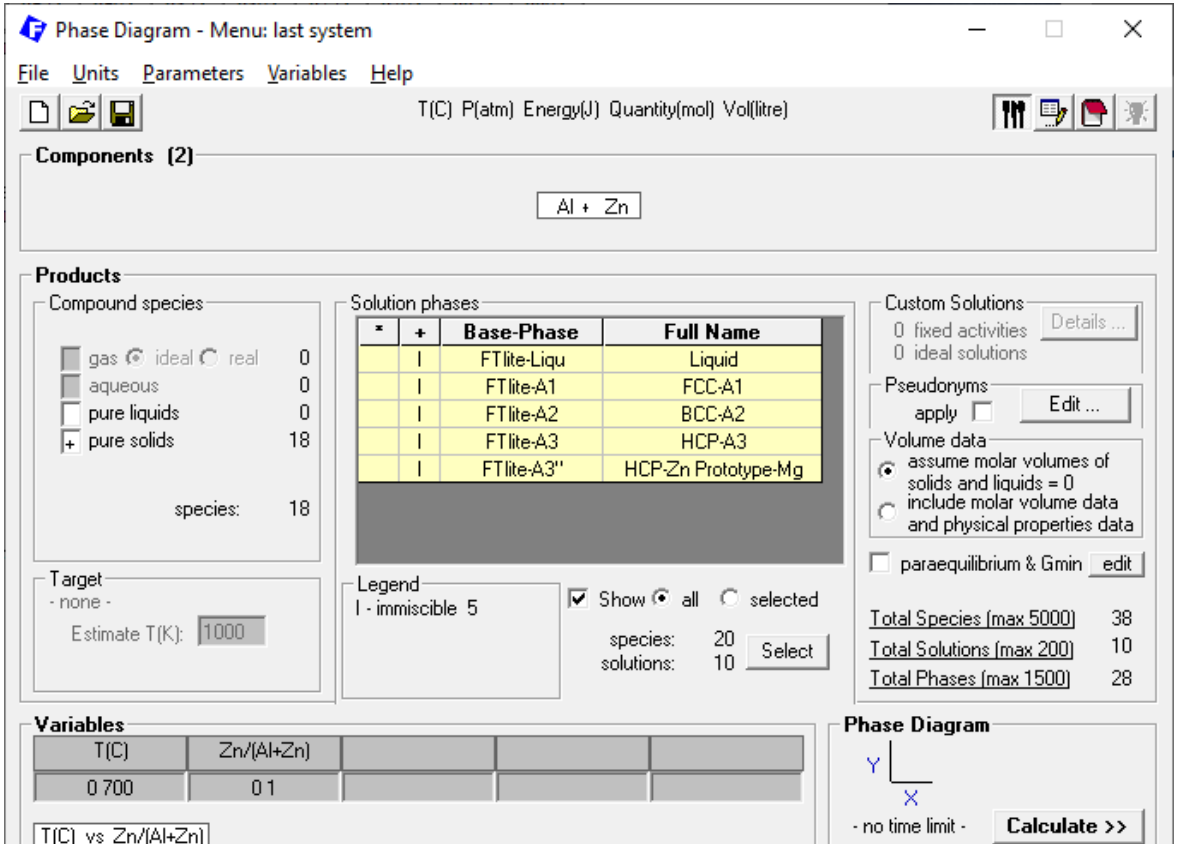
Scheil cooling calc.



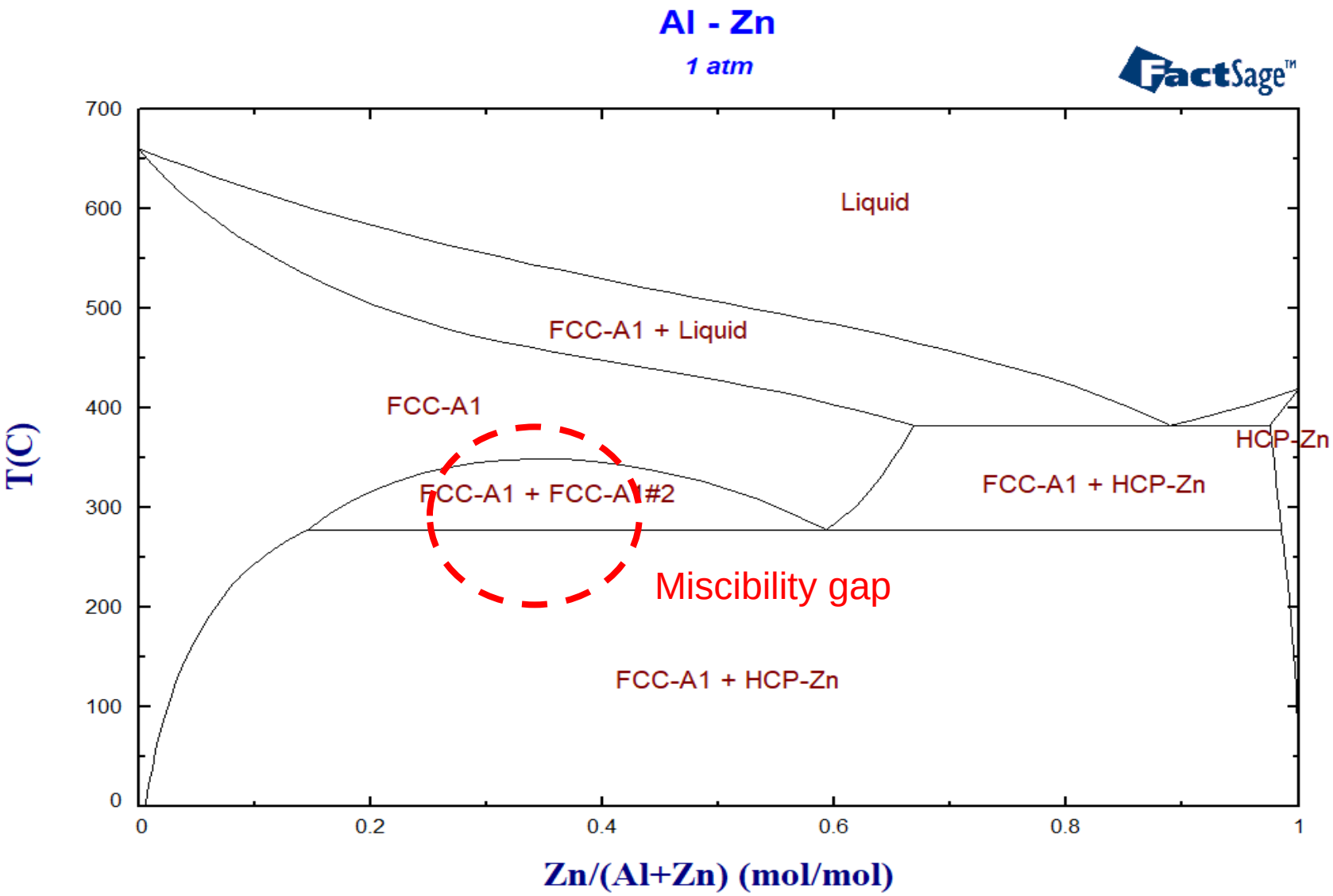
End of solidification

Scheil cooling calculation is terminated when liquid phase disappears

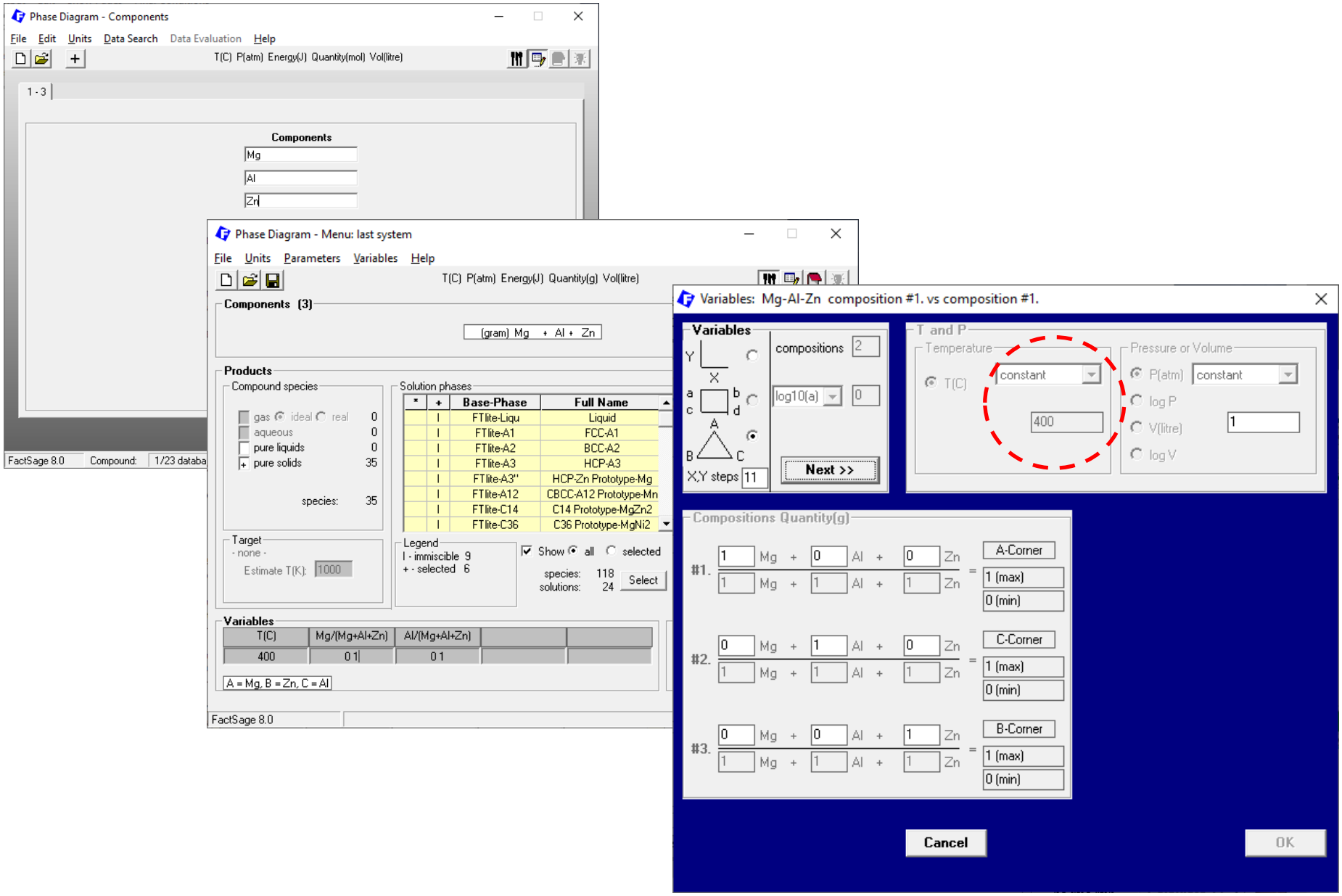
EX5. I option (miscibility gap)



"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.

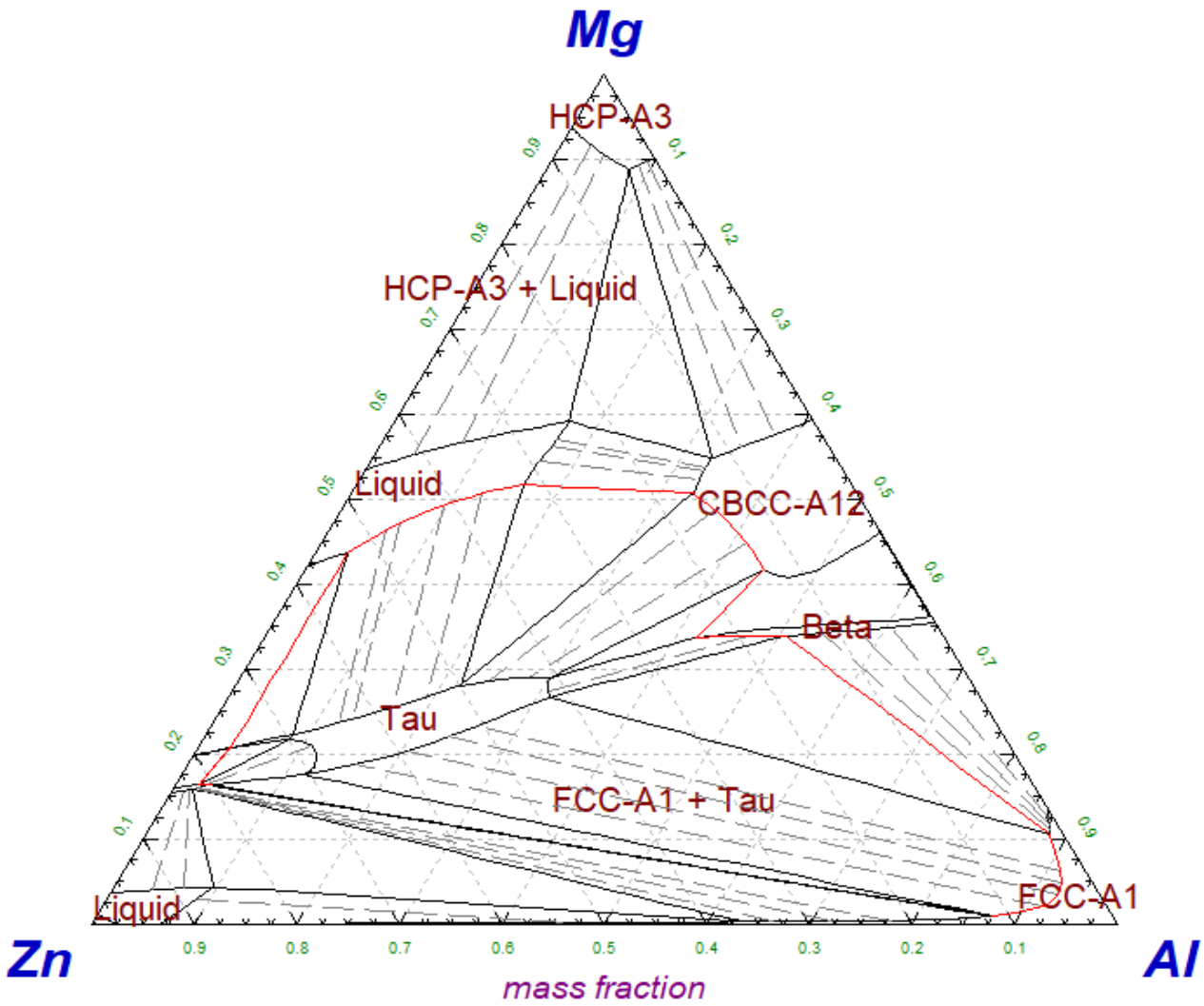

Al - Zn
1 atm
FactSage™
Liquid
FCC-A1 + Liquid
FCC-A1
FCC-A1 + FCC-A1#2
FCC-A1 + HCP-Zn
HCP-Zn
Miscibility gap
FCC-A1 + HCP-Zn
T(C)
Zn/(Al+Zn) (mol/mol)
0
100
200
300
400
500
600
700
0
0.2
0.4
0.6
0.8
1

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

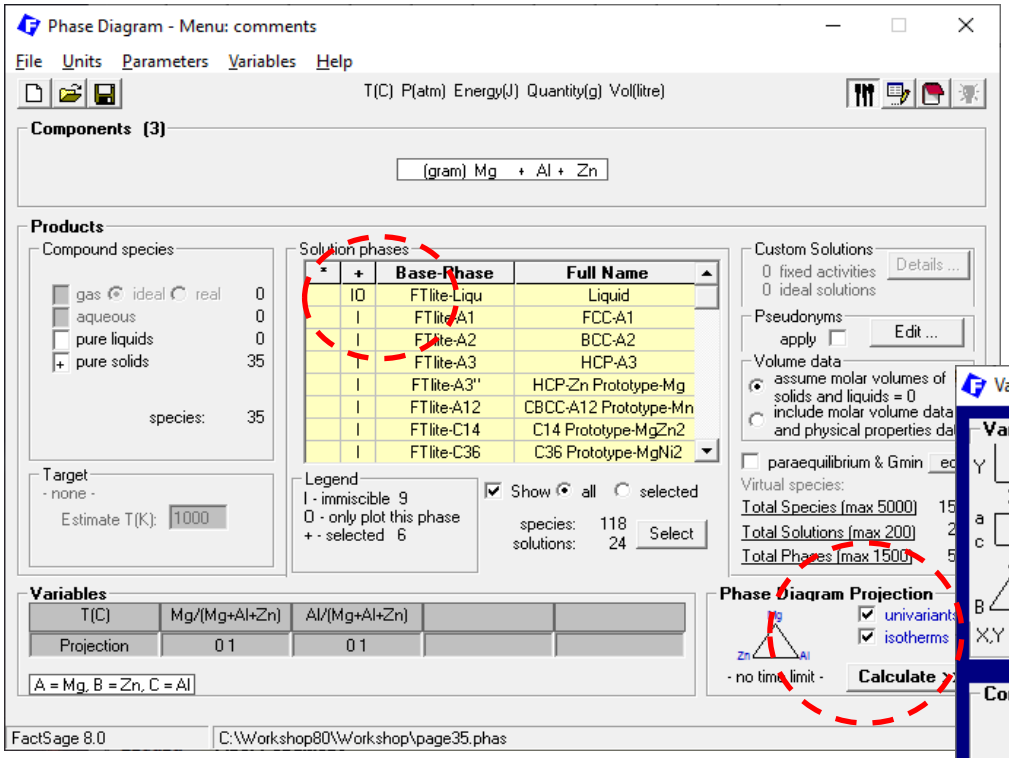


Mg - Al - Zn

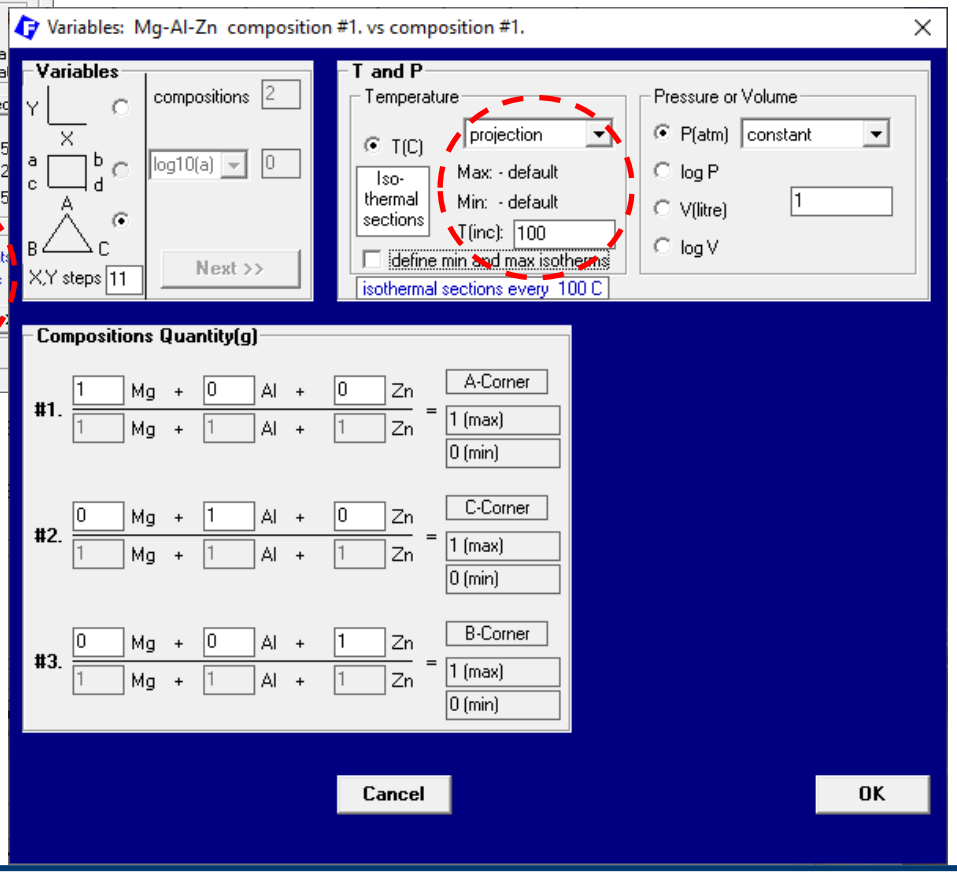
400°C, 1 atm



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)

Mg - Al - Zn

Projection (Liquid), 1 atm

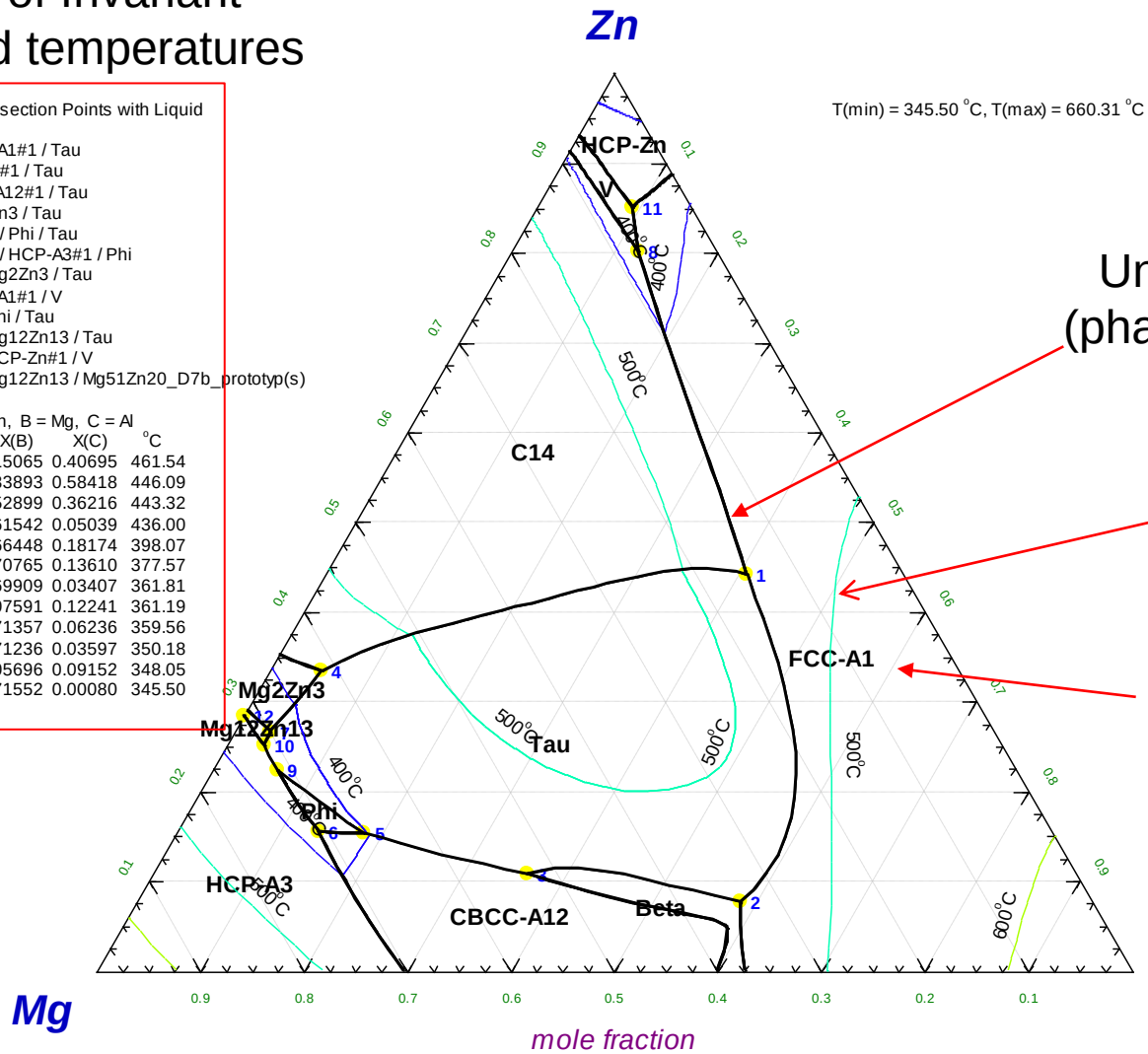
Summary of Invariant reactions and temperatures

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

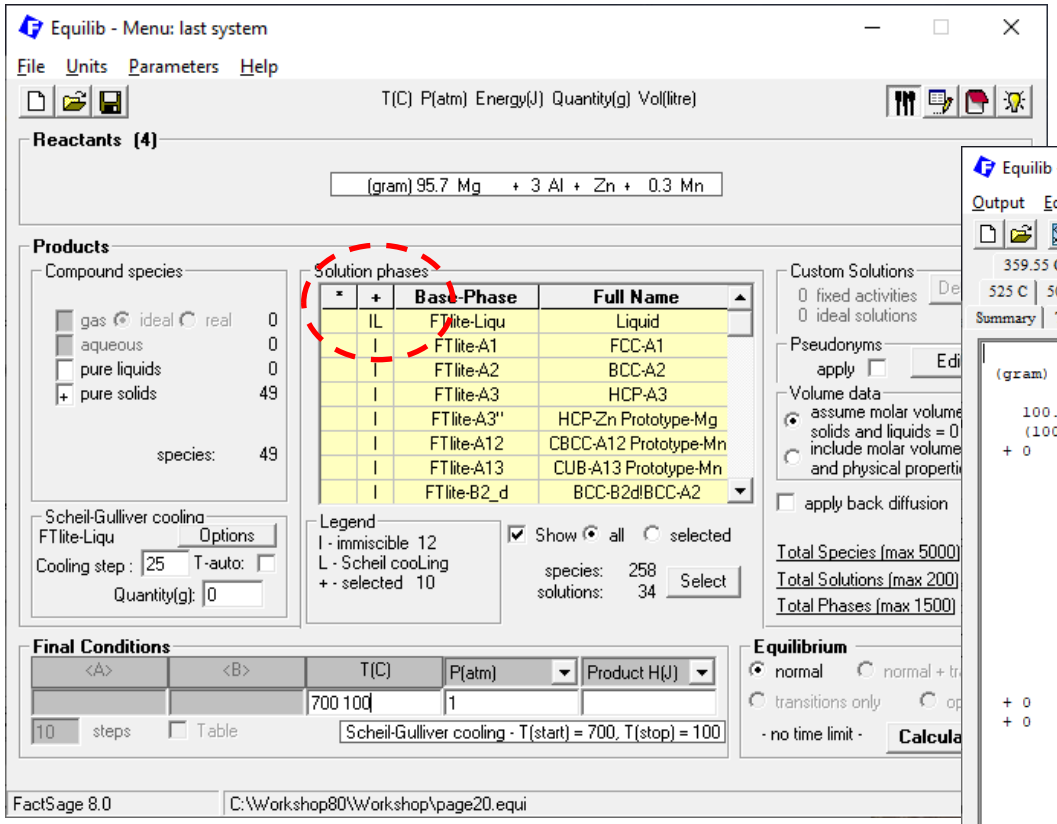


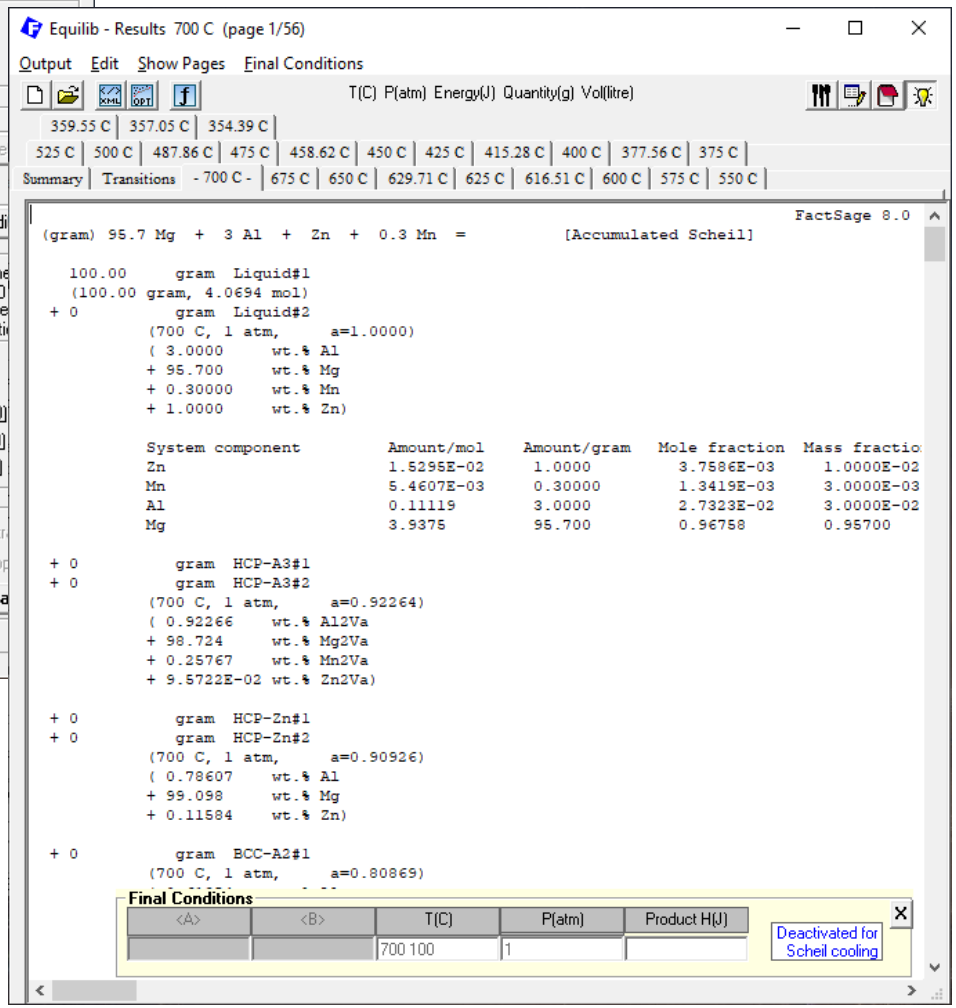
Univariant line (phase boundary)

Isotherms (liquidus)

Primary crystalline phase

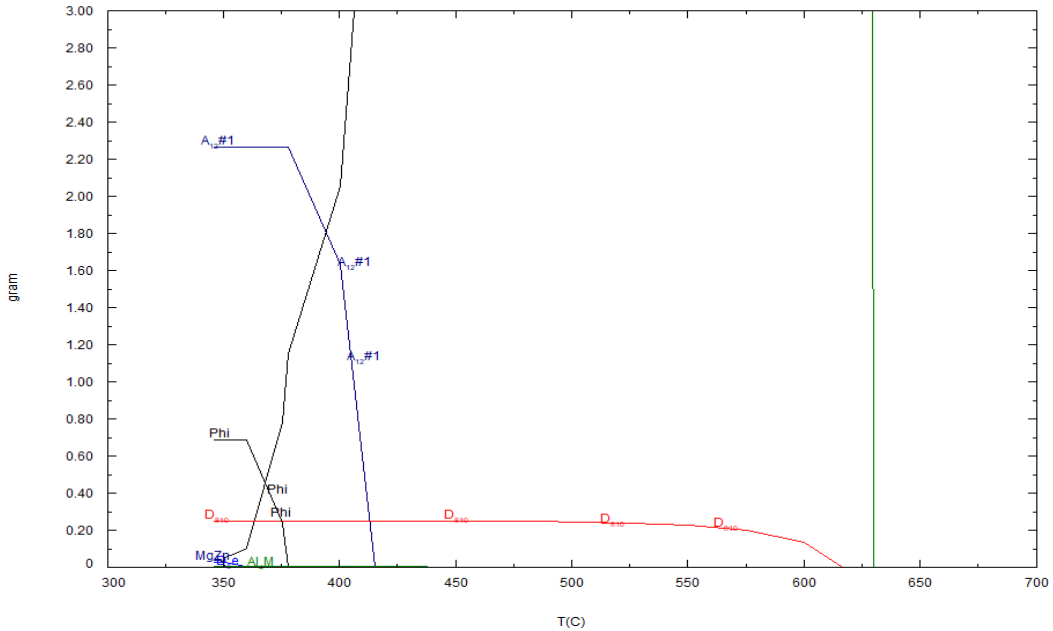
EX8. Scheil cooling calculation for AZ31 alloy (Mg-3Al-1Zn-0.3Mn)

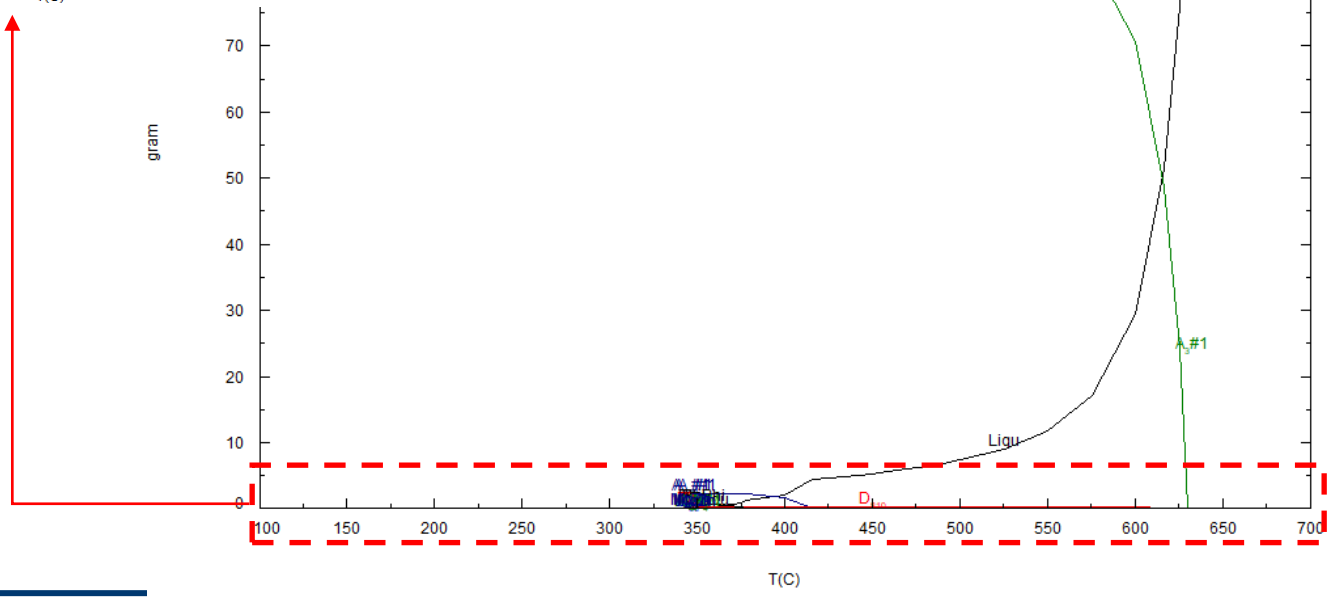




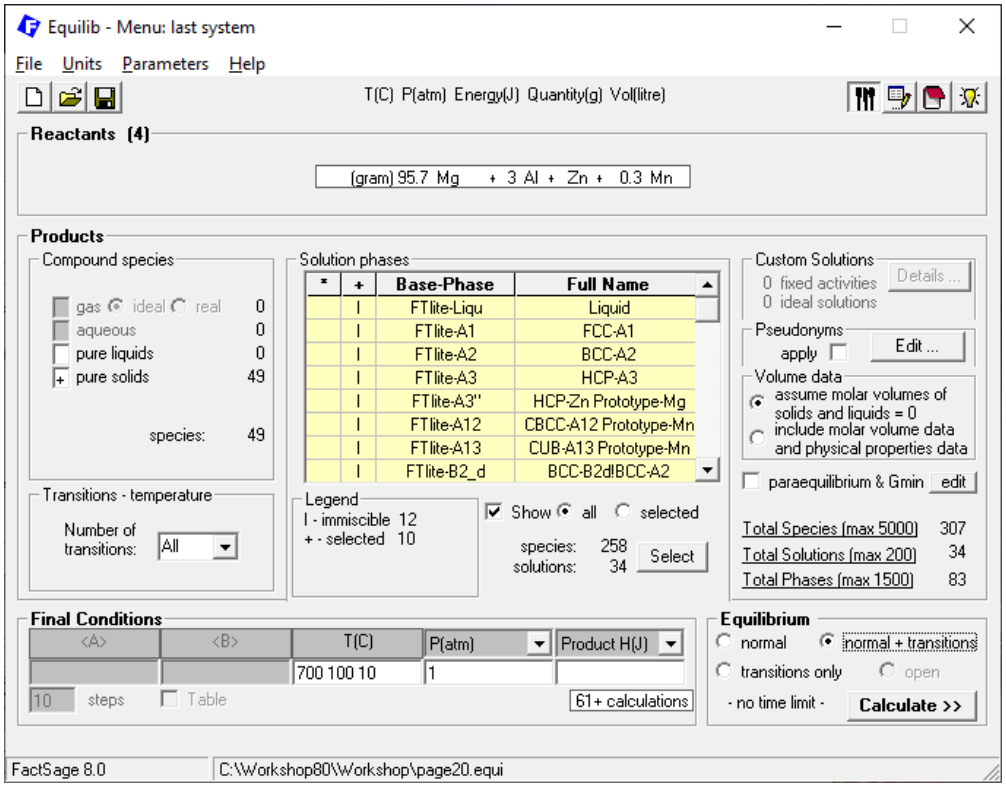
95.7 Mg + 3 Al + Zn + 0.3 Mn

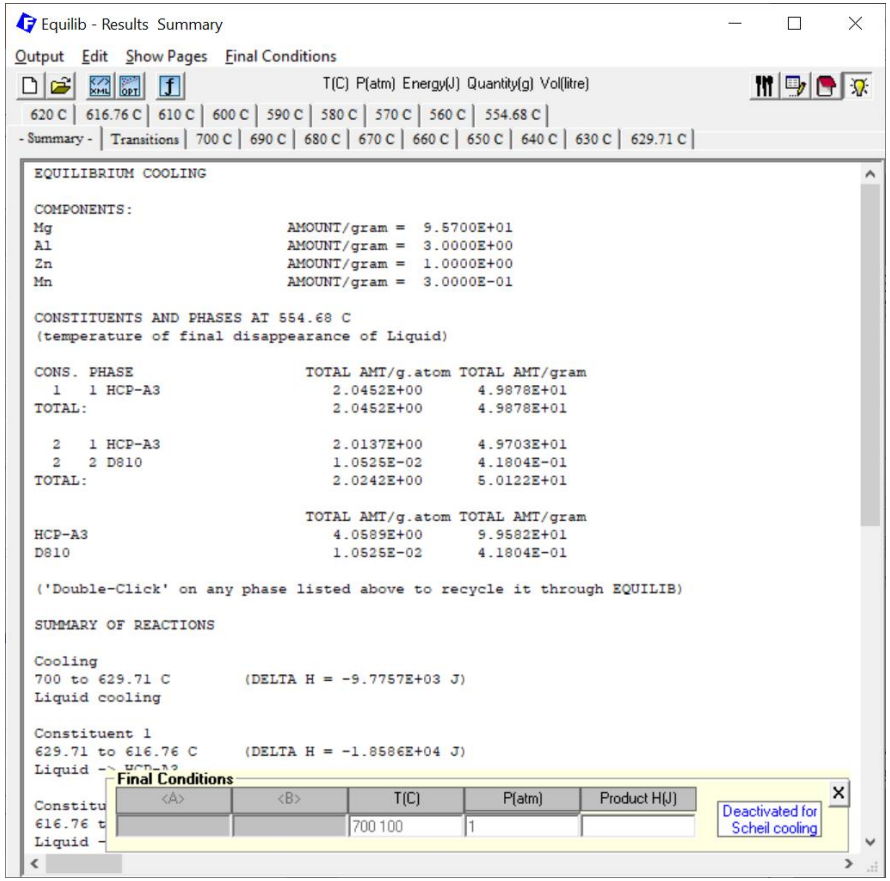
C:\Workshop80\Workshop\Equi0.res 19Dec19

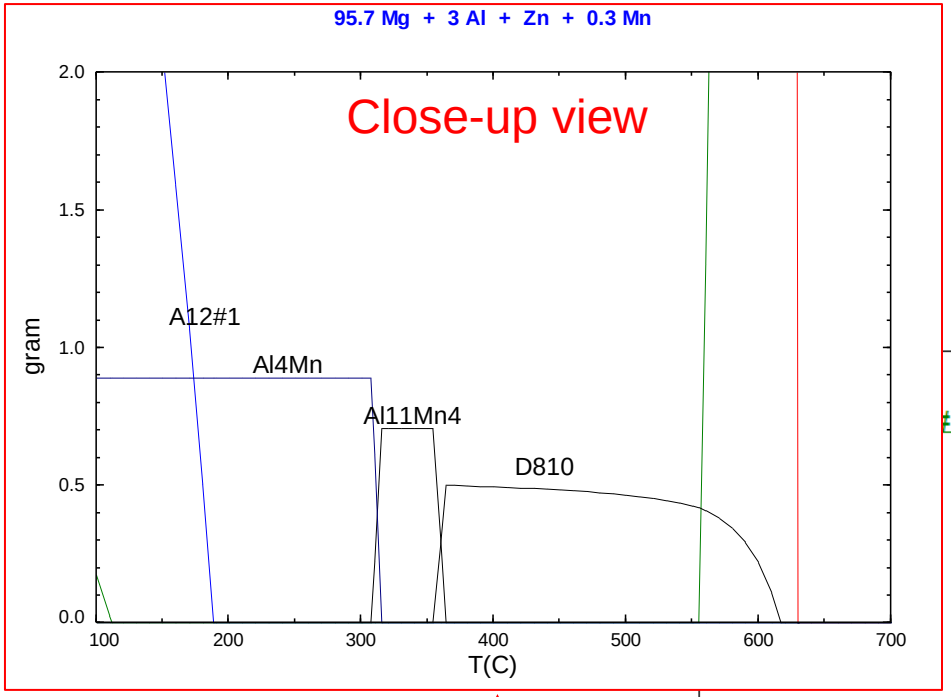


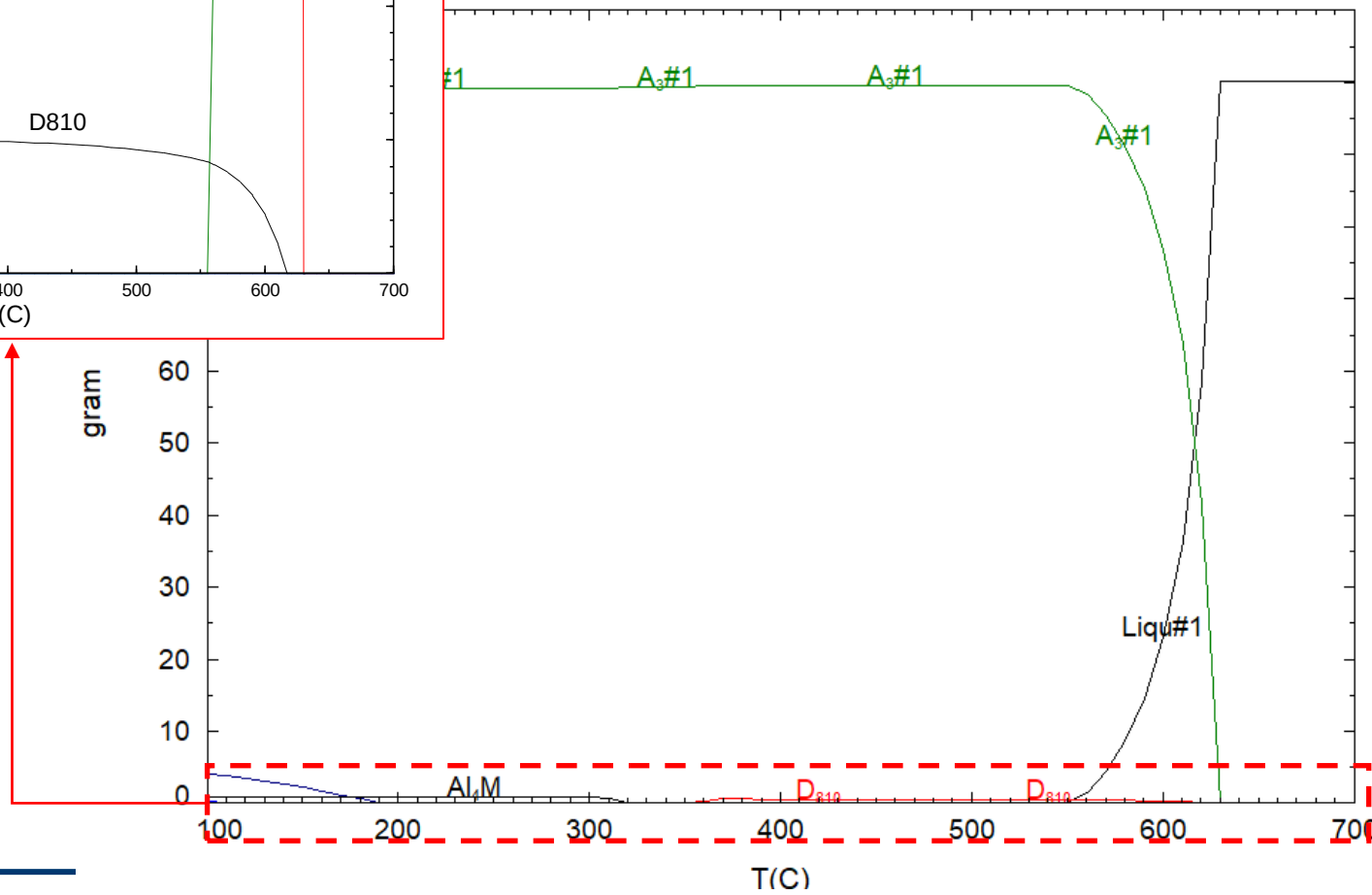


EX9. Equilibrium calculation for AZ31 alloy (Mg-3Al-1Zn-0.3Mn)

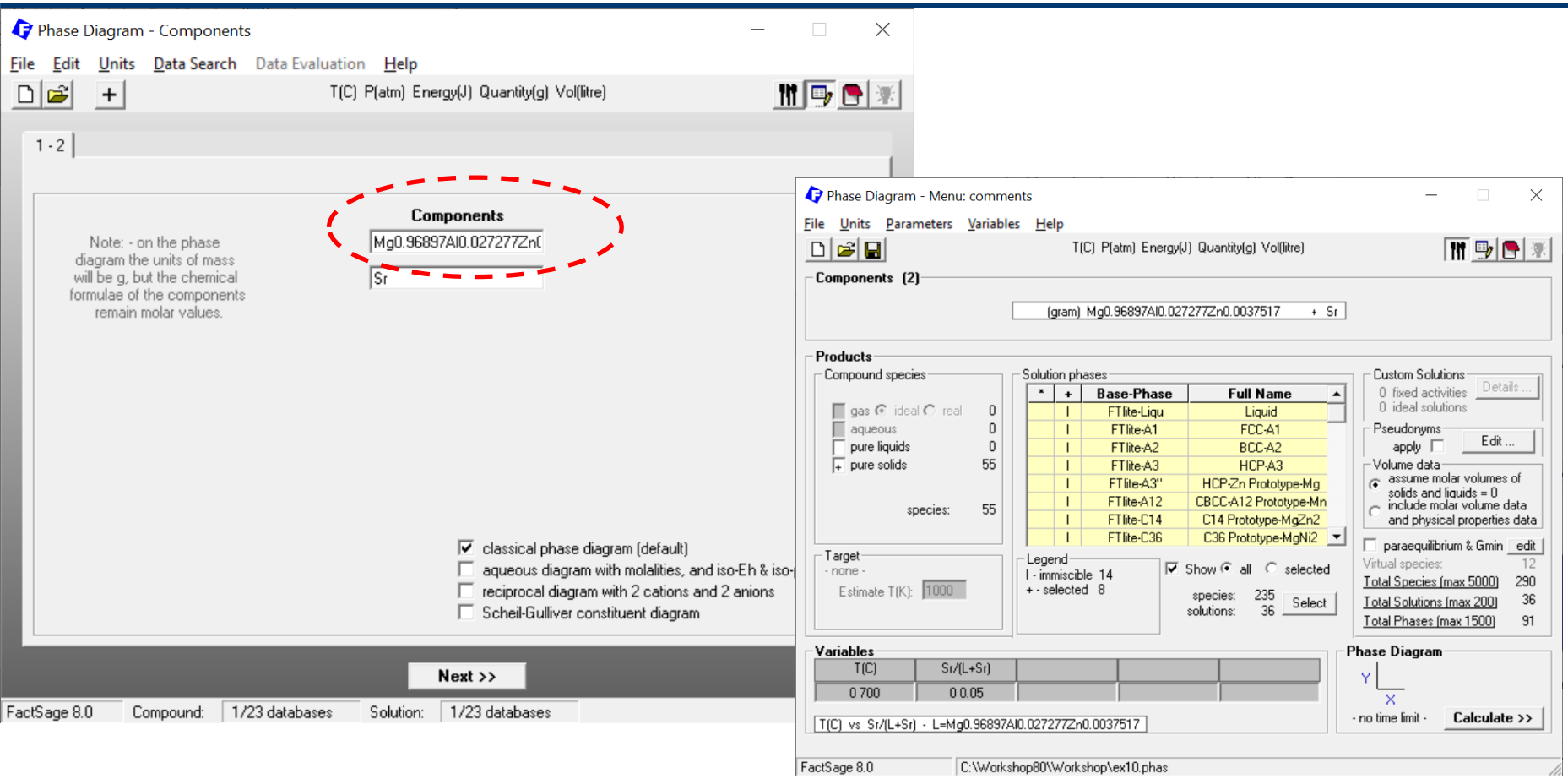





95.7 Mg + 3 Al + Zn + 0.3 Mn
Close-up view
gram
T(C)
A12#1
Al4Mn
Al11Mn4
D810

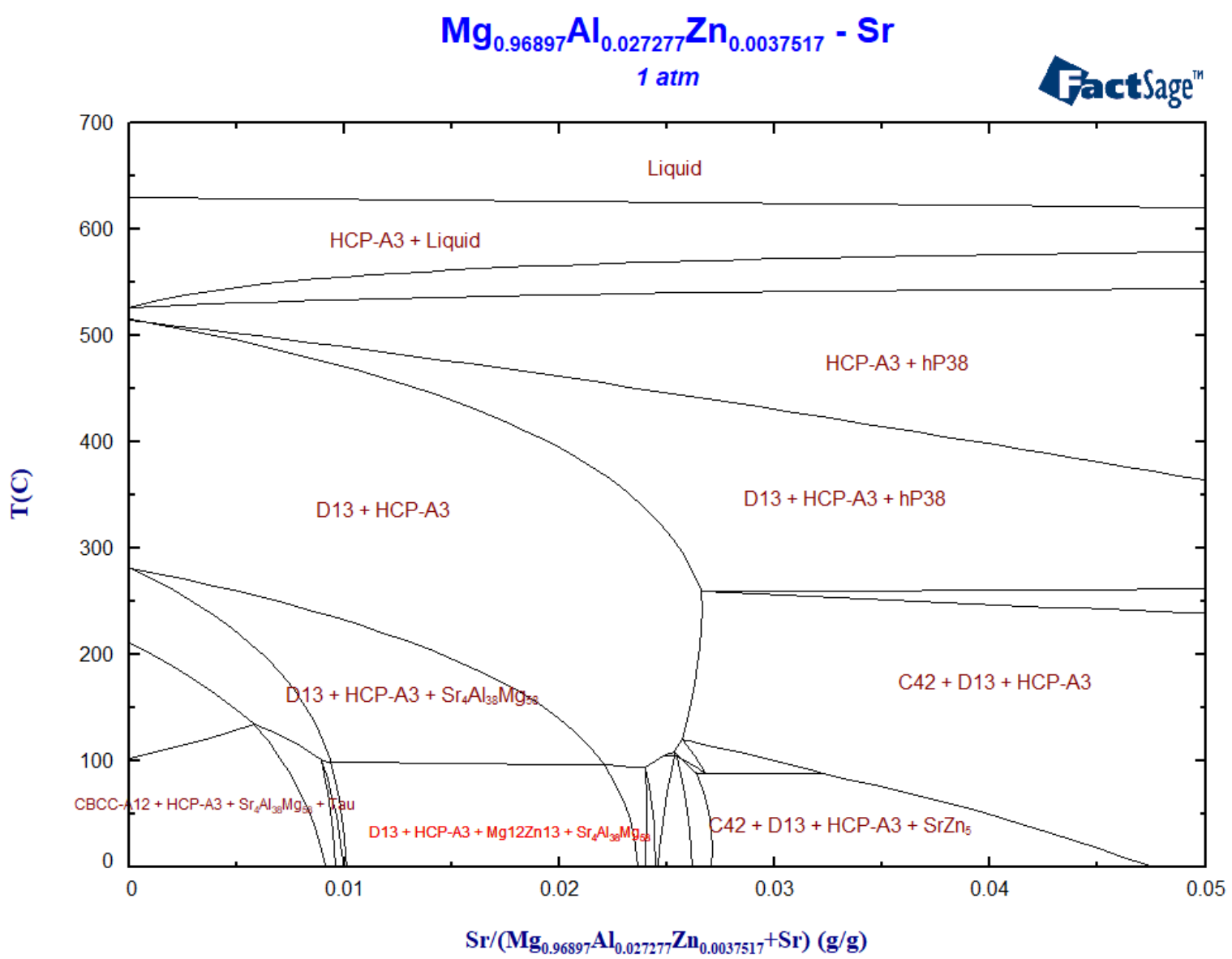

95.7 Mg + 3 Al + Zn + 0.3 Mn
C:\Workshop80\Workshop\Equi0.res 19Dec19
gram
T(C)
A3#1
Liqu#1
Al4M
D810

EX10. Phase diagram : AZ31 – Sr phase diagram

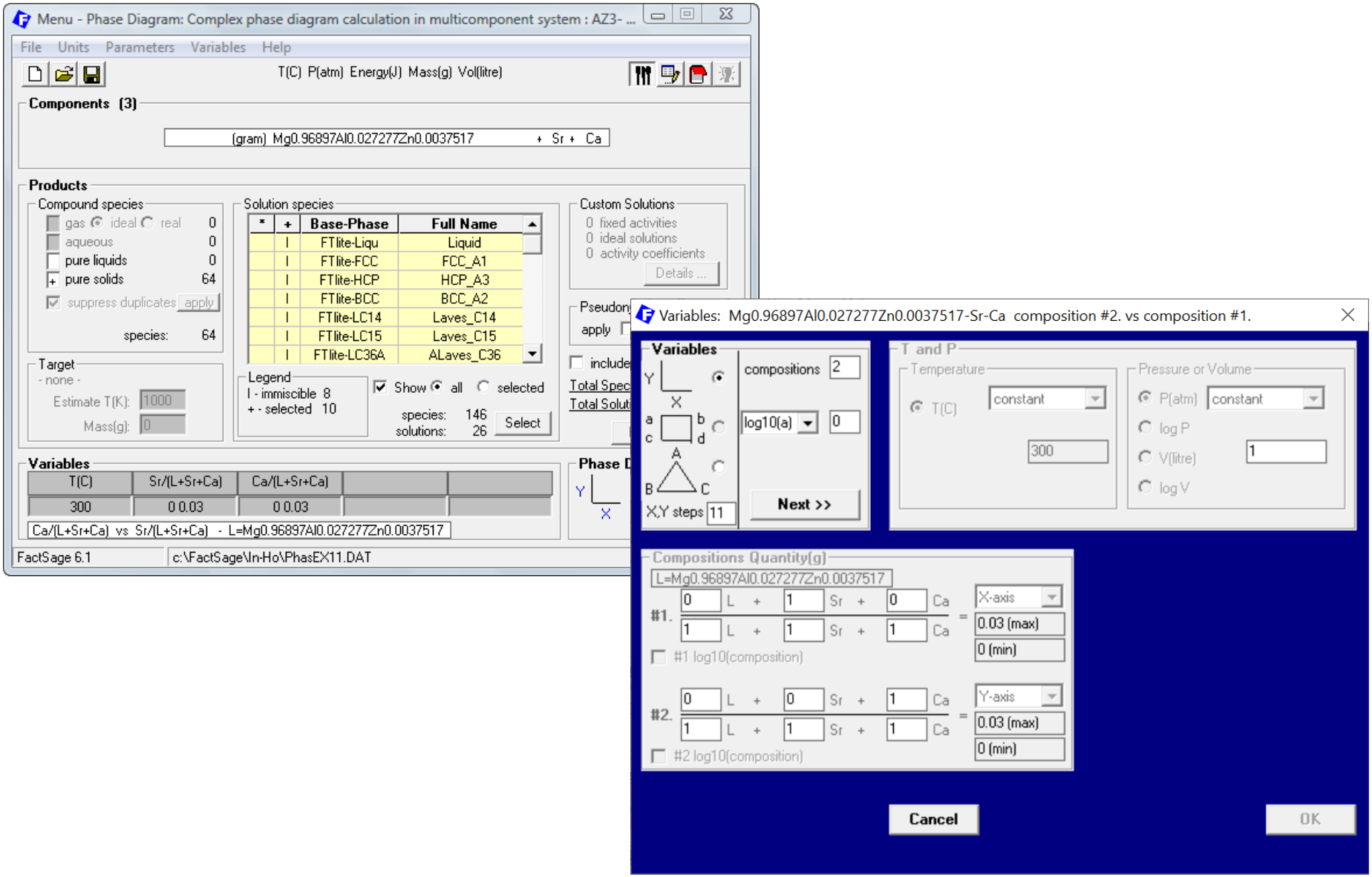


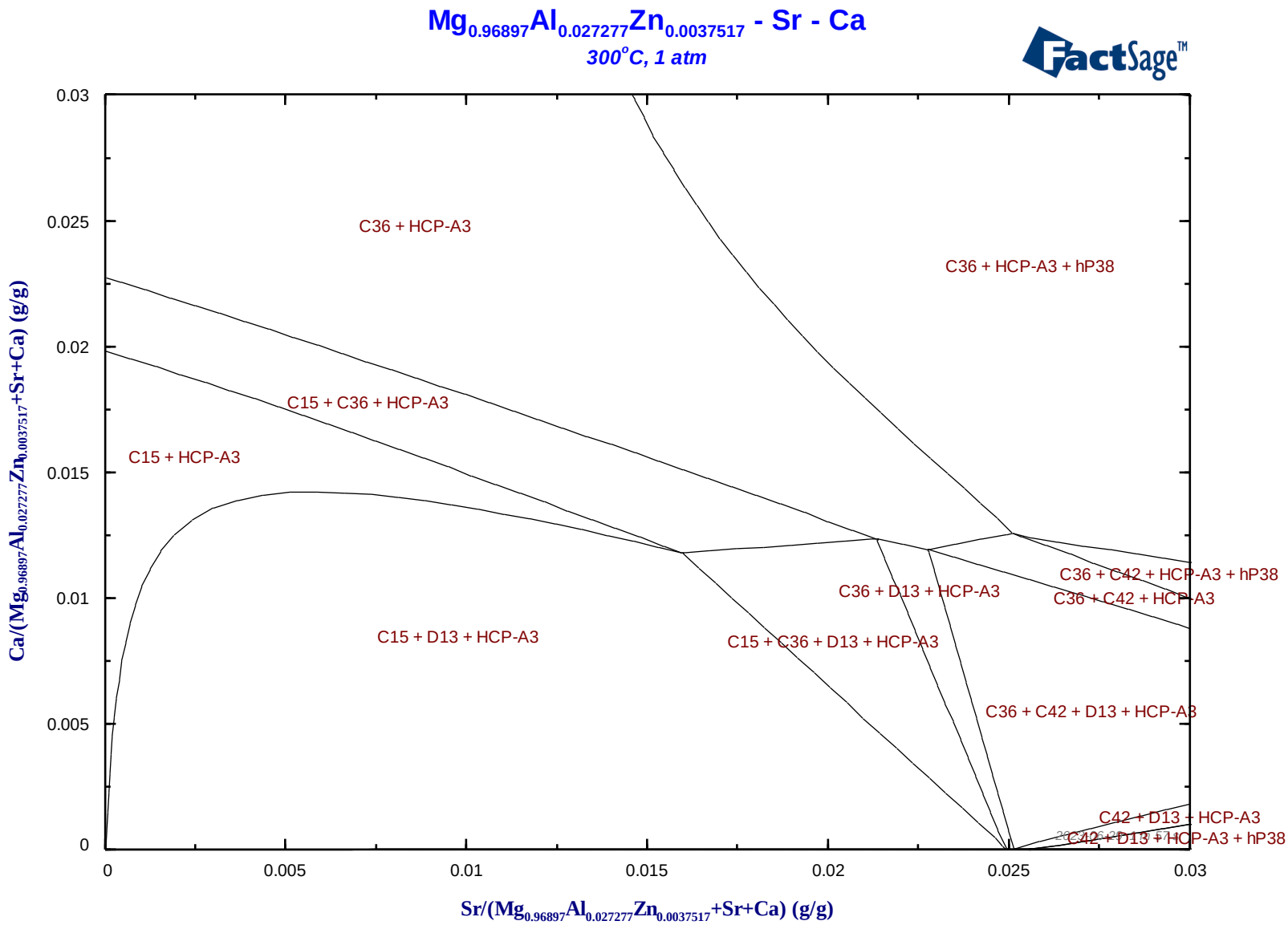
In FactSage, all the input is in molar formula.
Thus, in order to add AZ31 (97wt%Mg-3wt%Al-1wt%Zn), we have to do conversion of the composition into molar fraction first. Then, add this molar formula as input

97wt%Mg-3wt%Al-1wt%Zn -> 0.96897Mg-0.027277Al-0.0037517Zn

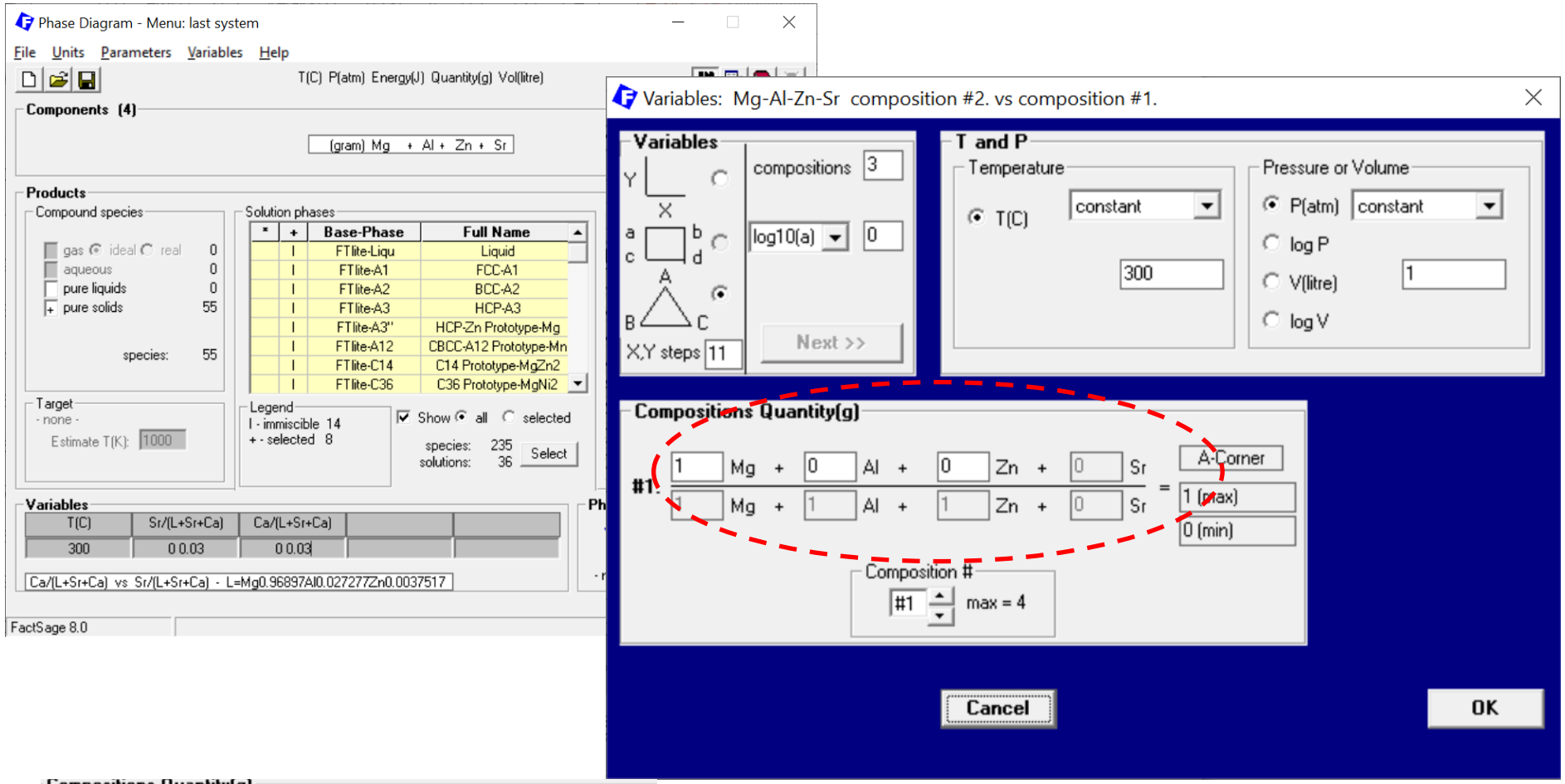

Mg0.96897Al0.027277Zn0.0037517 - Sr
1 atm
FactSage™
Liquid
HCP-A3 + Liquid
HCP-A3 + hP38
D13 + HCP-A3
D13 + HCP-A3 + hP38
D13 + HCP-A3 + Sr4Al38Mg58
C42 + D13 + HCP-A3
CBCC_A12 + HCP-A3 + Sr4Al38Mg58 + Tau
D13 + HCP-A3 + Mg12Zn13 + Sr4Al38Mg58
C42 + D13 + HCP-A3 + SrZn5
T(C)
700
600
500
400
300
200
100
0
0
0.01
0.02
0.03
0.04
0.05
Sr/(Mg0.96897Al0.027277Zn0.0037517+Sr) (g/g)

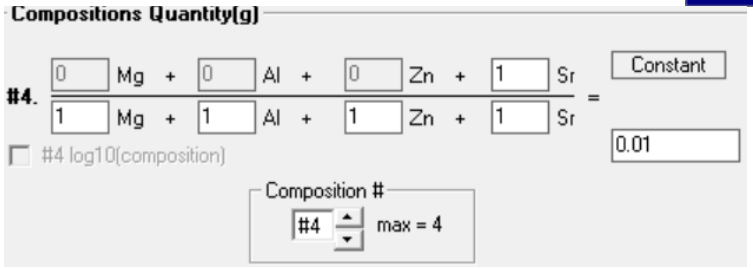
EX11. Phase diagram: AZ31 – Sr – Ca isothermal section




Mg0.96897Al0.027277Zn0.0037517 - Sr - Ca
300°C, 1 atm
FactSage™
C36 + HCP-A3
C36 + HCP-A3 + hP38
C15 + C36 + HCP-A3
C15 + HCP-A3
C36 + C42 + HCP-A3 + hP38
C36 + D13 + HCP-A3
C36 + C42 + HCP-A3
C15 + D13 + HCP-A3
C15 + C36 + D13 + HCP-A3
C36 + C42 + D13 + HCP-A3
C42 + D13 + HCP-A3
C42 + D13 + HCP-A3 + hP38
Ca/(Mg0.96897Al0.027277Zn0.0037517+Sr+Ca) (g/g)
Sr/(Mg0.96897Al0.027277Zn0.0037517+Sr+Ca) (g/g)
0
0.005
0.01
0.015
0.02
0.025
0.03

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

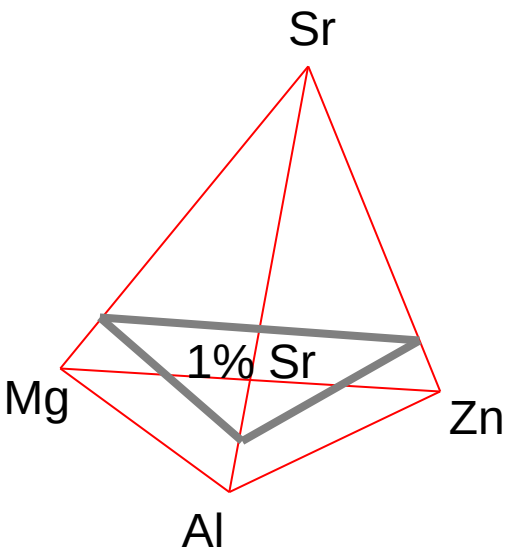


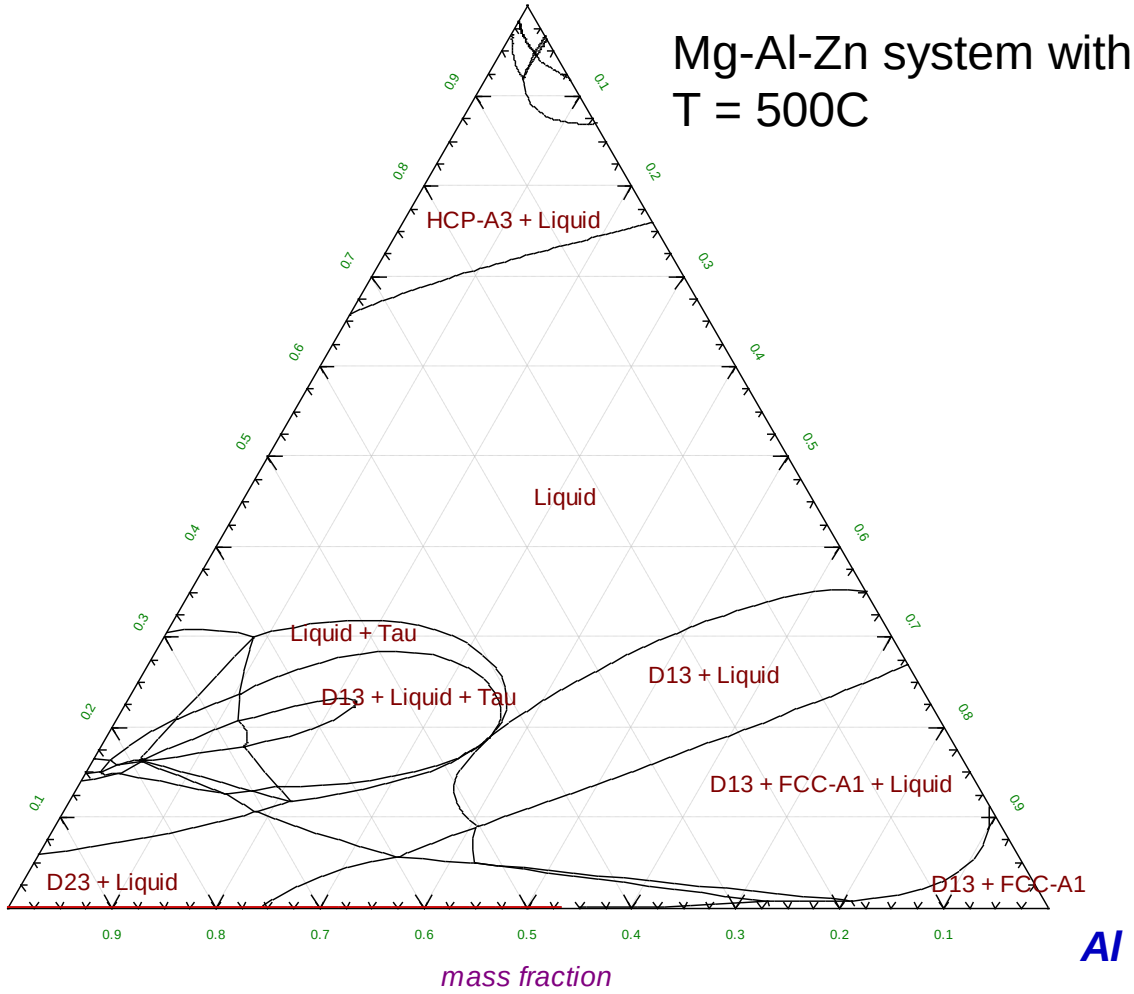


In the triangle diagram, the composition of 4th element is constant.

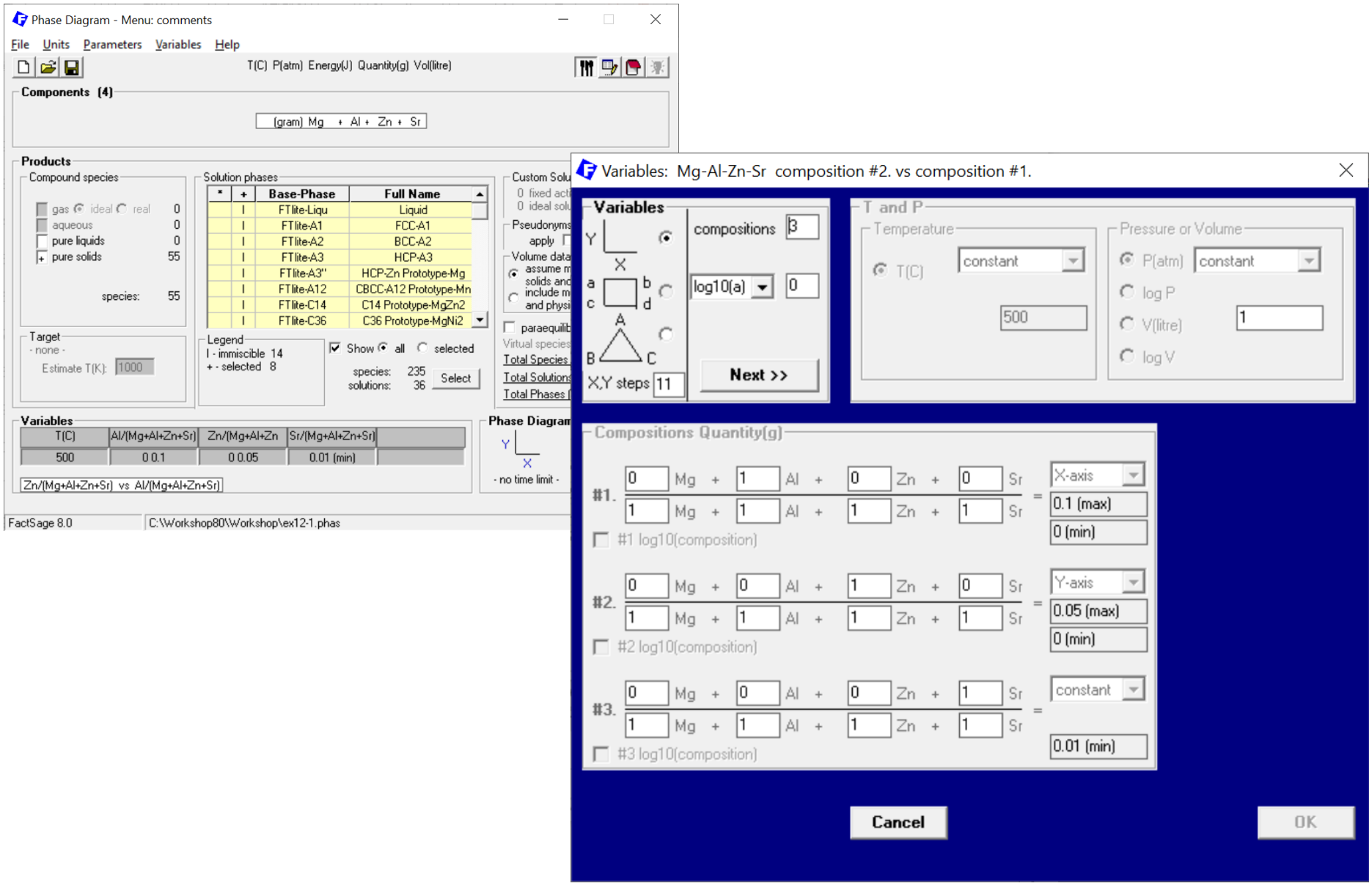
Mg - Al - Zn - Sr

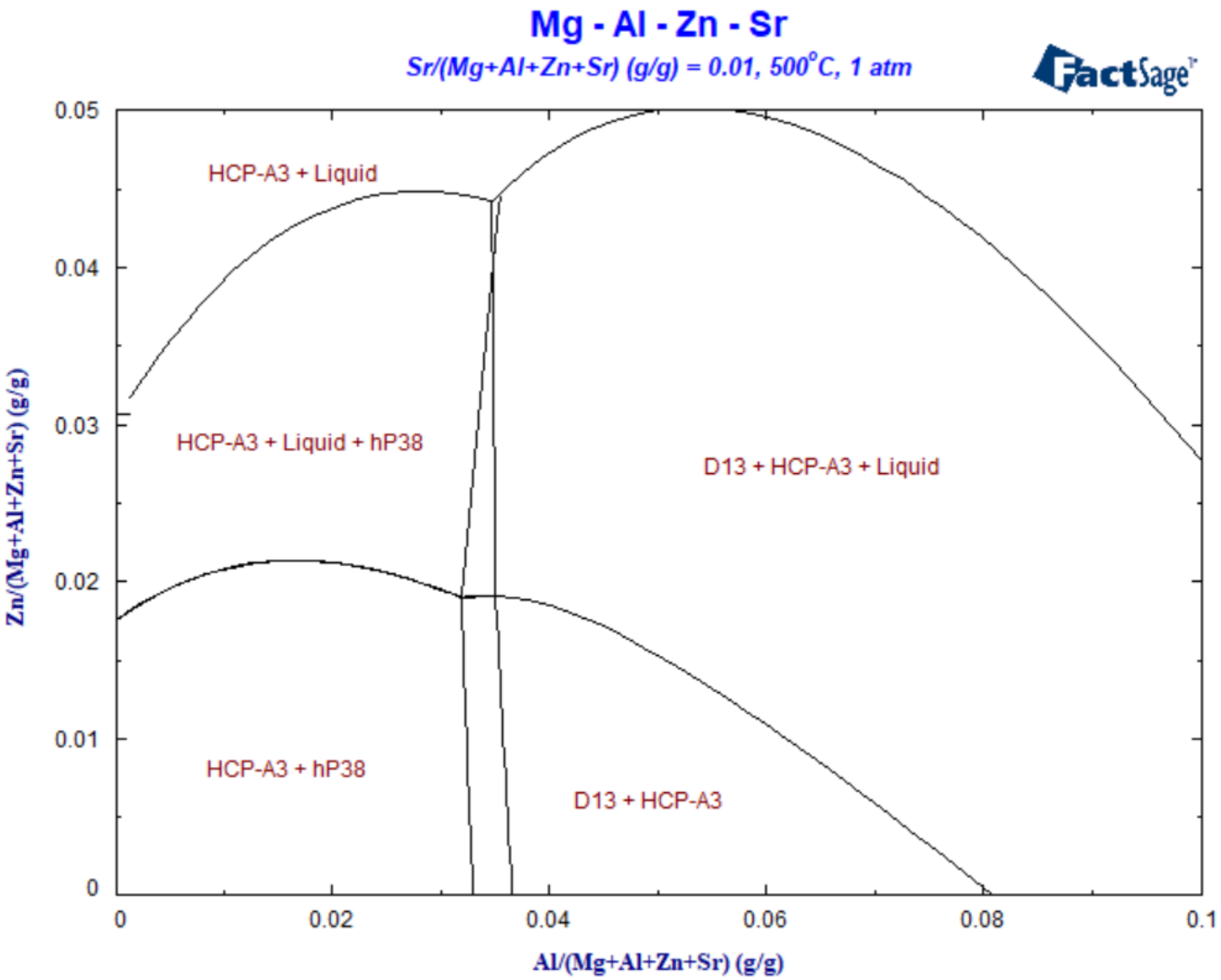
Sr/(Mg+Al+Zn+Sr) (g/g) = 0.01, 500°C, 1 atm



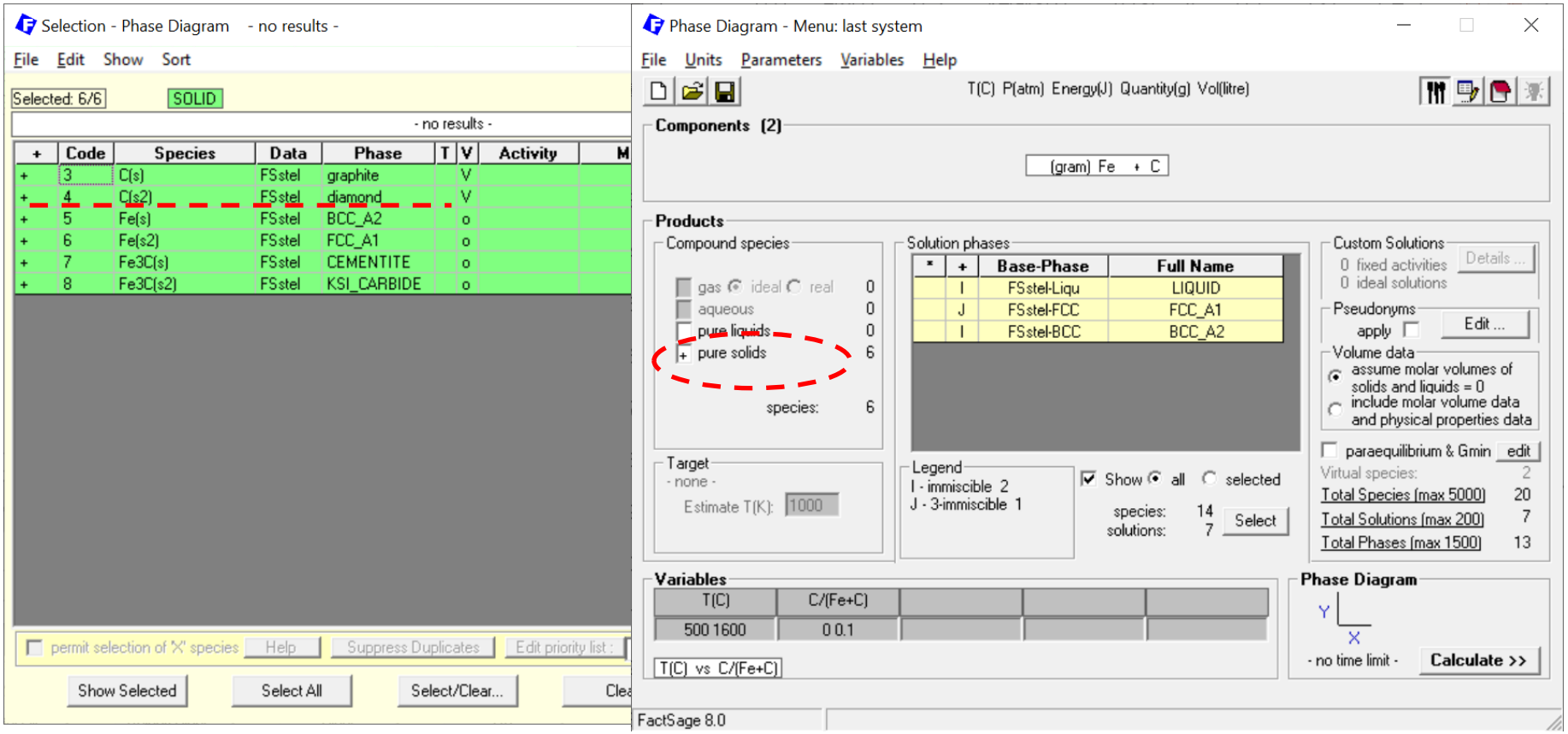


EX12-2. Mg-Al-Zn + 1% Sr triangle /rectangular isothermal section



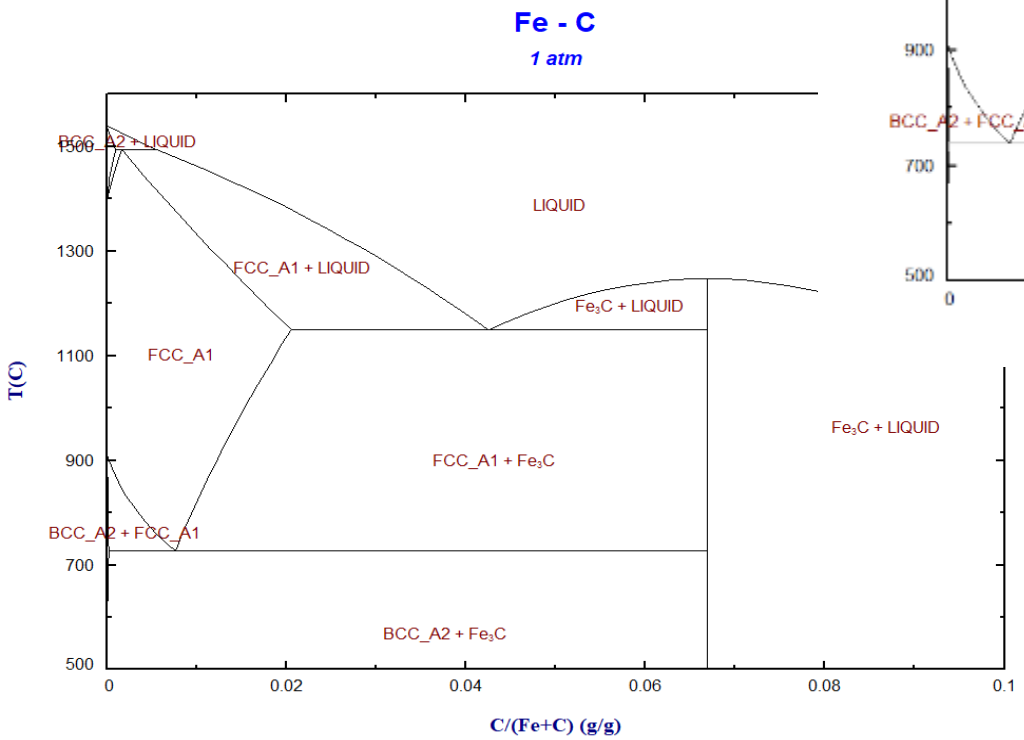

Mg - Al - Zn - Sr
Sr/(Mg+Al+Zn+Sr) (g/g) = 0.01, 500°C, 1 atm
FactSage
HCP-A3 + Liquid
HCP-A3 + Liquid + hP38
D13 + HCP-A3 + Liquid
HCP-A3 + hP38
D13 + HCP-A3
0.05
0.04
0.03
0.02
0.01
0
0
0.02
0.04
0.06
0.08
0.1
Zn/(Mg+Al+Zn+Sr) (g/g)
Al/(Mg+Al+Zn+Sr) (g/g)

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

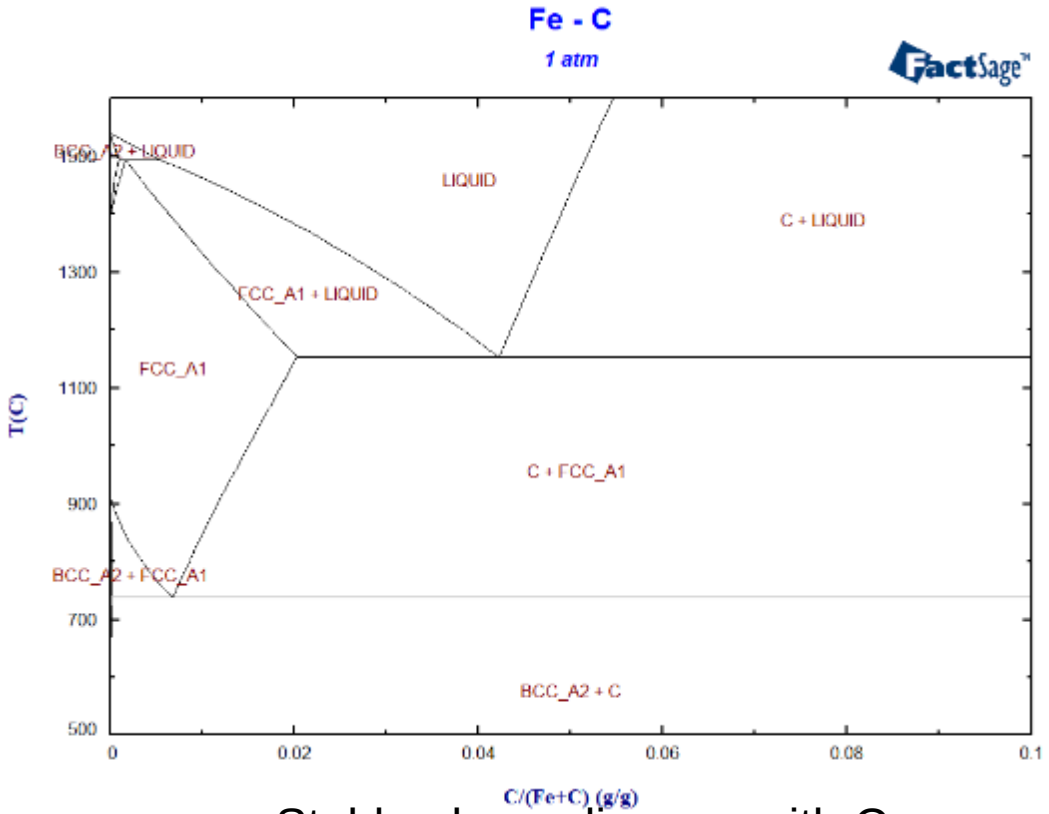


Although C (carbon) is thermodynamically stable phase than Fe3C, C is not appearing in most of low carbon steel. Thus, in order to do proper calculations, C should be removed from above compound list in particular in steel.

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.



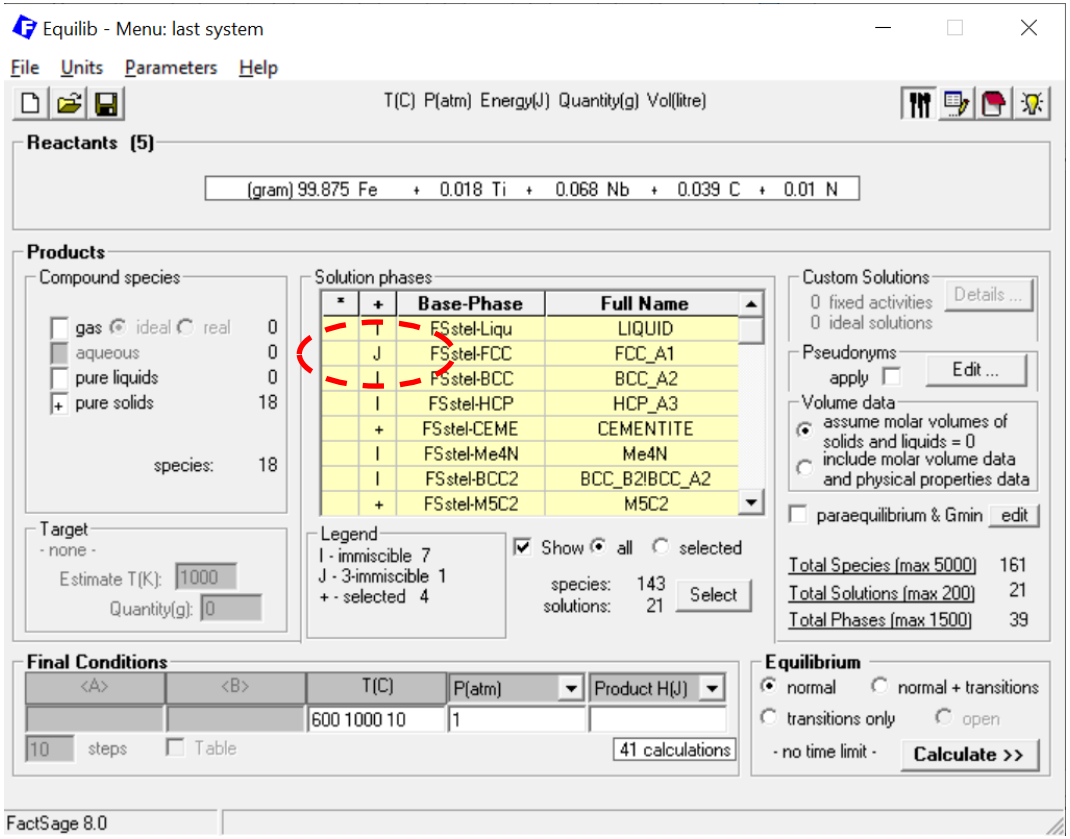
Metastable phase diagram without C



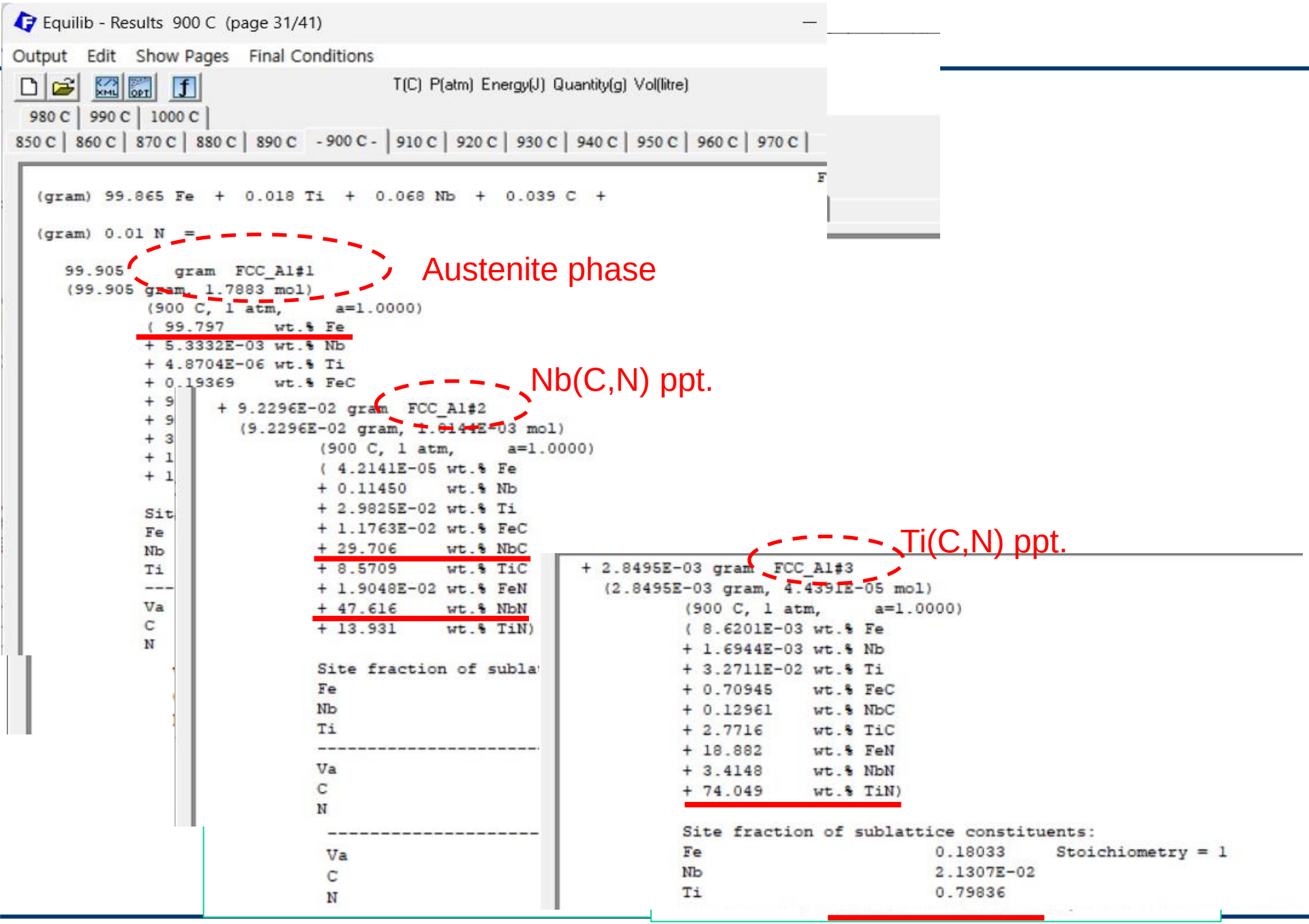
Stable phase diagram with C

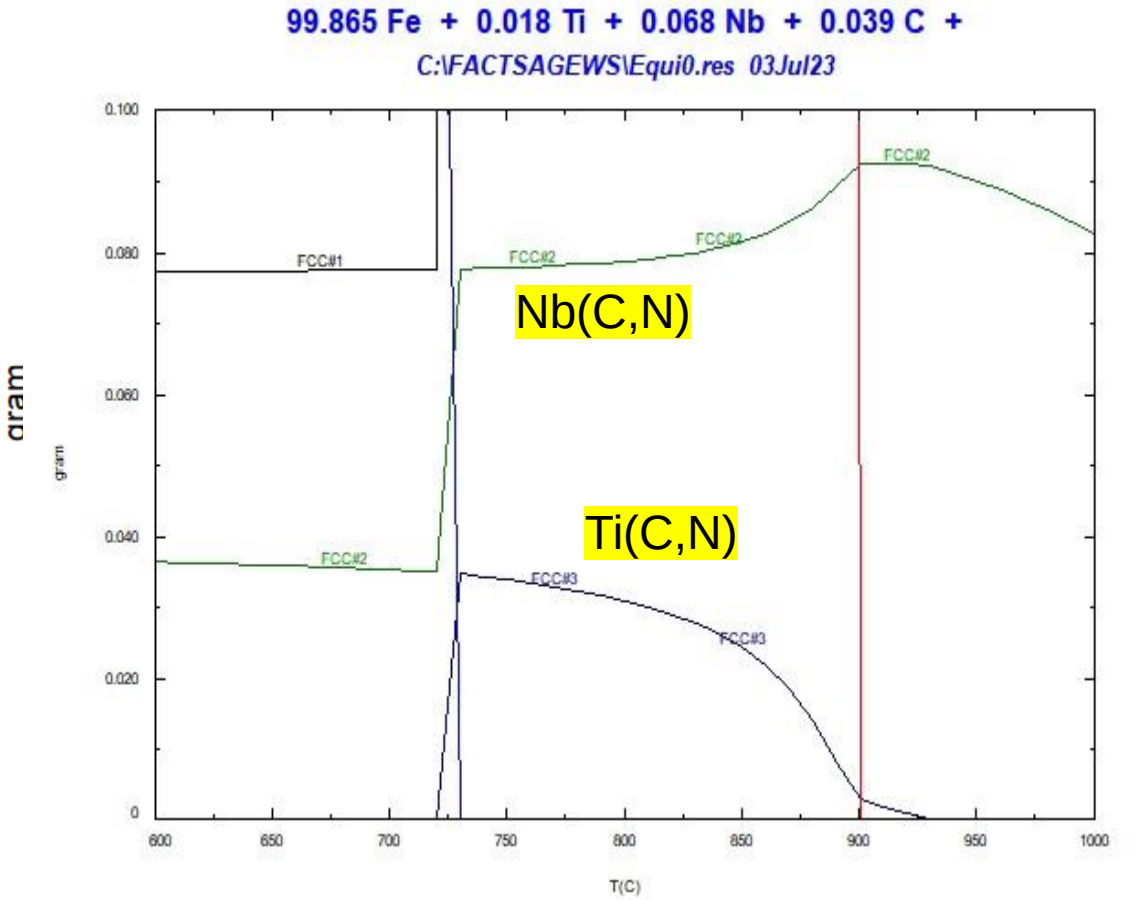
EX14-1. J option (3 possible miscibility gaps): Fe-Nb-Ti-C-N system

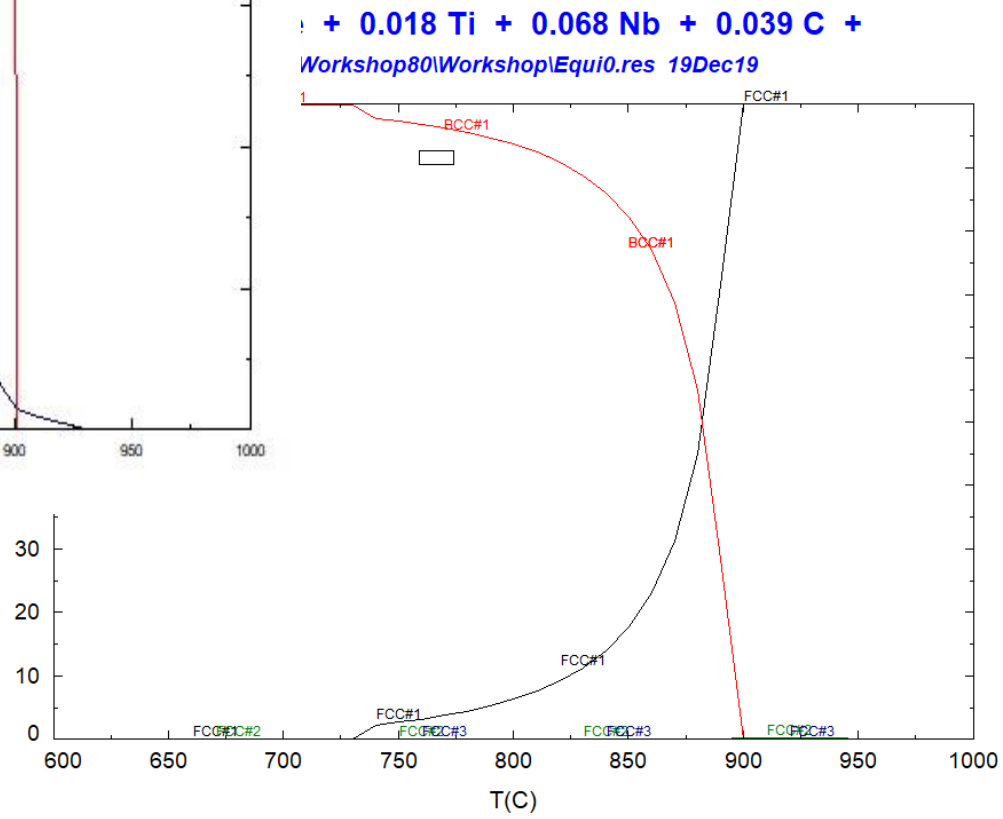
Unselect “C(s)”



“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.

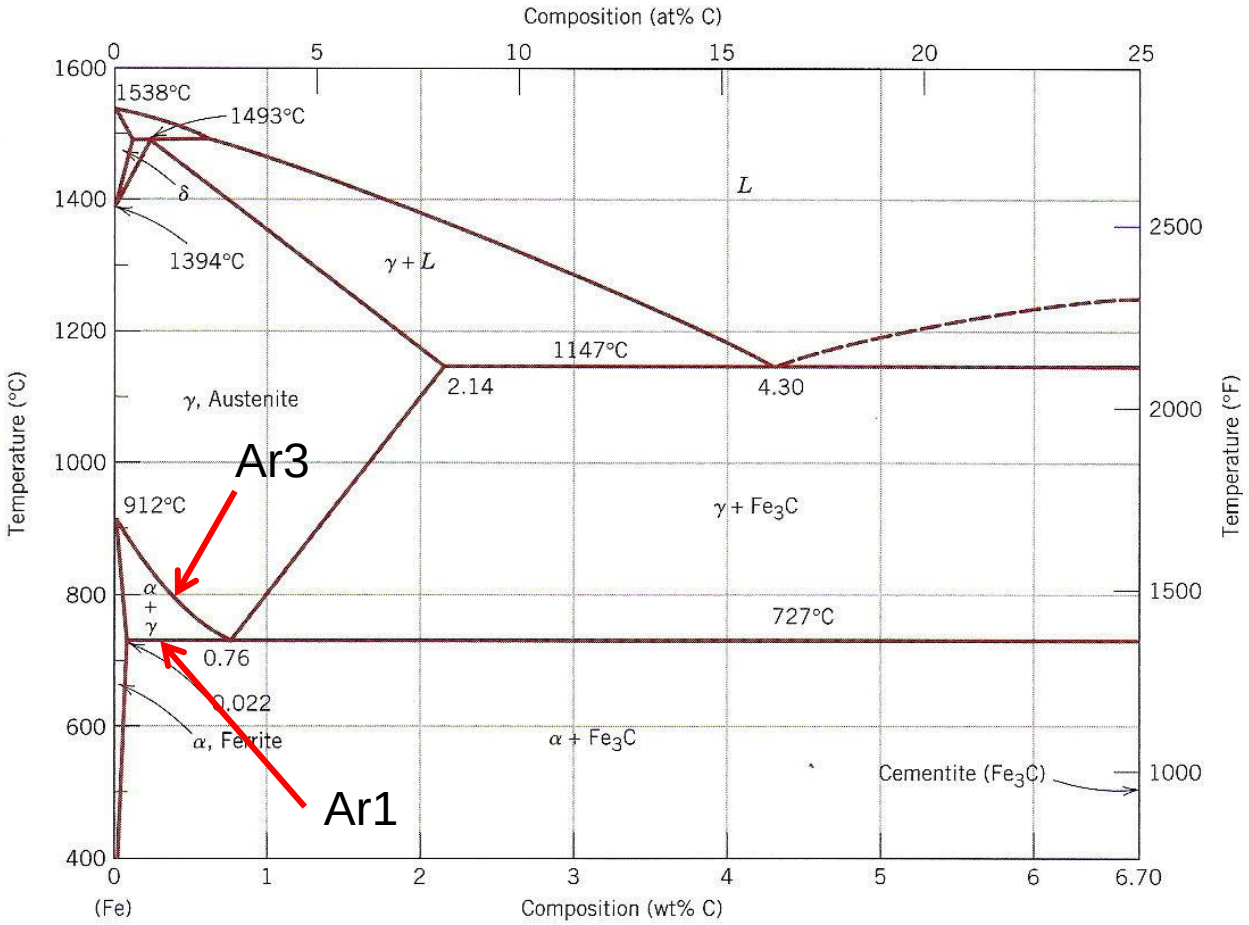

Equilib - Results 900 C (page 31/41)
Output Edit Show Pages Final Conditions
T(C) P(atm) Energy(J) Quantity(g) Vol(litre)
980 C | 990 C | 1000 C |
850 C | 860 C | 870 C | 880 C | 890 C | - 900 C - | 910 C | 920 C | 930 C | 940 C | 950 C | 960 C | 970 C |
(gram) 99.865 Fe + 0.018 Ti + 0.068 Nb + 0.039 C +
(gram) 0.01 N =
99.905 gram FCC_A1#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
+ 9.2296E-02 gram FCC_A1#2
(9.2296E-02 gram, 1.8144E-03 mol)
(900 C, 1 atm, a=1.0000)
(4.2141E-05 wt.% Fe
+ 0.11450 wt.% Nb
+ 2.9825E-02 wt.% Ti
+ 1.1763E-02 wt.% FeC
+ 29.706 wt.% NbC
+ 8.5709 wt.% TiC
+ 1.9048E-02 wt.% FeN
+ 47.616 wt.% NbN
+ 13.931 wt.% TiN)
Site fraction of subla
Fe
Nb
Ti
Va
C
N
Va
C
N
+ 2.8495E-03 gram FCC_A1#3
(2.8495E-03 gram, 4.4391E-05 mol)
(900 C, 1 atm, a=1.0000)
(8.6201E-03 wt.% Fe
+ 1.6944E-03 wt.% Nb
+ 3.2711E-02 wt.% Ti
+ 0.70945 wt.% FeC
+ 0.12961 wt.% NbC
+ 2.7716 wt.% TiC
+ 18.882 wt.% FeN
+ 3.4148 wt.% NbN
+ 74.049 wt.% TiN)
Site fraction of sublattice constituents:
Fe 0.18033 Stoichiometry = 1
Nb 2.1307E-02
Ti 0.79836
Austenite phase
Nb(C,N) ppt.
Ti(C,N) ppt.


99.865 Fe + 0.018 Ti + 0.068 Nb + 0.039 C +
C:\FACTSAGEWS\Equi0.res 03Jul23
gram
0.100
0.080
0.060
0.040
0.020
0
FCC#1
FCC#2
FCC#2
FCC#2
Nb(C,N)
Ti(C,N)
FCC#2
FCC#3
FCC#3
600
650
700
750
800
850
900
950
1000
T(C)


+ 0.018 Ti + 0.068 Nb + 0.039 C +
Workshop80\Workshop\Equi0.res 19Dec19
FCC#1
BCC#1
BCC#1
FCC#1
FCC#1
30
20
10
0
600
650
700
750
800
850
900
950
1000
T(C)

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.

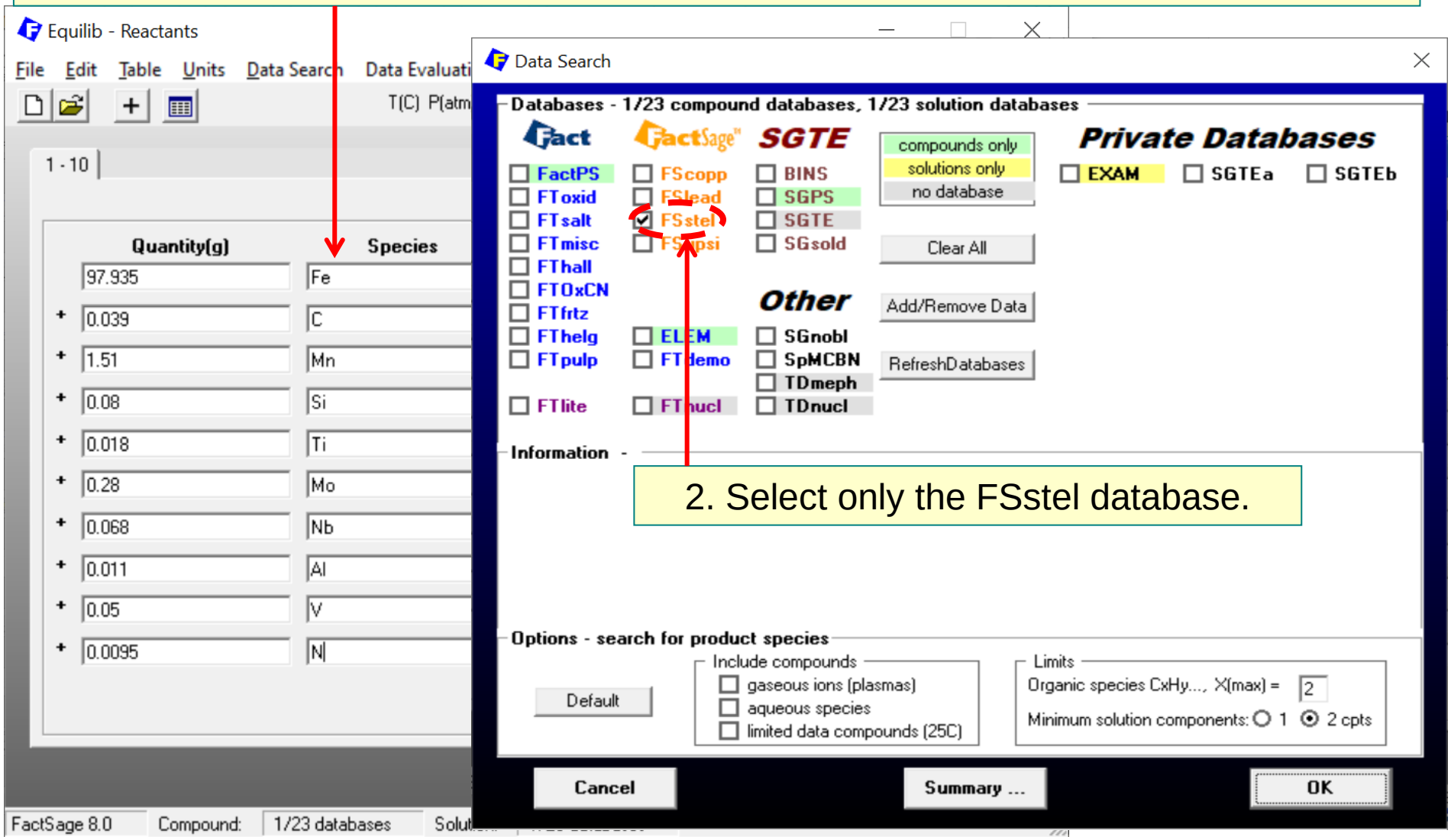


The steel is annealed in the austenite region an then cooled through the temperatures Ar3 and Ar1 temperatures (continuous cooling austenite to ferrite transformation start and finish.

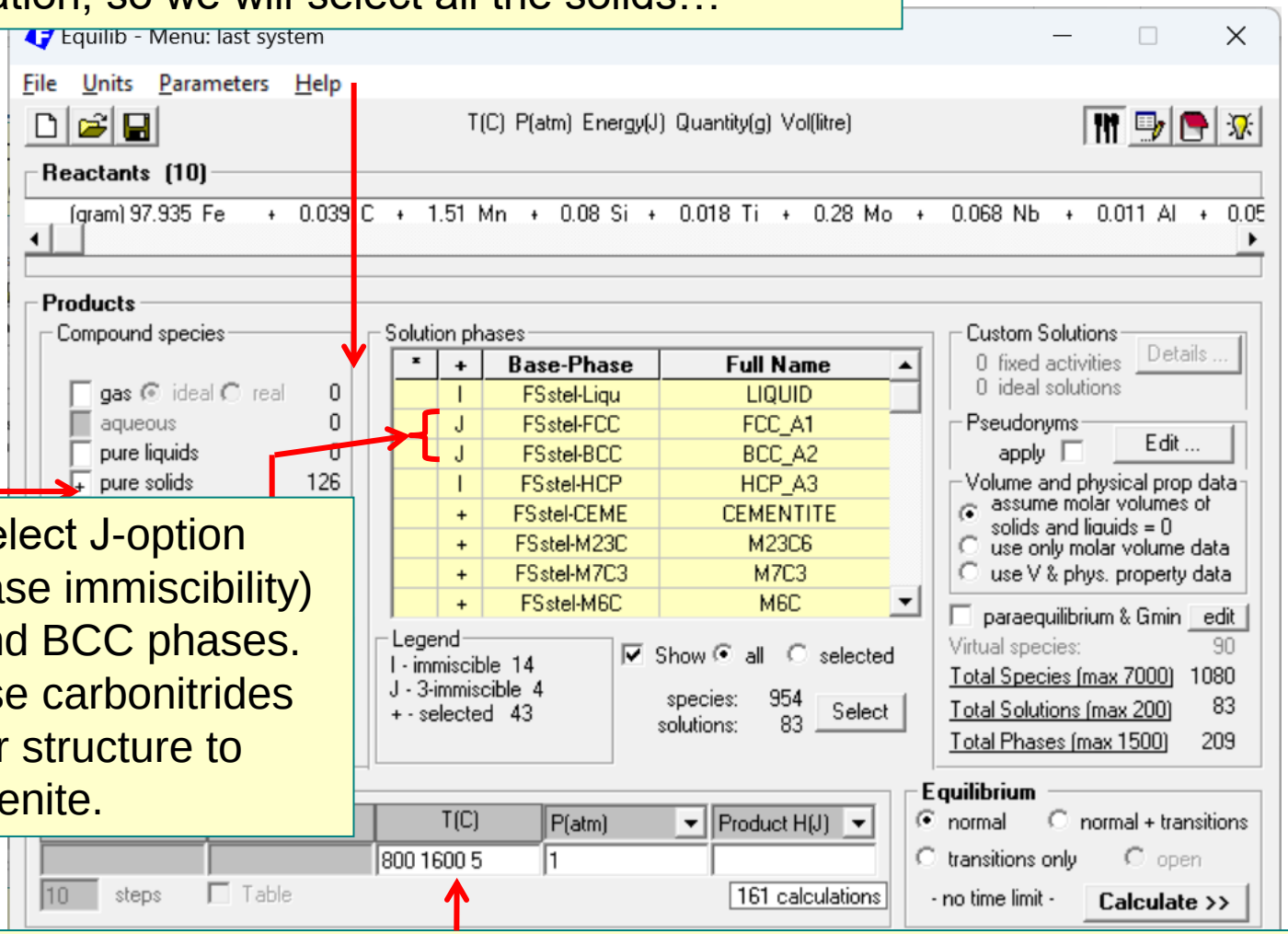
The goal of this study is to find the ideal annealing temperatures to avoid precipitation of Nb carbonitrides and promote precipitation of NbC

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)



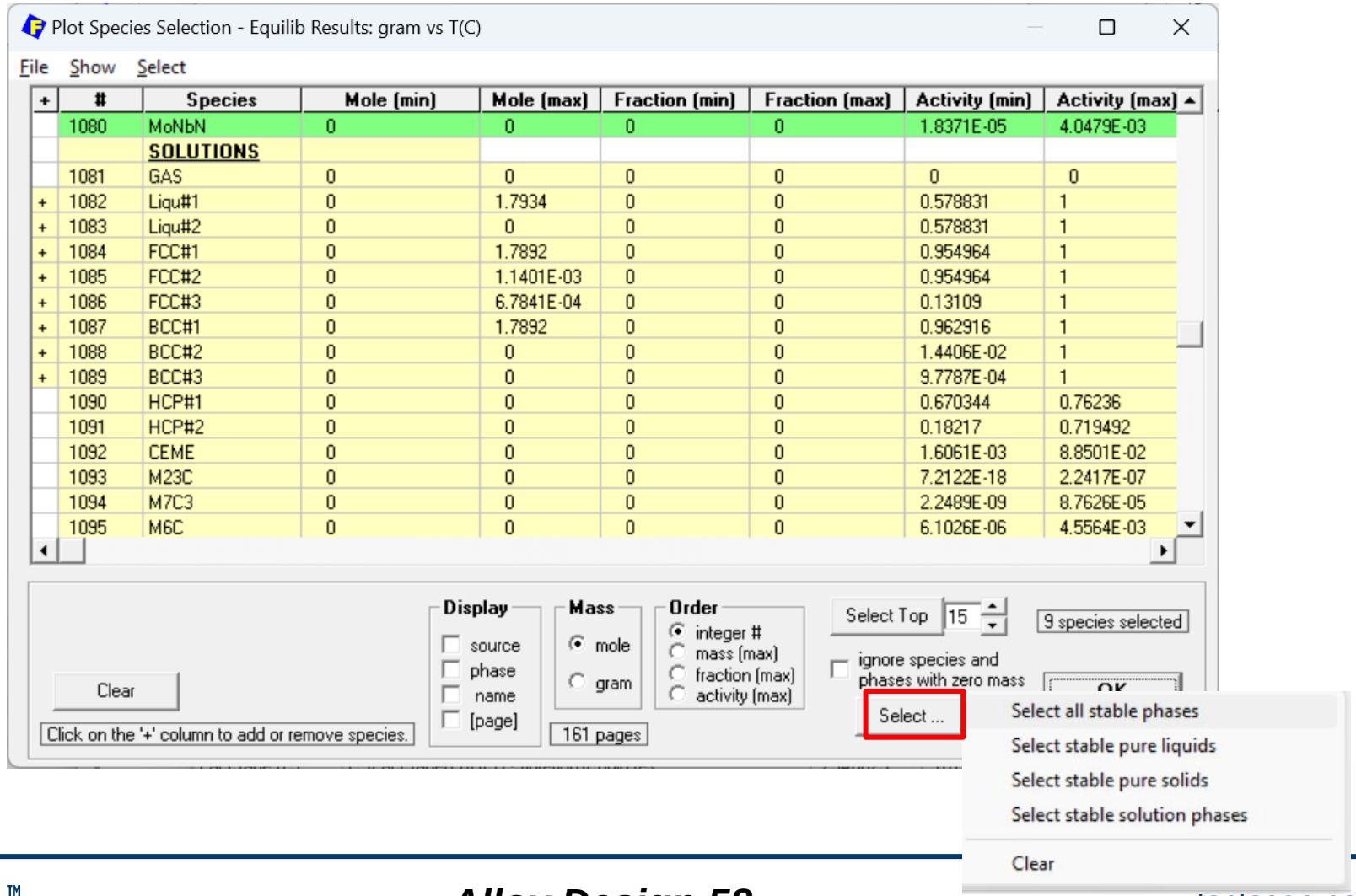
1. We are interested in carbide, nitride and carbonitride precipitation, so we will select all the solids…



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

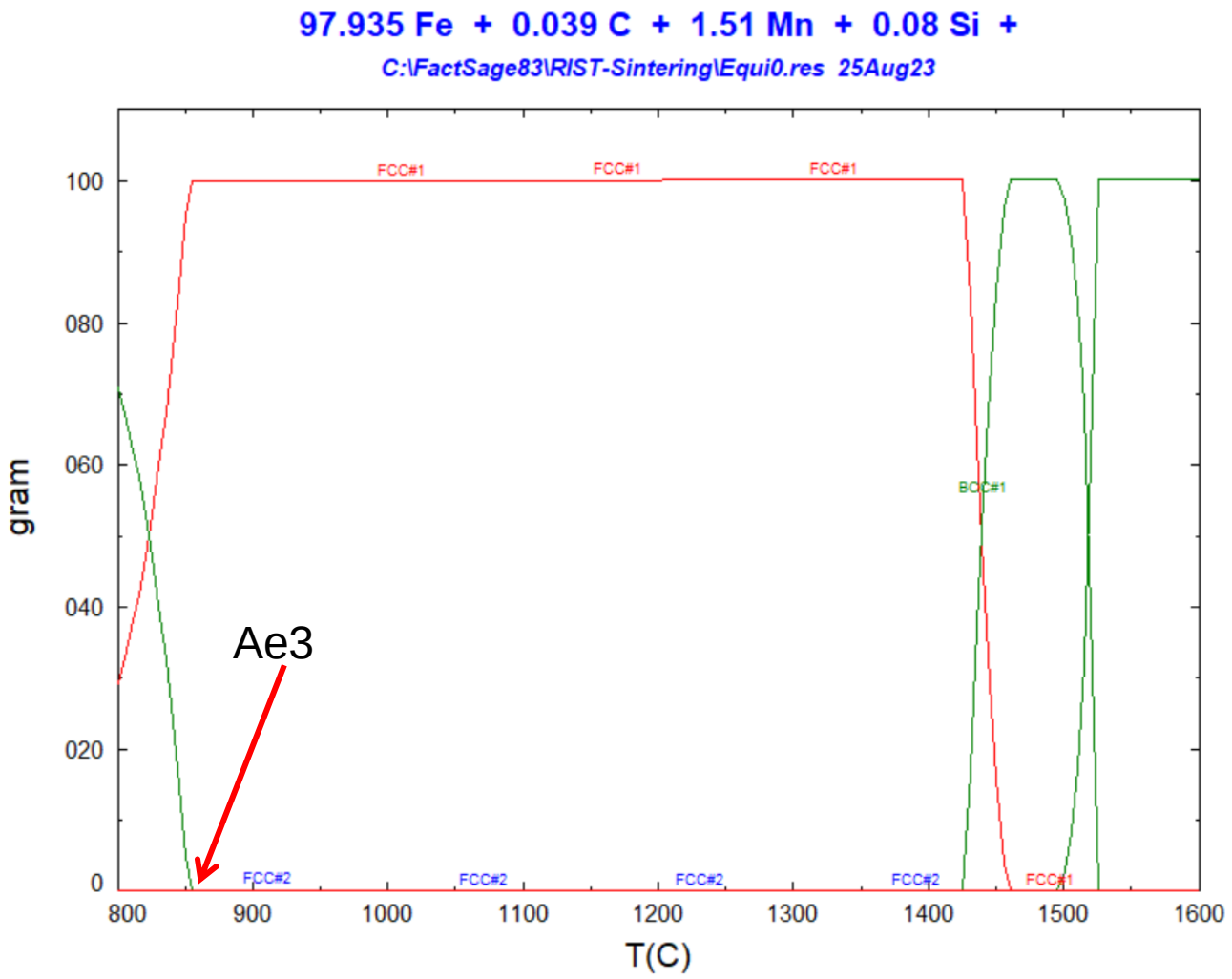
3. We will select a range of temperature encompassing the whole austenite phase.

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



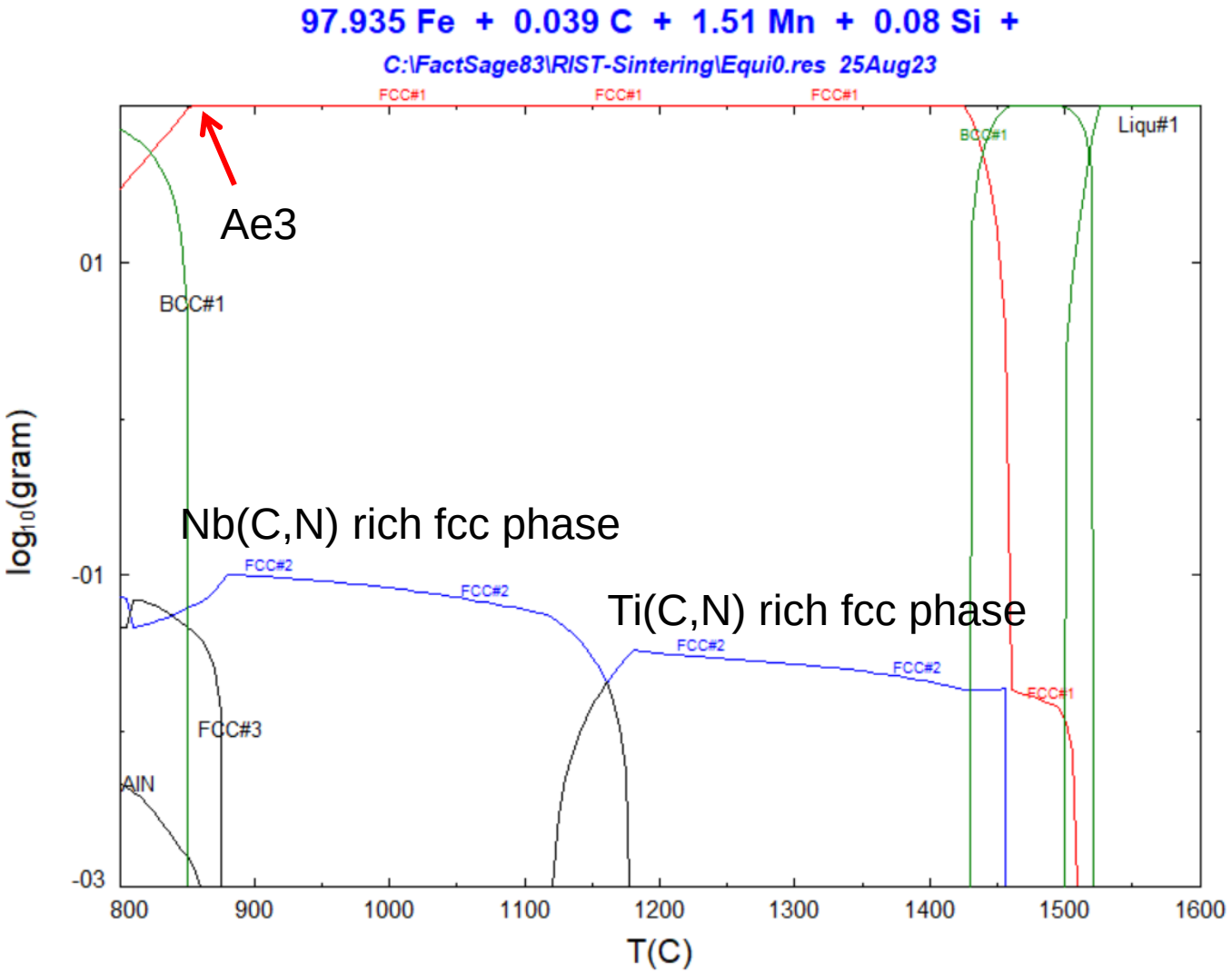
1. From the graph, we can deduce equilibrium transformation temperatures from austenite to ferrite.

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

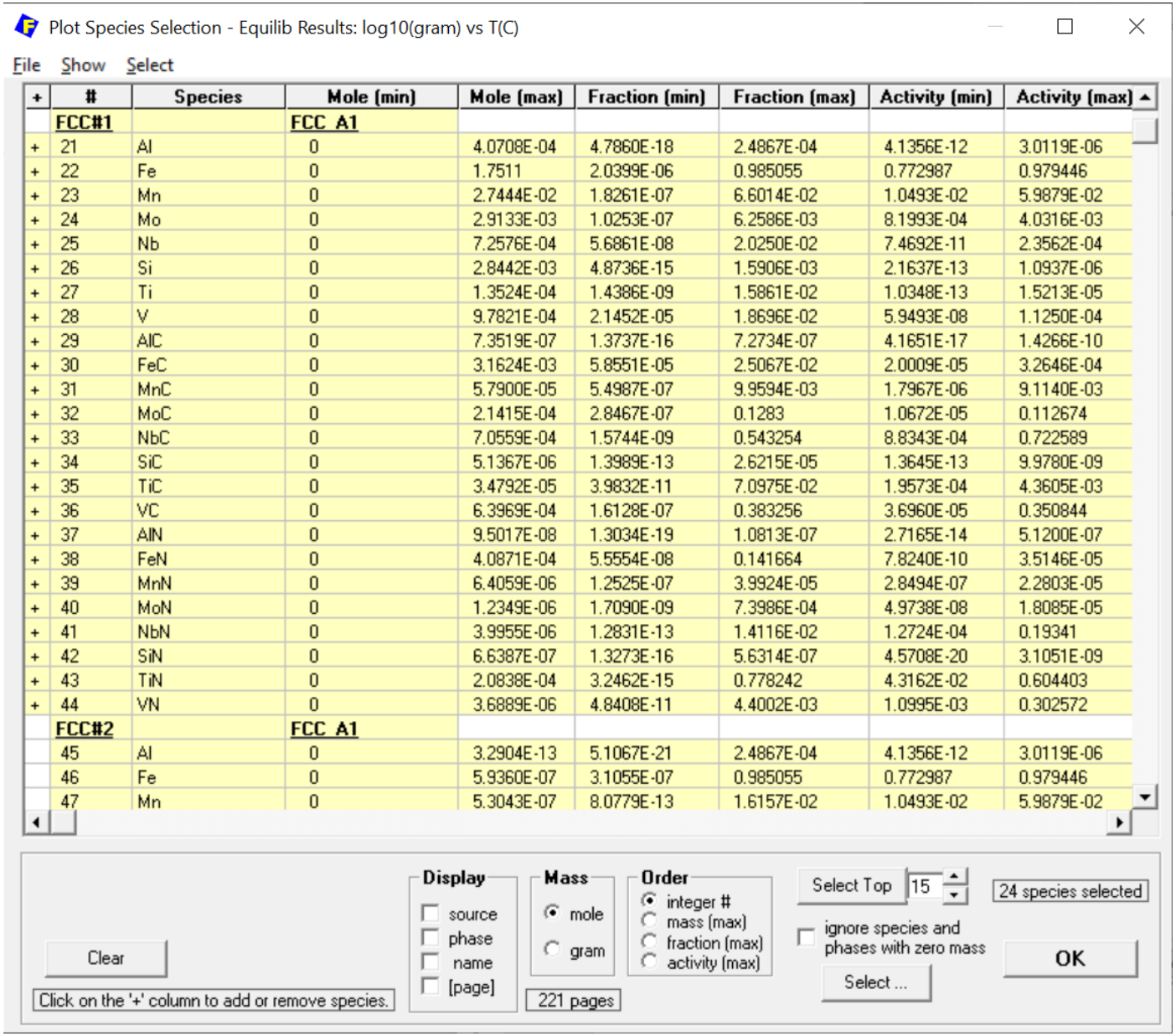


1. Using a log scale is very convenient for looking at the microalloyed elements.

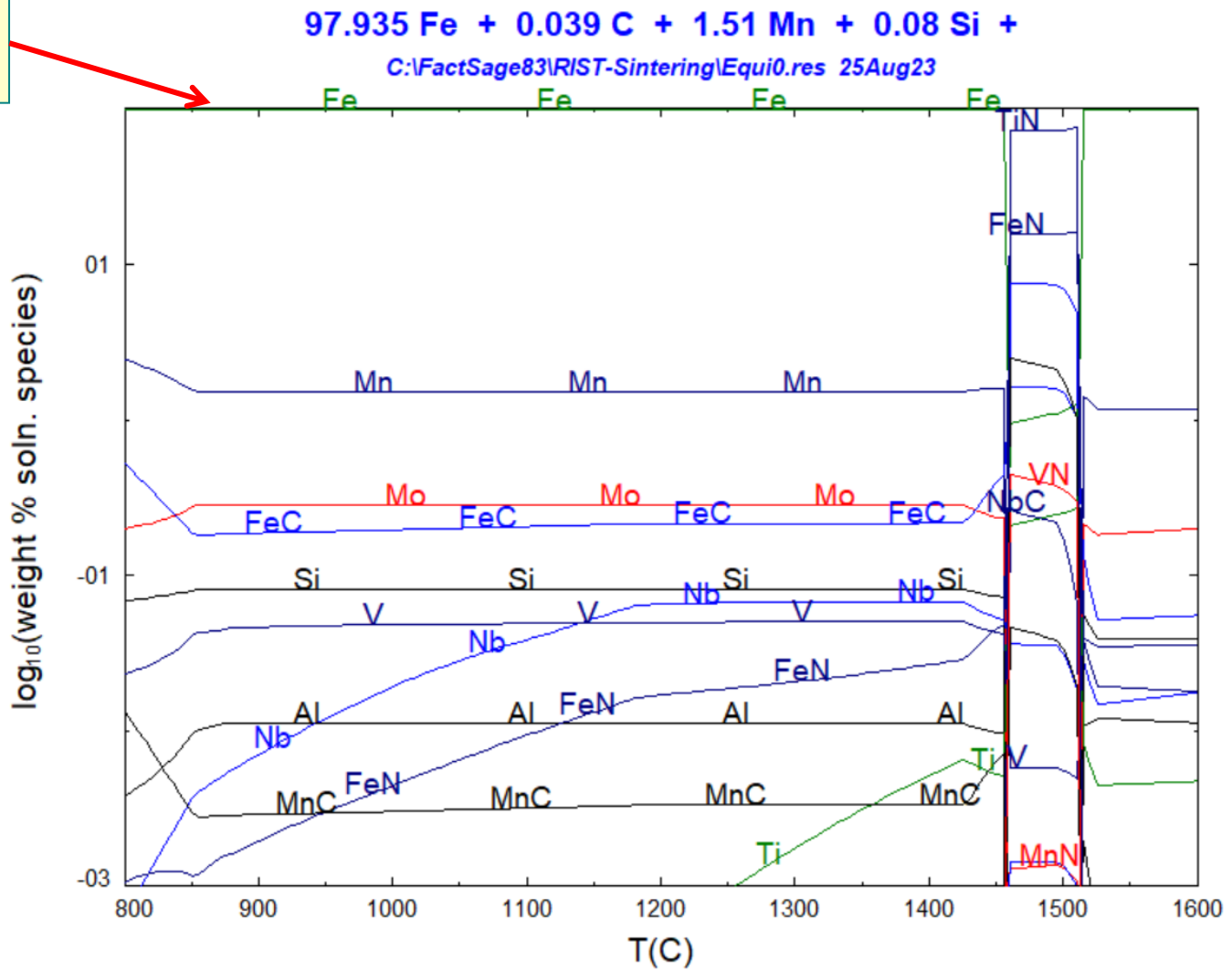
2. It is clearly seen that the FCC#1, #2 and #3 phases are forming. In this case, they are probably carbides and nitrides.
We can check this by plotting their composition with temperature



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

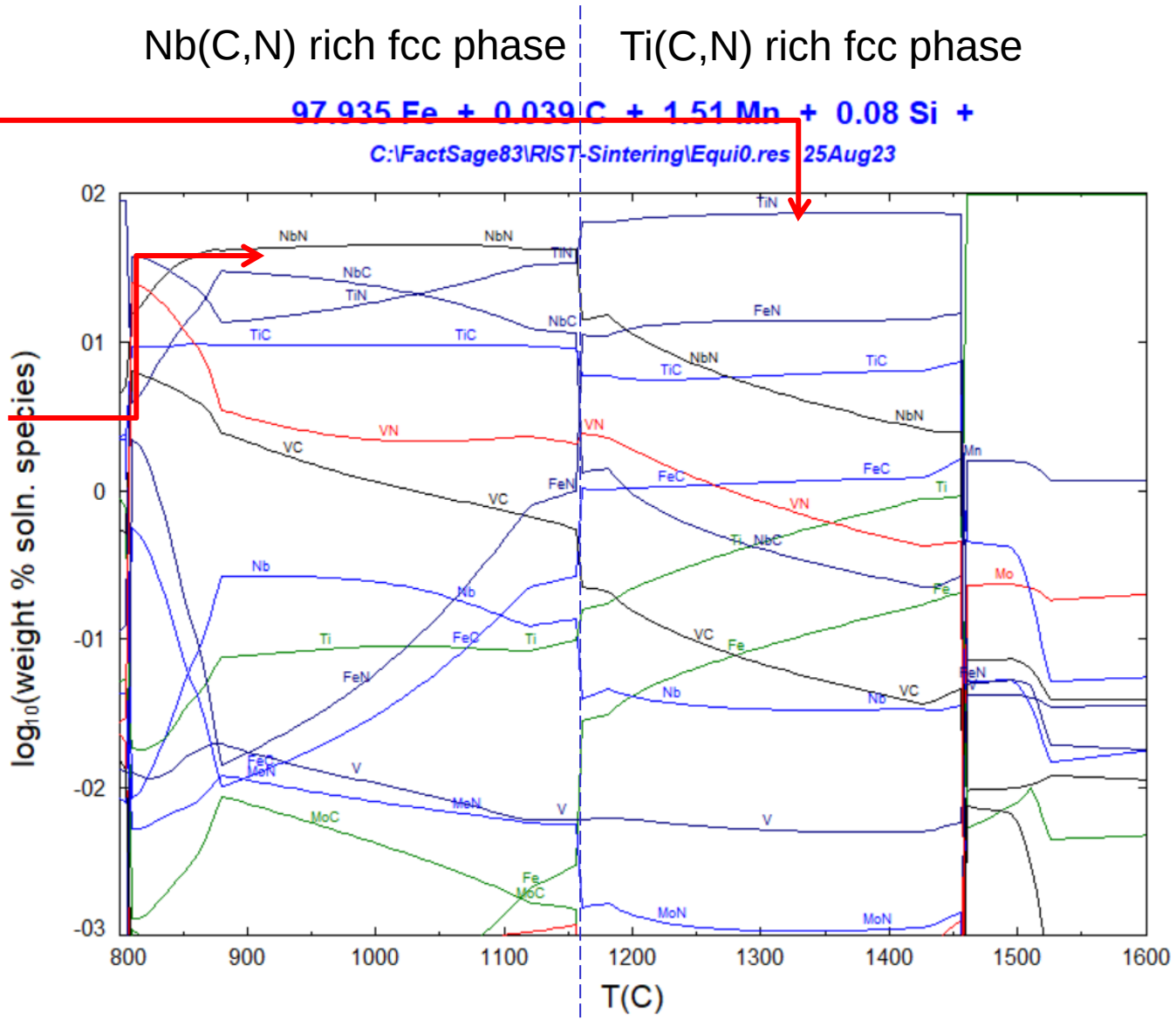


1. In the austenite region, the FCC#1 phase is composed mostly of iron (FeVa)

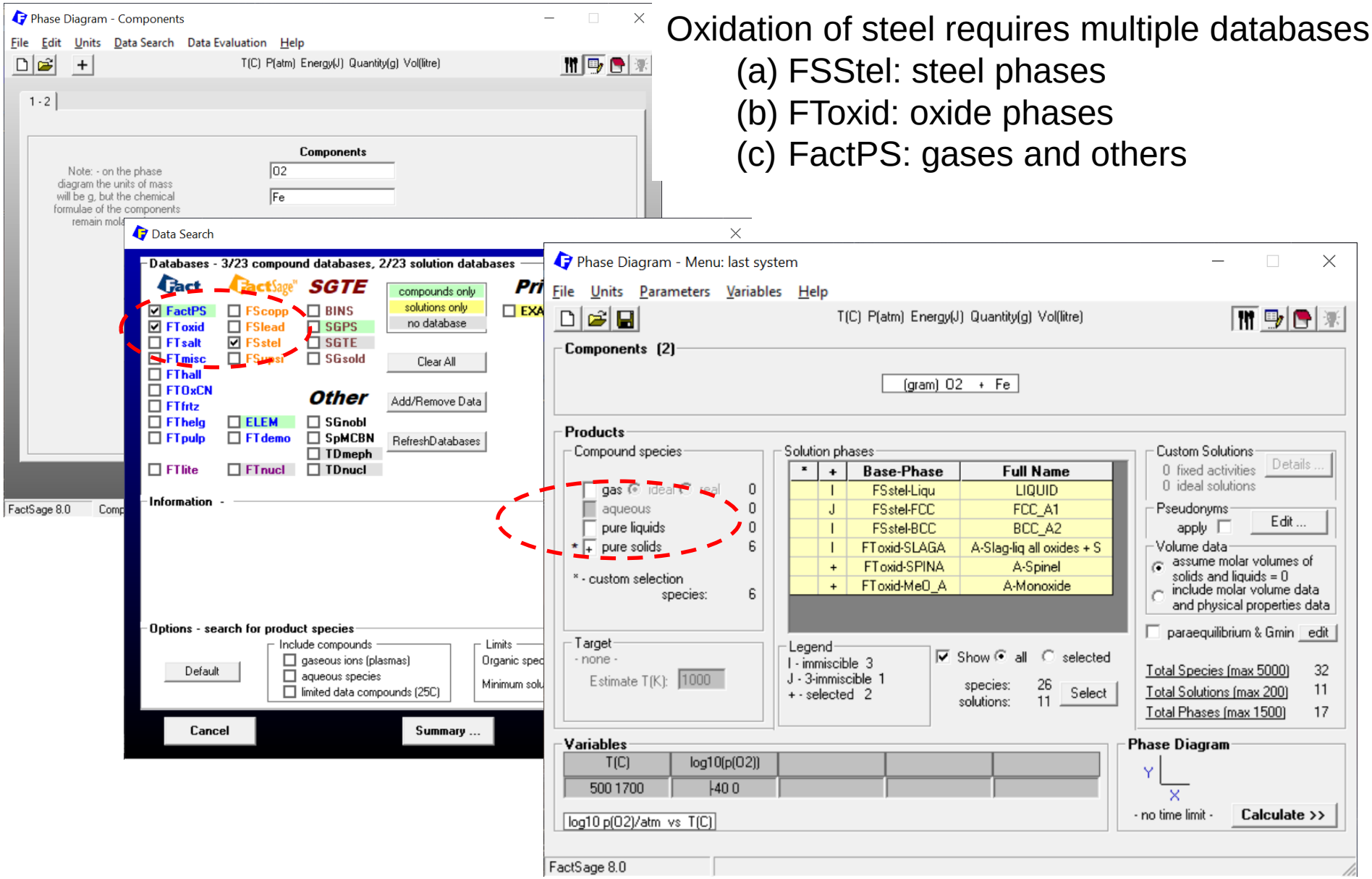


1. The FCC#2 phase is composed mainly of TiN and TiC at austenite temperatures…

2. Mainly composed of NbN and NbC



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

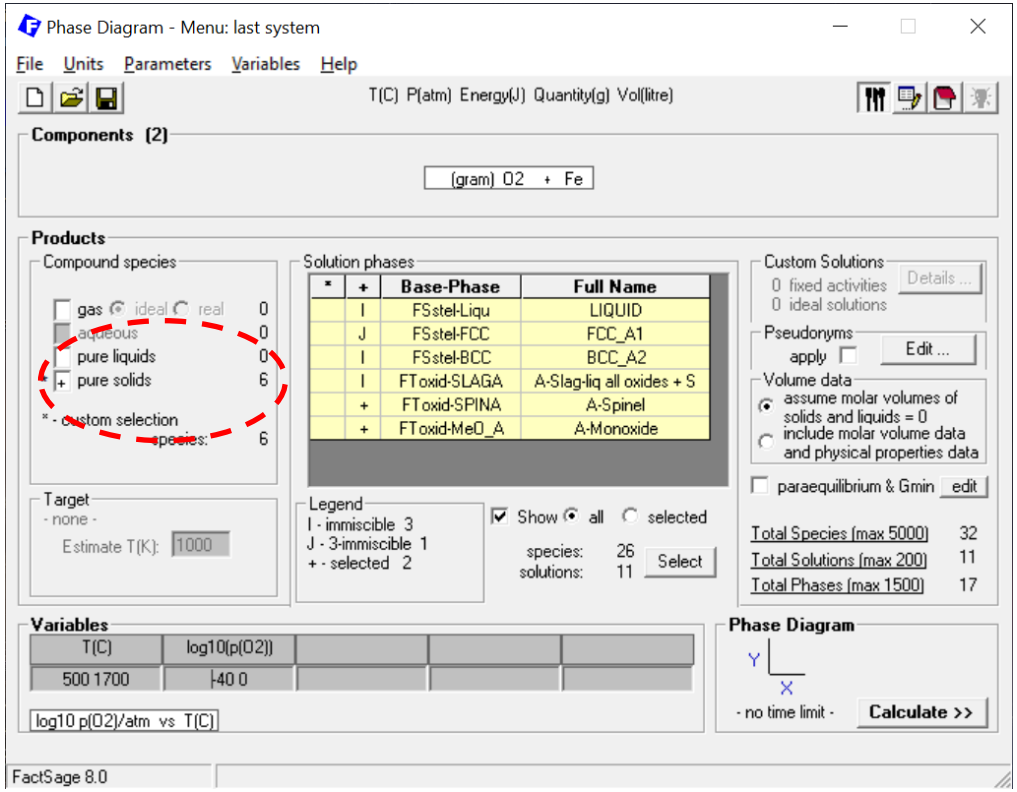


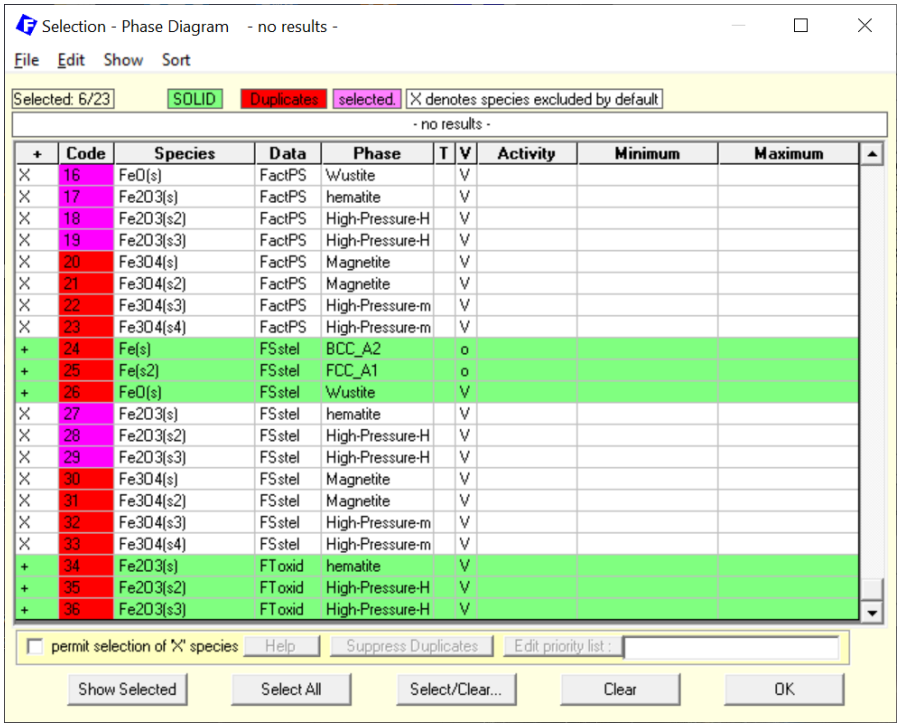
Oxidation of steel requires multiple databases

(a) FSStel: steel phases

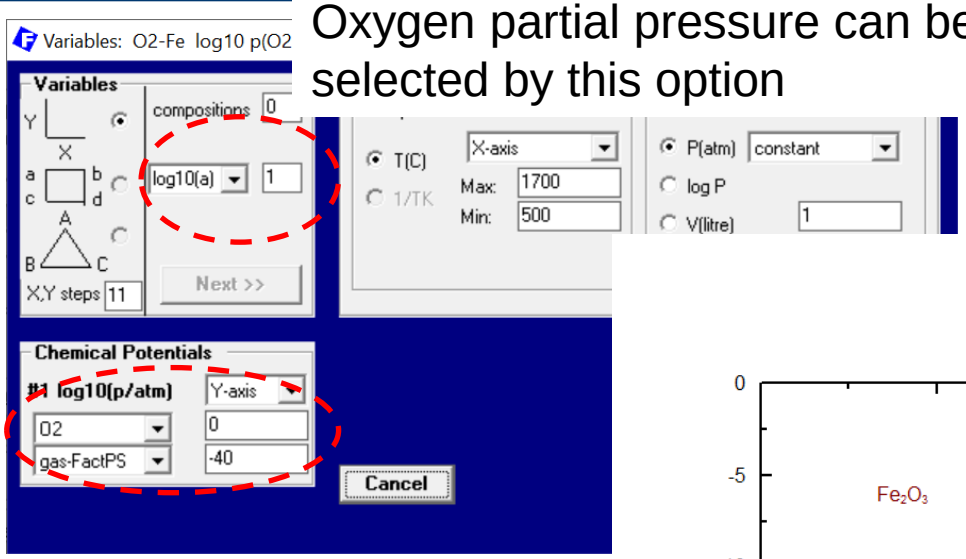
(b) FToxid: oxide phases

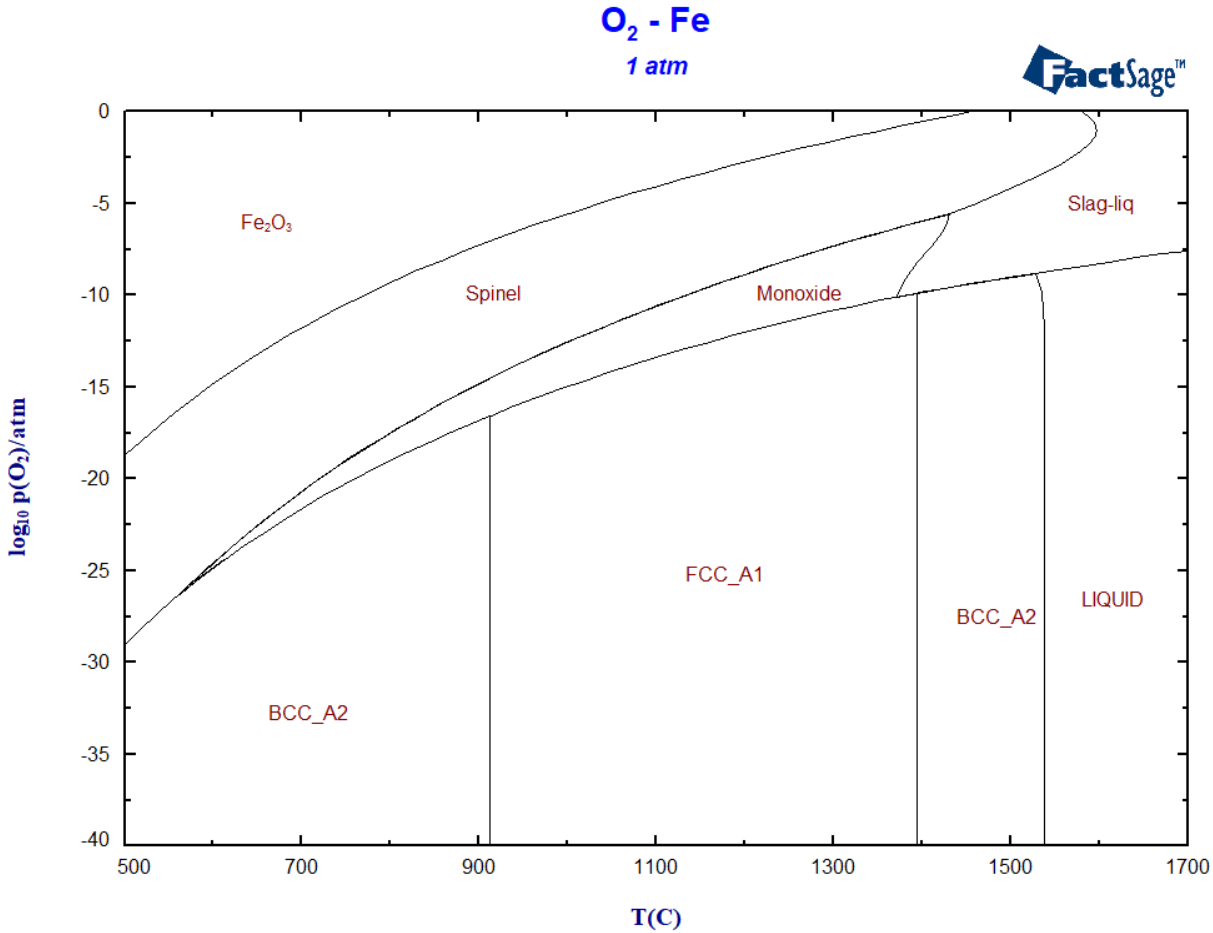
(c) FactPS: gases and others


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 real 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
Details ...
Pseudonyms
apply
Edit ...
Volume data
assume molar volumes of solids and liquids = 0
include molar volume data and physical properties data
paraequilibrium & Gmin edit
Target
- none -
Estimate T(K): 1000
Legend
I - immiscible 3
J - 3-immiscible 1
+ - selected 2
Show all selected
species: 26
solutions: 11
Select
Total Species (max 5000) 32
Total Solutions (max 200) 11
Total Phases (max 1500) 17
Variables
T(C) log10(p(O2))
500 1700 -40 0
log10 p(O2)/atm vs T(C)
Phase Diagram
Y
X
- no time limit -
Calculate >>
FactSage 8.0

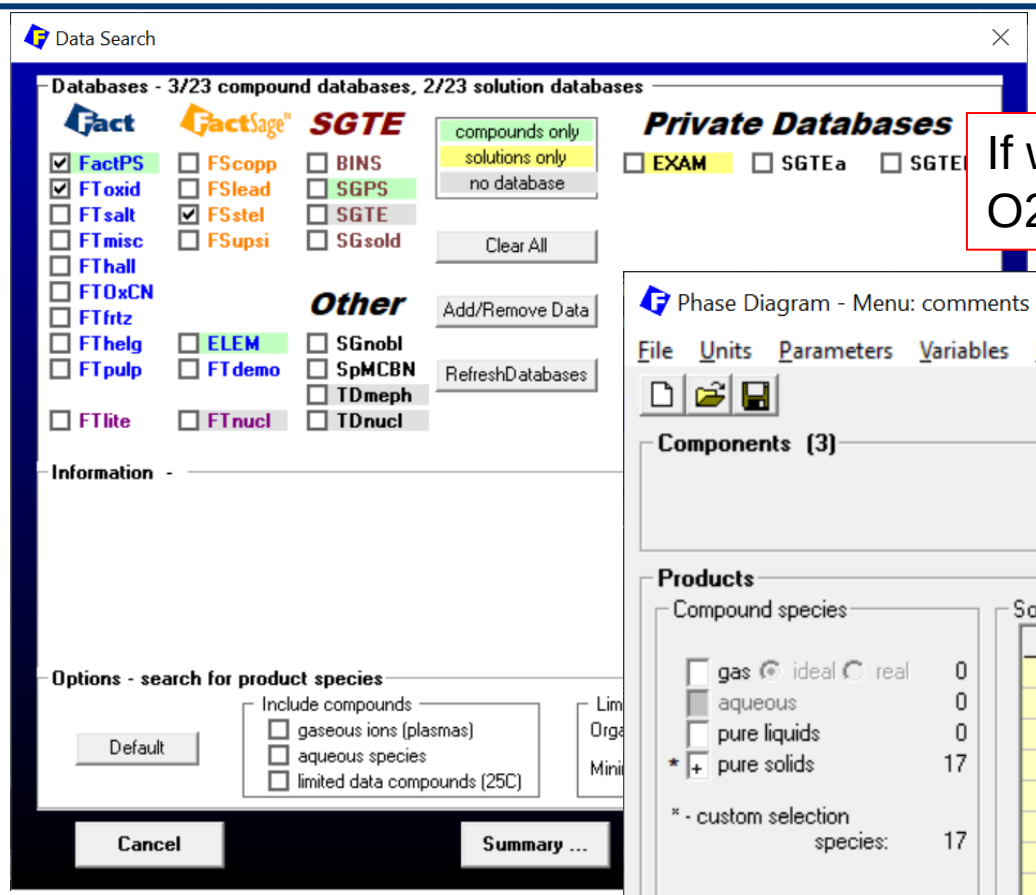

Selection - Phase Diagram - no results -
File Edit Show Sort
Selected: 6/23
SOLID
Duplicates
selected.
X denotes species excluded by default
- no results -
+ Code Species Data Phase T V Activity Minimum Maximum
X 16 FeO(s) FactPS Wustite V
X 17 Fe2O3(s) FactPS hematite V
X 18 Fe2O3(s2) FactPS High-Pressure-H 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 o
+ 25 Fe(s2) FSstel FCC_A1 o
+ 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

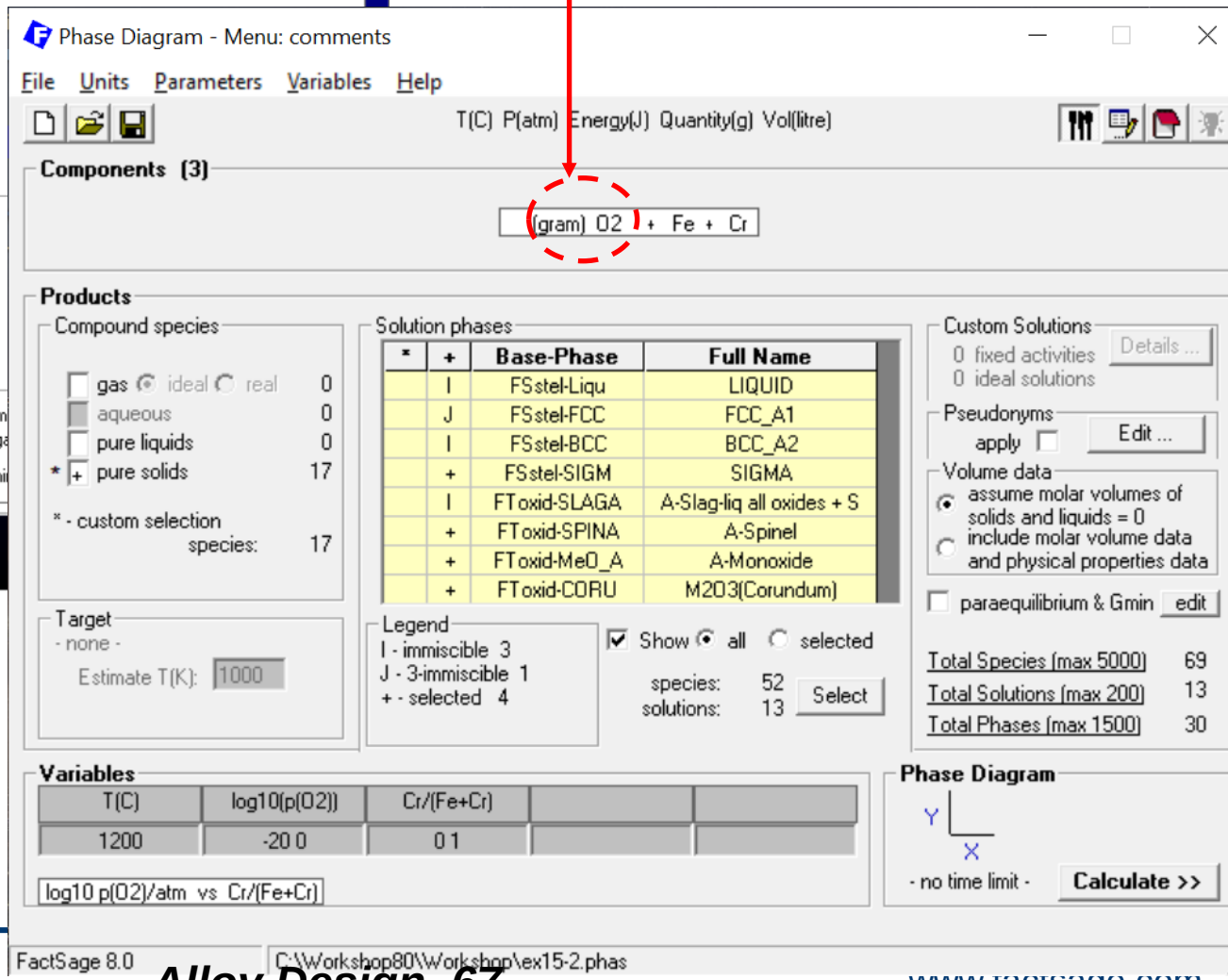


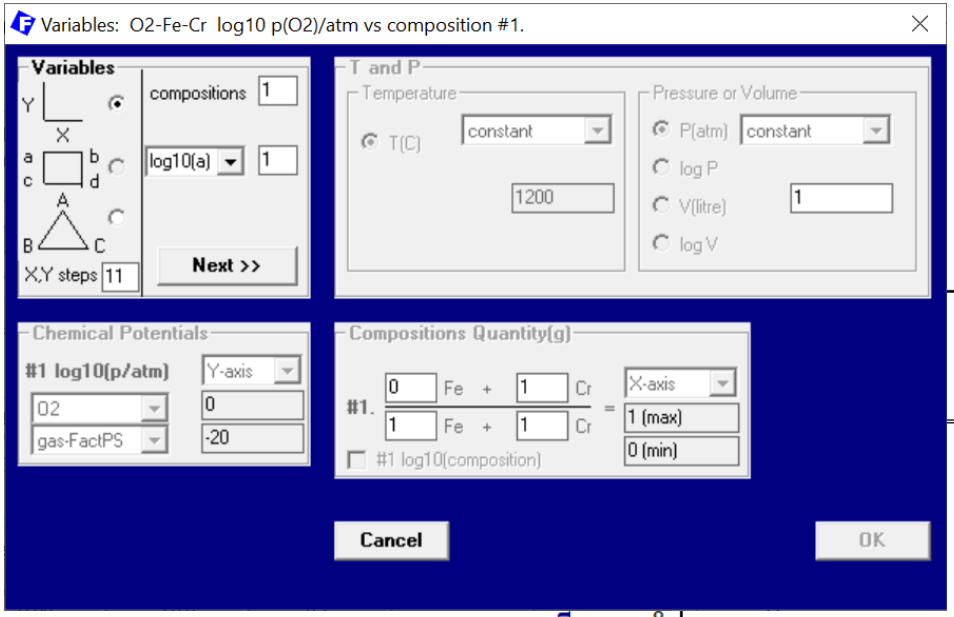


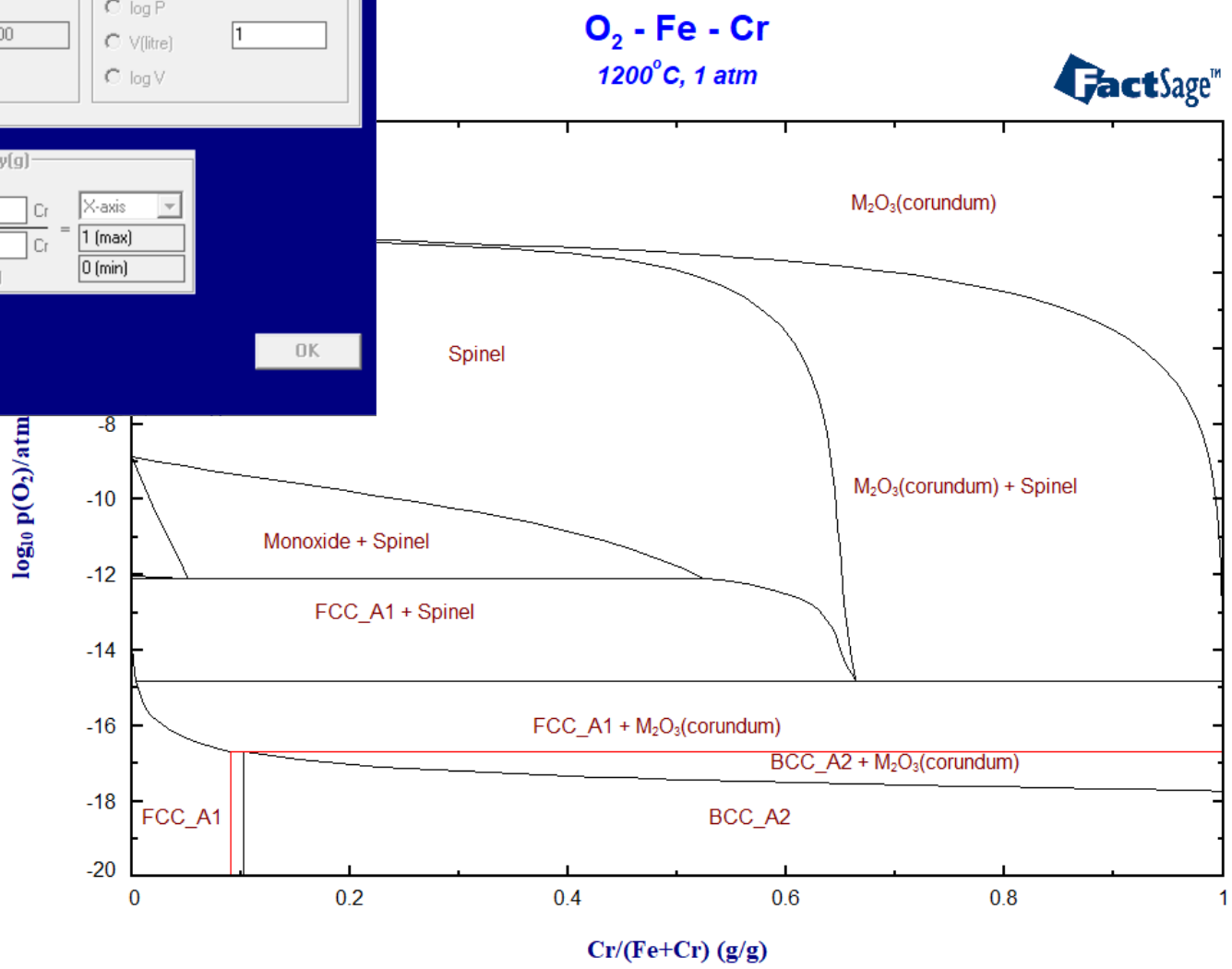
EX15-2. phase diagram PO2 – X: Oxidation of Fe-Cr



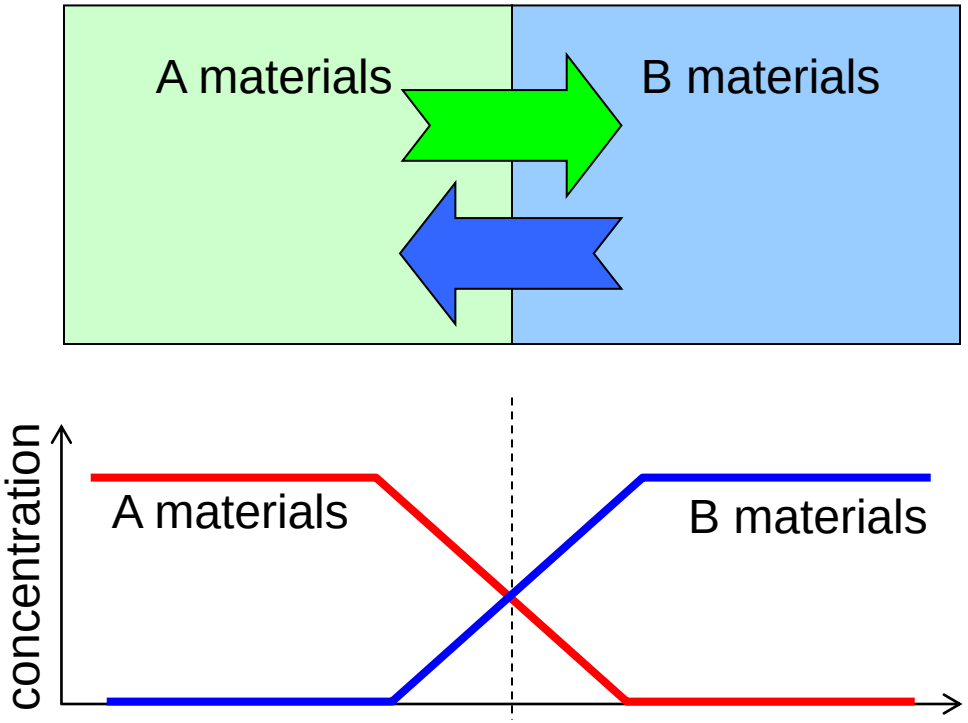
If we want to use oxygen as one of axes, O2 should be added as input component




Variables: O2-Fe-Cr log10 p(O2)/atm vs composition #1.
Variables
compositions 1
log10(a) 1
X,Y steps 11
Next >>
T and P
Temperature
T(C) constant
1200
Pressure or Volume
P(atm) constant
log P
V(litre) 1
log V
Chemical Potentials
#1 log10(p/atm) Y-axis
O2 0
gas-FactPS -20
Compositions Quantity(g)
#1. 0 Fe + 1 Cr / 1 Fe + 1 Cr = X-axis
1 (max)
0 (min)
#1 log10(composition)
Cancel
OK

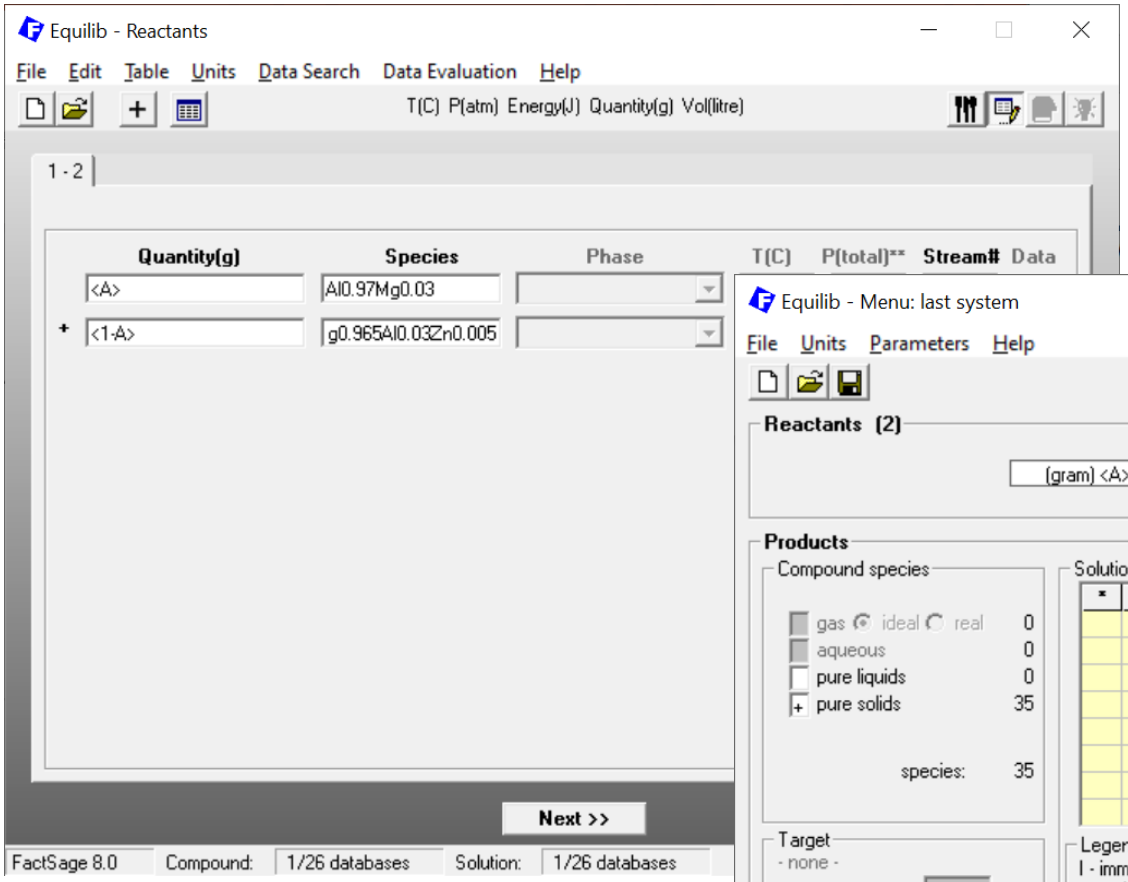

O2 - Fe - Cr
1200°C, 1 atm
FactSage™
M2O3(corundum)
Spinel
M2O3(corundum) + Spinel
Monoxide + Spinel
FCC_A1 + Spinel
FCC_A1 + M2O3(corundum)
BCC_A2 + M2O3(corundum)
FCC_A1
BCC_A2
log10 p(O2)/atm
-8
-10
-12
-14
-16
-18
-20
0
0.2
0.4
0.6
0.8
1
Cr/(Fe+Cr) (g/g)

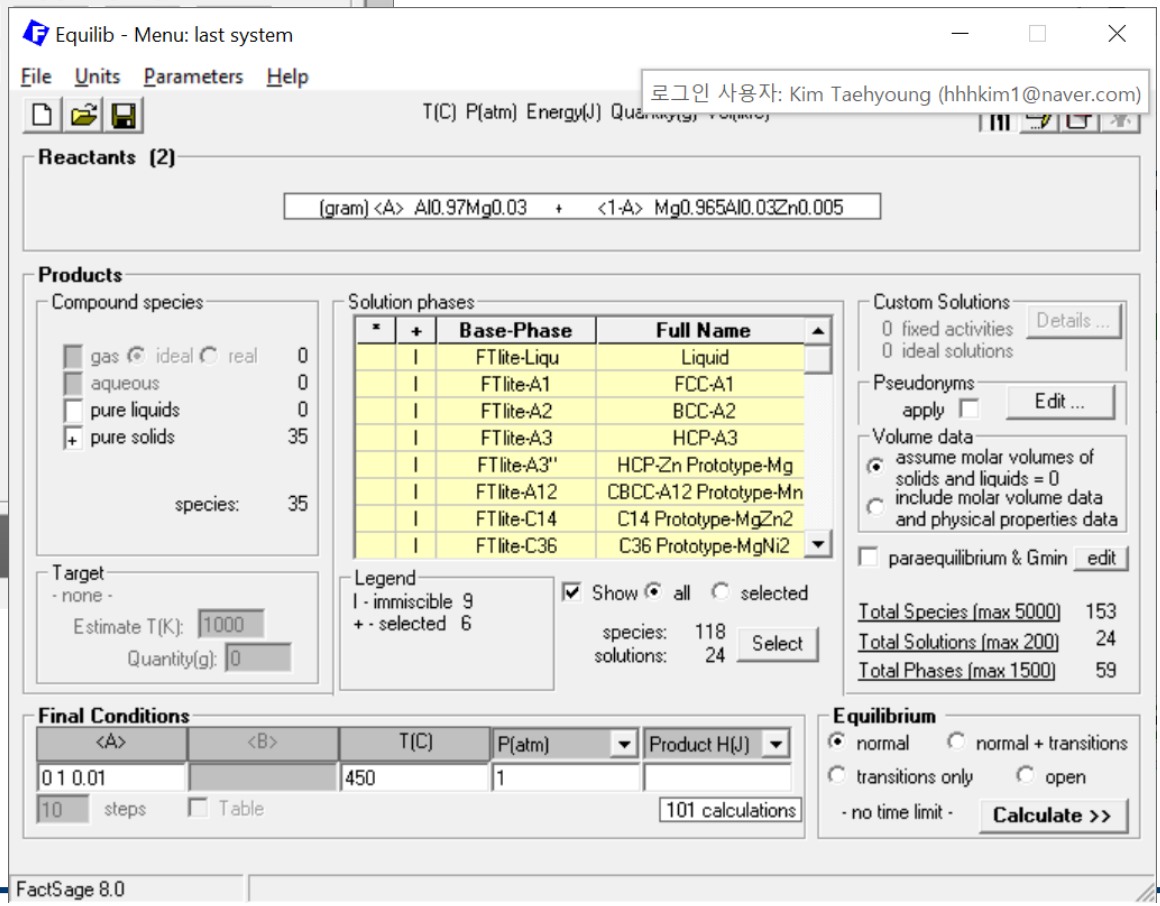
EX16. <A> option: Simple counter-cross inter-diffusion calc.



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 - Results A=0 (page 1/101)

Output Edit Show Pages Final Conditions

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

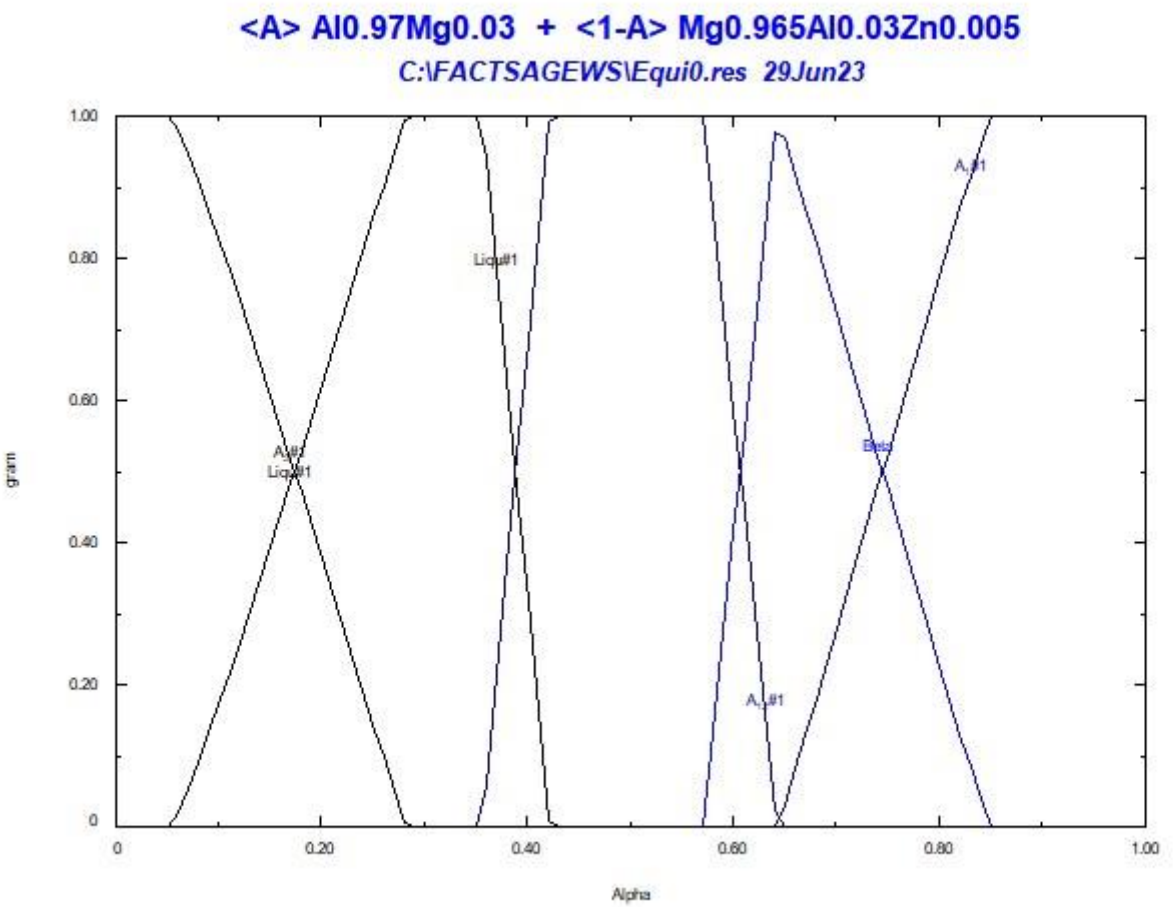
A=0.13 | A=0.14 | A=0.15 | A=0.16 | A=0.17 | A=0.18 | A=0.19 | A=0.2 | A=0.21 | A=0.22 | A=0.23 | A=0.24

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

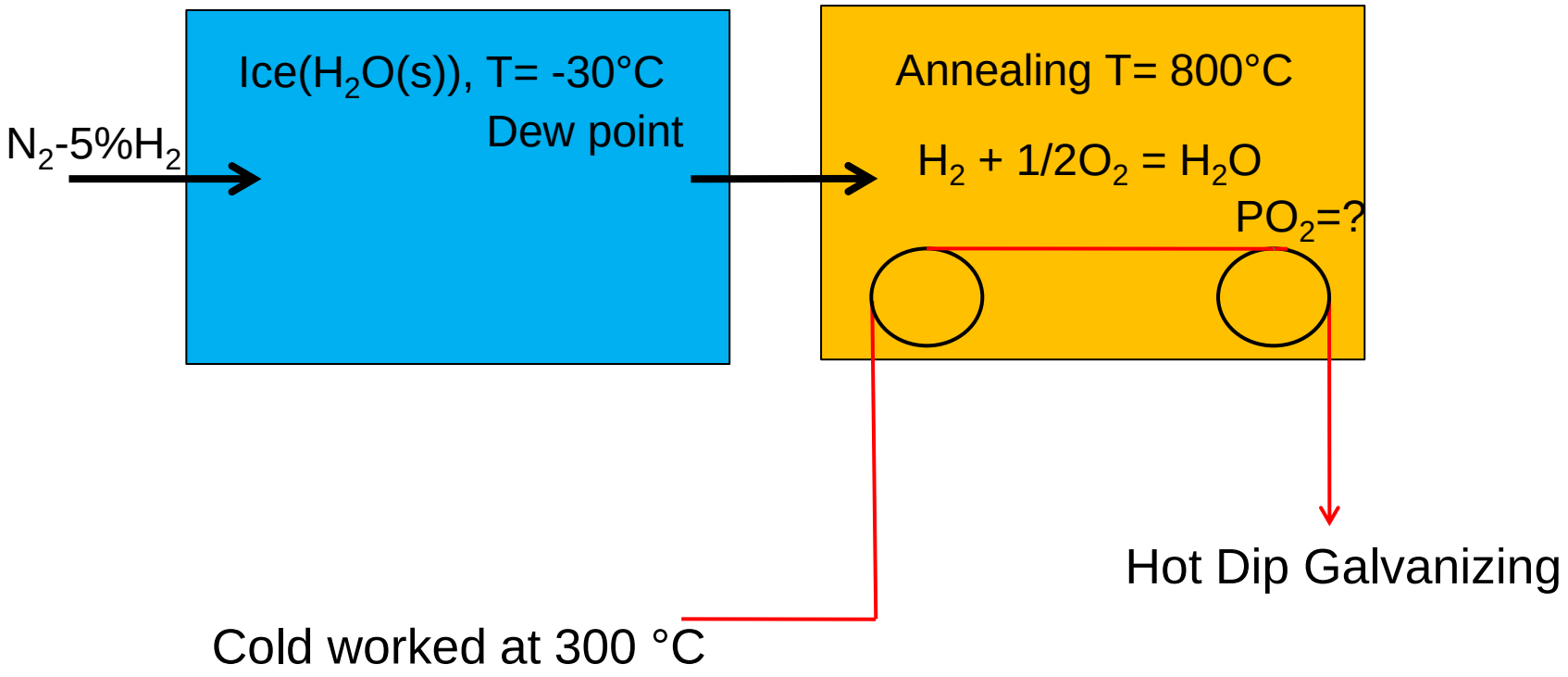
```
                                                                FactSage 8.3
(gram) <A> Al0.97Mg0.03  +  <1-A> Mg0.965Al0.03Zn0.005  =

   1.0000     gram  HCP-A3#1
   (1.0000 gram, 2.0333E-02 mol)
           (450 C, 1 atm,      a=1.0000)
           ( 3.2917     wt.% Al2Va
           + 95.379     wt.% Mg2Va
           + 1.3294     wt.% Zn2Va)

           System component         Amount/mol    Amount/gram   Mole fraction  Mass fractio
           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-A3#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
           + 73.985     wt.% Mg
           + 15.929     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

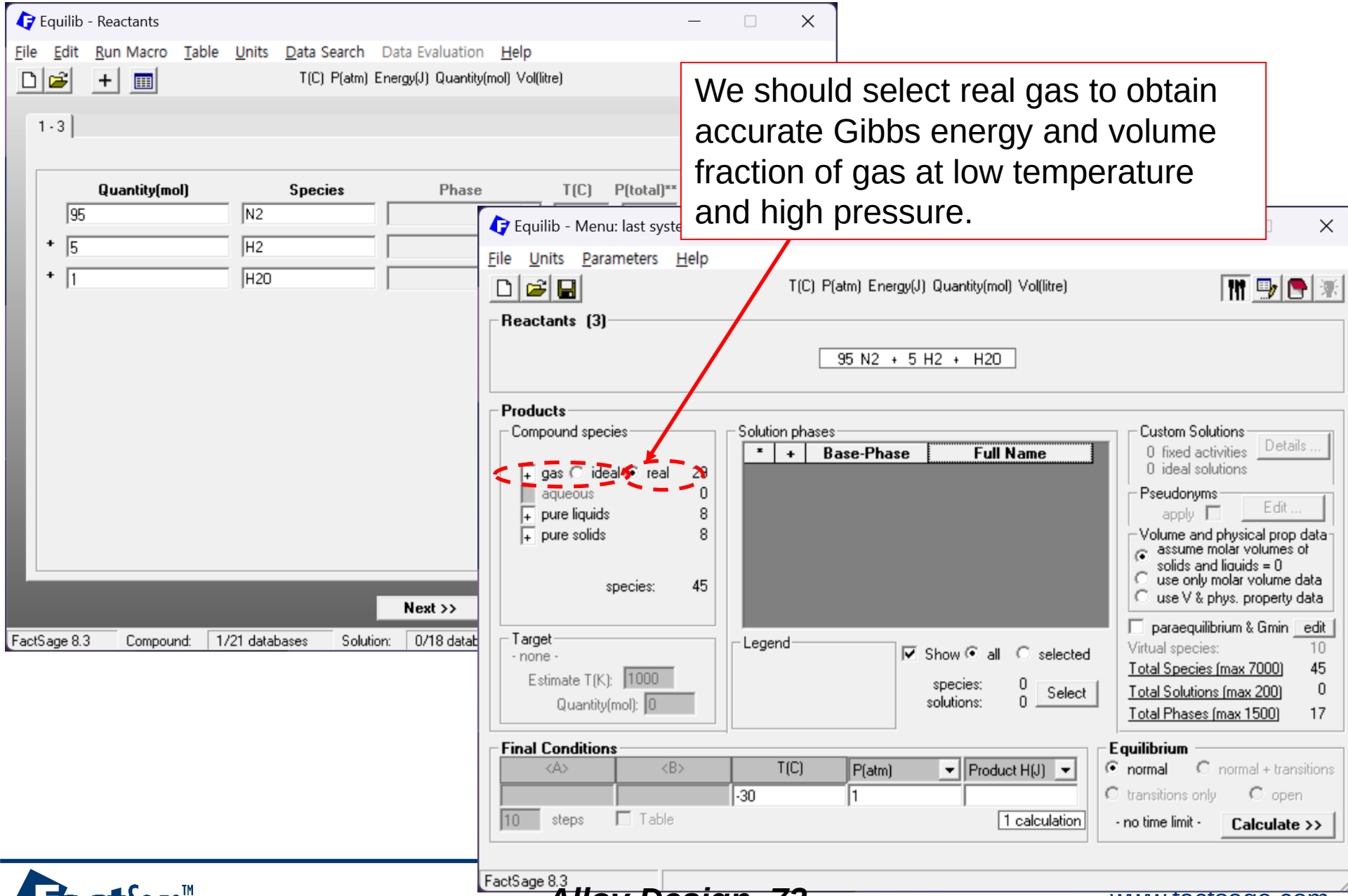
<A>	<B>	T(C)	P(atm)
0 1 0.01		450	1

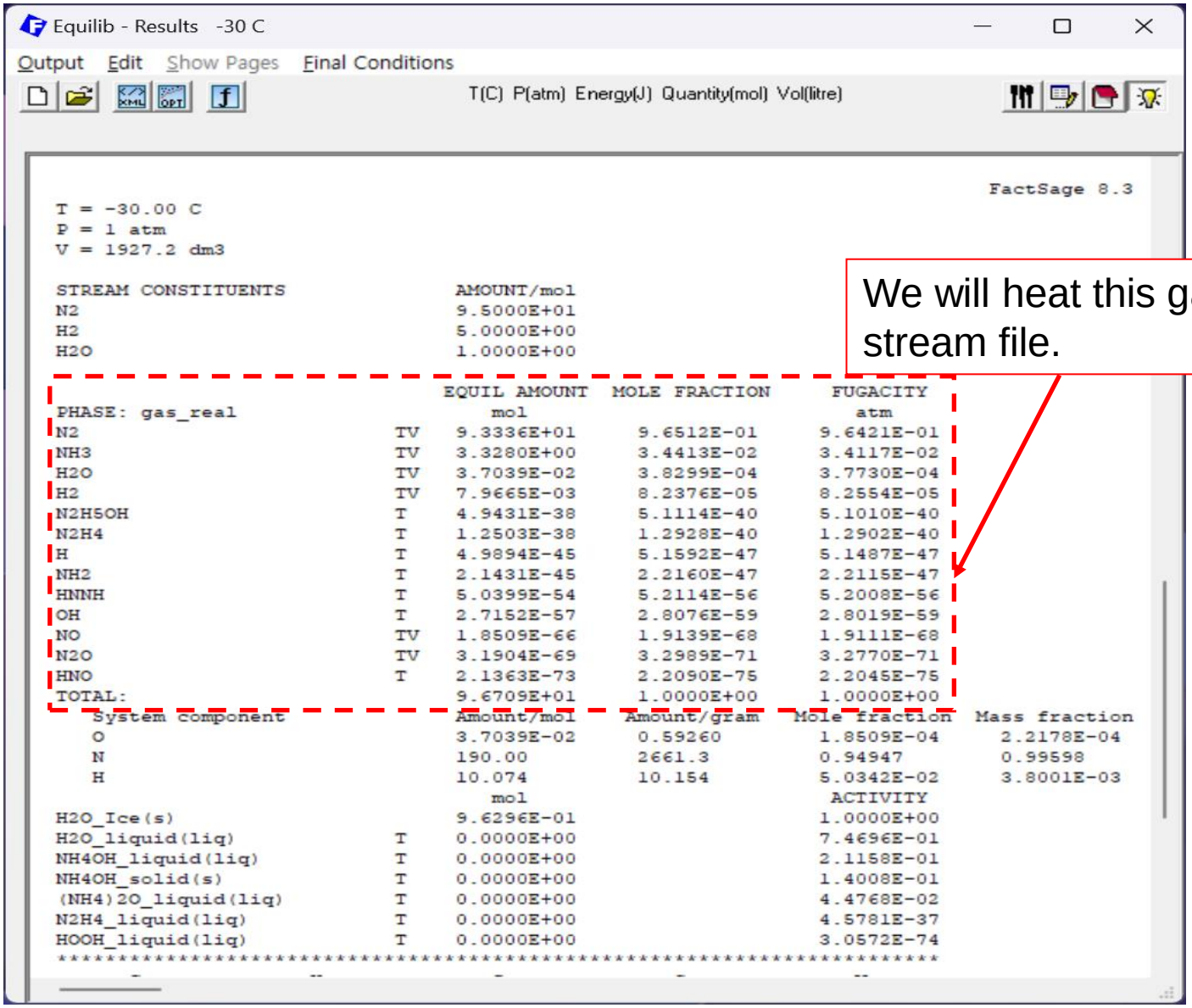


EX17. Oxygen partial pressure control for oxidation of metals



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





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

Creating stream file

Equilib - Results -30 C

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 ...

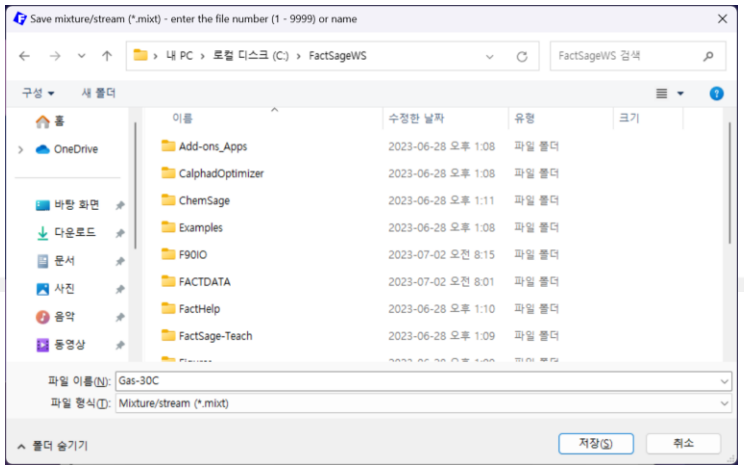
Recycle all streams ...
Save stream file
Stream file properties ...
Summary of streams
Directory (C:₩FACTSAGEWS₩) ...

Save gas phase ...
Save pure liquids ...
Save aqueous ...
Save pure solids ...
Save solutions

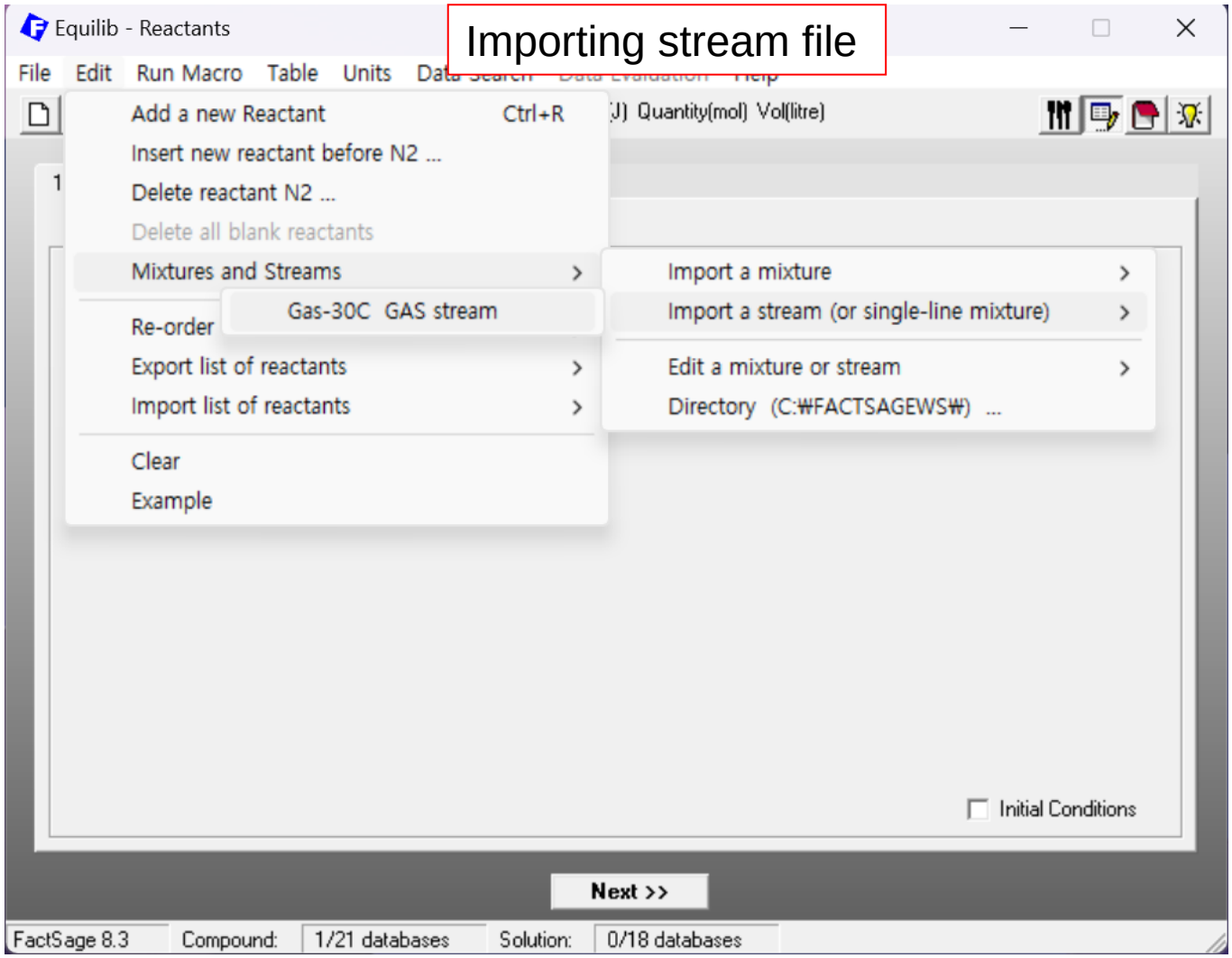
) Quantity(mol) Vol(litre)

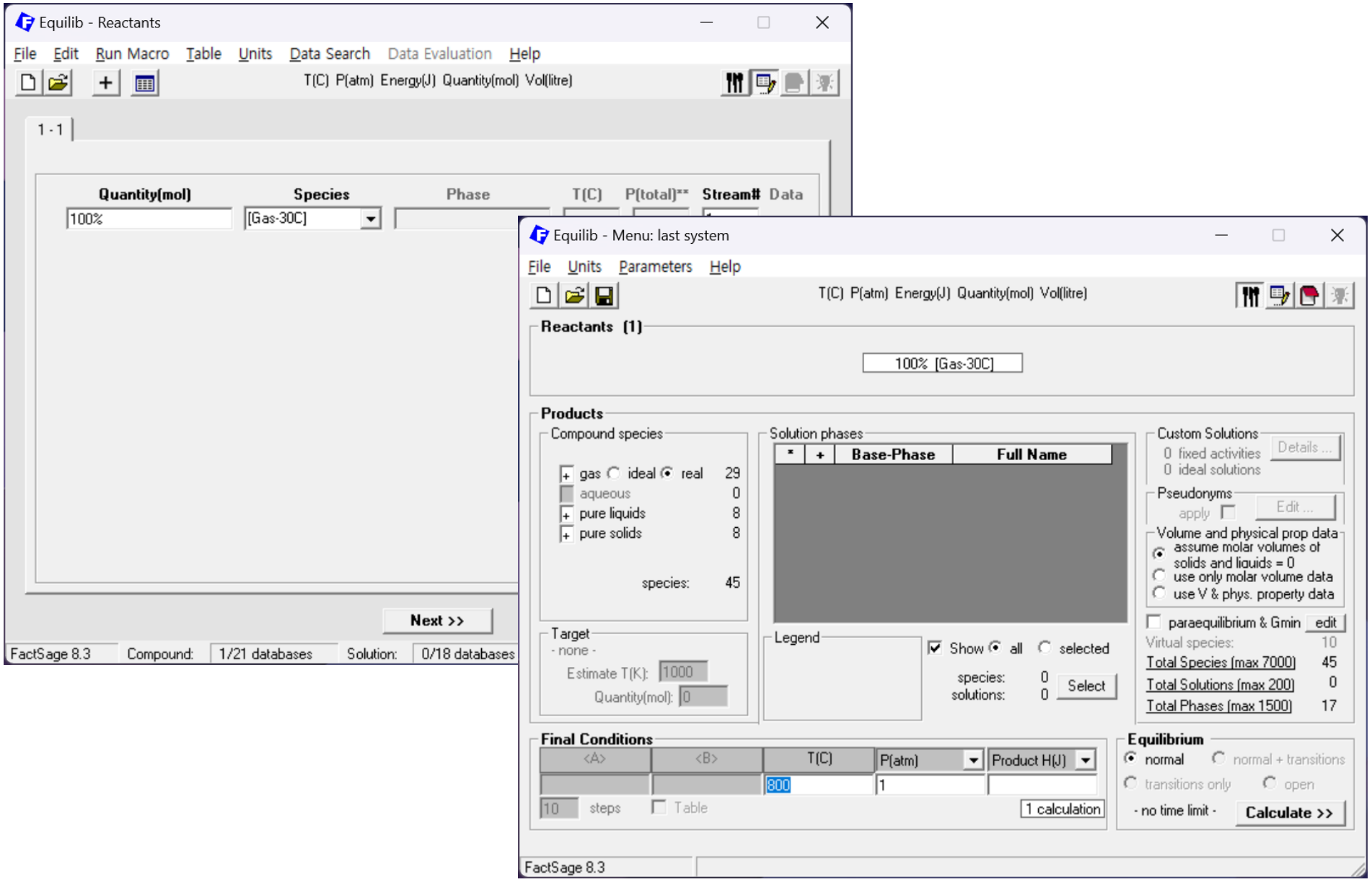
FactSage 8.3

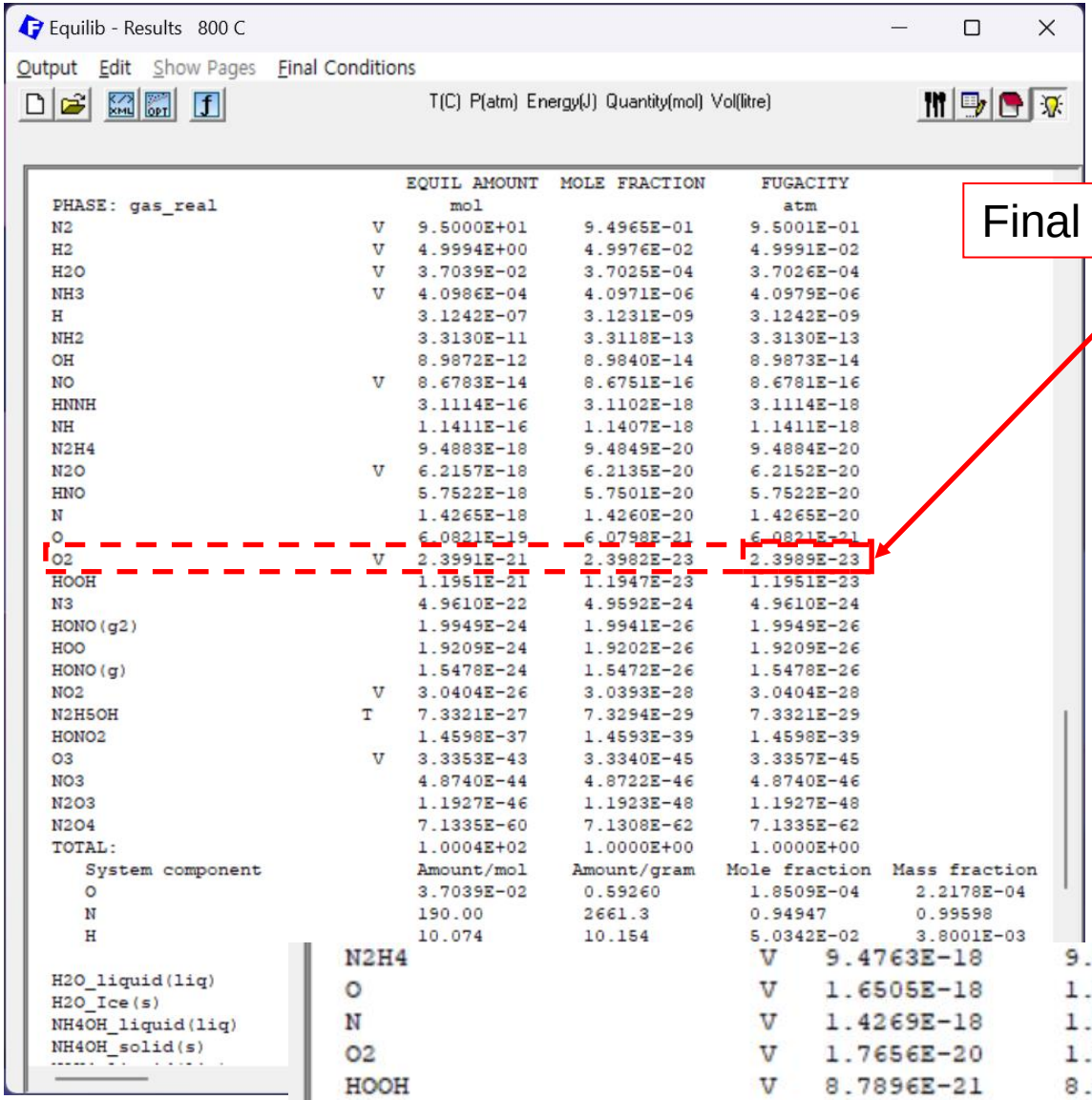
```
N2H4                                  T
H                                     T
NH2                                   T
HNNH                                  T
OH                                    T
+ 1.9139E-68    NO                   VT
+ 3.2989E-71    N2O                  VT
+ 2.2090E-75    HNO                   T)

+ 0.96296    mol   H2O_Ice
  (17.348 gram, 0.96296 mol)
         (-30.00 C, 1 atm, S1, a=1.0000)

+ 0          mol   H2O_liquid                    T
         (-30.00 C, 1 atm, L1, a=0.74696)

+ 0          mol   NH4OH_liquid                  T
         (-30.00 C, 1 atm, L1, a=0.21158)

+ 0          mol   NH4OH_solid                   T
         (-30.00 C, 1 atm, S1, a=0.14008)

+ 0          mol   (NH4)2O_liquid                T
         (-30.00 C, 1 atm, L1, a=4.4768E-02)

+ 0          mol   N2H4_liquid                   T
         (-30.00 C, 1 atm, L1, a=4.5781E-37)

+ 0          mol   HOOH_liquid                   T
         (-30.00 C, 1 atm, L1, a=3.0572E-74)

Cut-off limit for gaseous fractions/phase activities = 1.00E-75

Data on 19 product species identified with "T" have been extrapolated outside their valid temperature ranges

6 product species identified with "V" are modeled with an equation of state

*****************************************************************
      H             G             V             S            Cp
     (J)           (J)        (litre)         (J/K)        (J/K)
*****************************************************************
-6.02989E+05  -5.00390E+06   1.92722E+03   1.80996E+04   3.10032E+03

                                    H             G             S            Cp
                                   (J)           (J)         (J/K)        (J/K)
gas_real                    -3.19099E+05  -4.71132E+06  1.80638E+04  3.06542E+03
H2O_Ice                     -2.83890E+05  -2.92586E+05  3.57622E+01  3.49035E+01

Total mass/gram = 2689.4
Total mass/gram excluding gas_real = 17.348

Databases: FactPS 8.3
Data Search options: exclude gas ions; organic CxHy.. X(max) = 2; min soln cpts = 2
```



Importing stream file




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]
Next >>
FactSage 8.3 Compound: 1/21 databases Solution: 0/18 databases
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
Solution phases
* + Base-Phase Full Name
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
Virtual species: 10
Total Species (max 7000) 45
Total Solutions (max 200) 0
Total Phases (max 1500) 17
Target
- none -
Estimate T(K): 1000
Quantity(mol): 0
Legend
Show all selected
species: 0
solutions: 0
Select
Final Conditions
<A> <B> T(C) P(atm) Product H(J)
800 1
10 steps Table
1 calculation
Equilibrium
normal normal + transitions
transitions only open
- no time limit -
Calculate >>
FactSage 8.3

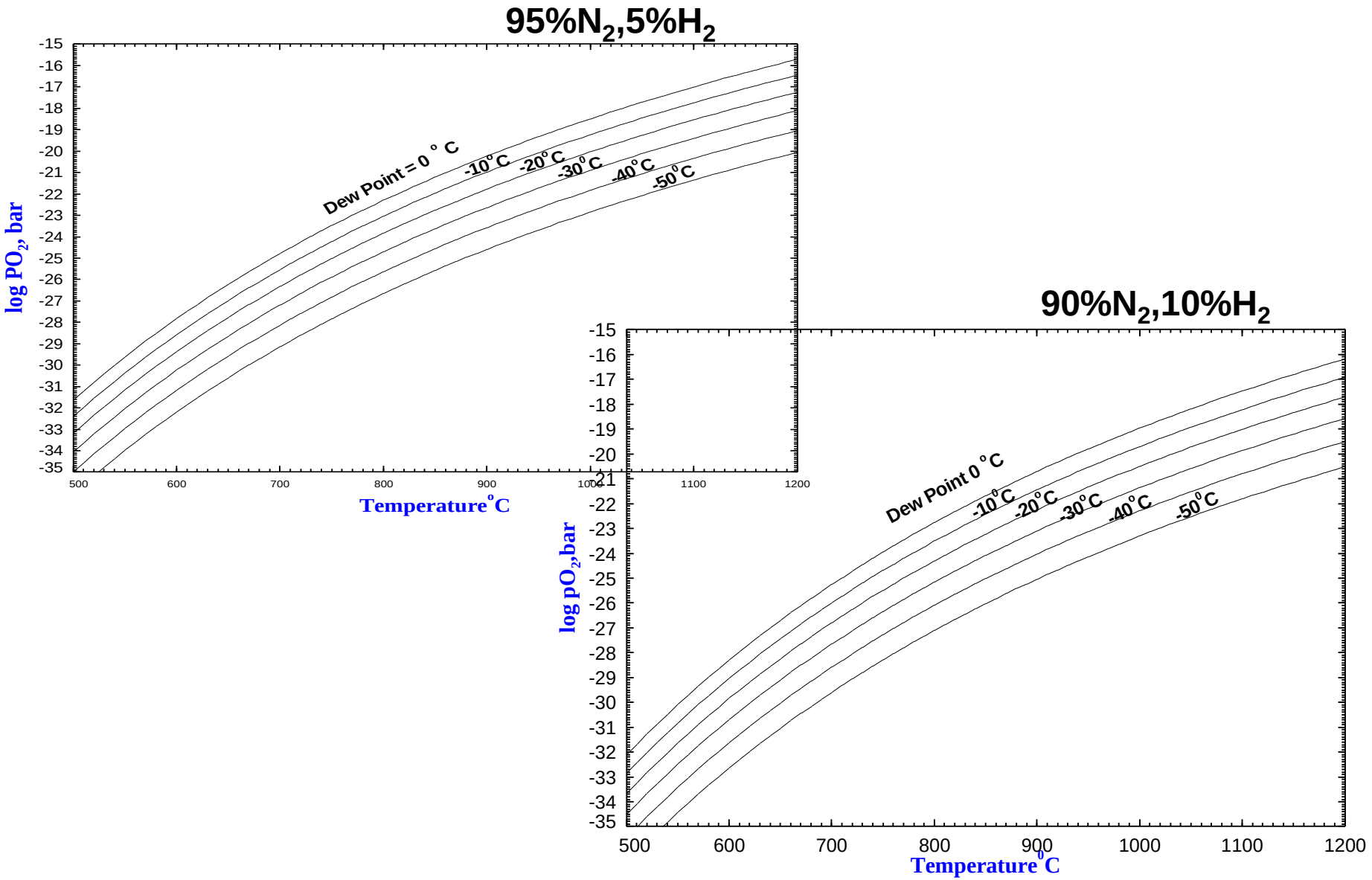


Final partial pressure of oxygen

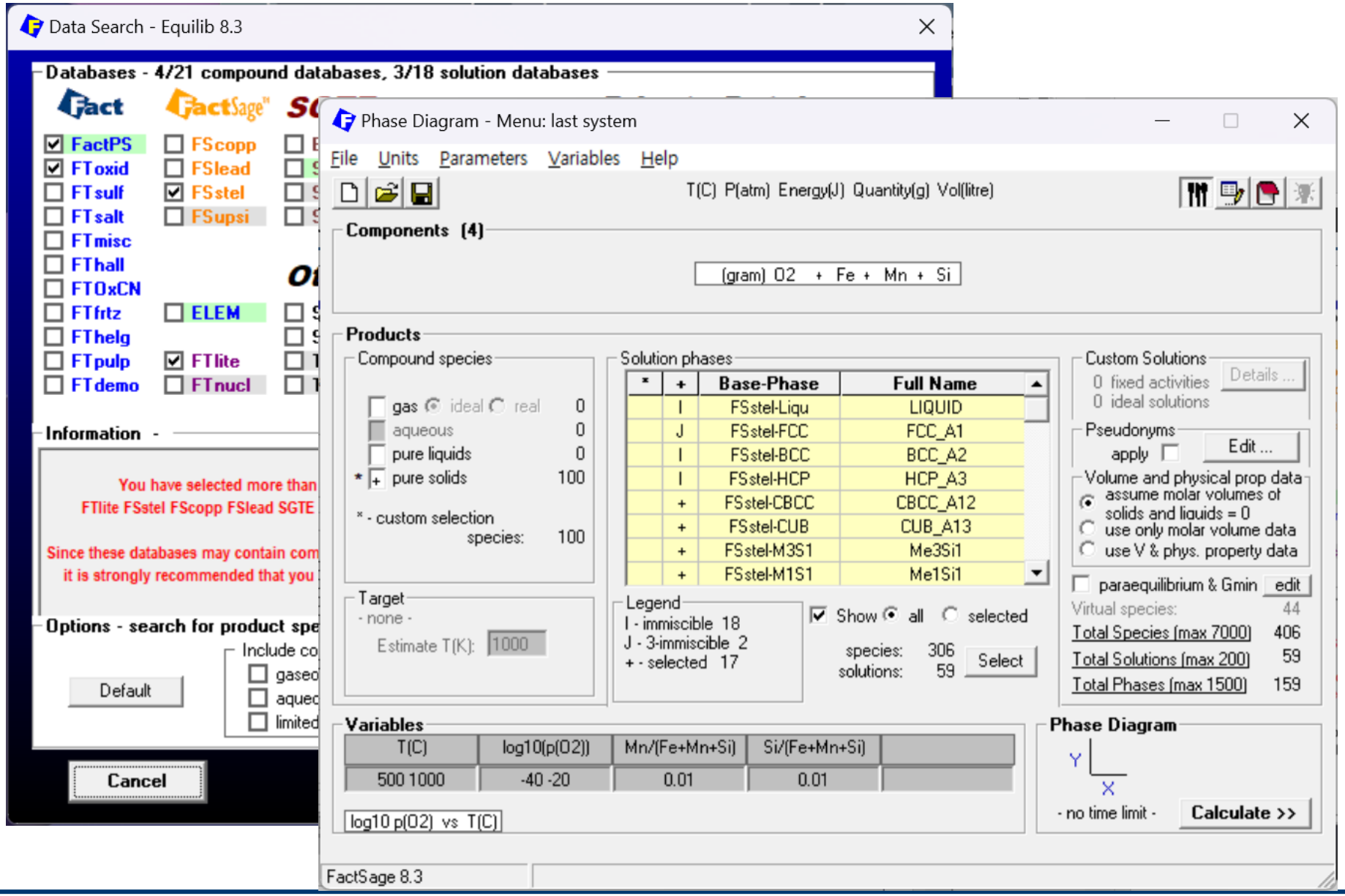
when the temperature of ice is -20°C

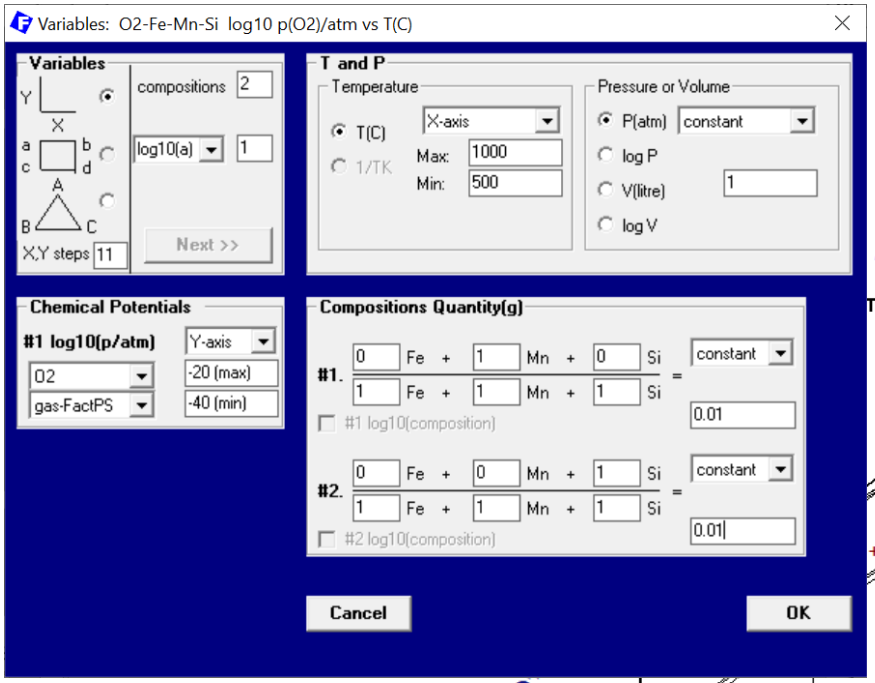
N2H4	V	9.4763E-18	9.4669E-20	9.4703E-20
O	V	1.6505E-18	1.6488E-20	1.6494E-20
N	V	1.4269E-18	1.4255E-20	1.4260E-20
O2	V	1.7656E-20	1.7638E-22	1.7643E-22
HOOH	V	8.7896E-21	8.7808E-23	8.7840E-23
N3	V	4.9595E-22	4.9545E-24	4.9563E-24
HONO(g2)	V	1.4672E-23	1.4657E-25	1.4662E-25

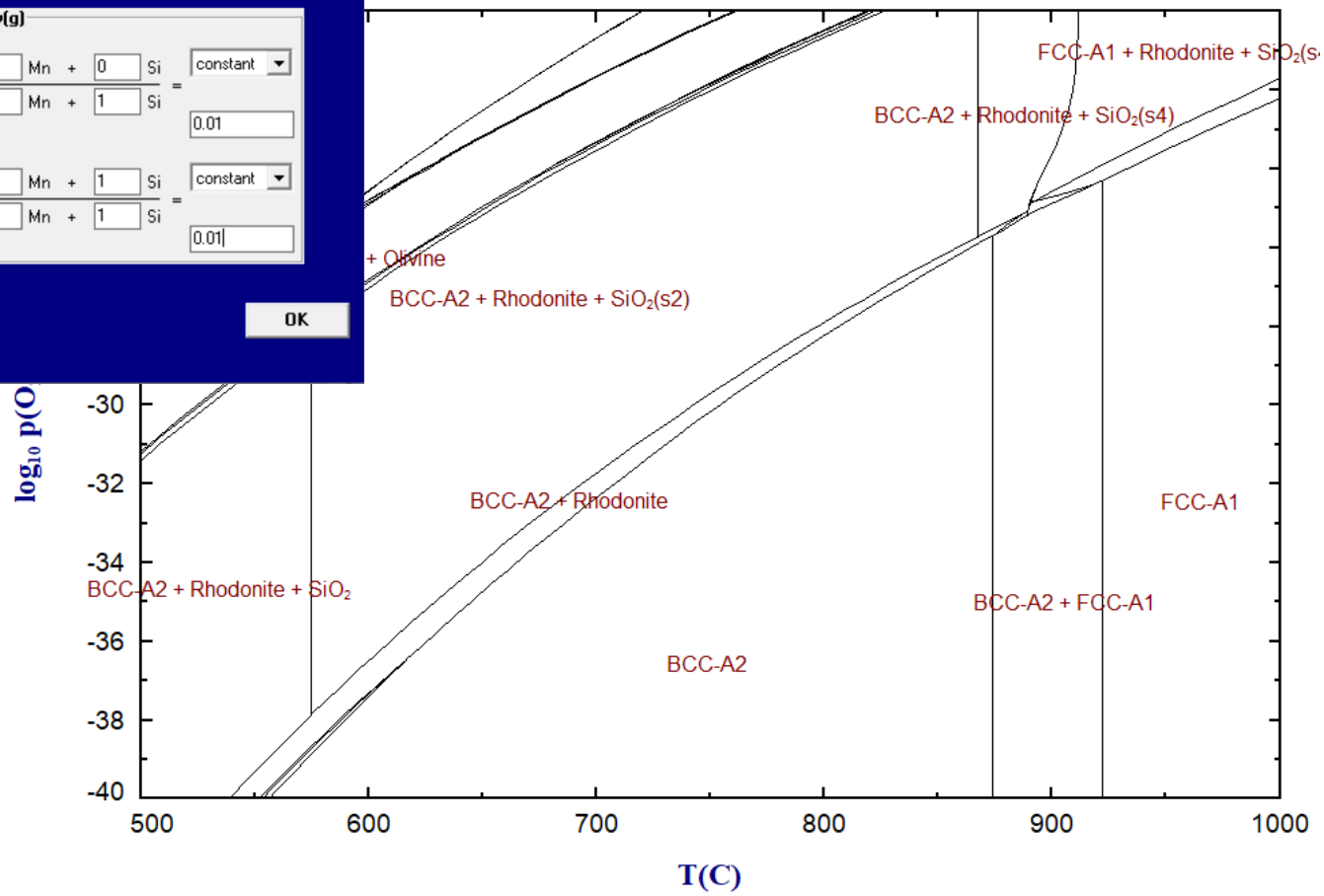
Dew points – PO_2/T Relationship



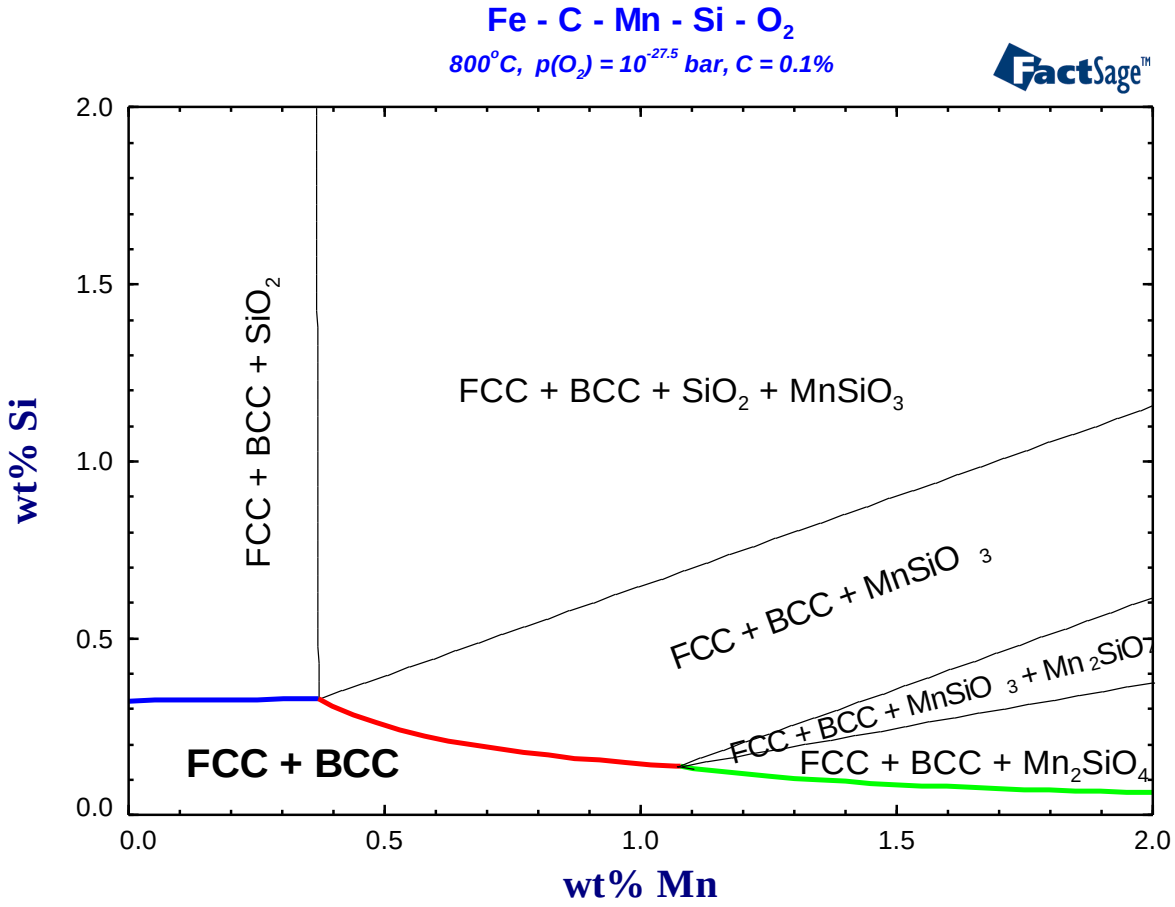
EX17-2. phase diagram PO_2 – T: Oxidation of Fe-1%Mn-1%Si




Variables: O2-Fe-Mn-Si log10 p(O2)/atm vs T(C)
Variables
compositions 2
log10(a) 1
X,Y steps 11
Next >>
T and P
Temperature
T(C)
1/TK
X-axis
Max: 1000
Min: 500
Pressure or Volume
P(atm) constant
log P
V(litre) 1
log V
Chemical Potentials
#1 log10(p/atm) Y-axis
O2
gas-FactPS
-20 (max)
-40 (min)
Compositions Quantity(g)
#1. 0 Fe + 1 Mn + 0 Si = constant
1 Fe + 1 Mn + 1 Si = 0.01
#1 log10(composition)
#2. 0 Fe + 0 Mn + 1 Si = constant
1 Fe + 1 Mn + 1 Si = 0.01
#2 log10(composition)
Cancel
OK


O2 - Fe - Mn - Si
Mn/Z (g/g) = 0.01, Si/Z (g/g) = 0.01, Z=(Fe+Mn+Si), 1 atm
FactSage™
FCC-A1 + Rhodonite + SiO2(s
BCC-A2 + Rhodonite + SiO2(s4)
+ Olivine
BCC-A2 + Rhodonite + SiO2(s2)
BCC-A2 + Rhodonite
FCC-A1
BCC-A2 + Rhodonite + SiO2
BCC-A2 + FCC-A1
BCC-A2
log10 p(O
-30
-32
-34
-36
-38
-40
500
600
700
800
900
1000
T(C)

EX17-3. Primary oxide formation diagram

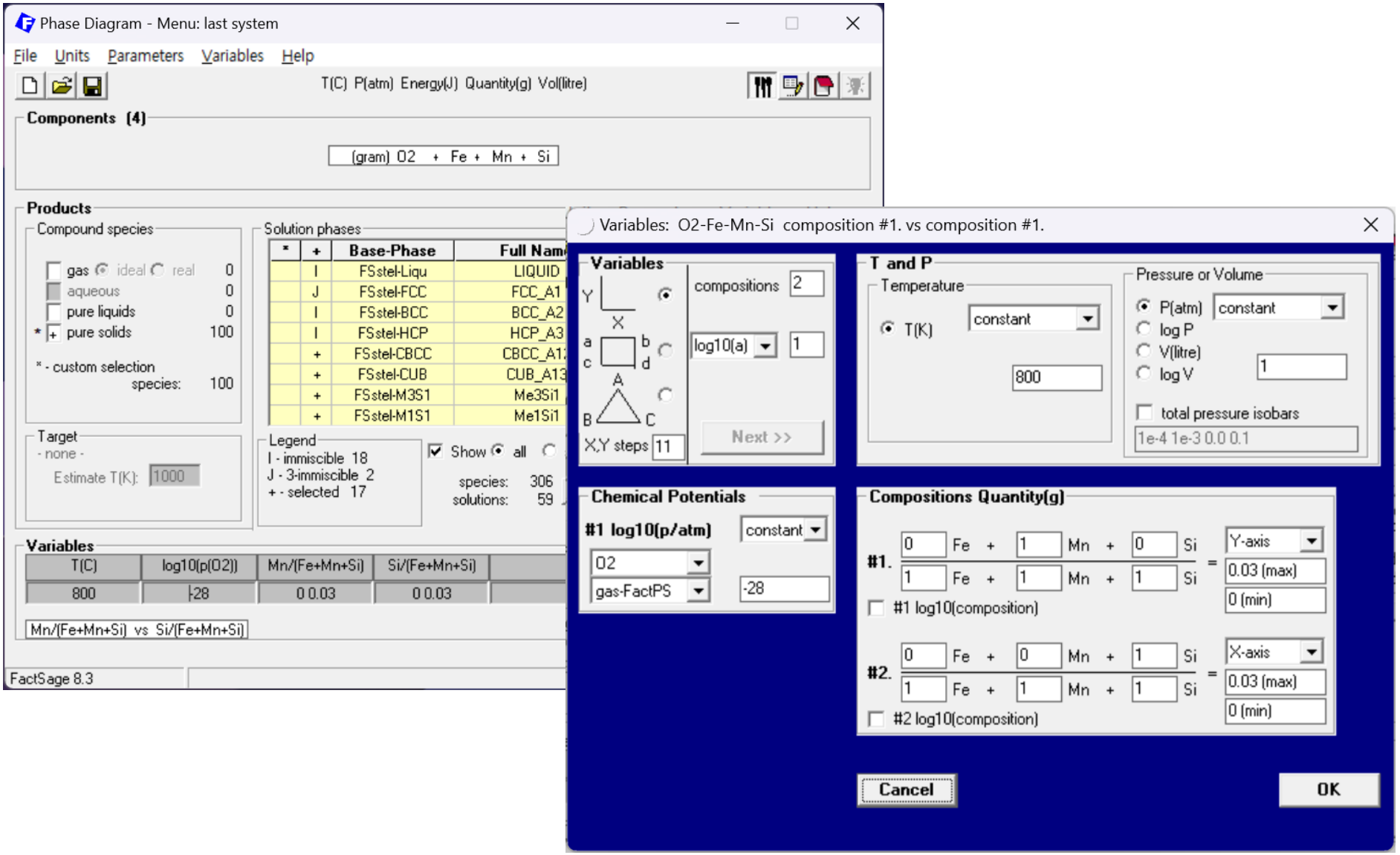


Drawing of the diagram:

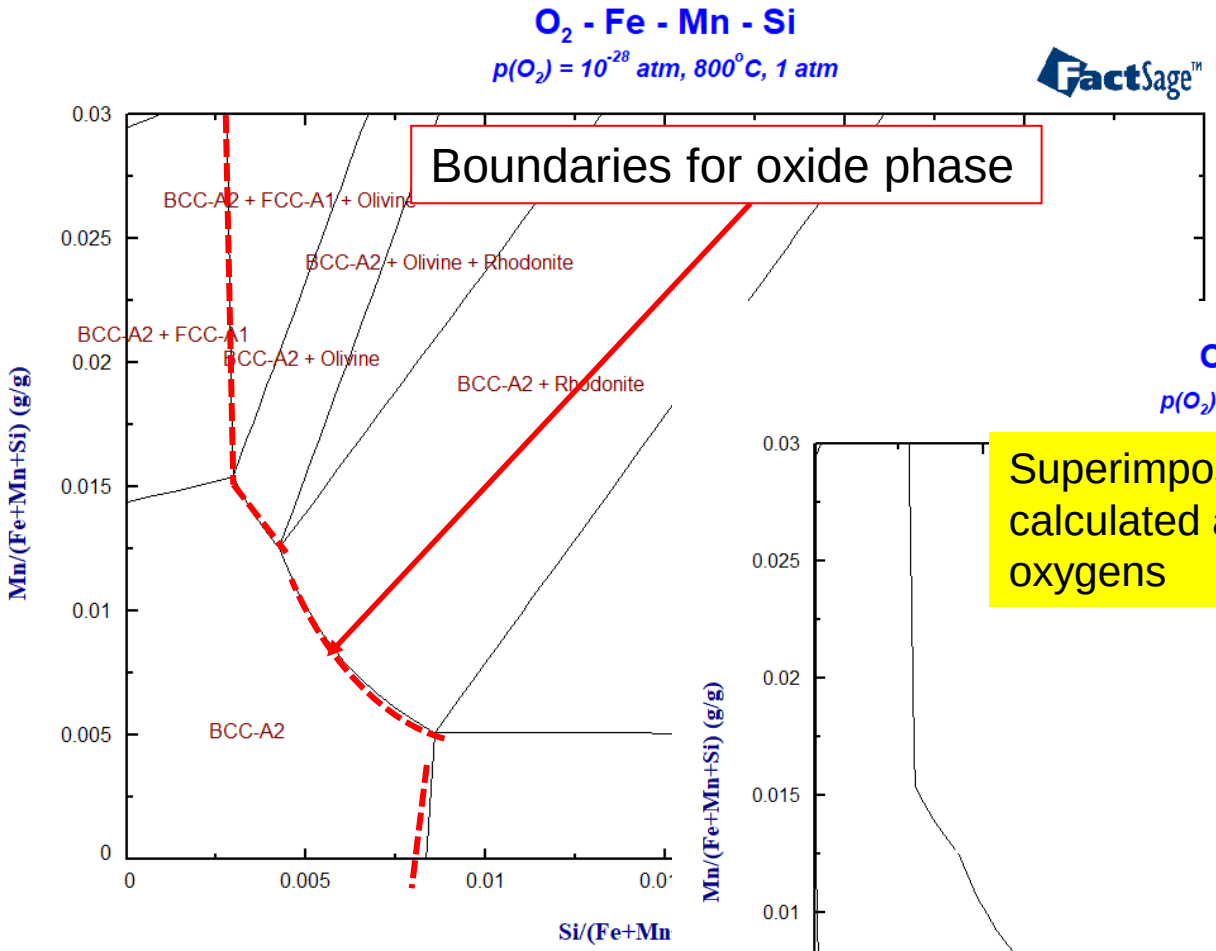
1) Collect all blue/red/green lines at different PO2 and superimpose them in one diagram.

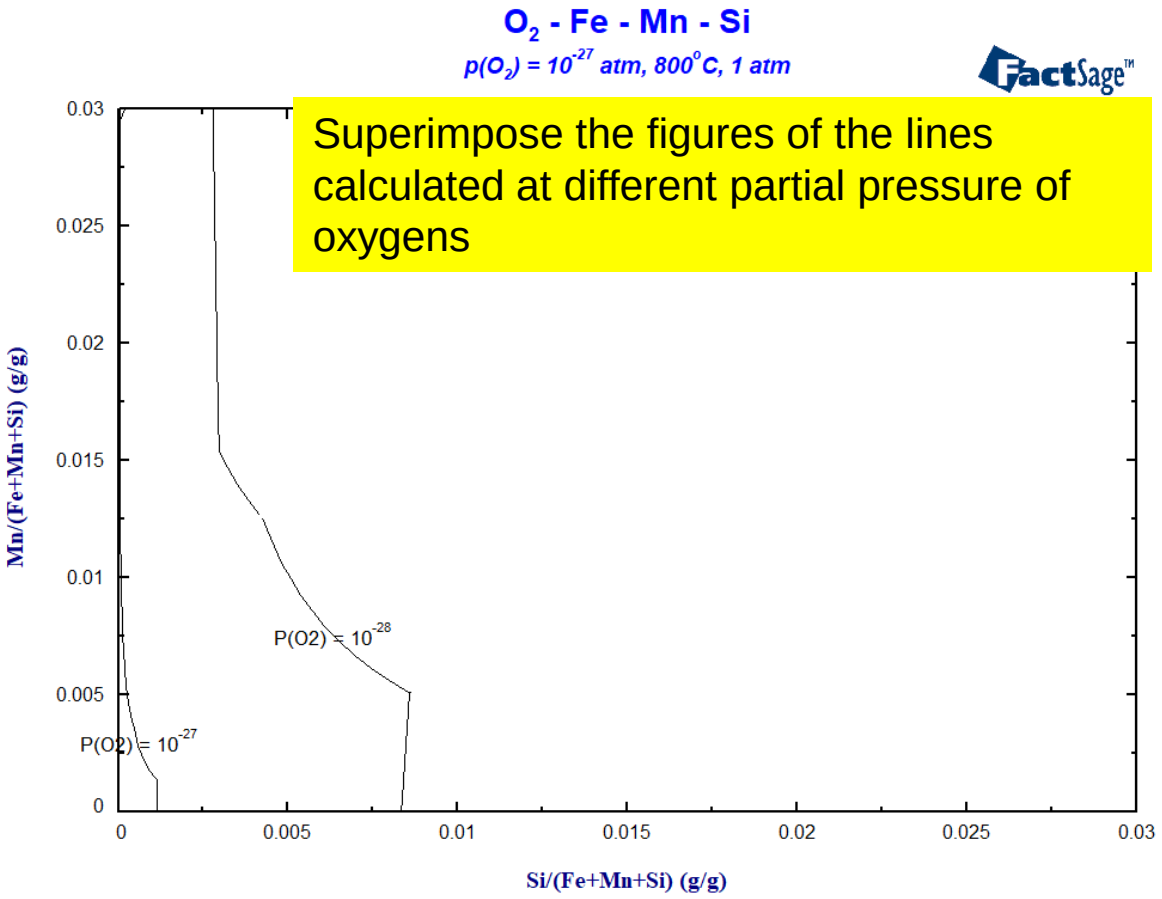
2) The boundary of each color line (different phase) is the phase boundary of the primary oxide phase in the diagram.

Fe-Mn-Si at $PO_2=10^{-28}$atm, T=800°C

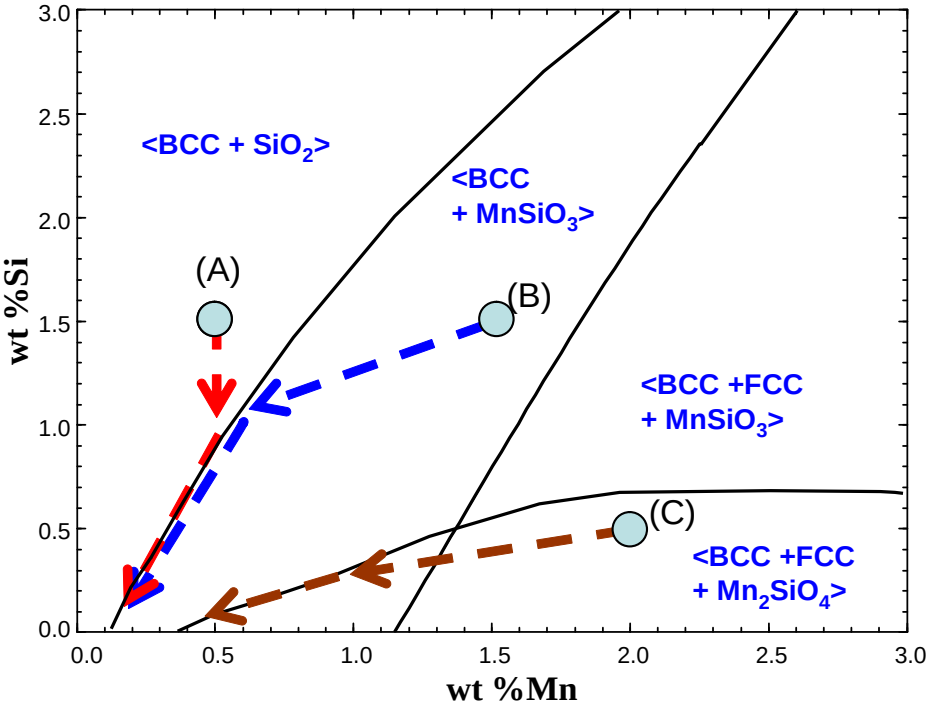


EX17-3. Primary oxide formation diagram

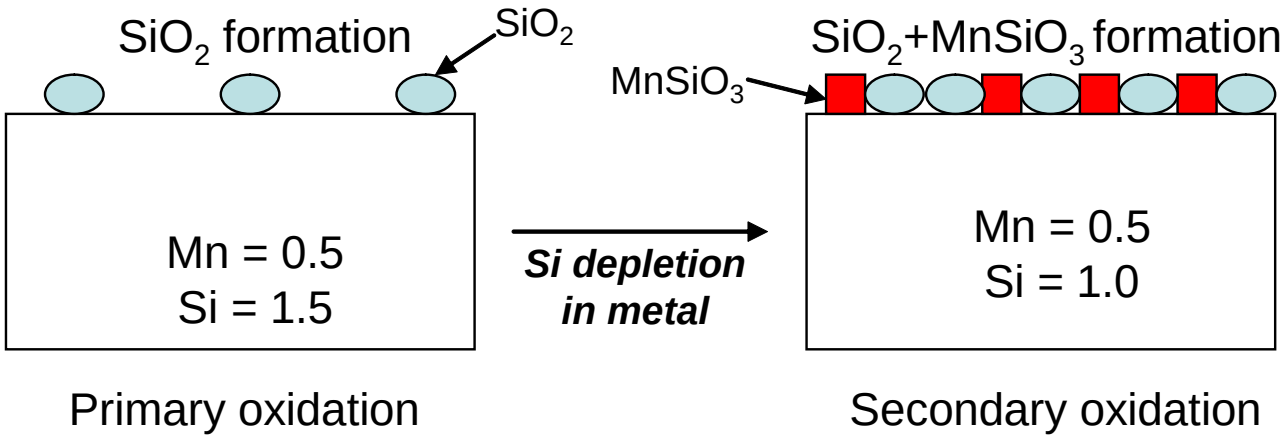




EX17-4. Primary and Secondary Oxidations

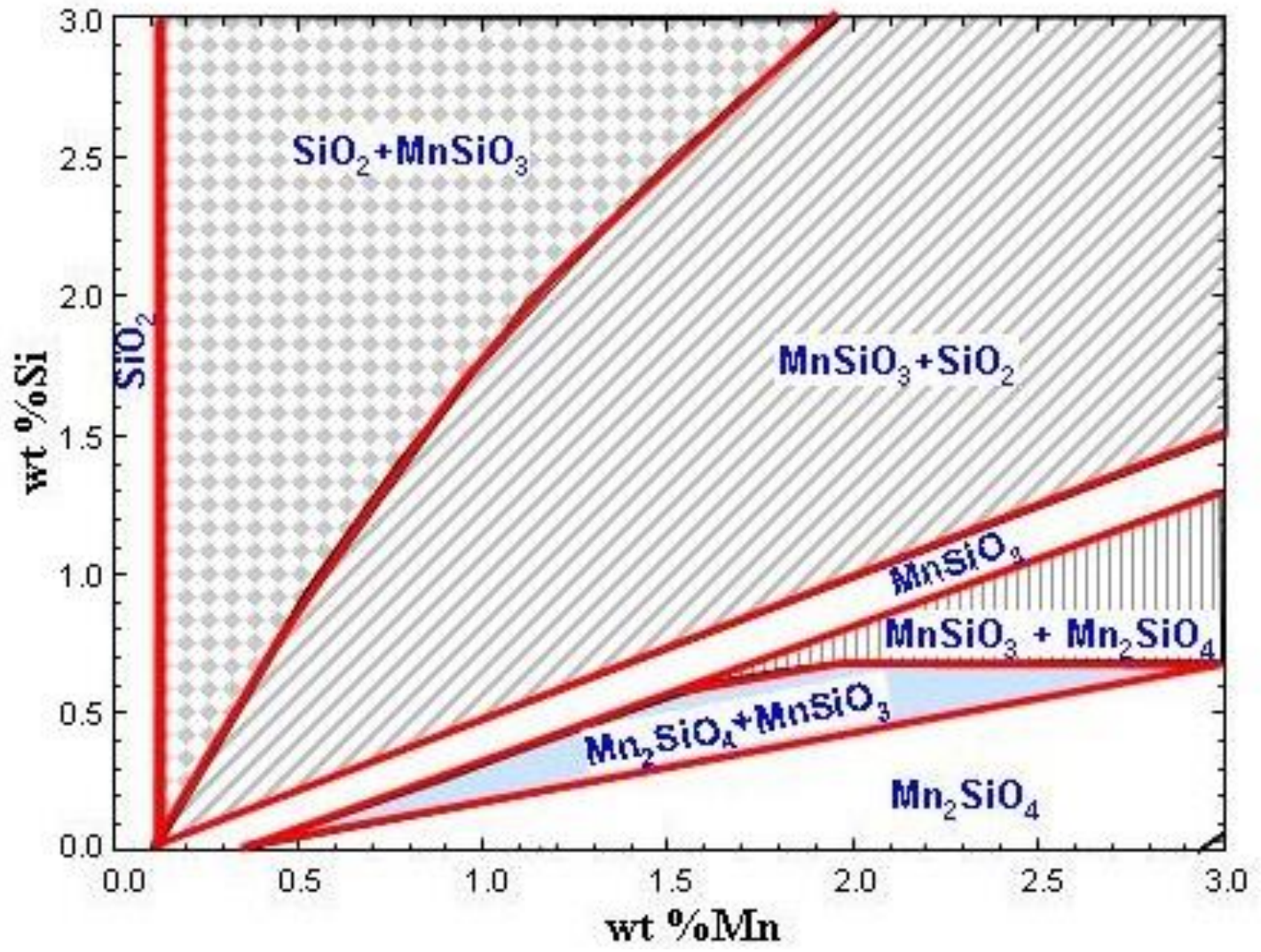


Concept of primary and secondary oxidations

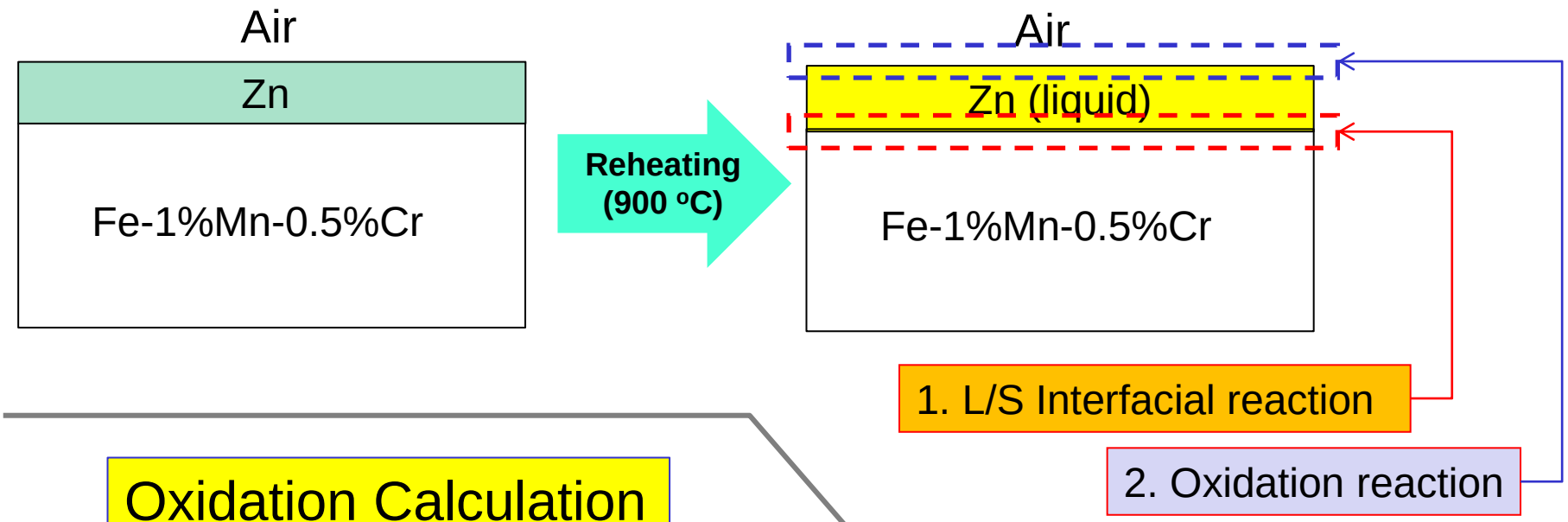


Oxidation phase diagram

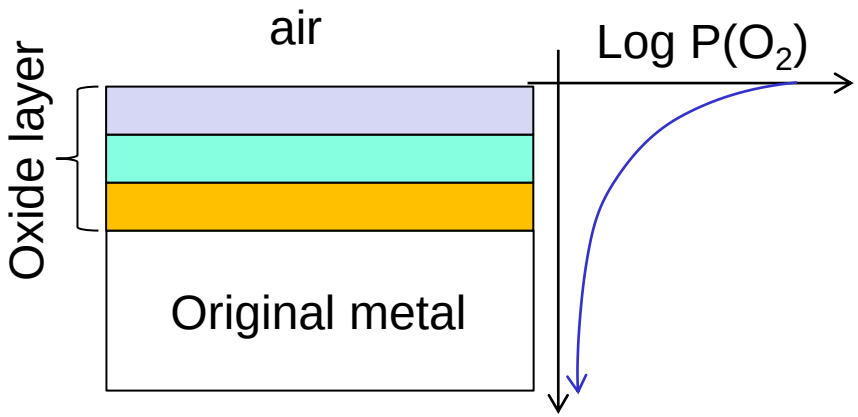
Oxidation phase diagram of the Fe-0.002%C-Mn-Si steel at 800°C



EX18. Remelting and oxidation of Zn galvanized steel



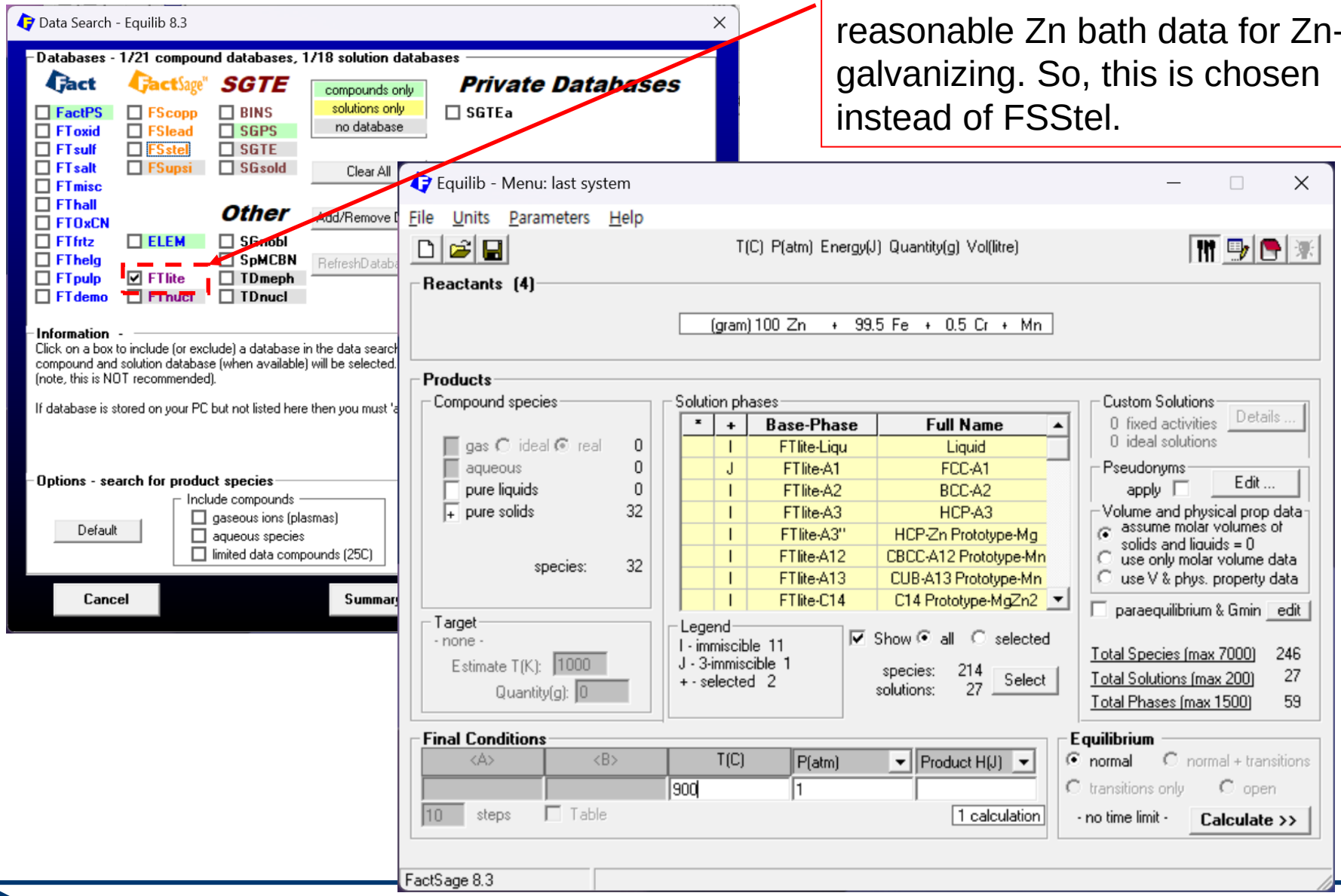
Oxidation Calculation



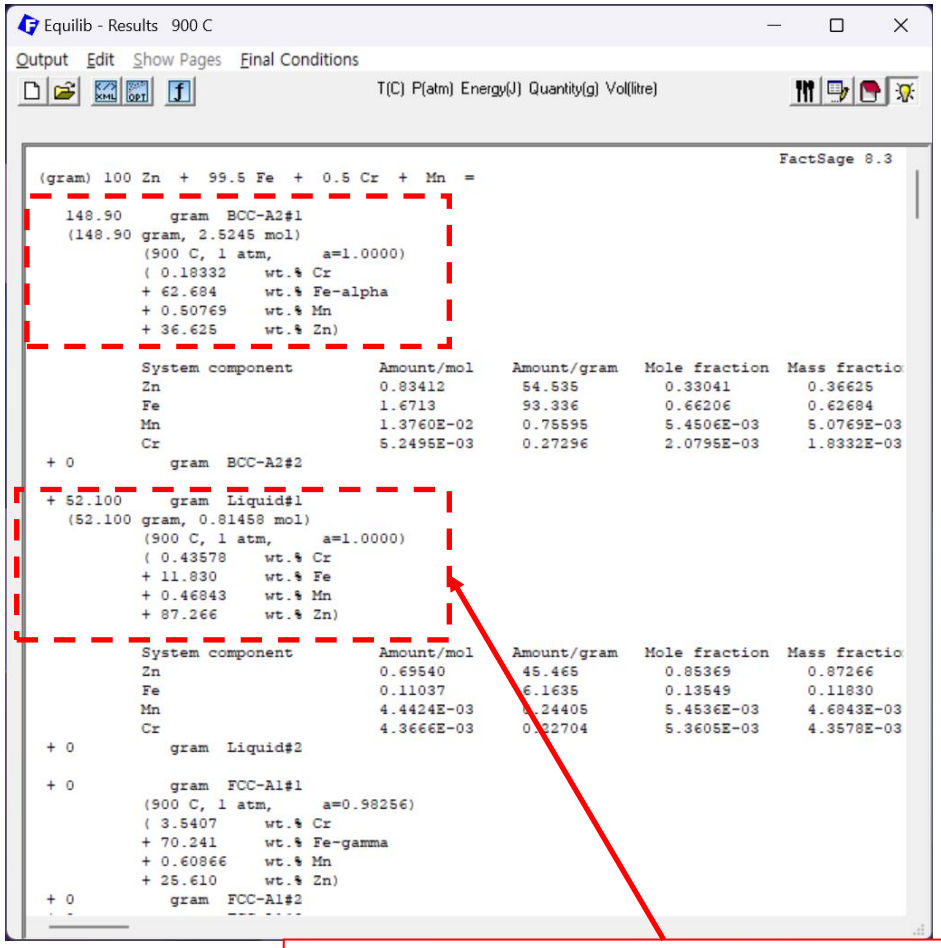
By controlling the partial pressure, different layer oxides can be calculated. But the partial pressure is not linearly decreasing with depth of oxide layer. So this type of calculation shows quantitative oxidation behavior

EX18-1. Interface reaction between liquid Zn and steel

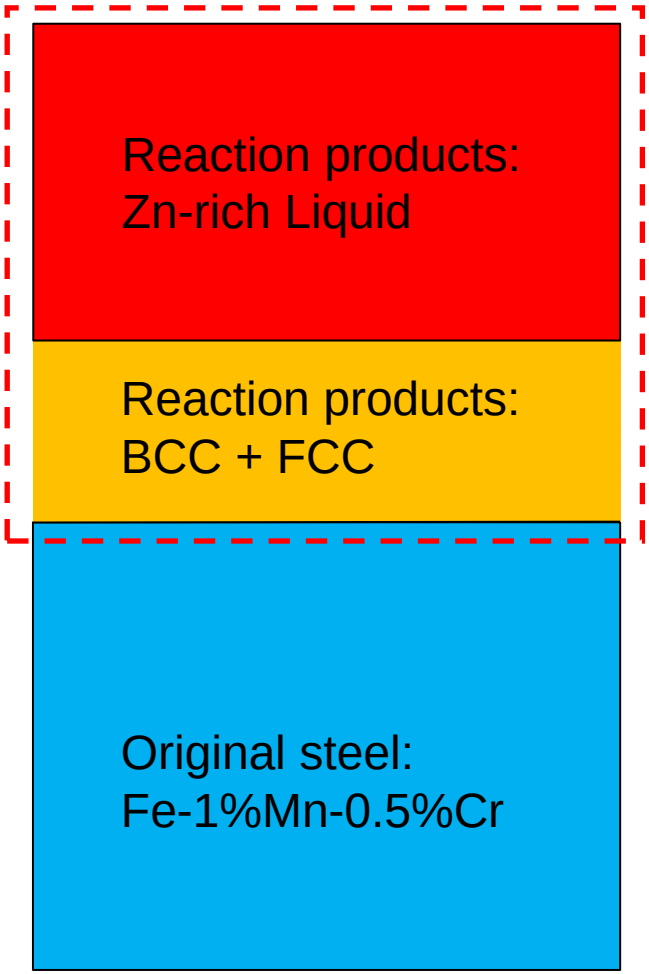
FTlite database contains reasonable Zn bath data for Zn-galvanizing. So, this is chosen instead of FSStel.



EX18-1. Interface reaction between liquid Zn and steel

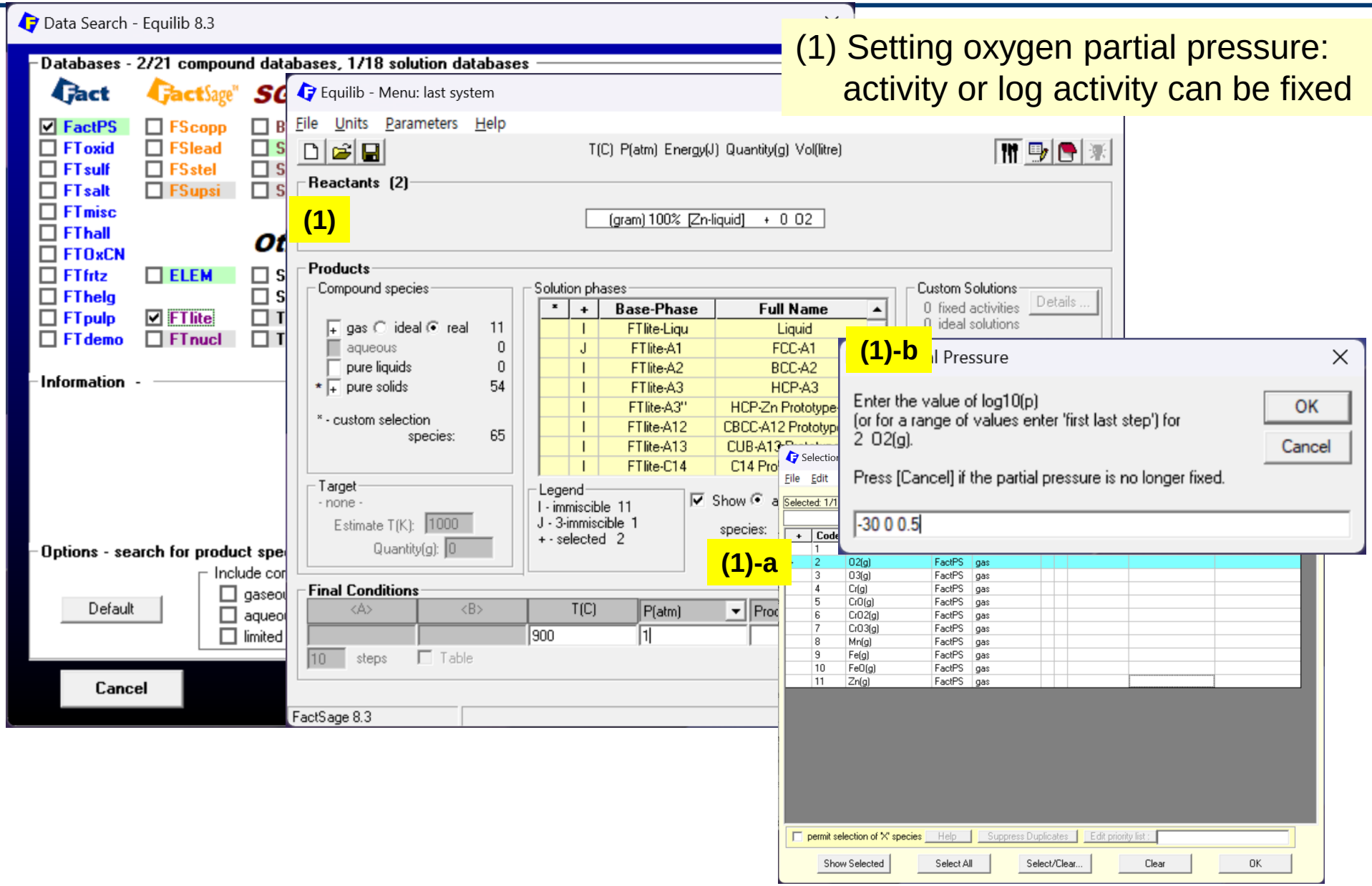


We need this liquid Zn for the oxidation reaction
→ Save it as stream

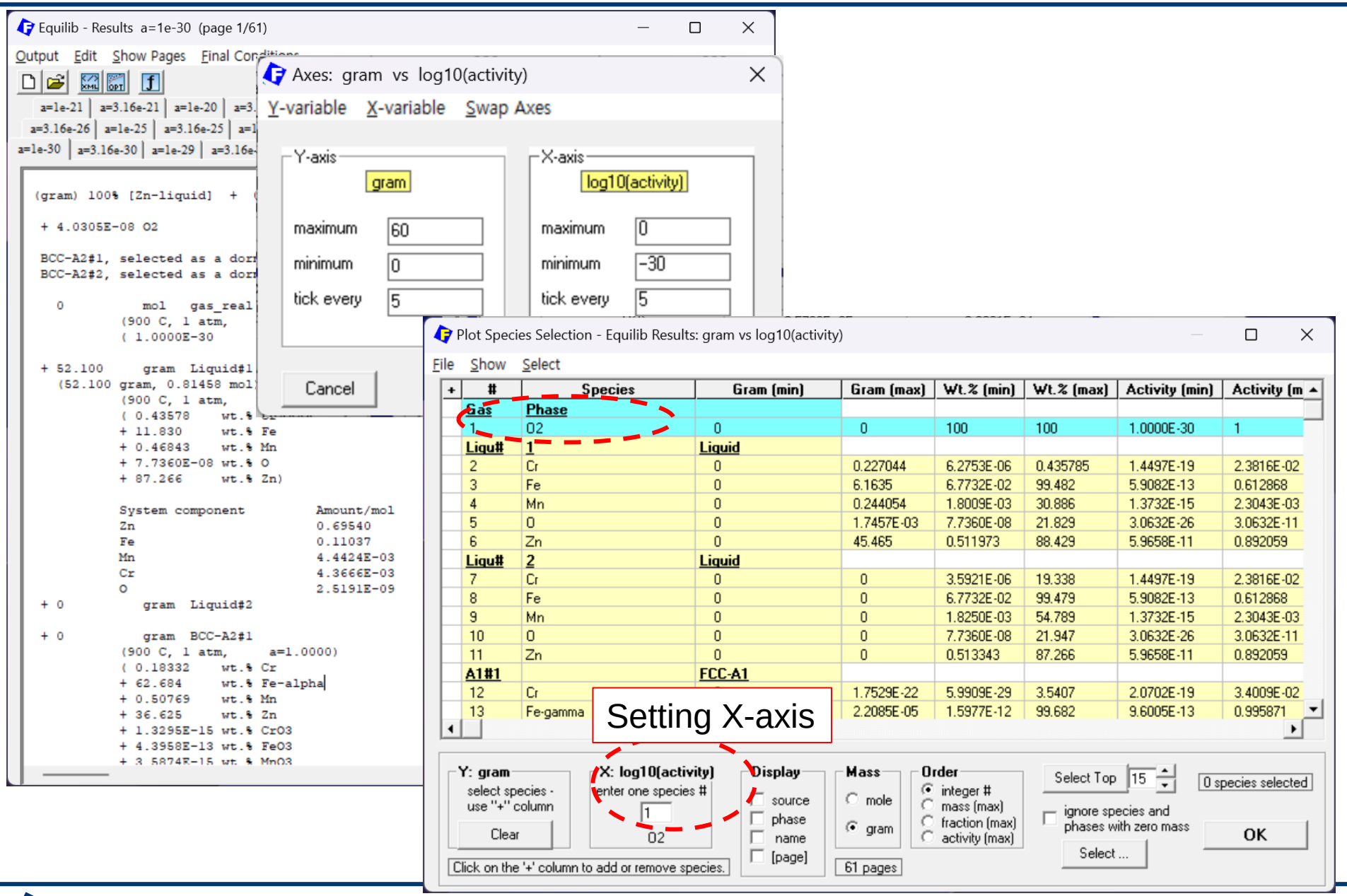


EX18-2. Oxidation reaction of liquid Zn

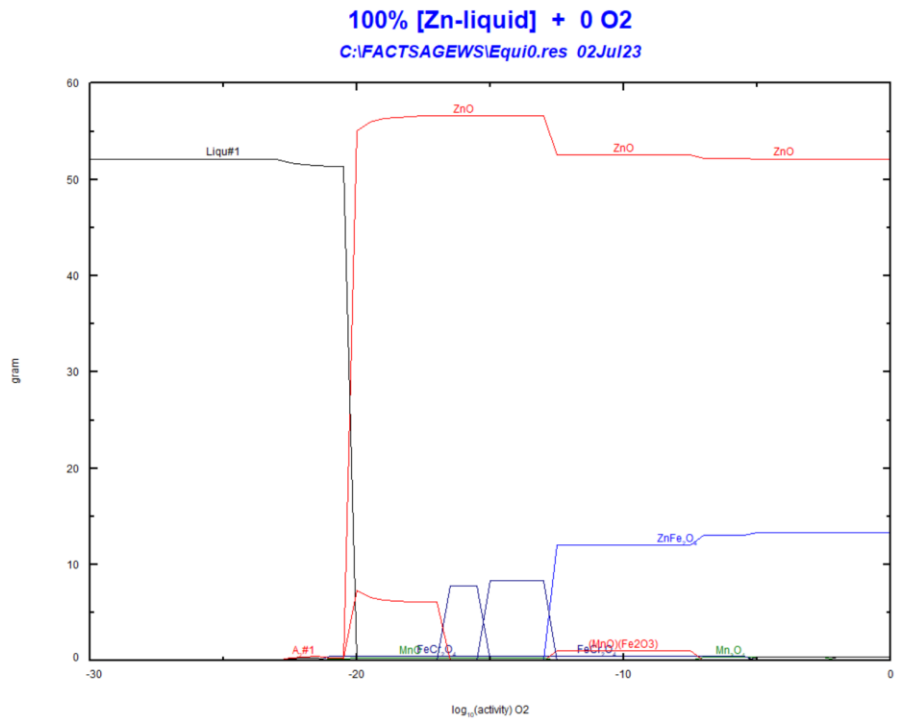
(1) Setting oxygen partial pressure: activity or log activity can be fixed

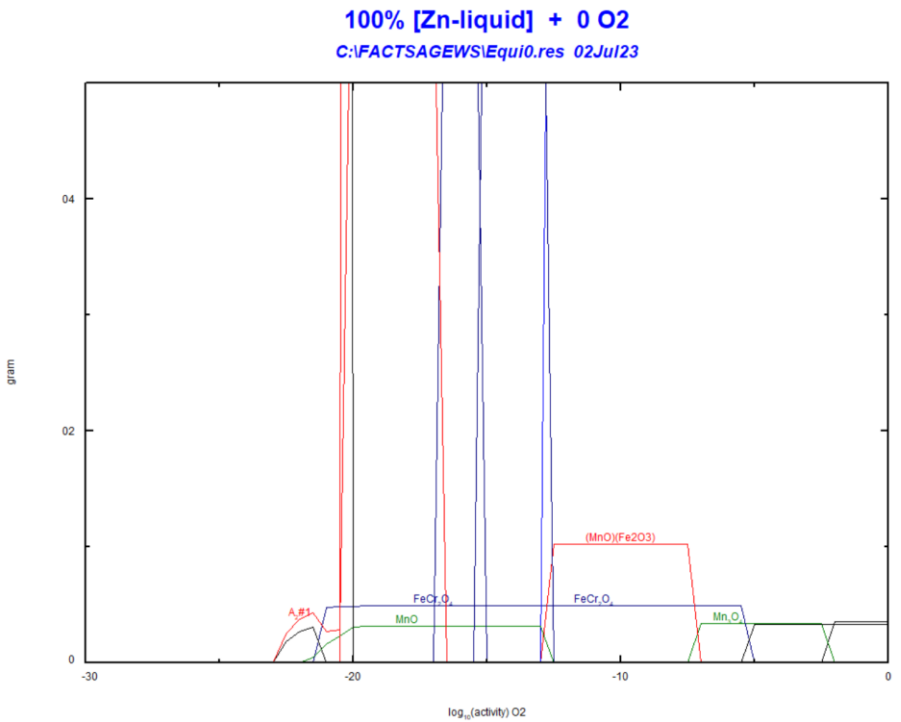


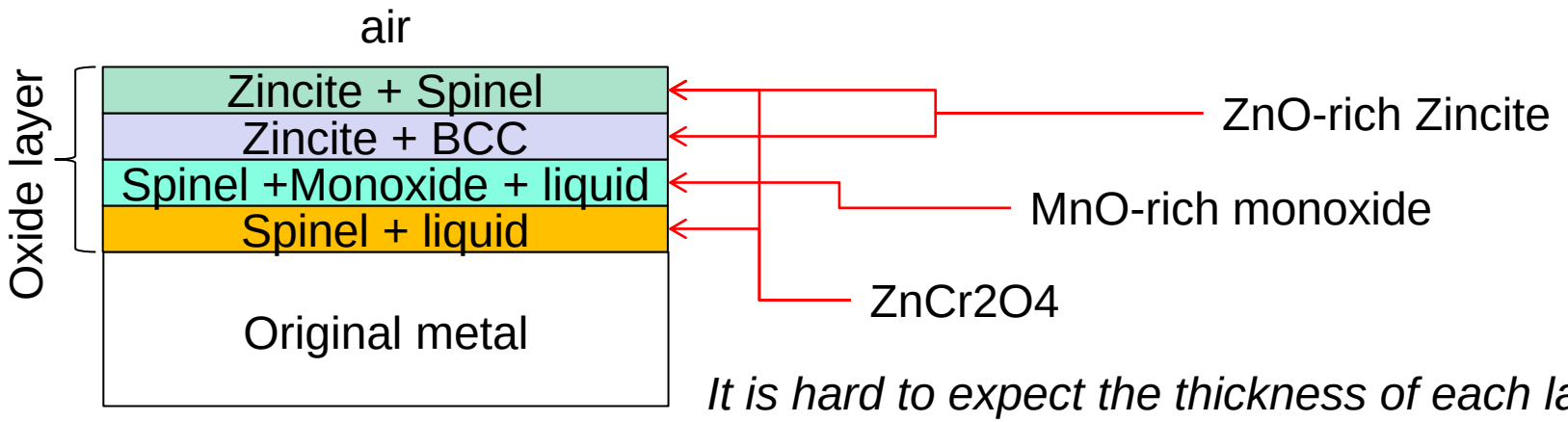
EX18-2. Oxidation reaction of liquid Zn



EX18-2. Oxidation reaction of liquid Zn

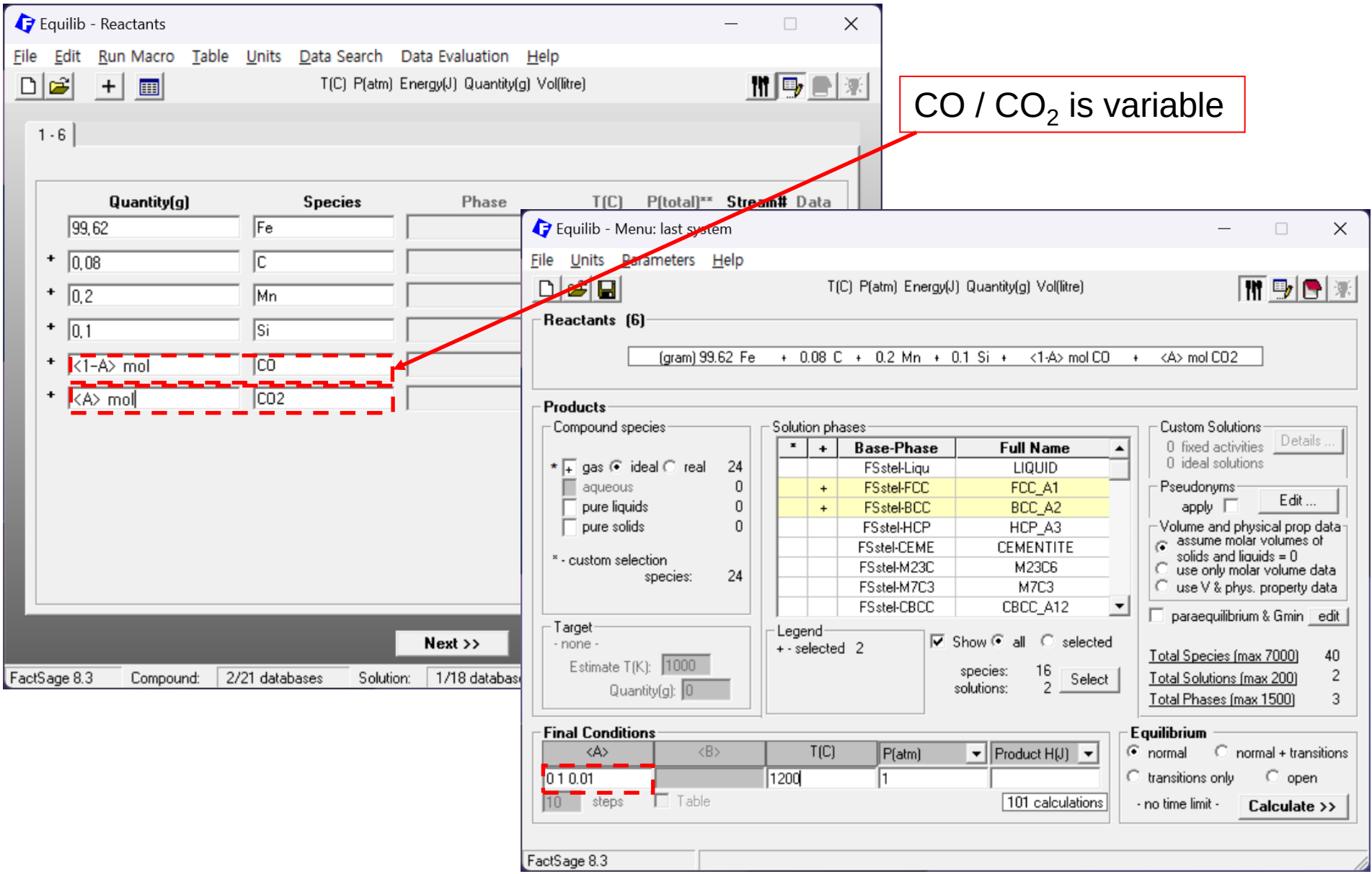




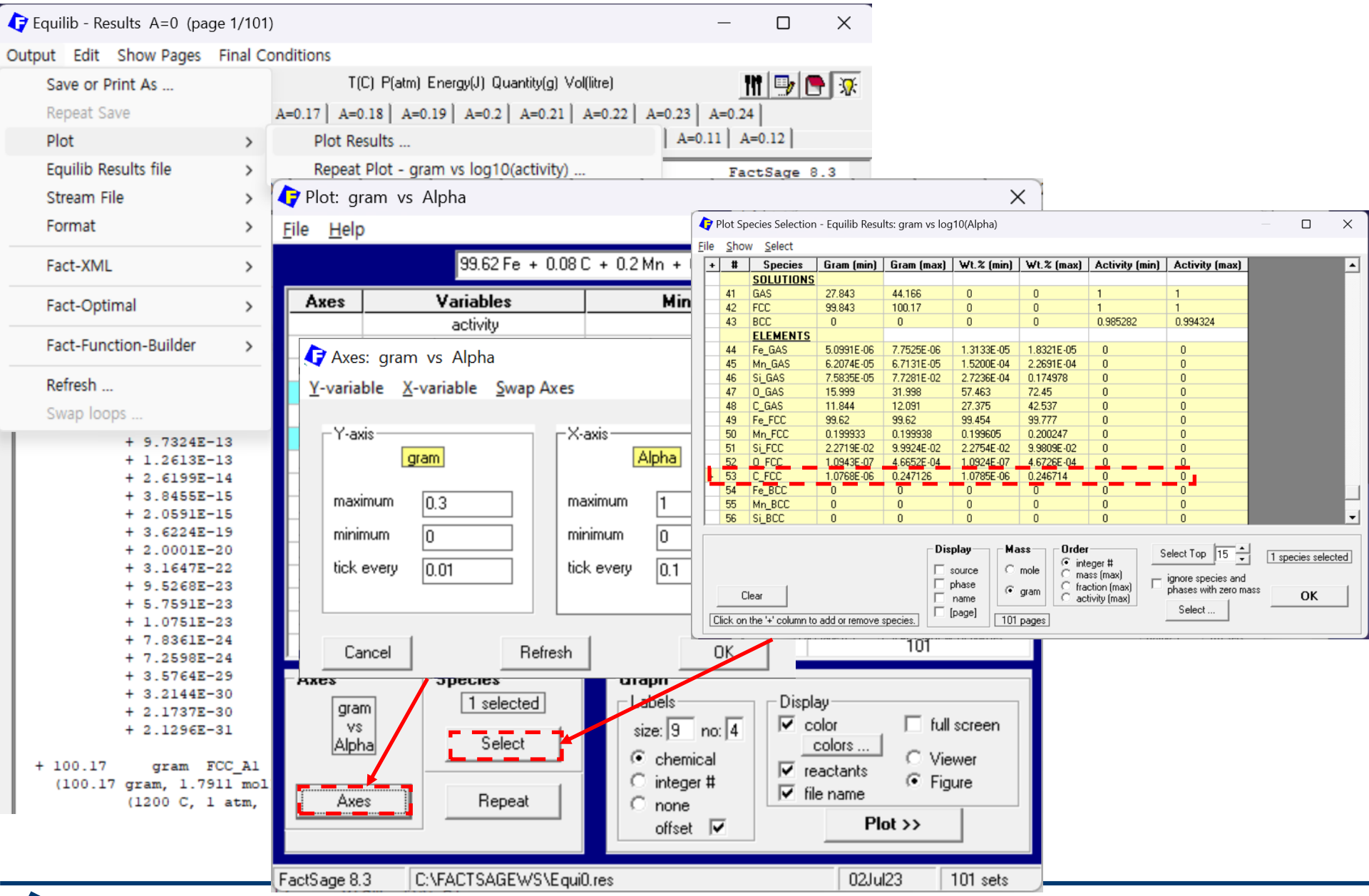


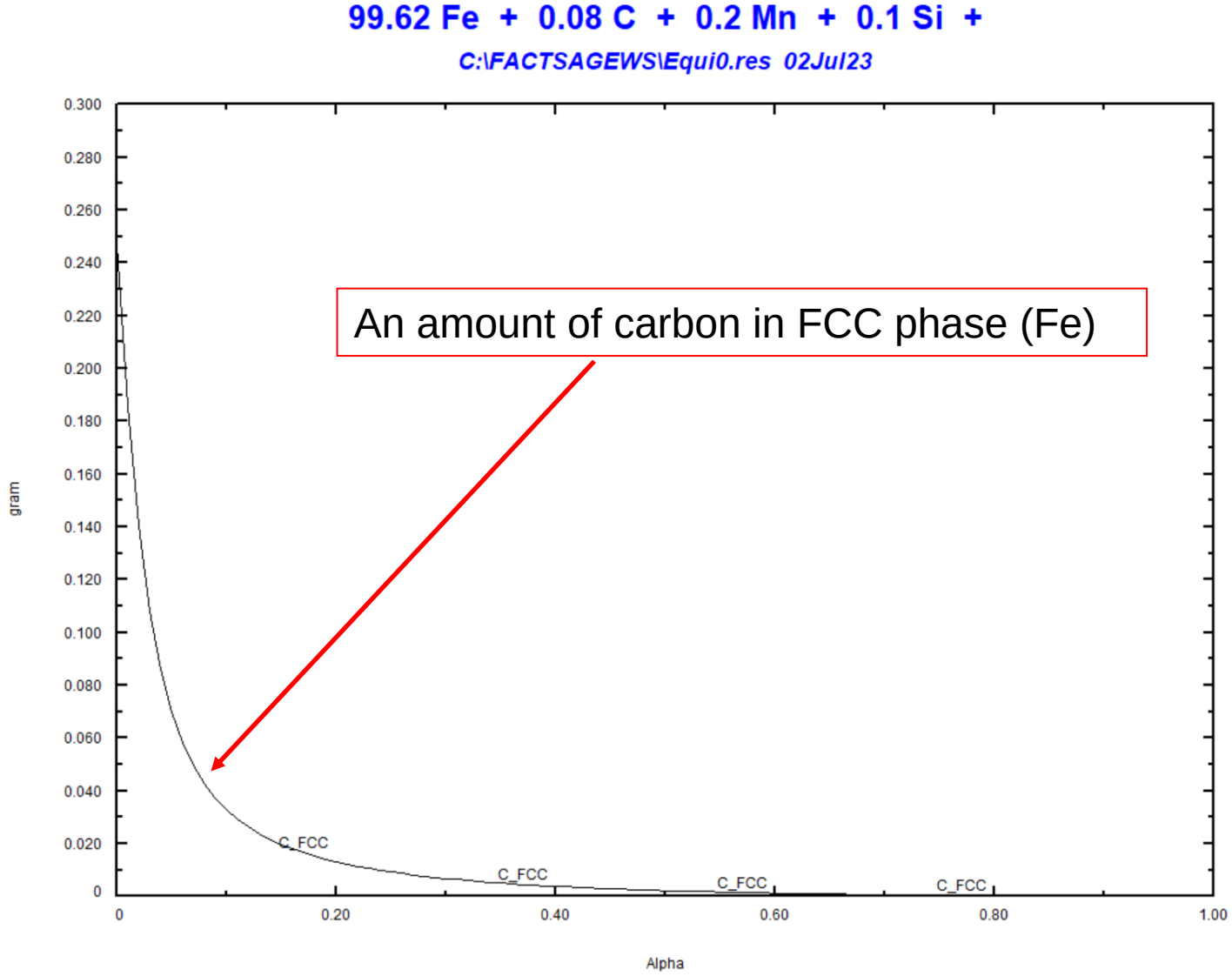
It is hard to expect the thickness of each layer

EX19. Carburization and Decarburization of Steel

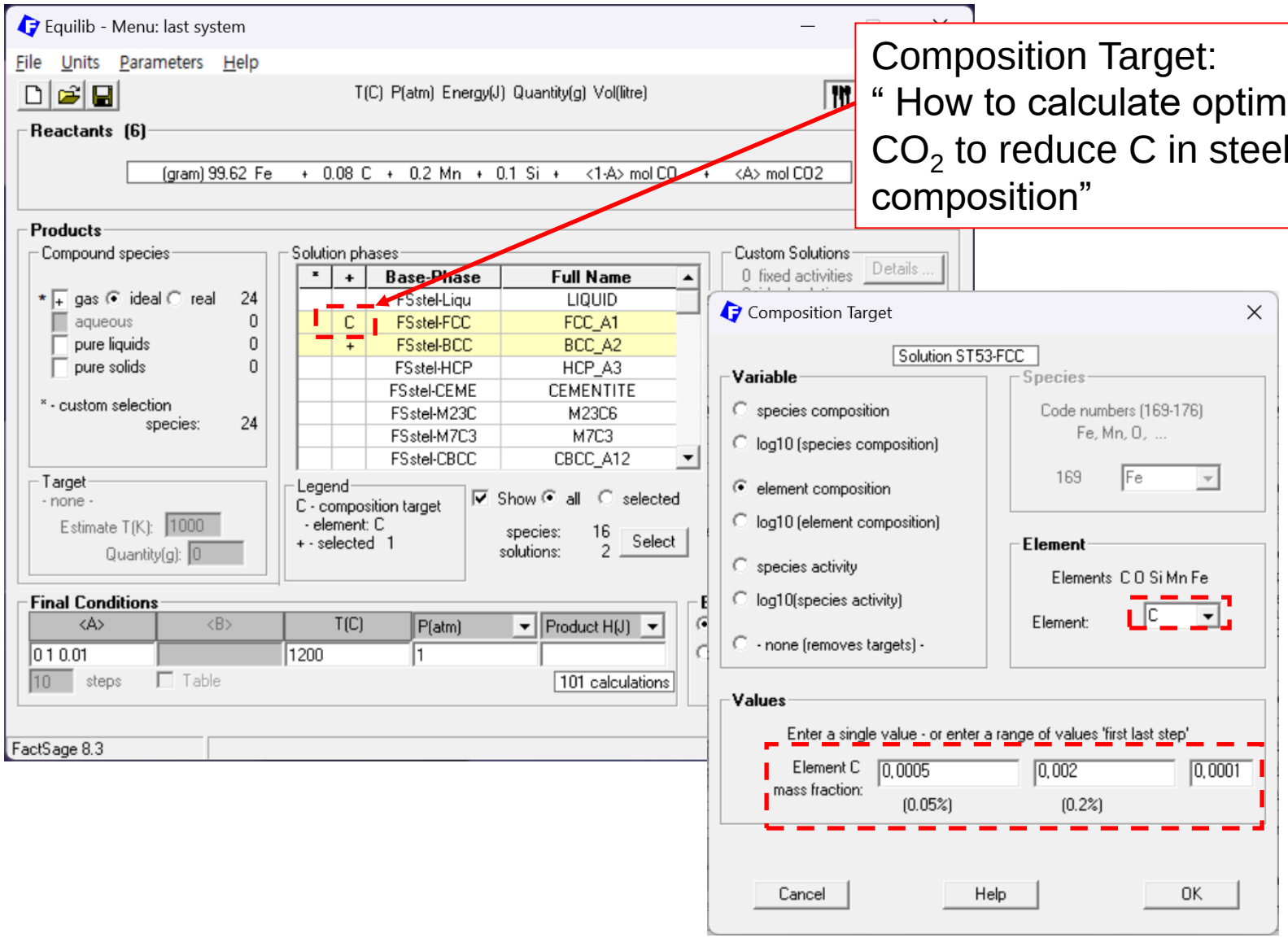


EX19. Carburization and Decarburization of Steel

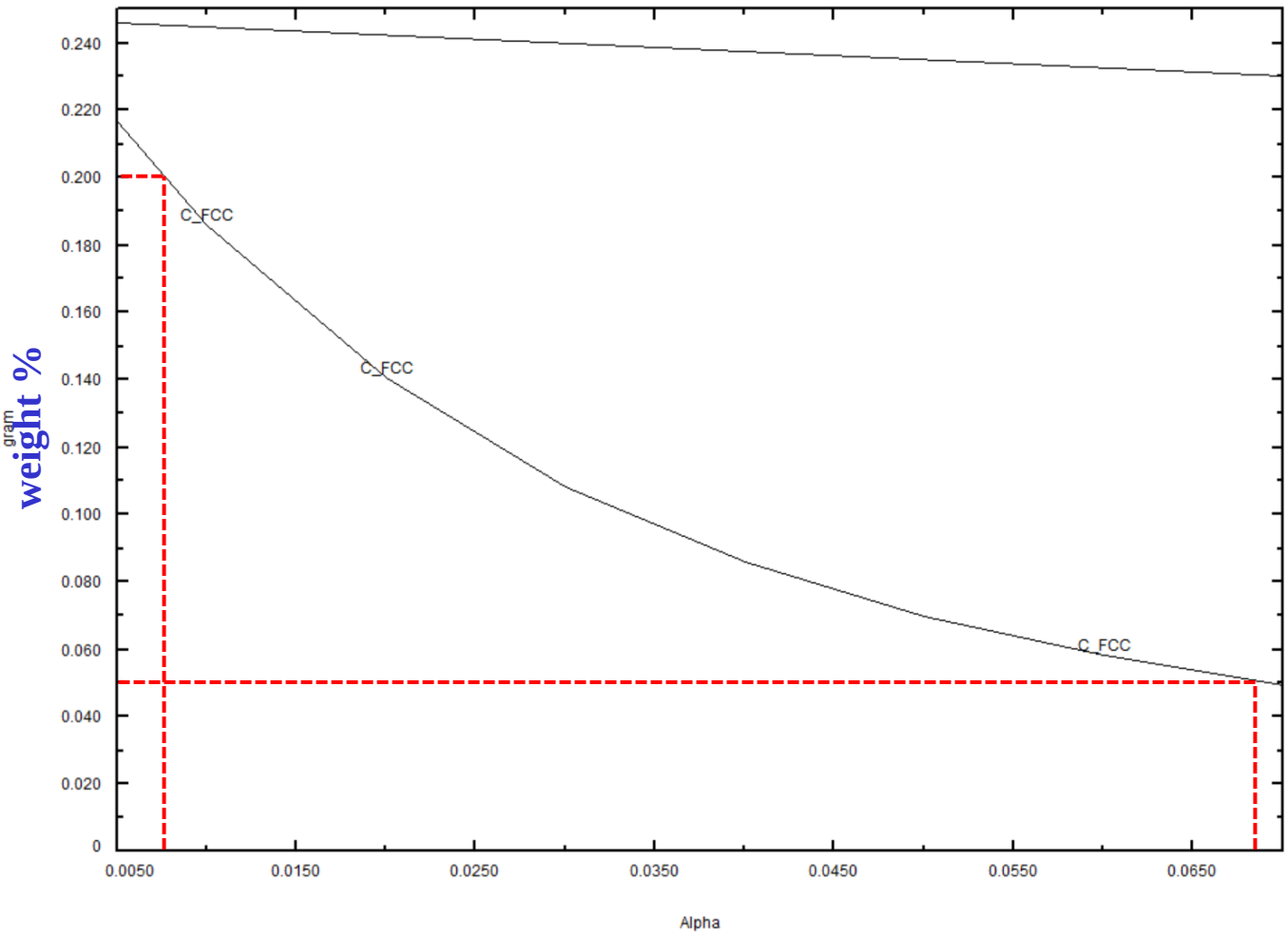



99.62 Fe + 0.08 C + 0.2 Mn + 0.1 Si +
C:\FACTSAGEWS\Equi0.res 02Jul23
An amount of carbon in FCC phase (Fe)
gram
Alpha
0.300
0.280
0.260
0.240
0.220
0.200
0.180
0.160
0.140
0.120
0.100
0.080
0.060
0.040
0.020
0
0.20
0.40
0.60
0.80
1.00
C_FCC
C_FCC
C_FCC
C_FCC

EX19. Carburization and Decarburization: Composition target

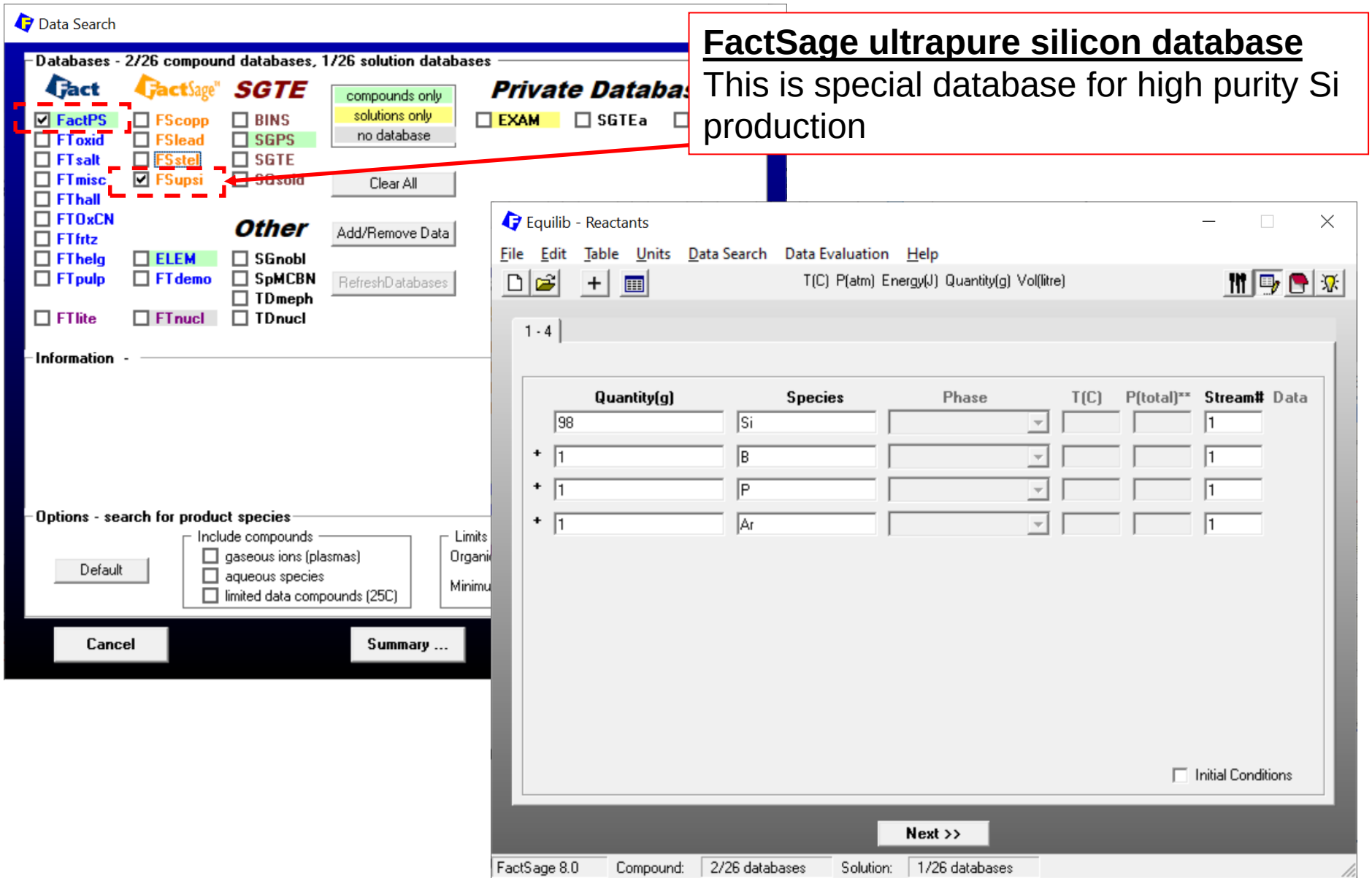


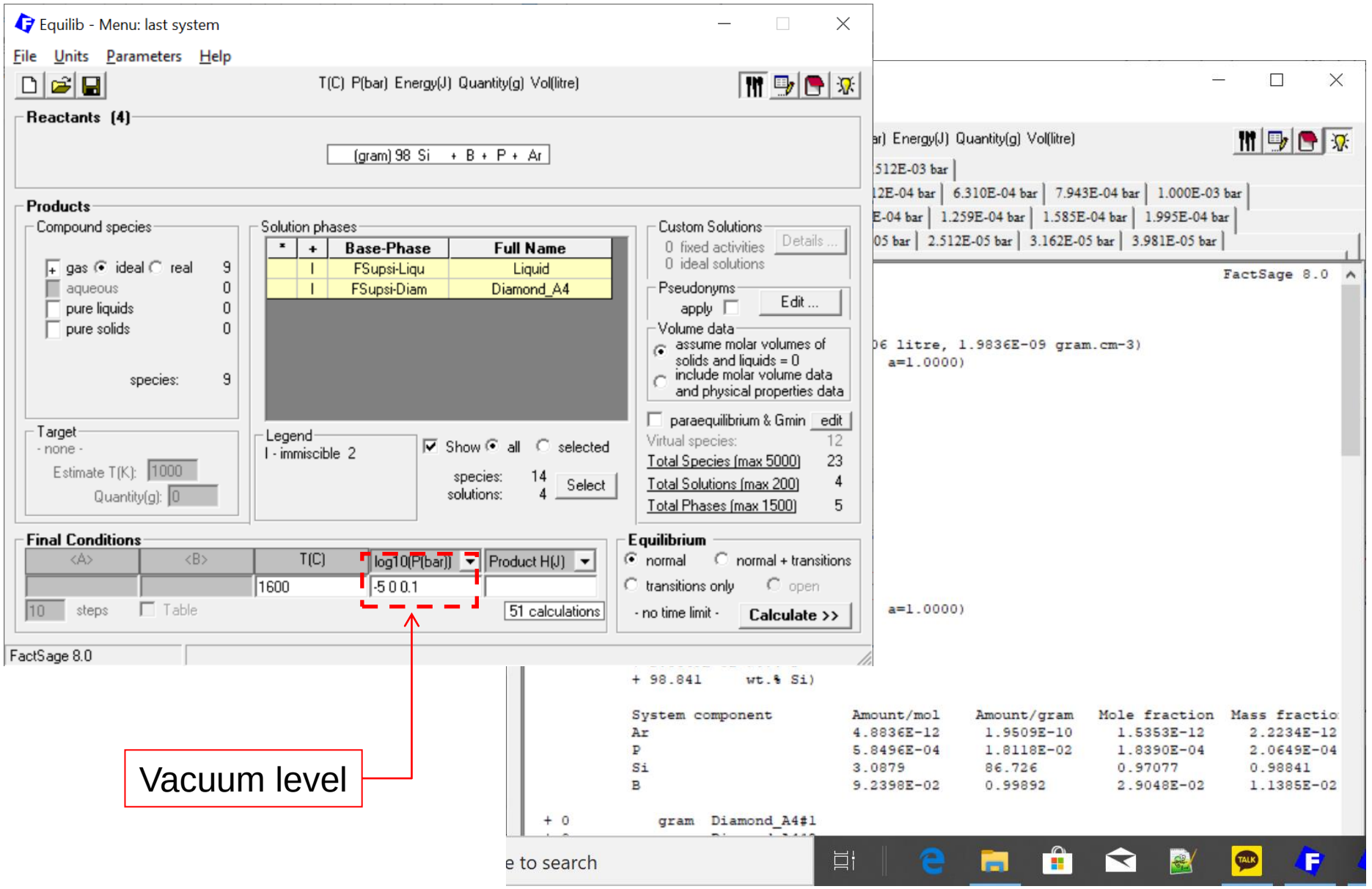
Composition Target:
" How to calculate optimum amount of CO_2 to reduce C in steel to a targeted composition"


99.62 Fe + 0.08 C + 0.2 Mn + 0.1 Si +
C:\FACTSAGEWS\Equi0.res 02Jul23
gram weight %
0.240
0.220
0.200
0.180
0.160
0.140
0.120
0.100
0.080
0.060
0.040
0.020
0
C_FCC
C_FCC
C_FCC
0.0050
0.0150
0.0250
0.0350
0.0450
0.0550
0.0650
Alpha

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

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




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
Solution phases
* + Base-Phase Full Name
I FSupsi-Liqu Liquid
I FSupsi-Diam Diamond_A4
Custom Solutions
0 fixed activities
0 ideal solutions
Details ...
Pseudonyms
apply
Edit ...
Volume data
assume molar volumes of solids and liquids = 0
include molar volume data and physical properties data
paraequilibrium & Gmin edit
Virtual species: 12
Total Species (max 5000) 23
Total Solutions (max 200) 4
Total Phases (max 1500) 5
Target
- none -
Estimate T(K): 1000
Quantity(g): 0
Legend
I - immiscible 2
Show all selected
species: 14
solutions: 4
Select
Final Conditions
<A> <B> T(C) log10(P(bar)) Product H(J)
1600 -5 0 0.1
10 steps Table
51 calculations
Equilibrium
normal normal + transitions
transitions only open
- no time limit -
Calculate >>
FactSage 8.0
Vacuum level
FactSage 8.0
+ 98.841 wt.% Si)
System component Amount/mol Amount/gram Mole fraction Mass fractio
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

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

Y-variable X-variable Swap Axes

Y-axis: weight % soln. species — maximum 1, minimum 0, tick every 0.2

X-axis: log10(P(bar)) — maximum 0, minimum -5, tick every 0.5

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

File Show Select

+	#	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.
	Liqu#	1	Liquid					
	10	Ar	1.9509E-10	3.7460E-04	2.2234E-10	3.7460E-04	1.4794E-12	2.
	11	B	0.998915	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	86.726	98	98.001	98.918	0.96692	0.
	Liqu#	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.

Clear

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

Display: source, phase, name, [page]

Mass: mole, gram

51 pages

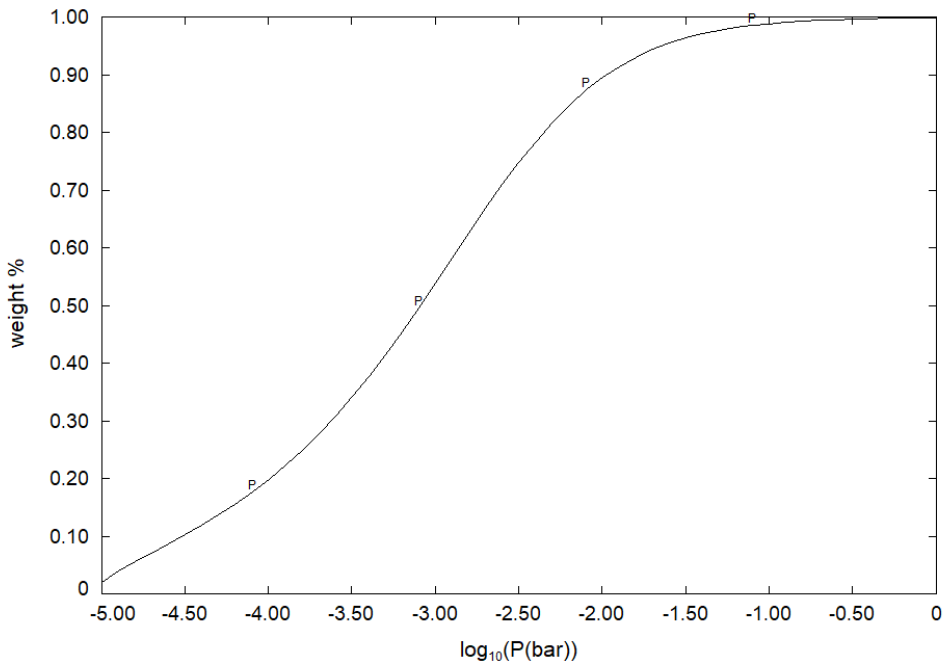
Order: integer #, mass (max), fraction (max), activity (max)

Select T

ignore phase

Sel

P content in liquid Si



EX20-2. B reduction in high purity Si using H_2-H_2O mixture

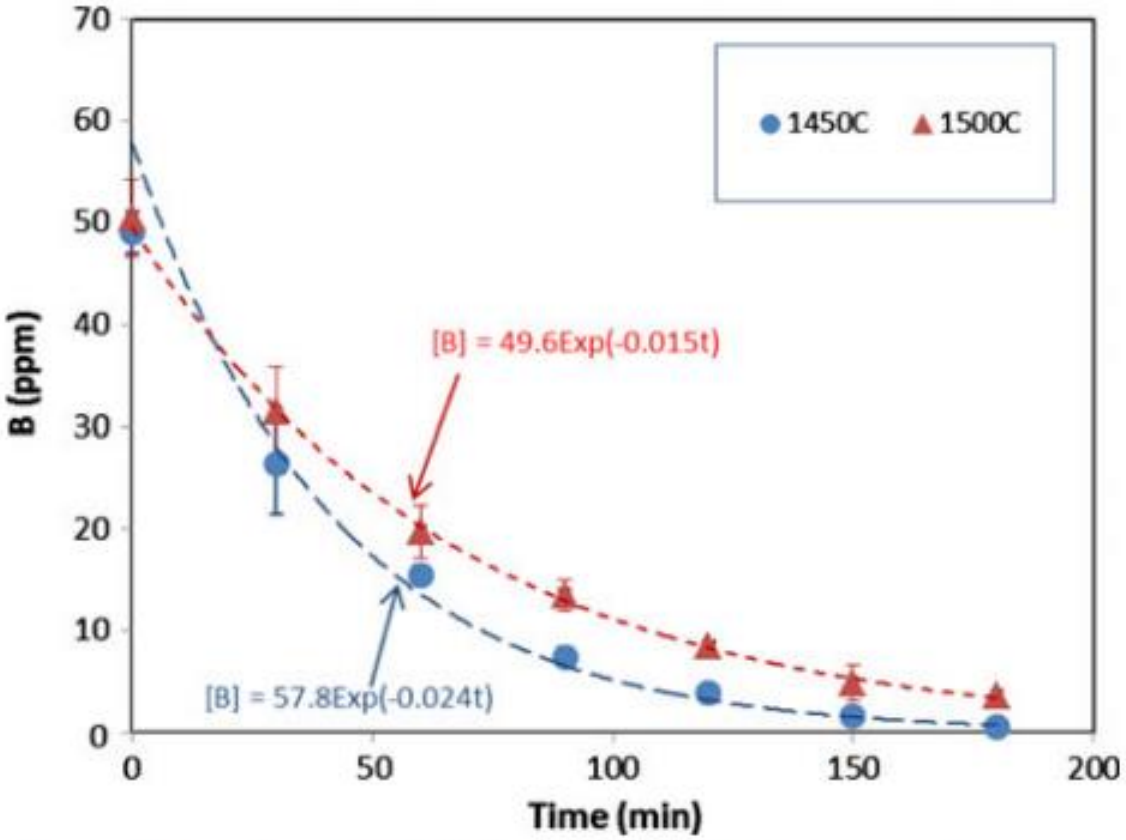


Fig. 1. B concentration changes in H_2-H_2O blowing determined by the resistivity meter

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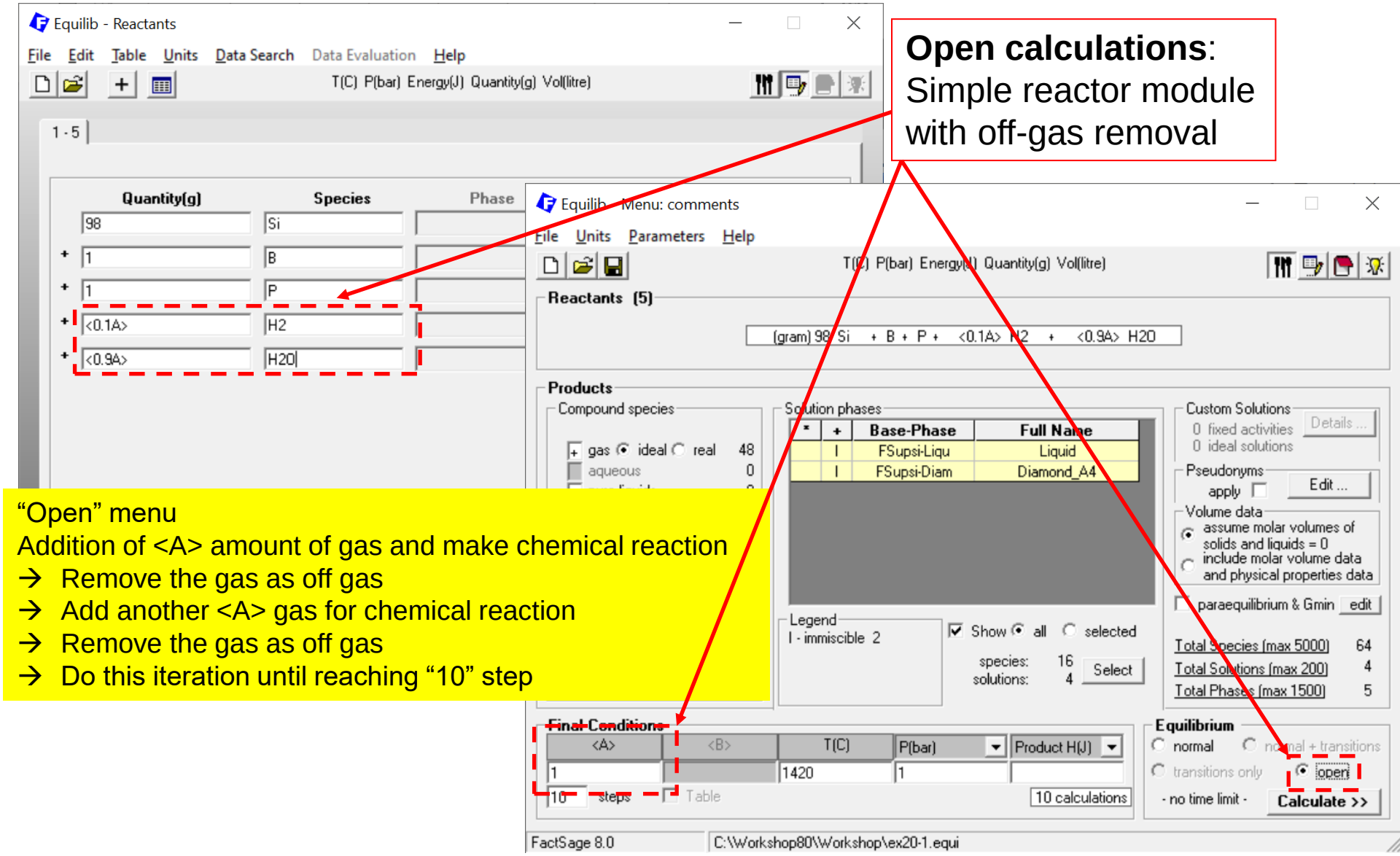
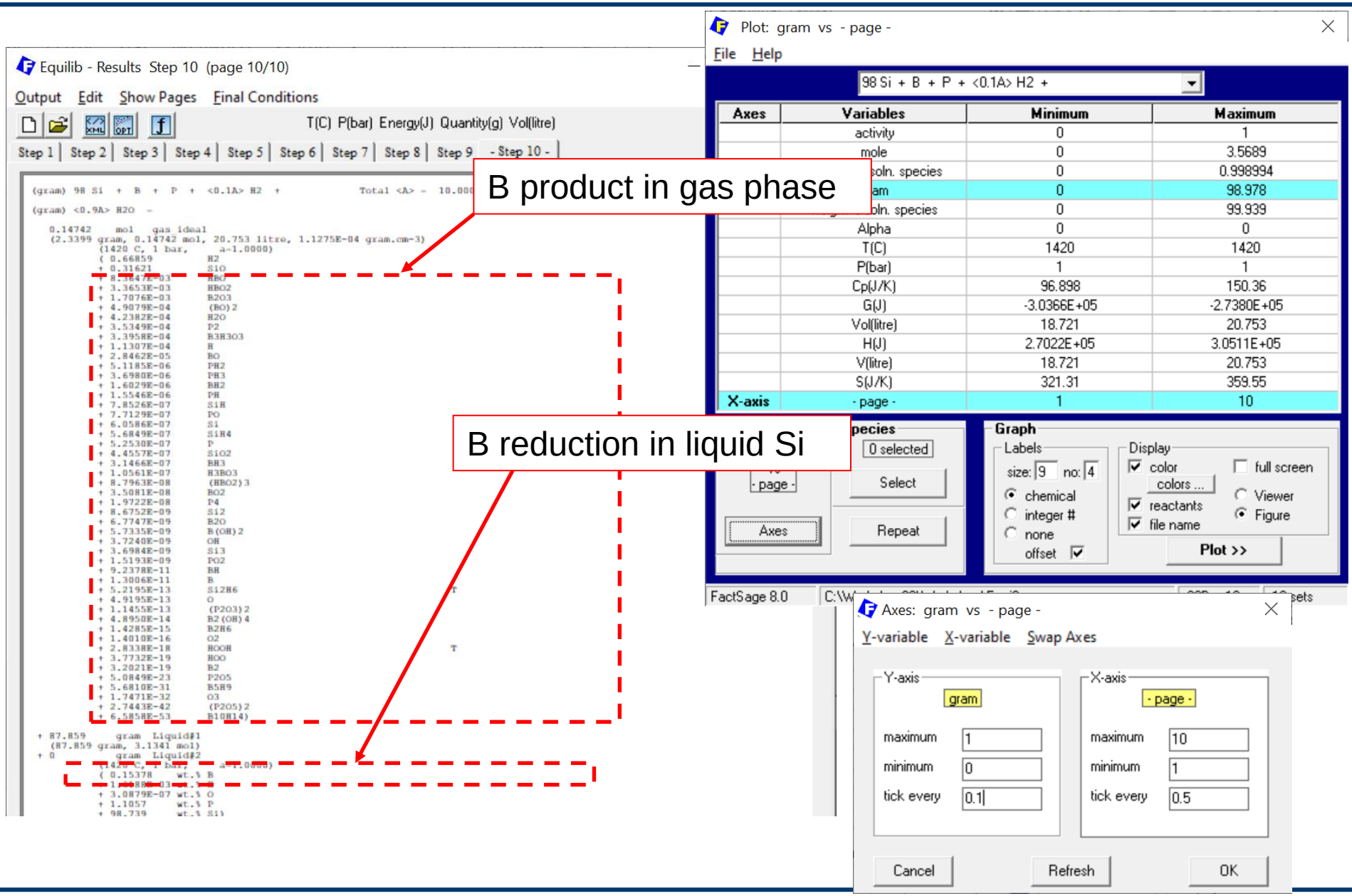
Volume 64, Number 8 (2012), 952-956



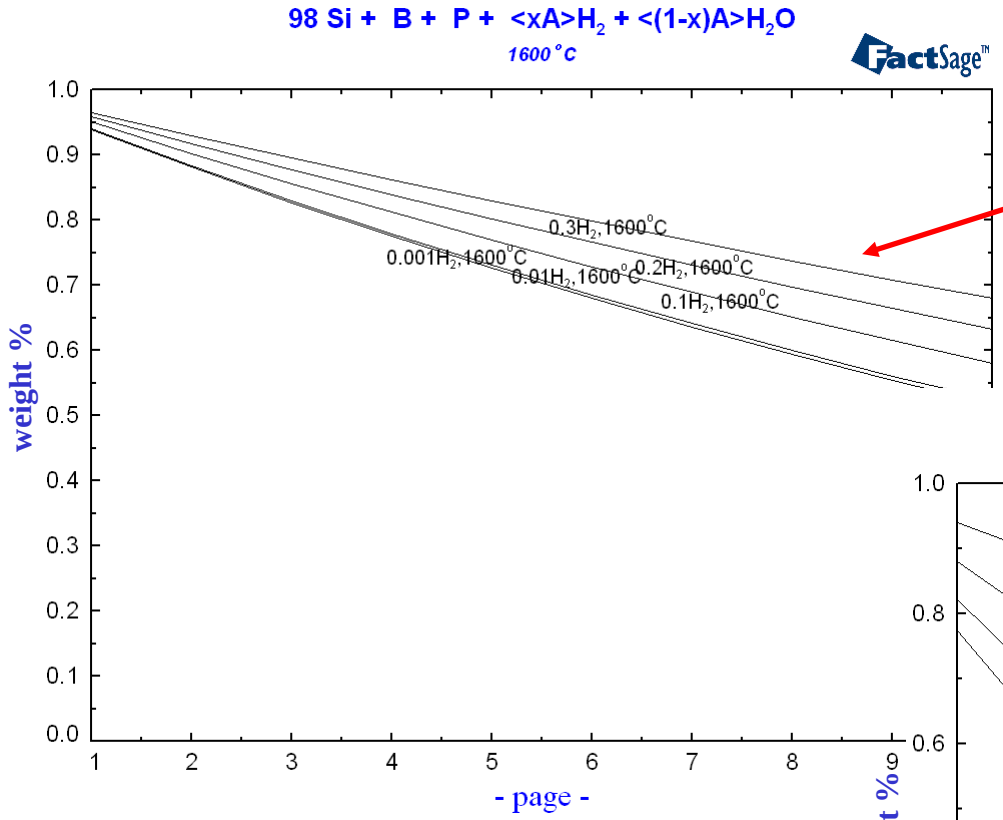
Open calculations:
Simple reactor module with off-gas removal

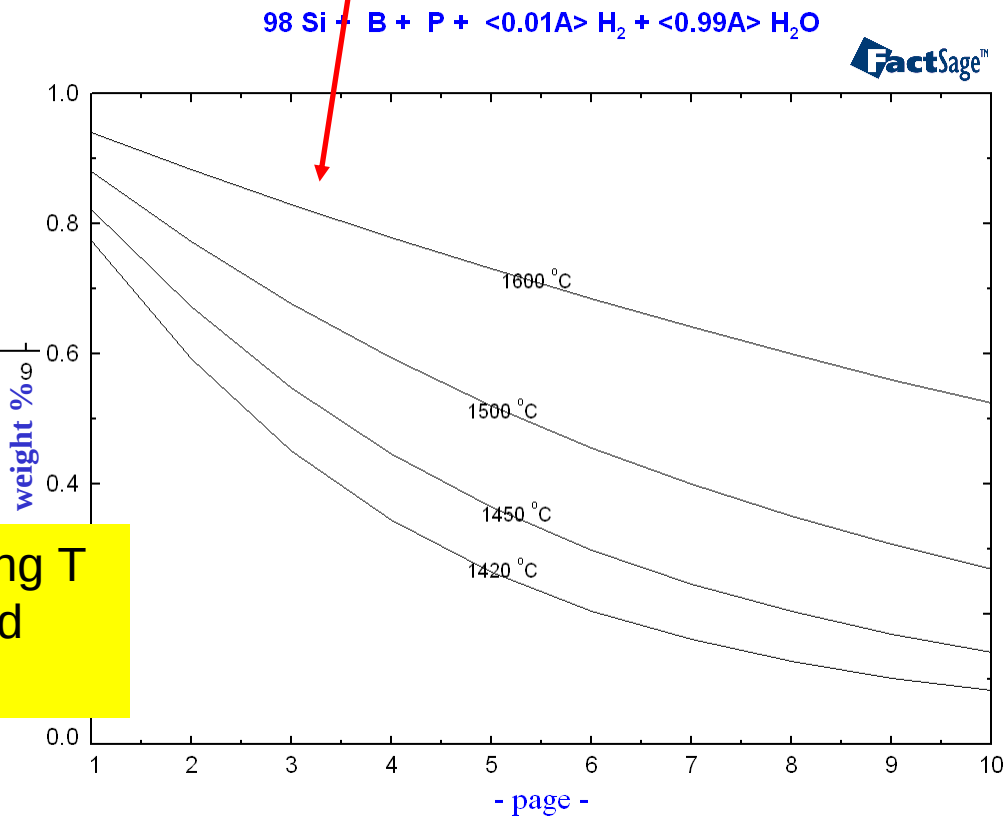
"Open" menu
Addition of <A> amount of gas and make chemical reaction

→ 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 -
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
0 0.998994
0 98.978
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
0 selected
Select
Repeat
Axes
Graph
Labels
size: 9 no: 4
chemical
integer #
none
offset
Display
color
colors ...
reactants
file name
full screen
Viewer
Figure
Plot >>
FactSage 8.0
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

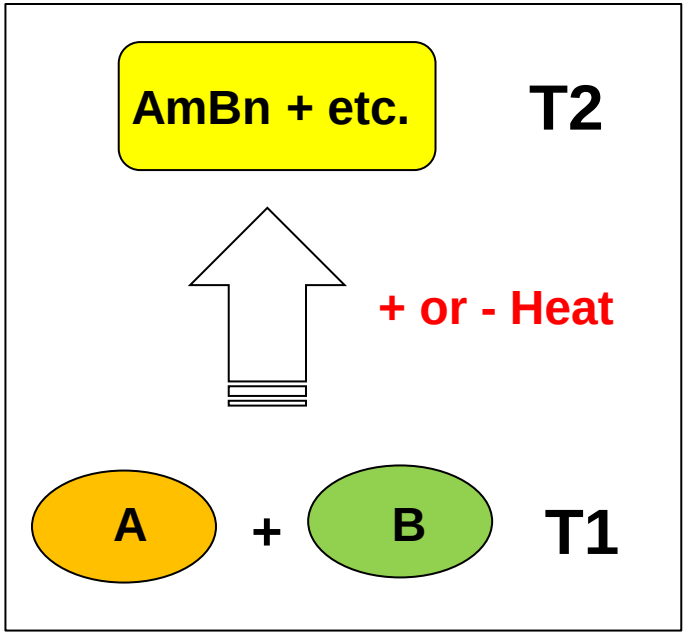
B content in liquid Si



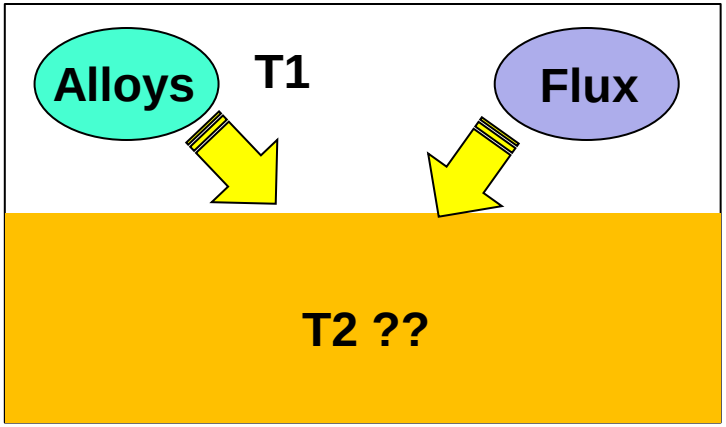


B content can be reduced with decreasing T
"page" in x-axis is amount of gas injected
(or considered as the degassing time)

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

Use two stream

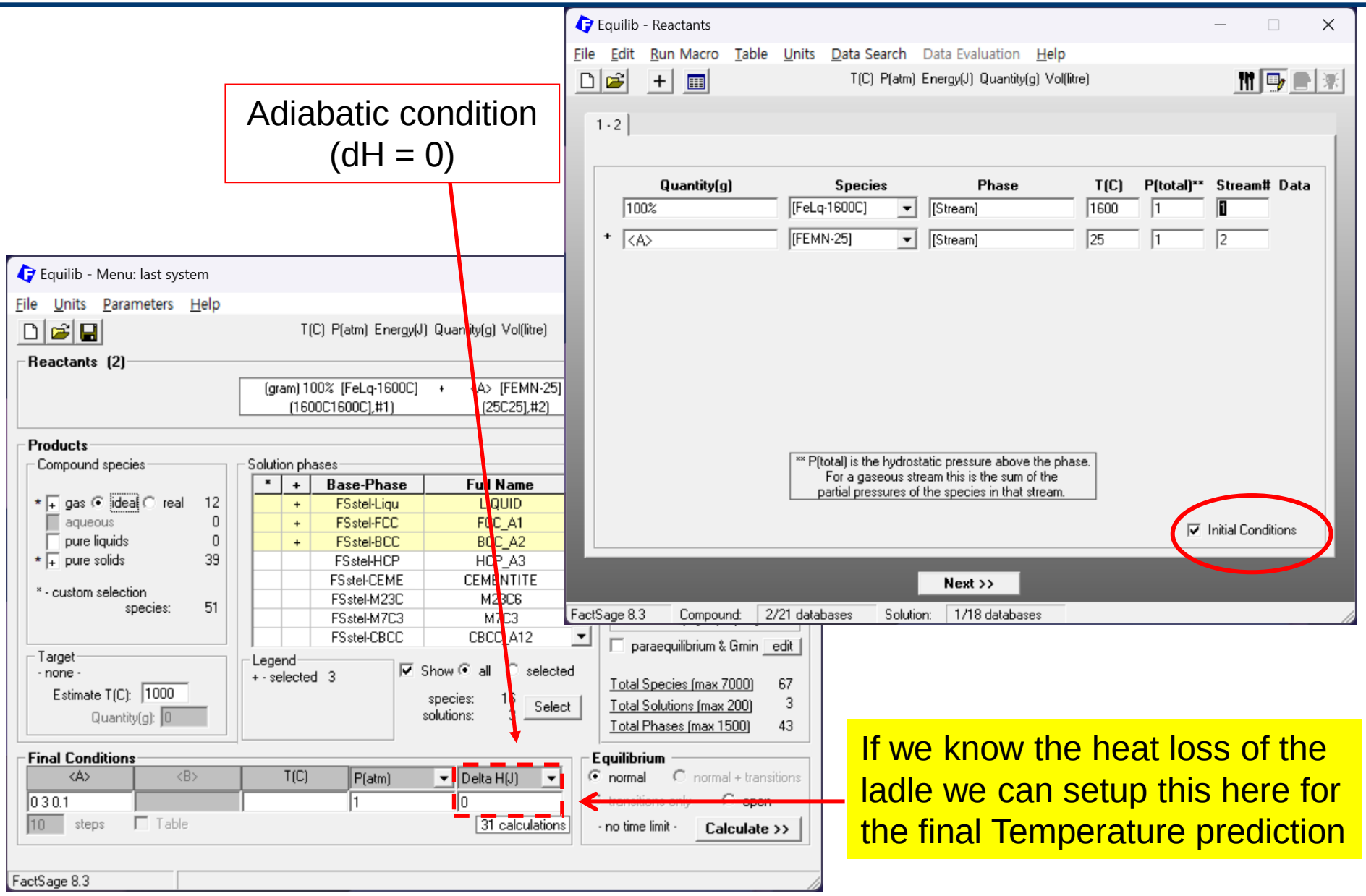
1.

```
(gram) 98.2 Fe  +  Al  +  0.8 C  =

  0          mol   gas_ideal
           (1600 C, 1 atm,      a=7.8931E-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
```

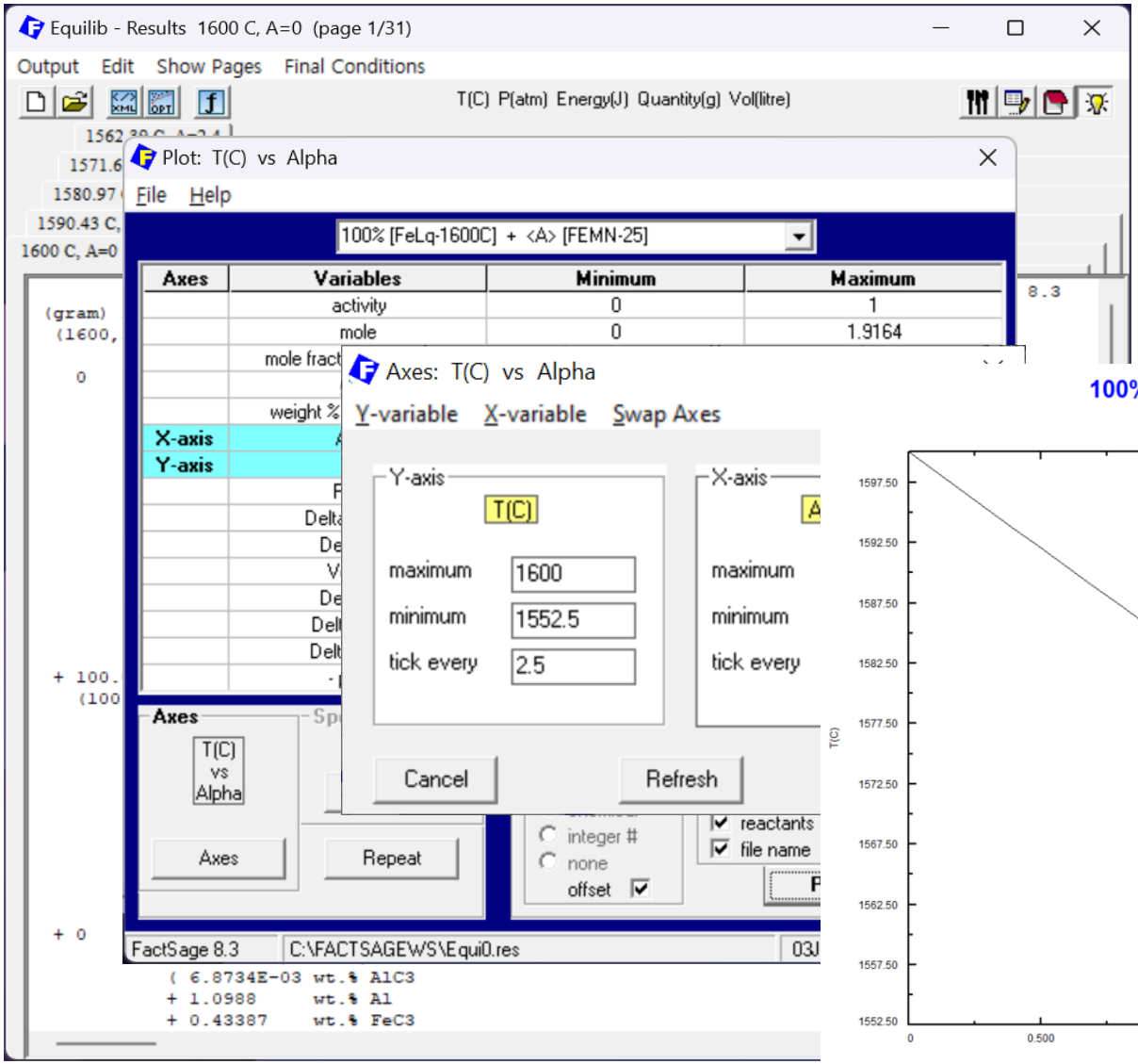
2.

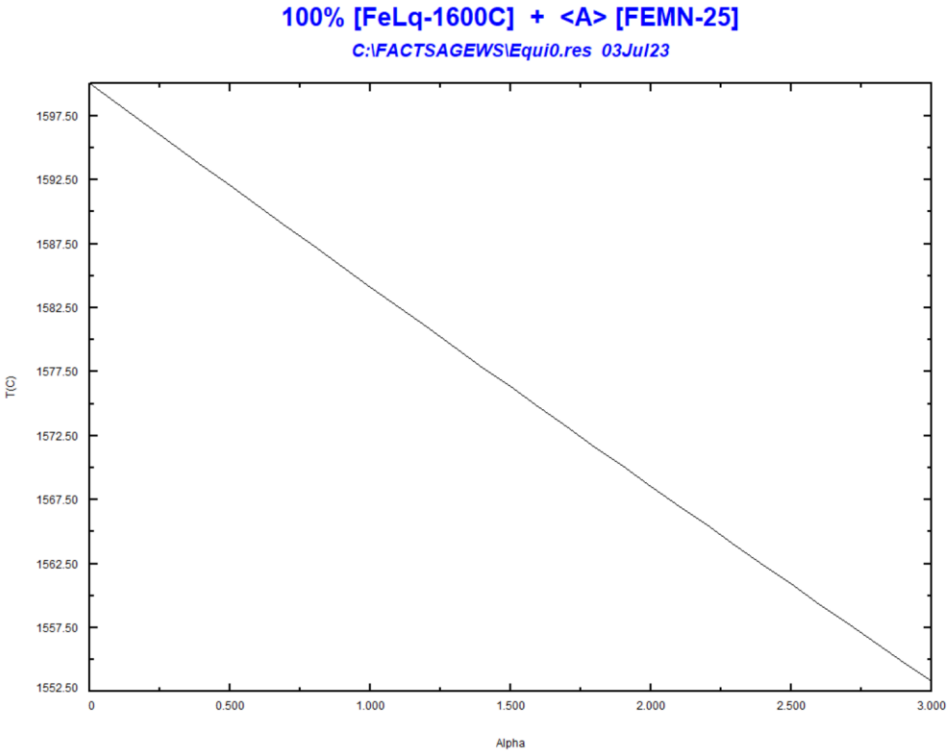
```
(gram) 65 Mn  +  35 Fe  =

  0          mol   gas_ideal
           (25 C, 1 atm,      a=4.1207E-43)
           ( 4.1207E-43       Mn
           + 2.7767E-64       Fe)

+ 79.544      gram  CBCC_A12
  (79.544 gram, 1.4436 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    4.8648E-03     4.7861E-03
```

Adiabatic condition
(dH = 0)

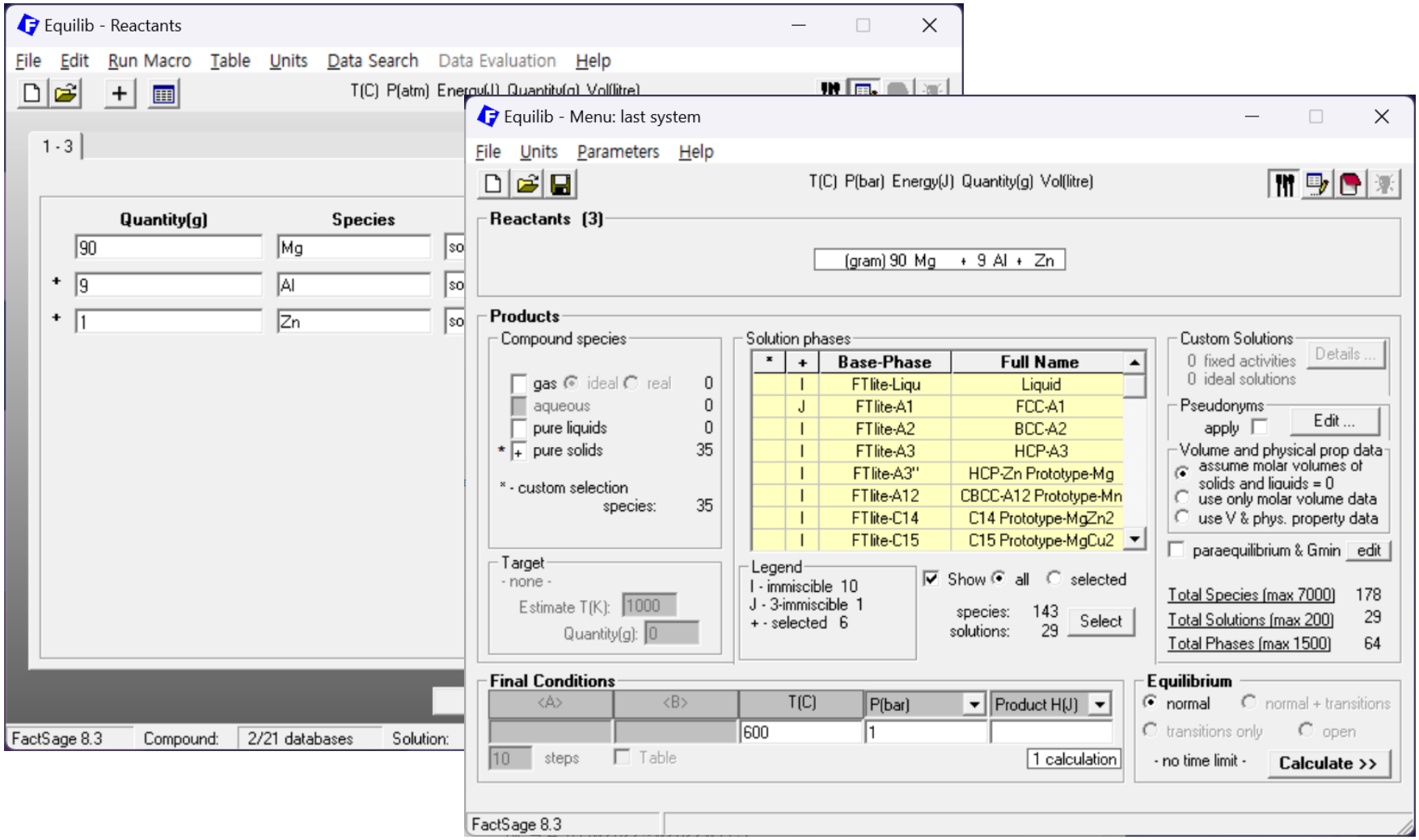


If we know the heat loss of the ladle we can setup this here for the final Temperature prediction


Equilib - Results 1600 C, A=0 (page 1/31)
Output Edit Show Pages Final Conditions
T(C) P(atm) Energy(J) Quantity(g) Vol(litre)
Plot: T(C) vs Alpha
File Help
100% [FeLq-1600C] + <A> [FEMN-25]
Axes Variables Minimum Maximum
activity 0 1
mole 0 1.9164
Axes: T(C) vs Alpha
Y-variable X-variable Swap Axes
Y-axis
T(C)
maximum 1600
minimum 1552.5
tick every 2.5
X-axis
maximum
minimum
tick every
Cancel
Refresh
Axes
T(C) vs Alpha
Axes
Repeat
integer #
none
offset
reactants
file name
FactSage 8.3
C:\FACTSAGEWS\Equi0.res
(6.8734E-03 wt.% AlC3
+ 1.0988 wt.% Al
+ 0.43387 wt.% FeC3


100% [FeLq-1600C] + <A> [FEMN-25]
C:\FACTSAGEWS\Equi0.res 03Jul23
T(C)
1597.50
1592.50
1587.50
1582.50
1577.50
1572.50
1567.50
1562.50
1557.50
1552.50
0
0.500
1.000
1.500
2.000
2.500
3.000
Alpha

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



Stream : AZ31 alloy at 600 °C

Equilib - Menu: last system

File Units Parameters Help

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

Reactants (1)

(gram) 100% [AZ91-600C]

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
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

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

Legend
I - immiscible 10
J - 3-immiscible 1
+ - selected 6

☑ Show ◉ all ○ selected
species: 143
solutions: 29
Select

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

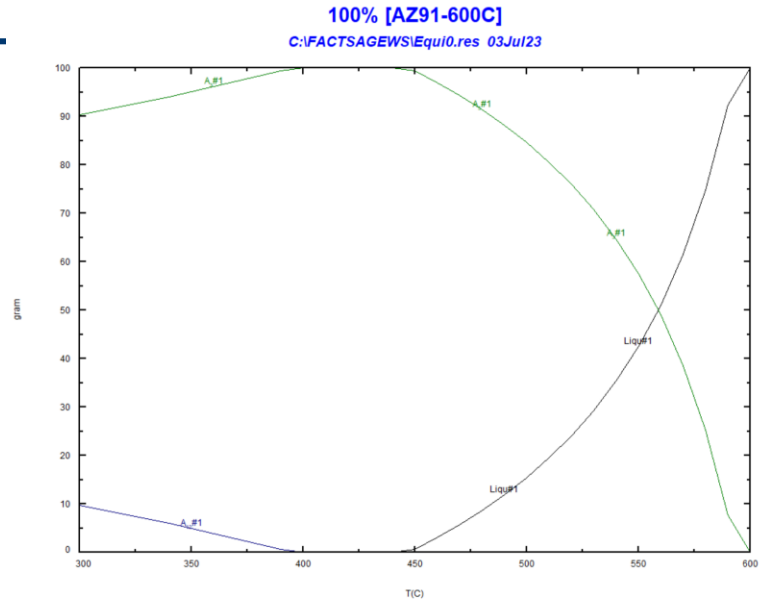
Final Conditions

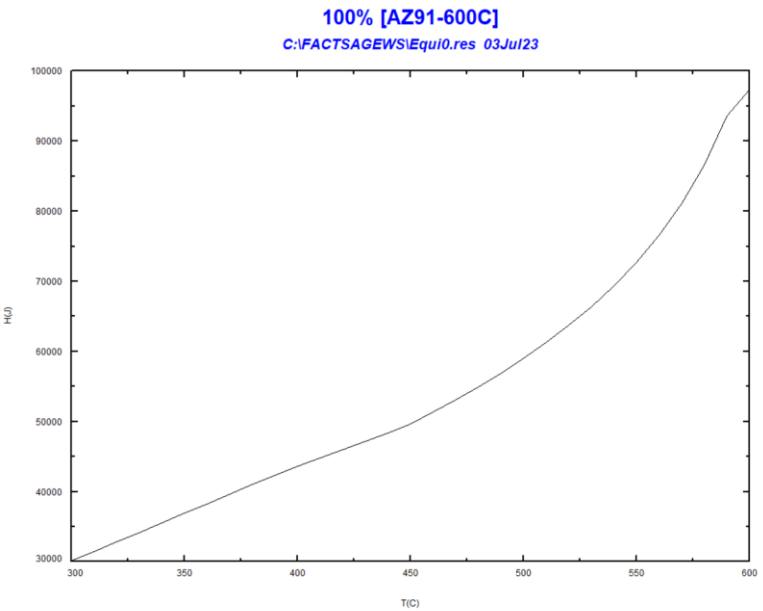
<A>	<B>	T(C)	P(bar)	Product H(J)
		600 300 10	1	

10 steps ☐ Table 31 calculations

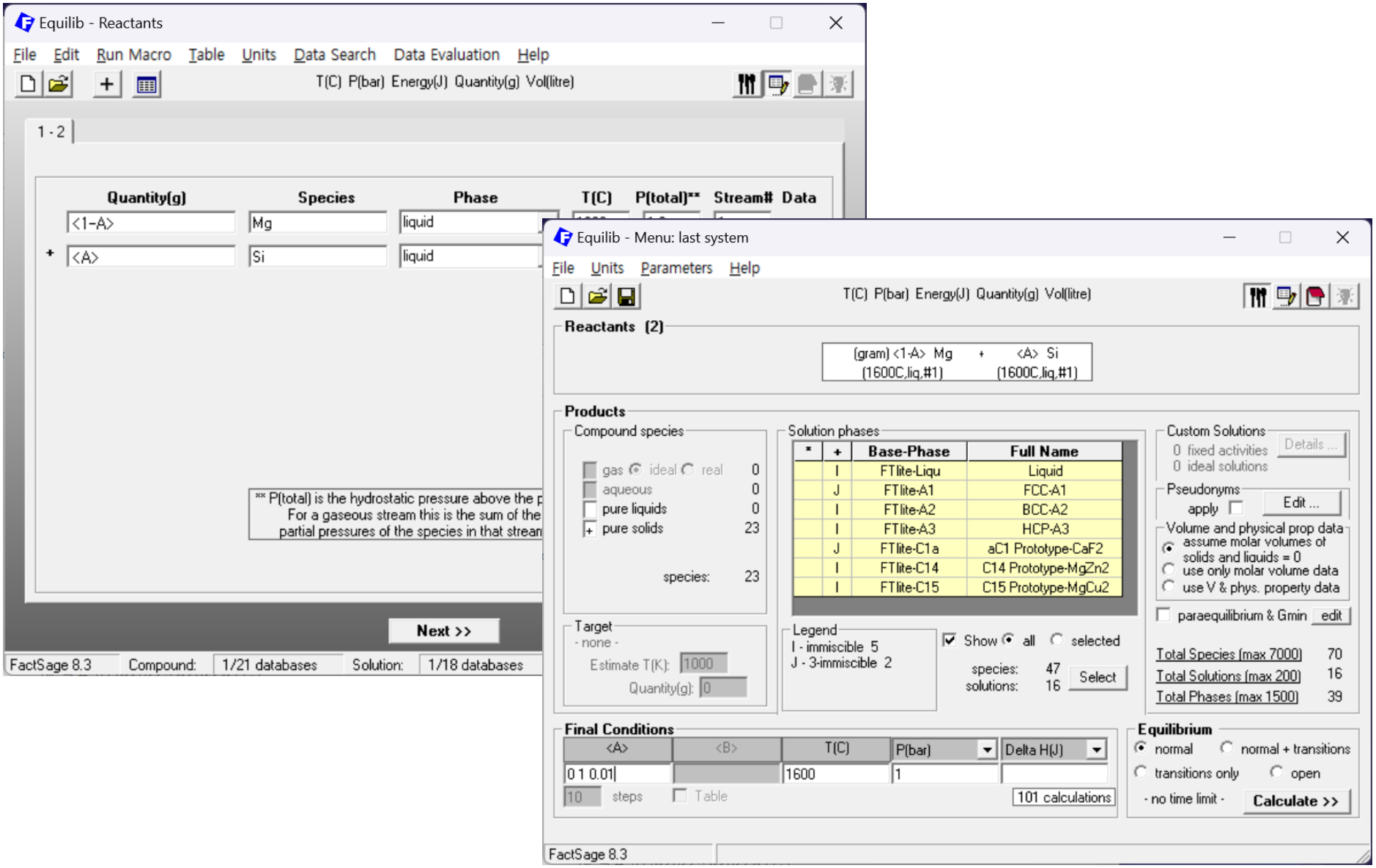
Equilibrium
- ◉ normal ○ normal + transitions
- ○ transitions only ○ open
- no time limit - Calculate >>

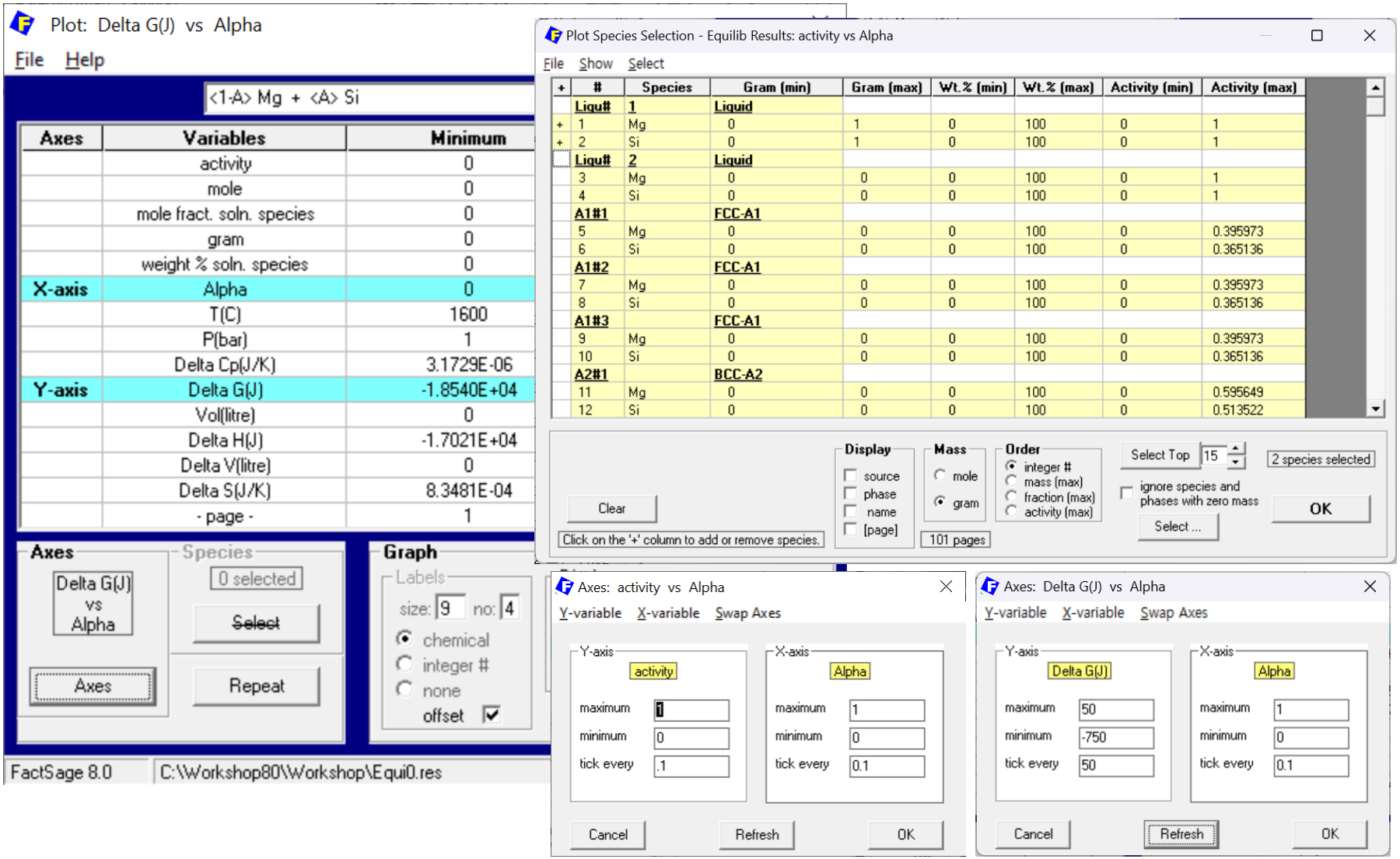
FactSage 8.3

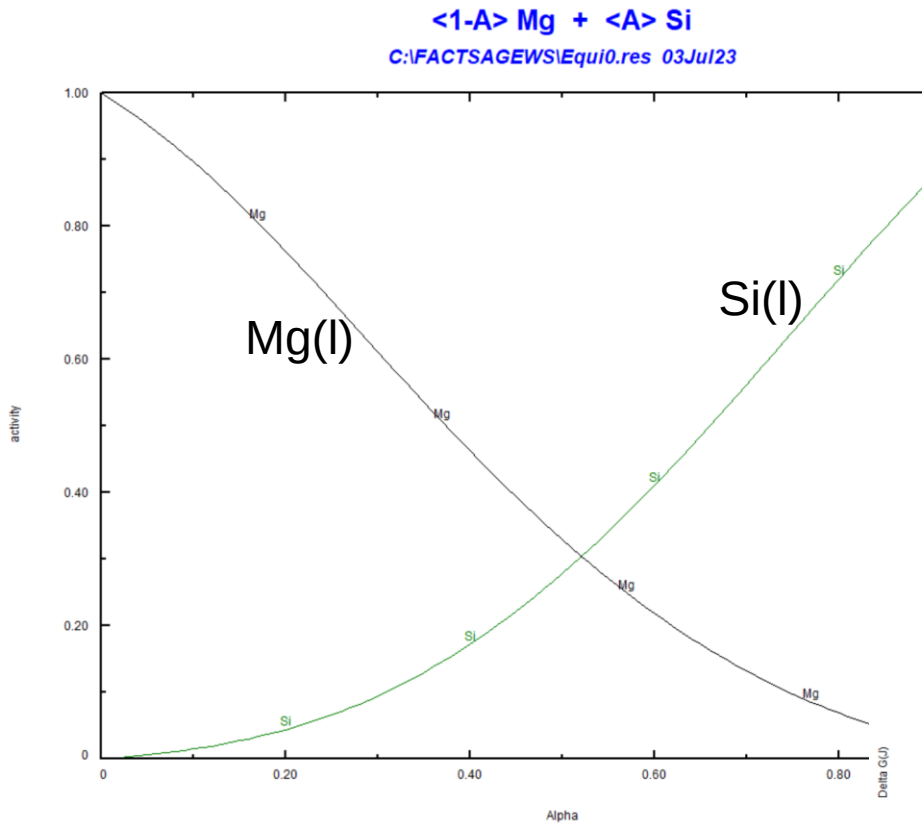


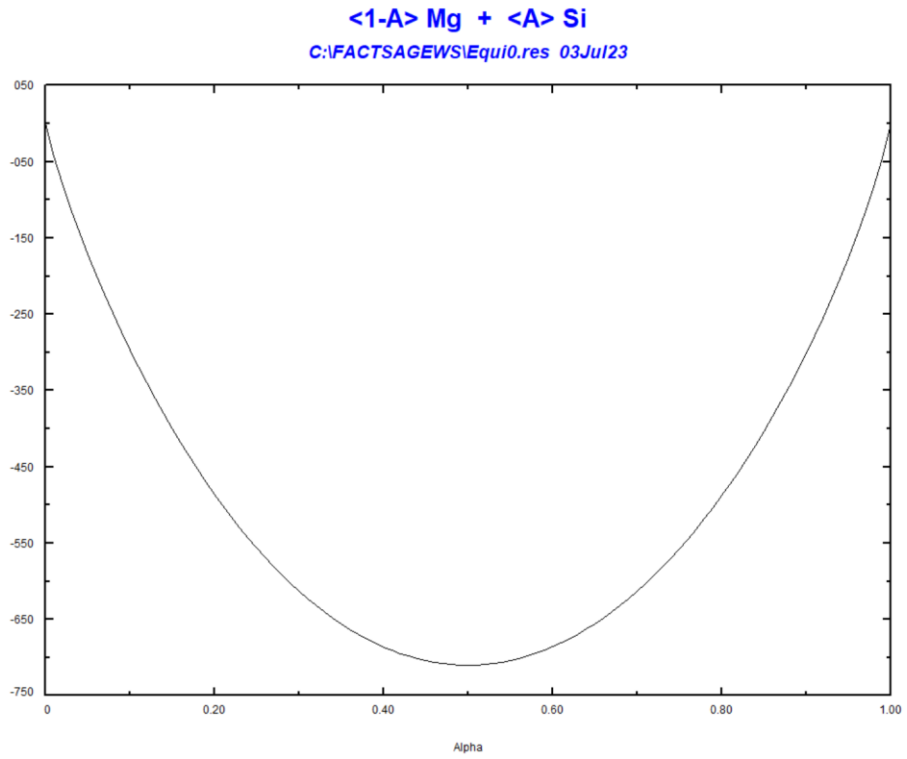


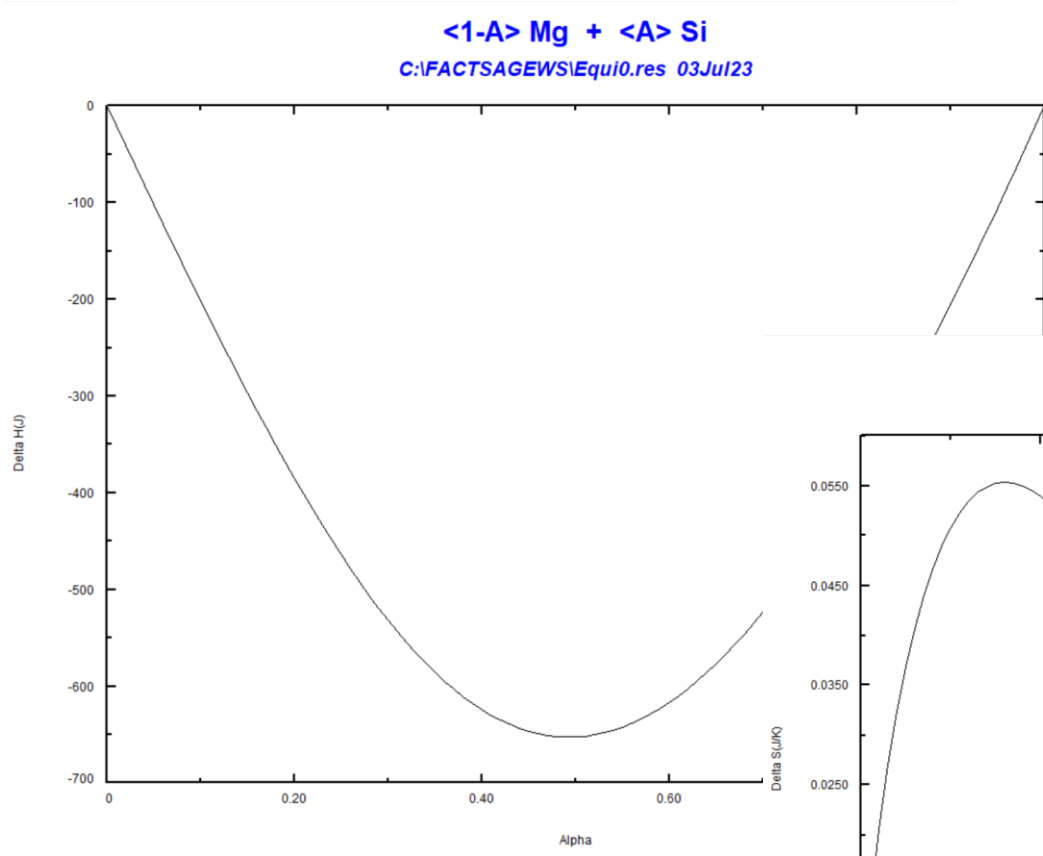
EX22-1. Thermodynamic properties: Activity, ΔG, ΔH, ΔS etc.

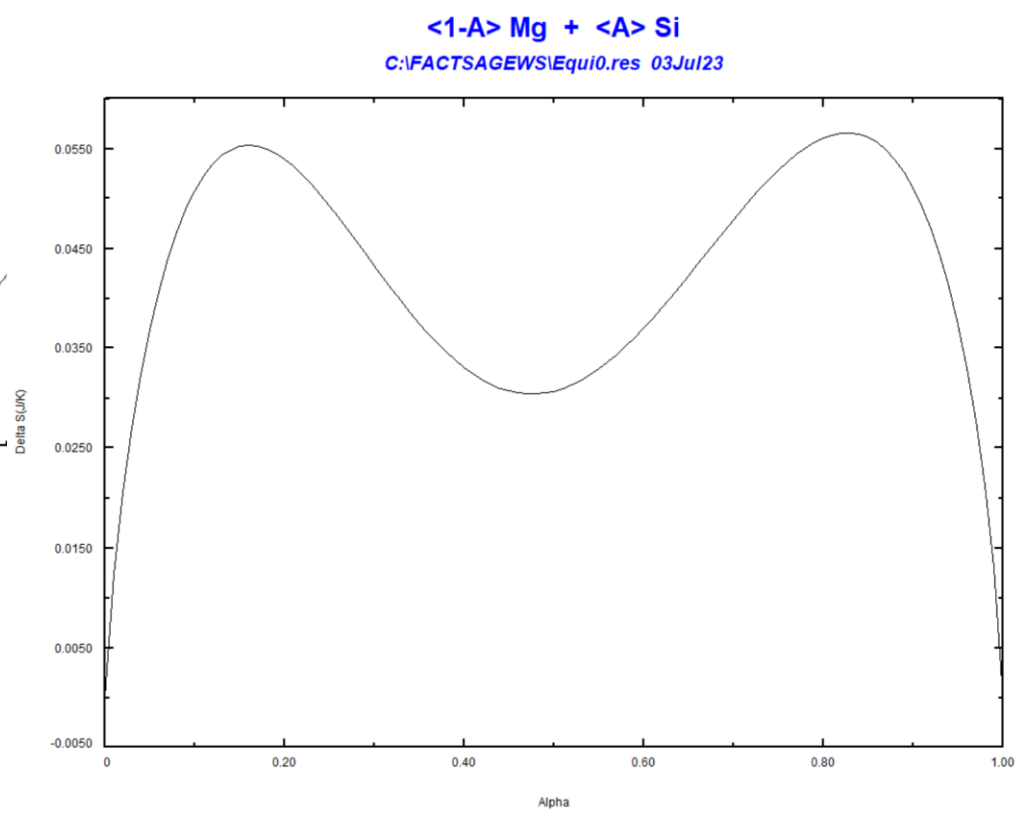



Plot: Delta G(J) vs Alpha
File Help
<1-A> Mg + <A> Si
Axes | Variables | Minimum
activity 0
mole 0
mole fract. soln. species 0
gram 0
weight % soln. species 0
X-axis Alpha 0
T(C) 1600
P(bar) 1
Delta Cp(J/K) 3.1729E-06
Y-axis Delta G(J) -1.8540E+04
Vol(litre) 0
Delta H(J) -1.7021E+04
Delta V(litre) 0
Delta S(J/K) 8.3481E-04
- page - 1
Axes
Delta G(J) vs Alpha
Axes
Species
0 selected
Select
Repeat
Graph
Labels
size: 9 no: 4
chemical
integer #
none
offset
FactSage 8.0
C:\Workshop80\Workshop\Equi0.res
Plot Species Selection - Equilib Results: activity vs Alpha
File Show Select
+ # Species Gram (min) Gram (max) Wt.% (min) Wt.% (max) Activity (min) Activity (max)
Liqu# 1 Liquid
1 Mg 0 1 0 100 0 1
2 Si 0 1 0 100 0 1
Liqu# 2 Liquid
3 Mg 0 0 0 100 0 1
4 Si 0 0 0 100 0 1
A1#1 FCC-A1
5 Mg 0 0 0 100 0 0.395973
6 Si 0 0 0 100 0 0.365136
A1#2 FCC-A1
7 Mg 0 0 0 100 0 0.395973
8 Si 0 0 0 100 0 0.365136
A1#3 FCC-A1
9 Mg 0 0 0 100 0 0.395973
10 Si 0 0 0 100 0 0.365136
A2#1 BCC-A2
11 Mg 0 0 0 100 0 0.595649
12 Si 0 0 0 100 0 0.513522
Clear
Click on the '+' column to add or remove species.
Display
source
phase
name
[page]
Mass
mole
gram
101 pages
Order
integer #
mass (max)
fraction (max)
activity (max)
Select Top 15
2 species selected
ignore species and phases with zero mass
Select ...
OK
Axes: activity vs Alpha
Y-variable X-variable Swap Axes
Y-axis
activity
maximum 1
minimum 0
tick every .1
X-axis
Alpha
maximum 1
minimum 0
tick every 0.1
Cancel Refresh OK
Axes: Delta G(J) vs Alpha
Y-variable X-variable Swap Axes
Y-axis
Delta G(J)
maximum 50
minimum -750
tick every 50
X-axis
Alpha
maximum 1
minimum 0
tick every 0.1
Cancel Refresh OK

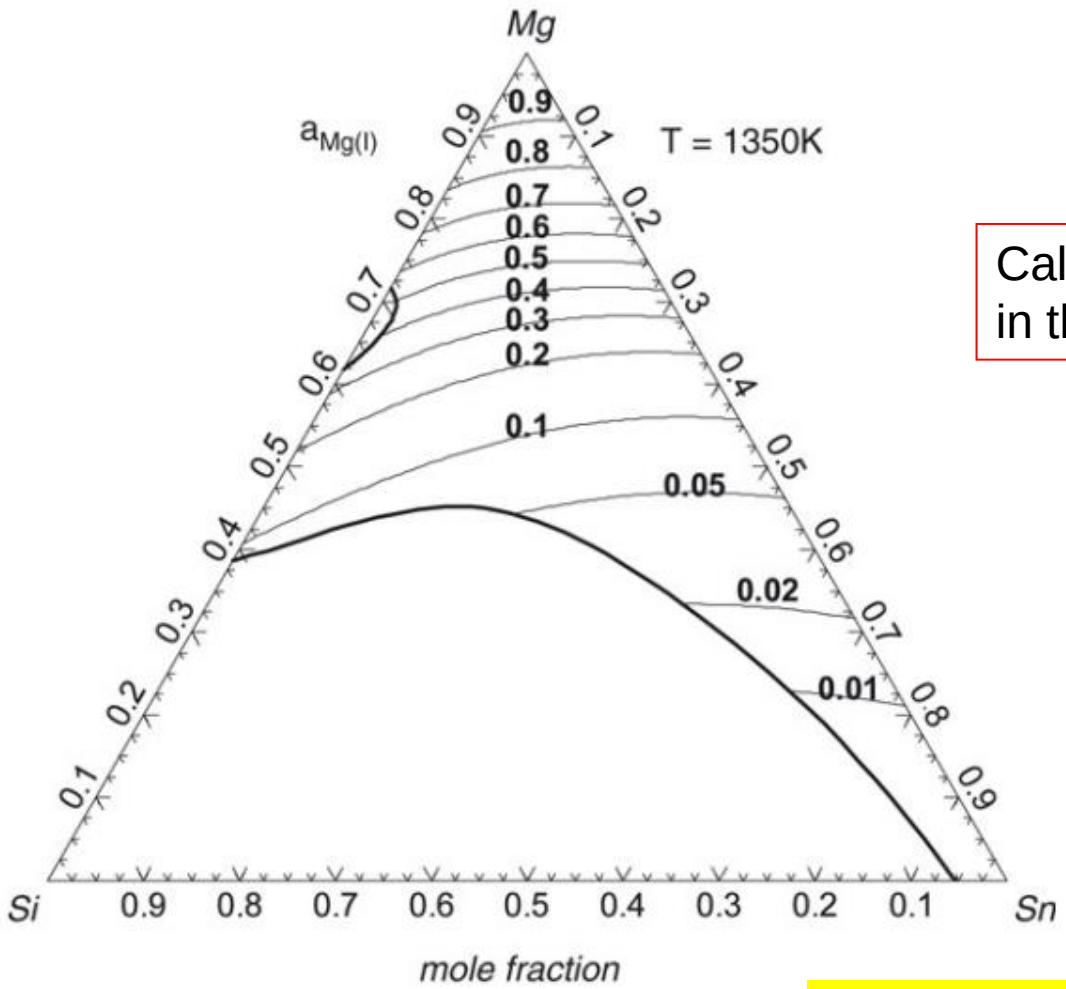

<1-A> Mg + <A> Si
C:\FACTSAGEWS\Equi0.res 03Jul23
Mg(l)
Si(l)
activity
Alpha
Mg
Si
1.00
0.80
0.60
0.40
0.20
0
0.20
0.40
0.60
0.80


<1-A> Mg + <A> Si
C:\FACTSAGEWS\Equi0.res 03Jul23
Delta GJ)
Alpha
050
-050
-150
-250
-350
-450
-550
-650
-750
0
0.20
0.40
0.60
0.80
1.00


<1-A> Mg + <A> Si
C:\FACTSAGEWS\Equi0.res 03Jul23
0
-100
-200
-300
-400
-500
-600
-700
Delta H(J)
0
0.20
0.40
0.60
Alpha


<1-A> Mg + <A> Si
C:\FACTSAGEWS\Equi0.res 03Jul23
0.0550
0.0450
0.0350
0.0250
0.0150
0.0050
-0.0050
Delta S(J/K)
0
0.20
0.40
0.60
0.80
1.00
Alpha

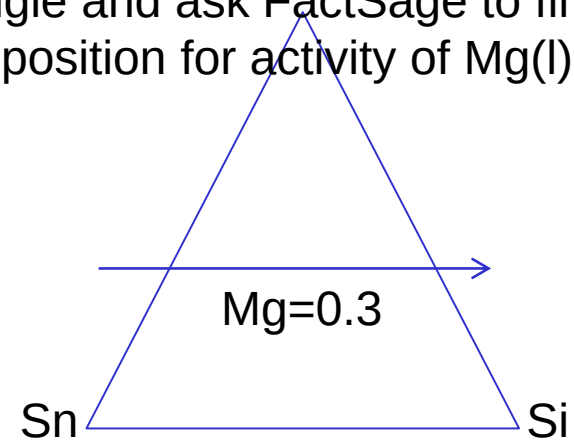
EX22-2. Iso-activity line in ternary system



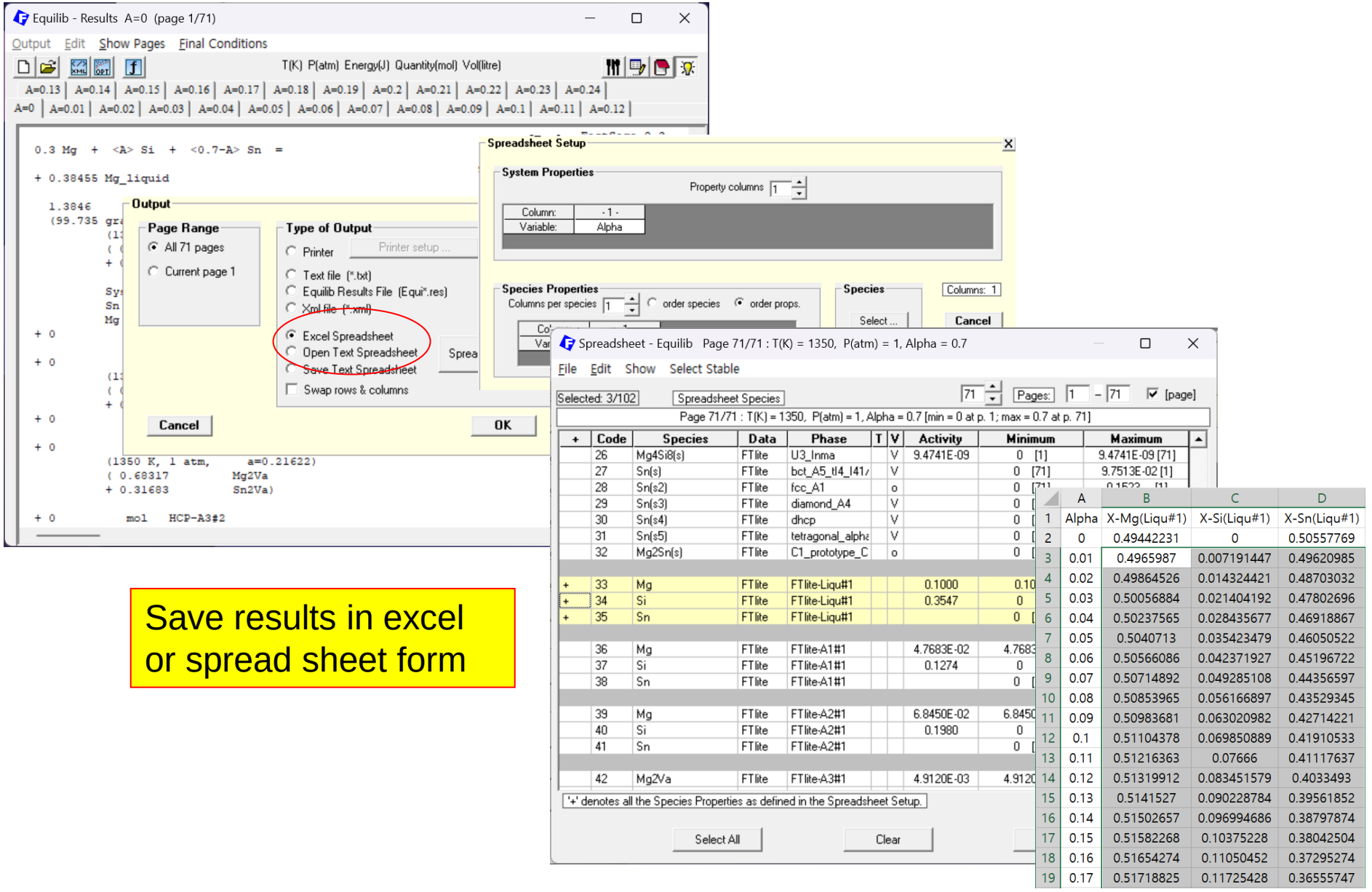
Calculation of iso-activity line of Mg(l) in the Mg-Si-Sn system at T=1350 K

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

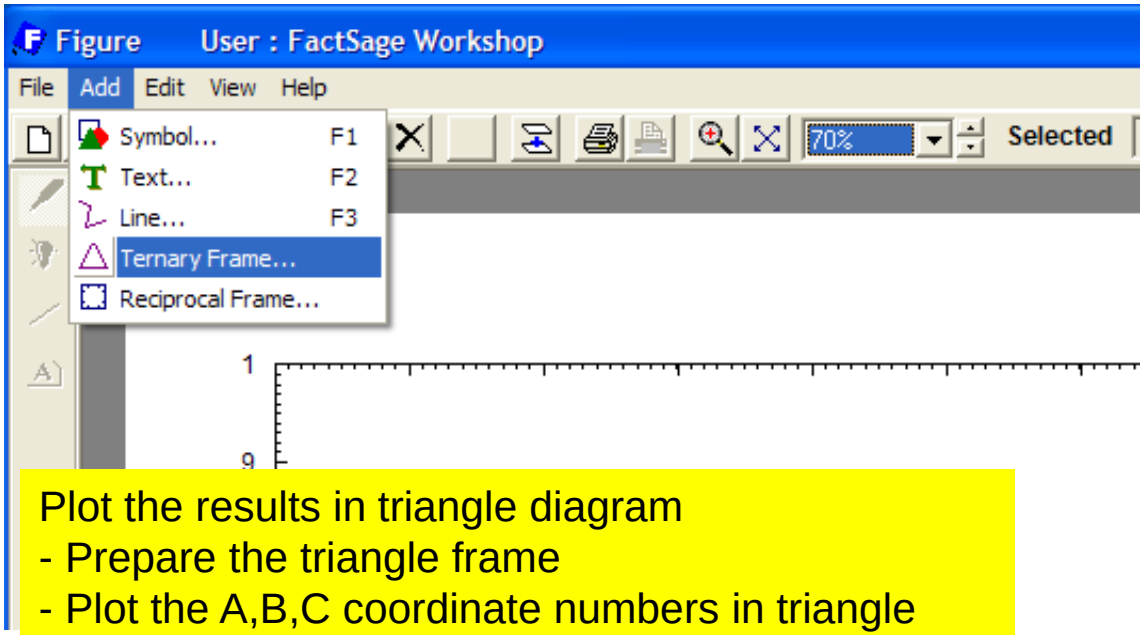
scan X_{Mg} = 0.3 from left to right of this triangle and ask FactSage to find out composition for activity of Mg(l) = 0.1



(1) Click mouth right button on “pure liquids” →
(2) Click “+” button to (3) setup activity of element (this case is for Mg)

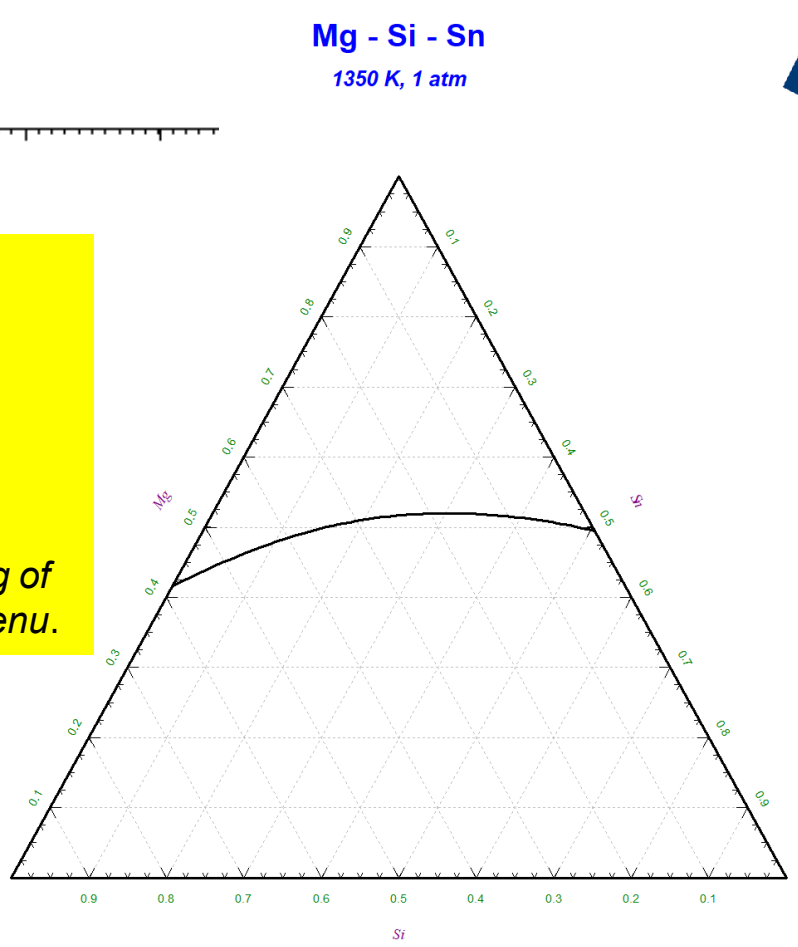


Save results in excel or spread sheet form

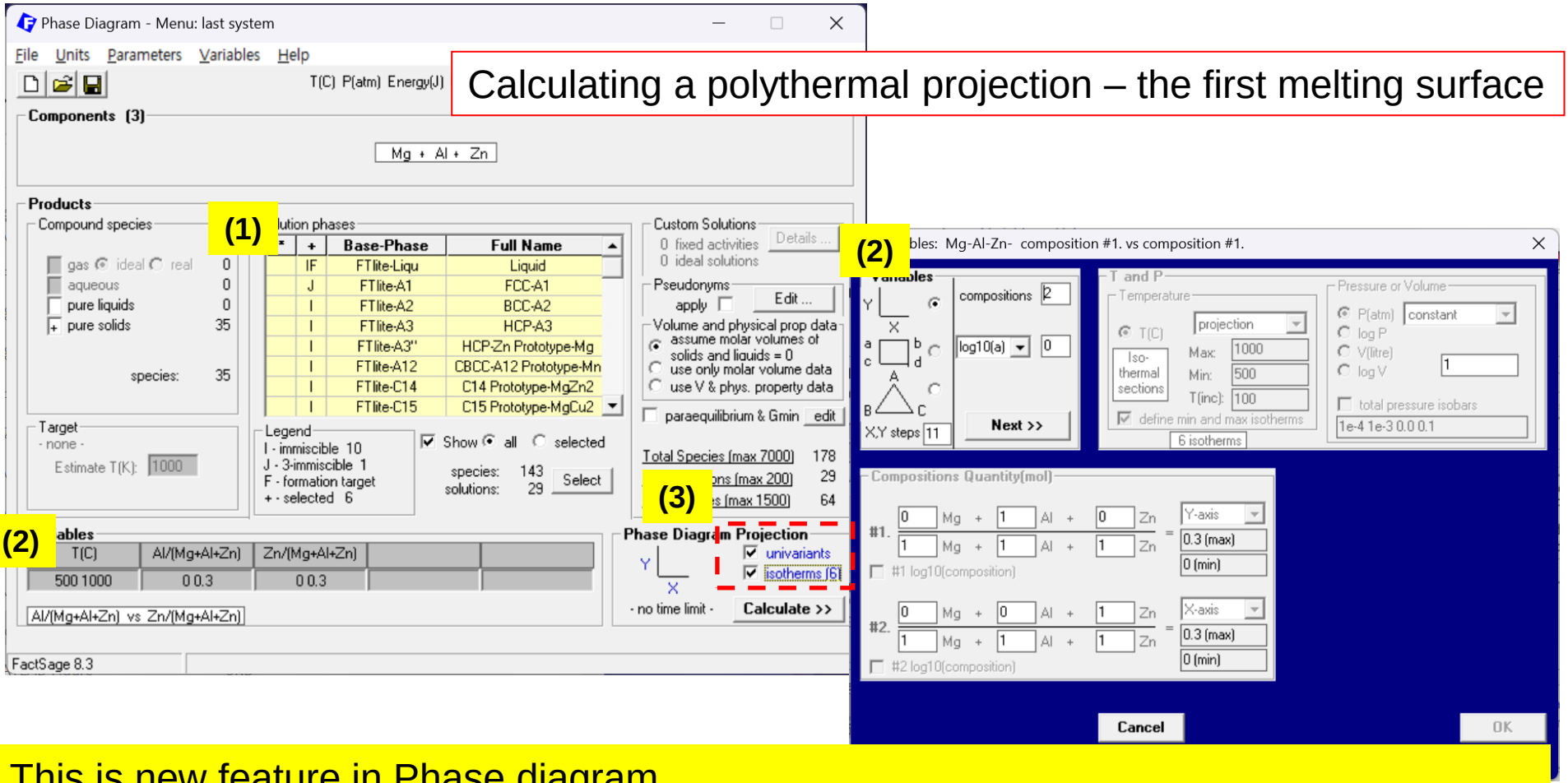


Plot the results in triangle diagram
- Prepare the triangle frame
- Plot the A,B,C coordinate numbers in triangle diagram
"Cont+C" → "Cont+V" or "copy" and "paste".

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



EX23. Calculation for Solidus lines (Solidus projection)

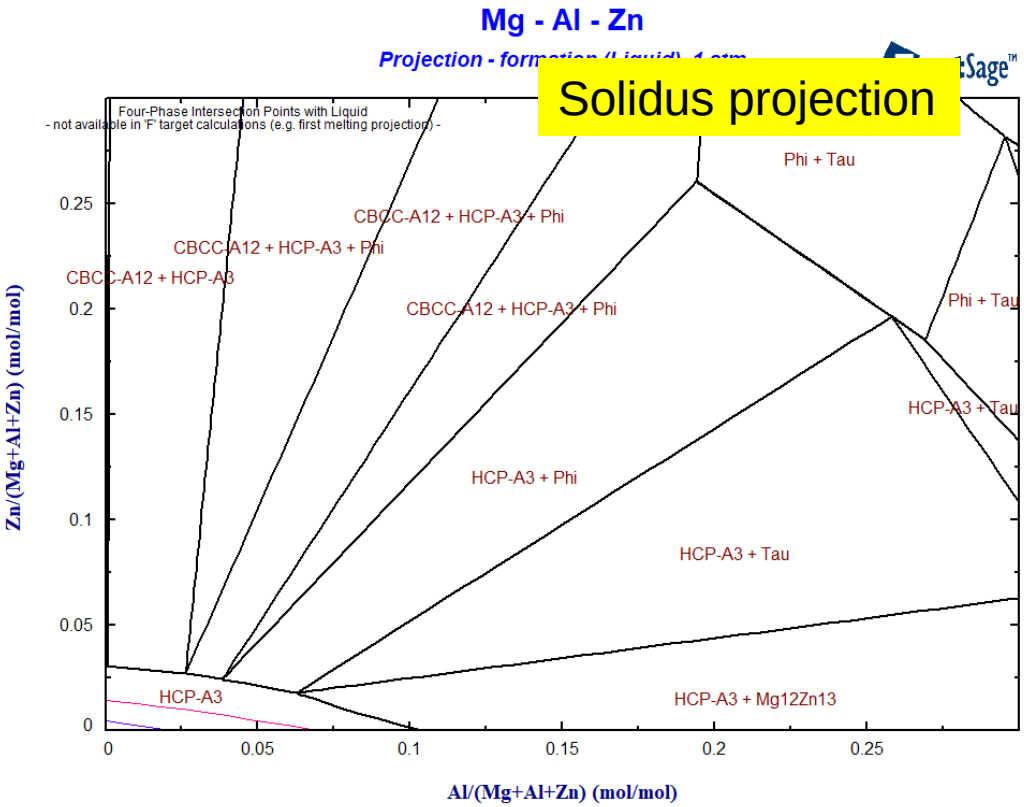


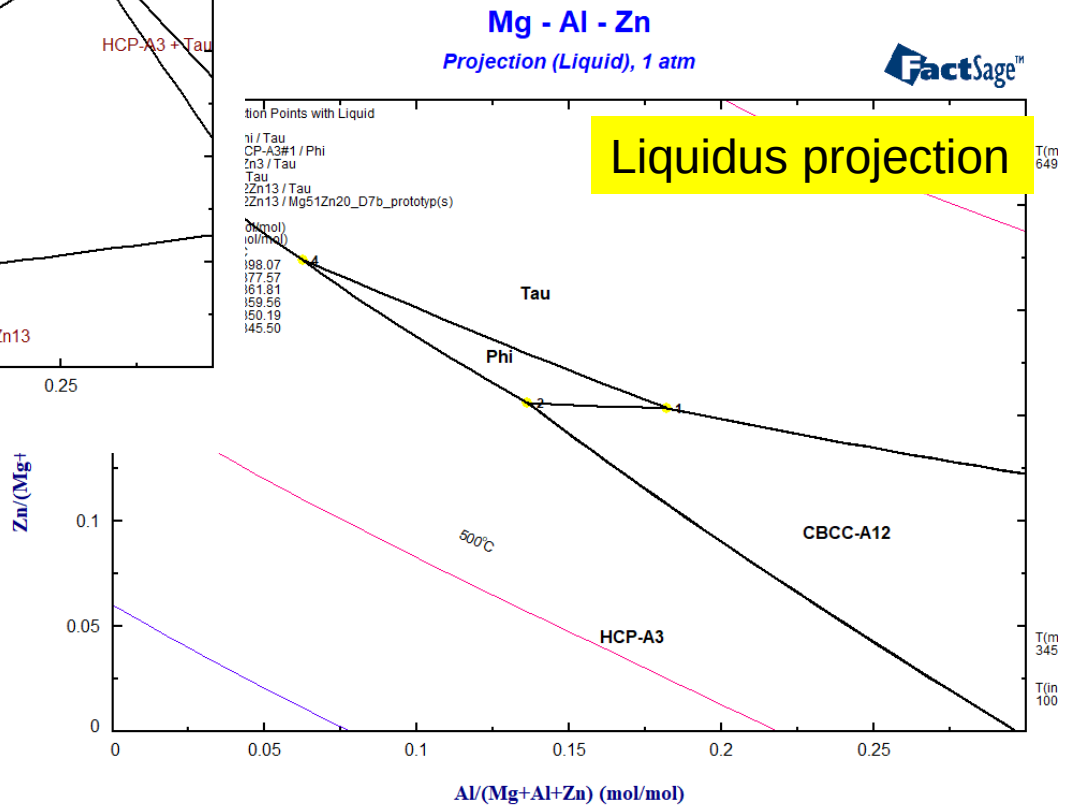
Calculating a polythermal projection – the first melting surface

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)

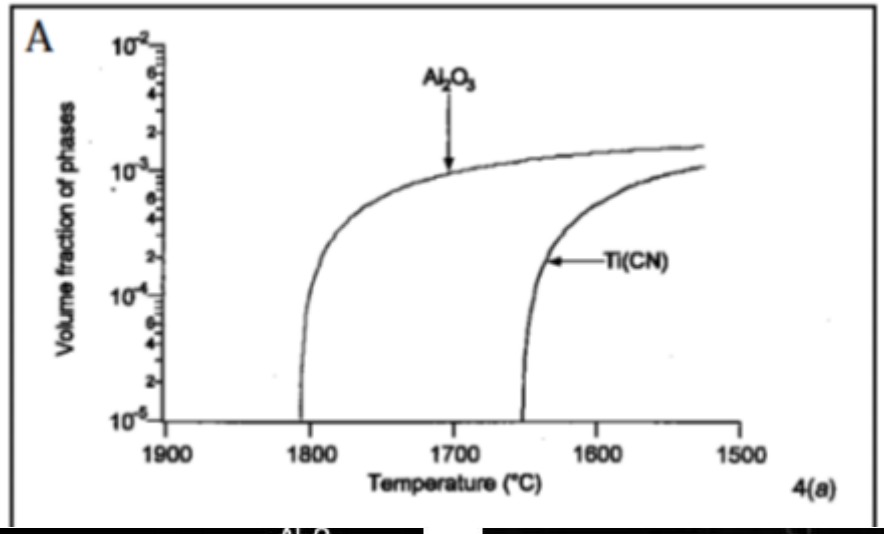


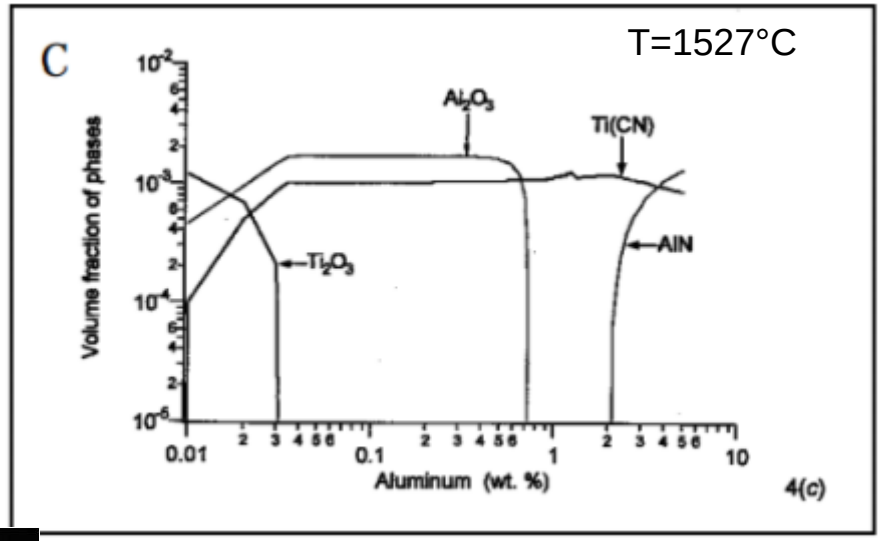


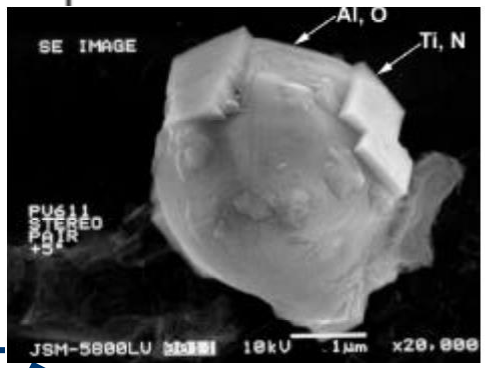
EX24. Non-metallic Inclusion formation during metal solidification

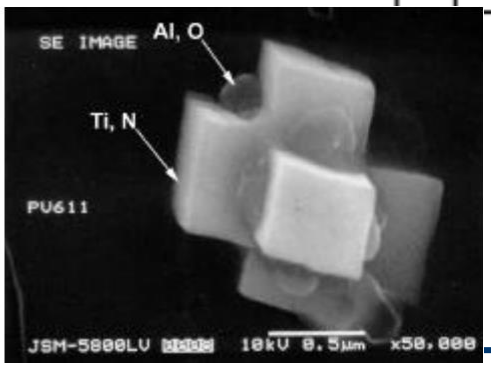
Table 3 — Chemical Test Summary

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





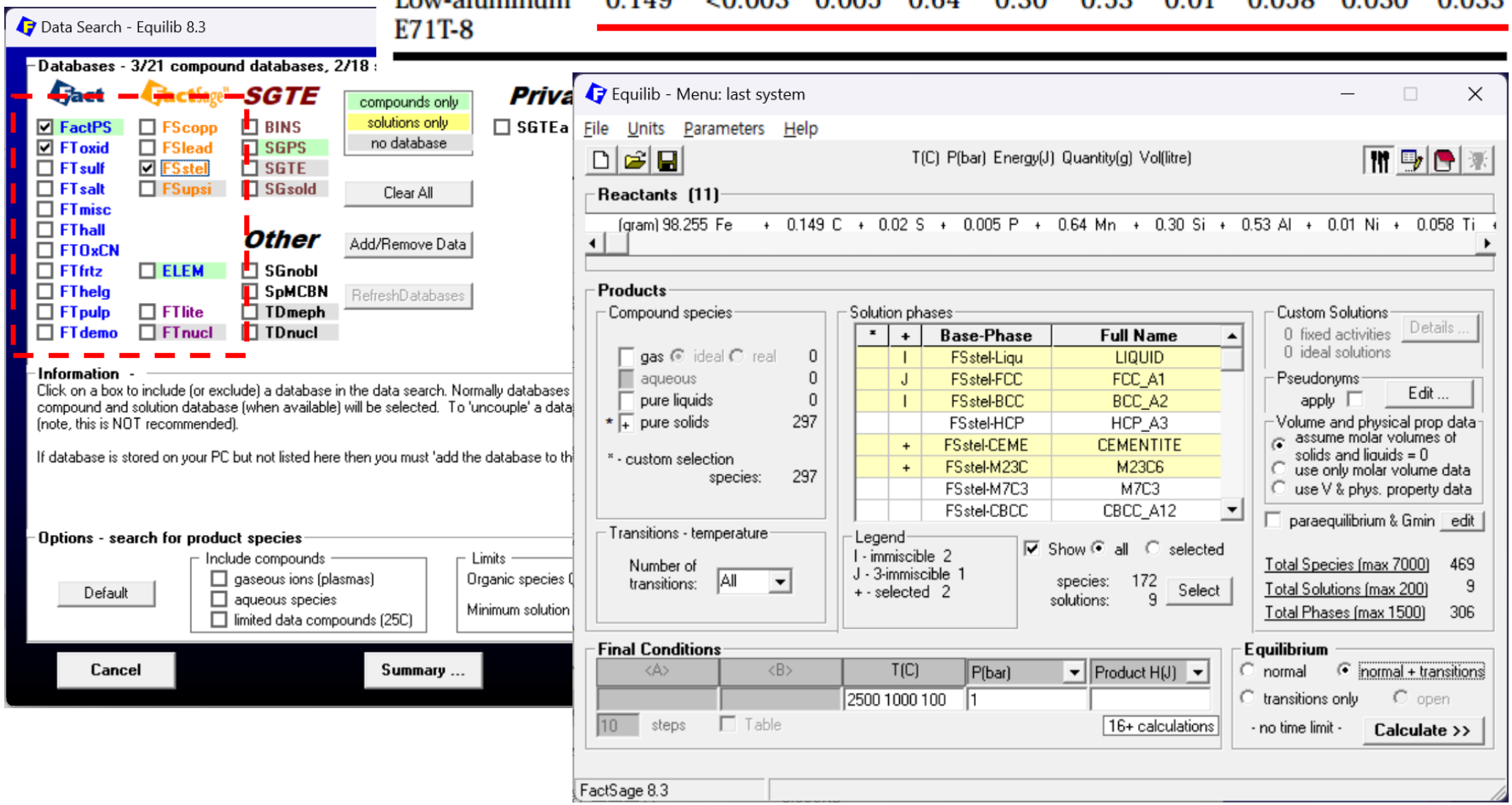




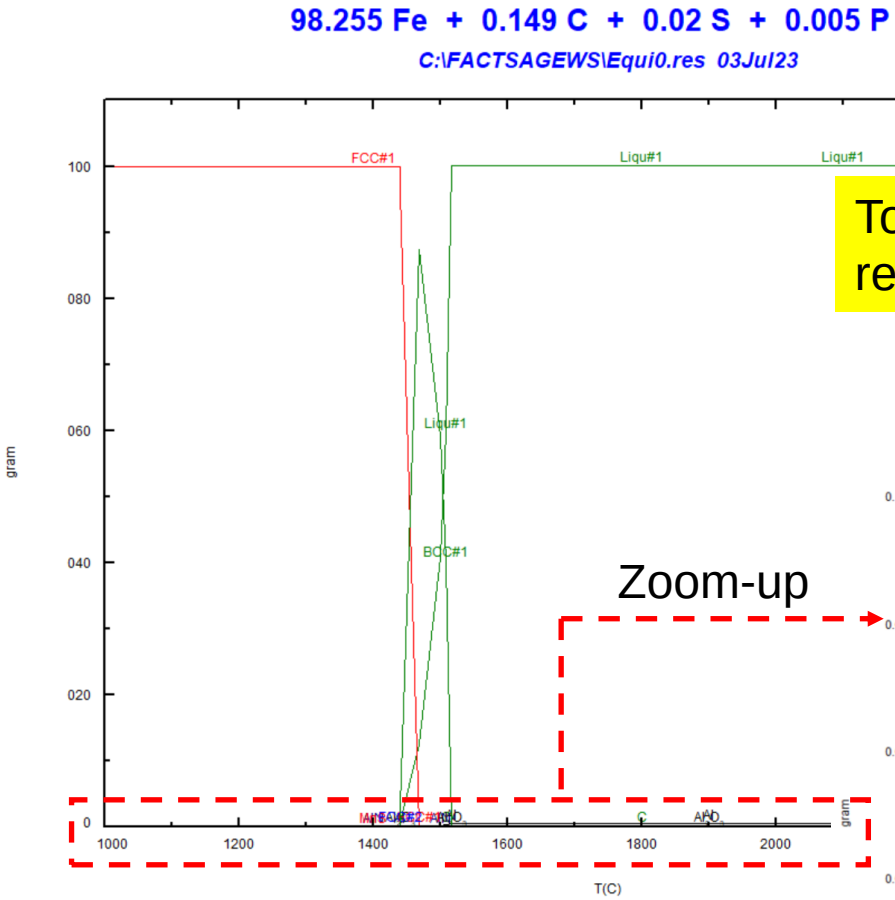
AWS 80th Annual Meeting, April 12–15, 1999, St. Louis, Mo. Page 98-s to 105-s

Table 3 — Chemical Test Summary

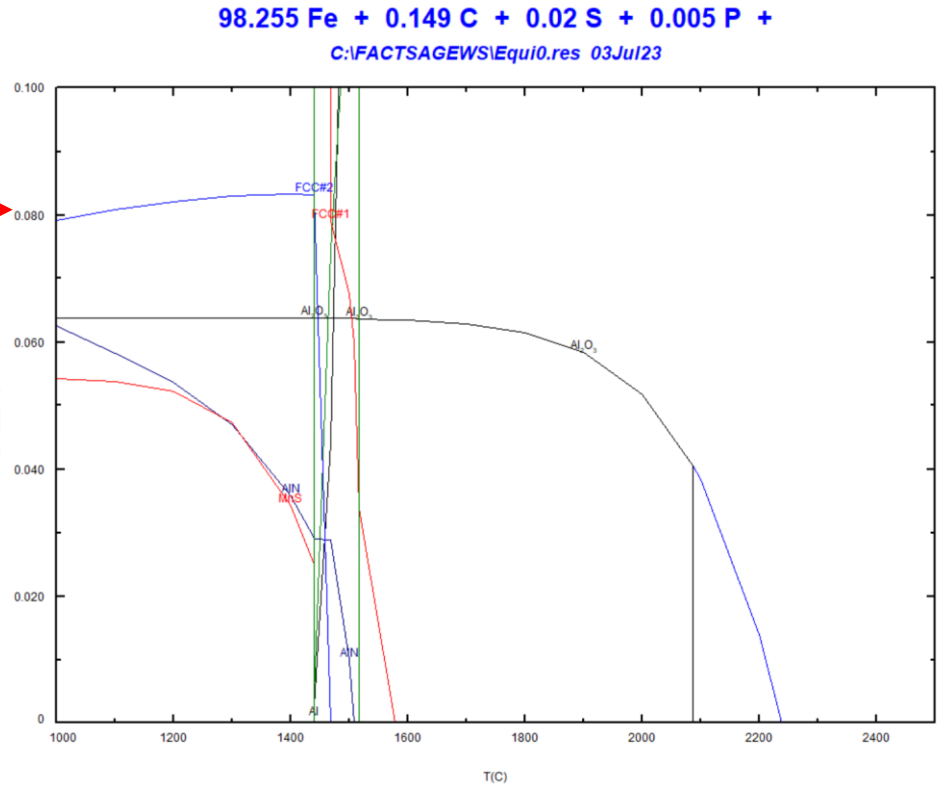
Weld	C	S	P	Mn	Si	Al	Ni	Ti	O	N
High-aluminum E70T-4	0.234	<0.003	0.011	0.50	0.28	1.70	0.02	0.003	0.006	0.064
Low-aluminum E71T-8	0.149	<0.003	0.005	0.64	0.30	0.53	0.01	0.058	0.030	0.033



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

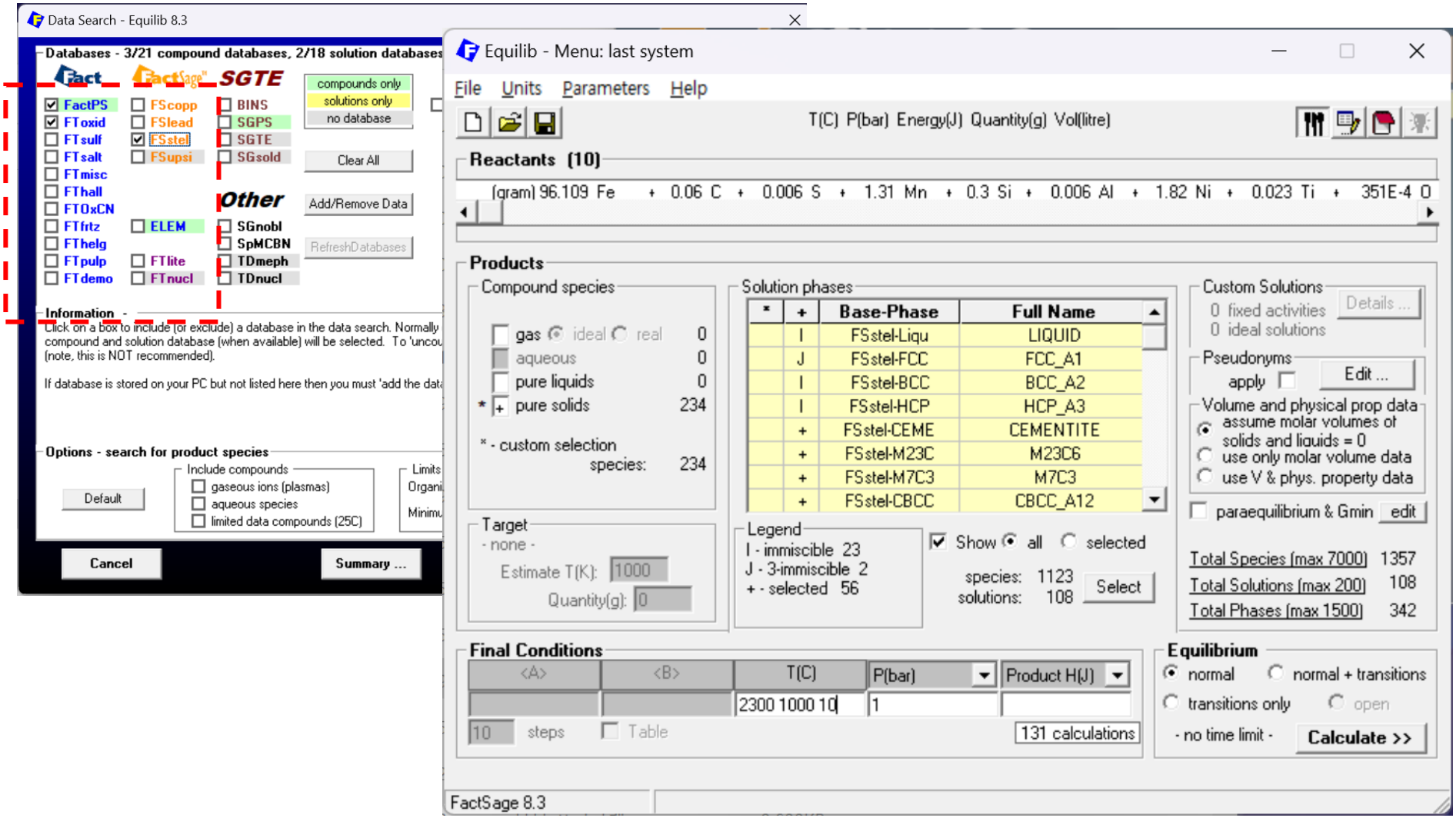


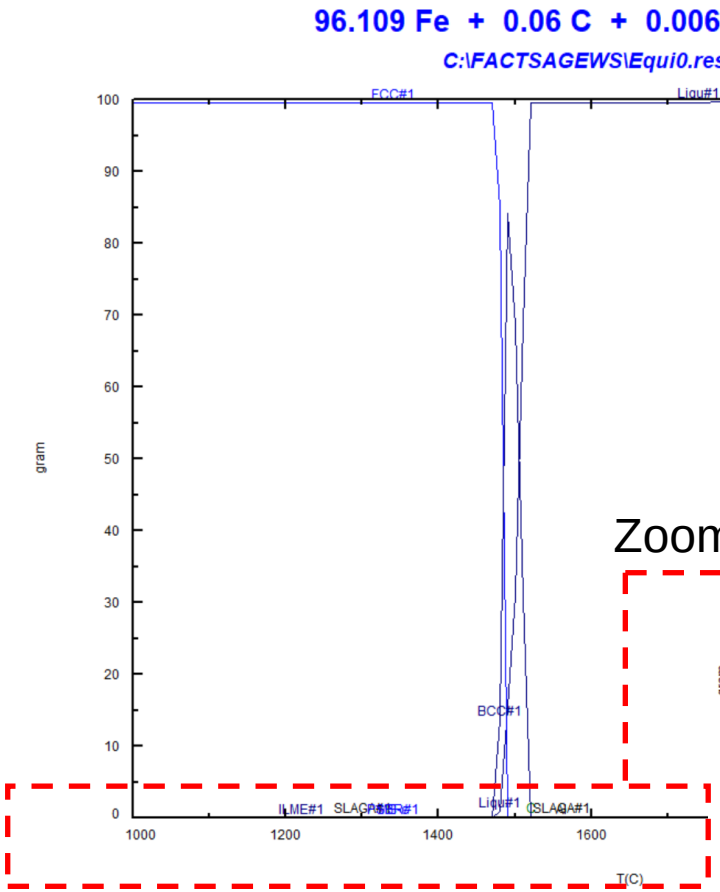
Zoom-up



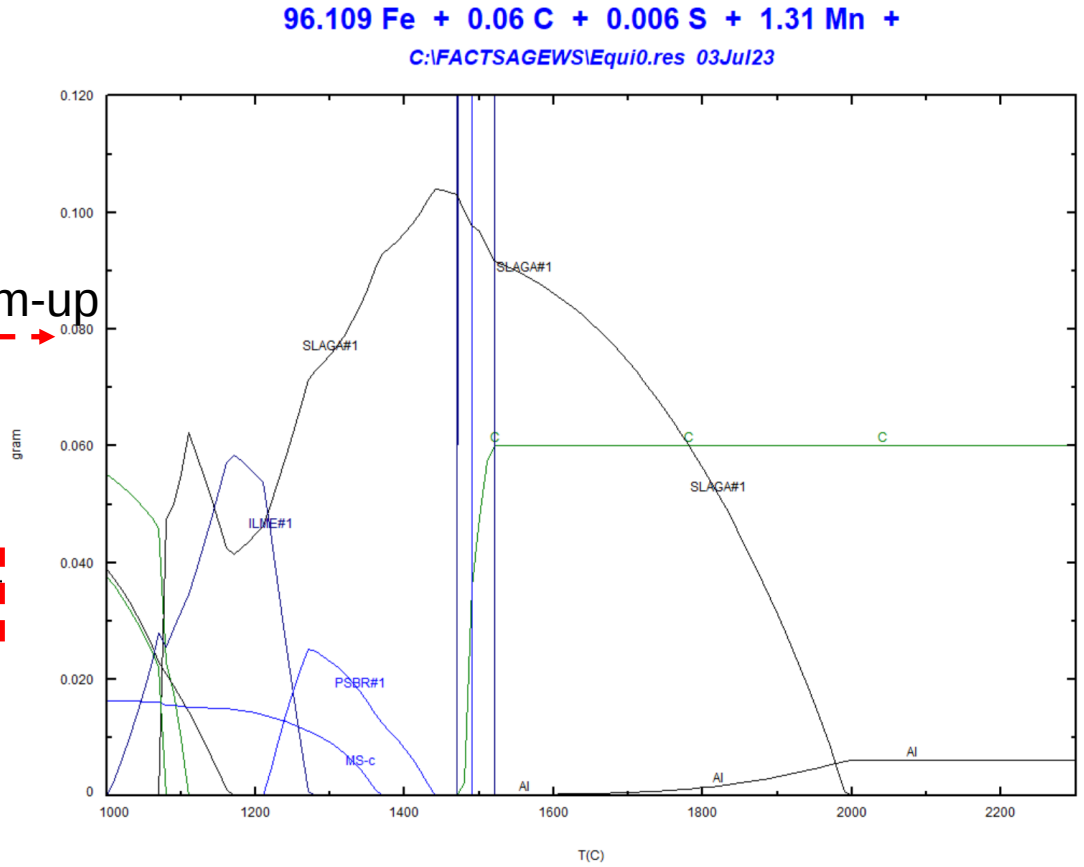
EX24. Non-metallic Inclusion formation during metal solidification

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



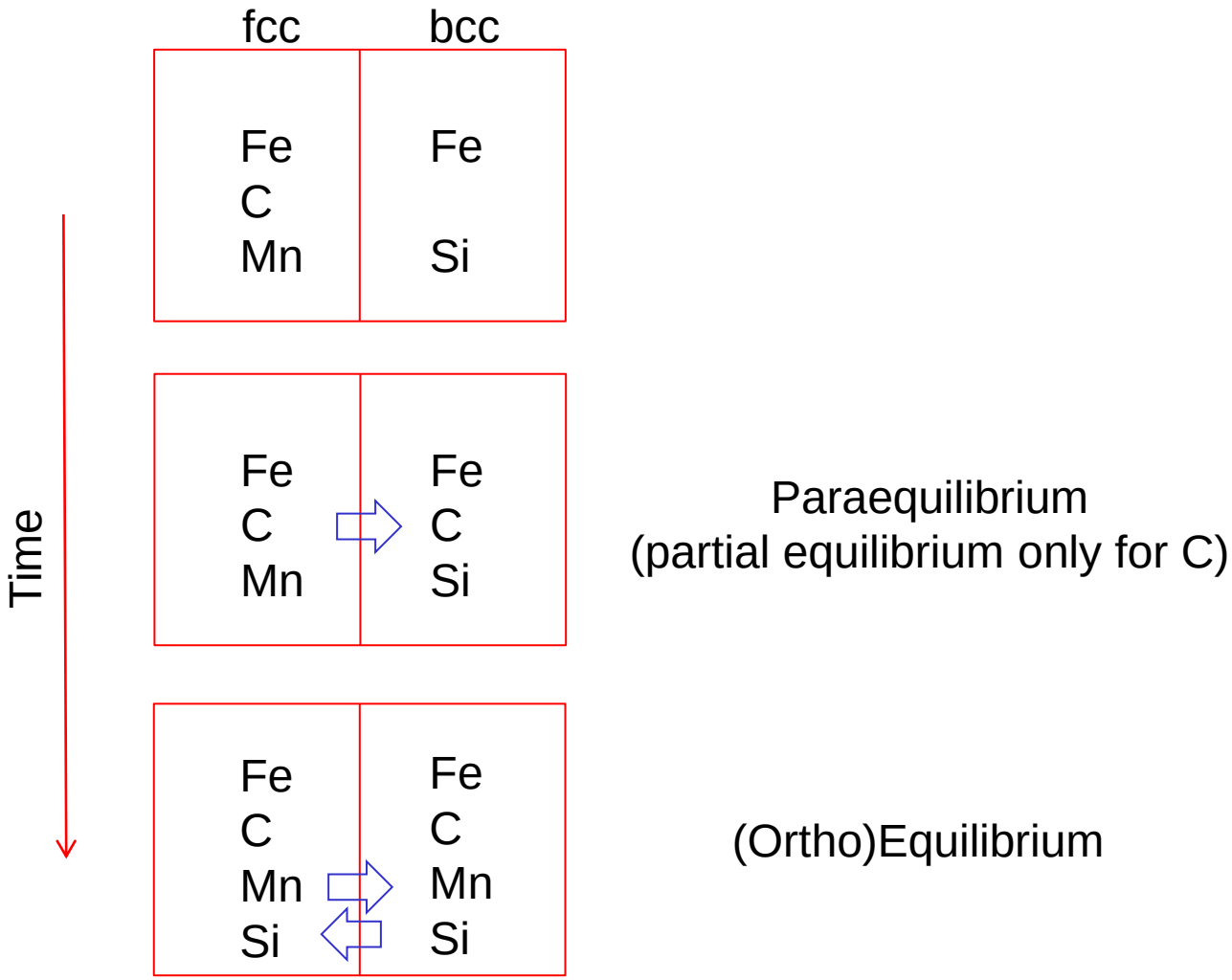

96.109 Fe + 0.06 C + 0.006 S + 1.31 Mn +
C:\FACTSAGEWS\Equi0.res 03Jul23
FCC#1
Liqu#1
Liqu#1
BCC#1
ILME#1
Liqu#1
SLAGA#1
gram
T(C)

Zoom-up

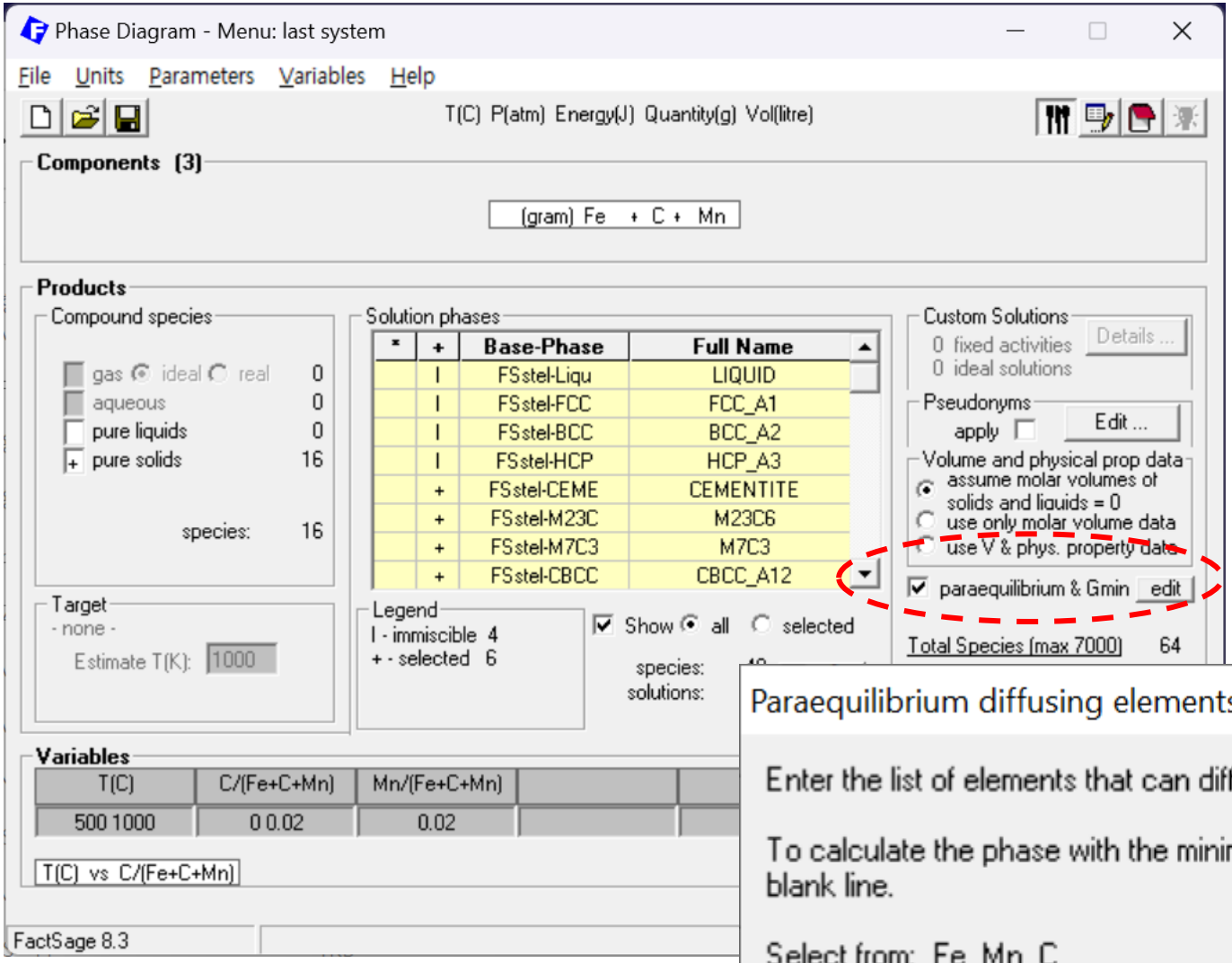

96.109 Fe + 0.06 C + 0.006 S + 1.31 Mn +
C:\FACTSAGEWS\Equi0.res 03Jul23
SLAGA#1
SLAGA#1
SLAGA#1
C
C
C
ILME#1
PSBR#1
MS-c
Al
Al
Al
gram
T(C)

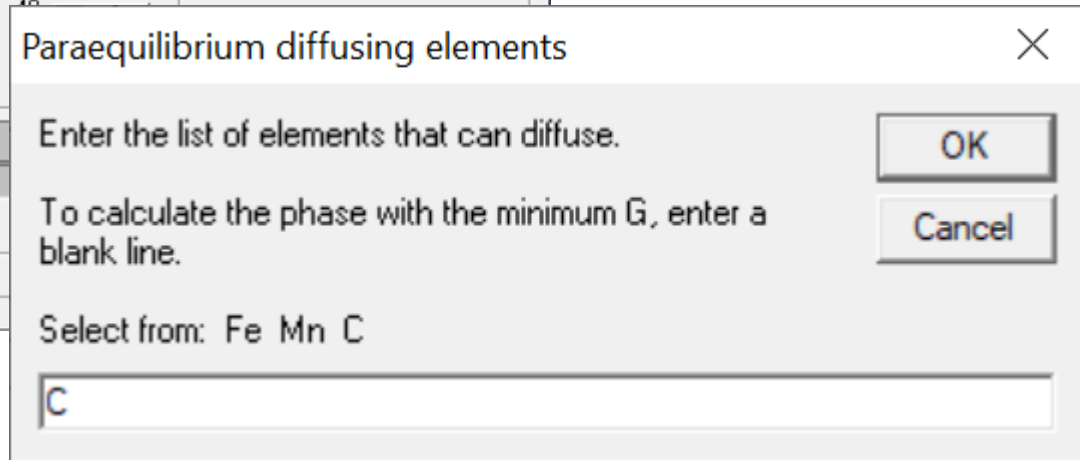
Paraequilibrium (Partial equilibrium) vs Orthoequilibrium (Fully equilibrium)

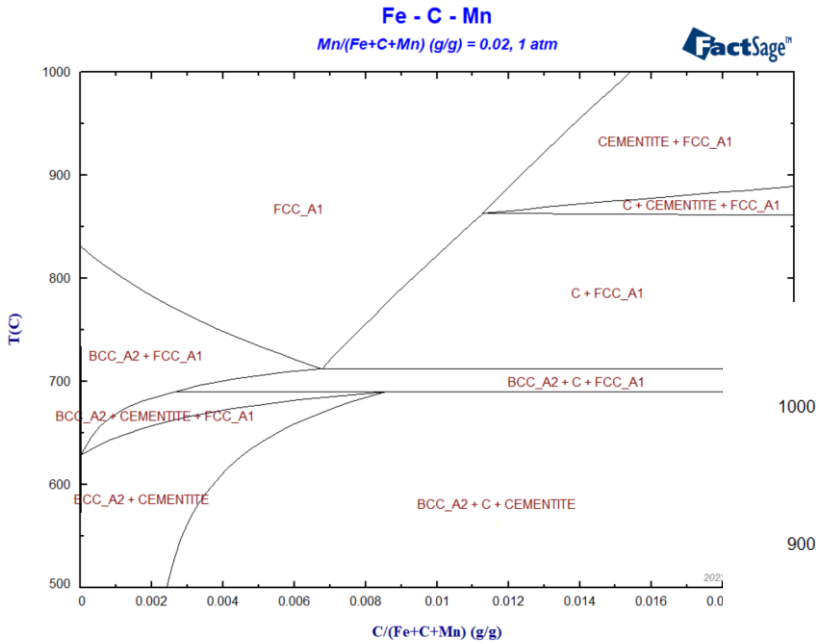
Diffusion of C is much faster than Mn or Si



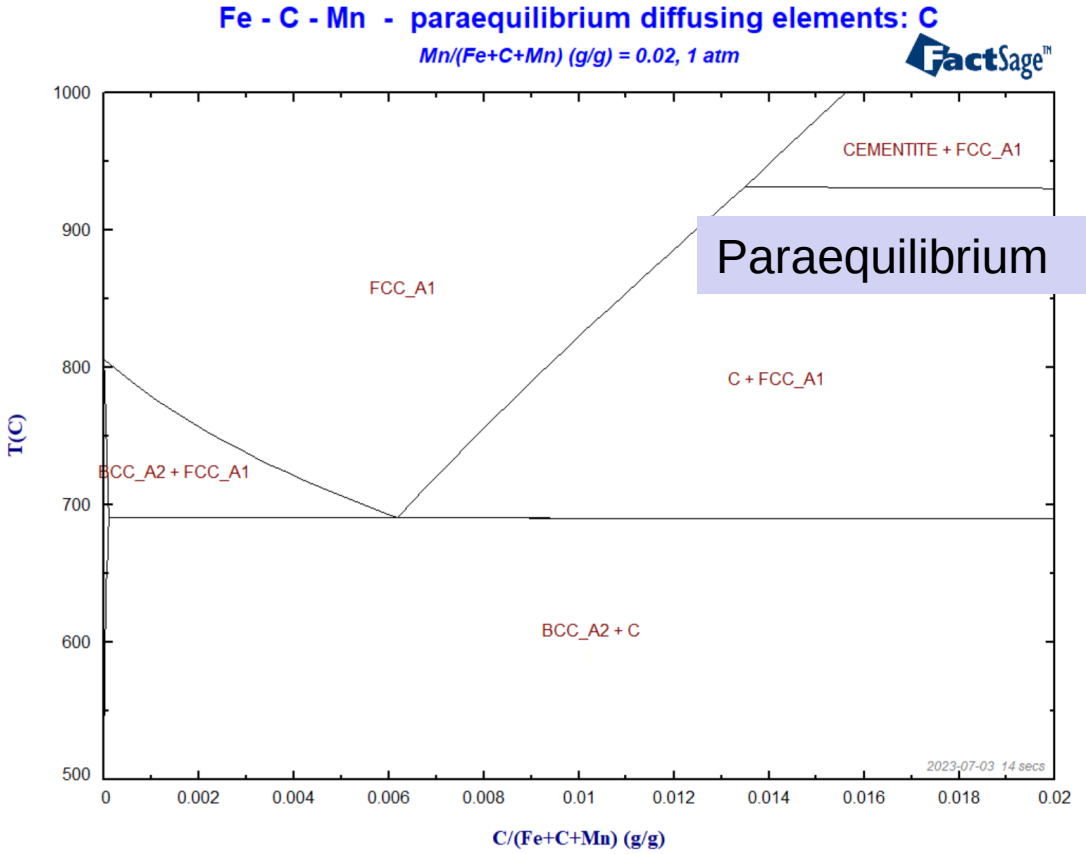
EX25-1. Paraequilibrium: Steel A3 temperature





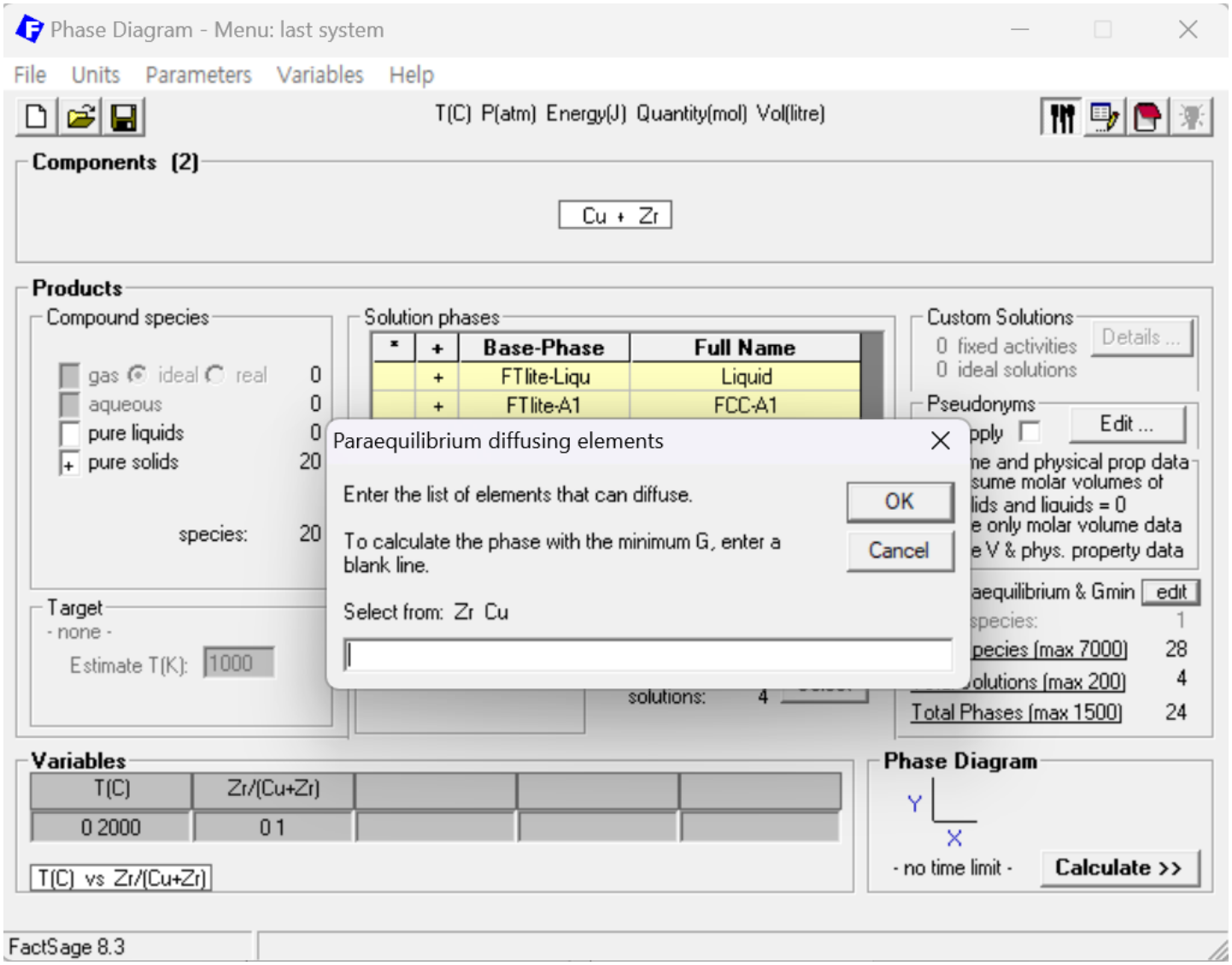


Full equilibrium

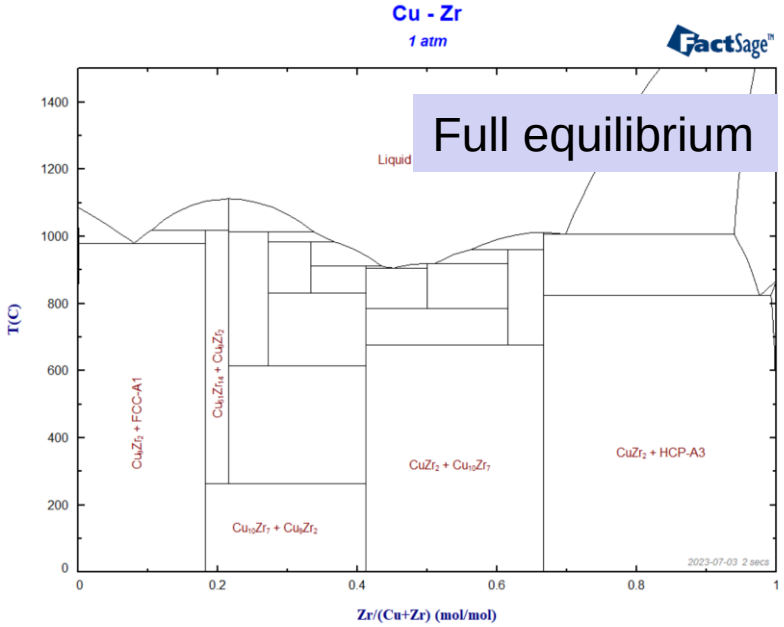


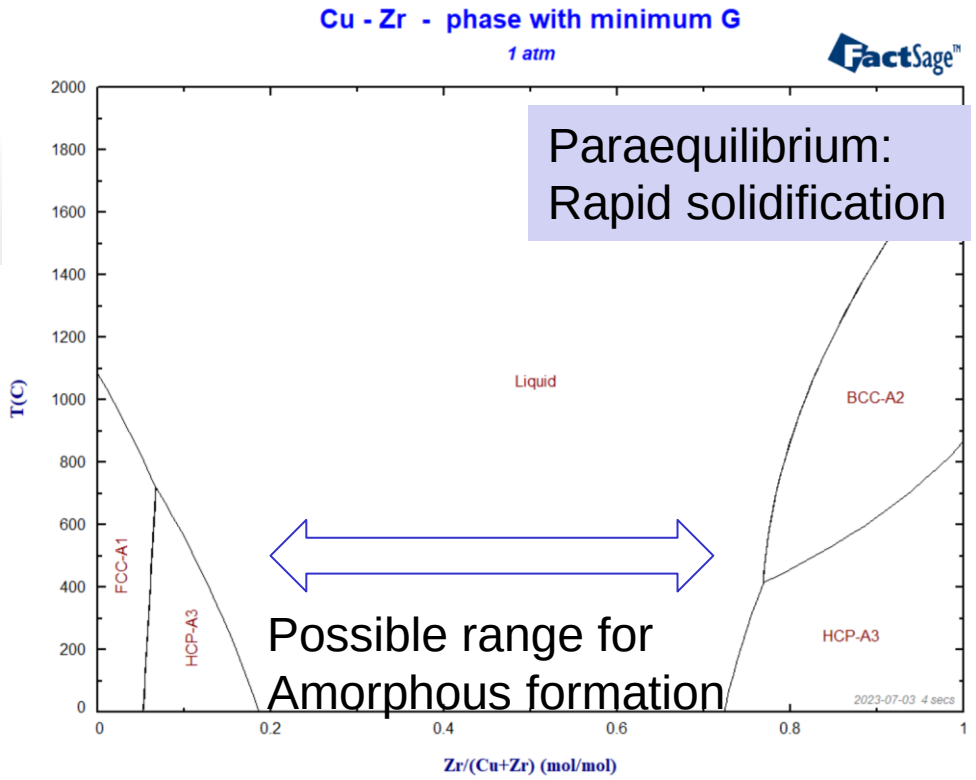
Paraequilibrium

EX25-2. Paraequilibrium: Rapid solidification for amorphous metal



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


Cu - Zr
1 atm
FactSage
Full equilibrium
Liquid
T(C)
Zr/(Cu+Zr) (mol/mol)
2023-07-03 2 secs


Cu - Zr - phase with minimum G
1 atm
FactSage
Paraequilibrium:
Rapid solidification
Liquid
BCC-A2
FCC-A1
HCP-A3
HCP-A3
Possible range for
Amorphous formation
T(C)
Zr/(Cu+Zr) (mol/mol)
2023-07-03 4 secs

Cu - Zr - Mg - phase with minimum G

300°C, 1 atm