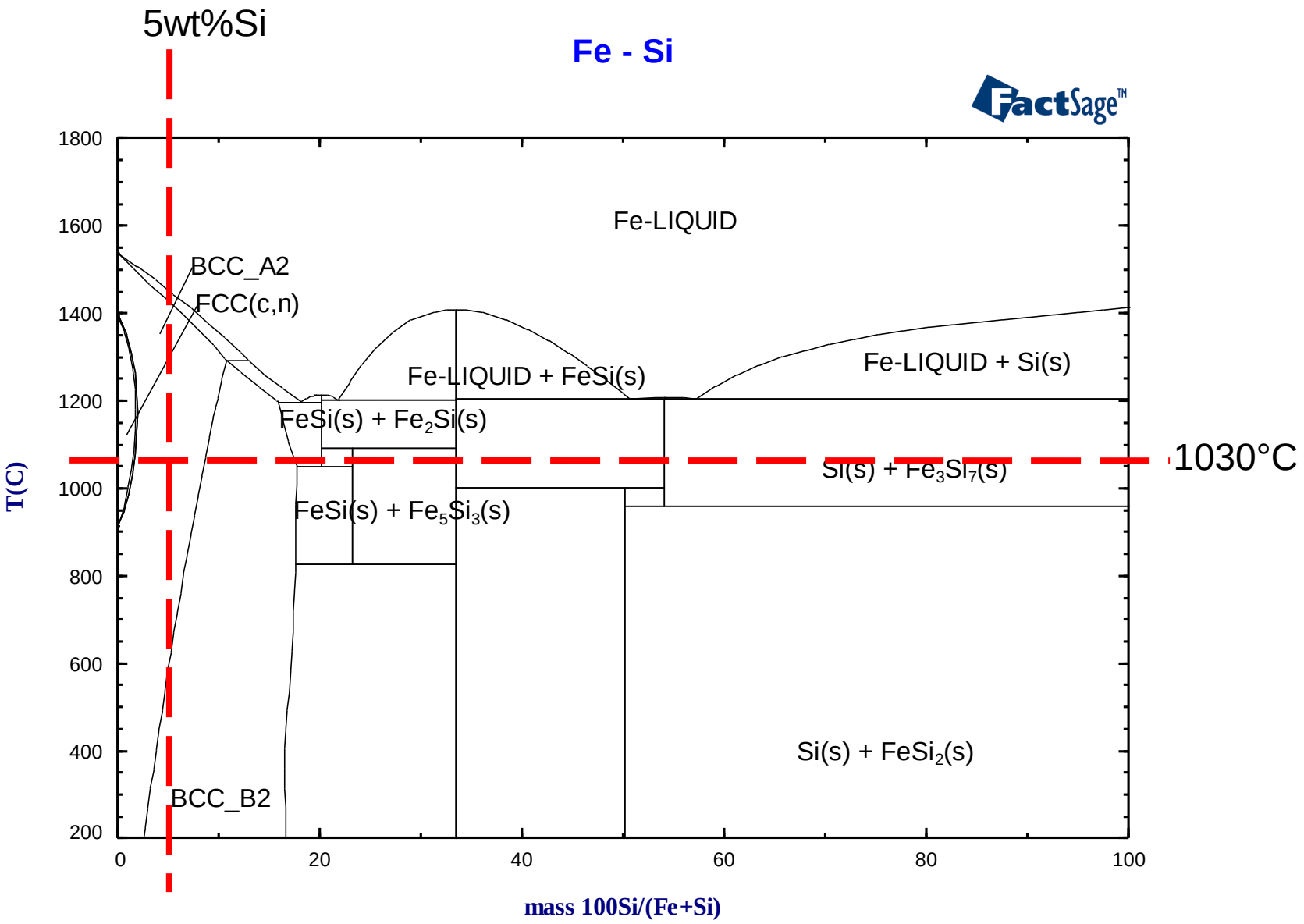
Ferrous Application I

Contents

Contents

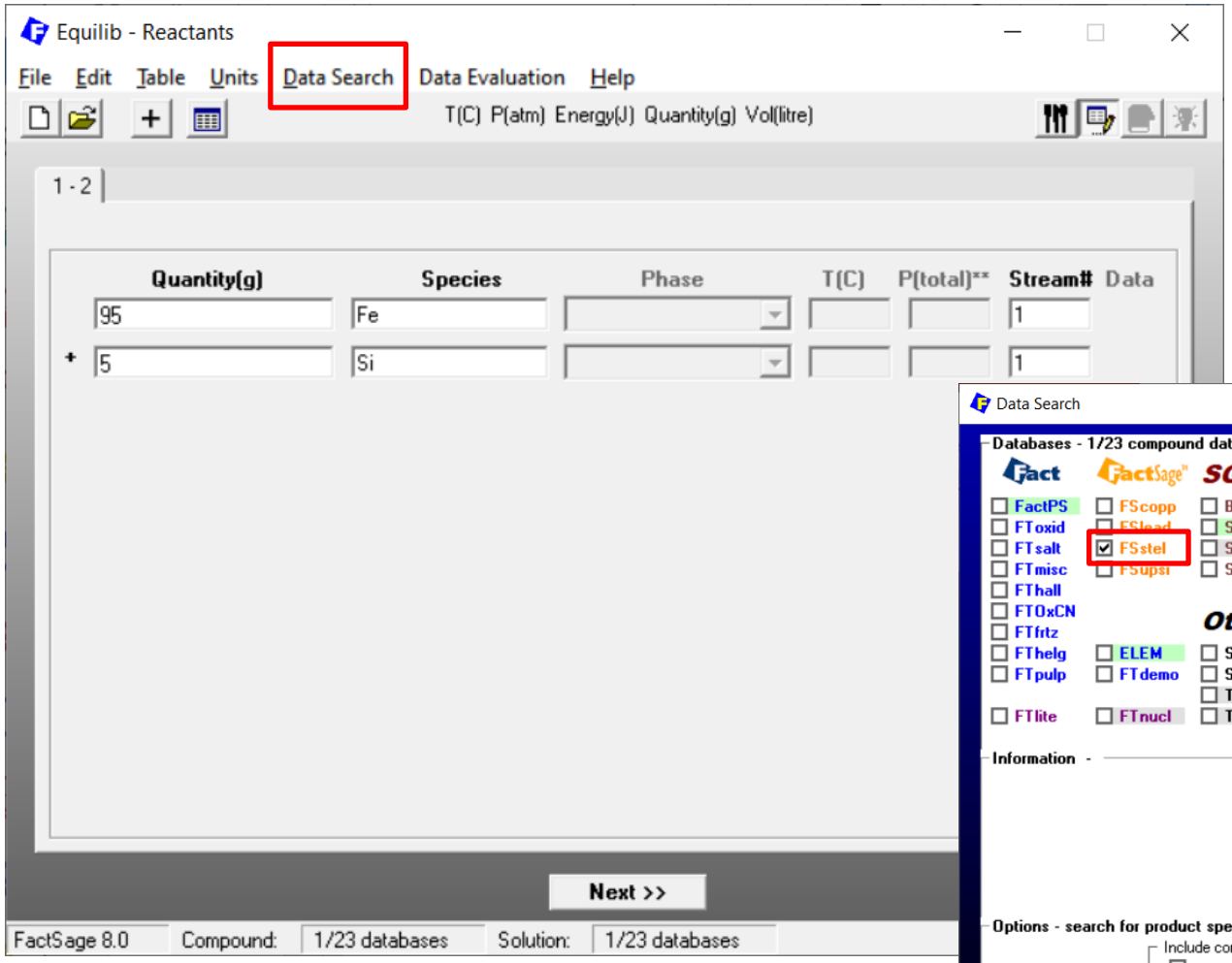
Simple calculation examples of Equilib module

Fe-Si binary phase diagram - Fe-5wt.% Si at 1030 °C

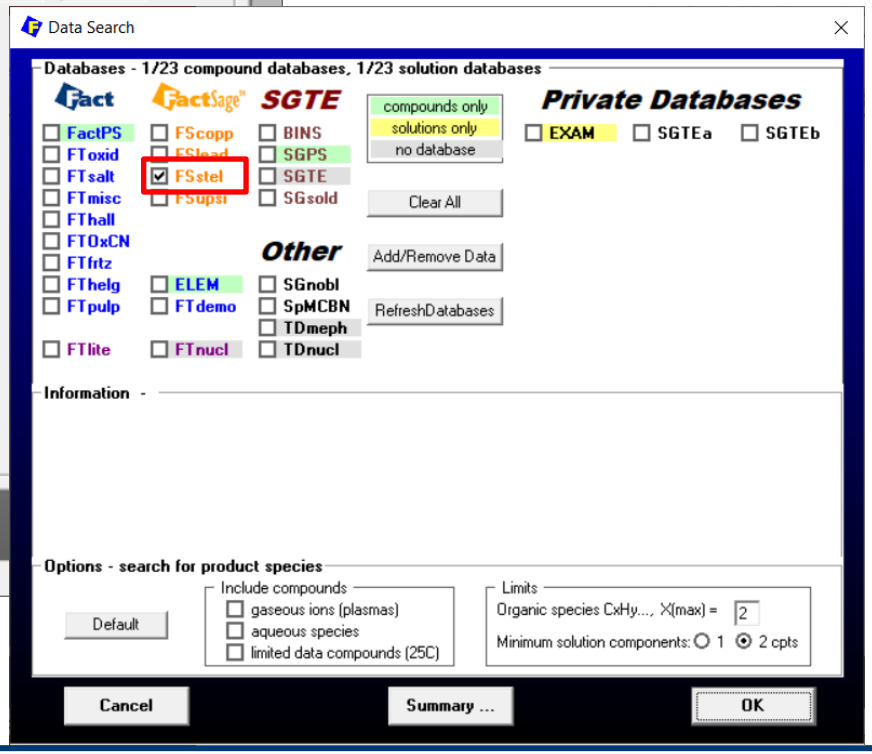


Reactants Window - Fe-Si at Fe-5wt.% Si

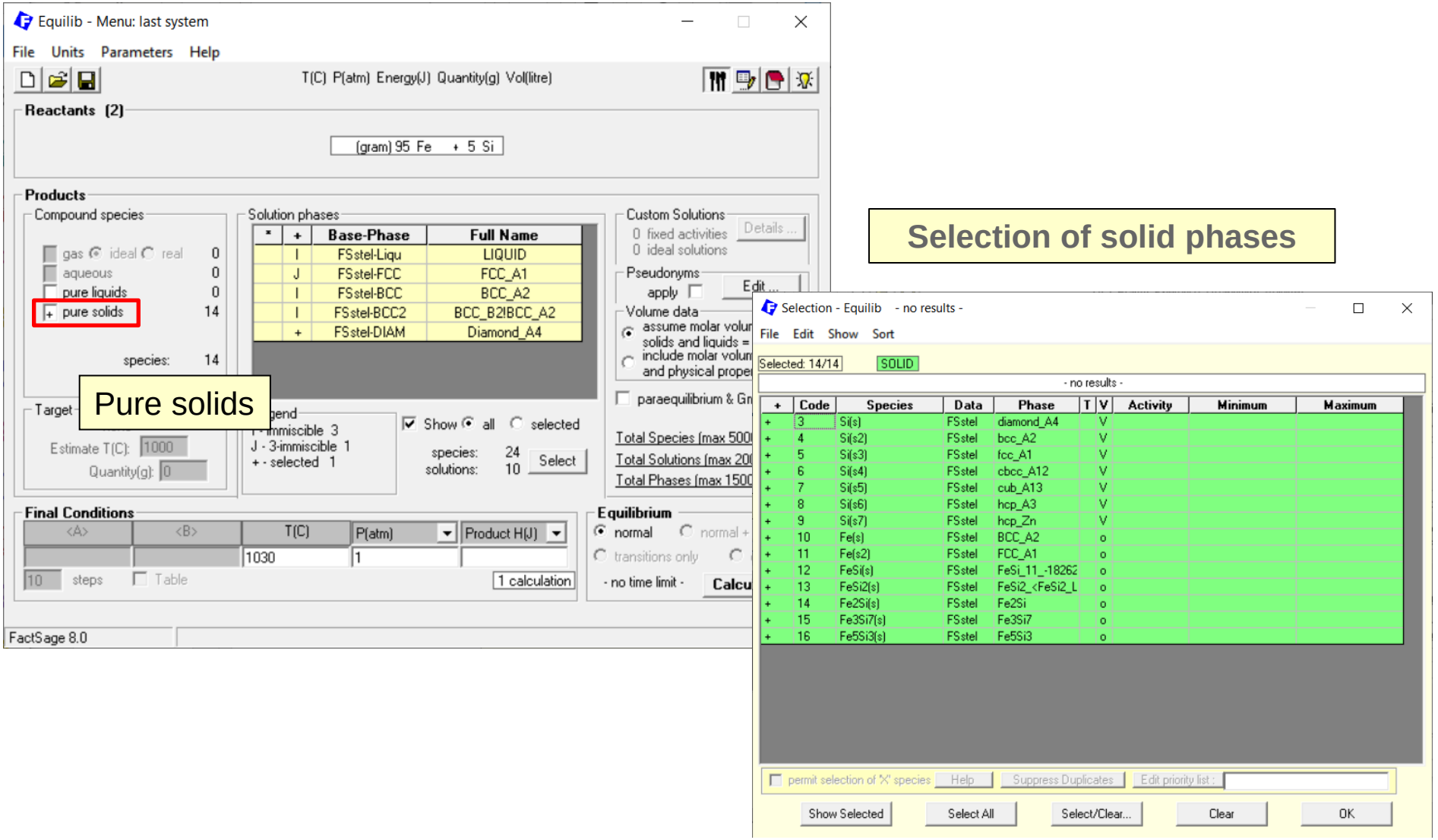
Reactants Window



Data Search

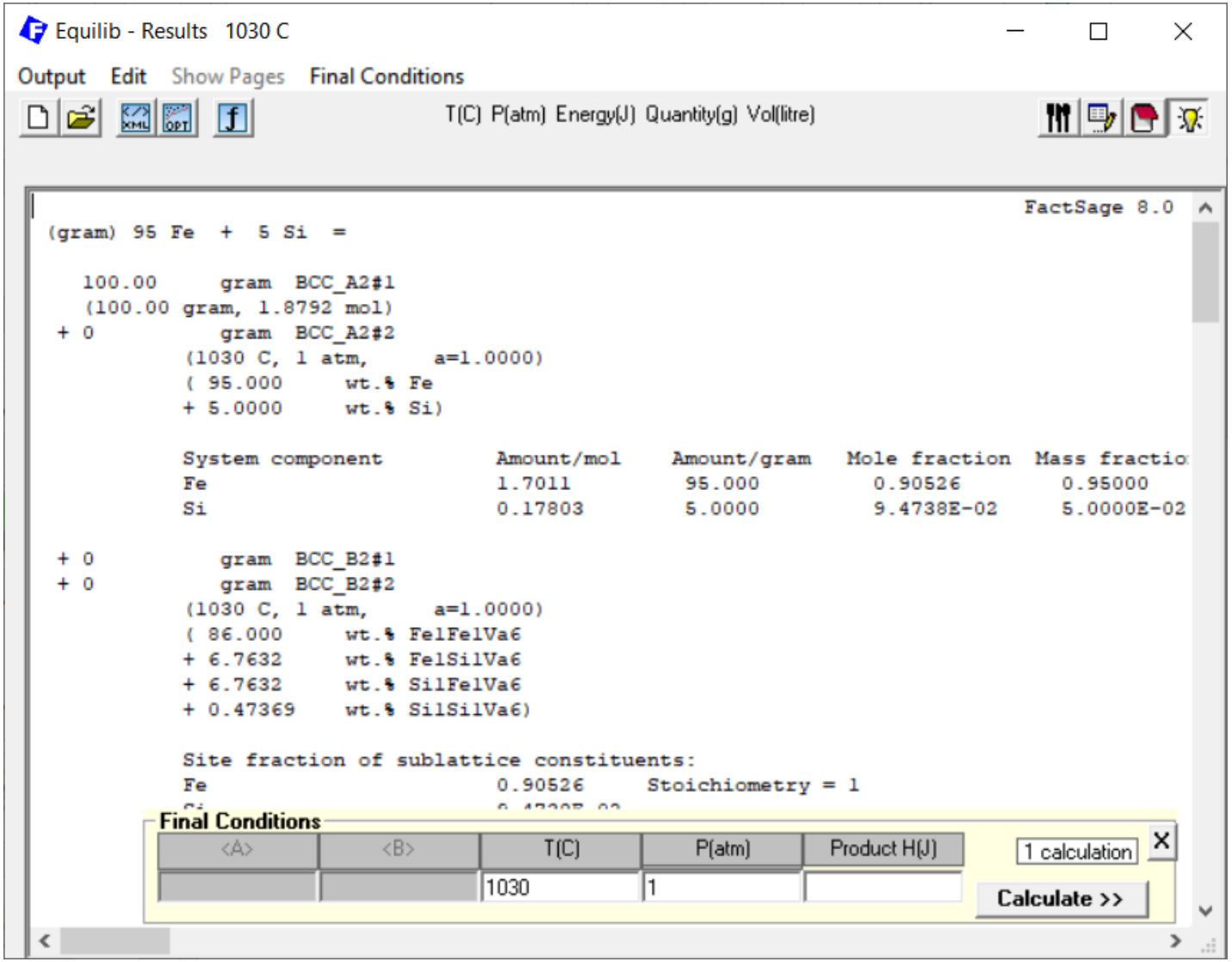


Menu Window - Fe-5wt.% Si at 1030 °C

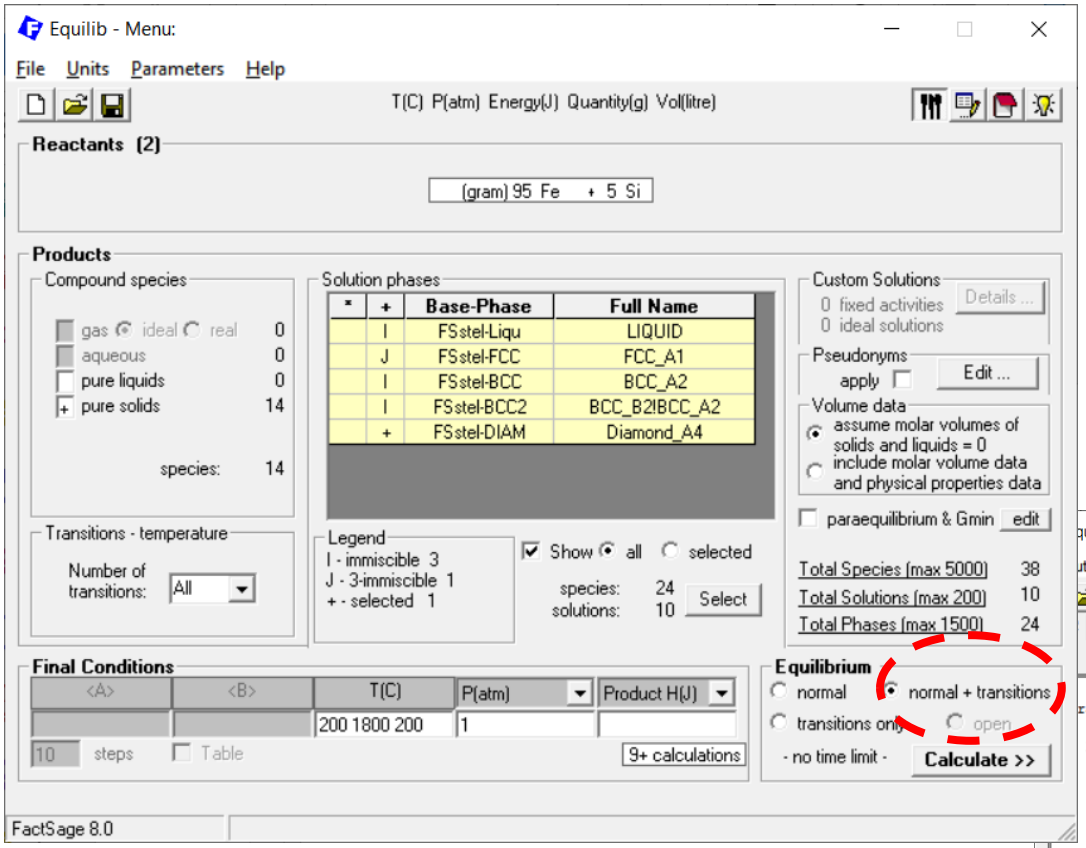


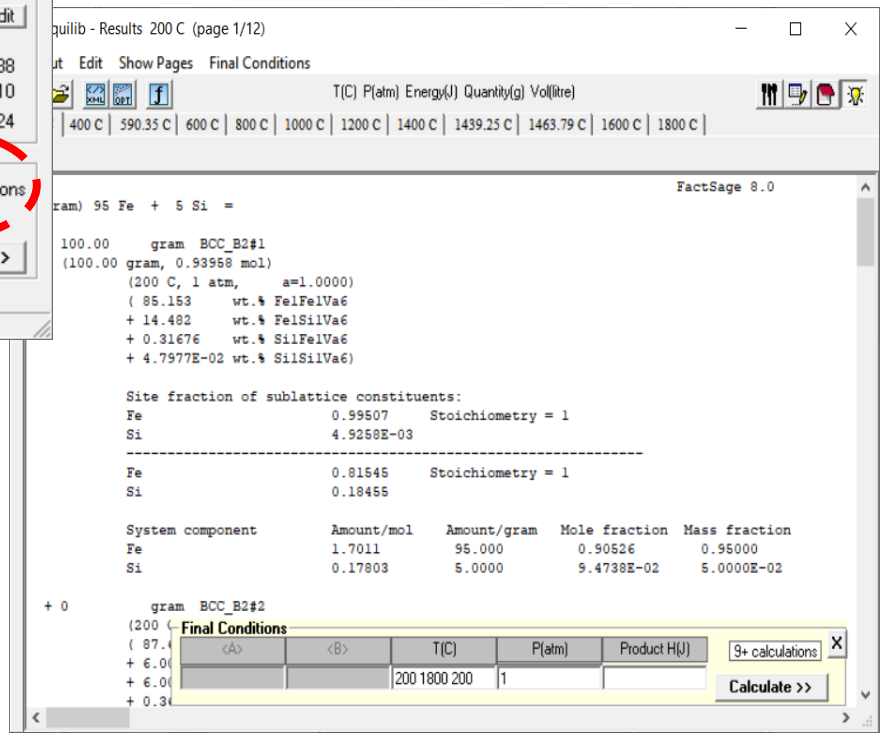
Selection of solid phases

Results Window - Fe-5wt.% Si at 1030 °C



Fe-5wt.% Si transition calculations: “Transition”





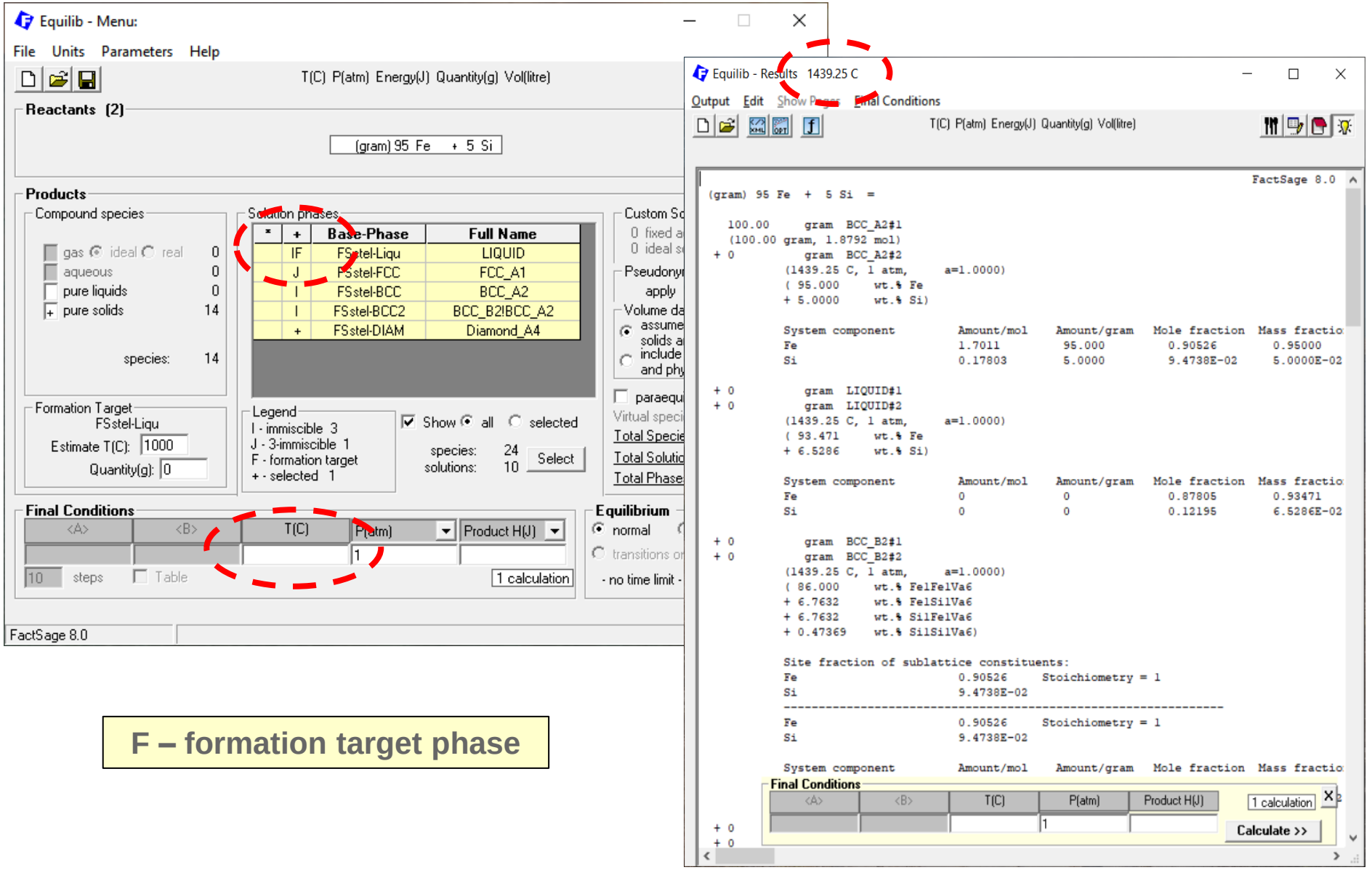
Fe-5wt.% Si from 200 °C to 1800 °C every 200 °C

Phase transformation calculations

- "Transition":
  - select "Transition" for calculation mode.
  - most simple way to calculate all transition of T or X at given range set by user.

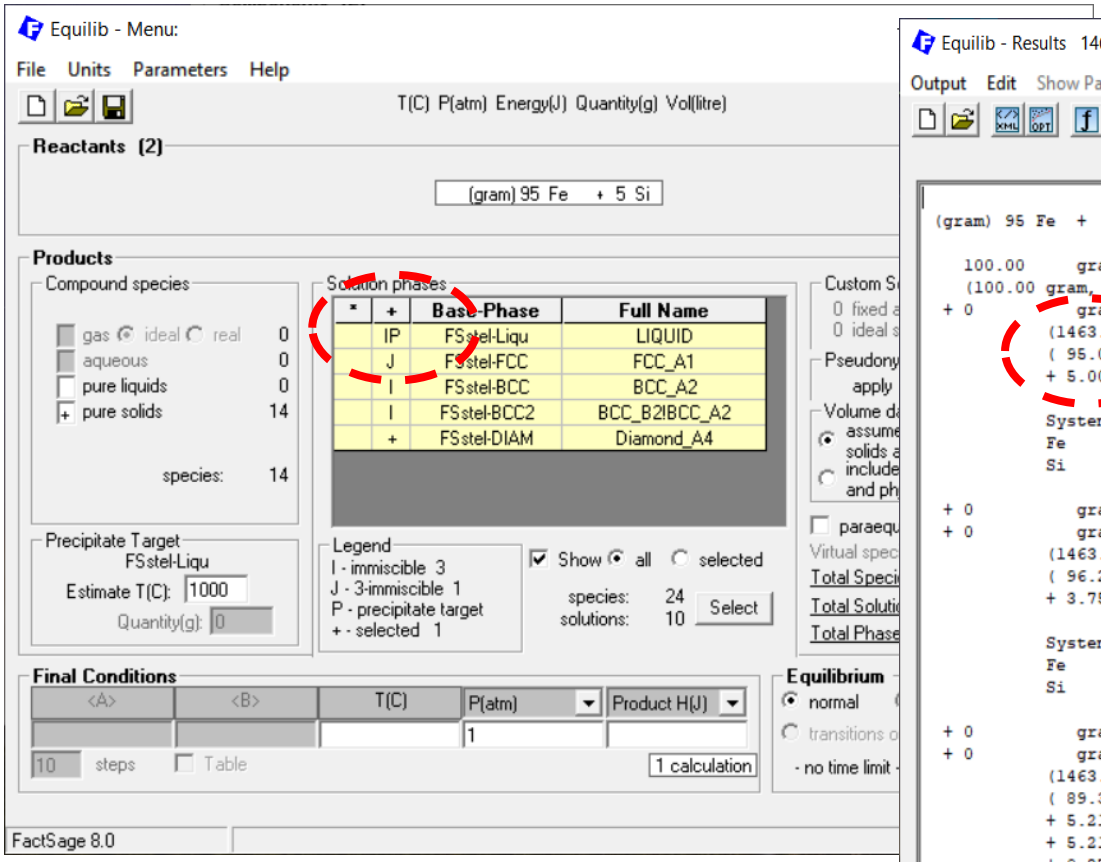
    for X (composition), set <A> to component in Reactant window.
  - FactSage will show all specific conditions when transitions occur.
- "Precipitation" target:
  - Set "P" option for target phase.
  - FactSage will decrease temperature and find at which temperature another phase starts to form from the target phase. For example, if Liquid is target phase, "P" target will give liquidus temperature.
- "Formation" target:
  - Set "F" option for target phase.
  - FactSage will increase temperature and find at which temperature the target phase begin to form. For example, if Liquid is target phase, "F" target will give solidus temperature.

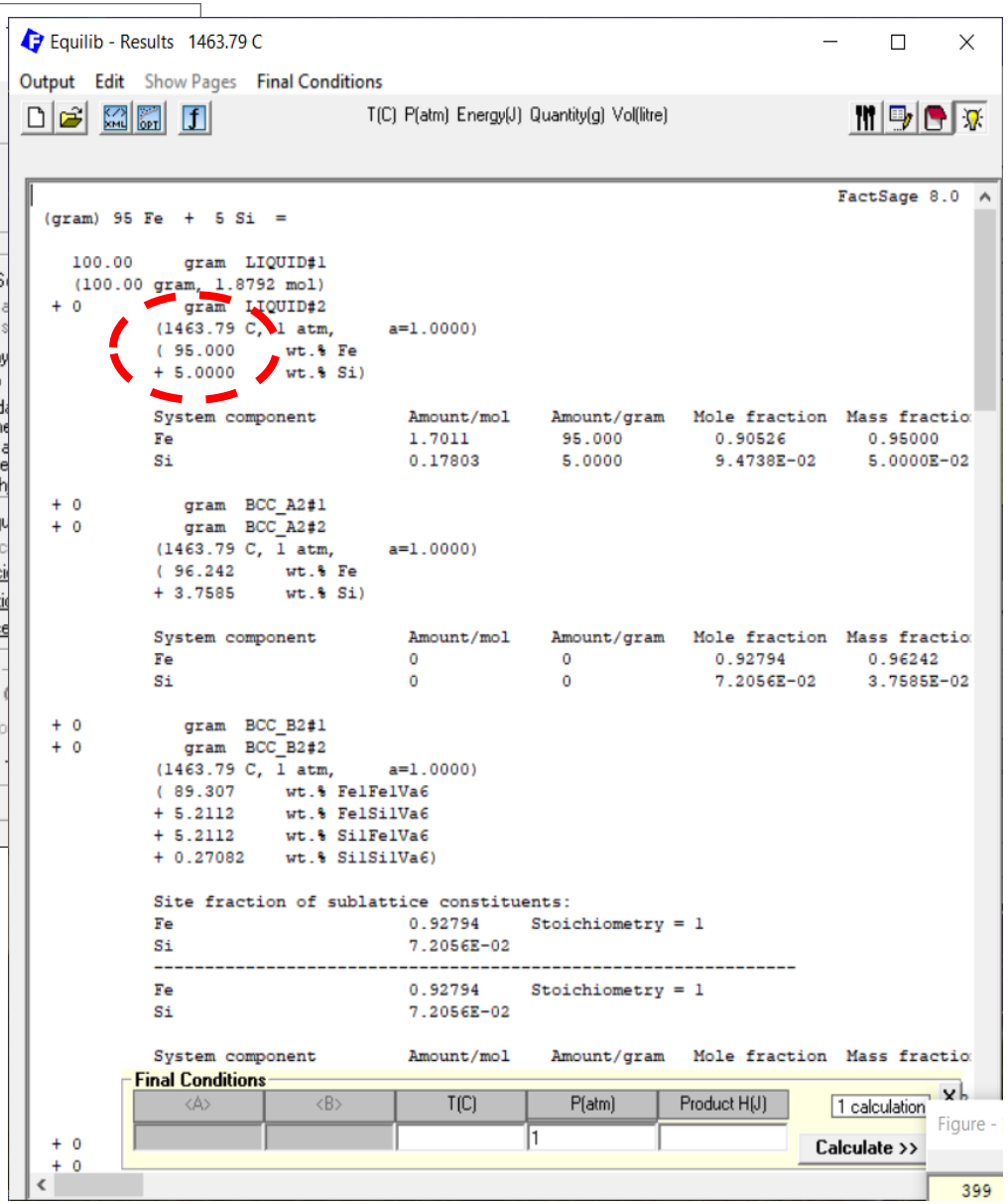
Fe-5wt.%Si target for liquid phase: “Formation target”



F – formation target phase

Fe-5wt.%Si target for liquid phase: “Precipitation target”



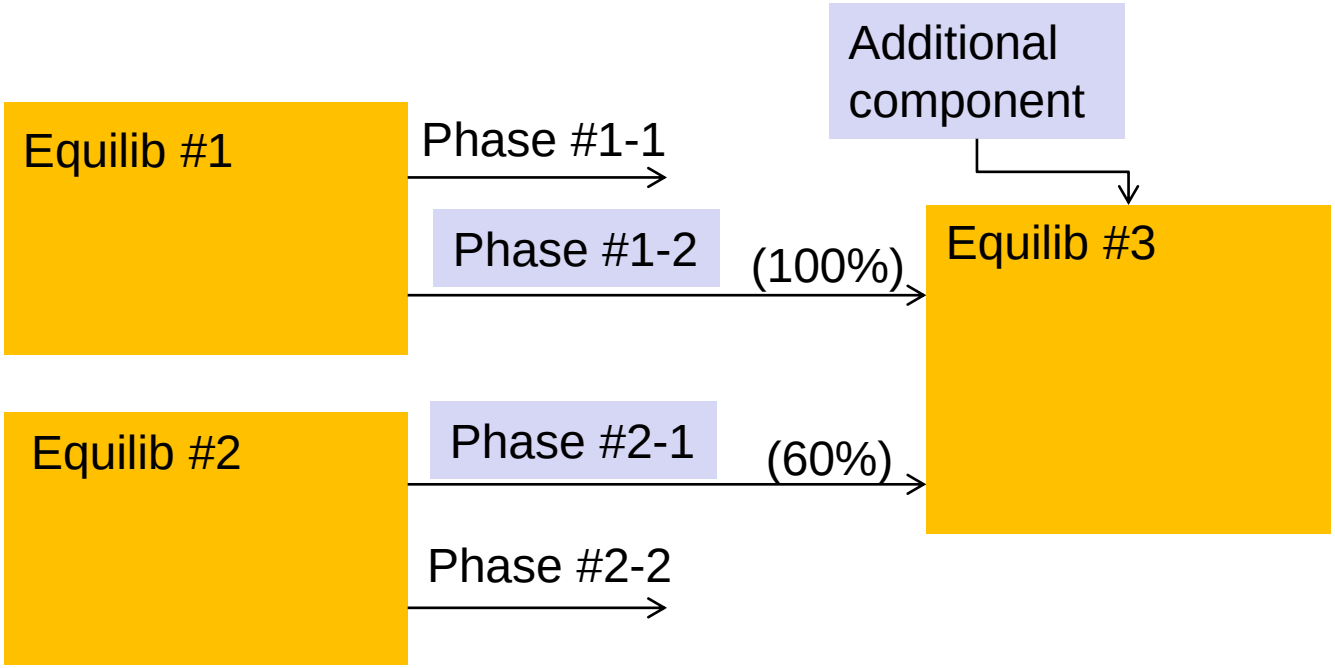


P – precipitate target phase

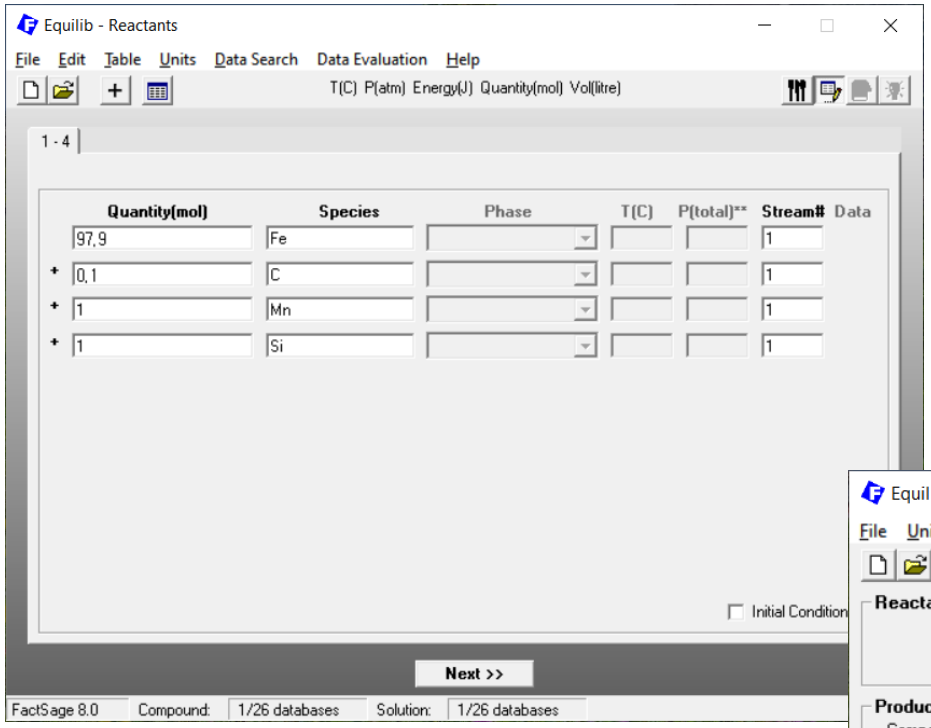
- What is stream and why we need this?

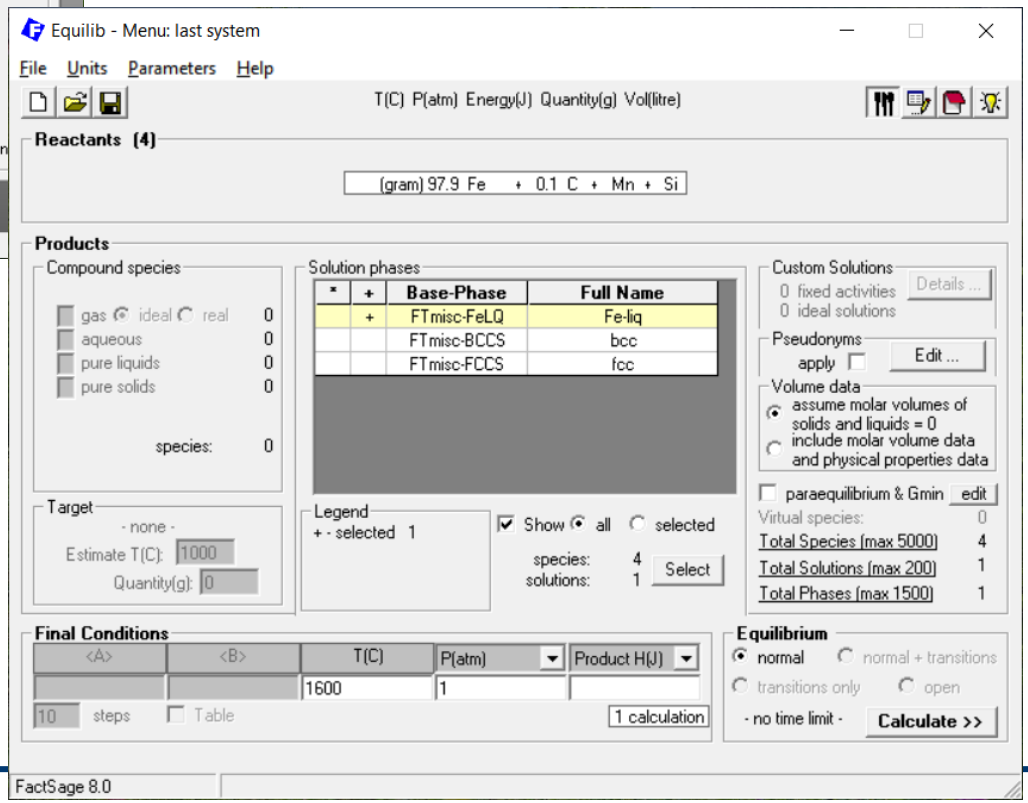
In industrial process, solutions (or mixtures) can be added as reactants. This is called as “stream” (or “mixture”) in FactSage. In order to easily create and add such solutions as input, “stream” can be created from Equilib and it can be added as reactant for next Equilib calculation. Heat and mass of solution(s) are conserved in stream.

** “mixture” can be generated in “Mixture” module in FactSage*

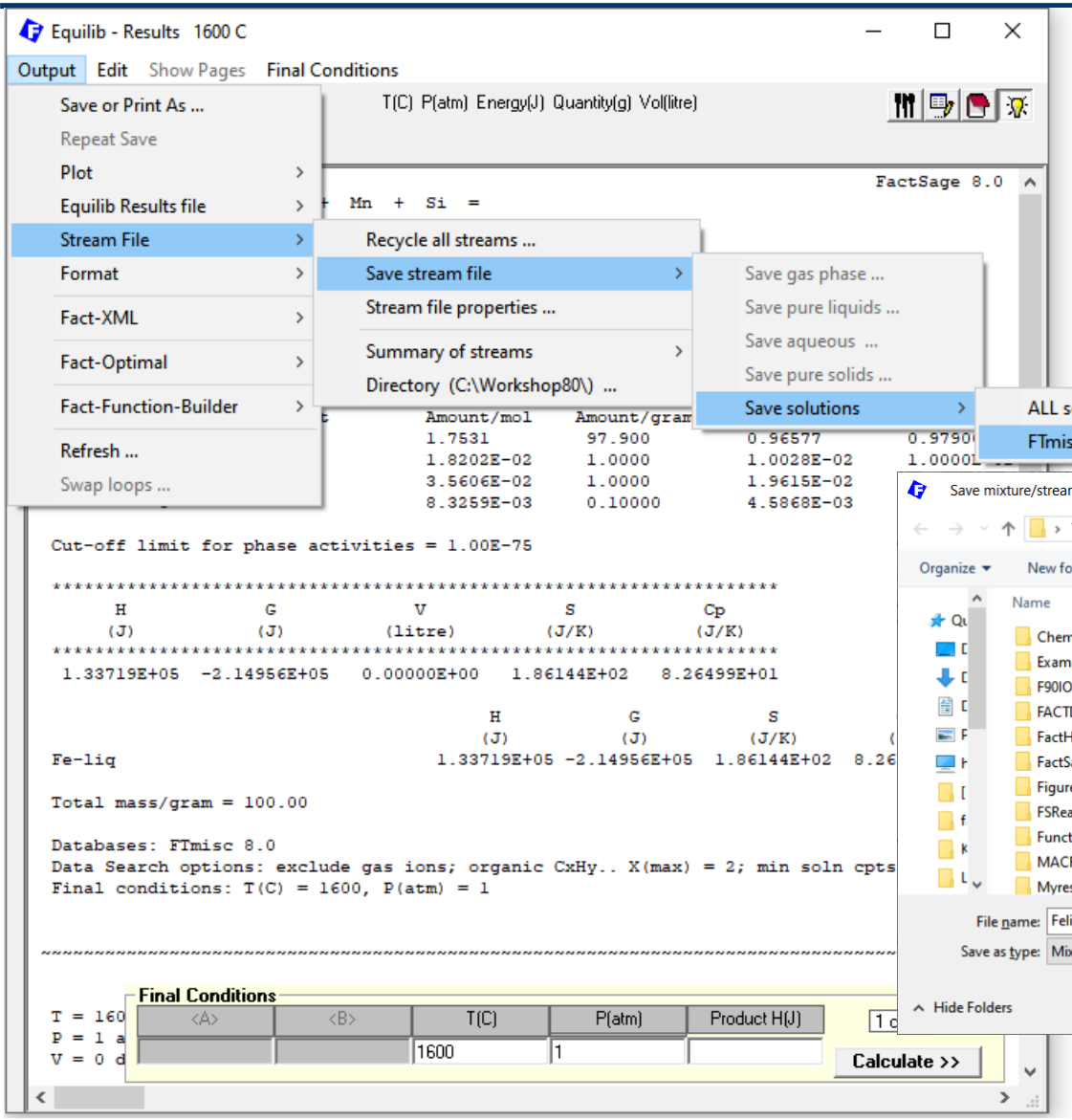


Creating new stream : Fe-0.1C-1Mn-1Si at 1600°C

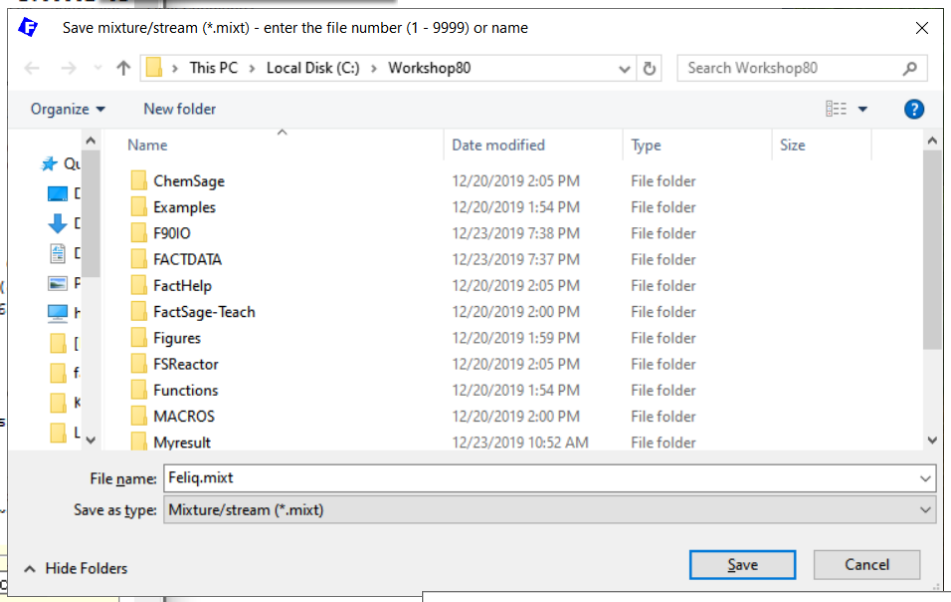


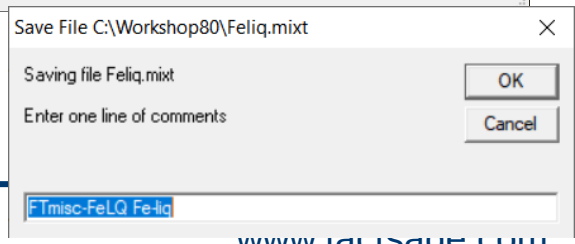


Creating new stream : Fe-0.1C-1Mn-1Si at 1600°C

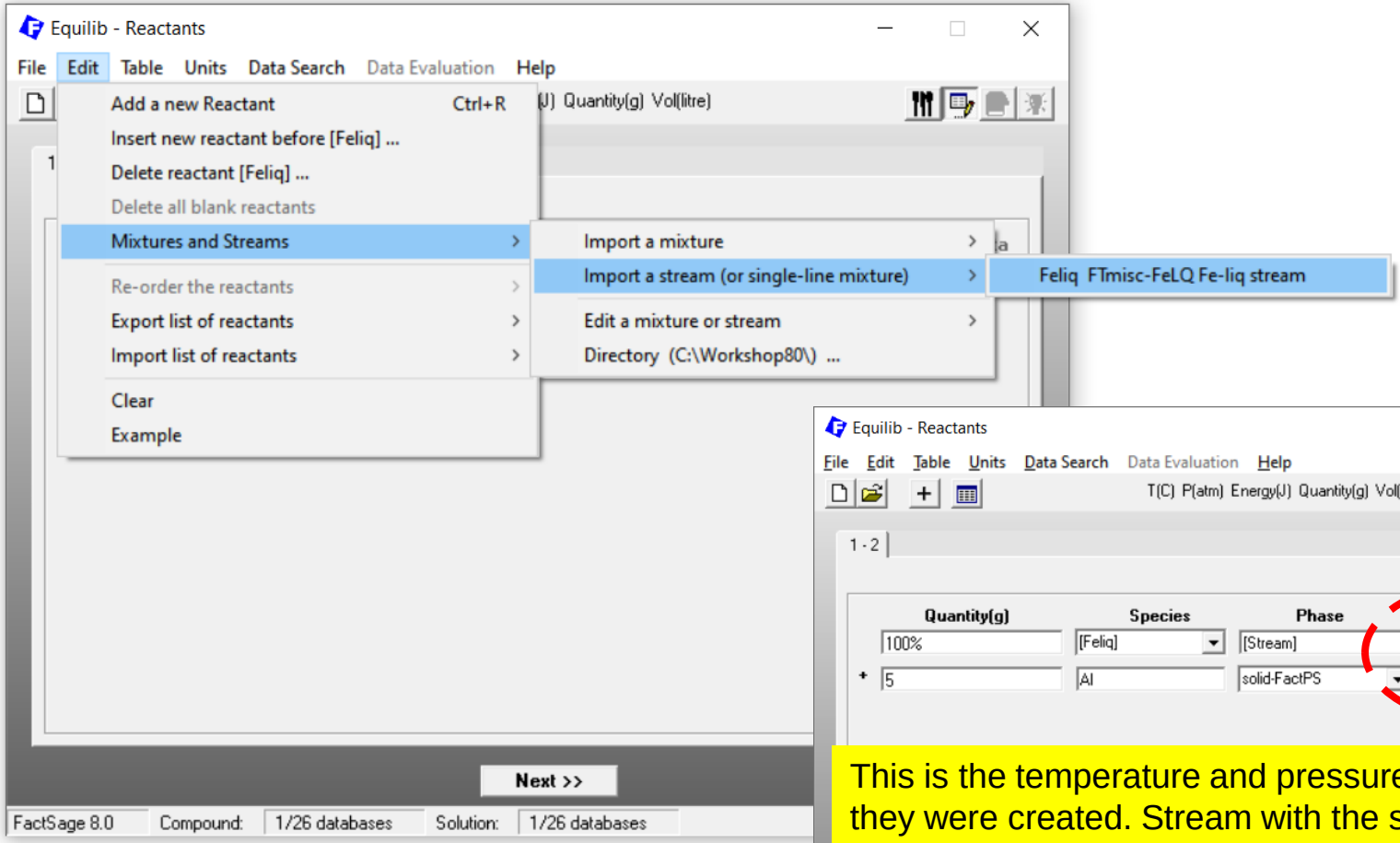


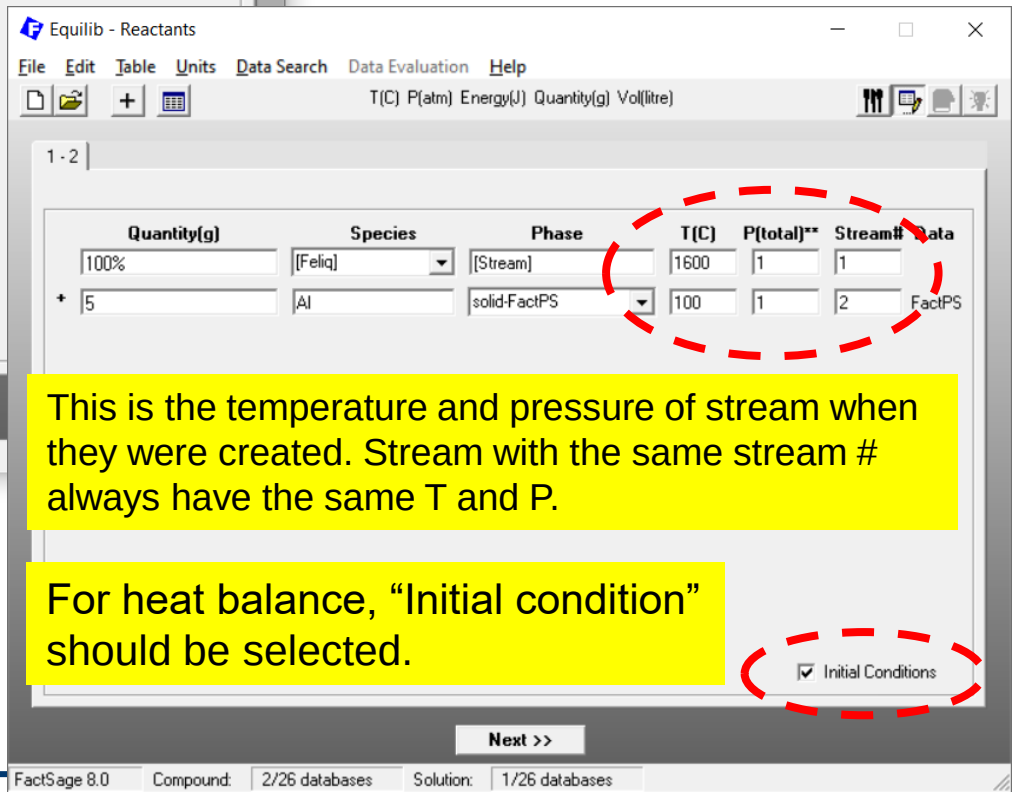
Save the liquid FeLQ phase as a stream



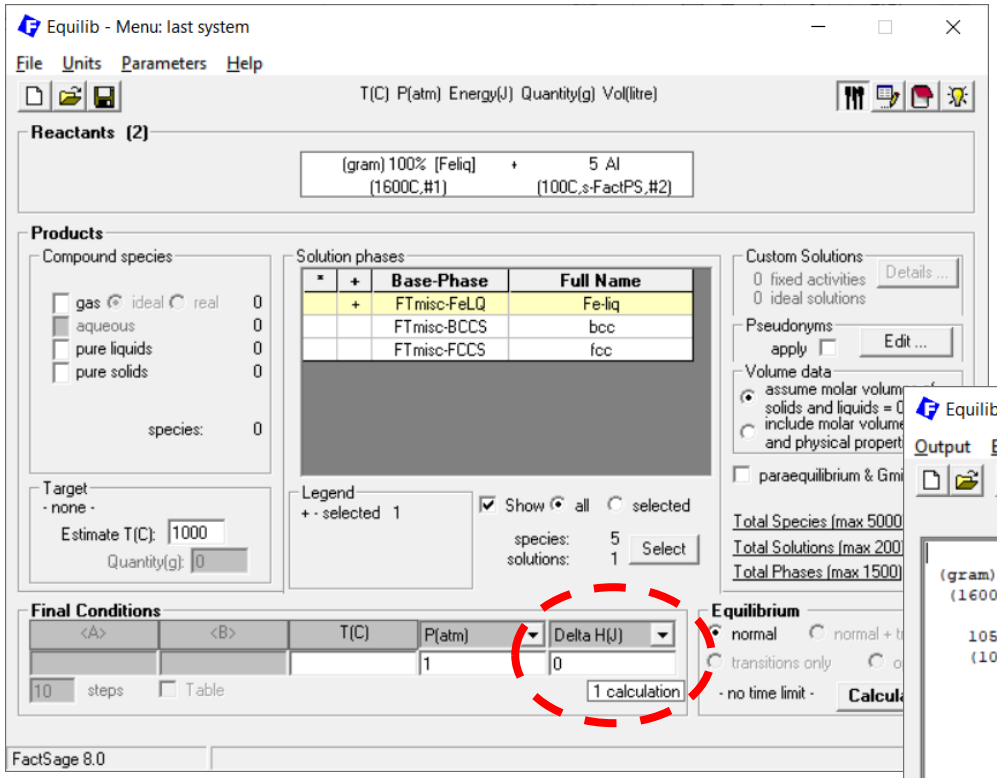


Import stream : Fe-0.1C-1Mn-1Si at 1600°C



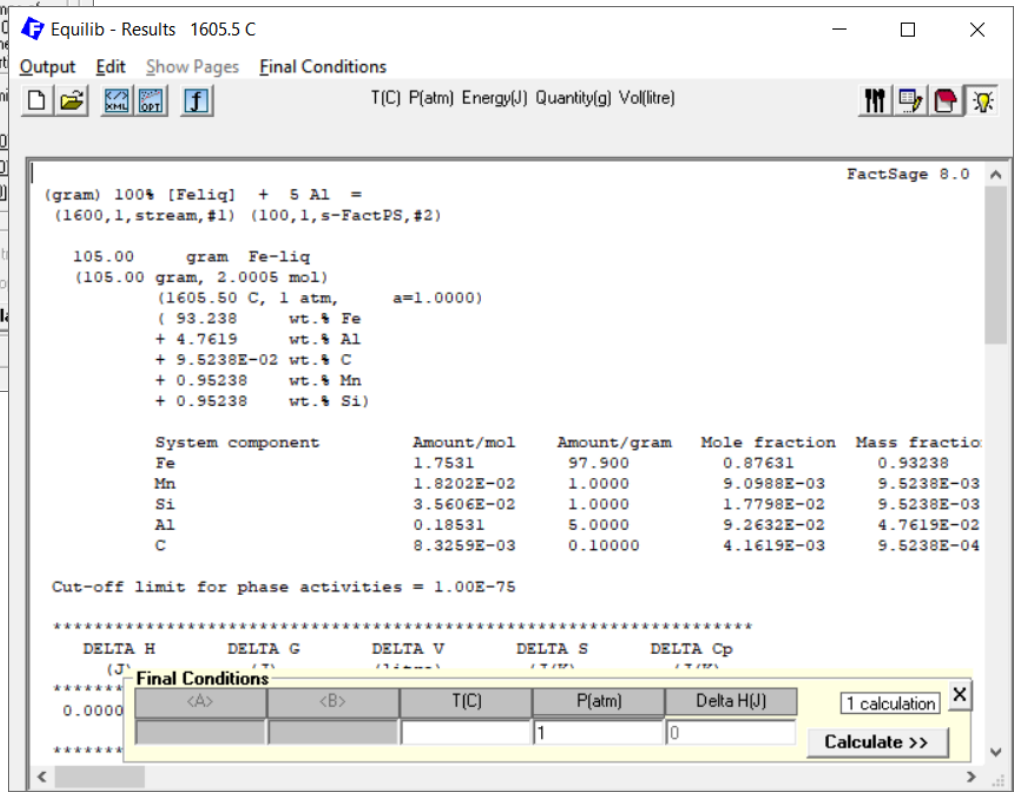


Heat balance: Fe-0.1C-1Mn-1Si(1600°C) + Al (25°C)



Adiabatic calculation :
Delta(H) = 0

Delta(H) > 0: heat loss
Delta(H) < 0: heat gain



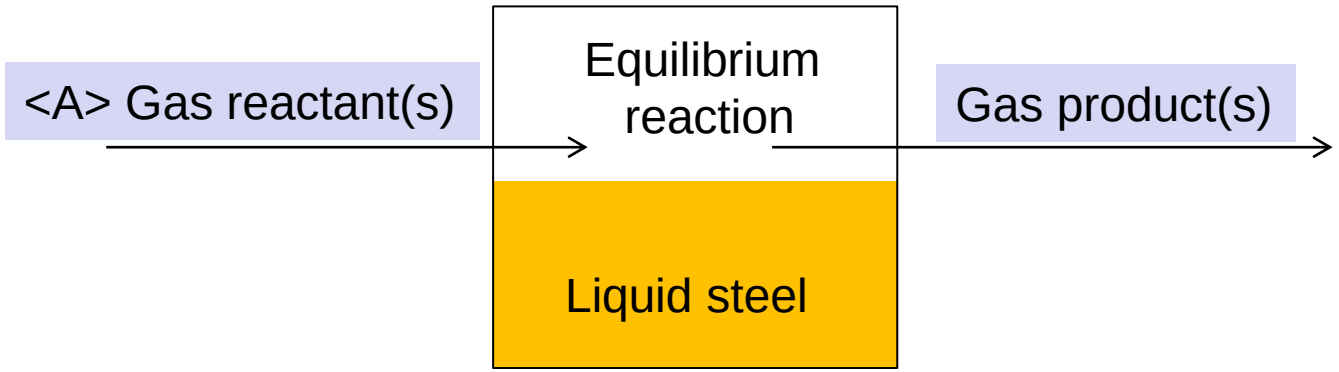
Calculated adiabatic temperature = 1605.5 °C

- What is open and why we need this?

In many industrial process, gas are continuously injected and it come out after the reaction with the materials in reactors.

This process can be simulated by “Open” calculation mode.

For activating this <A> for gas species should be assigned in Reactant window.



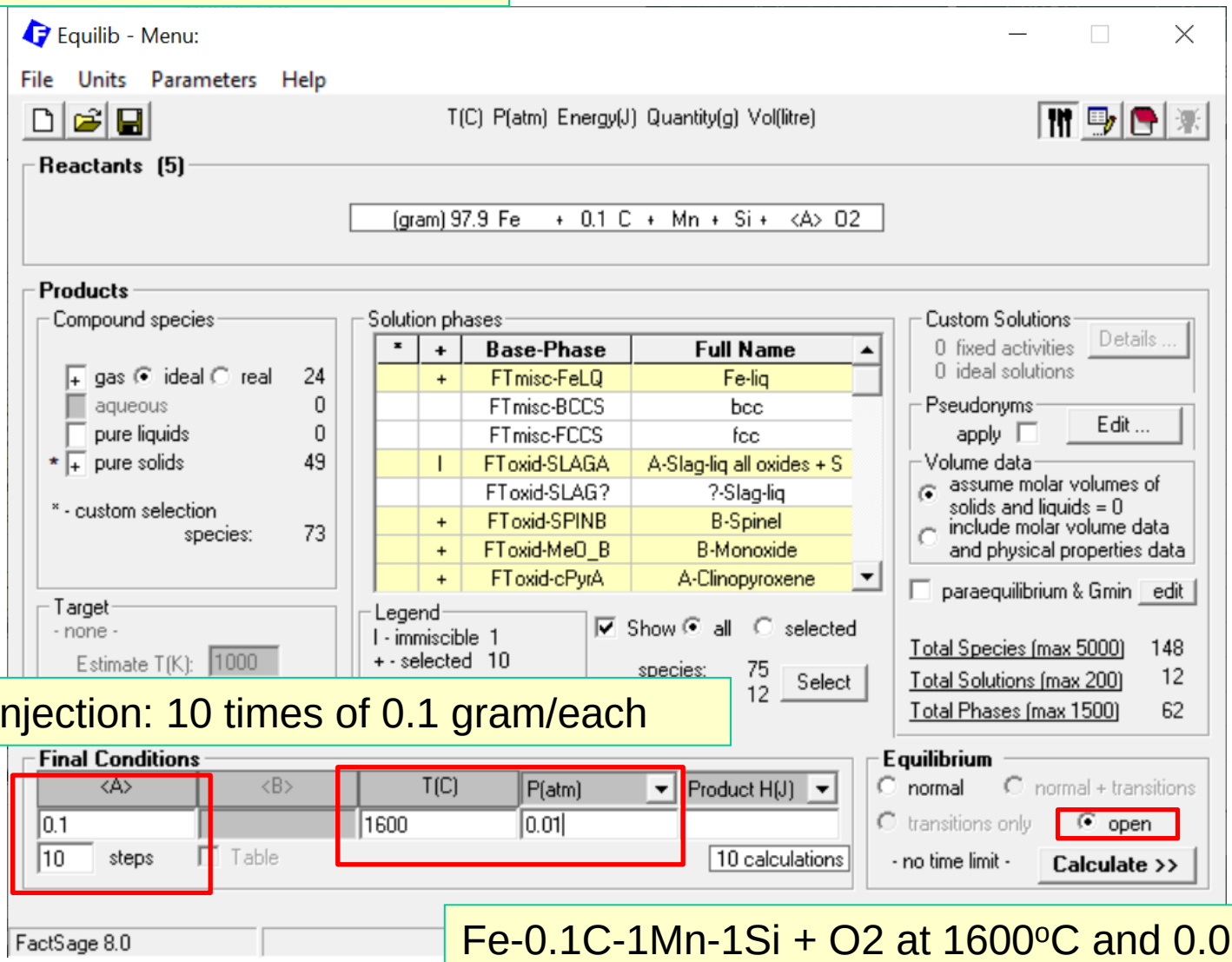
Repeat this calculation for “Step” times and find the evolution of chemical composition of gas or materials in reactor

No heat balance calculation can be done. Temperature of reactor should be specified by user. Reaction in reactor reaches full equilibrium at each step.

** Open calculation is NOT working with “Stream”*

Open Calculation - off-gas removal

RH – Vacuum degassing process



Oxygen injection: 10 times of 0.1 gram/each

Fe-0.1C-1Mn-1Si + O2 at 1600°C and 0.01 atm

Open Calculation - results

Equilib - Results Step 10 (page 10/10)

Output Edit Show Pages Final Conditions

T(C) P(atm) 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 -

```
          + 4.5715E-23      O3
          + 1.8641E-31      C4
          + 4.1137E-33      Fe(CO)5
          + 2.4932E-35      C5)

+ 98.839     gram  Fe-liq
  (98.839 gram, 1.7765 mol)
          (1600 C, 1.0000E-02 atm,     a=1.0000)
          ( 98.992     wt.% Fe
          + 2.2278E-03 wt.% C
          + 0.65443    wt.% Mn
          + 7.5768E-03 wt.% O
          + 0.34245    wt.% Si
          + 1.5068E-04 wt.% SiO
          + 8.3395E-04 wt.% MnO)

          System component         Amount/mol    Amount/gram   Mole fraction
          Fe                       1.7520         97.843         0.98621
          Mn                       1.1786E-02      0.64747       6.6339E-03
          Si                       1.2055E-02      0.33856       6.7855E-03
          O                        4.8307E-04      7.7288E-03    2.7191E-04
          C                        1.8333E-04      2.2020E-03    1.0320E-04

+ 1.0279     gram  Slag-liq#1
  (1.0279 gram, 1.5840E-02 mol)
          (1600 C, 1.0000E-02 atm,     a=1.0000)
          ( 52.051     wt.% SiO2
          + 6.6205     wt.% FeO
          + 4.2485E-03 wt.% Fe2O3
          + 41.320     wt.% MnO
          + 4.1169E-03 wt.% Mn2O3)

          Site fraction of sublattice constituents:
          Si                       0.56215
          Fe2+                     5.9798E-02
          Fe3+                     3.4529E-05
          Mn2+                     0.37798
          Mn3+                     3.3844E-05
```

Carbon content decreases due to the reactions:

$$\underline{C} + O_2 = CO_2$$

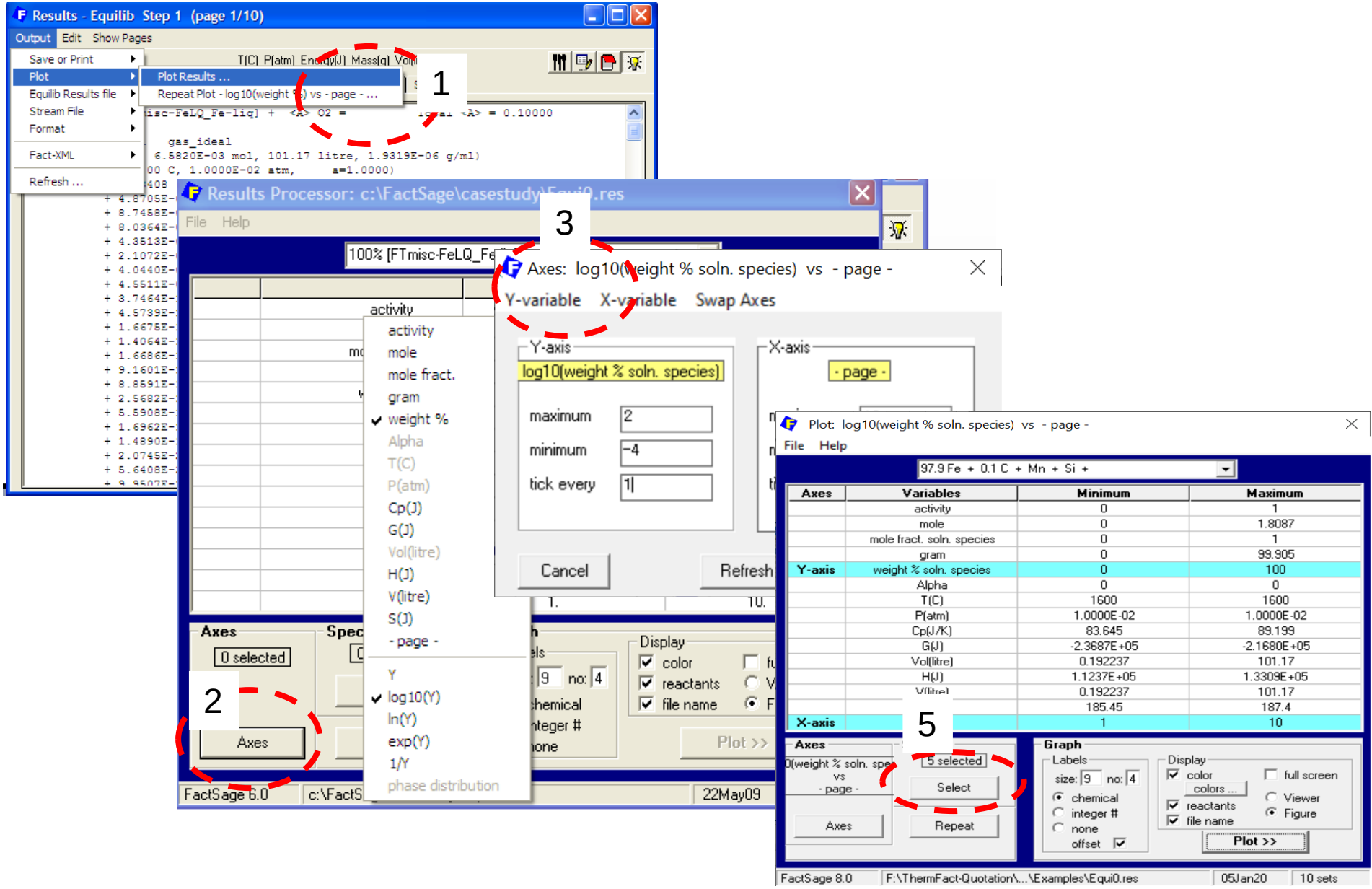
$$\underline{C} + 0.5O_2 = CO$$

New slag formed due to Si and Mn oxidation:

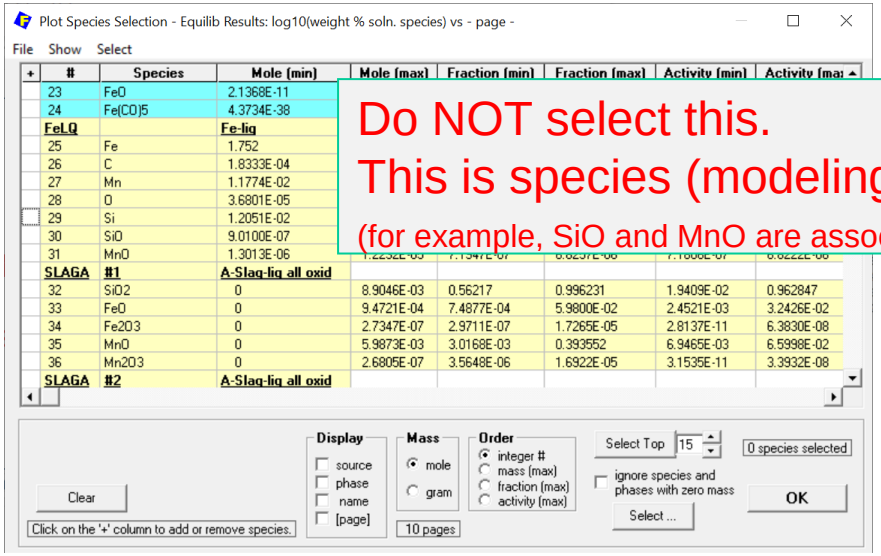
$$\underline{Mn} + 0.5O_2 = MnO$$

$$\underline{Si} + O_2 = SiO_2$$

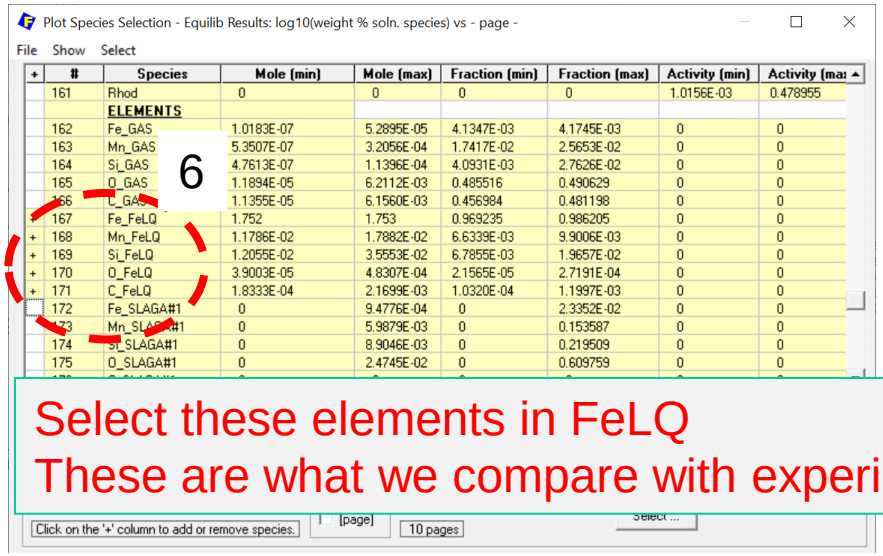
Open Calculation - plot of log(wt% liquid steel)

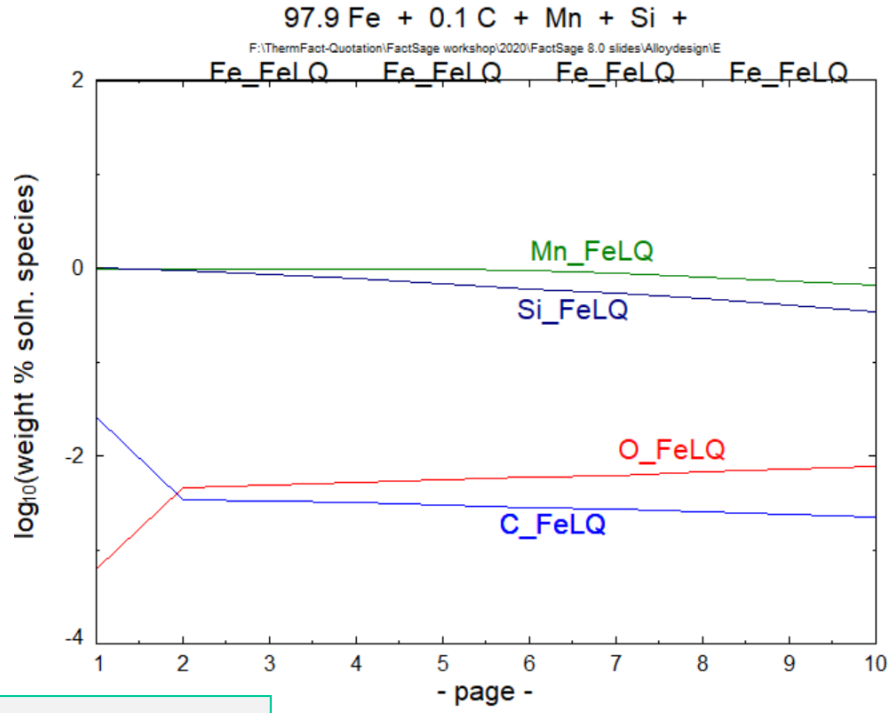


Open Calculation - log(wt%) vs page



Do NOT select this.
This is species (modeling) in FeLQ
(for example, SiO and MnO are associate model species)





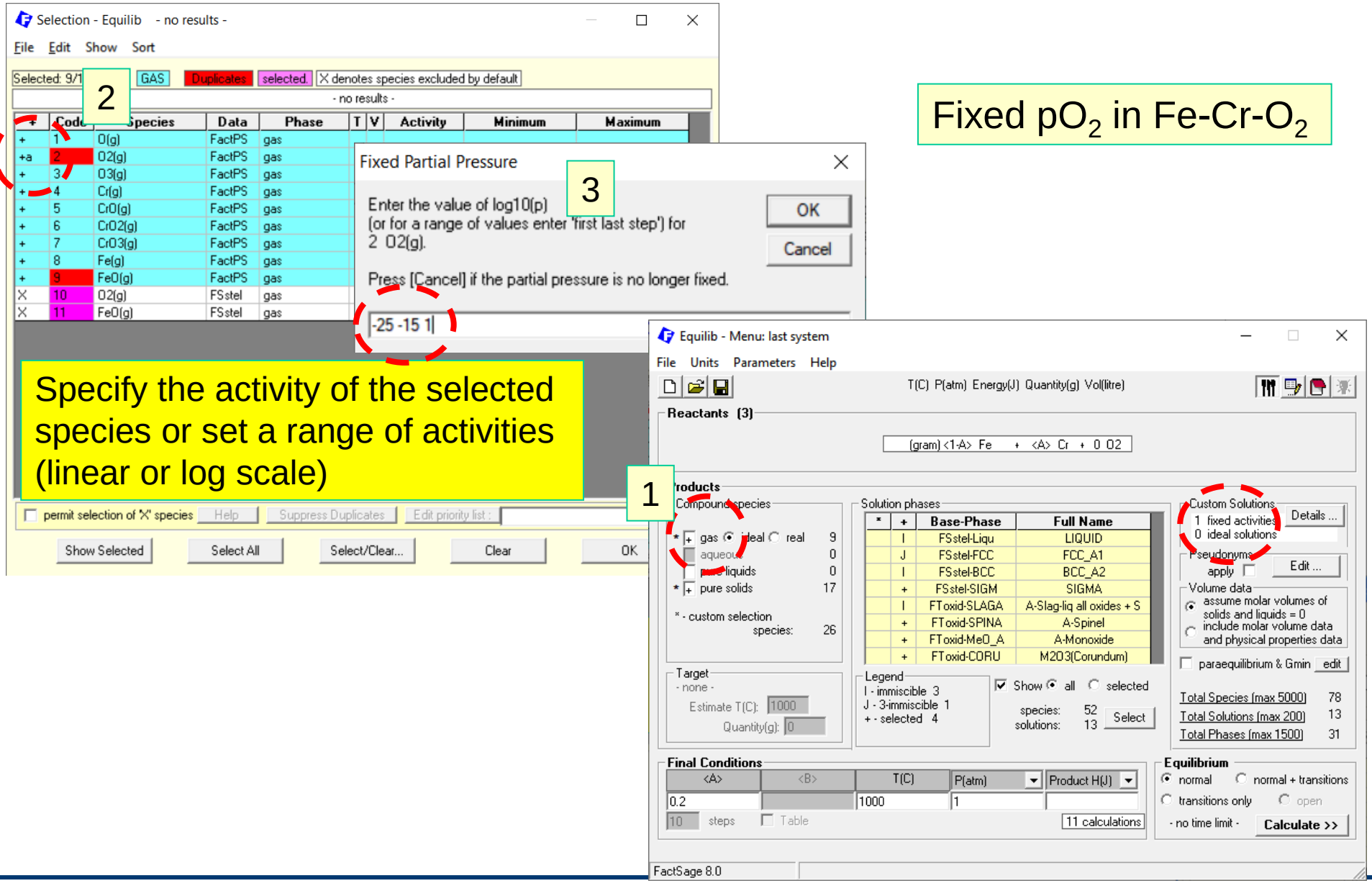
Select these elements in FeLQ
These are what we compare with experimental analysis

When we need to fix activity or partial pressure ?

Only a couple of cases when you need to fix activity or partial pressures are listed below. There could be numerous cases other than these.

- In steelmaking process or other pyrometallurgical process, “Slags” play important roles. Slags can contain oxide components having more than 2 oxidation states (for example, iron oxide, FeO and Fe2O3). In some case, FactSage cannot determine how much Fe2+ and Fe3+ exist in molten slags. The best way to resolve this problem is to fix the oxygen partial pressure of oxygen.
- Any case when you have oxides (solid or liquid state) with more than 2 oxidation states, it is better to fix oxygen partial pressure.
- When you study the solubility of gas species in slag, for example sulfur, it is better to fix the partial pressure of S2 or SO2 gas like in experiments.
- *If you equilibrate liquid steel (containing O or S) and slag, this can automatically fixing the oxygen or sulfur partial pressure. So, you don’t have to fix the partial pressure of gas species.*
- If you want to saturate the slag with Fe, you can fix the activity of Fe = 1 or enter small amount of Fe in the calculations.
- If you want to calculate iso-activity of SiO2 (or any other component) composition of slag, you can set activity of SiO2.

Fixed activity of gas and solid species

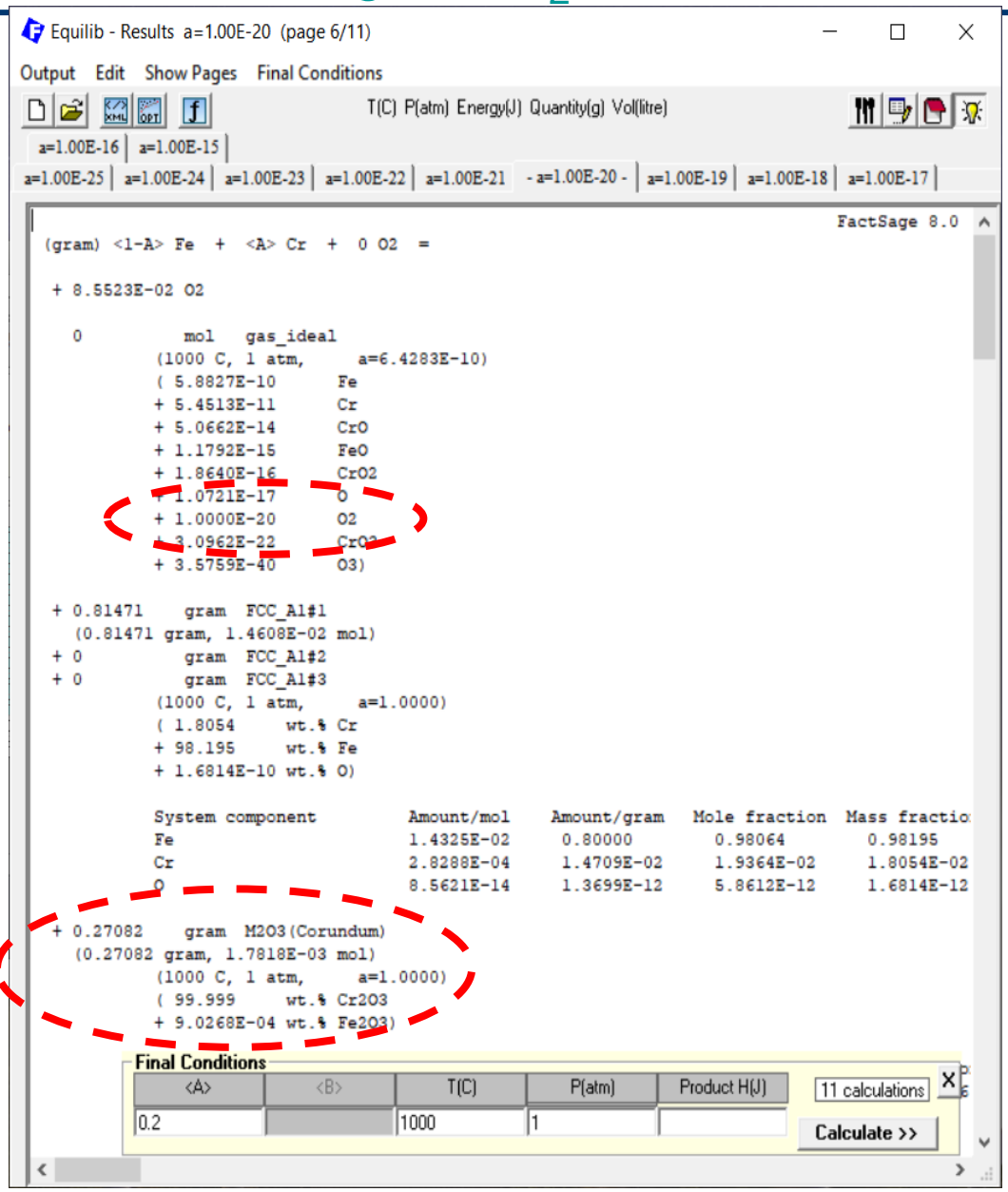


Fixed pO_2 in Fe-Cr-O_2

Fixed partial pressure of a gas : O_2

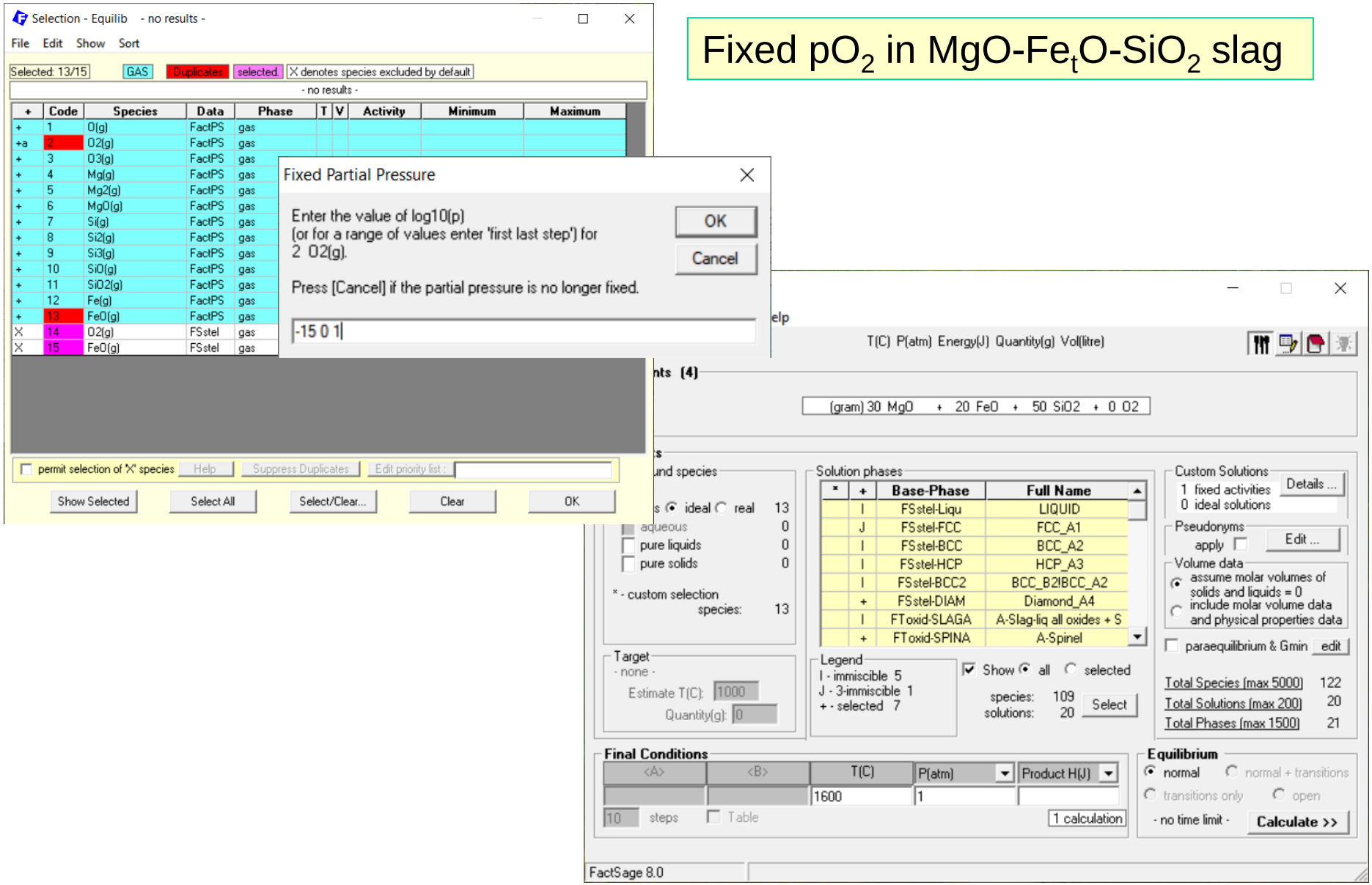
Results at log(pO_2) = -20

Small amount of Cr_2O_3 can form on top of the Fe-20%Cr alloy



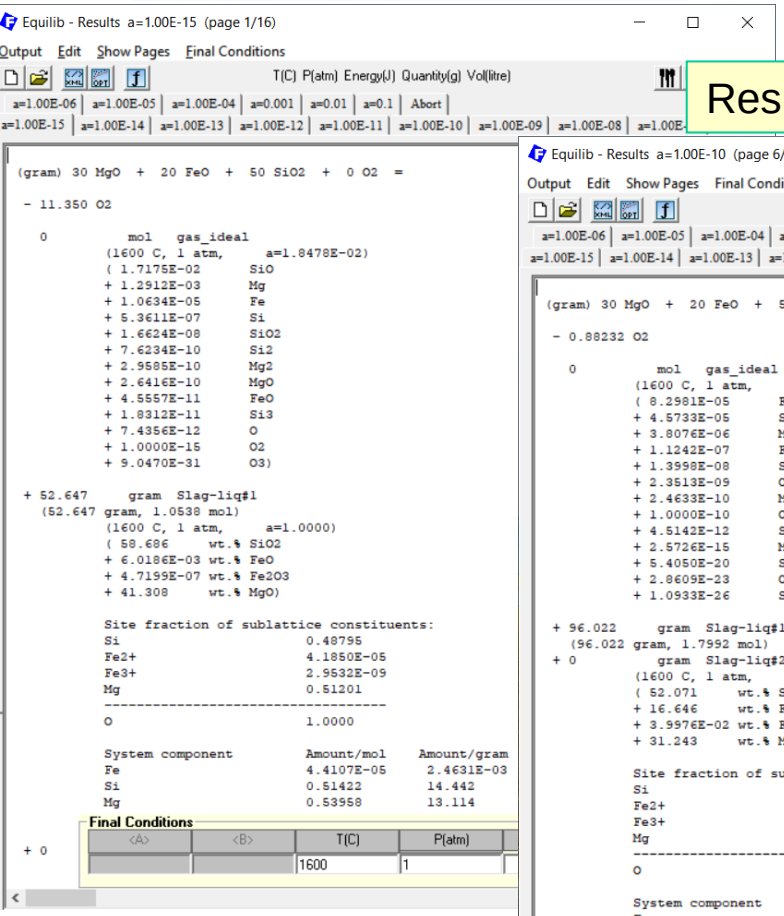
Fixed partial pressure of a gas : O_2

Fixed pO_2 in $MgO\text{-}Fe_tO\text{-}SiO_2$ slag

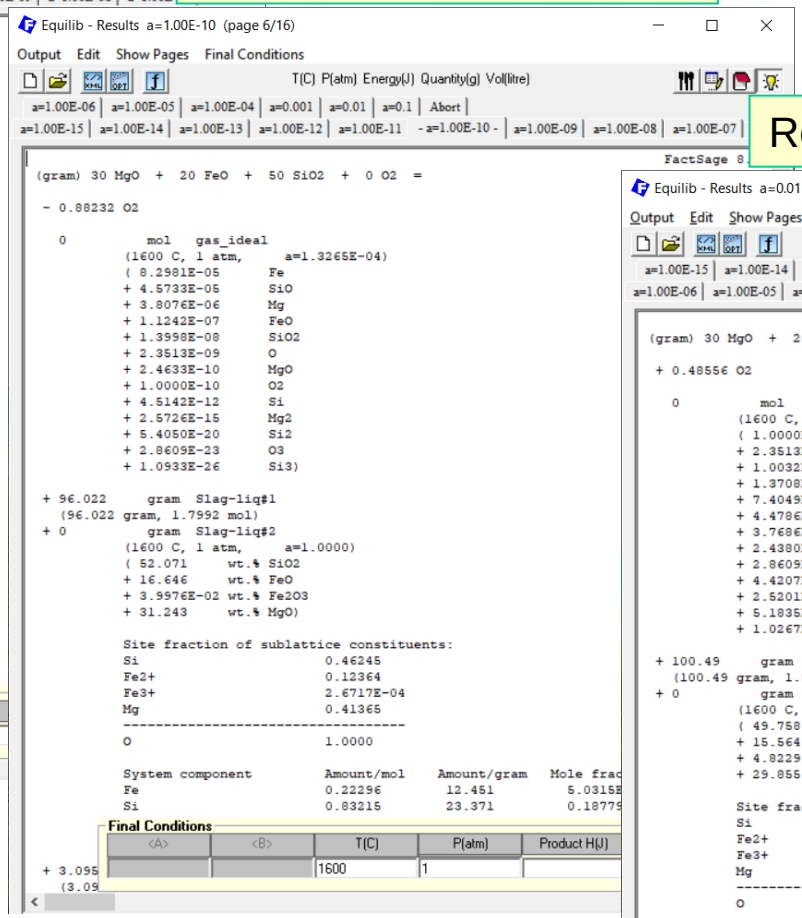


Fixed partial pressure of a gas : O_2

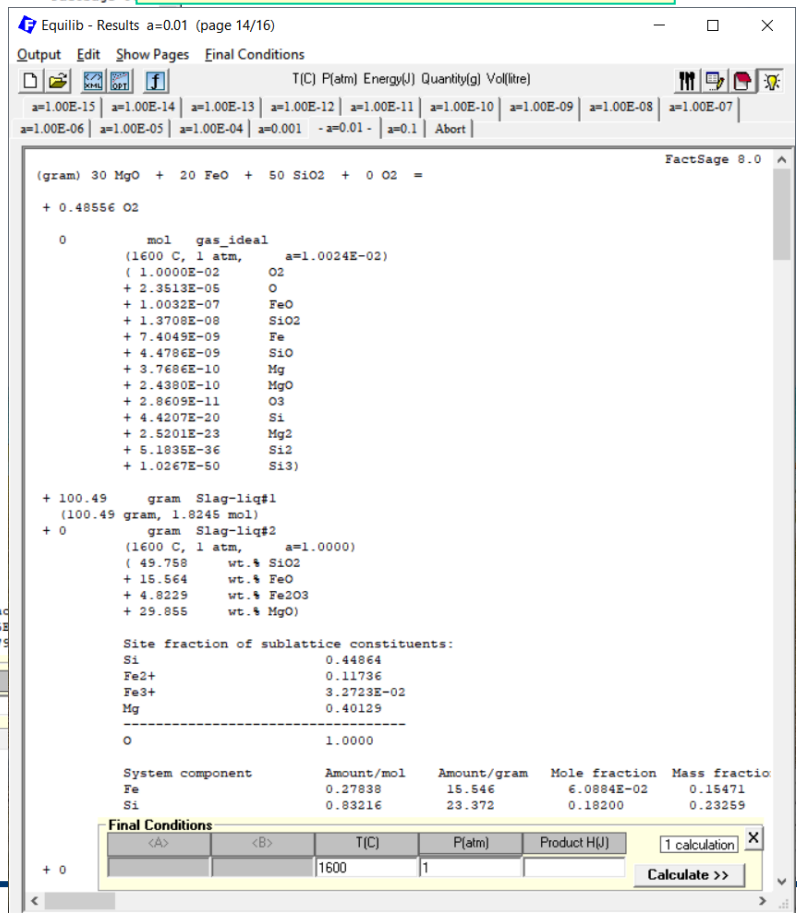
Results at $\log(pO_2) = -15$



Results at $\log(pO_2) = -10$



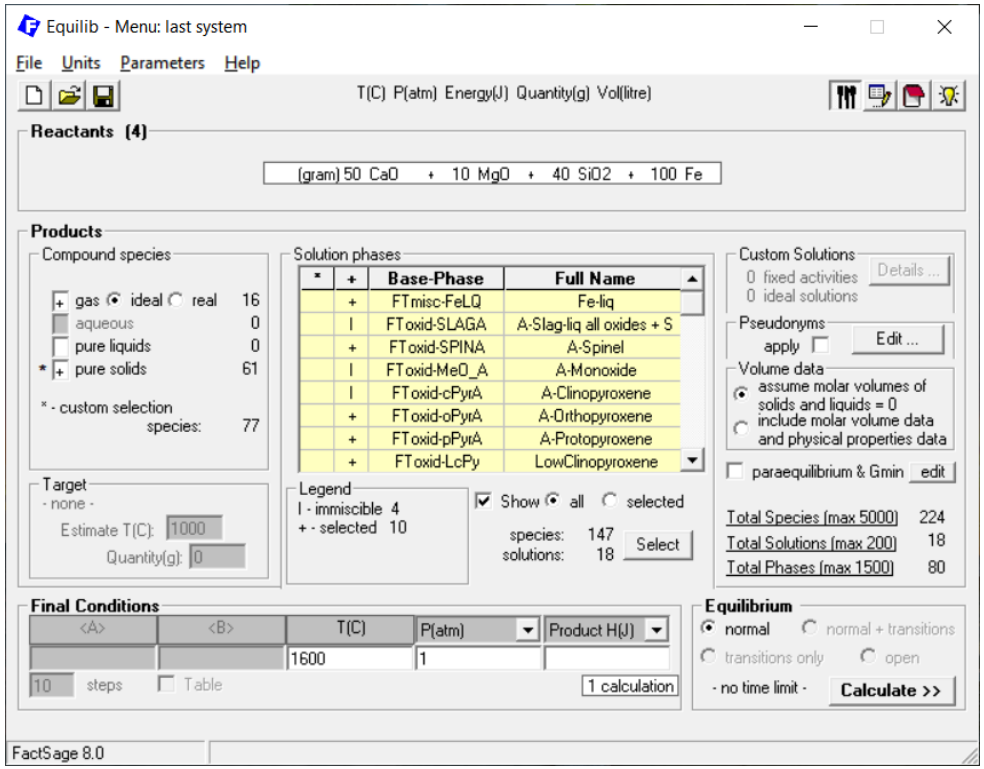
Results at $\log(pO_2) = -2$

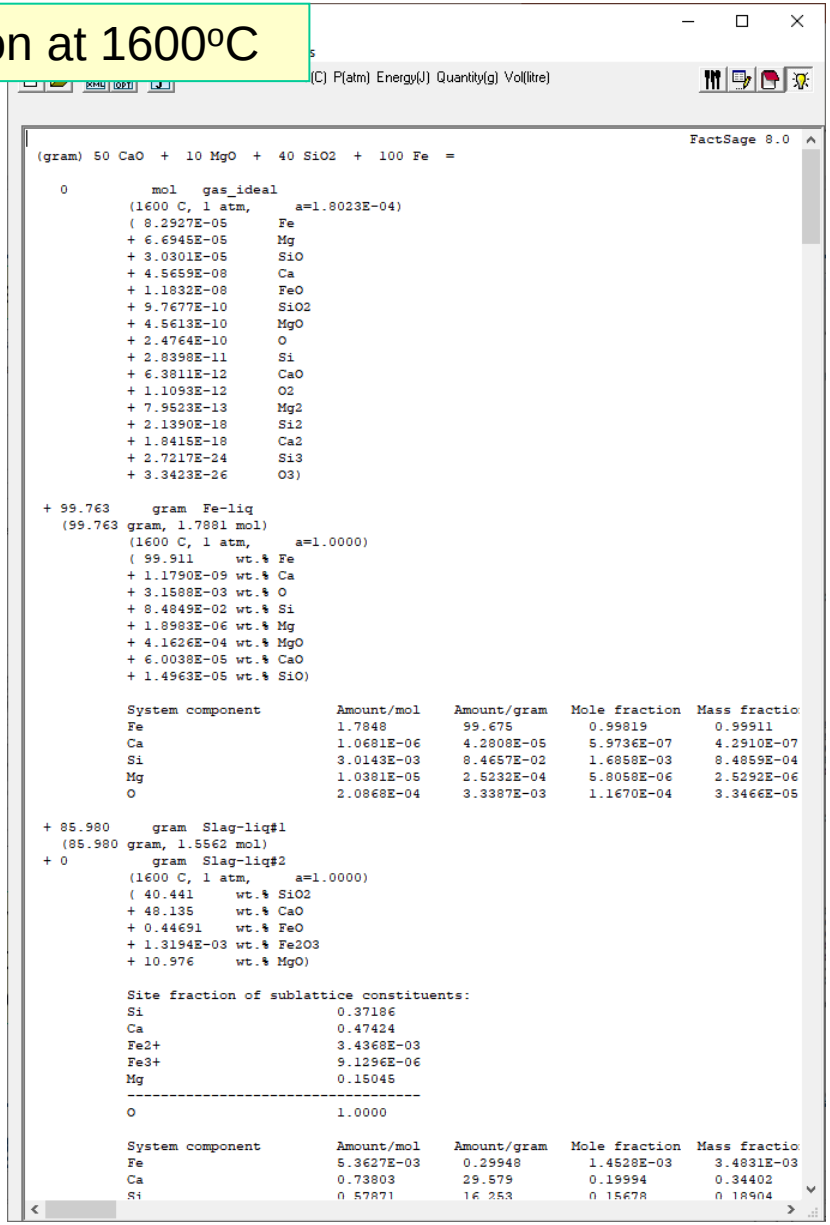


The amounts of FeO and Fe_2O_3 change with pO_2

Fixed activity of Fe: Fe saturation

Slag ($CaO-MgO-SiO_2$) and liquid Fe equilibration at 1600°C

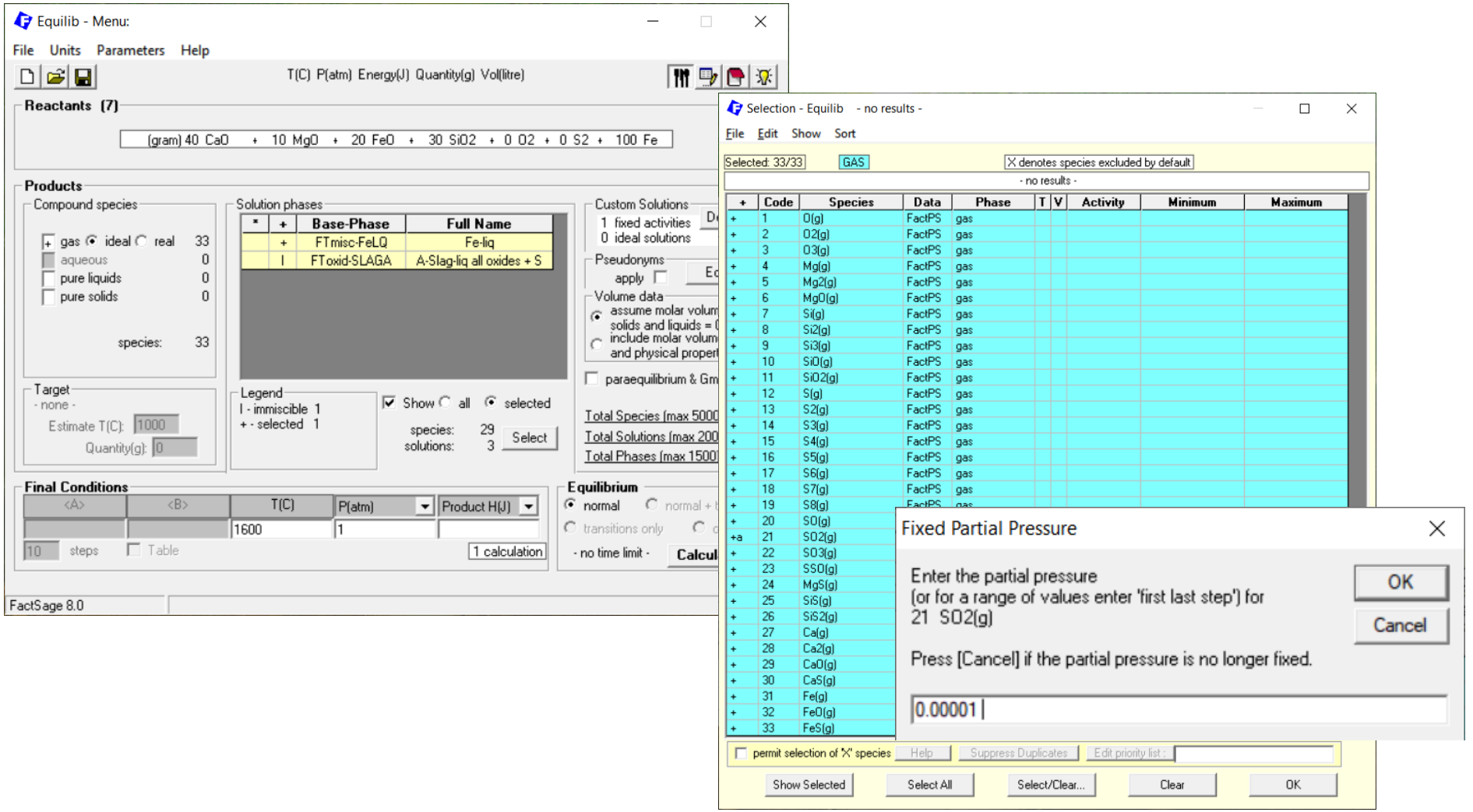




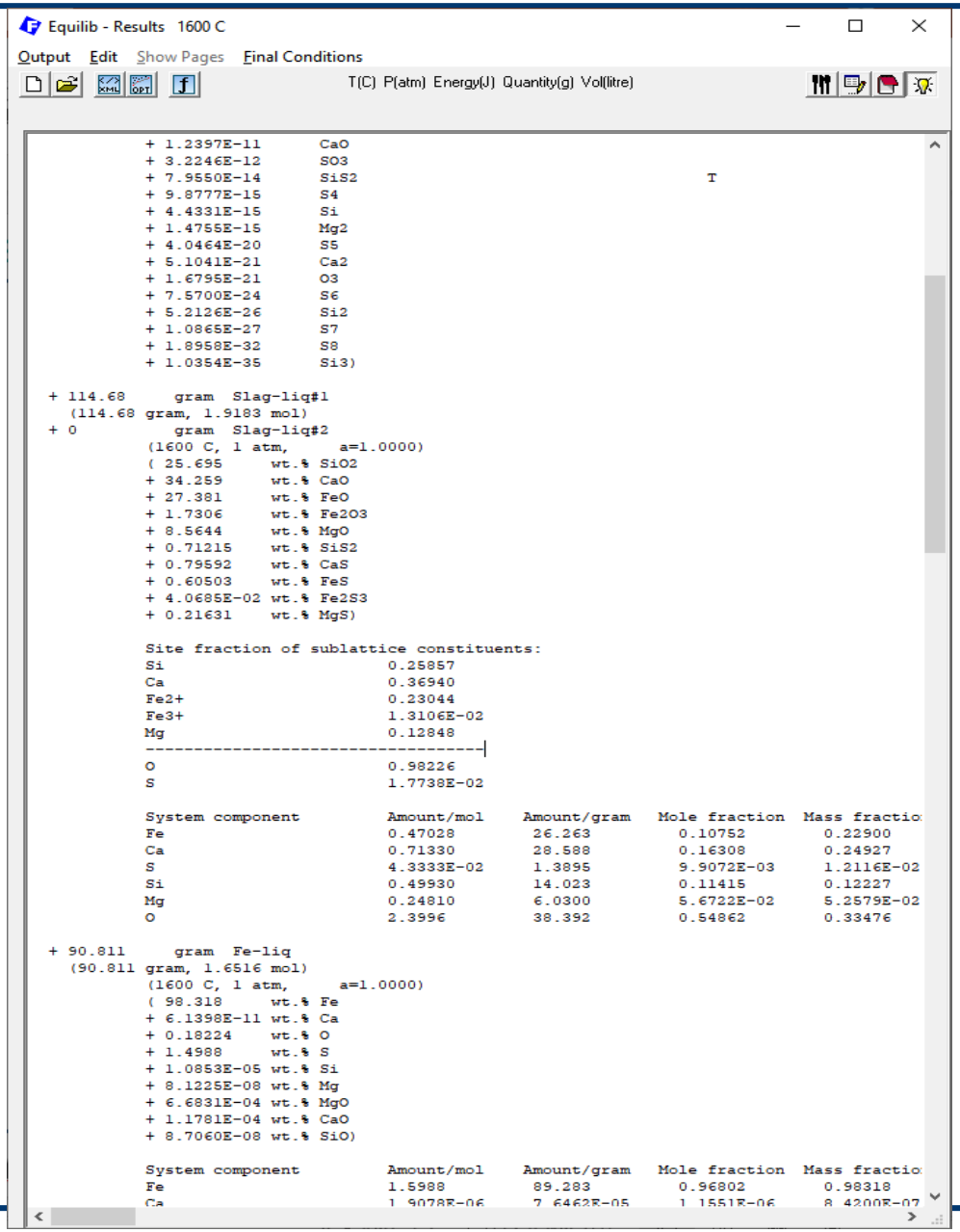
One way to fix Fe saturation in steelmaking calculations is to add a small amount of Fe as an input component

Fixed partial pressure of a gas : Fe saturation and fixed SO_2

Gas / Slag (CaO-MgO-FeO-SiO_2) / Liquid Fe equilibration



Fixed partial pressure of a gas : Fe saturation and SO_2



Gas (SO_2, S_2, O_2, etc.)
Slag (CaO, MgO, FeO, … CaS, MgS, FeS, etc.)
Fe-Lq (O, S, etc.)

Equilibration reactions include:

$CaO + SO_2 = CaS + 2\underline{O}$

$SO_2 = 2\underline{O} + \underline{S}$

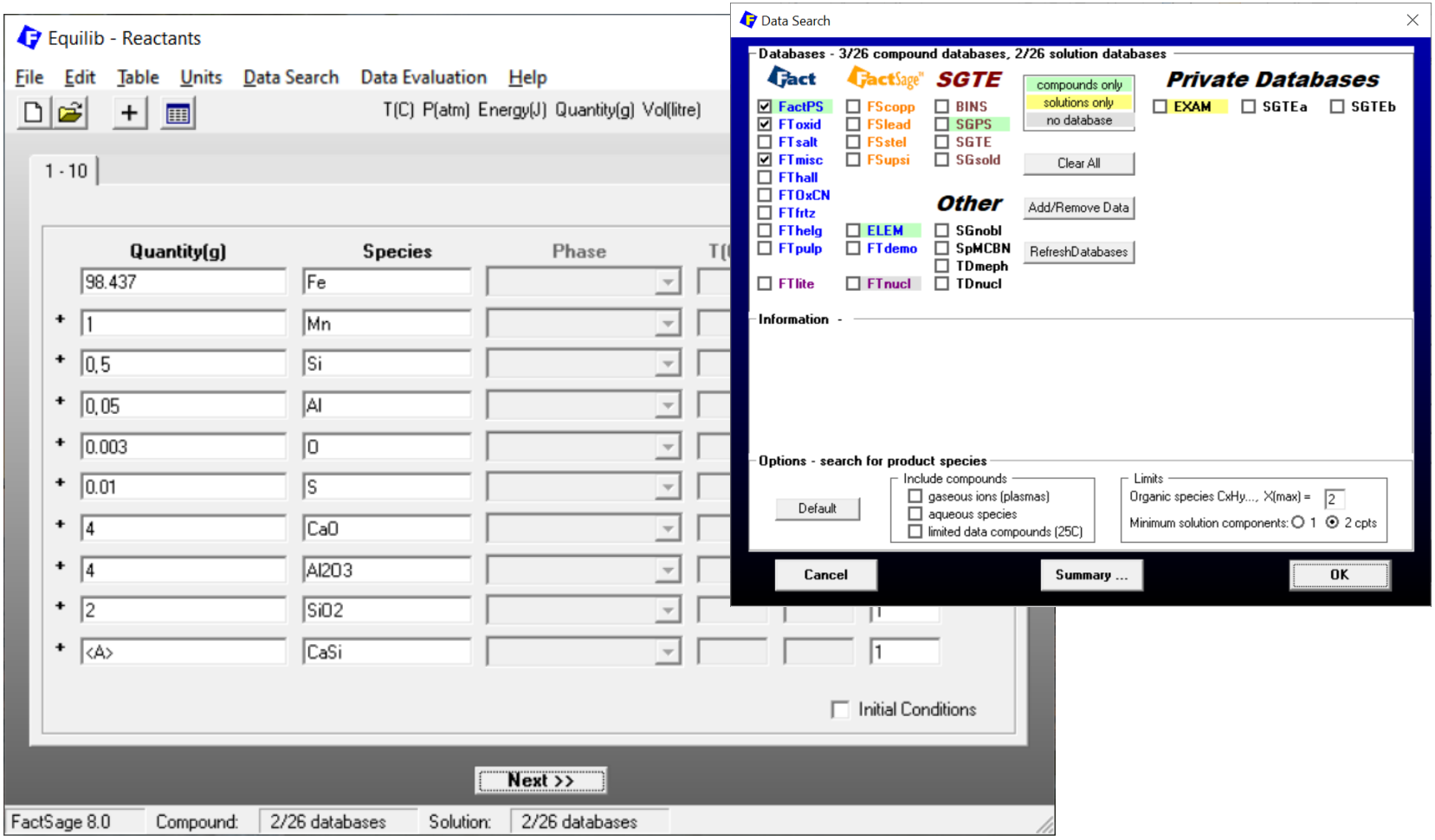
$CaO + FeS = CaS + FeO$

……

Composition target: target S content in liquid steel

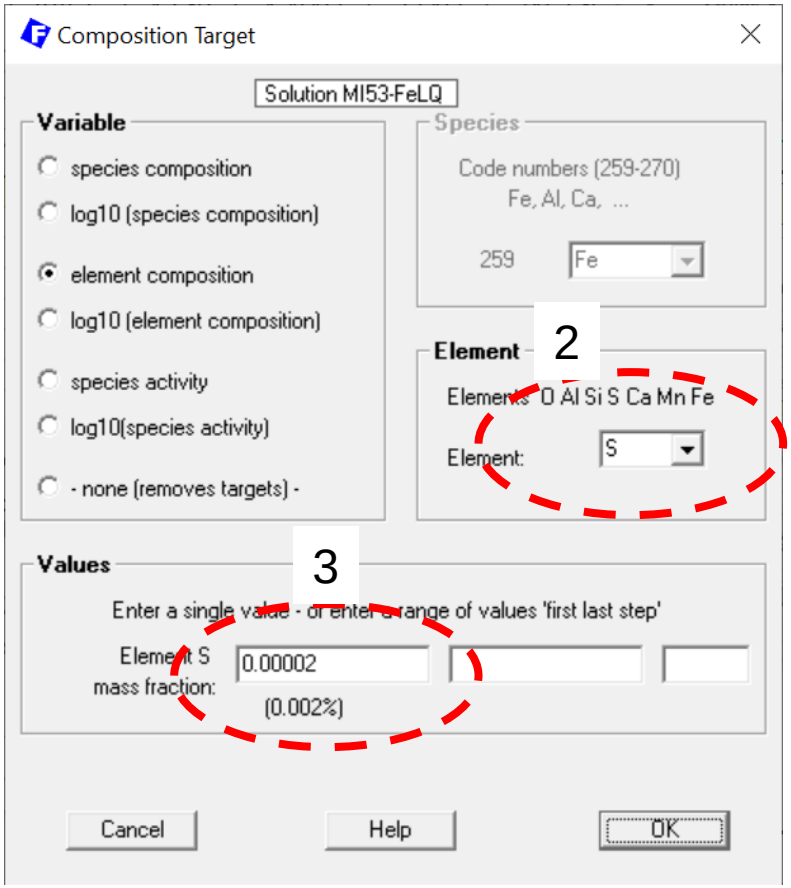
Composition Target: slag / liquid steel equilibrium

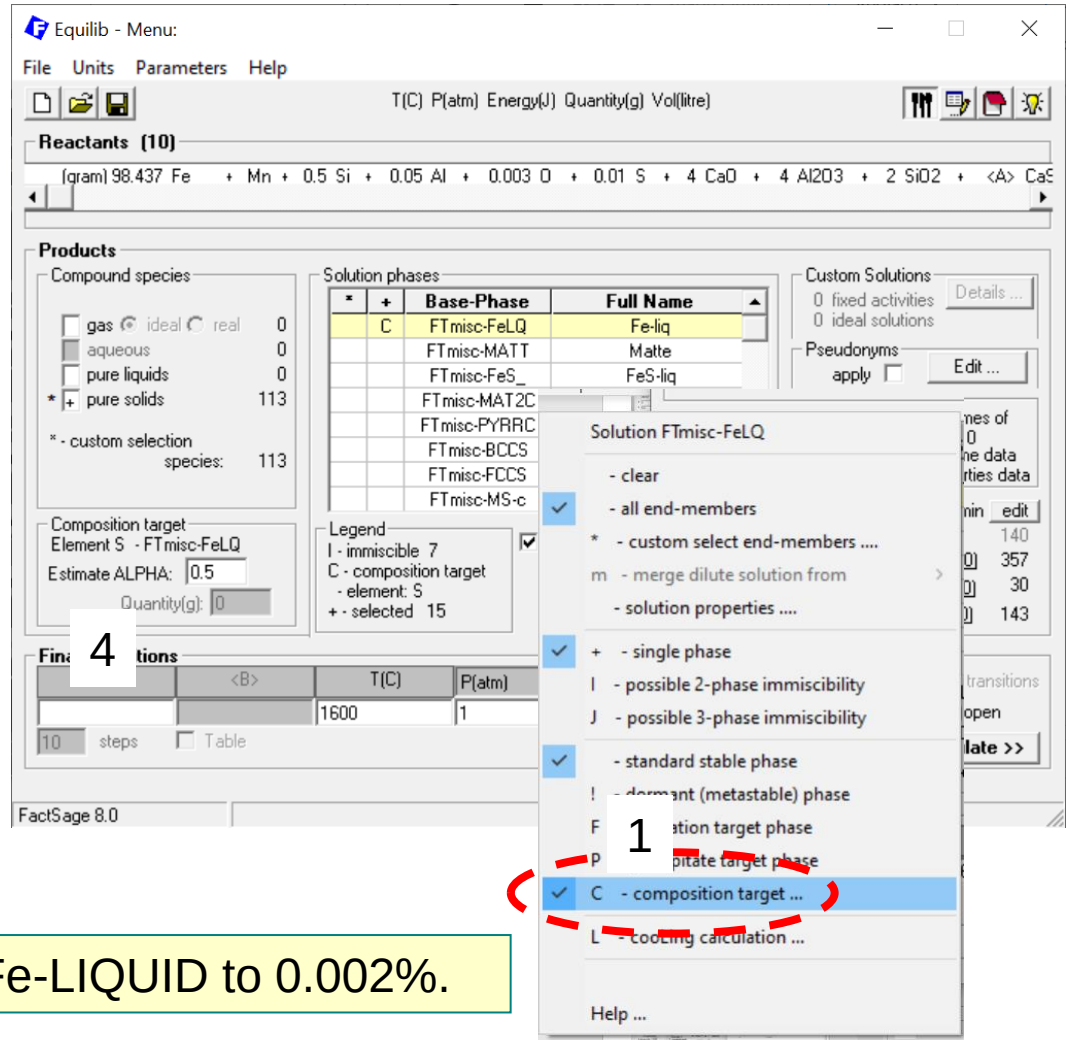
" How to calculate optimum amount of CaSi to reduce S in liquid steel to a targeted composition"



Composition target: target S content in liquid steel

Selecting target element (species)





Add CaSi (<A>) to reduce [%S] in Fe-LIQUID to 0.002%.

Composition target: target S content in liquid steel

Amount of CaSi = 0.9674 gram to obtain [%S] = 0.002%

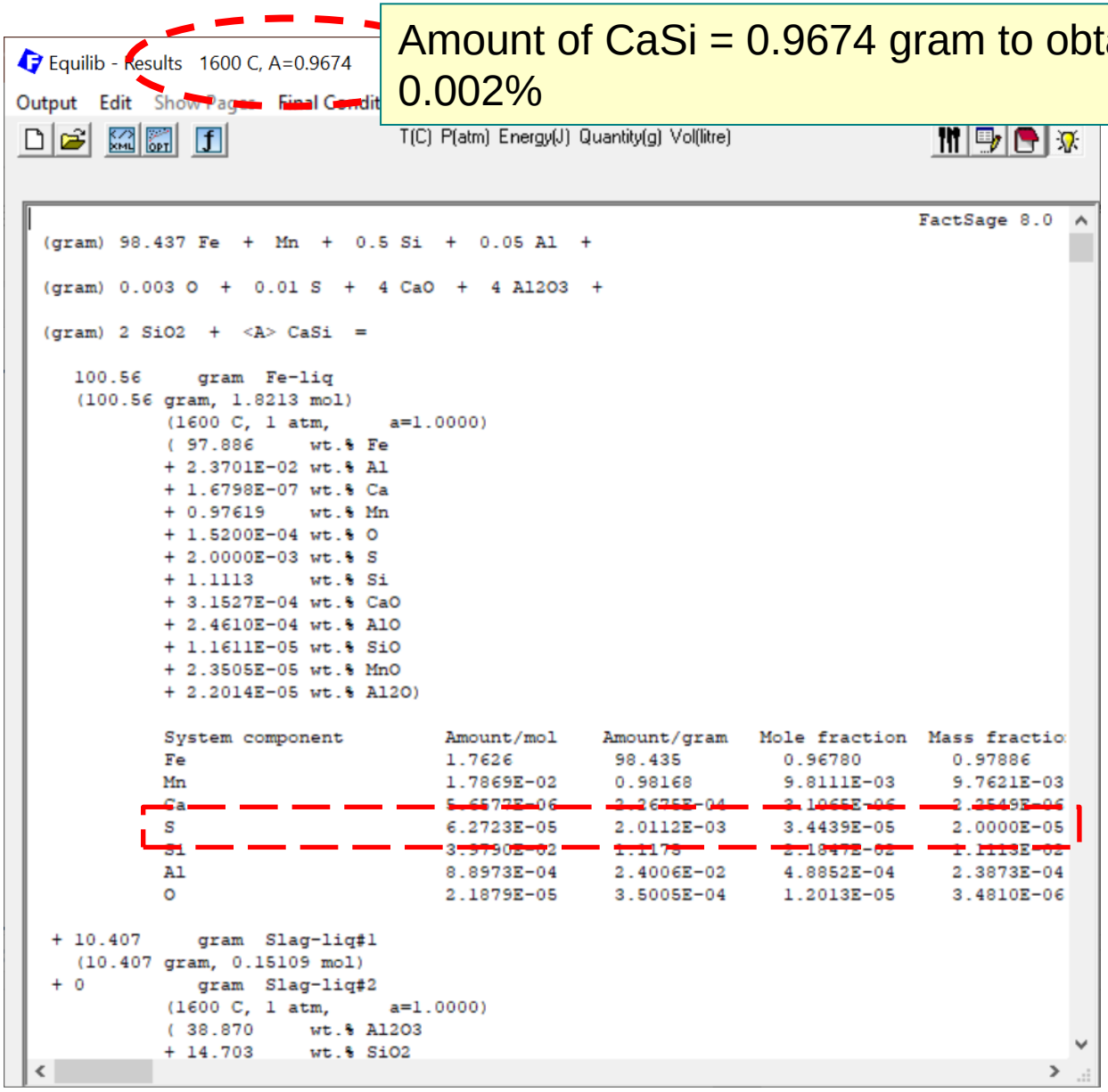


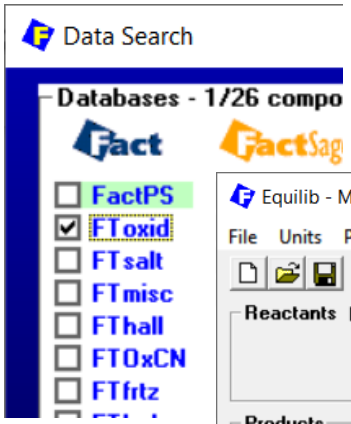
Table calculations: multi-calculation using EXCEL sheet

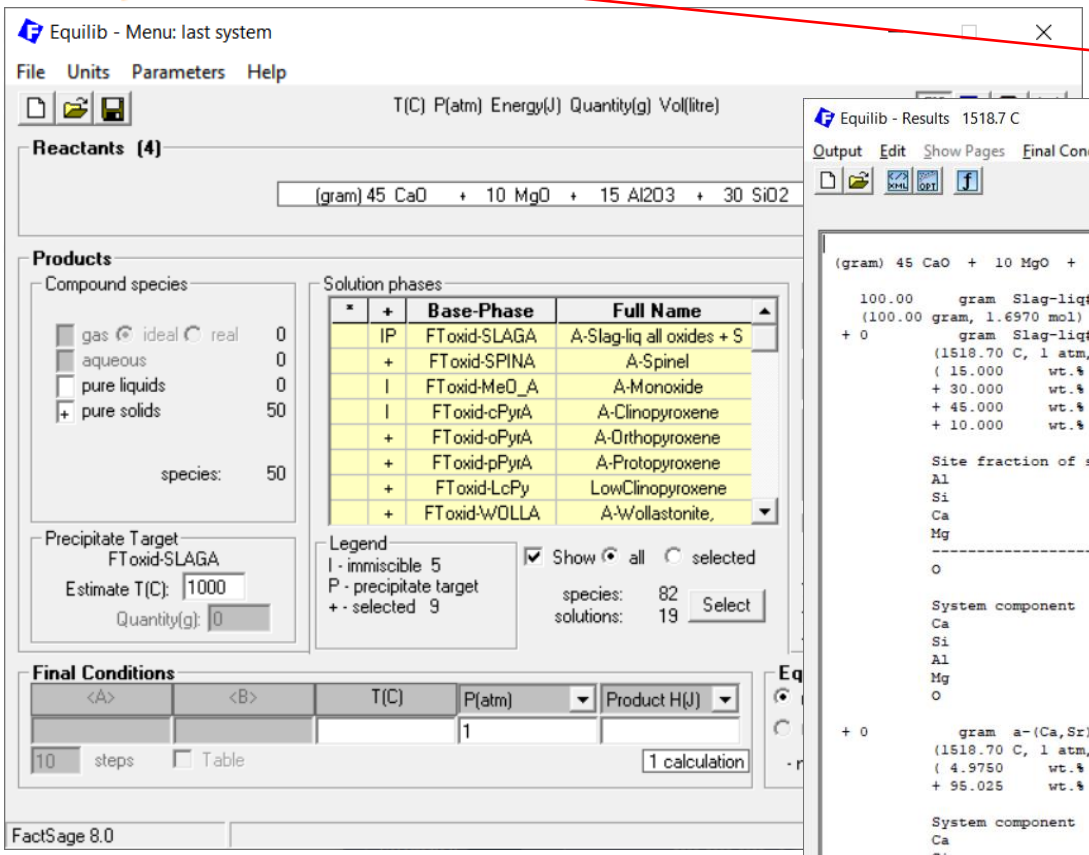
For example, calculations for liquidus temperatures for many slag compositions

→ One by one in Equilib using Precipitation target for liquid slag

→ Or using **Table** calculation

Perform one calculation to make sure that your calculation is working





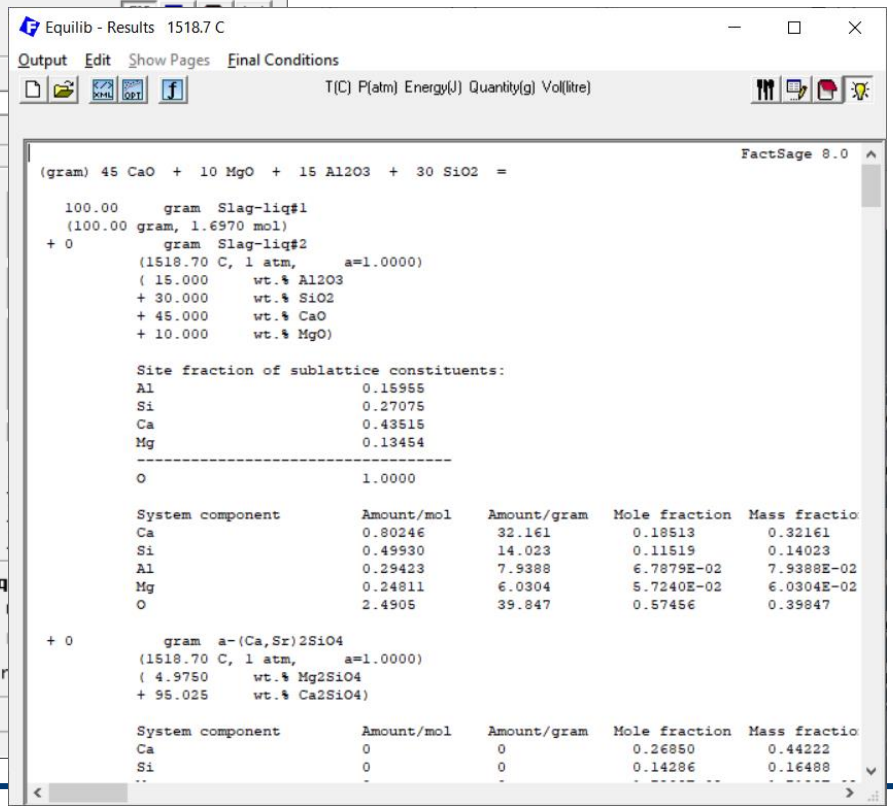


Table calculations: multi-calculation using EXCEL sheet

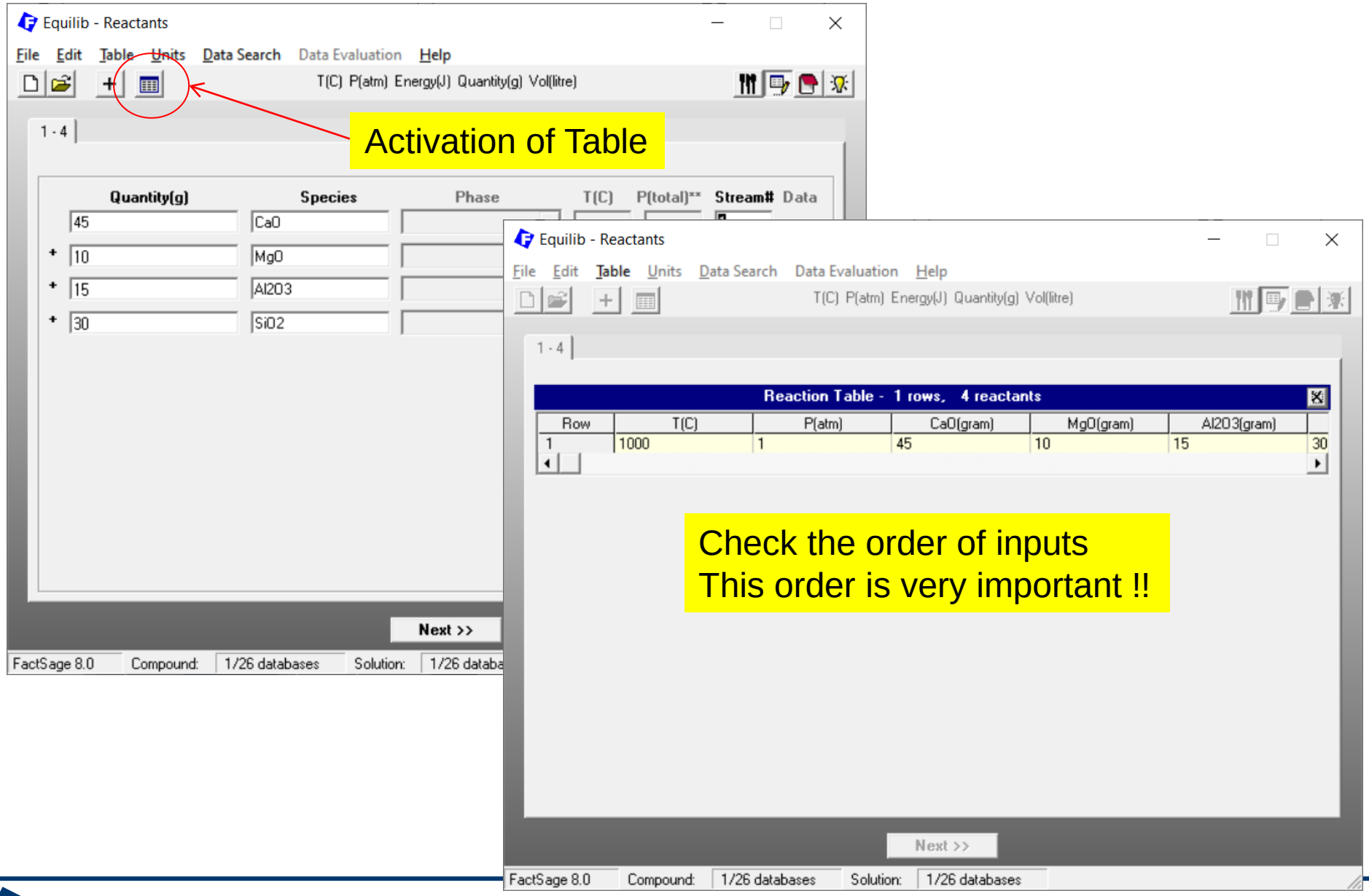
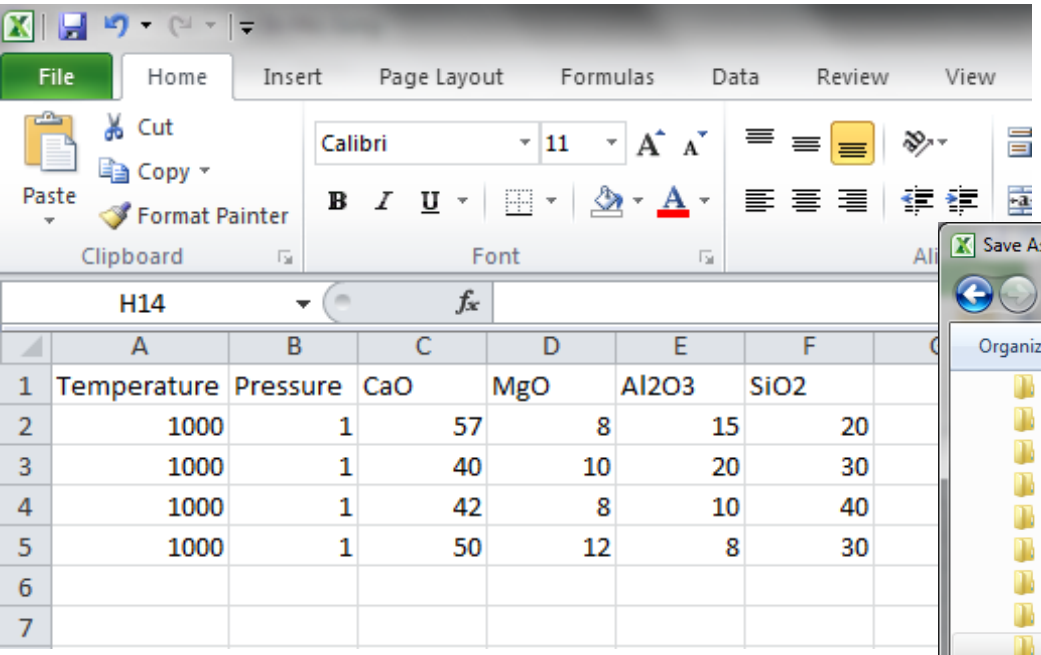


Table calculations: multi-calculation using EXCEL sheet

Prepare data in excel spread sheet (input order is the same as the input displayed in FactSage table mode; see previous slide)
and then save it as “txt” file



	A	B	C	D	E	F
1	Temperature	Pressure	CaO	MgO	Al2O3	SiO2
2	1000	1	57	8	15	20
3	1000	1	40	10	20	30
4	1000	1	42	8	10	40
5	1000	1	50	12	8	30
6						
7						

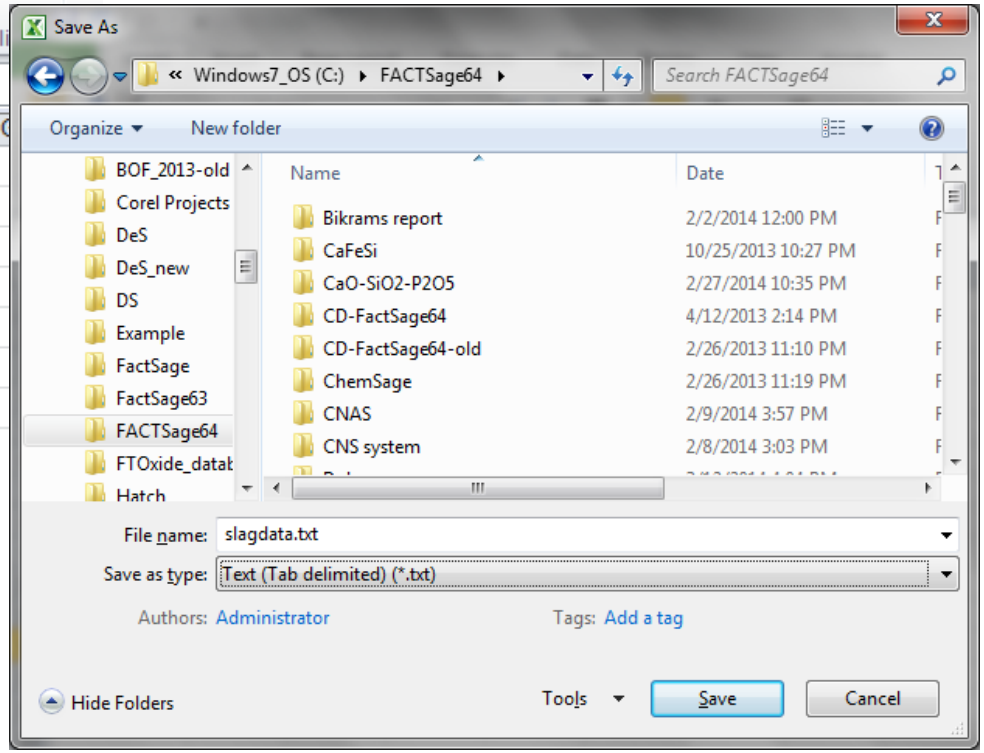
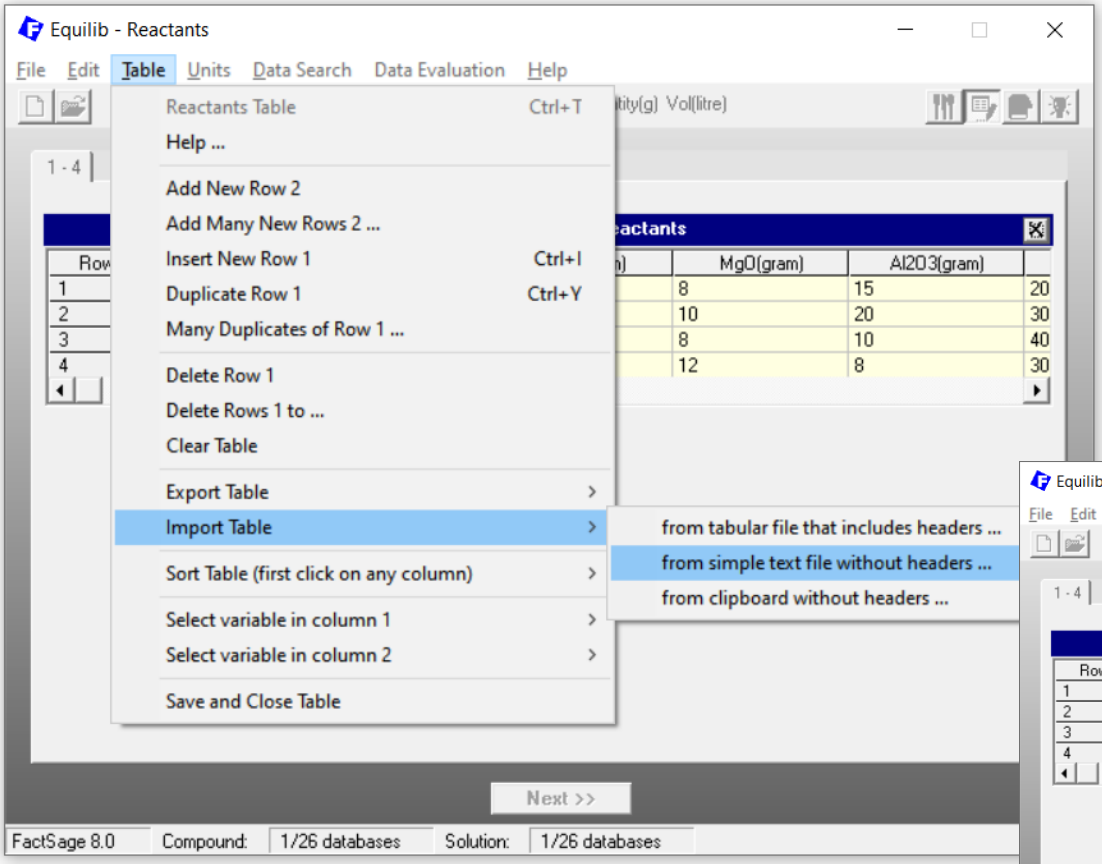


Table calculations: multi-calculation using EXCEL sheet

Import table from text file



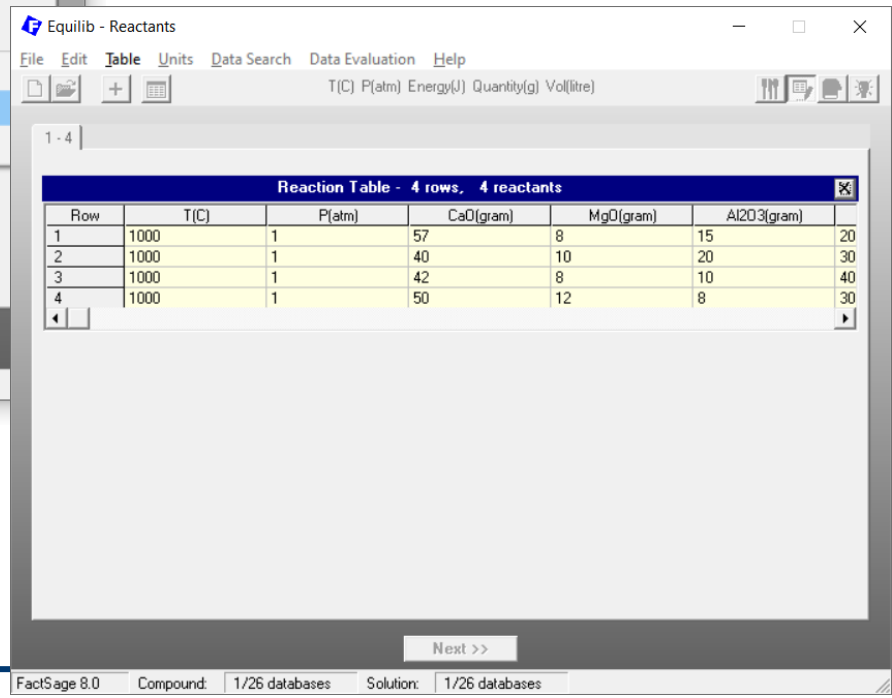
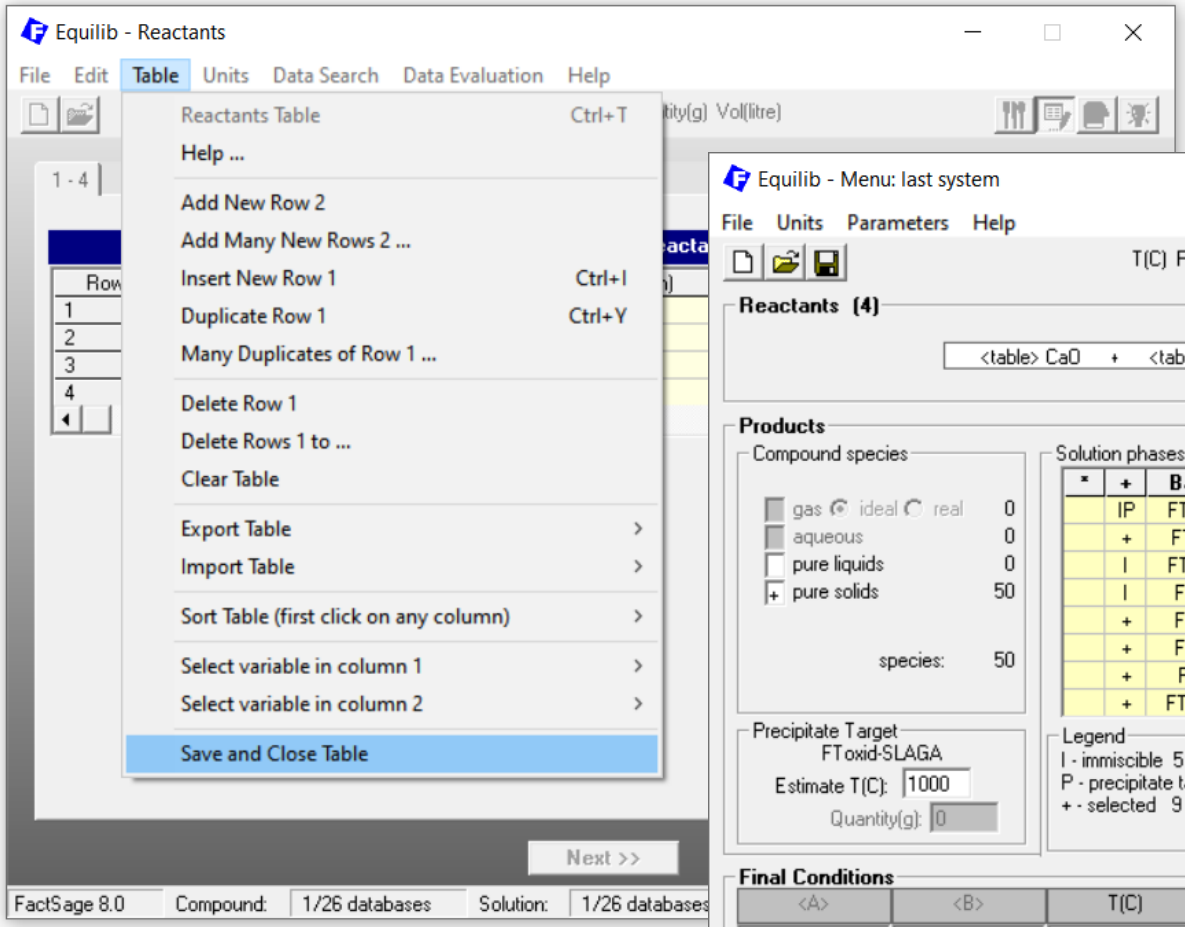
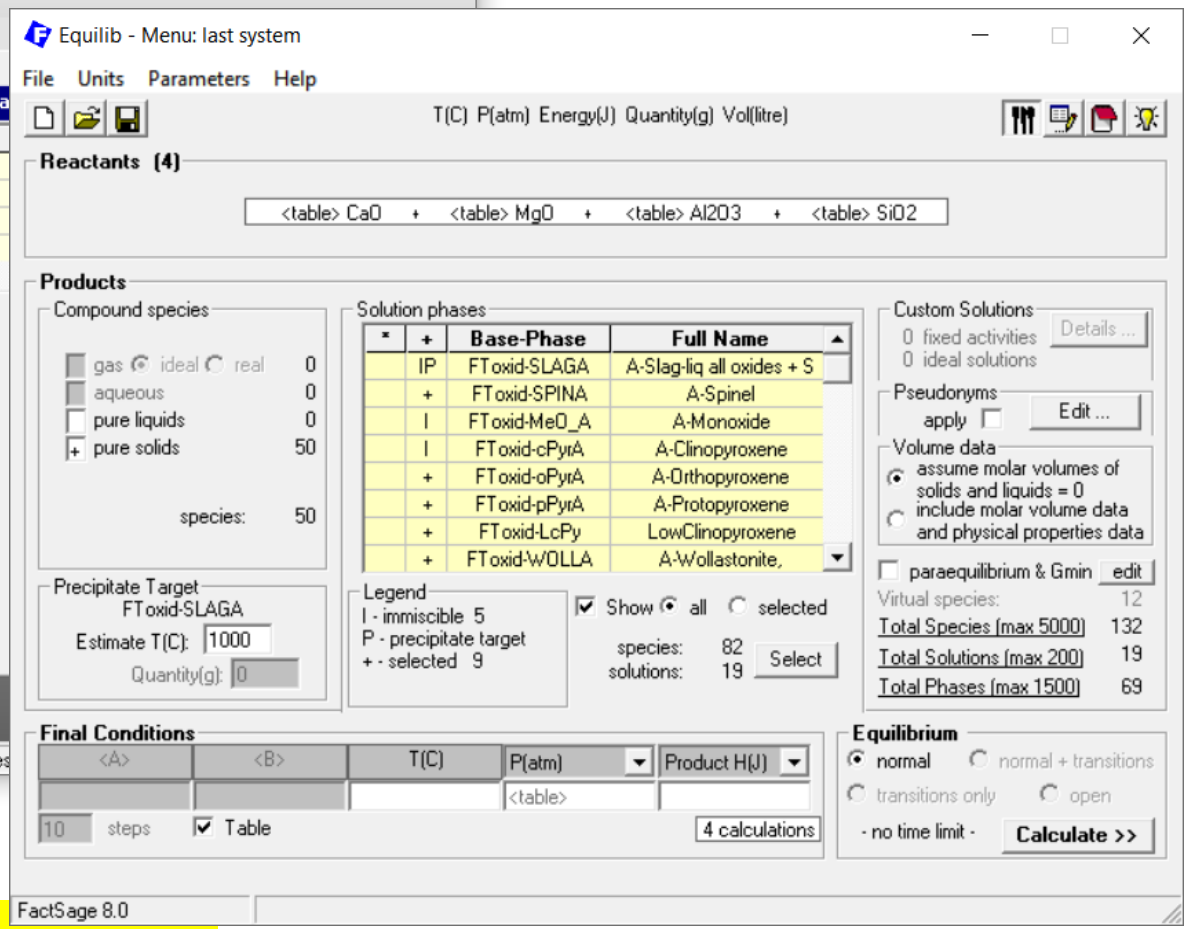


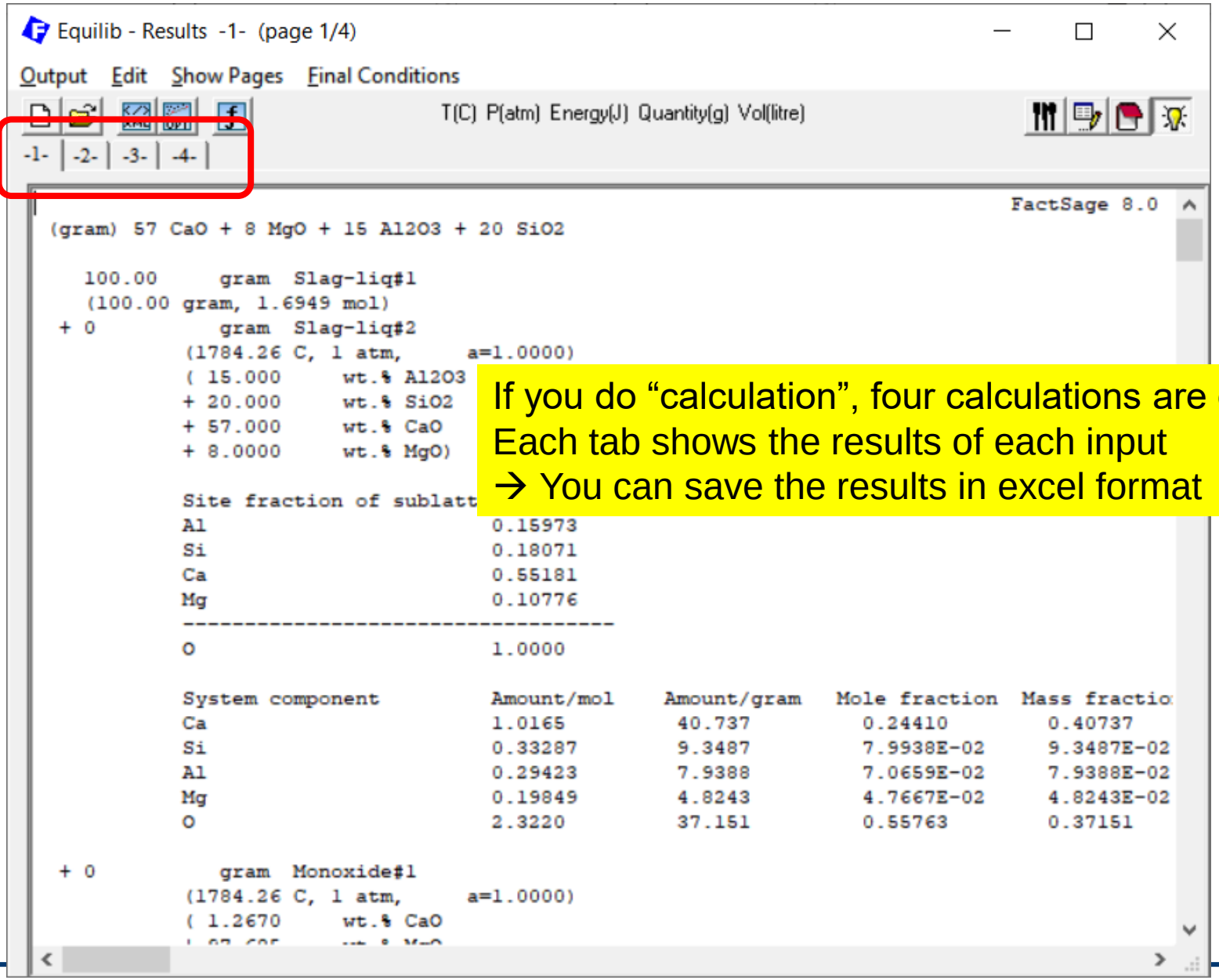
Table calculations: multi-calculation using EXCEL sheet





Close table input mode
→ Now in the calculation, activate “Table”

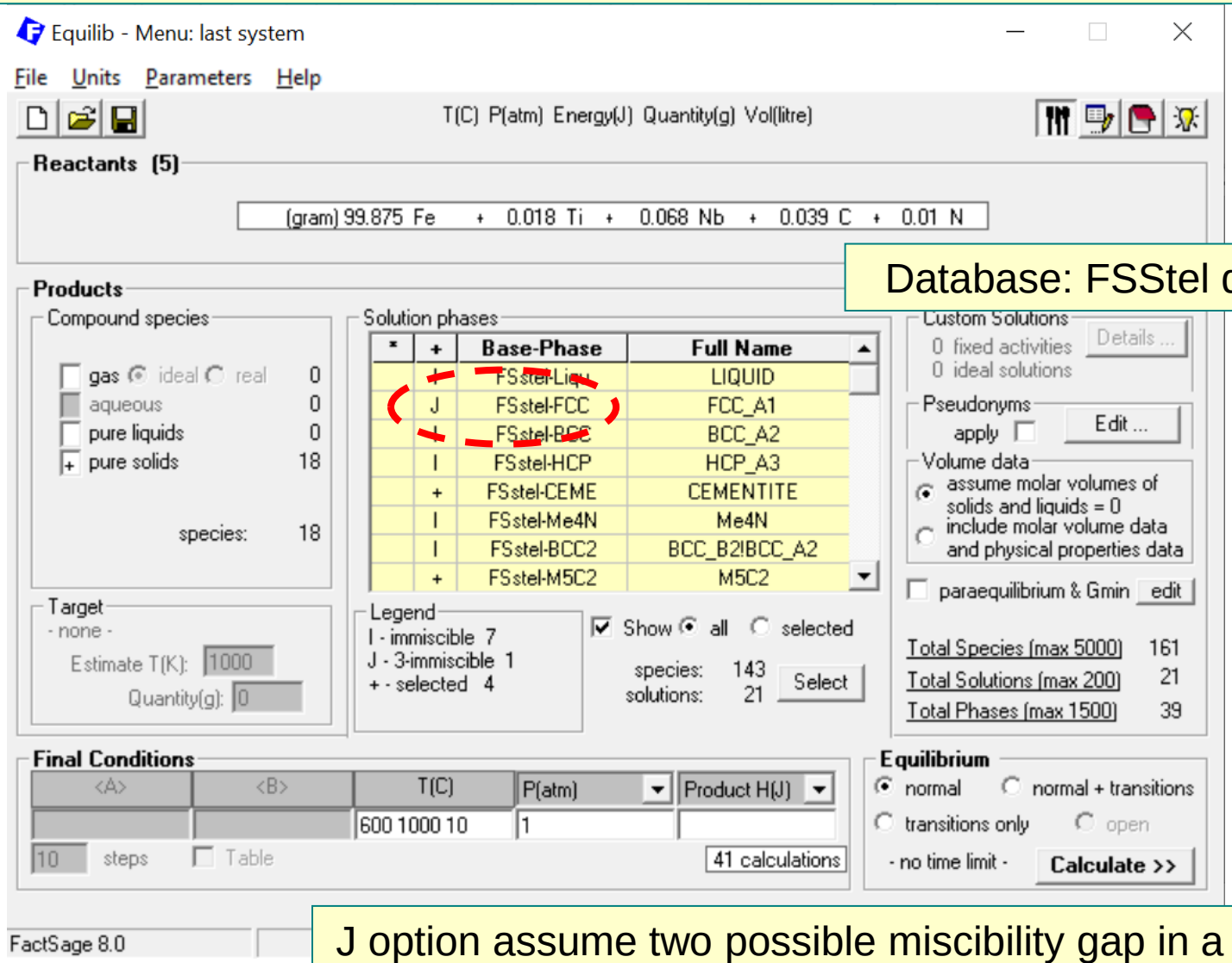
Table calculations: multi-calculation using EXCEL sheet



If you do “calculation”, four calculations are done:
Each tab shows the results of each input
→ You can save the results in excel format

J option for FCC phase: Fe steel containing (Ti,Nb)(C,N) ppts

Fe-0.039C-0.01N-0.068Nb-0.018Ti: three possible FCC phases



Database: FSStel database

J option assume two possible miscibility gap in a solution

J option for FCC phase: Fe steel containing (Ti,Nb)(C,N) ppts

Austenite, Ti and Nb carbo-nitrides are all FCC. In the FSStel database, all these fcc phases are modeled as a single FCC_A1 solution with three possible miscibility gaps.

Equilib - Results 900 C (page 34/44)

Output Edit Show Pages Final Conditions

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

930 C | 940 C | 950 C | 960 C | 970 C | 980 C | 990 C | 1000 C |

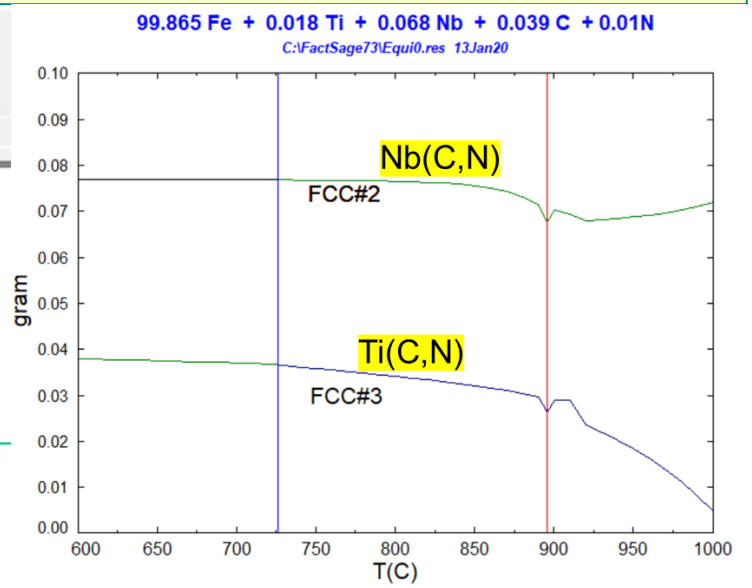
830 C | 840 C | 850 C | 860 C | 870 C | 880 C | 890 C | 895.31 C | - 900 C - | 910 C | 920 C |

Austenite phase

```
99.901      gram  FCC_A1#1
(99.901 gram, 1.7882 mol)
        (900 C, 1 atm,      a=1.0000)
        ( 99.798      wt.% Fe
        + 6.0158E-03 wt.% Nb
        + 2.3491E-06 wt.% Ti
        + 0.18941     wt.% FeC
        + 1.0611E-05 wt.% NbC
        + 4.5898E-09 wt.% TiC
```

Nb(C,N) ppt.

```
+ 7.0138E-02 gram  FCC_A1#2
  (7.0138E-02 gram, 6.8433E-04 mol)
        (900 C, 1 atm,      a=1.0000)
        ( 1.0260E-03 wt.% Fe
        + 6.5424      wt.% Nb
        + 0.16044     wt.% Ti
        + 1.0799E-02 wt.% FeC
        + 64.000      wt.% NbC
        + 1.7385      wt.% TiC
        + 4.5688E-03 wt.% FeN
        + 26.804      wt.% NbN
        + 0.73833     wt.% TiN)

        Site fraction of sublattice co
        Fe                          2.489
        Nb                          0.954
        Ti                          4.542
        ------------------------------
        Va                          7.562
        C                           0.655
        N                           0.269
```

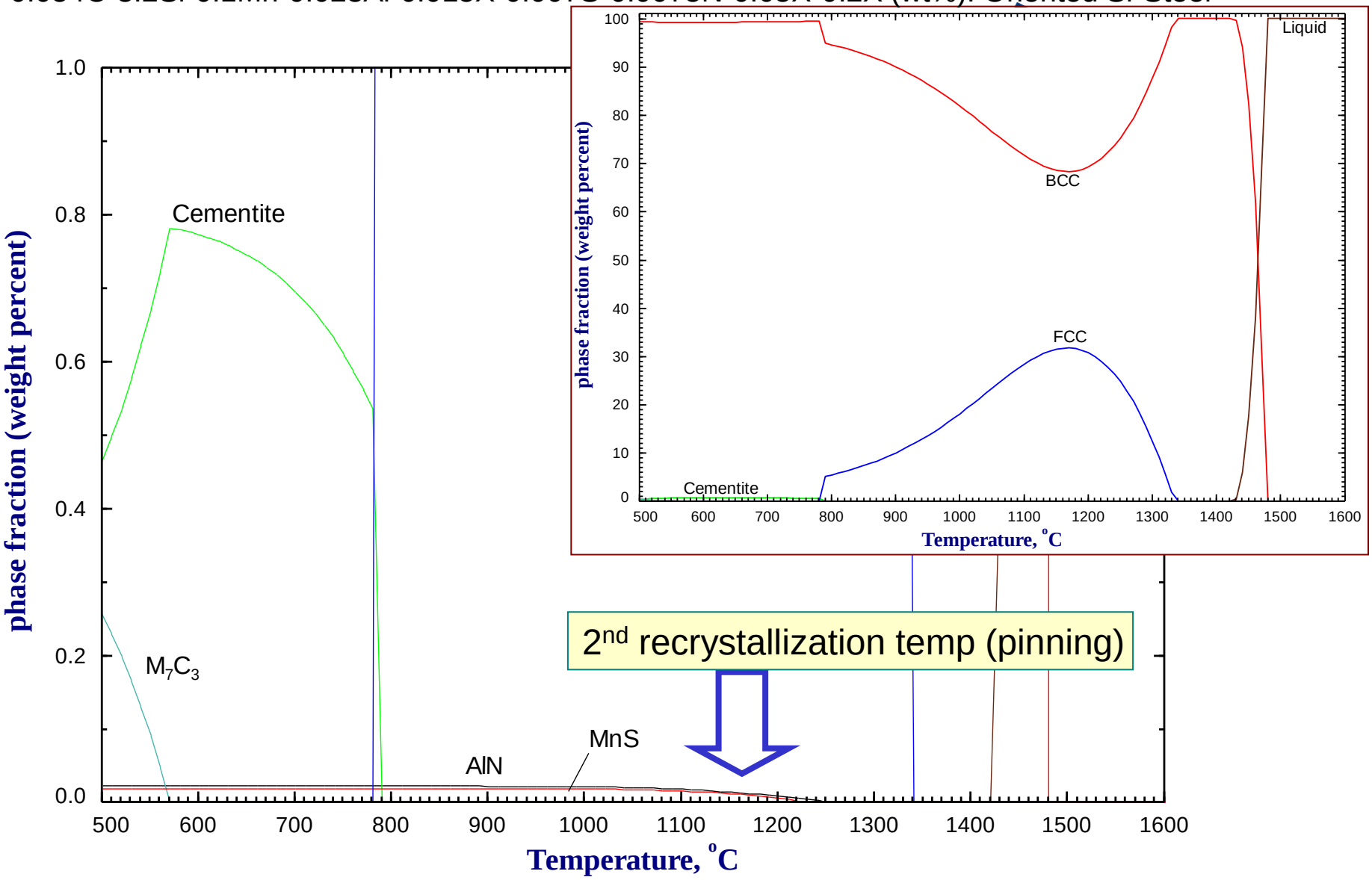


Ti(C,N) ppt.

```
+ 2.8907E-02 gram  FCC_A1#3
  (2.8907E-02 gram, 4.4612E-04 mol)
        (900 C, 1 atm,      a=1.0000)
        ( 1.0067E-02 wt.% Fe
        + 2.7001E-03 wt.% Nb
        + 3.4144E-02 wt.% Ti
        + 0.46550     wt.% FeC
        + 0.11604     wt.% NbC
        + 1.6255      wt.% TiC
        + 20.570      wt.% FeN
        + 5.0759      wt.% NbN
        + 72.101      wt.% TiN)
```

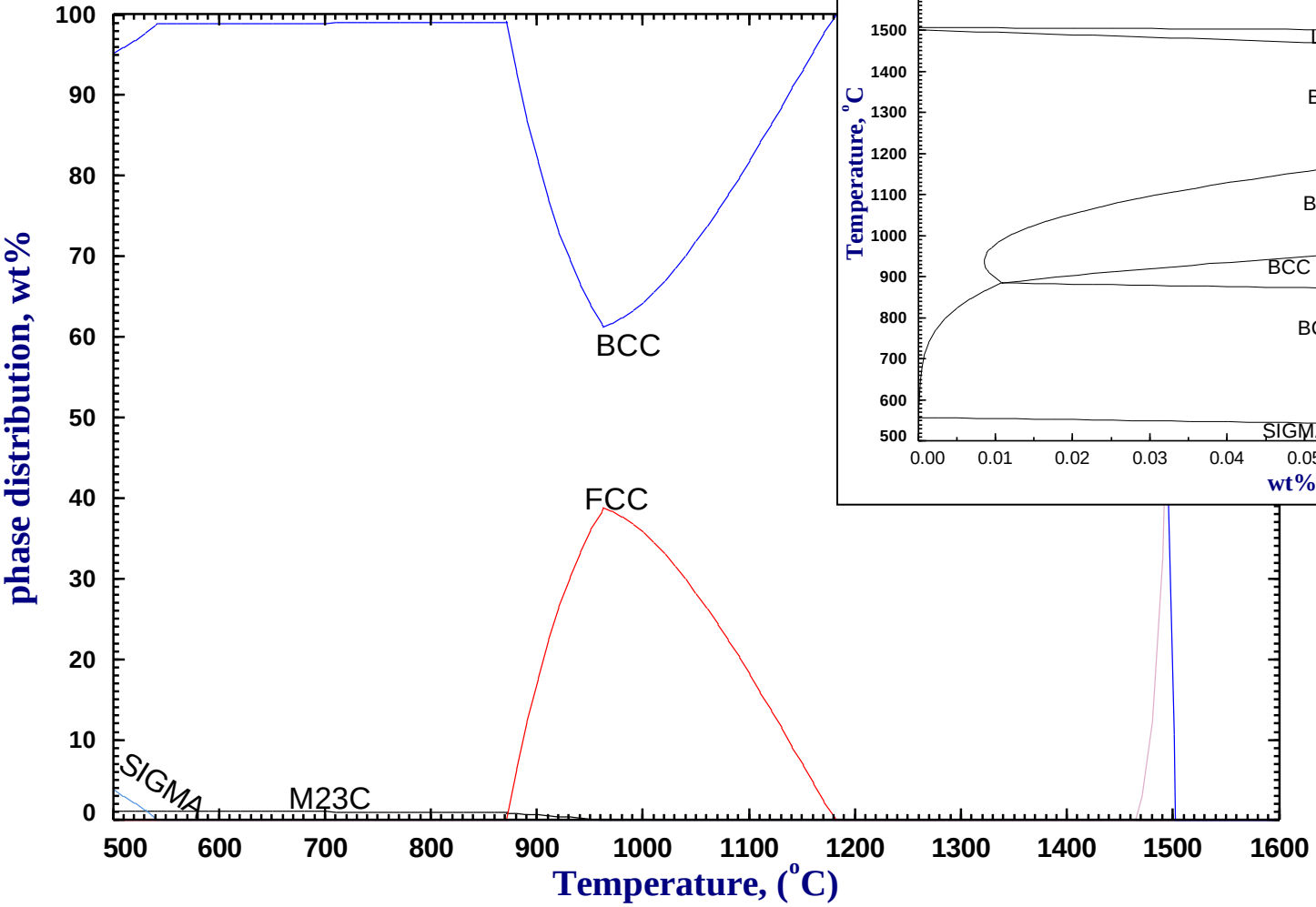
Precipitation of AlN and MnS in a commercial Si-steel

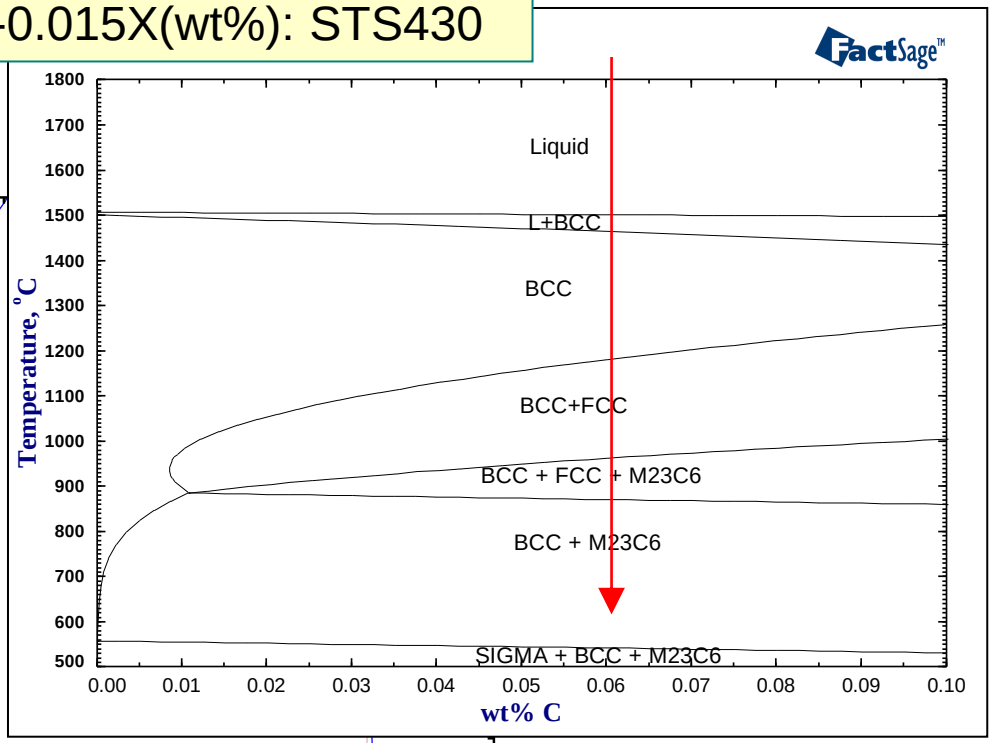
Fe-0.054C-3.2Si-0.1Mn-0.028Al-0.015X-0.007S-0.0075N-0.05X-0.2X (wt%): Oriented Si-Steel



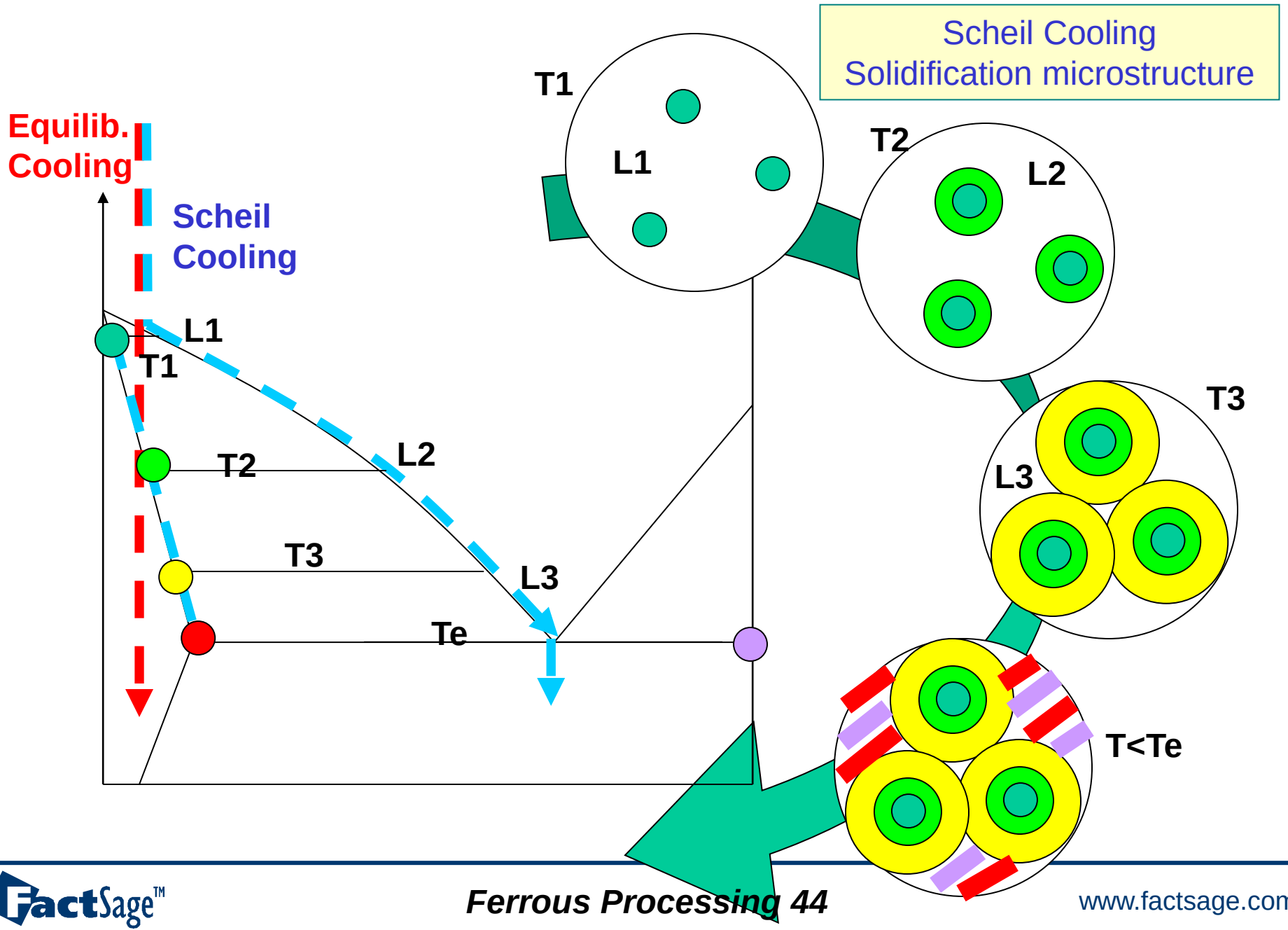
Phase diagram / Phase fraction of 430 Stainless Steel

Fe-16.2Cr-0.06C-0.3Si-0.4Mn-0.3Ni-0.015X(wt%): STS430



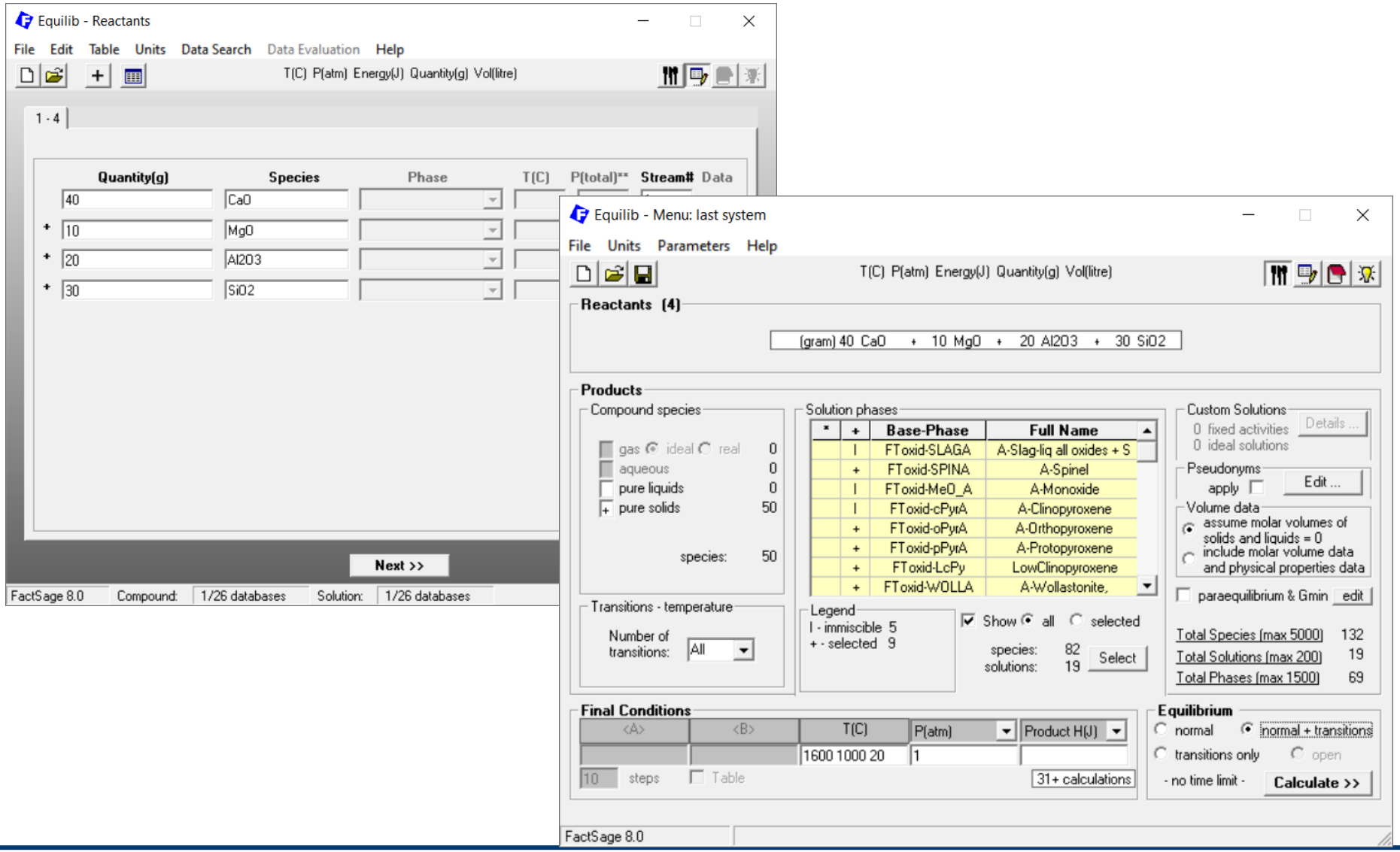


Equilibrium cooling and Scheil cooling

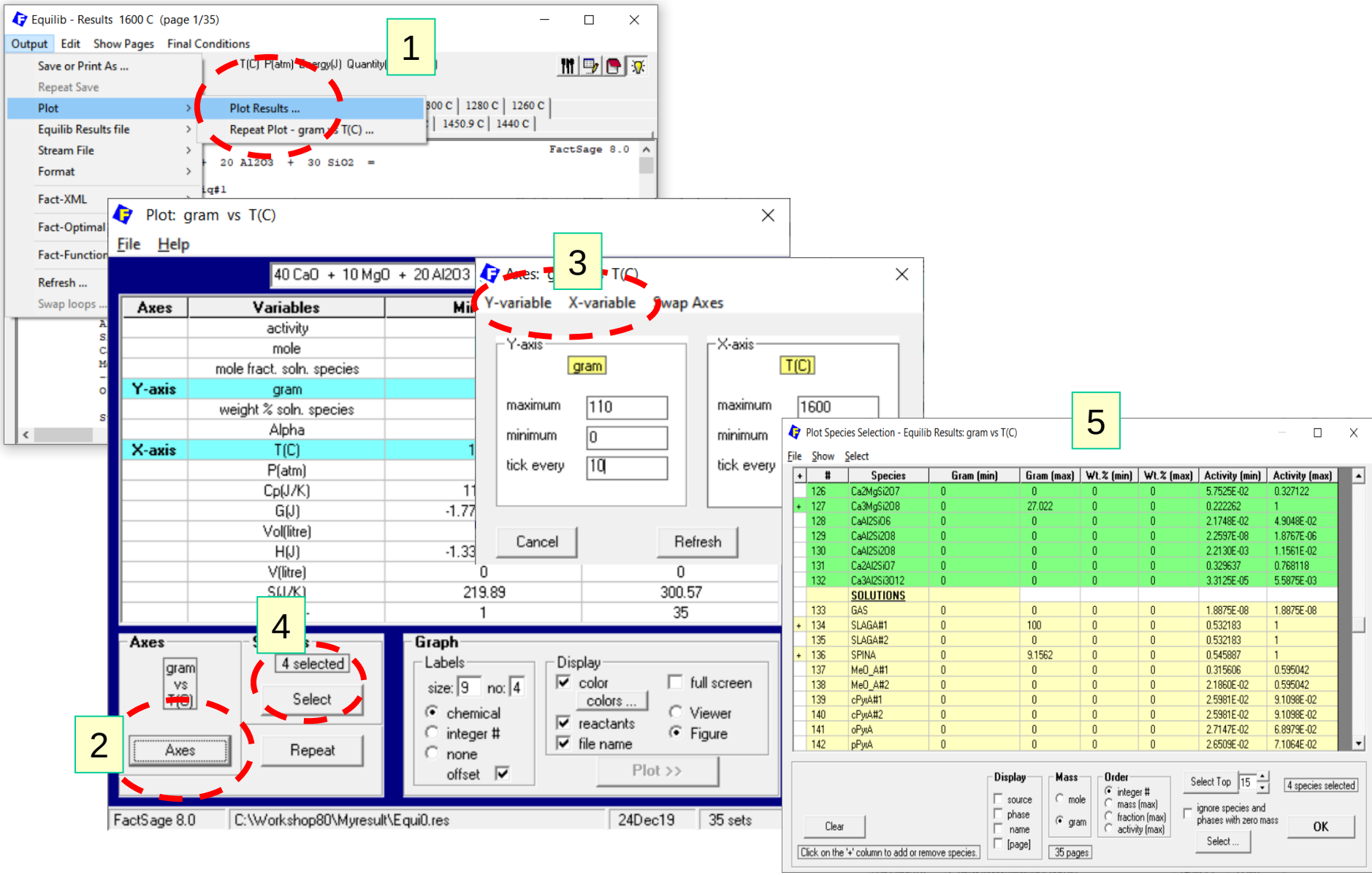


Equilibrium solidification of slag

Equilibrium cooling of the CaO-SiO_2-Al_2O_3-MgO slag

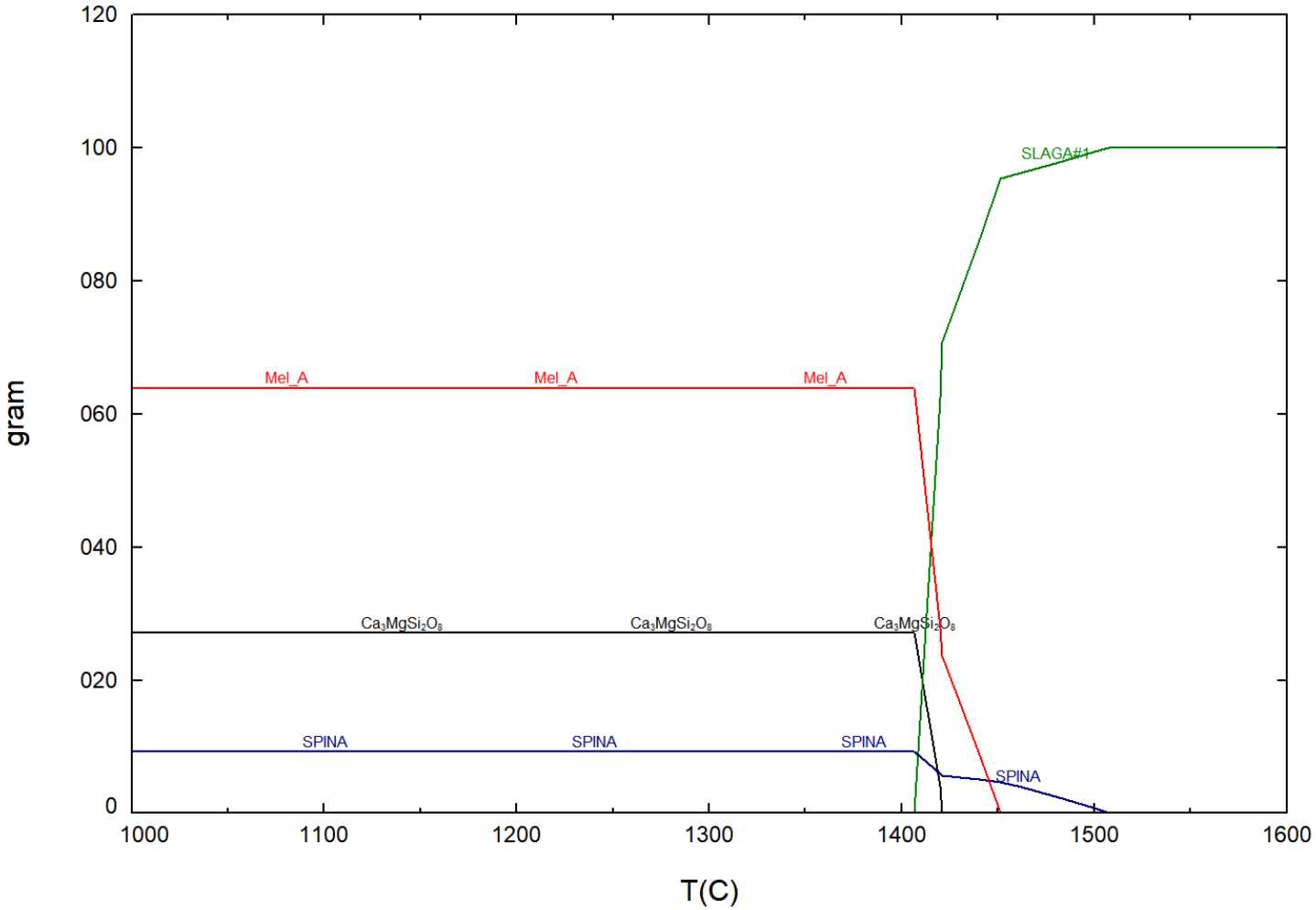


Equilibrium solidification of slag: plot amount vs. temperature



Equilibrium solidification of slag: plot amount vs. temperature

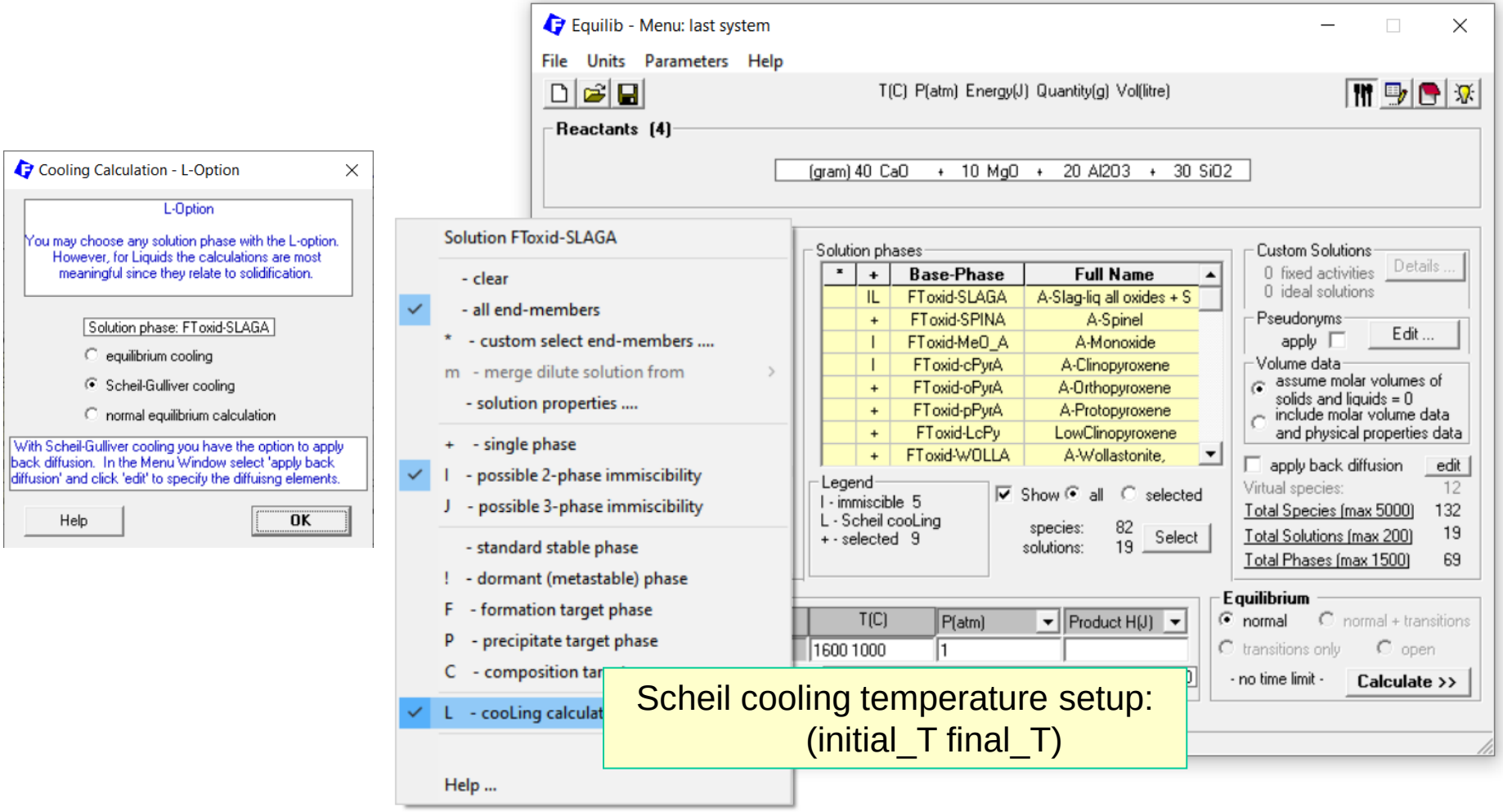
40 CaO + 10 MgO + 20 Al2O3 + 30 SiO2



Equilibrium solidification is completed at ~ 1410°C

Scheil cooling solidification of slag

Scheil cooling of the CaO-SiO_2-Al_2O_3-MgO slag



Equilibrium solidification of slag: plot amount vs. temperature

Equilib - Results Summary

Output Edit Show Pages Final Conditions

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

1245.96 C | 1245.96 C

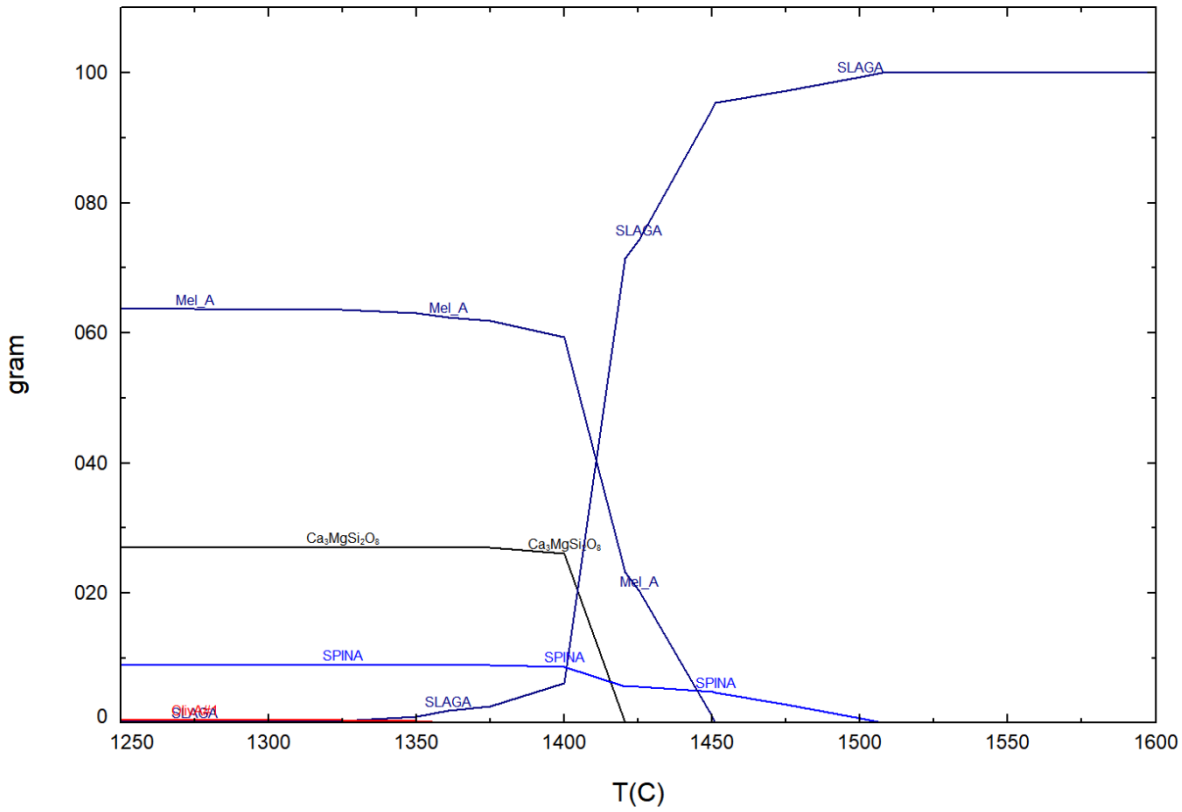
1425 C | 1420.44 C | 1400 C | 1375 C | 1360.62 C | 1350 C | 1325 C | 1300 C | 1275 C | 1250 C | 1246.54 C

Summary | Transitions | 1600 C | 1575 C | 1550 C | 1525 C | 1507.44 C | 1500 C | 1475 C | 1450 C | 1450 C

```
SCHEIL-GULLIVER COOLING

COMPONENTS:
CaO                     AMOUNT/gram =  4.0000E+01
MgO                     AMOUNT/gram =  1.0000E+01
Al2O3                   AMOUNT/gram =  2.0000E+01
SiO2                    AMOUNT/gram =  3.0000E+01

CONSTITUENTS AND PHASES AT 1245.96 C
(temperature of final disappearance of Slag-liq)

CONS.  PHASE                  TOTAL AMT/g.atom  TOTAL AMT/gram
  1    1 Spinel                 2.2900E-01       4.6542E+00
TOTAL:                          2.2900E-01       4.6542E+00

  2    1 Spinel                 4.5054E-02       9.1566E-01
  2    2 Melilite               1.0104E+00       2.3048E+01
TOTAL:                          1.0555E+00       2.3963E+01

  3    1 Spinel                 1.6012E-01       3.2542E+00
  3    2 Melilite               1.7268E+00       3.9346E+01
```

Scheil cooling solidification is completed at ~ 1320°C

40 CaO + 10 MgO + 20 Al2O3 + 30 SiO2



Solidification of mould flux

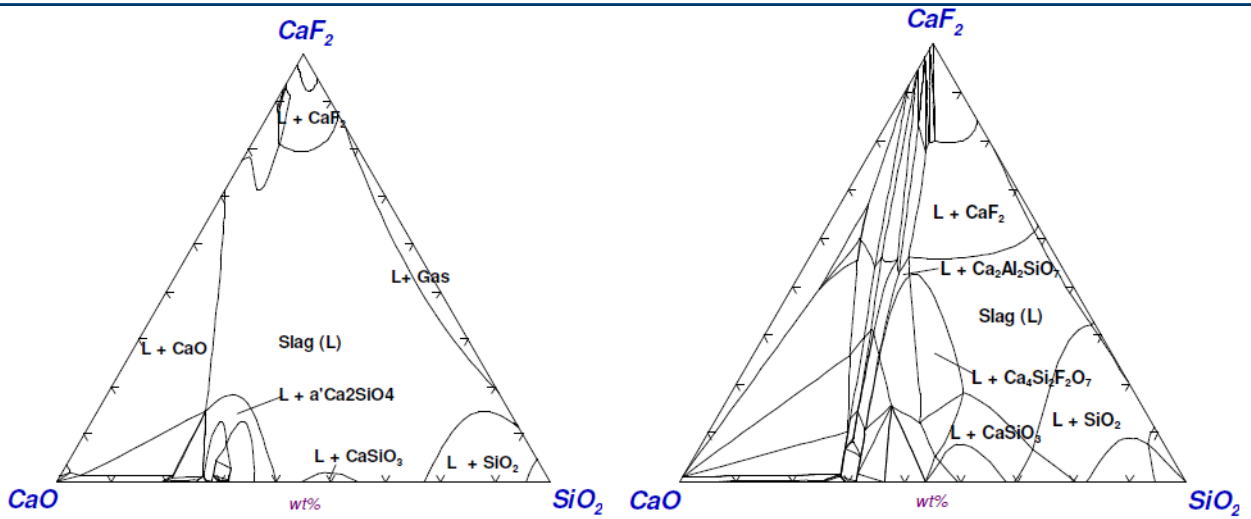


Figure 6. Calculated isothermal phase diagrams for the CaO-SiO_2-CaF_2-10 wt. % Al_2O_3 system at 1 bar [54]. (a) 1400 °C and (b) 1200 °C.

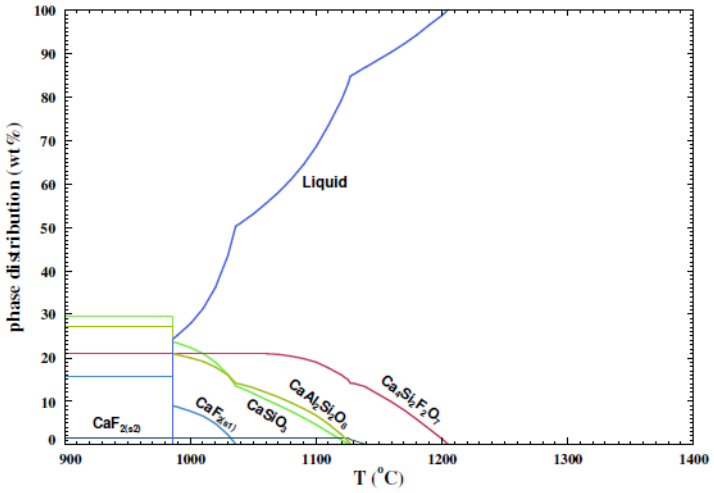
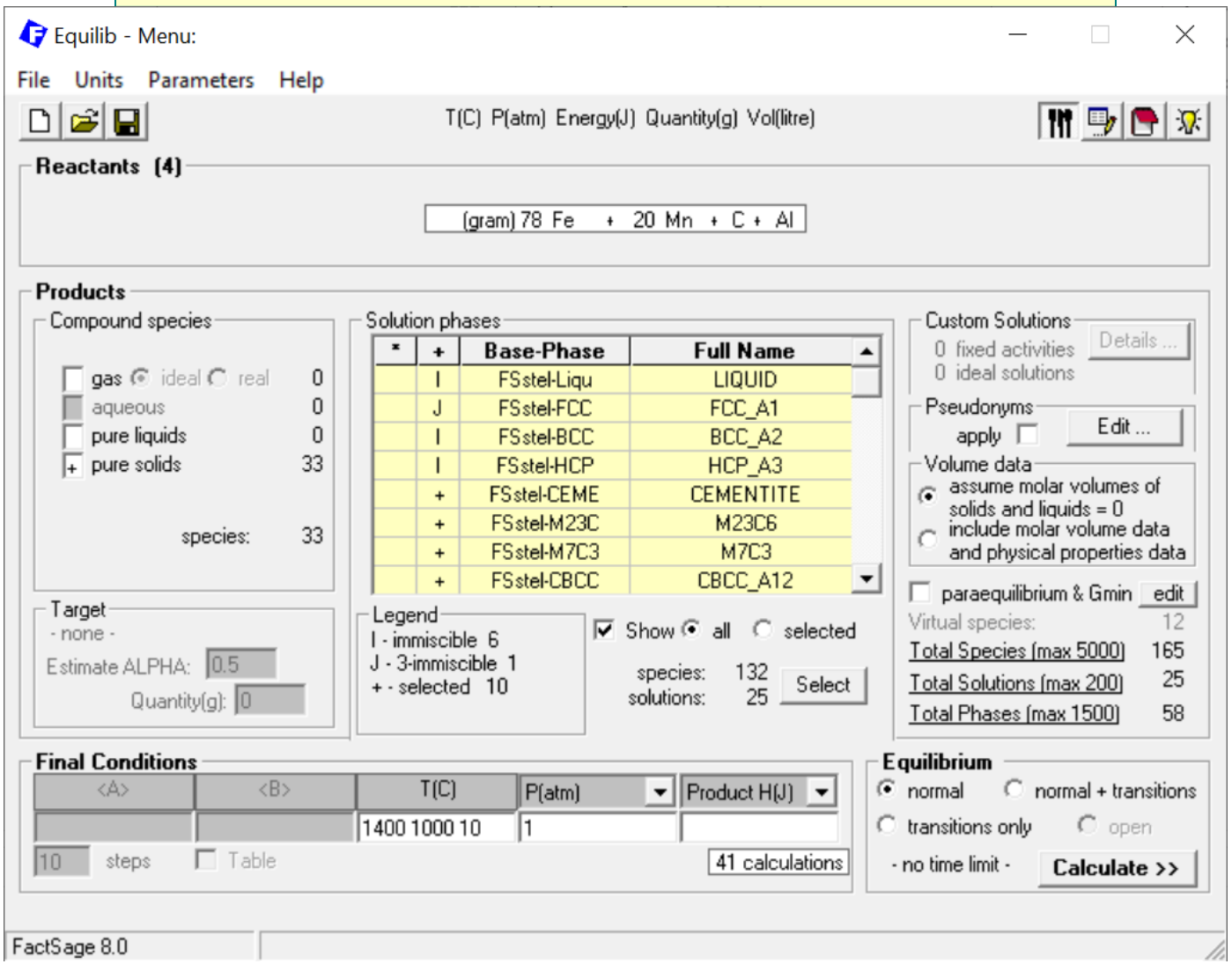


Figure 7. Solidification simulation of the 30CaO-10Al_2O_3-40SiO_2-20CaF_2 (in wt. %) mould flux using the Scheil cooling calculation [16].

Equilibrium solidification of steel: TWIP steel

Equilibrium cooling of Fe-20Mn-1C-1Al TWIP steel



Equilibrium solidification of steel: TWIP steel

Equilib - Results 1400 C (page 1/81)

Output Edit Show Pages Final Conditions

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

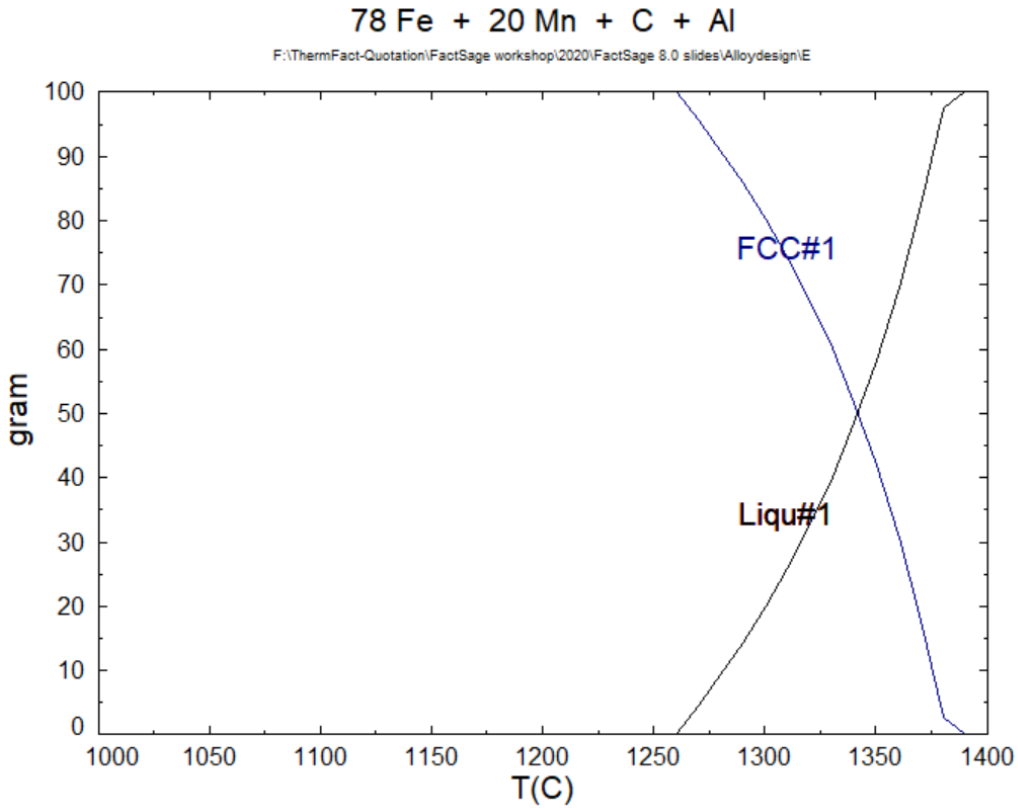
1270 C | 1260 C | 1250 C | 1240 C | 1230 C | 1220 C | 1210 C | 1200 C | 1190 C | 1180 C | 1170 C | 1160 C |
1400 C | 1390 C | 1380 C | 1370 C | 1360 C | 1350 C | 1340 C | 1330 C | 1320 C | 1310 C | 1300 C | 1290 C | 1280 C |

FactSage 8.0

```
(gram) 78 Fe  +  20 Mn  +  C  +  Al  =

   100.00     gram  LIQUID#1
   (100.00 gram, 1.8811 mol)
+ 0           gram  LIQUID#2
          (1400 C, 1 atm,      a=1.0000)
          ( 1.0000     wt.% Al
          + 1.0000     wt.% C
          + 78.000     wt.% Fe
          + 20.000     wt.% Mn)

          System component         Amount/mol    Amount/gram   Mole fraction  Mass fractio
          Fe                       1.3967         78.000         0.74251        0.78000
          Mn                       0.36405        20.000         0.19353        0.20000
          Al                       3.7062E-02     1.0000         1.9703E-02     1.0000E-02
          C                        8.3259E-02     1.0000         4.4261E-02     1.0000E-02

+ 0           gram  FCC_A1#1
+ 0           gram  FCC_A1#2
+ 0           gram  FCC_A1#3
          (1400 C, 1 atm,      a=0.98774)
          ( 1.0004     wt.% Al
          + 82.322     wt.% Fe
          + 14.976     wt.% Mn
          + 2.0551E-02 wt.% AlC
          + 1.4220     wt.% FeC
          + 0.25944    wt.% MnC)

+ 0           gram  BCC_A2#1
+ 0           gram  BCC_A2#2
          (1400 C, 1 atm,      a=0.97742)
          ( 4.8208E-03 wt.% AlC3
          + 1.2805     wt.% Al
          + 0.22282    wt.% FeC3
          + 84.018     wt.% Fe
          + 3.8533E-02 wt.% MnC3
          + 14.436     wt.% Mn)

+ 0           gram  BCC_B2#1
+ 0           gram  BCC_B2#2
          (1400 C, 1 atm,      a=0.94610)
          ( 3.5787E-02 wt.% Al1Al1Va6
          + 1.6883     wt.% Al1Fe1Va6
          + 0.28845    wt.% Al1Mn1Va6
          + 1.6883     wt.% Fe1Al1Va6
          + 69.977     wt.% Fe1Fe1Va6
          + 11.990     wt.% Fe1Mn1Va6
          + 0.28845    wt.% Mn1Al1Va6
          + 11.990     wt.% Mn1Fe1Va6
          + 2.0542     wt.% Mn1Mn1Va6)

+ 0           gram  CUB_A13
          (1400 C, 1 atm,      a=0.81702)
          ( 1.2558E-03 wt.% AlC
          + 0.82079    wt.% AlVa
          + 9.9046E-02 wt.% FeC
          + 76.997     wt.% FeVa
          + 2.8451E-02 wt.% MnC
```

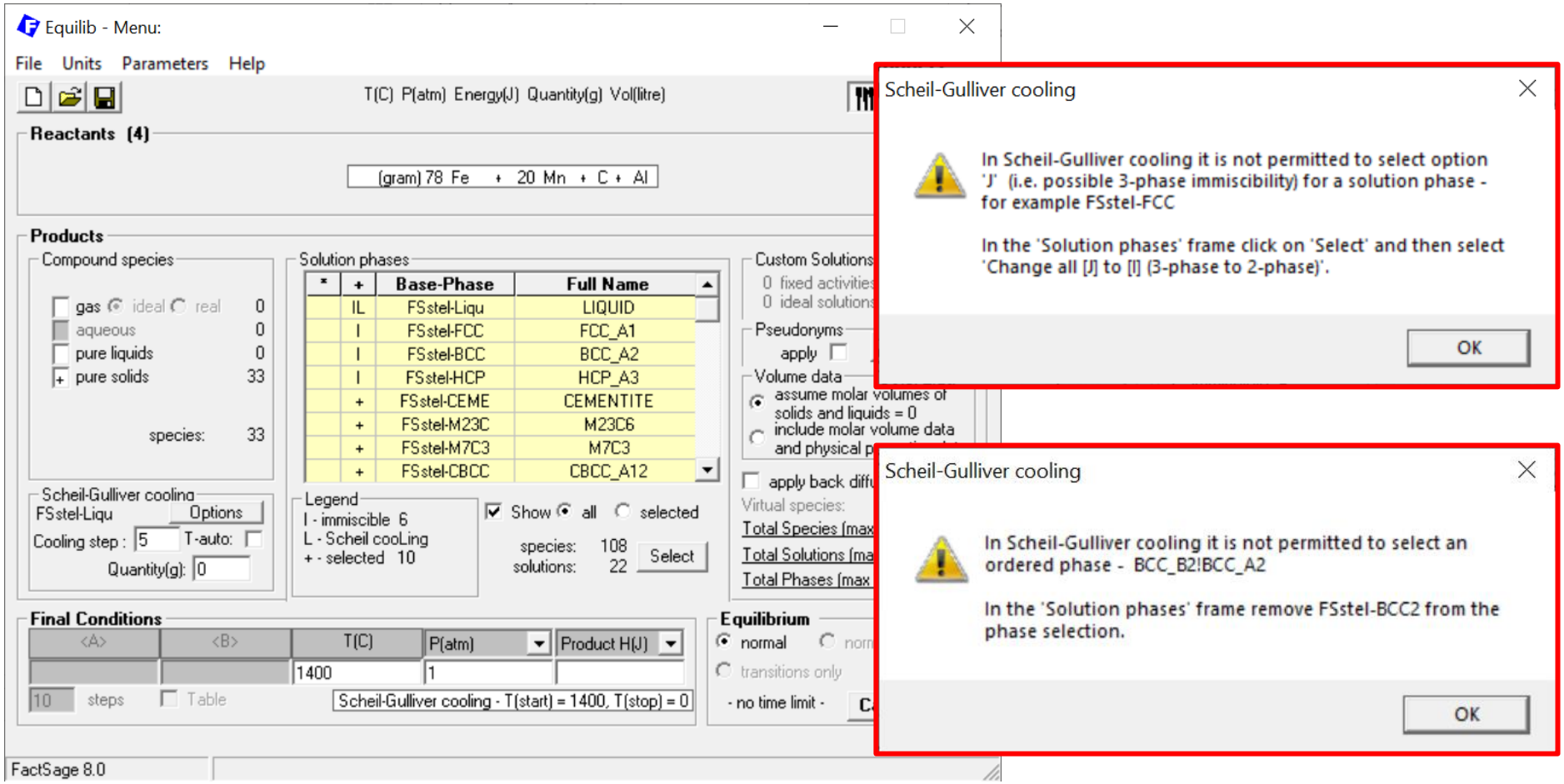
Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)	81 calculations
		1400 600 10	1		Calculate >>



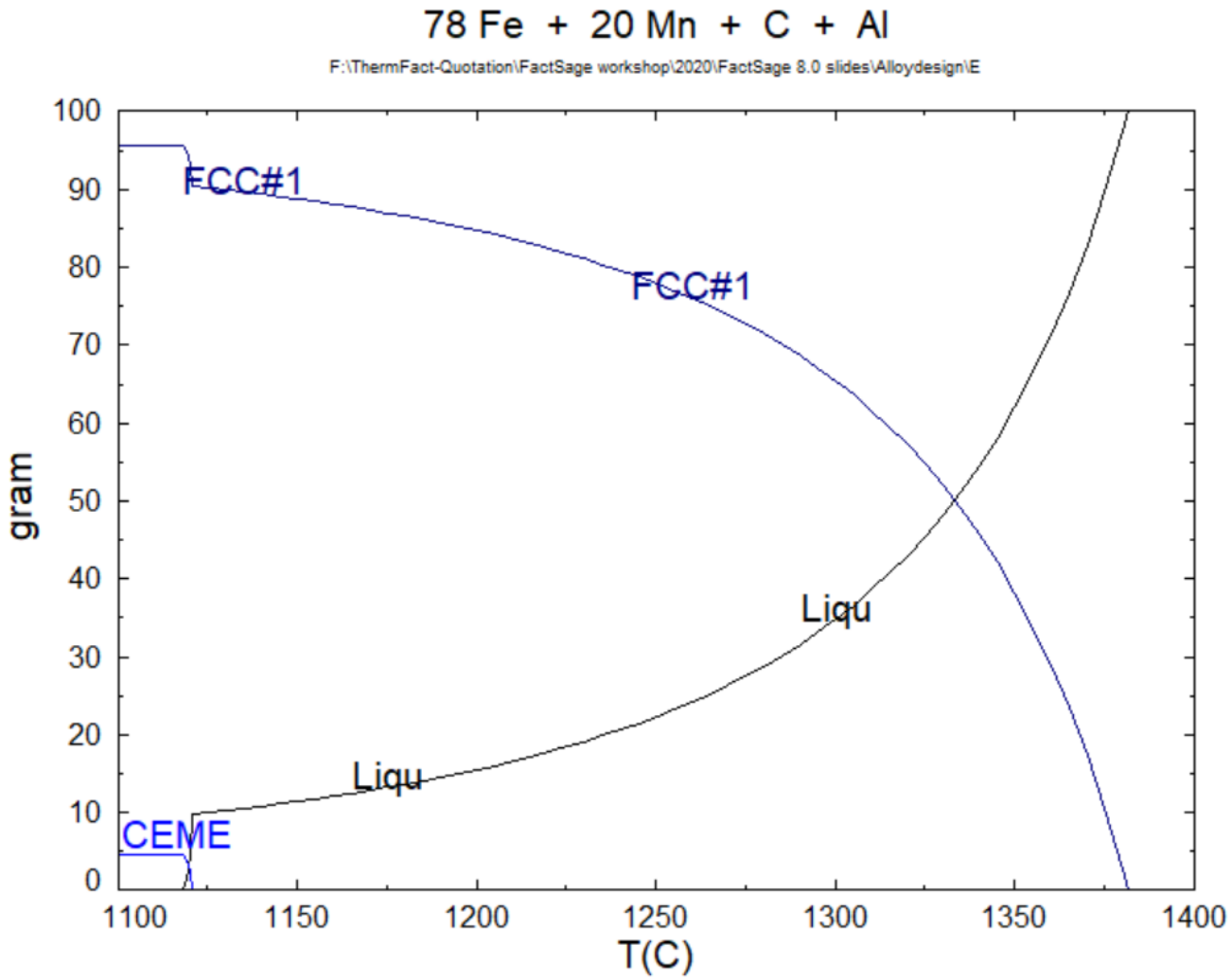
Scheil cooling solidification of steel: TWIP steel

Scheil cooling of Fe-20Mn-1C-1Al TWIP steel

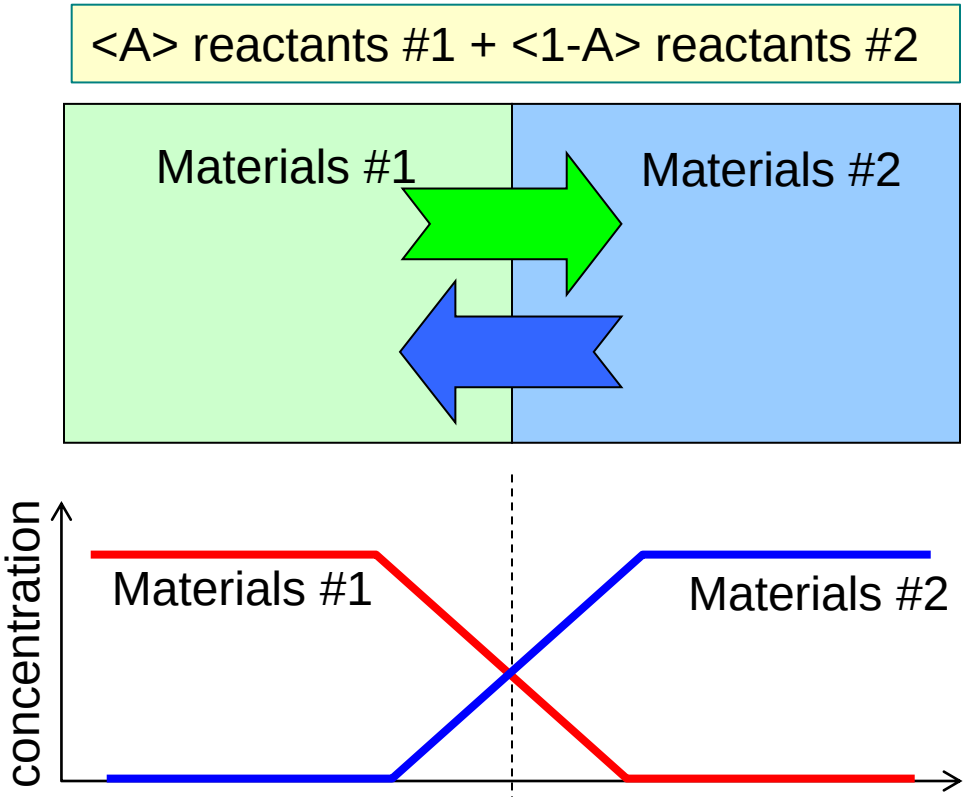


Scheil solidification of steel: TWIP steel

Solidification is completed at ~ 1116°C which is almost 150°C lower than equilibrium calculation.



Simple counter-cross inter-diffusion calculation: <A> option

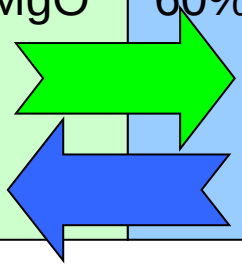


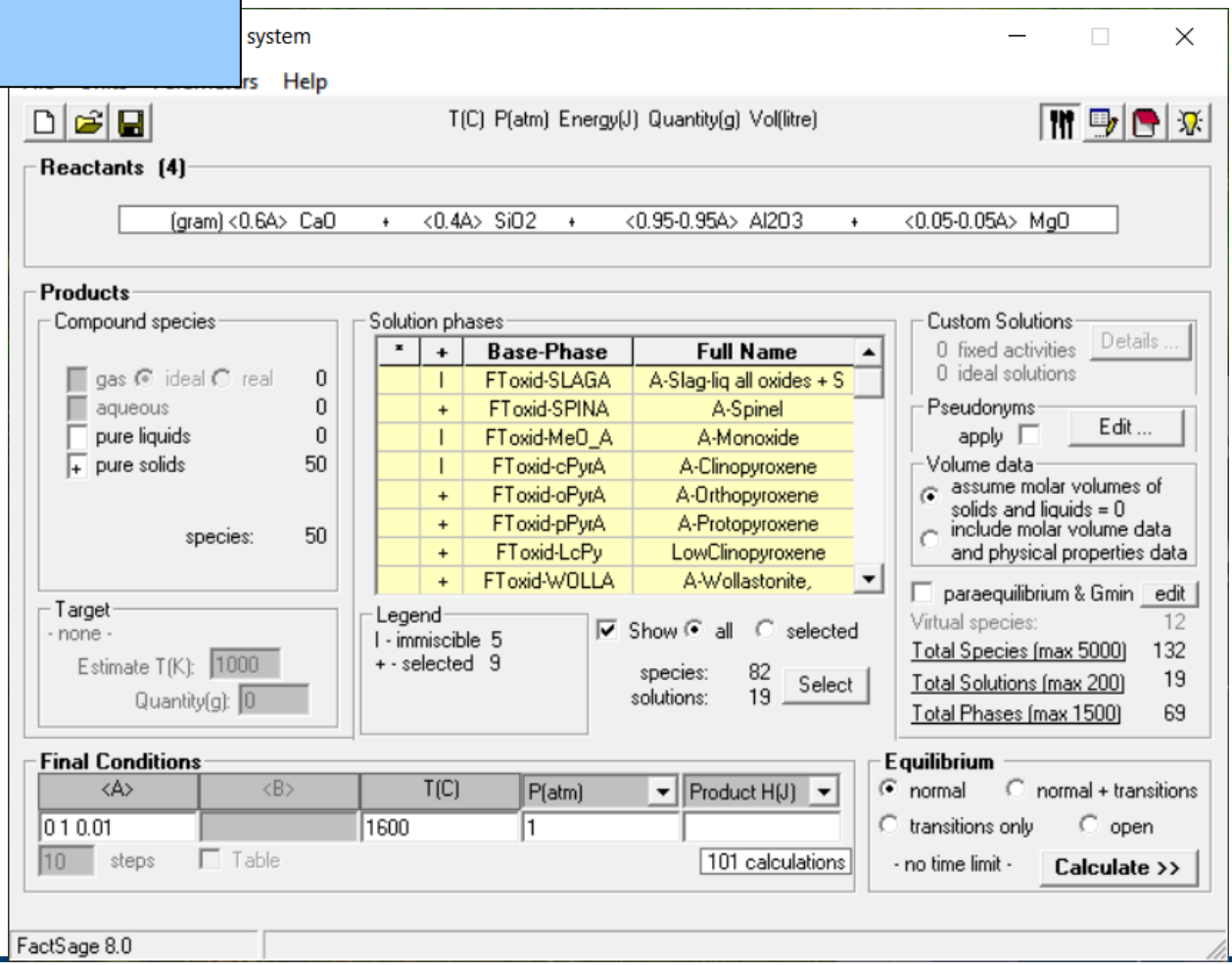
Counter-cross inter-diffusion reactions at interface can be simulated with the <A> option in Equilib. This assumes the diffusivities of all components in both materials are the same.

Counter-cross reaction: refractory / slag

Refractory
95%Al_2O_3-5%MgO

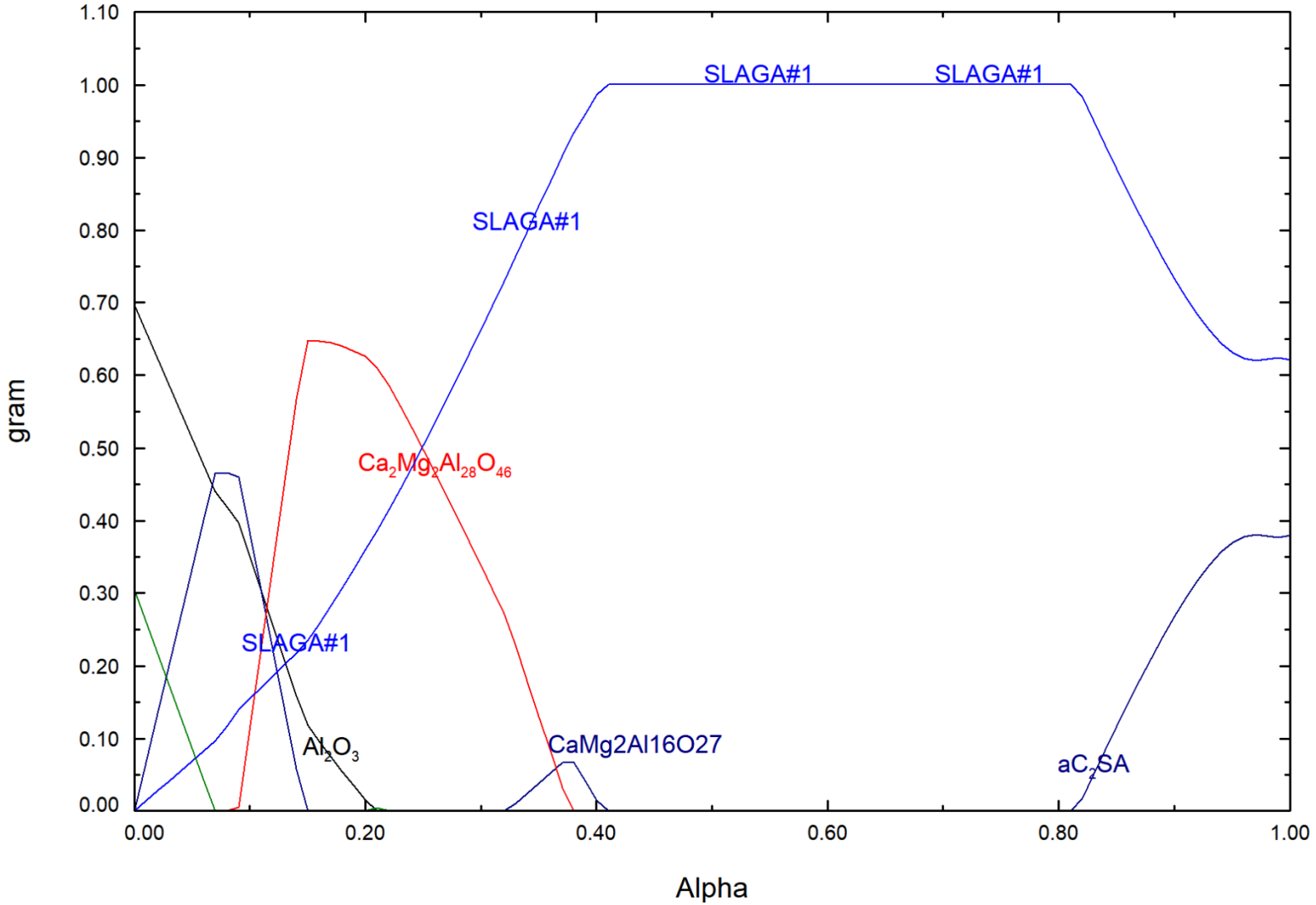
Slag
60%CaO-40%SiO_2



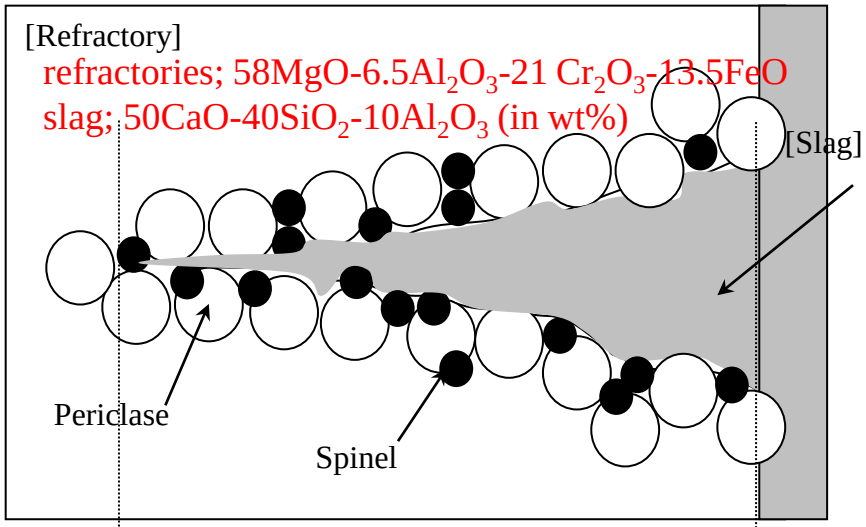


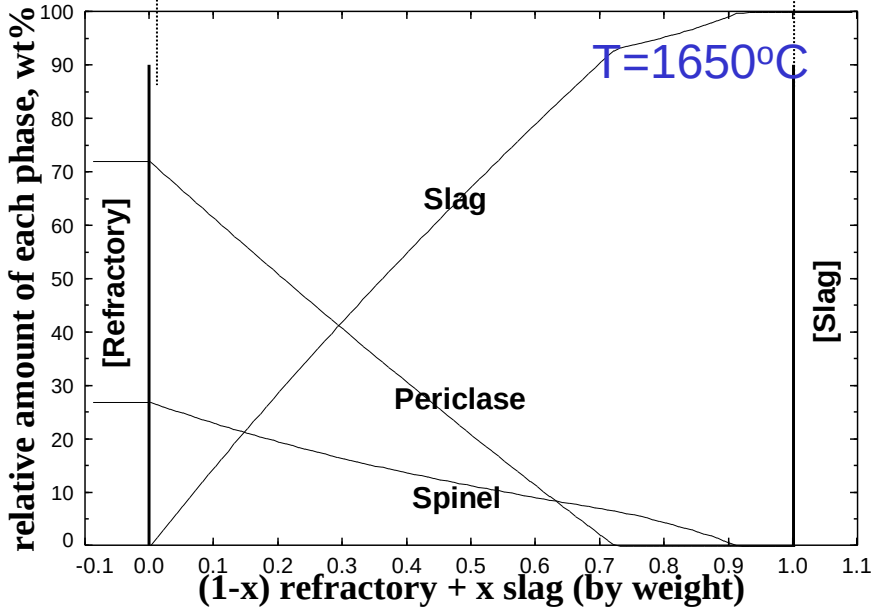
Counter-cross reaction: refractory / slag

<0.6A> CaO + <0.4A> SiO2 + <0.95-0.95A> Al2O3 + <0.05-0.05A> MgO

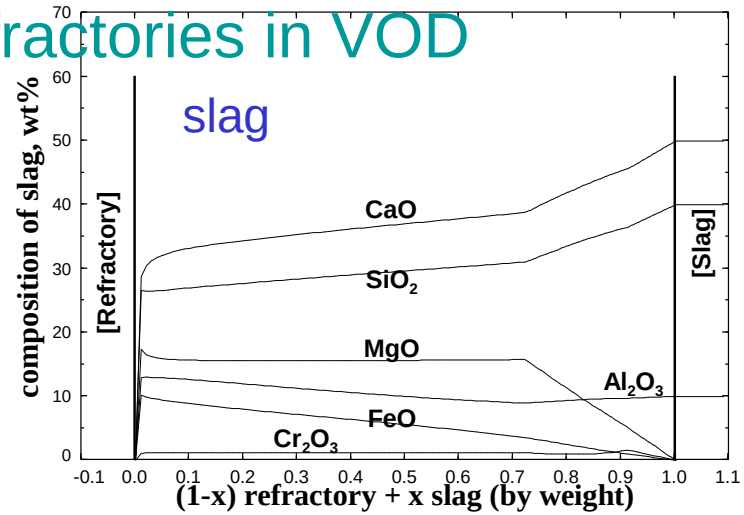


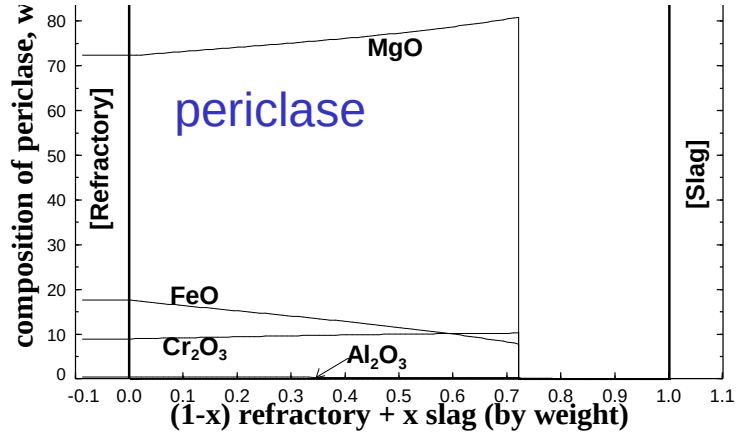
Counter-cross reaction: Refractories in VOD

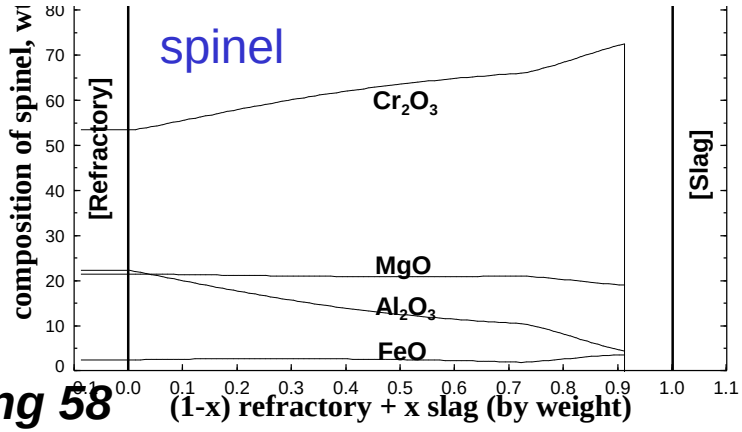




Jung et al., Taikabutsu, vol. 56, 2004, pp. 382-386.





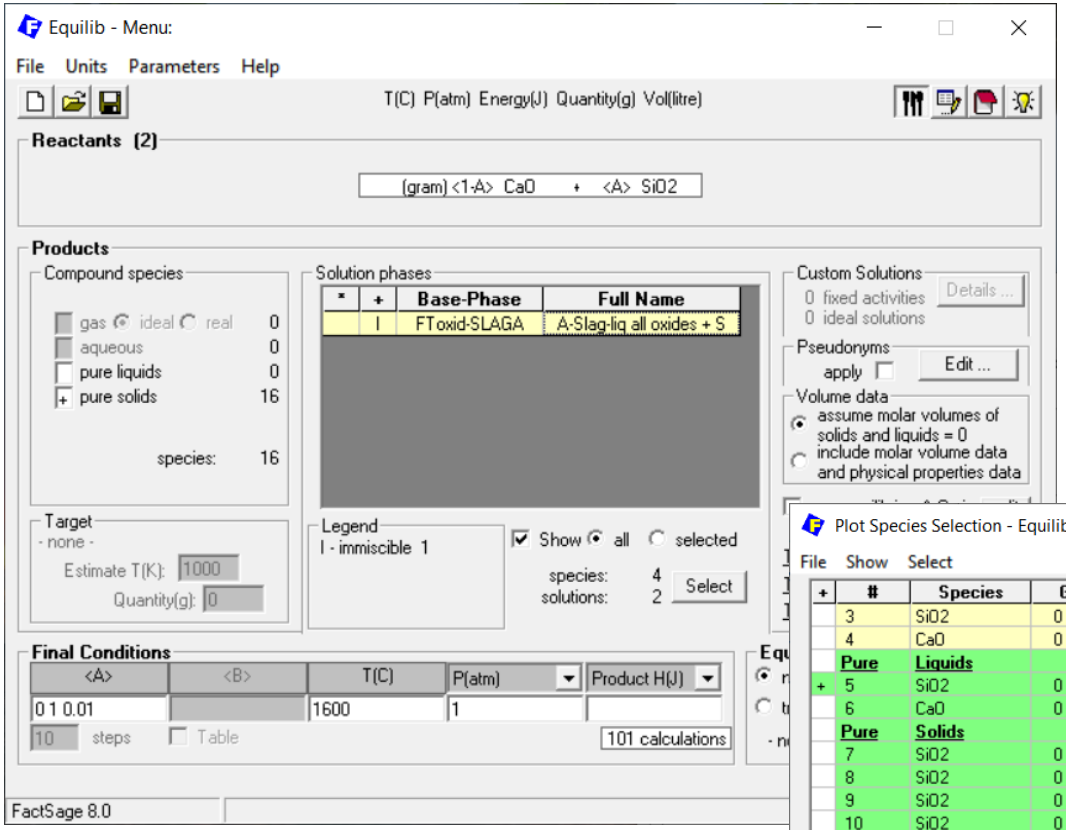


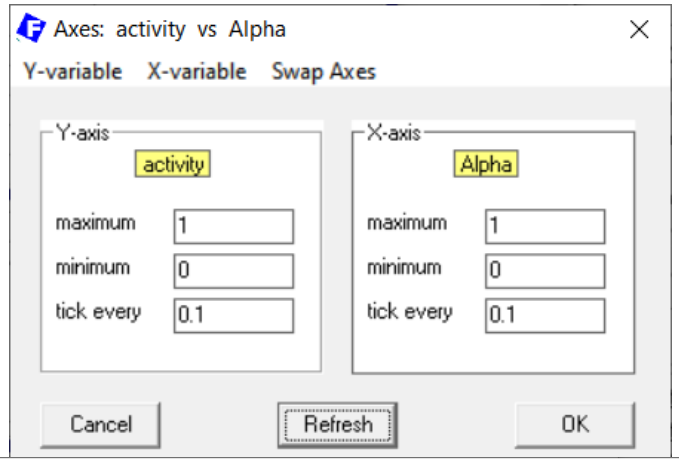
Application: Activity calculations

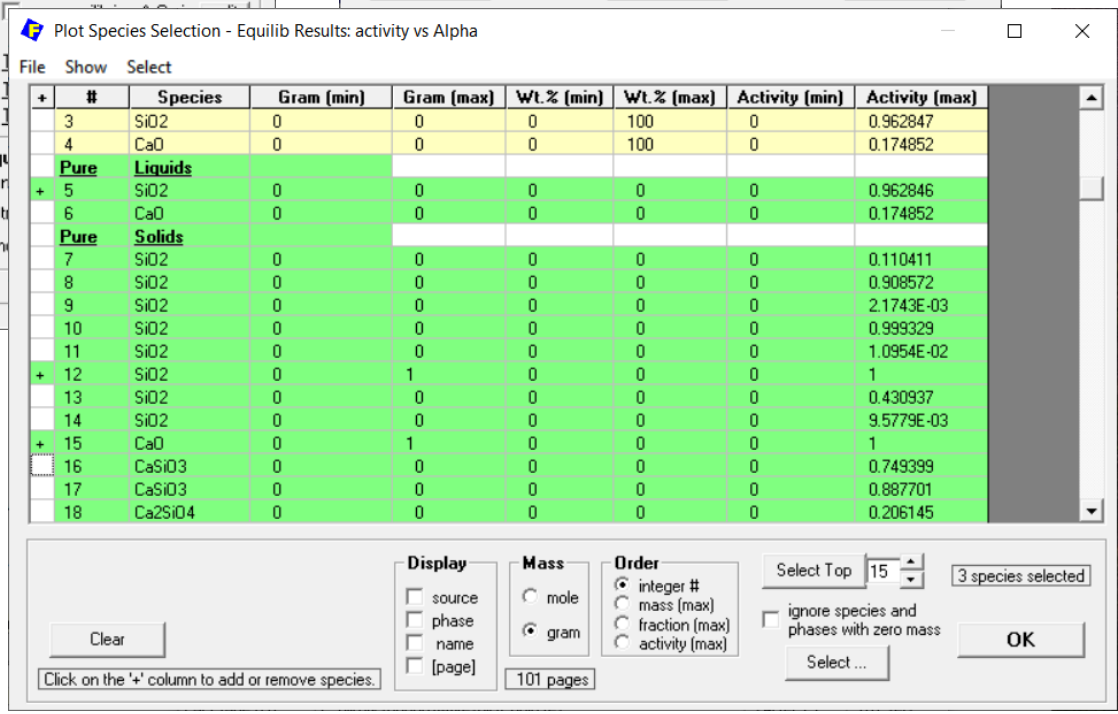
Slag: binary, ternary and multi-component systems
FeLq : oxygen and alloying elements

Now in FactSage 70, iso-activity lines in ternary or higher order system can be easily calculated using Phase Diagram module

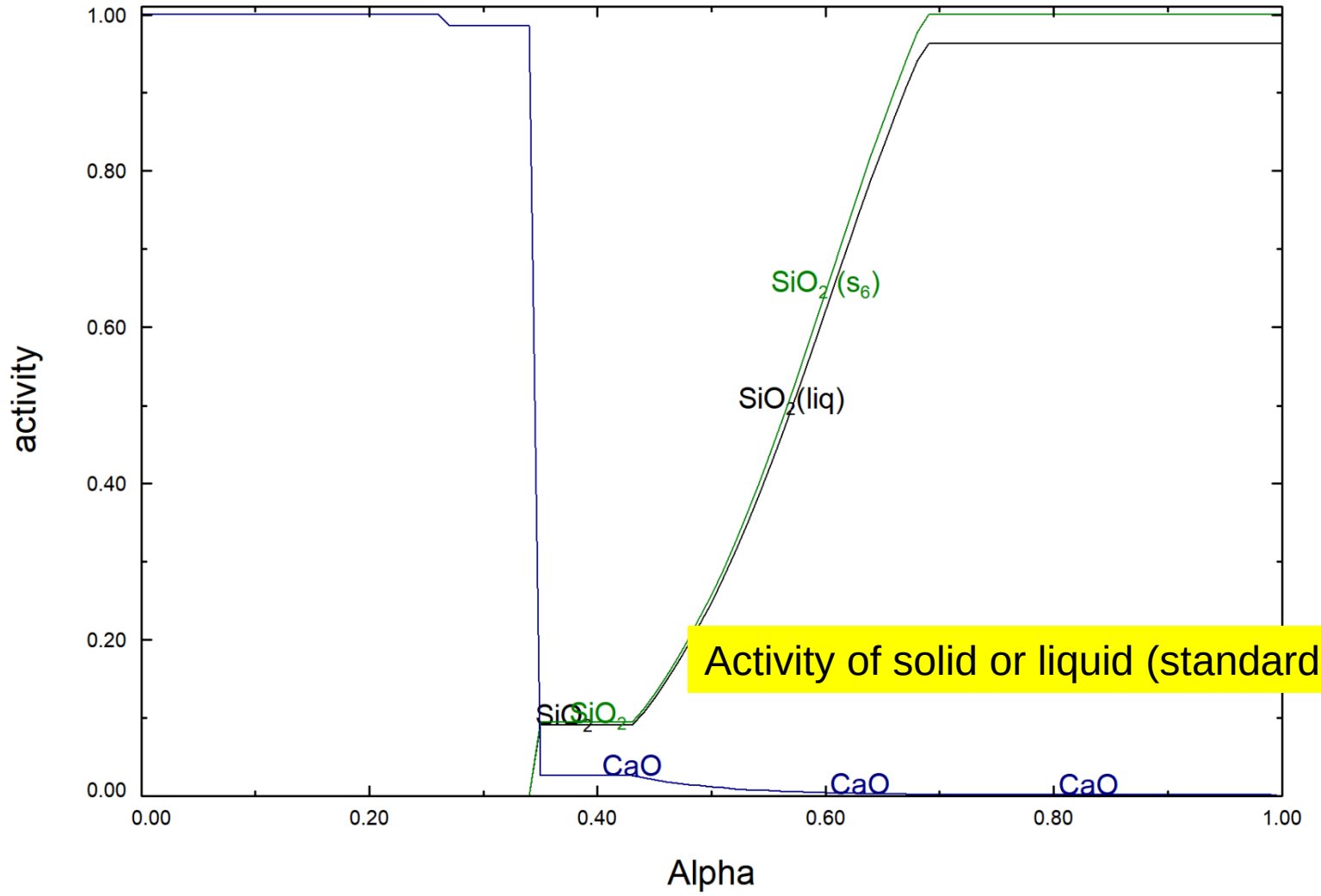
Activity calculations – Binary system







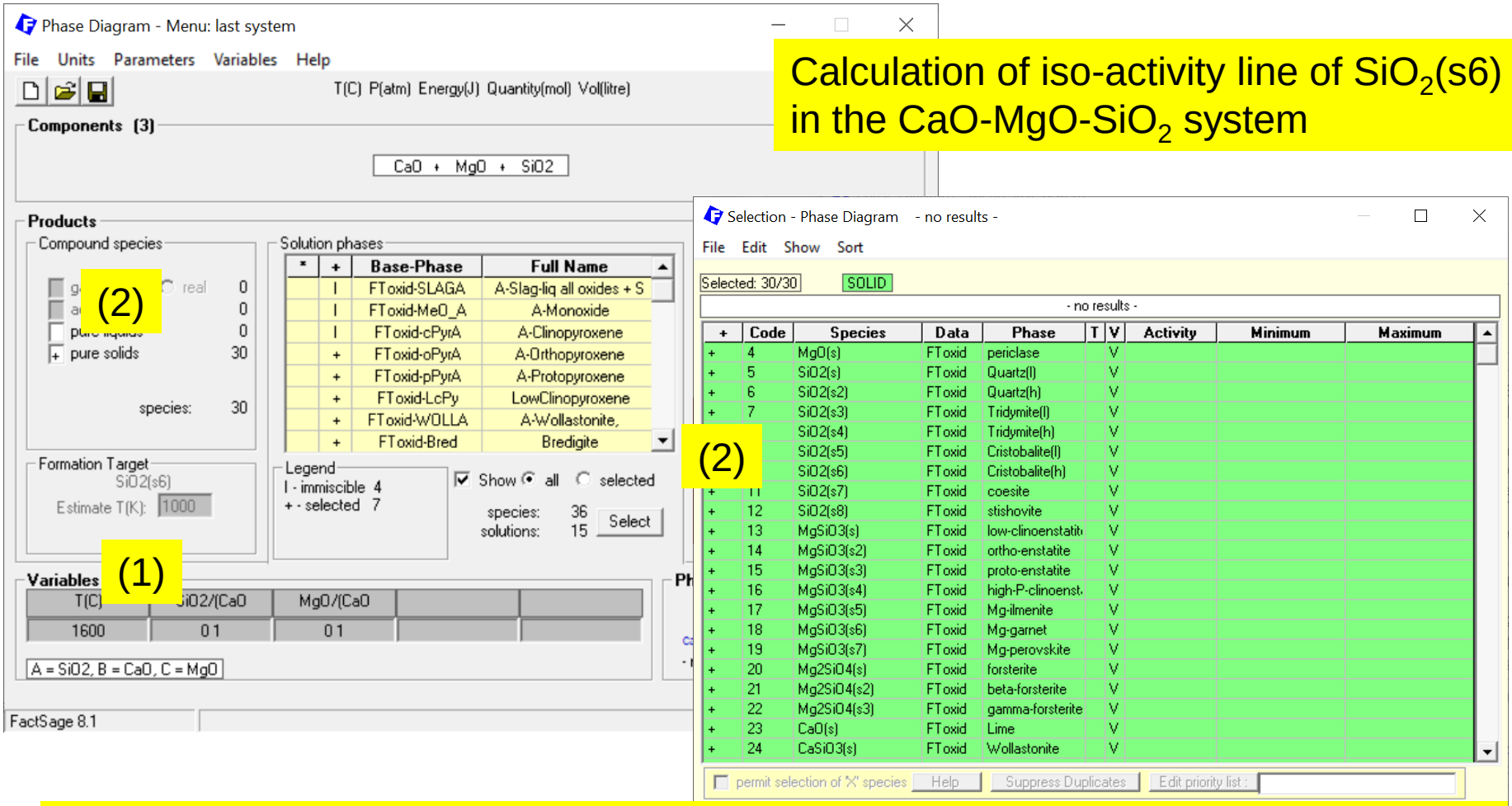
Activity calculations – Binary system



Activity of solid or liquid (standard state) ?

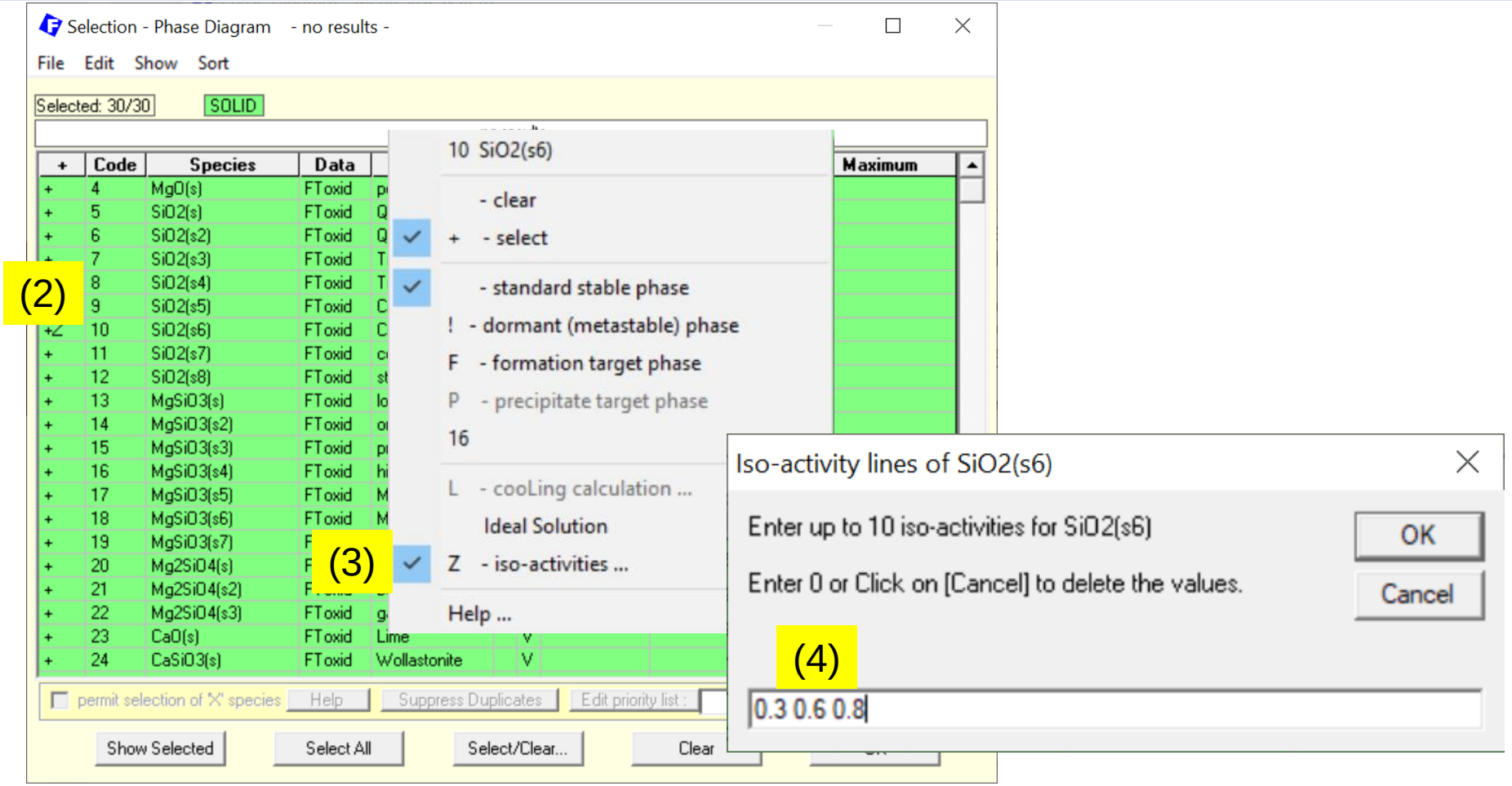
Activity calculations – Ternary system

Calculation of iso-activity line of SiO_2(s6) in the CaO-MgO-SiO_2 system



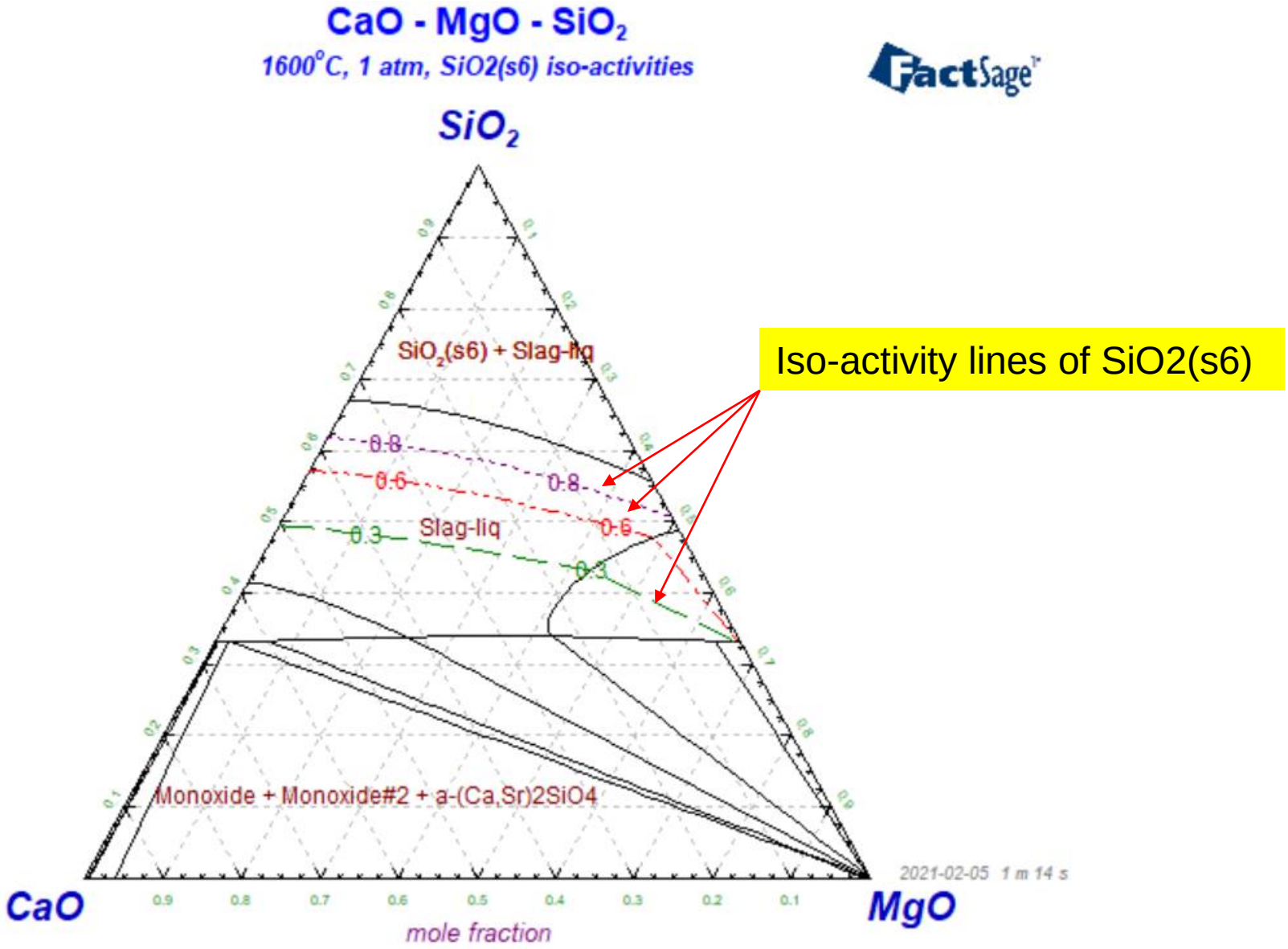
(1) Run phase diagram and select the axis and temperature.
(2) Click the solid or liquid phase you want to set its activity. For example, select "SiO2(s6)" in this example

Activity calculations – Ternary system



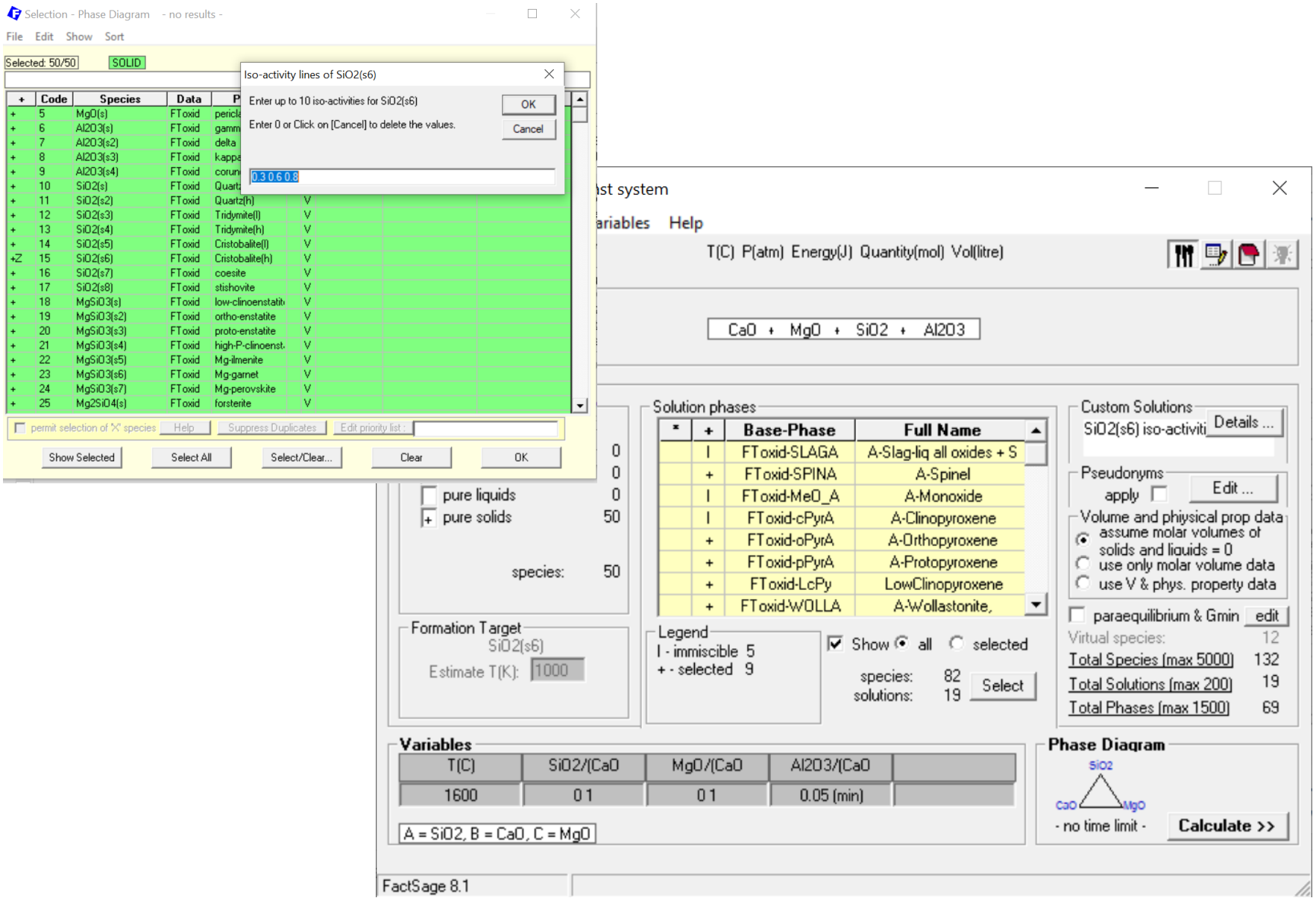
(2) Click the solid or liquid phase you want to set its activity. For example, select "liquid Mg" in this example
(3) Click "Z - iso-activities"
(4) Set the activity values to plot in phase diagram – up to 10 values

Activity calculations – Ternary system

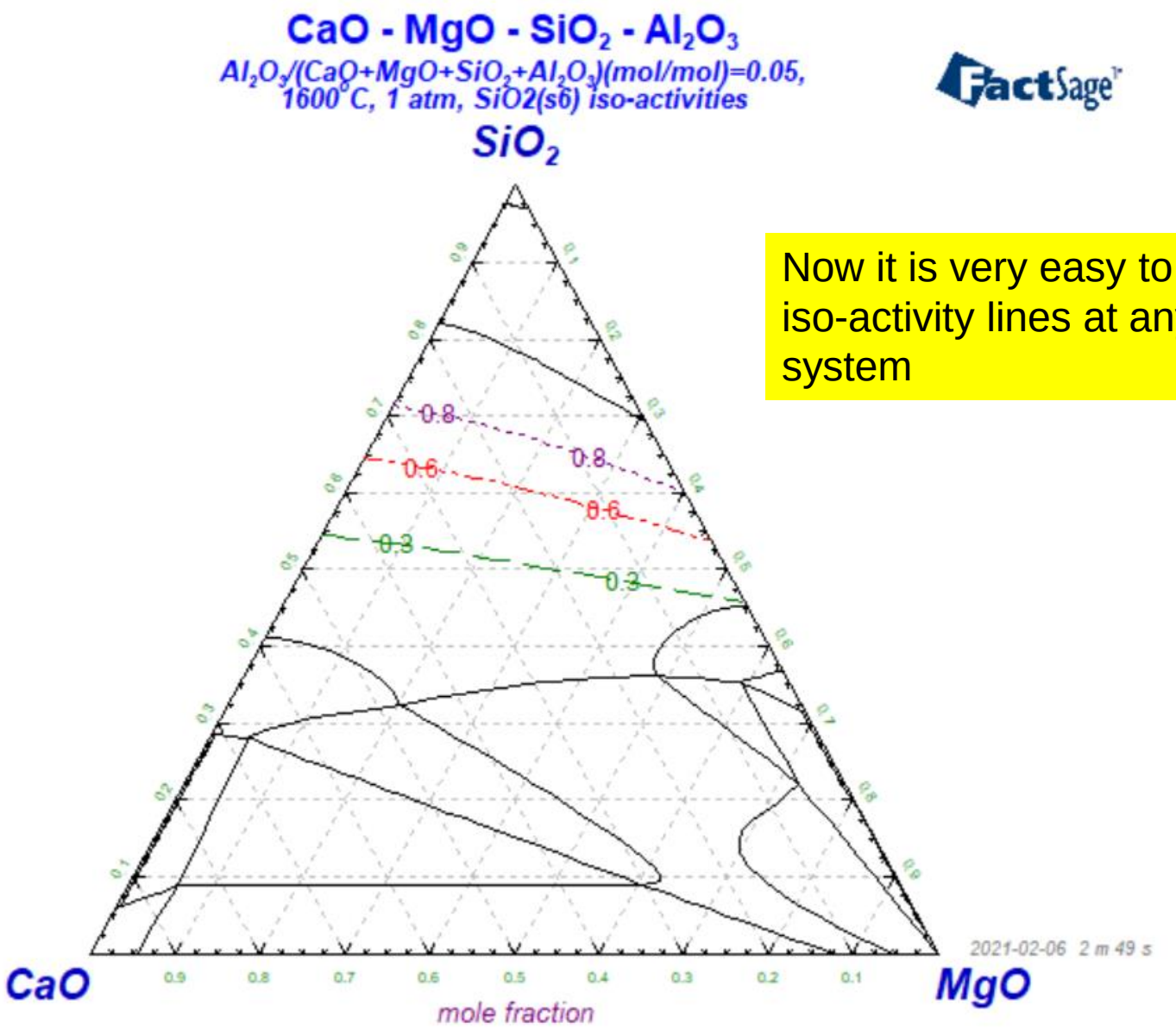


Iso-activity lines of SiO2(s6)

Activity calculations – Quaternary or higher order system



Activity calculations – Quaternary or higher order system



Now it is very easy to calculate iso-activity lines at any high order system

Activity of oxygen (wt% standard state) in liquid steel

$$RT \ln \gamma_M^o = g_{M\,(\text{Henrian S.S.})}^o - g_{M\,(\text{Pure Element S.S.})}^o$$

$$\Rightarrow a_{M\,(\text{pure Element S.S.})} = \gamma_M^o \, a_{M\,(\text{Henrian s.s.})}$$

$a_{O \text{ in FeLq}}$

$\ln \gamma_O^o = -15280/T + 3.5$: value used in FeLq database; slightly different depending on assessments

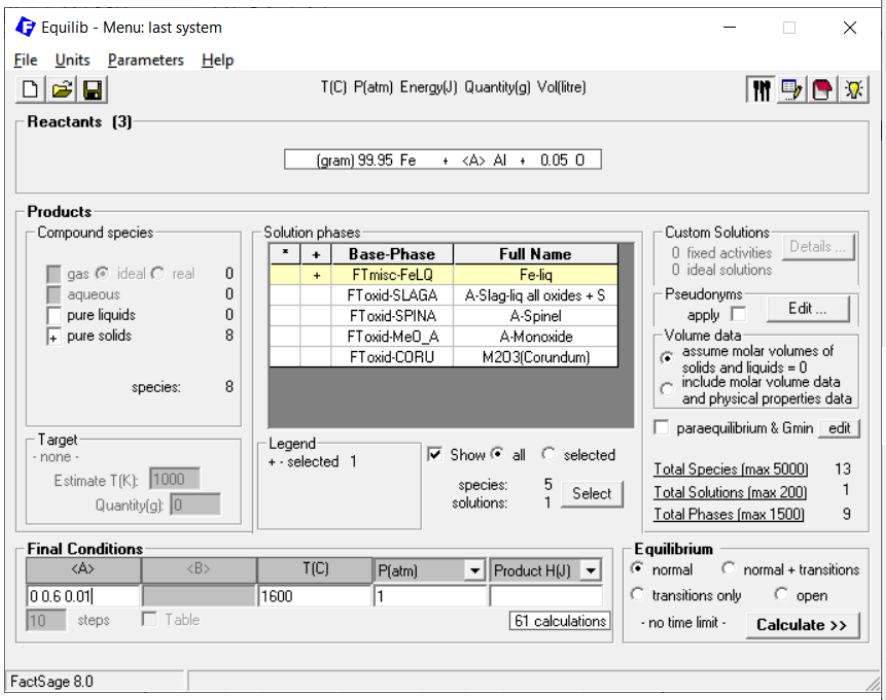
Reference pure element standard state of O in FeLq : Gas (0.5 O_2)

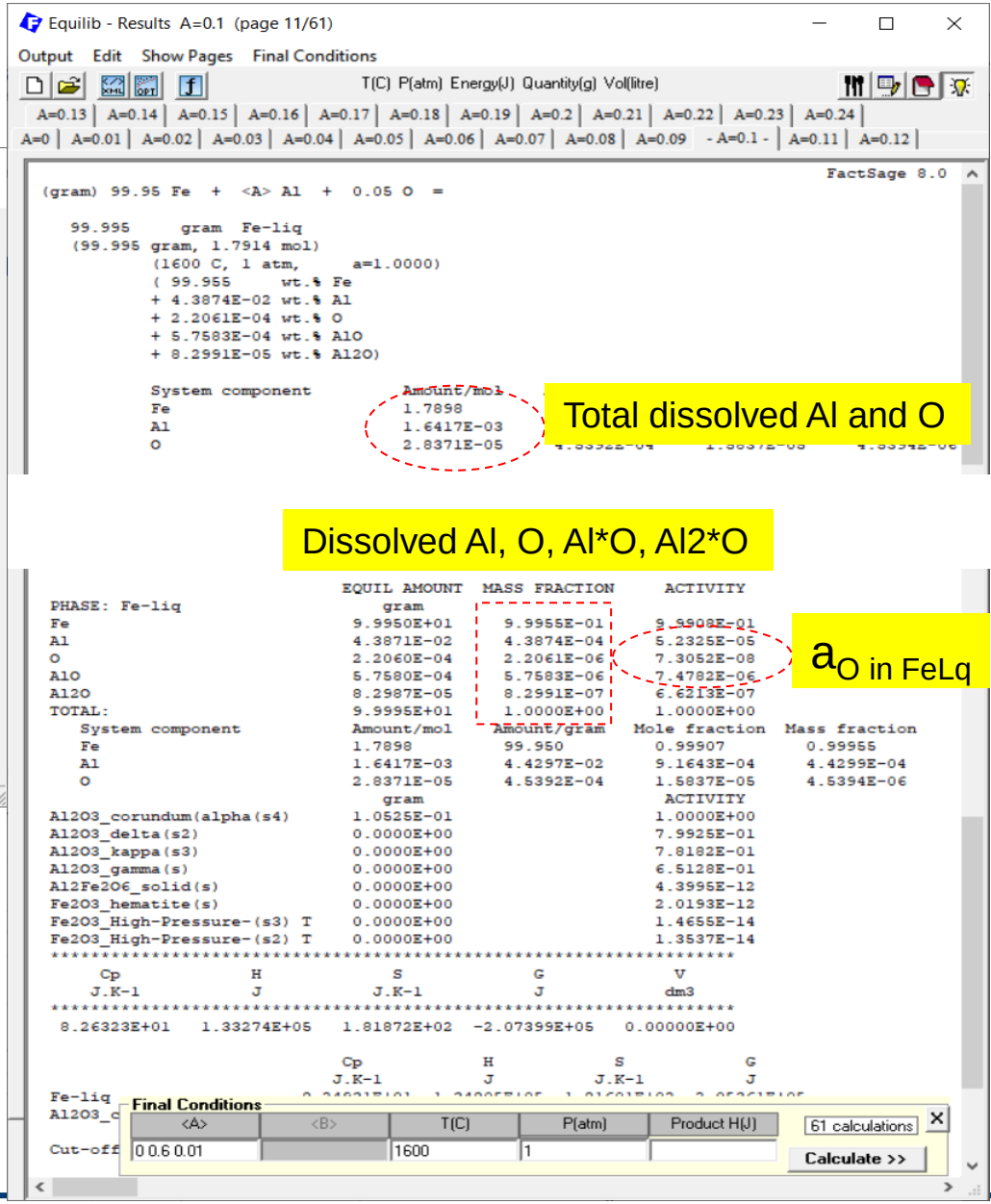
$$a_i(\text{wt\% std. state}) = \frac{100 M_i}{M_{Fe}} a_i(\text{Henrian std. state})$$

Log $a_{O(wt\%)}$ = Log($a_{O \text{ in FeLq}}$) - Log((EXP(-15280/T+3.5)*55.847/100/16))

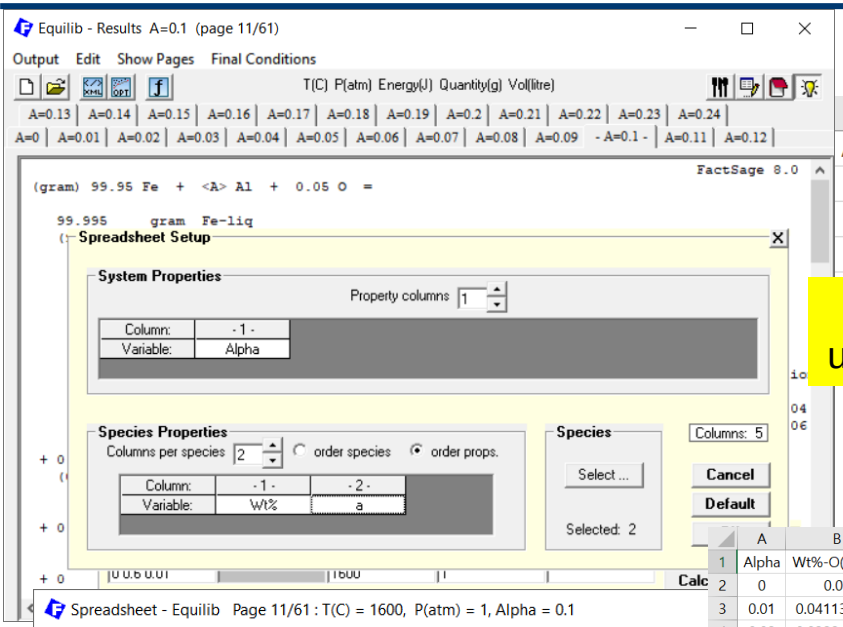
where T in Kelvin

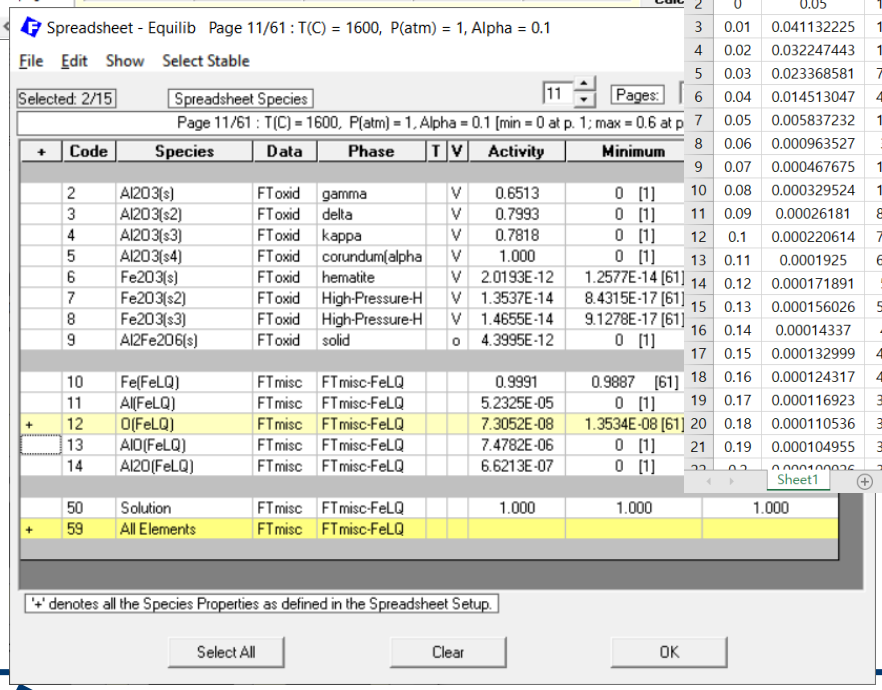
Activity of oxygen (wt% standard state) in liquid steel





Activity of oxygen (wt% standard state) in liquid steel





+	Code	Species	Data	Phase	T	V	Activity	Minimum	
	2	Al2O3(s)	FToxid	gamma		V	0.6513	0 [1]	
	3	Al2O3(s2)	FToxid	delta		V	0.7993	0 [1]	
	4	Al2O3(s3)	FToxid	kappa		V	0.7818	0 [1]	
	5	Al2O3(s4)	FToxid	corundum(alpha		V	1.000	0 [1]	
	6	Fe2O3(s)	FToxid	hematite		V	2.0193E-12	1.2577E-14 [61]	
	7	Fe2O3(s2)	FToxid	High-Pressure-H		V	1.3537E-14	8.4315E-17 [61]	
	8	Fe2O3(s3)	FToxid	High-Pressure-H		V	1.4655E-14	9.1278E-17 [61]	
	9	Al2Fe2O6(s)	FToxid	solid		o	4.3995E-12	0 [1]	
	10	Fe(FeLQ)	FTmisc	FTmisc-FeLQ			0.9991	0.9887 [61]	
	11	Al(FeLQ)	FTmisc	FTmisc-FeLQ			5.2325E-05	0 [1]	
+	12	O(FeLQ)	FTmisc	FTmisc-FeLQ			7.3052E-08	1.3534E-08 [61]	
	13	AlO(FeLQ)	FTmisc	FTmisc-FeLQ			7.4782E-06	0 [1]	
	14	Al2O(FeLQ)	FTmisc	FTmisc-FeLQ			6.6213E-07	0 [1]	
	50	Solution	FTmisc	FTmisc-FeLQ			1.000	1.000	1.000
+	59	All Elements	FTmisc	FTmisc-FeLQ					

$a_{O\ in\ FeLQ}$

Total dissolved Al and O

A	B	C	D	E	F
Alpha	Wt%-O(FeLQ)	a-O(FeLQ)	Wt%-Fe_FTmisc-FeLQ	Wt%-Al_FTmisc-FeLQ	Wt%-O_FTmisc-FeLQ
0	0.05	1.65438E-05	99.95	0	0.05
0.01	0.041132225	1.36127E-05	99.958808	4.37926E-05	0.041147937
0.02	0.032247443	1.06746E-05	99.96768	5.48179E-05	0.032265182
		3722E-06	99.976535	7.54777E-05	0.023389413

Dissolved unassociated O

	A	B	C	D	E	F	G	H	I	J
1	Alpha	Wt%-O(FeLQ)	a-O(FeLQ)	Wt%-Fe_FTmisc-FeLQ	Wt%-Al_FTmisc-FeLQ	Wt%-O_FTmisc-FeLQ	a-Fe_FTmisc-FeLQ	a-Al_FTmisc-FeLQ	a-O_FTmisc-FeLQ	
2	0	0.05	1.65438E-05	99.95	0	0.05	<-not-calctd.->	<-not-calctd.->	<-not-calctd.->	
3	0.01	0.041132225	1.36127E-05	99.958808	4.37926E-05	0.041147937	<-not-calctd.->	<-not-calctd.->	<-not-calctd.->	
4	0.02	0.032247443	1.06746E-05	99.96768	5.48179E-05	0.032265182	<-not-calctd.->	<-not-calctd.->	<-not-calctd.->	
5	0.03	0.023368581	7.73722E-06	99.976535	7.54777E-05	0.023389413	<-not-calctd.->	<-not-calctd.->	<-not-calctd.->	
6	0.04	0.014513047	4.80625E-06	99.985334	0.00012696	0.014539475	<-not-calctd.->	<-not-calctd.->	<-not-calctd.->	
7	0.05	0.005837232	1.93351E-06	99.993728	0.000393134	0.00587891	<-not-calctd.->	<-not-calctd.->	<-not-calctd.->	
8	0.06	0.000963527	3.1918E-07	99.993945	0.004987647	0.001067027	<-not-calctd.->	<-not-calctd.->	<-not-calctd.->	
9	0.07	0.000467675	1.54909E-07	99.984894	0.014487143	0.000619046	<-not-calctd.->	<-not-calctd.->	<-not-calctd.->	
10	0.08	0.000329524	1.09138E-07	99.975117	0.024369484	0.000513357	<-not-calctd.->	<-not-calctd.->	<-not-calctd.->	
11	0.09	0.00026181	8.67022E-08	99.965206	0.034322168	0.000472016	<-not-calctd.->	<-not-calctd.->	<-not-calctd.->	
12	0.1	0.000220614	7.30519E-08	99.955247	0.044299009	0.000453944	<-not-calctd.->	<-not-calctd.->	<-not-calctd.->	
13	0.11	0.0001925	6.37357E-08	99.945267	0.054286291	0.000446942	<-not-calctd.->	<-not-calctd.->	<-not-calctd.->	
14	0.12	0.000171891	5.6906E-08	99.935275	0.064278482	0.000446089	<-not-calctd.->	<-not-calctd.->	<-not-calctd.->	
15	0.13	0.000156026	5.16482E-08	99.925278	0.074272916	0.000449013	<-not-calctd.->	<-not-calctd.->	<-not-calctd.->	
16	0.14	0.00014337	4.7454E-08	99.915277	0.084268152	0.000454433	<-not-calctd.->	<-not-calctd.->	<-not-calctd.->	
17	0.15	0.000132999	4.40165E-08	99.905275	0.094263343	0.000461593	<-not-calctd.->	<-not-calctd.->	<-not-calctd.->	
18	0.16	0.000124317	4.11386E-08	99.895272	0.10425796	0.000470022	<-not-calctd.->	<-not-calctd.->	<-not-calctd.->	
19	0.17	0.000116923	3.86877E-08	99.885269	0.11425165	0.00047941	<-not-calctd.->	<-not-calctd.->	<-not-calctd.->	
20	0.18	0.000110536	3.65706E-08	99.875266	0.12424418	0.000489544	<-not-calctd.->	<-not-calctd.->	<-not-calctd.->	
21	0.19	0.000104955	3.47201E-08	99.865264	0.13423538	0.000500274	<-not-calctd.->	<-not-calctd.->	<-not-calctd.->	

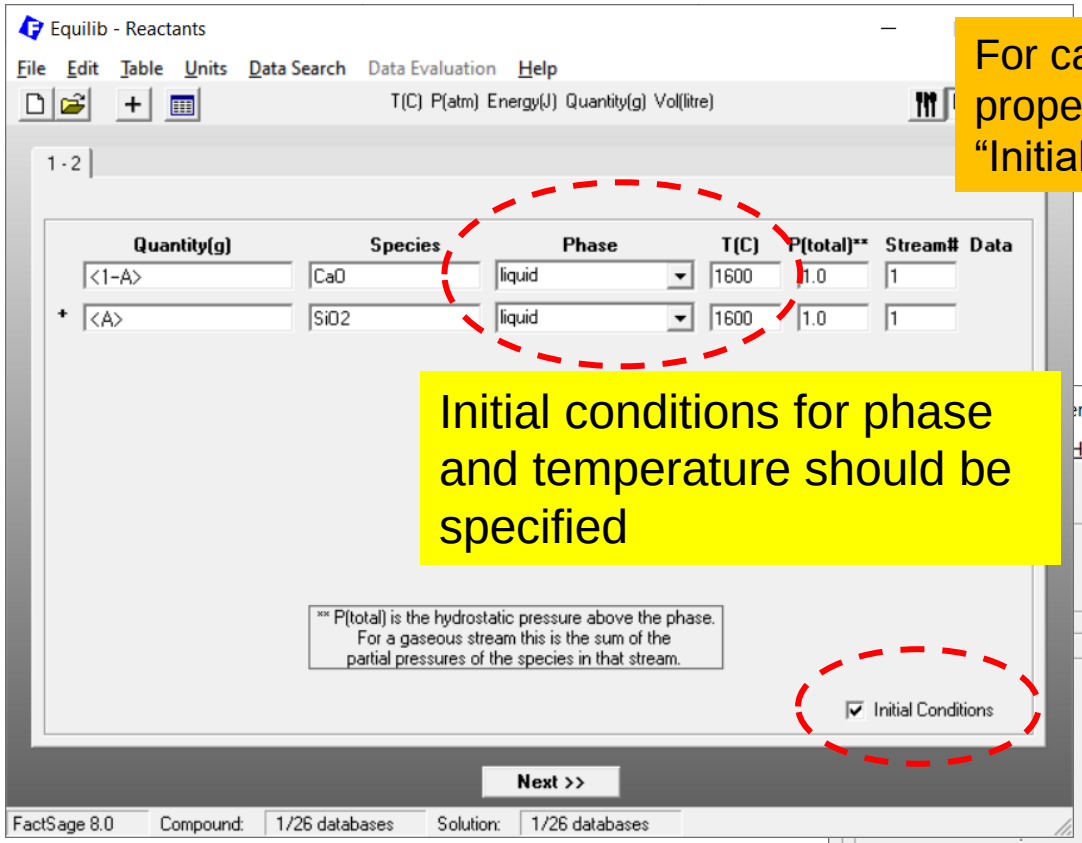
Sheet1

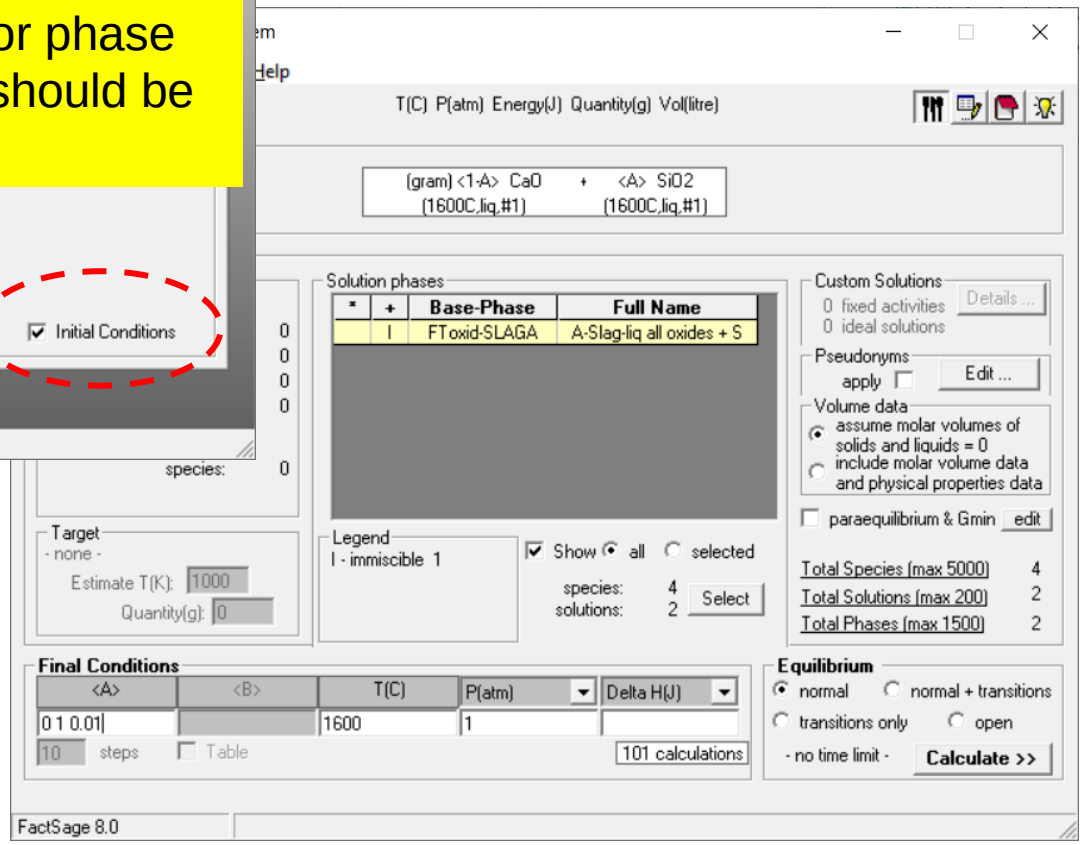
→ Then, convert $a_{O\ in\ FeLq}$ to $a_{O\ wt\%\ s.s.}$

Thermodynamic properties: ΔG, ΔH, ΔS etc.

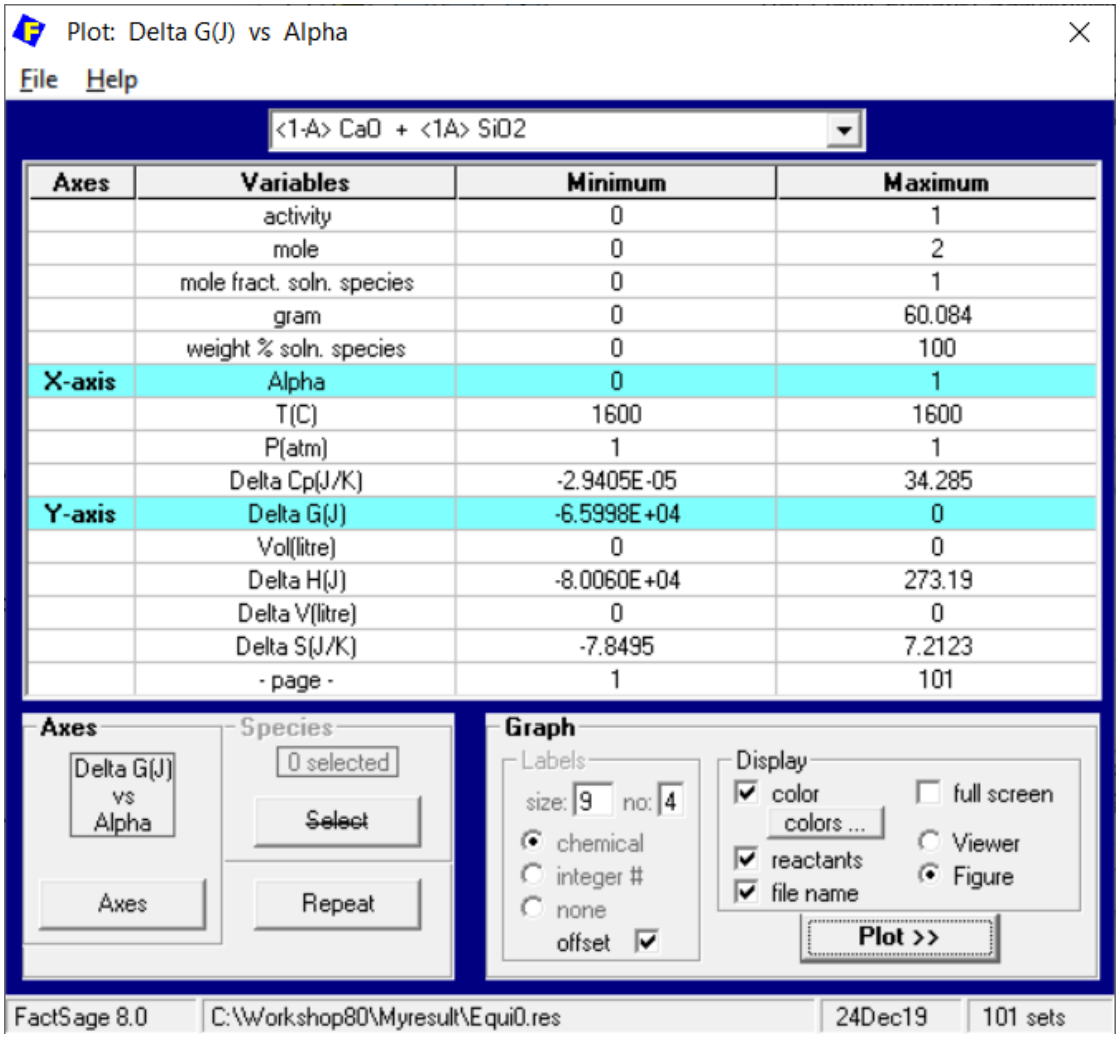
For calculating the difference of thermodynamic properties from the initial state to the final state, “Initial Conditions” should be activated.

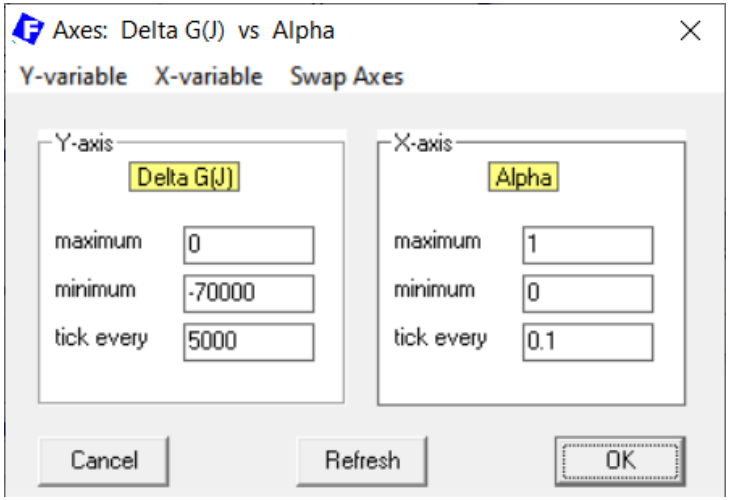
Initial conditions for phase and temperature should be specified



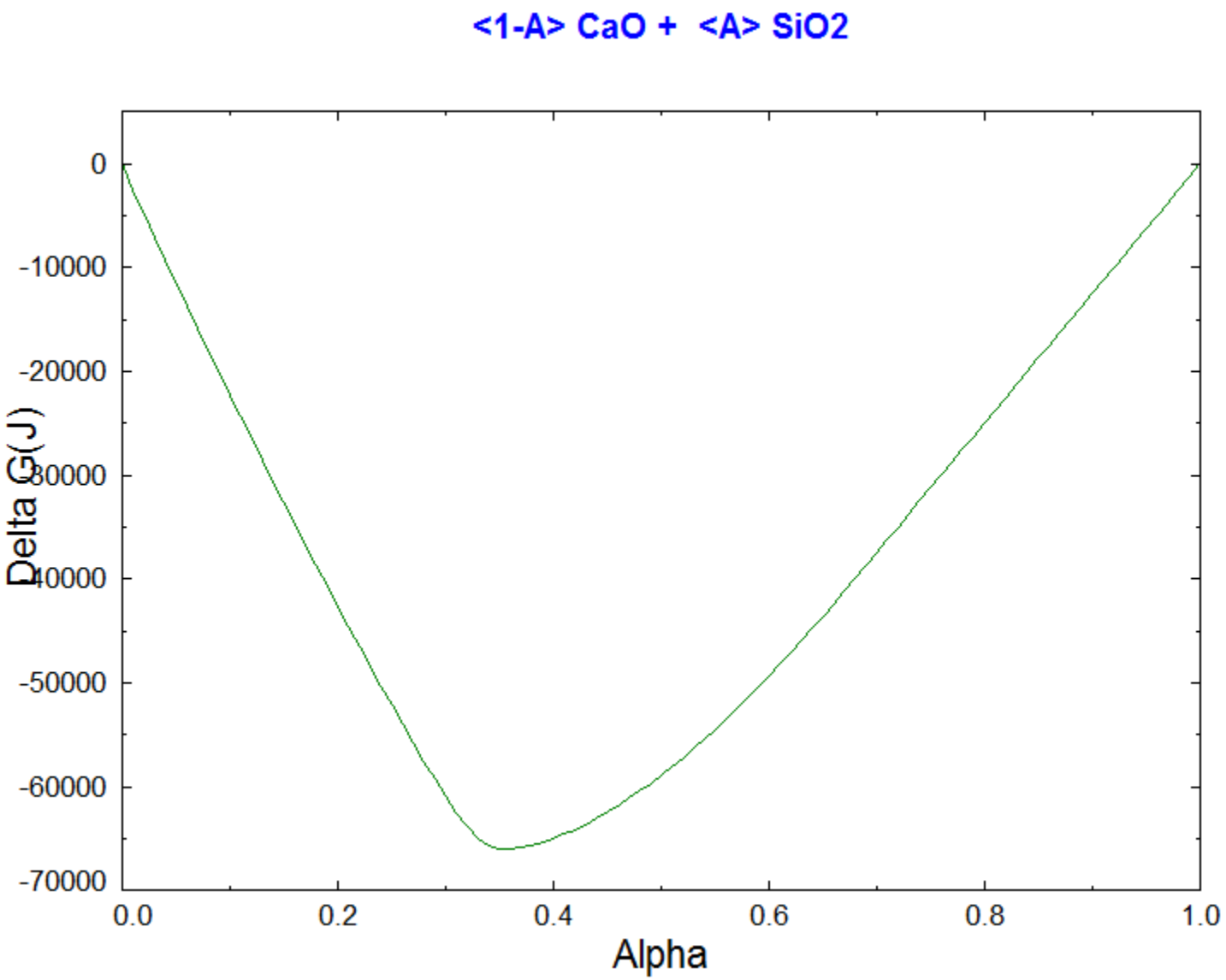


Thermodynamic properties: Activity, ΔG, ΔH, ΔS etc.

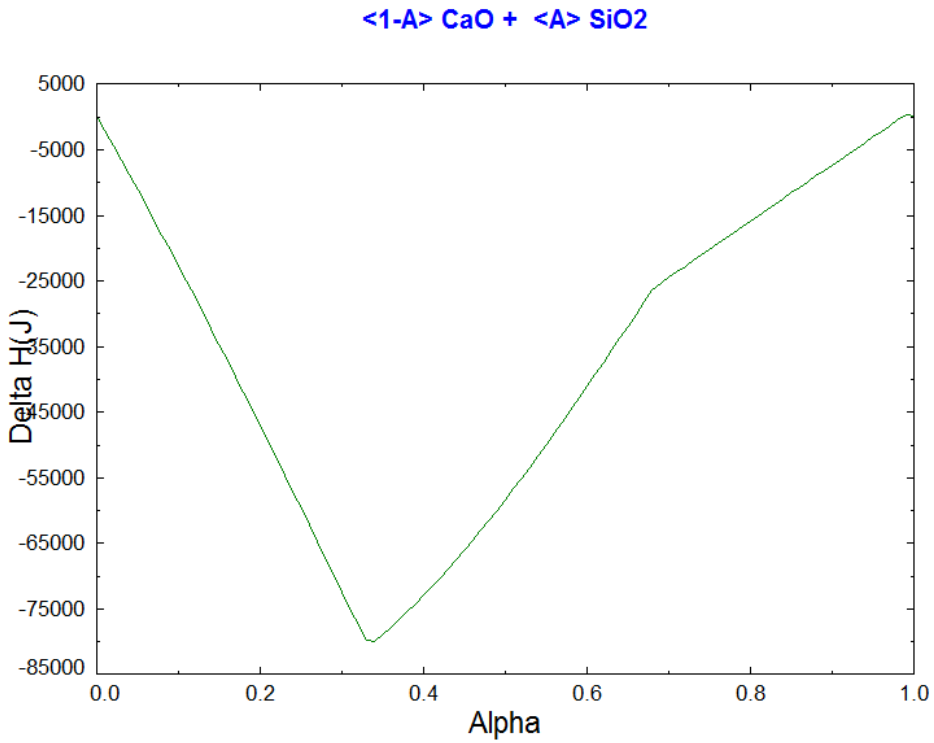


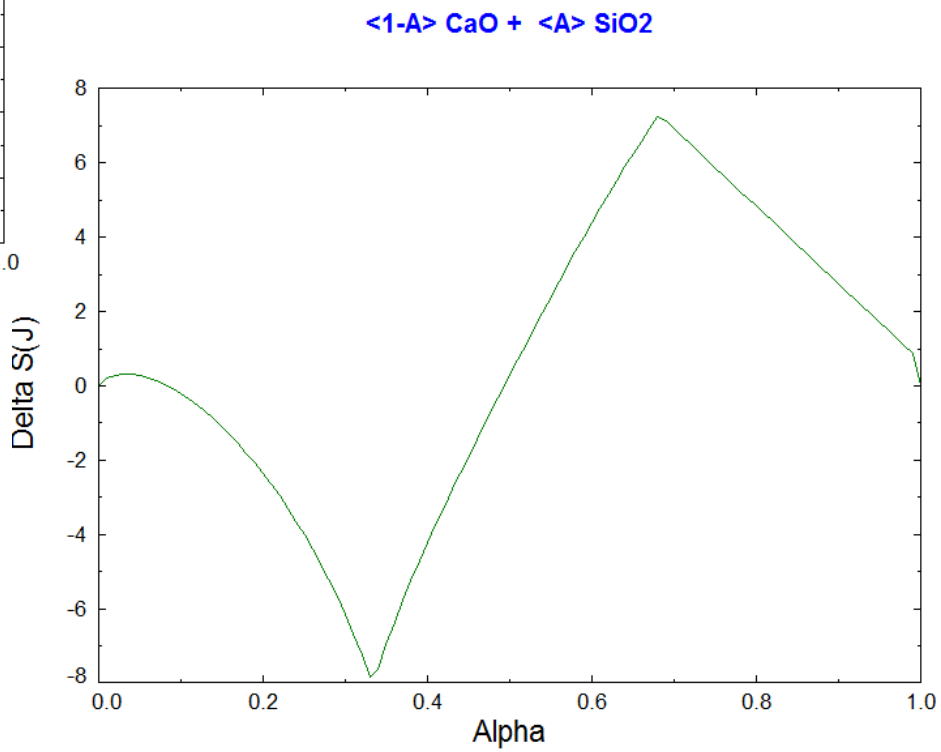


Thermodynamic properties: ΔG, ΔH, ΔS etc.



Thermodynamic properties: Activity, ΔG, ΔH, ΔS etc.



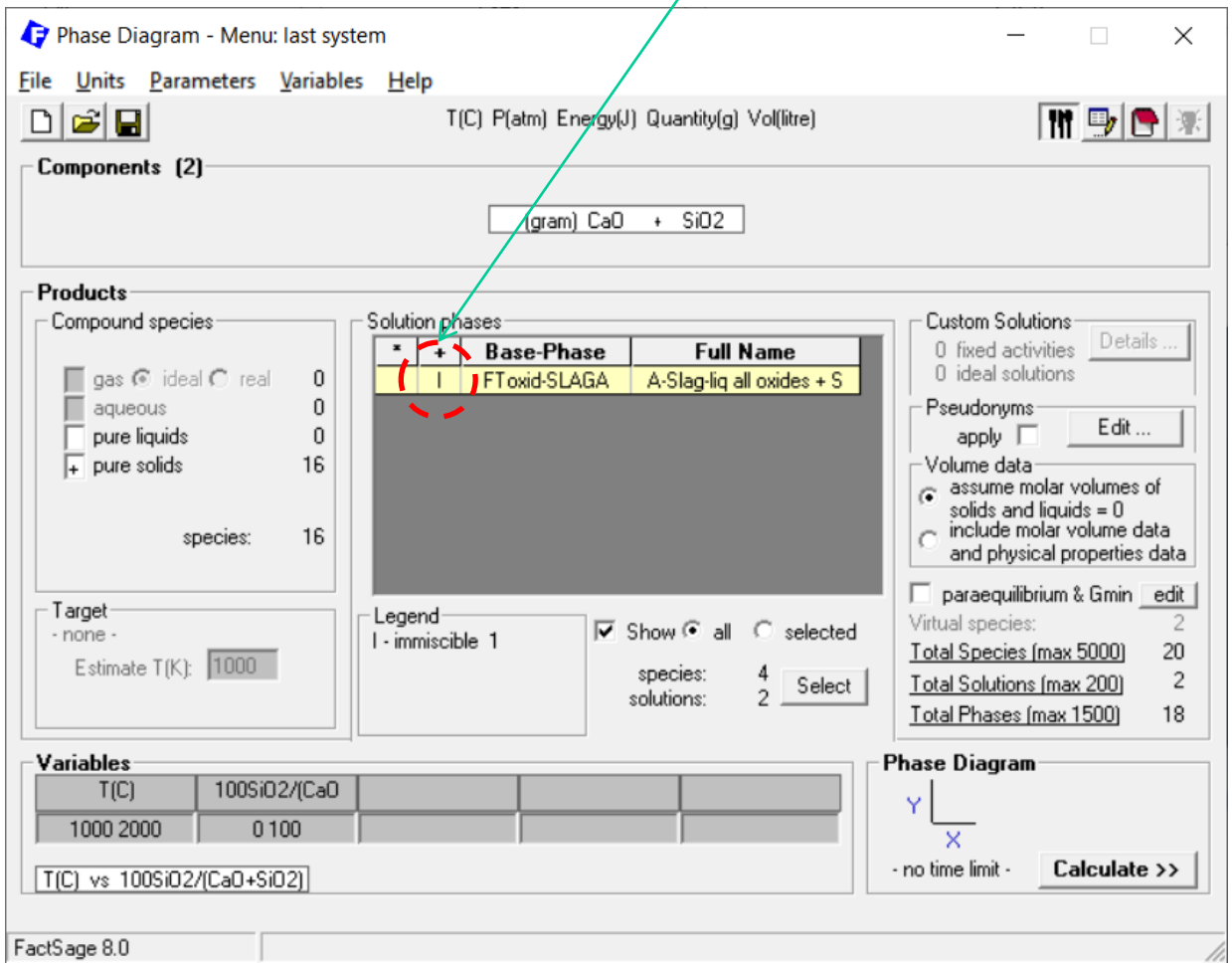


Simple examples of Phase diagram

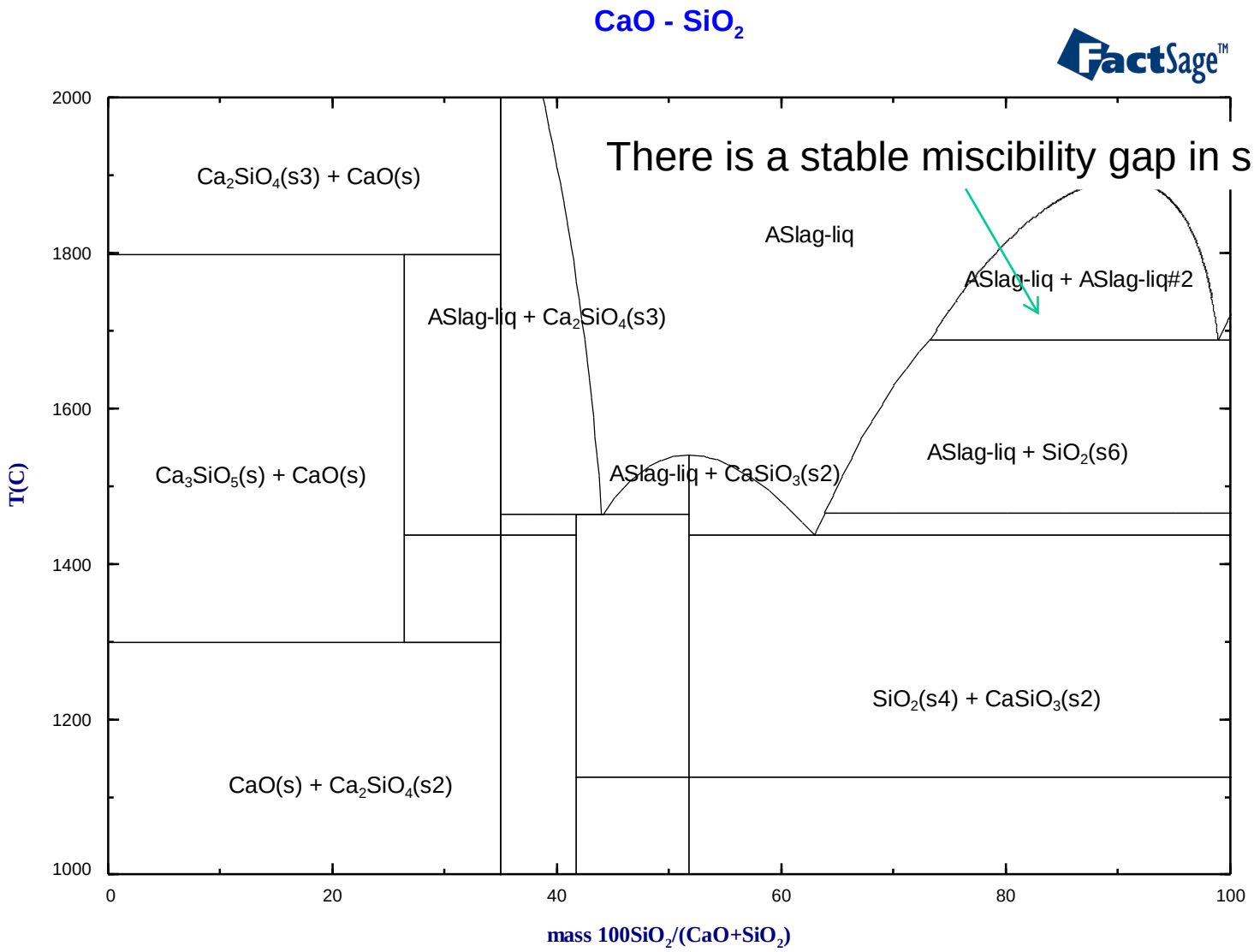
Binary phase diagram
Ternary and multi-component systems

Binary phase diagram: CaO-SiO2

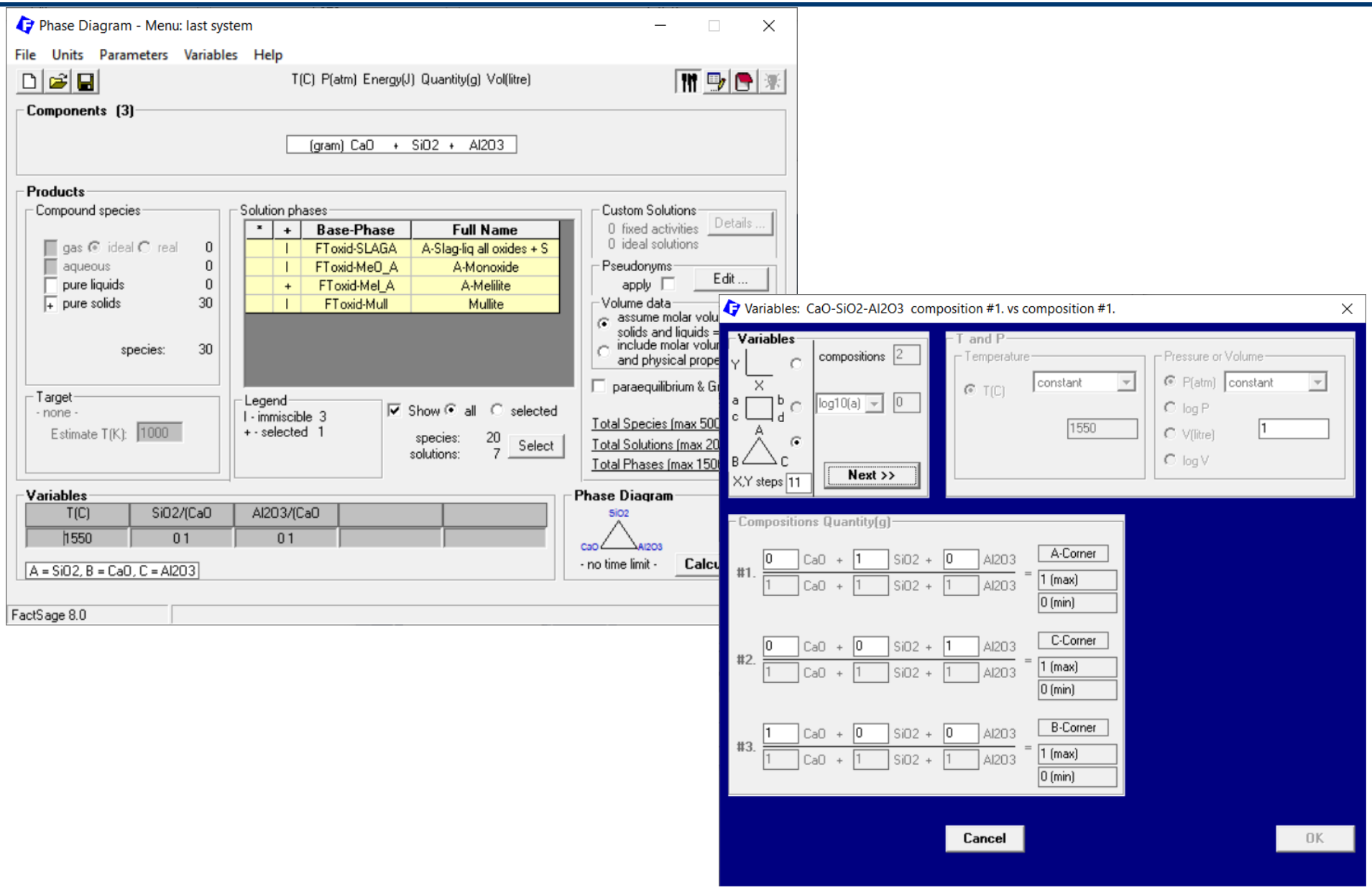
There is a stable miscibility gap in slag; automatic selection by FactSage



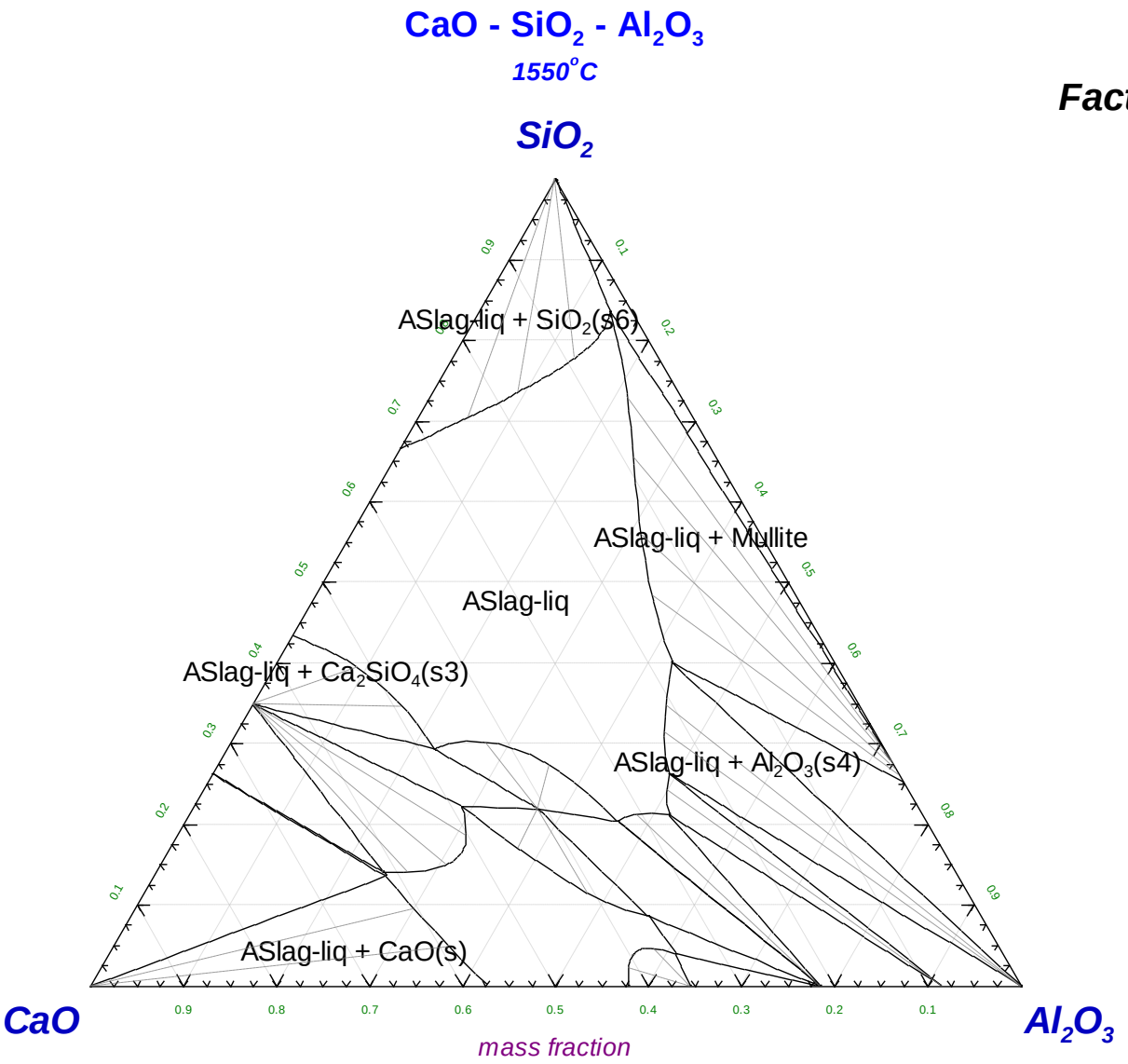
Binary phase diagram: CaO-SiO2



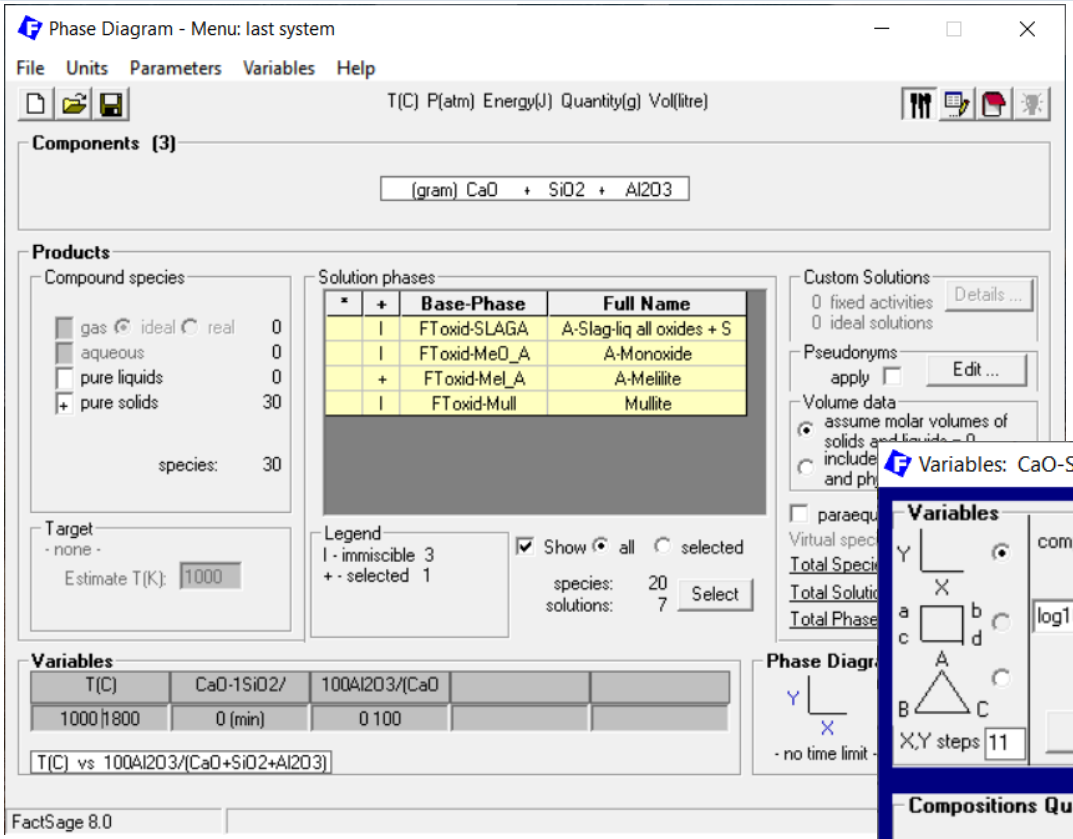
Ternary phase diagram: CaO-SiO2-Al2O3 isothermal section

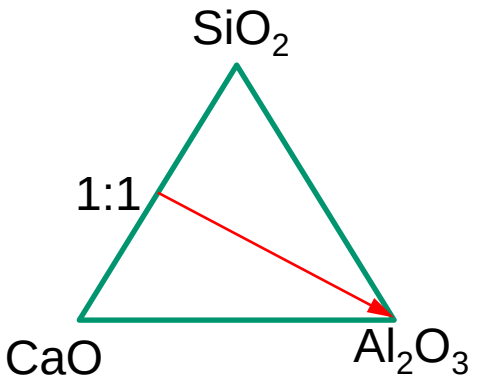


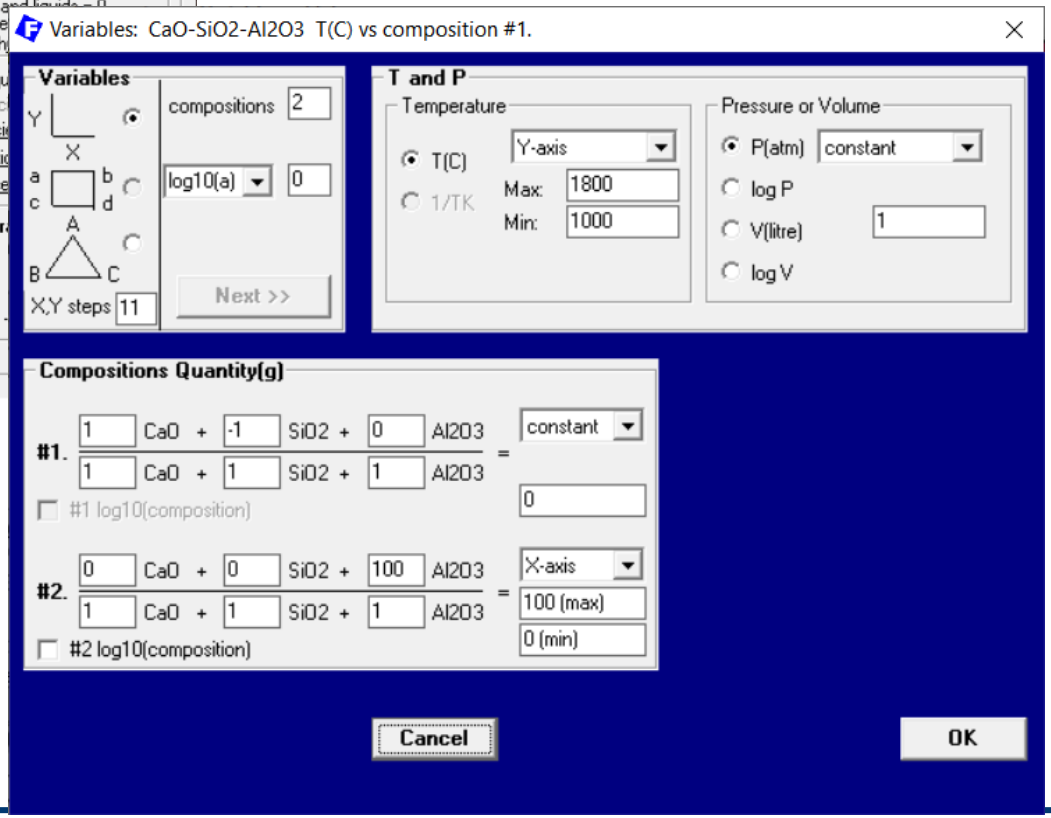
Ternary phase diagram: CaO-SiO2-Al2O3 isothermal section



Ternary system: section in ternary (isopleth)

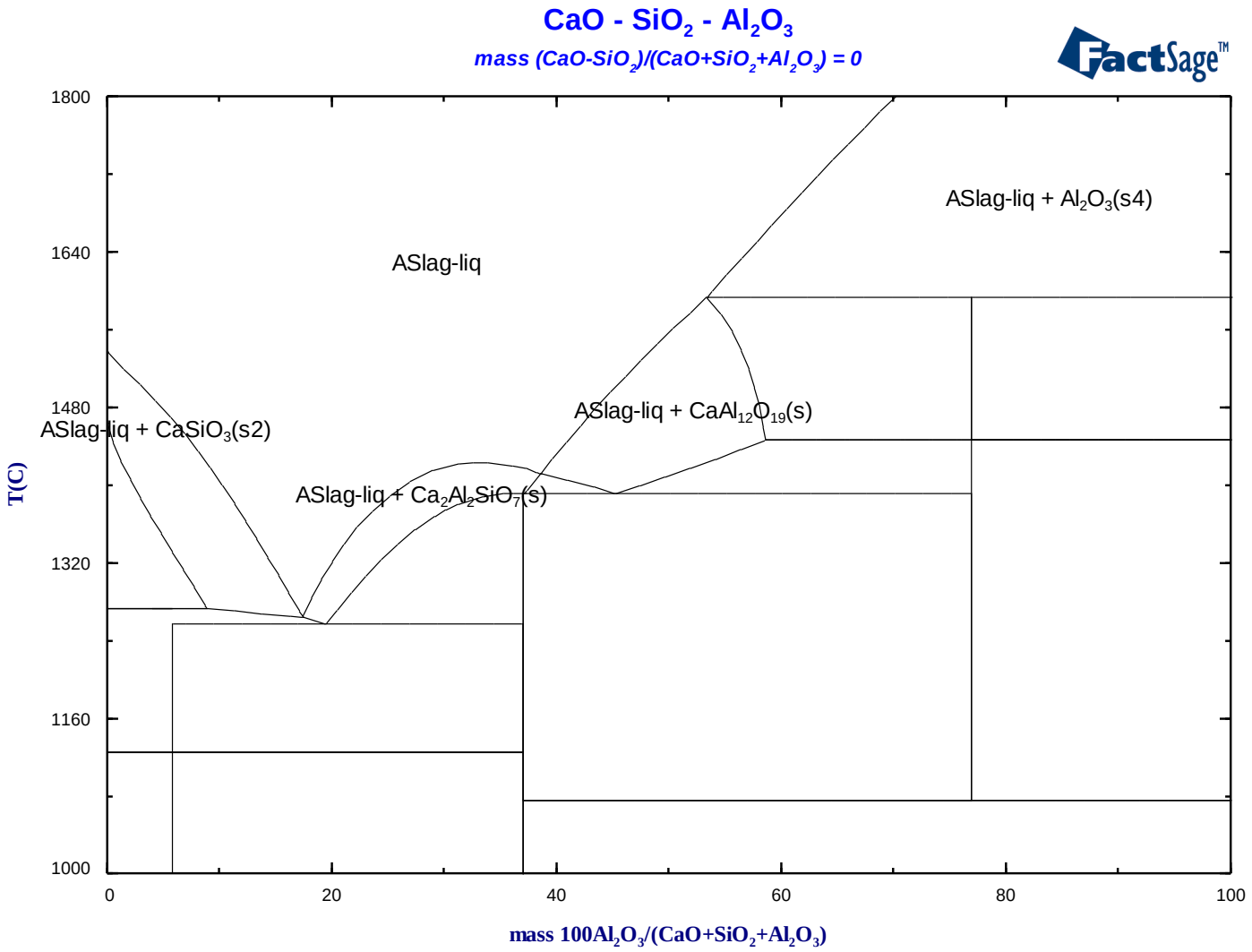




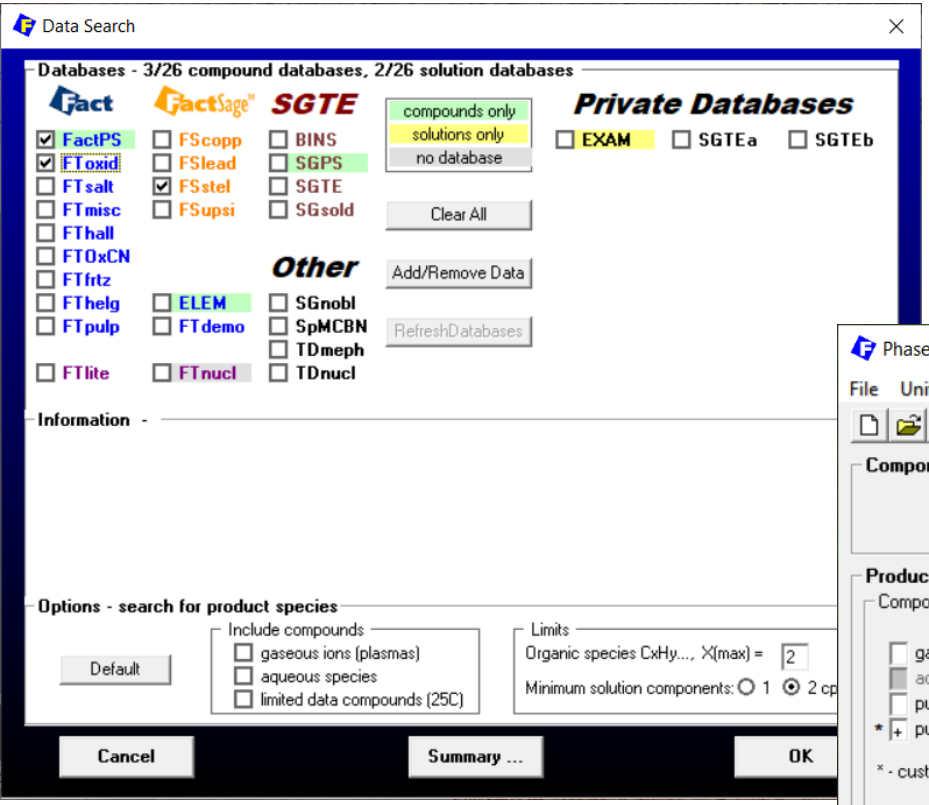


Ternary system: section in ternary (isopleth)

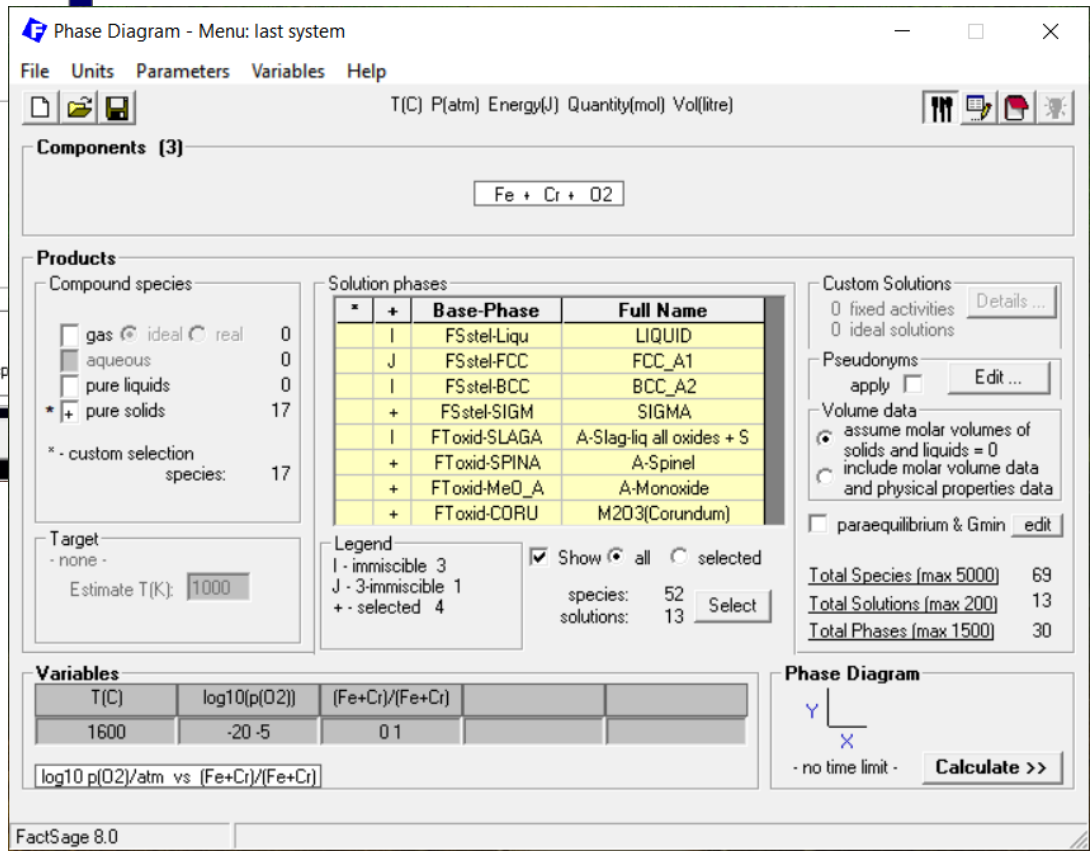
$CaO\text{-}SiO_2\text{-}Al_2O_3$ Vertical section at $(wt\%CaO/wt\%SiO_2) = 1$



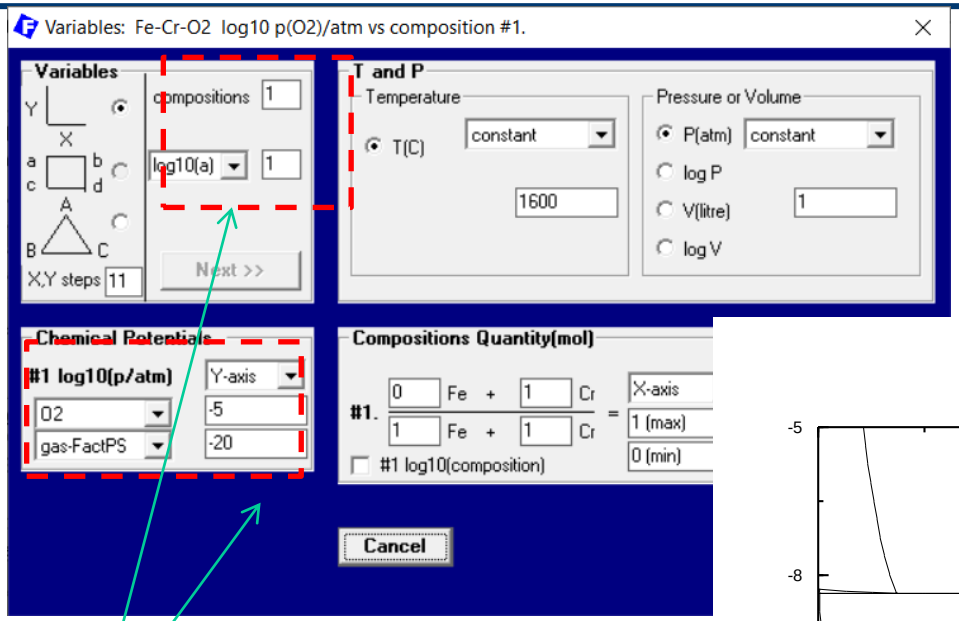
Oxidation diagram: Fe-Cr-O2



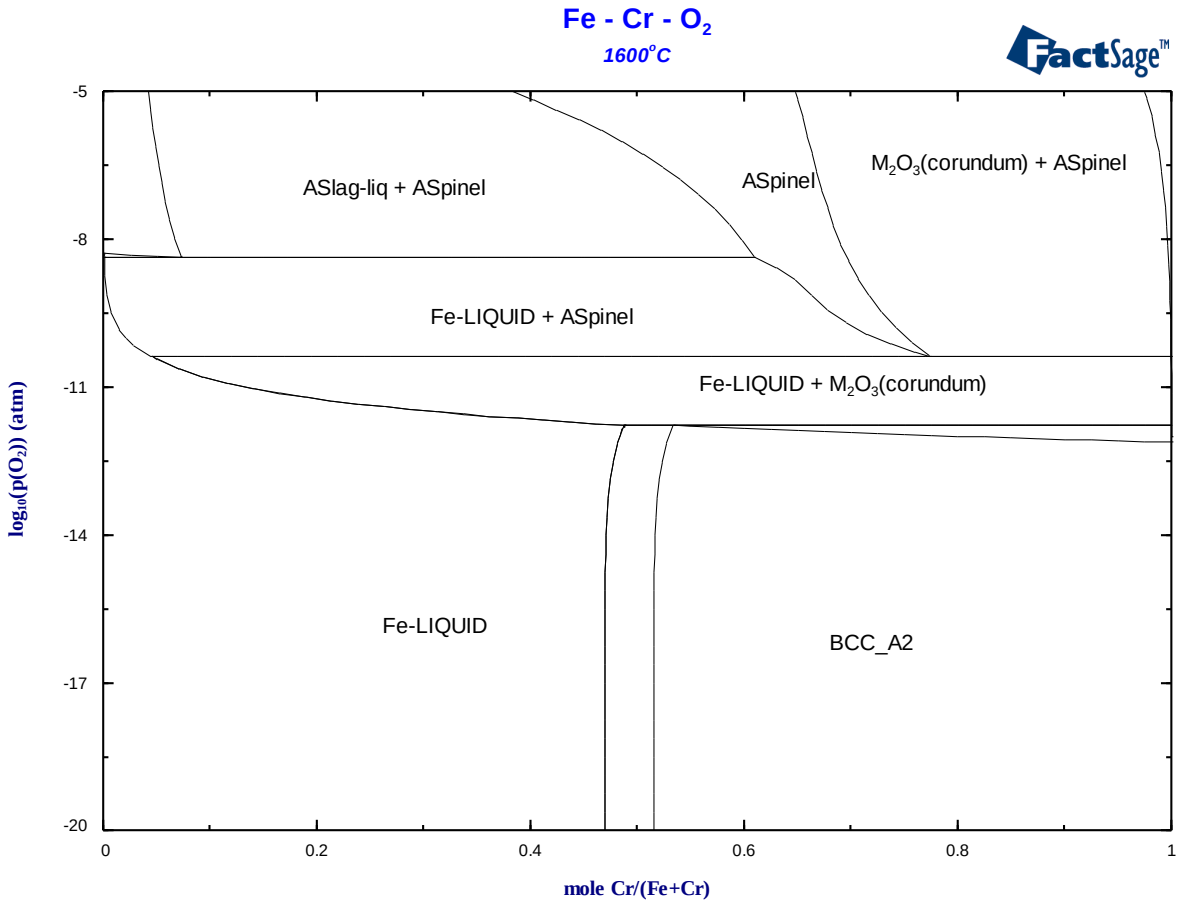
Combination of many databases:
FACT53: gases (if necessary)
FToxid: oxide phases
FSStel: fcc, bcc and other metallic phases



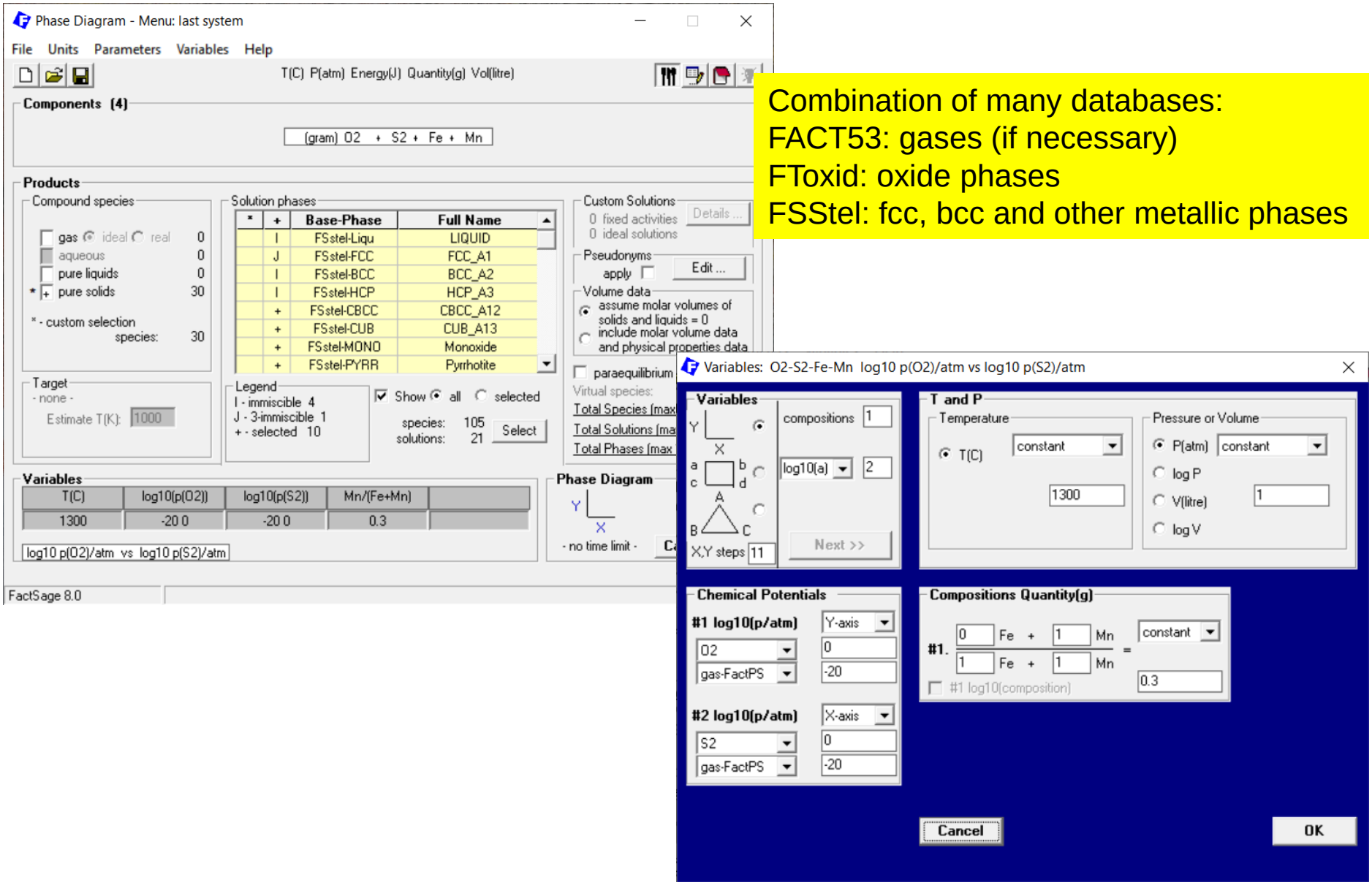
Oxidation diagram: Fe-Cr-O2



Log pO_2 for y-axis variable

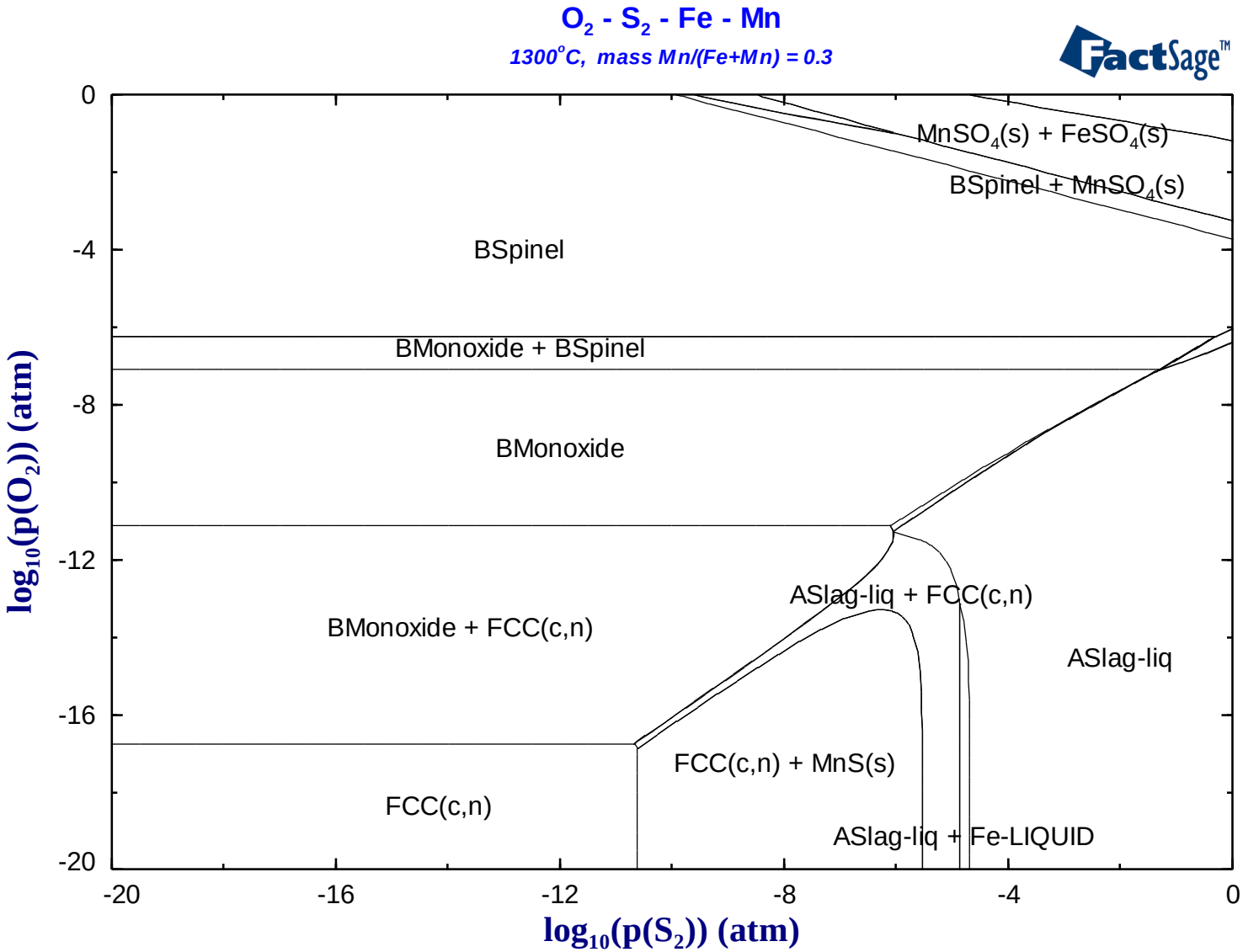


Predominance diagram: Fe-Mn-O2-S2

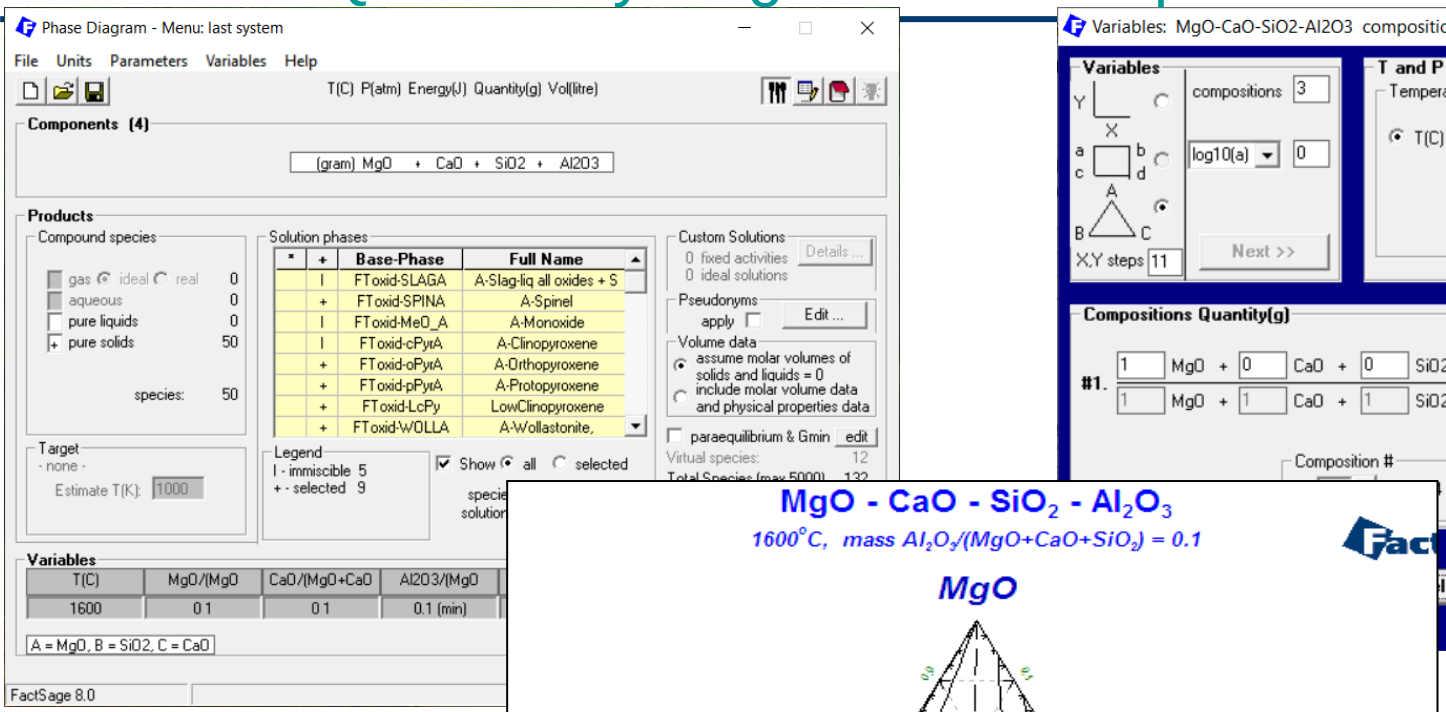


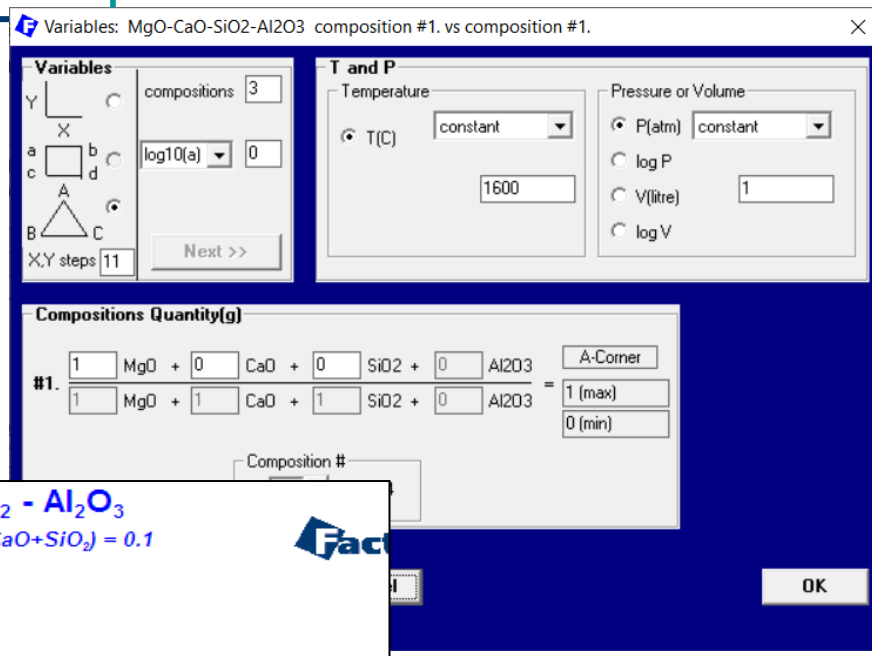
Combination of many databases:
FACT53: gases (if necessary)
FToxid: oxide phases
FSStel: fcc, bcc and other metallic phases

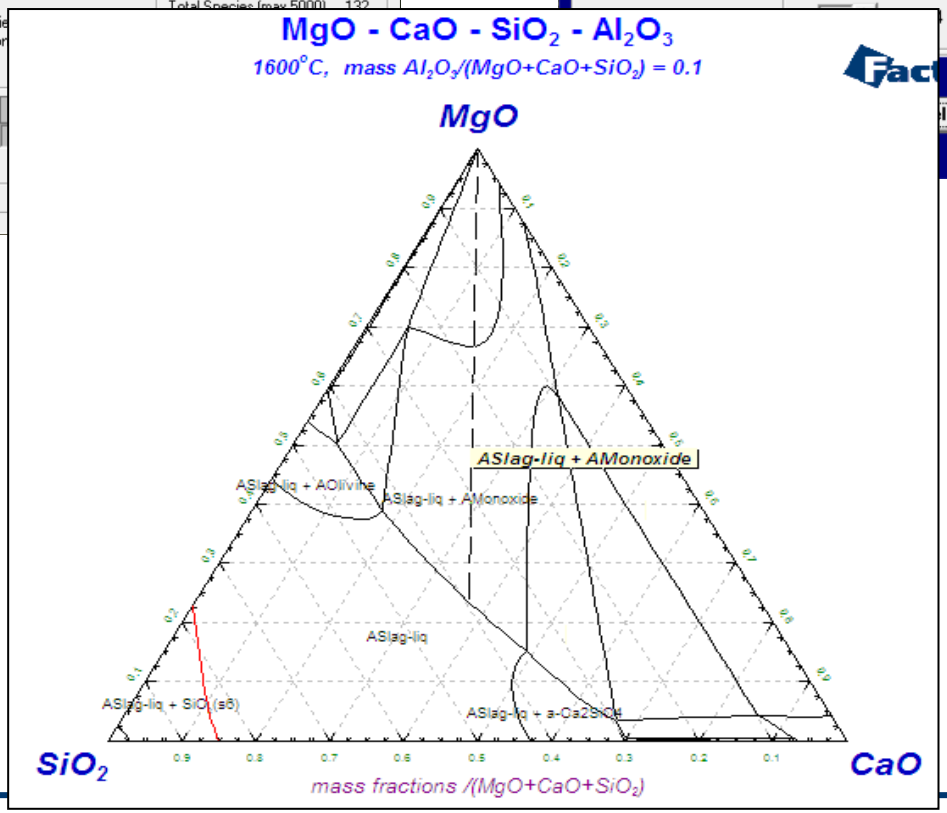
Predominance diagram: Fe-Mn-O2-S2



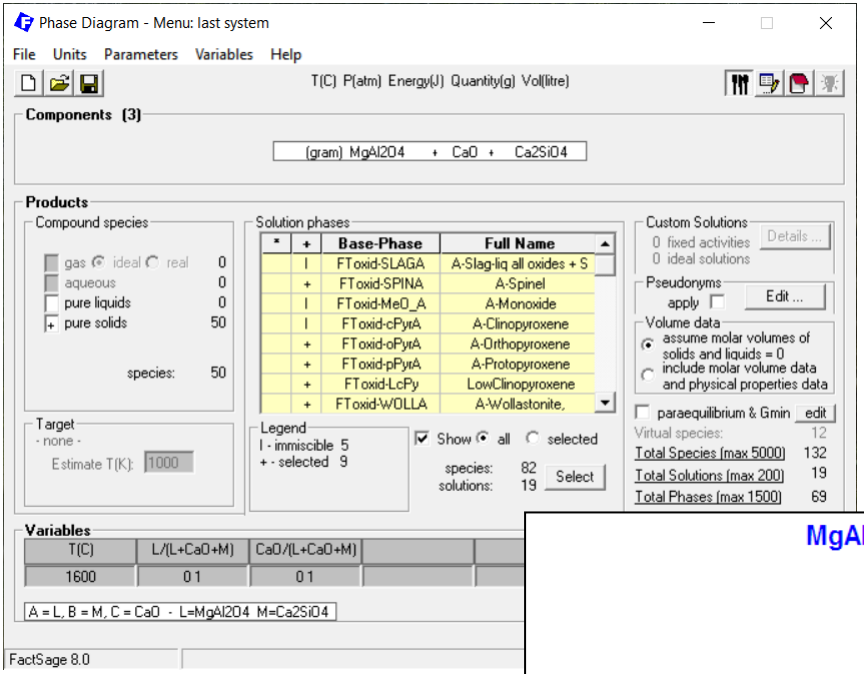
Quaternary diagram: iso-composition section

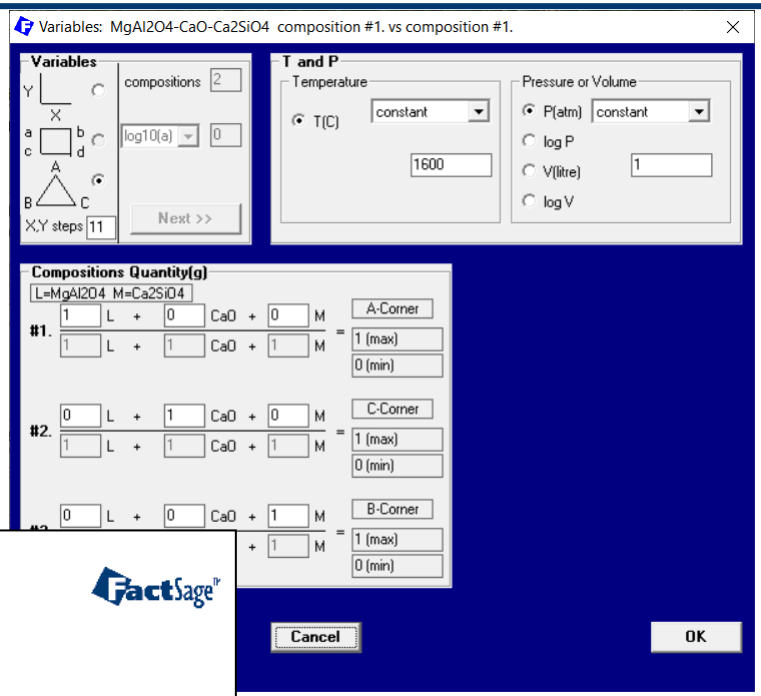


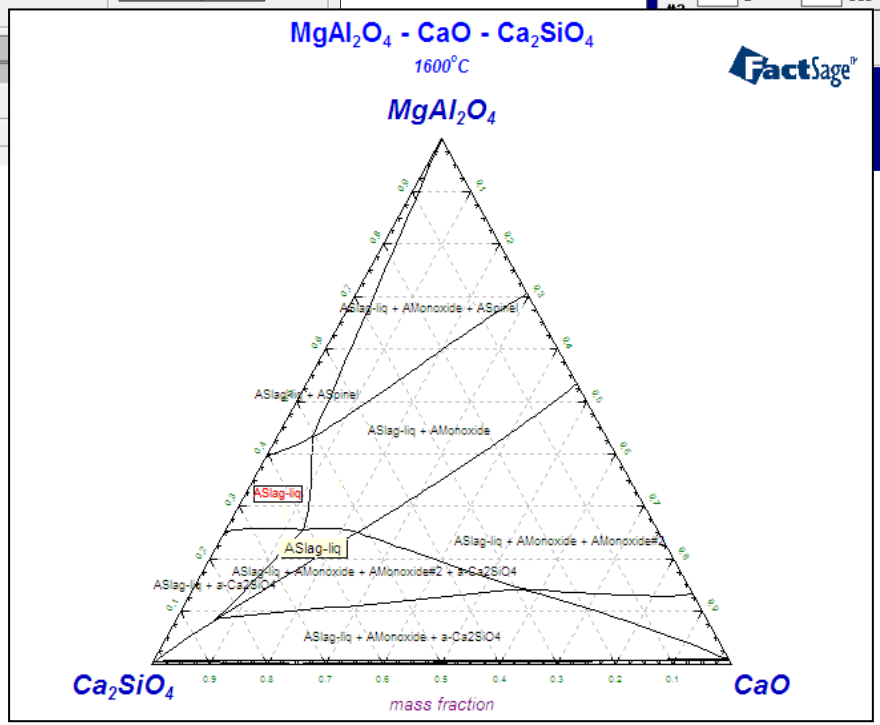




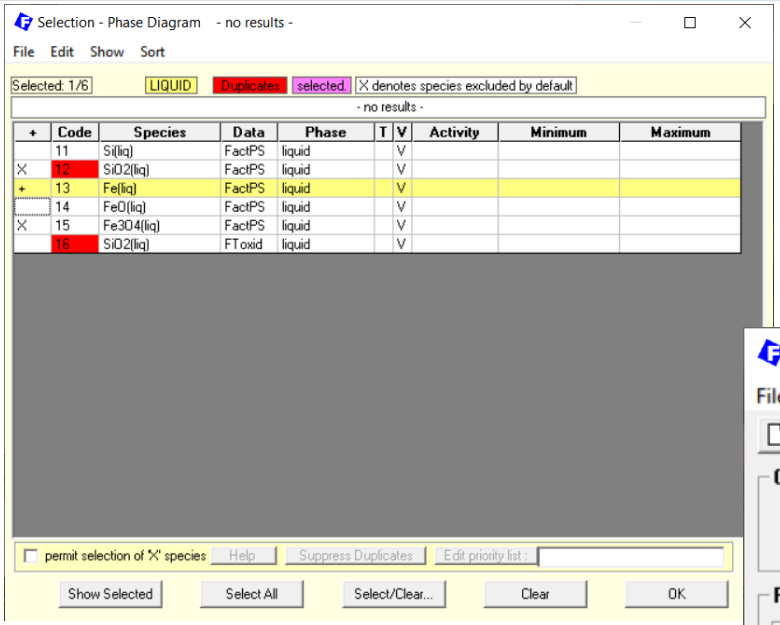
Quaternary system: CaO-Ca2SiO4-MgAl2O4



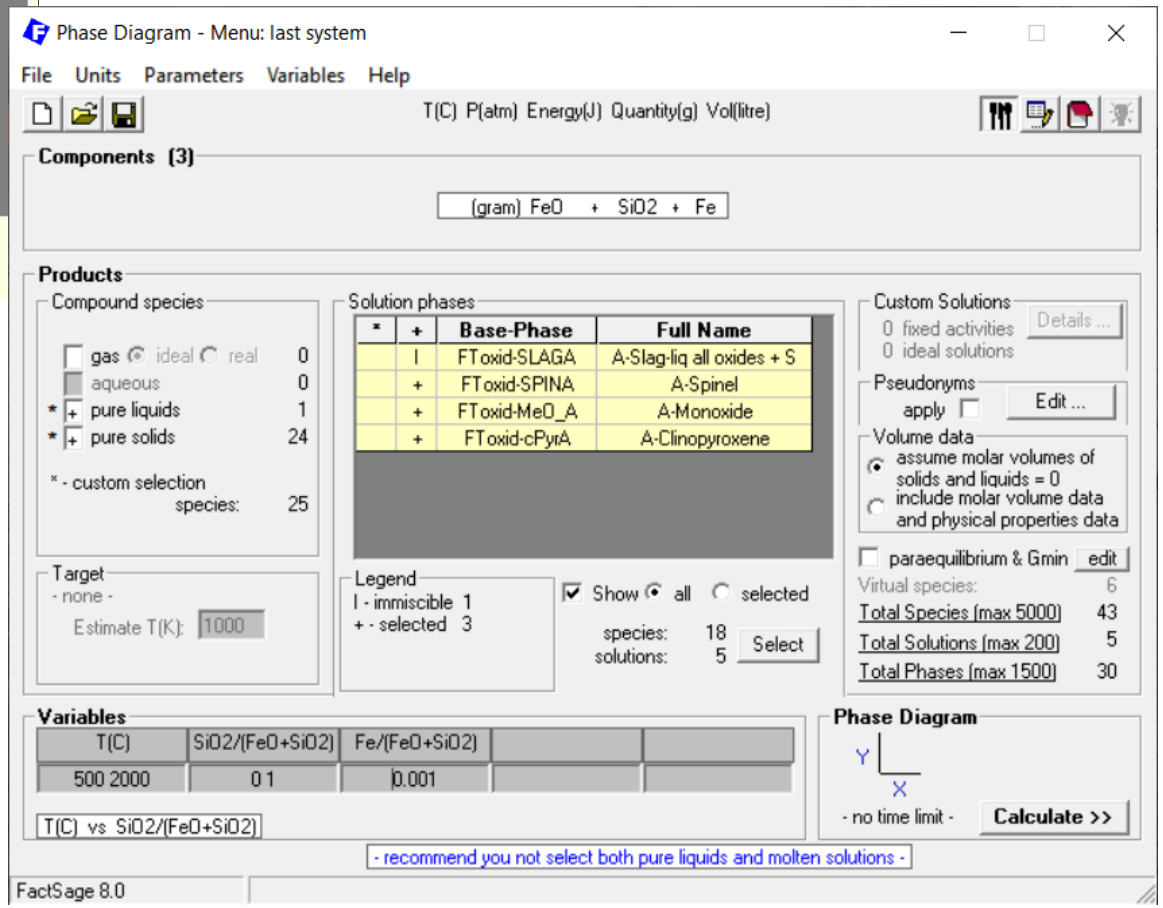




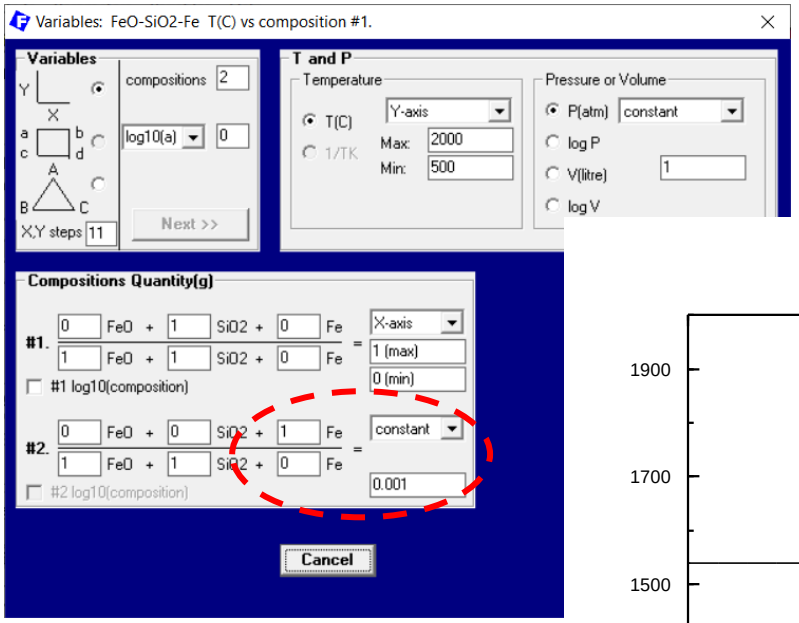
Fe oxide containing system: Fe saturation



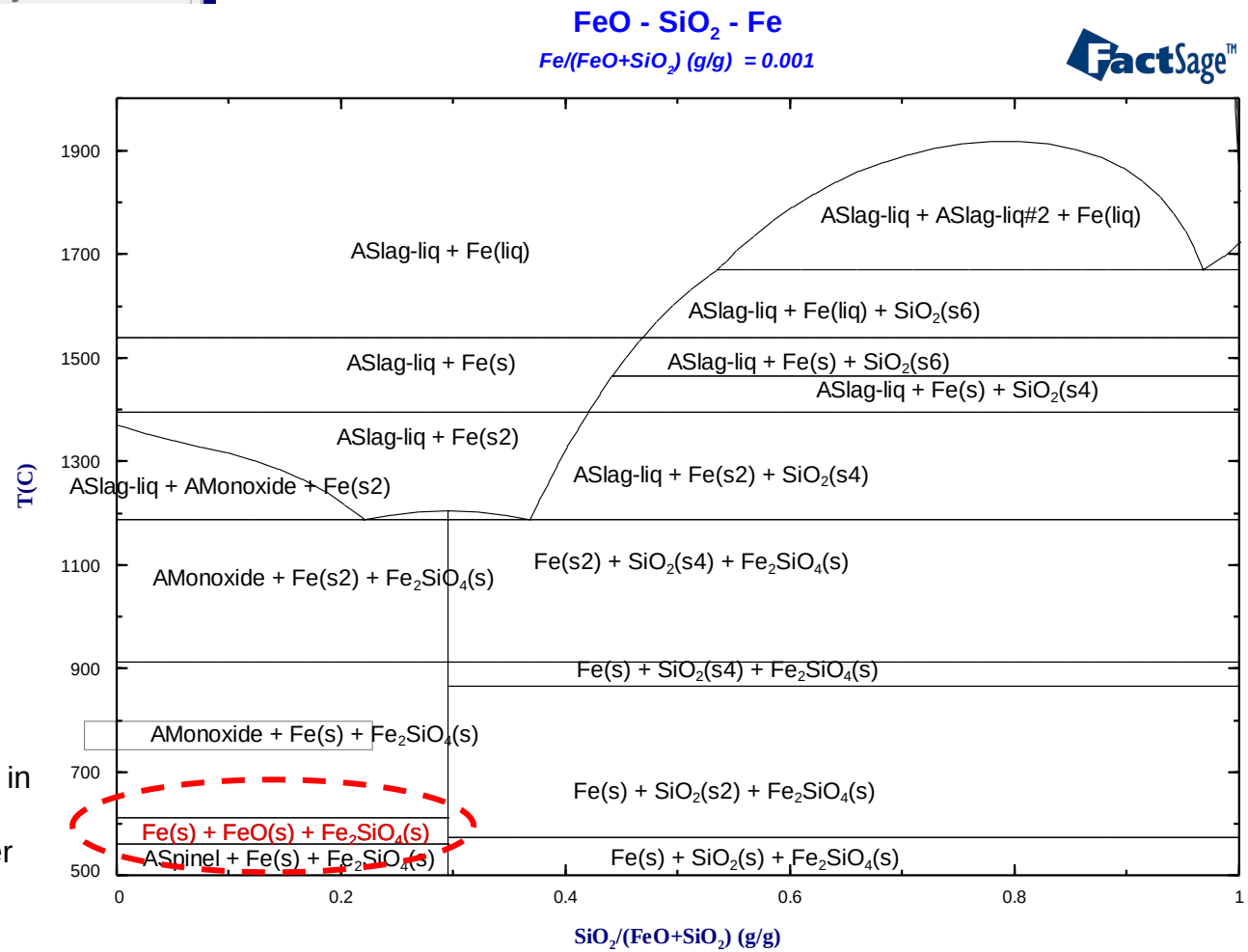
Intentional addition of Fe to make Fe saturation



Fe oxide containing system: Fe saturation

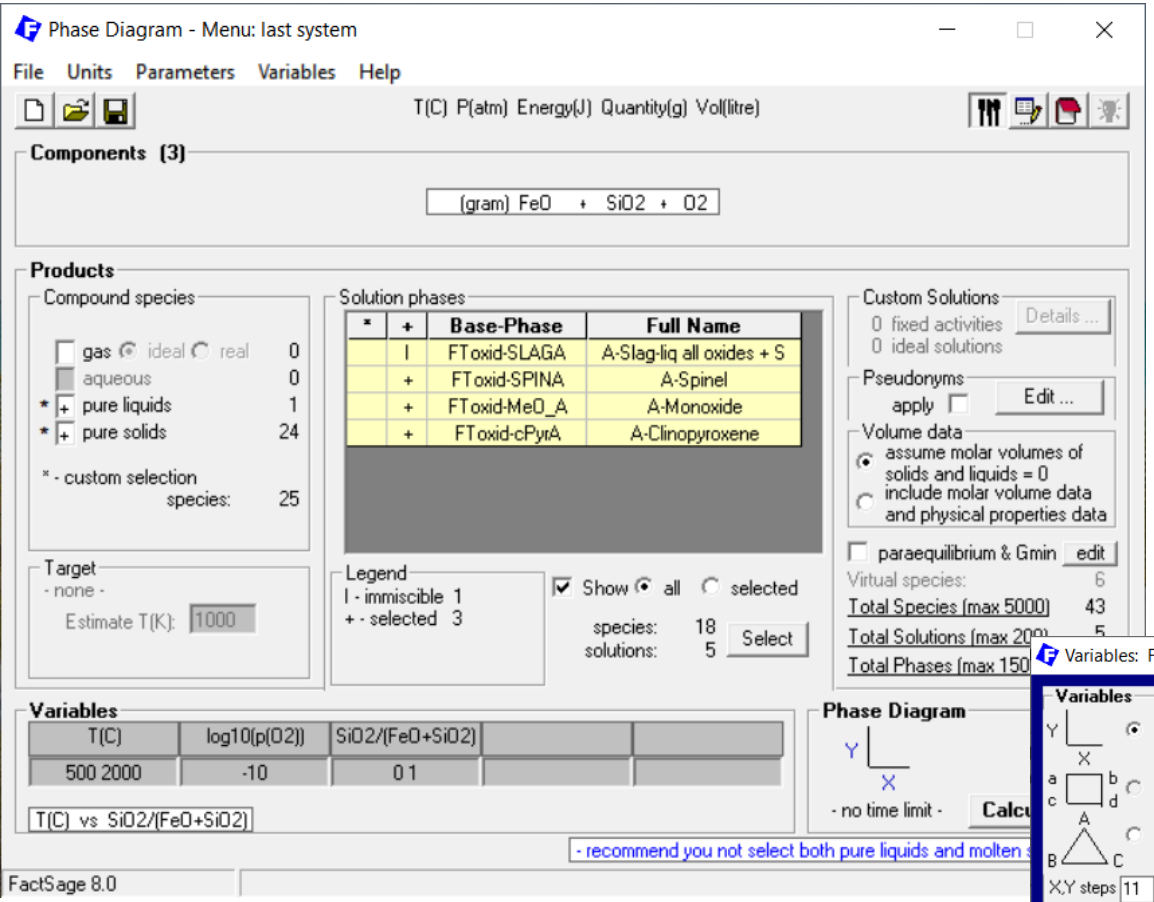


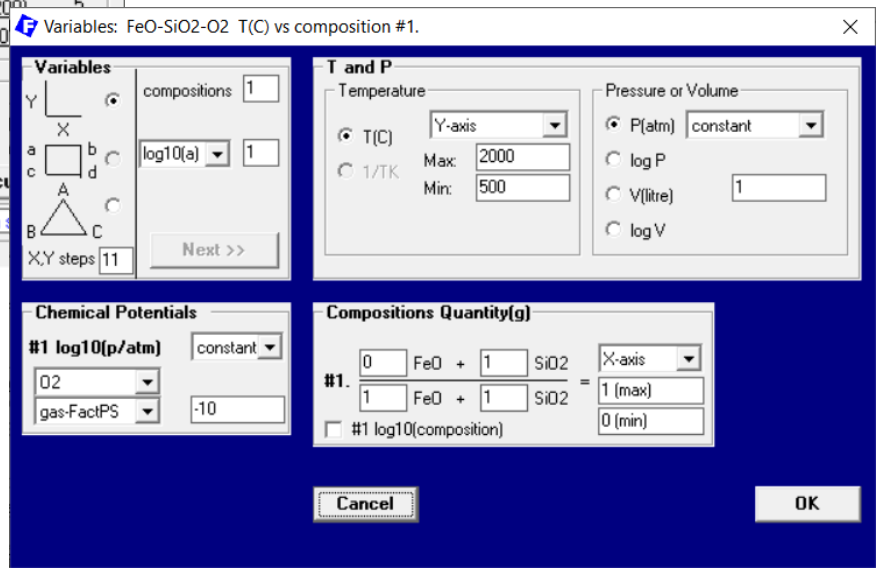
Intentional addition of Fe to make Fe saturation



Monoxide = FeO. But due to slightly different Gibbs energies of FeO stored in two databases, FeO from FACT53 appears in the calculation. → for better calcs, remove FeO(s) from database selection

Fe oxide containing system: fixed PO2

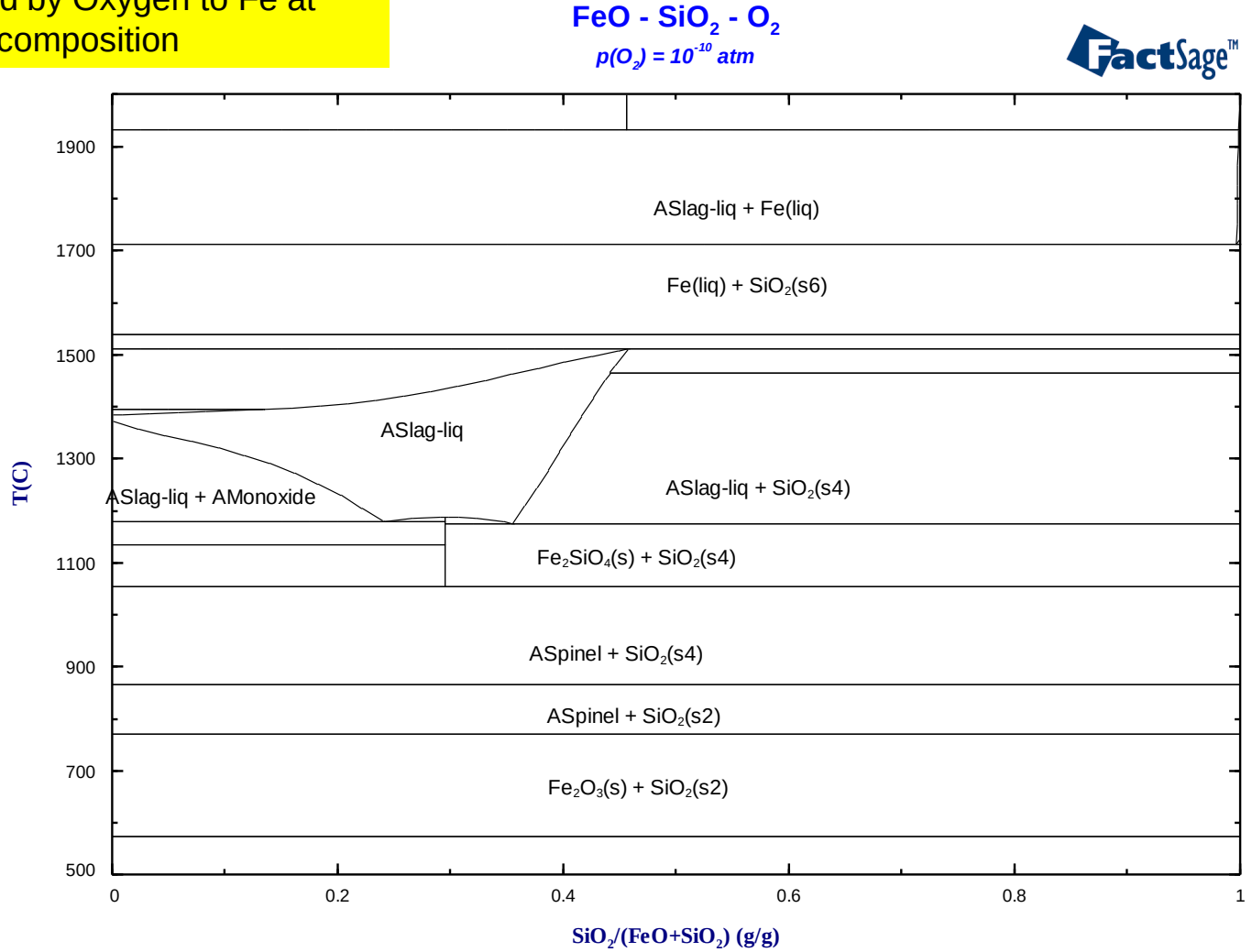




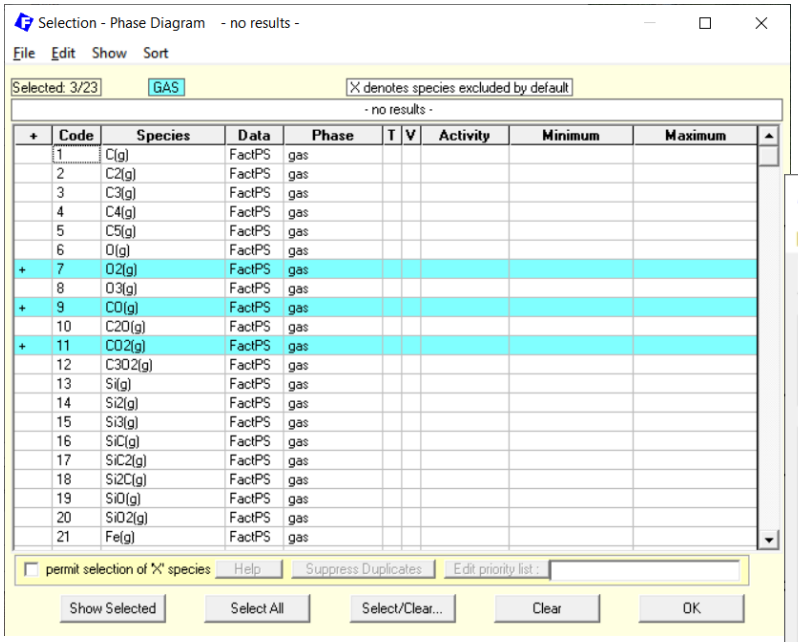
Fixing PO_2 to control the oxidation state of Fe

Fe oxide containing system: fixed PO2

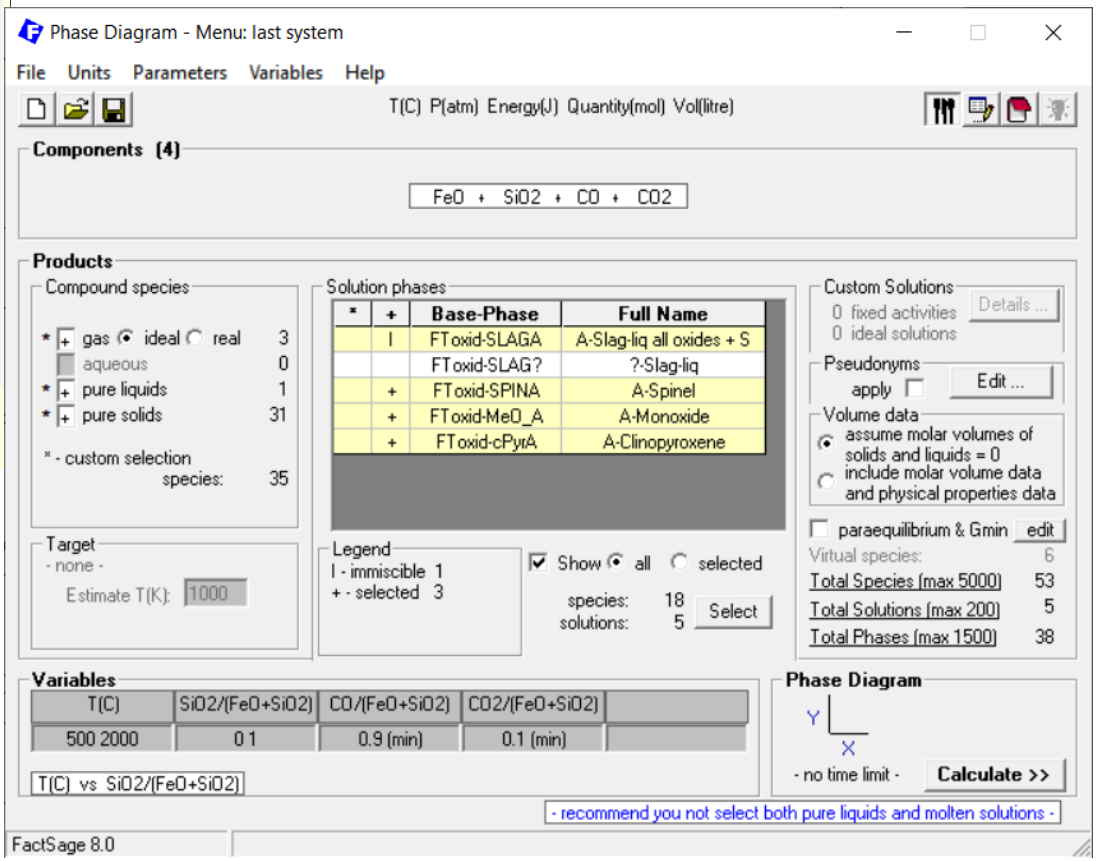
When PO2 is fixed with selection of Fe, slag and Fe oxides can be reduced by Oxygen to Fe at certain temperature and composition



Fe oxide containing system: fixed CO/CO2 gas

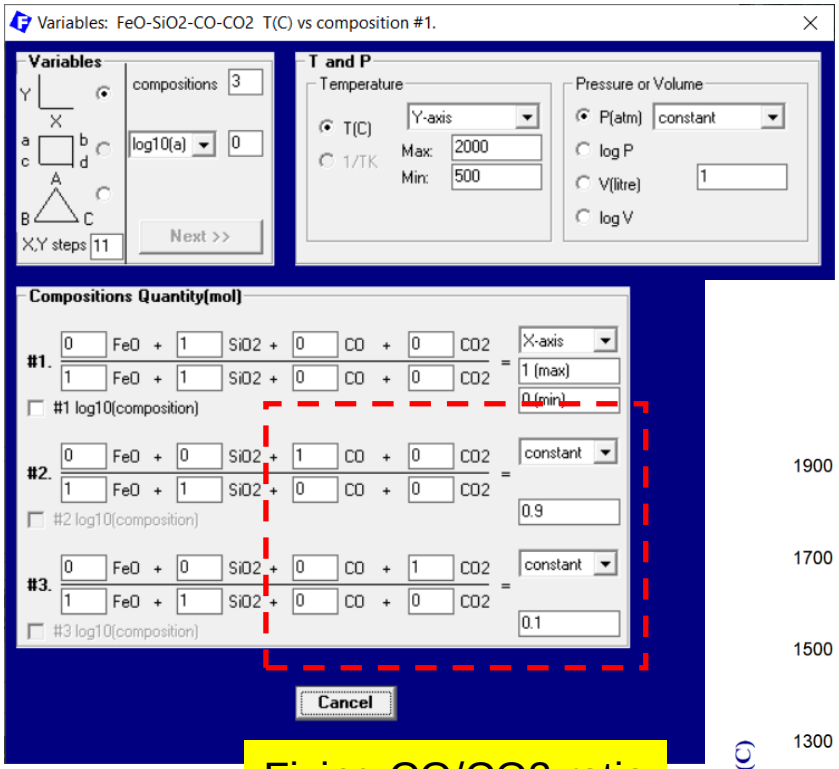


Fixing PO_2 by CO/CO2 gas mixture

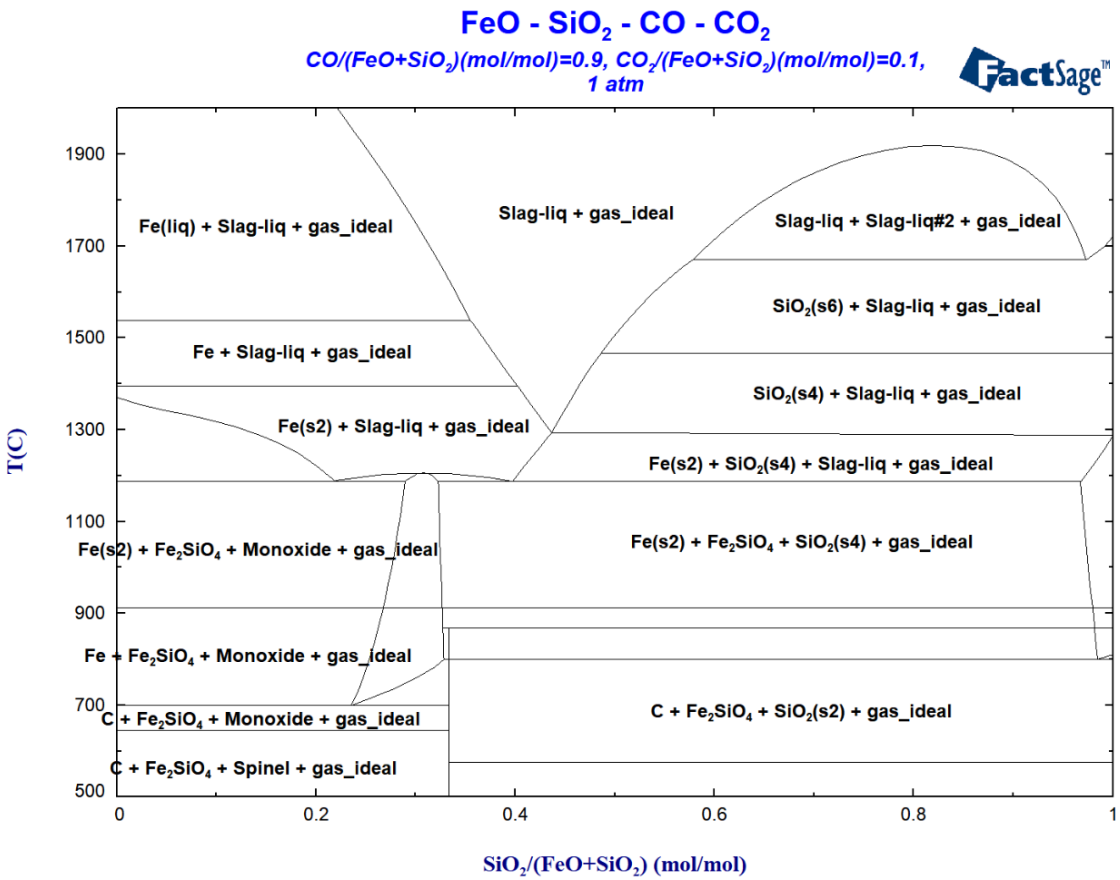


Select only CO, CO2 and O2 gas to simulate real experiment of oxide/gas equilibration.
→ If we select all gases, some amount of oxides can be evaporated depending on the relative amount of gas and oxide in the calculations

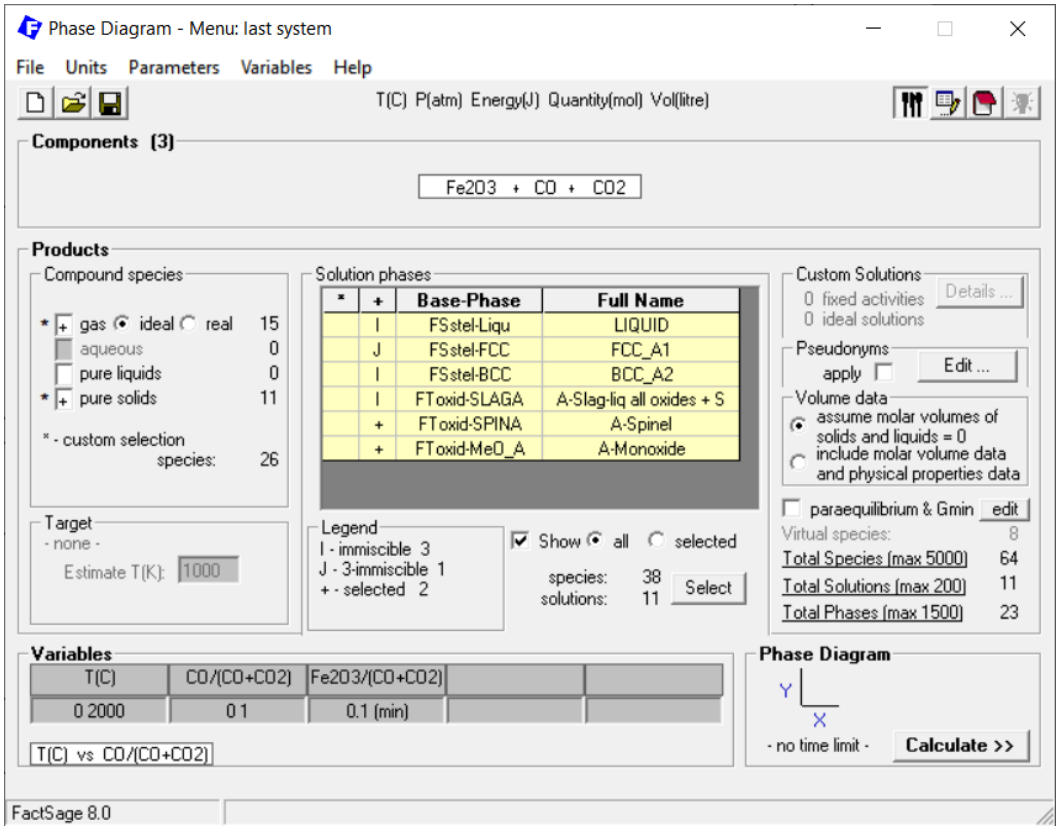
Fe oxide containing system: fixed CO/CO2 gas

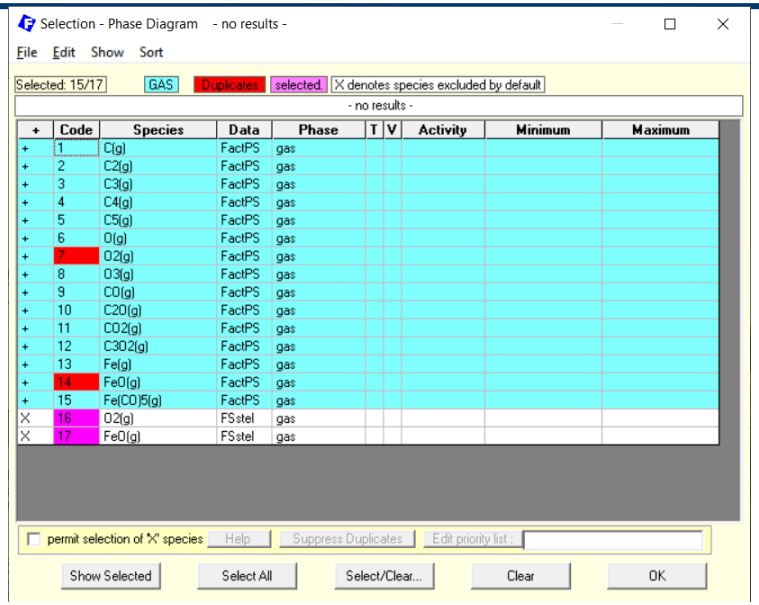


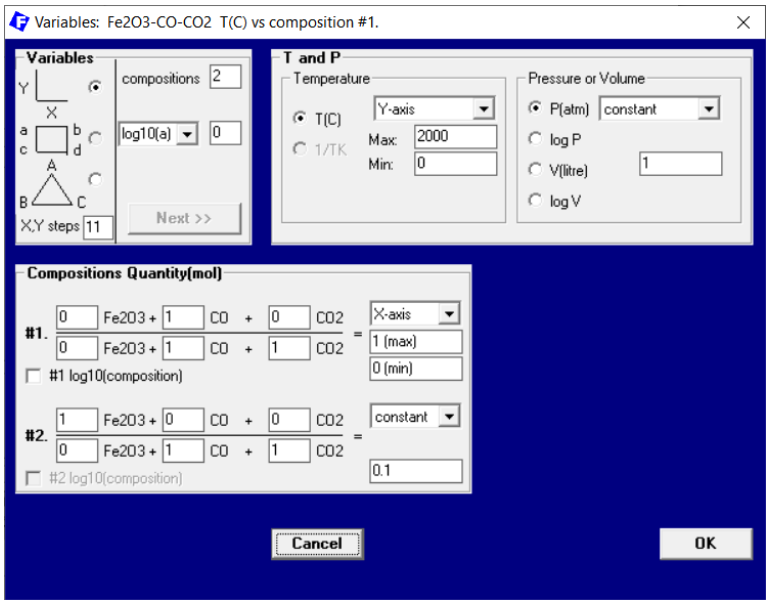
Fixing CO/CO2 ratio



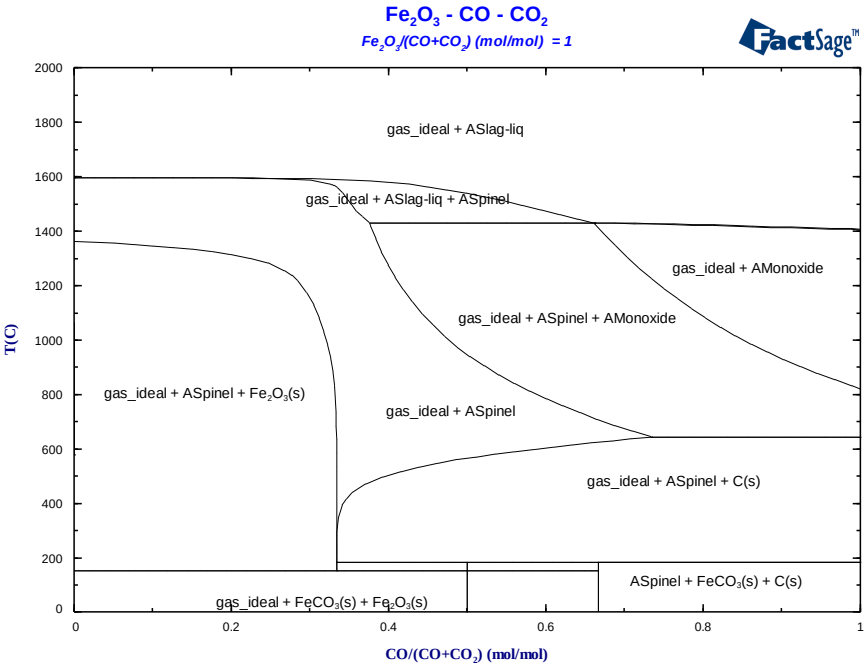
Fe oxide containing system: fixed CO/CO2 gas







Fe oxide containing system: fixed CO/CO2 gas



1mole
CO-CO2 gas
1mole
Fe2O3

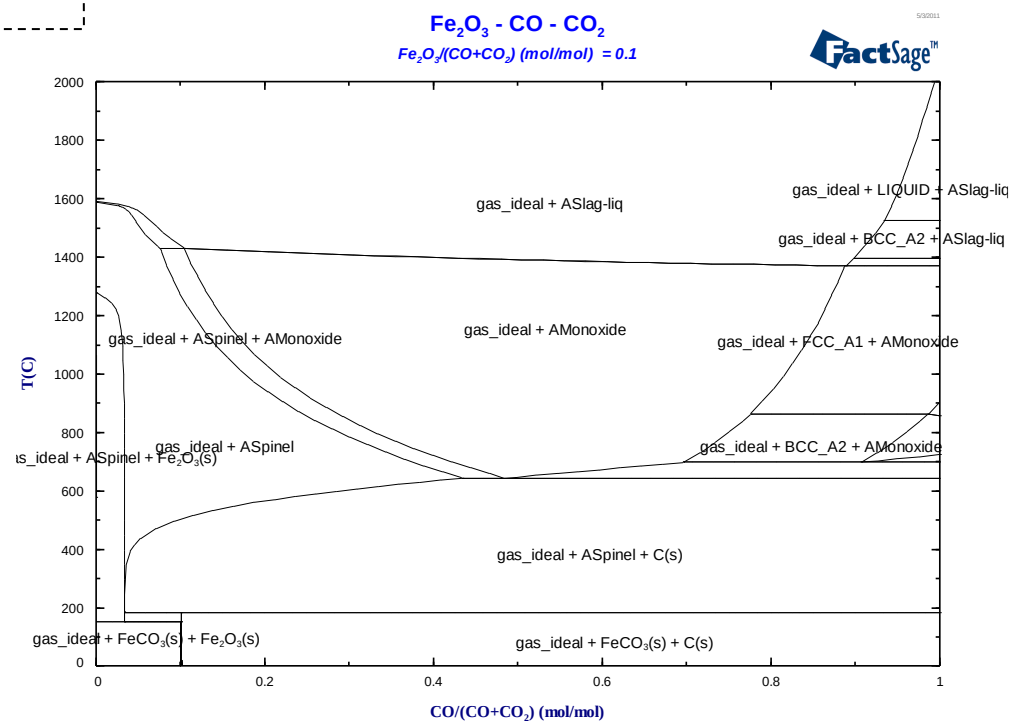
<Closed system>

10mole
CO-CO2 gas
1mole
Fe2O3

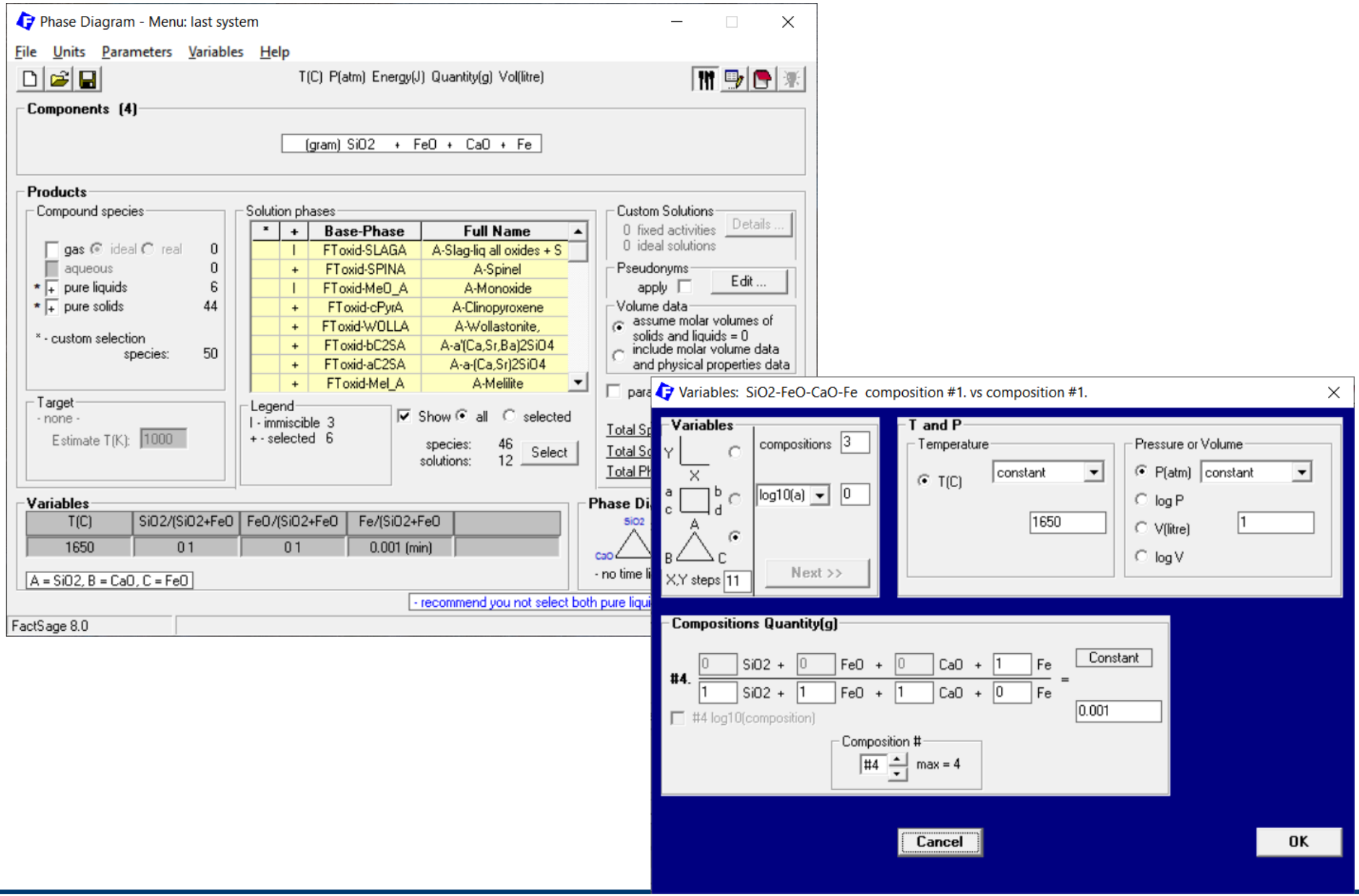
<Closed system>

10mole CO-CO2 gas
1mole
Fe2O3

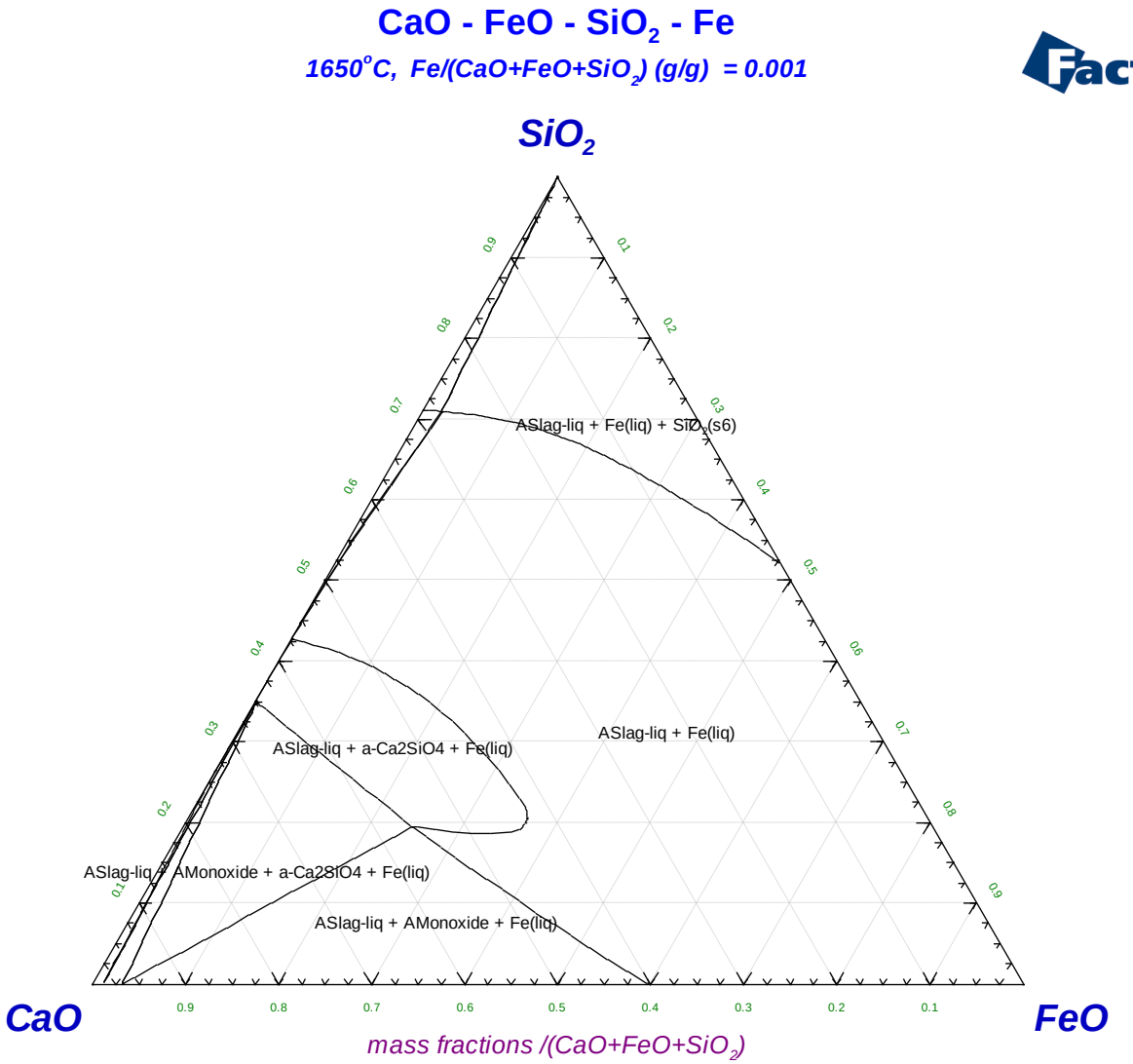
<Open system>



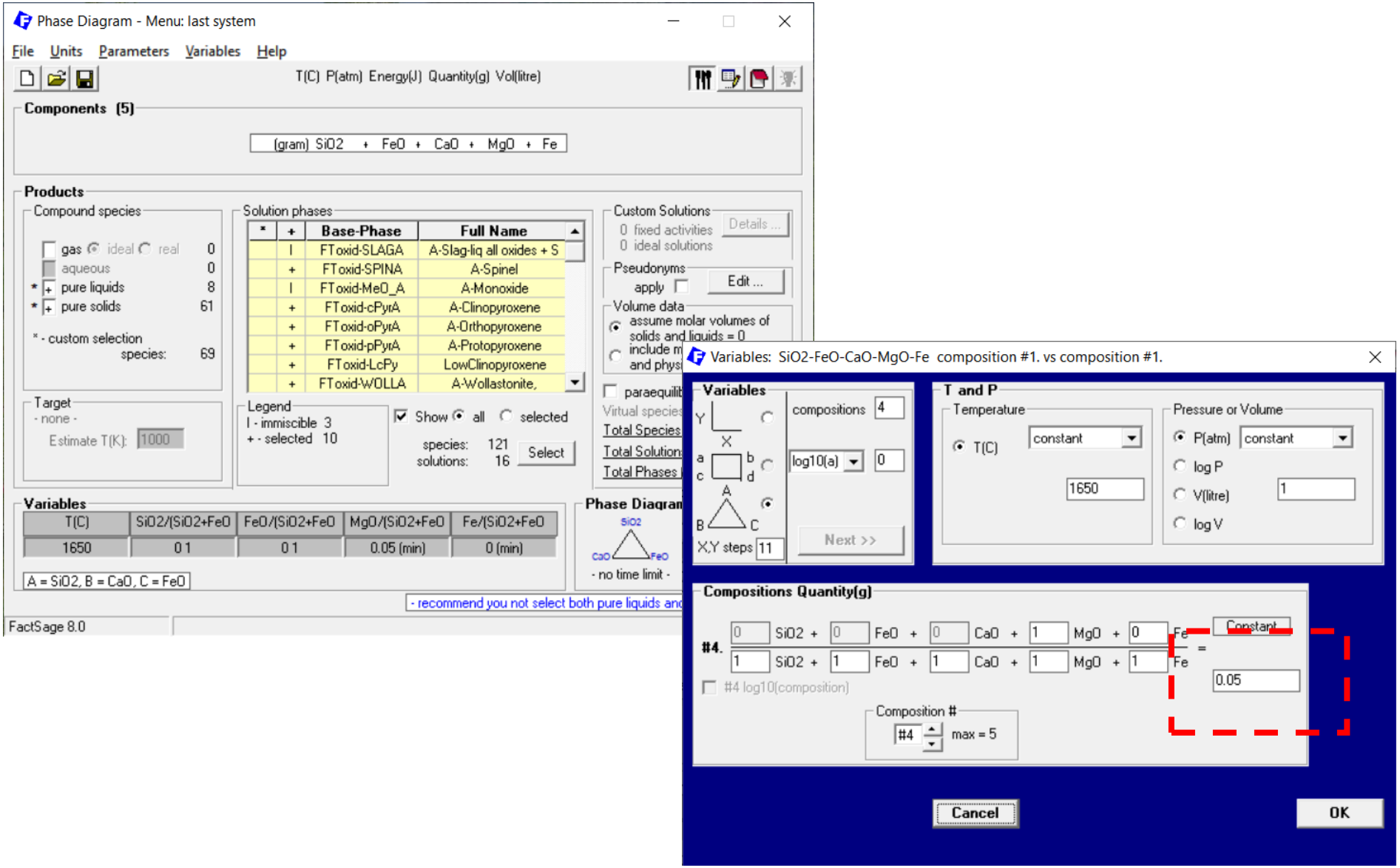
CaO-FetO-SiO2 system with Fe saturation



CaO-FetO-SiO2 system with Fe saturation



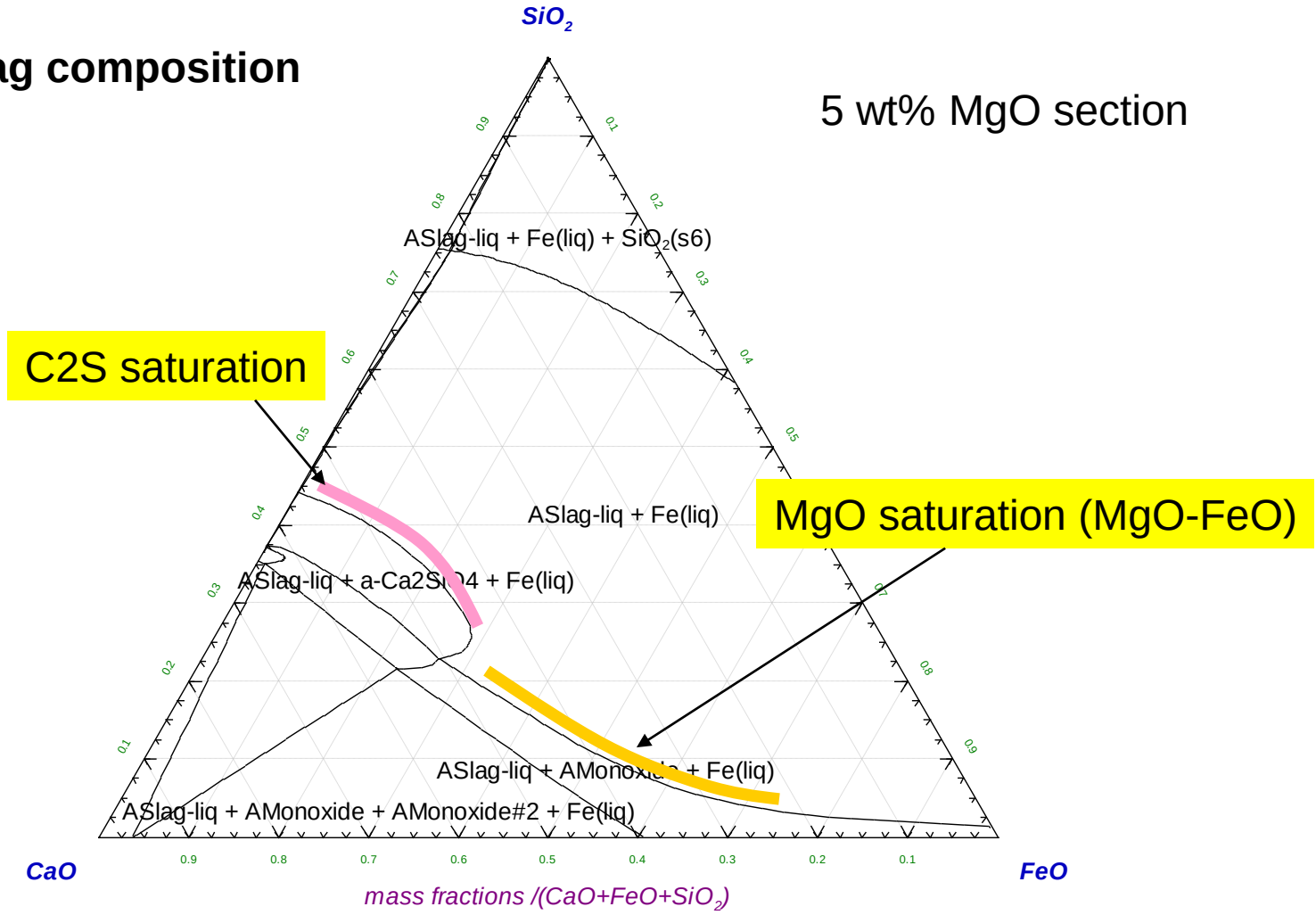
CaO-FetO-SiO2-5wt%MgO system with Fe saturation



CaO-FetO-SiO2-5wt%MgO system with Fe saturation

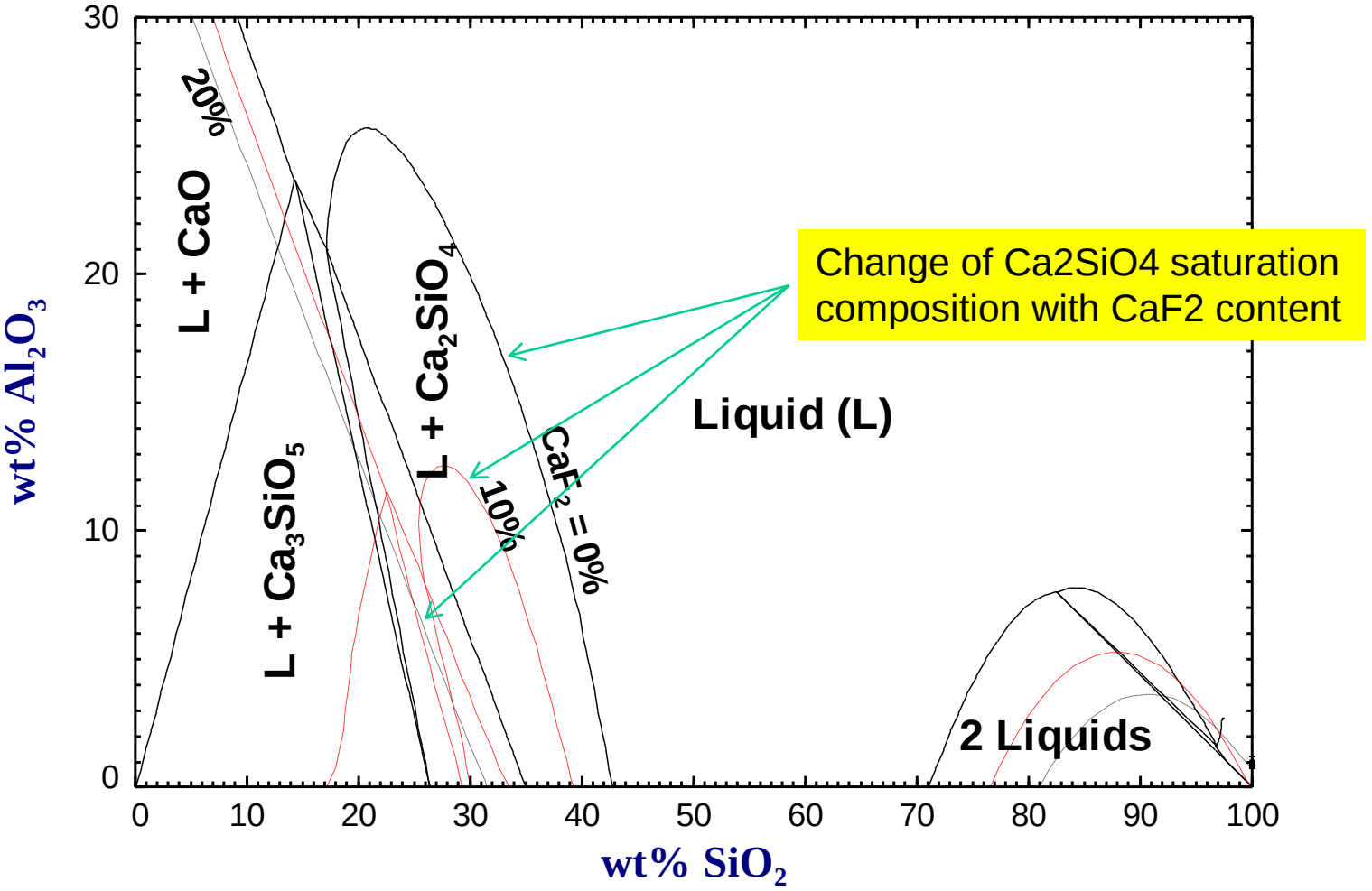
BOF slag composition

5 wt% MgO section



$CaO-SiO_2-Al_2O_3$ + F slags for refining flux

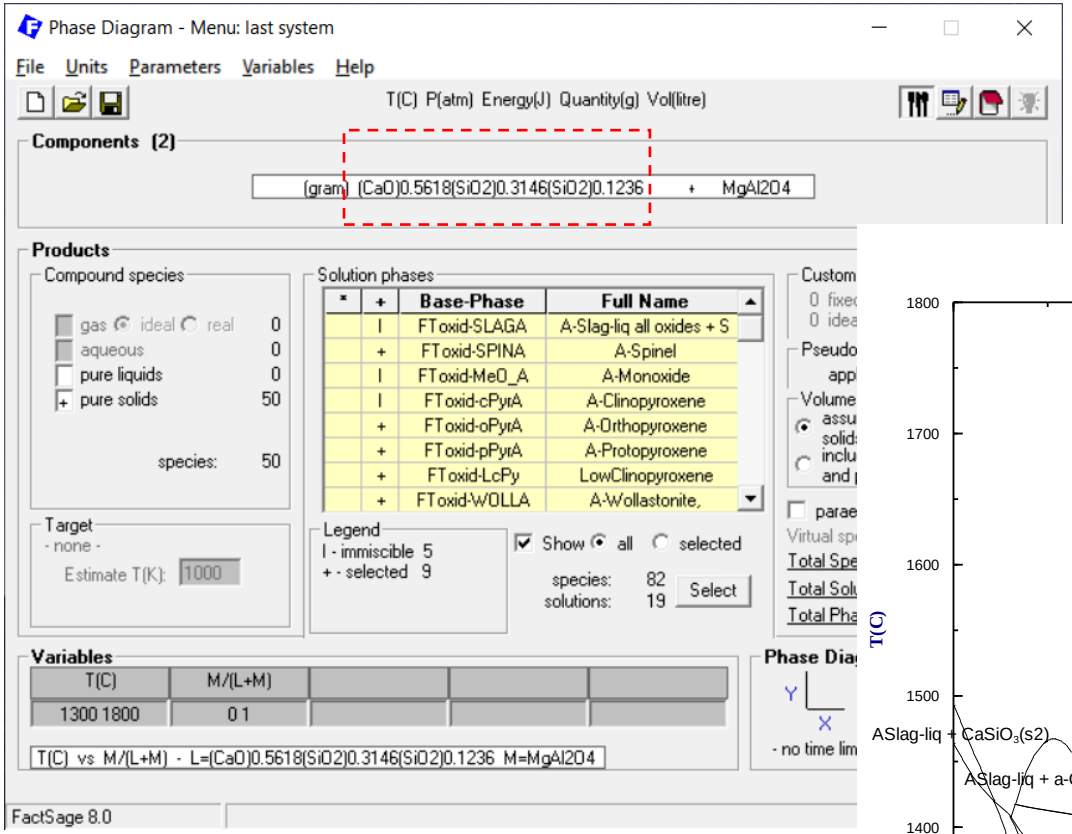
$CaO-Al_2O_3-SiO_2$ with various CaF_2 content at 1650°C.



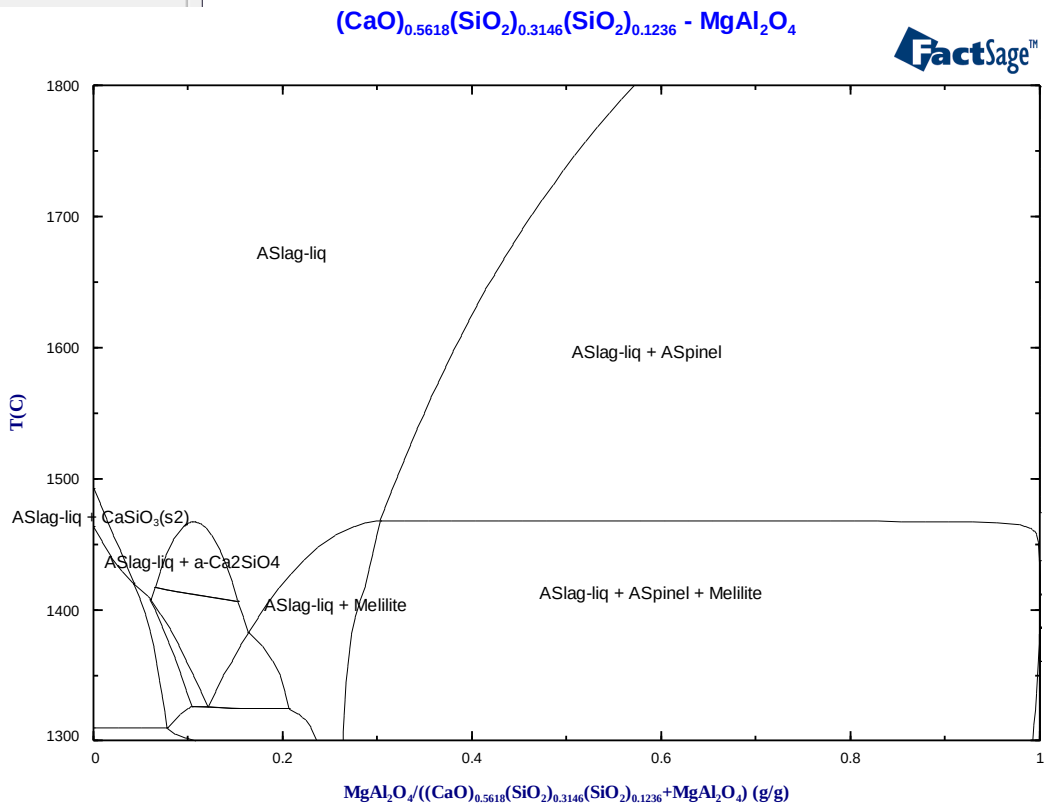
At 20% CaF_2: Slag can directly equilibrated with CaO (no Ca_2SiO_4)

CaO-Al2O2-SiO2 slag – MgAl2O4 refractory

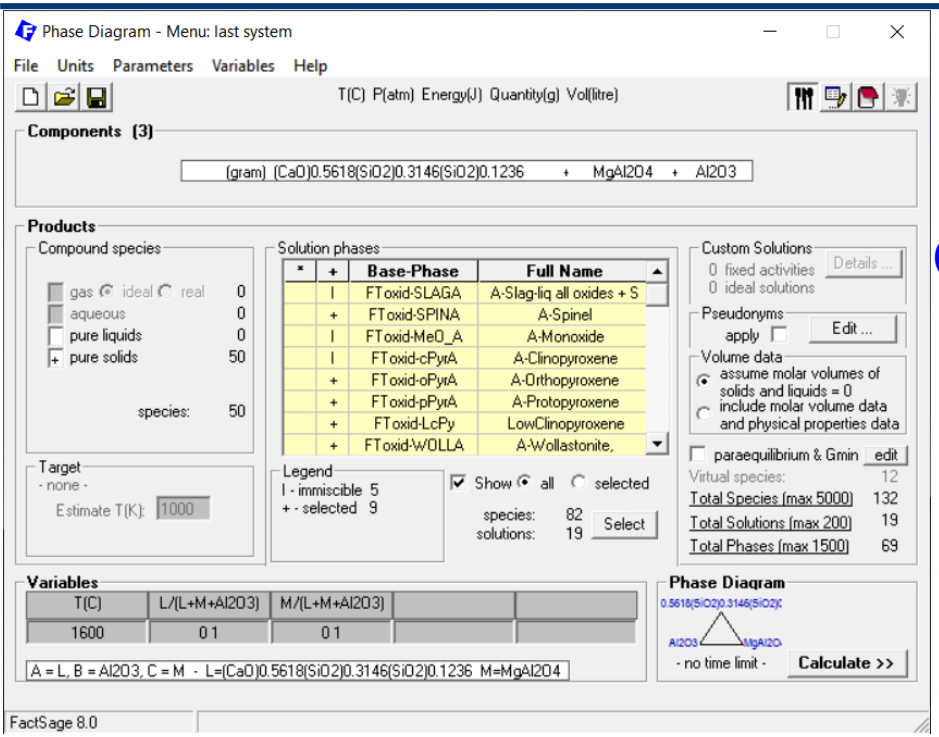
50%CaO-30%SiO2-20%Al2O3 slag → in mole: $(CaO)_{0.5618}(SiO2)_{0.3146}(Al2O3)_{0.1236}$
(Equilib or Phase Diagram's components are in molar base)



Dissolution of spinel inclusion into slag



CaO-Al2O2-SiO2 slag – MgAl2O4/Al2O3 refractories

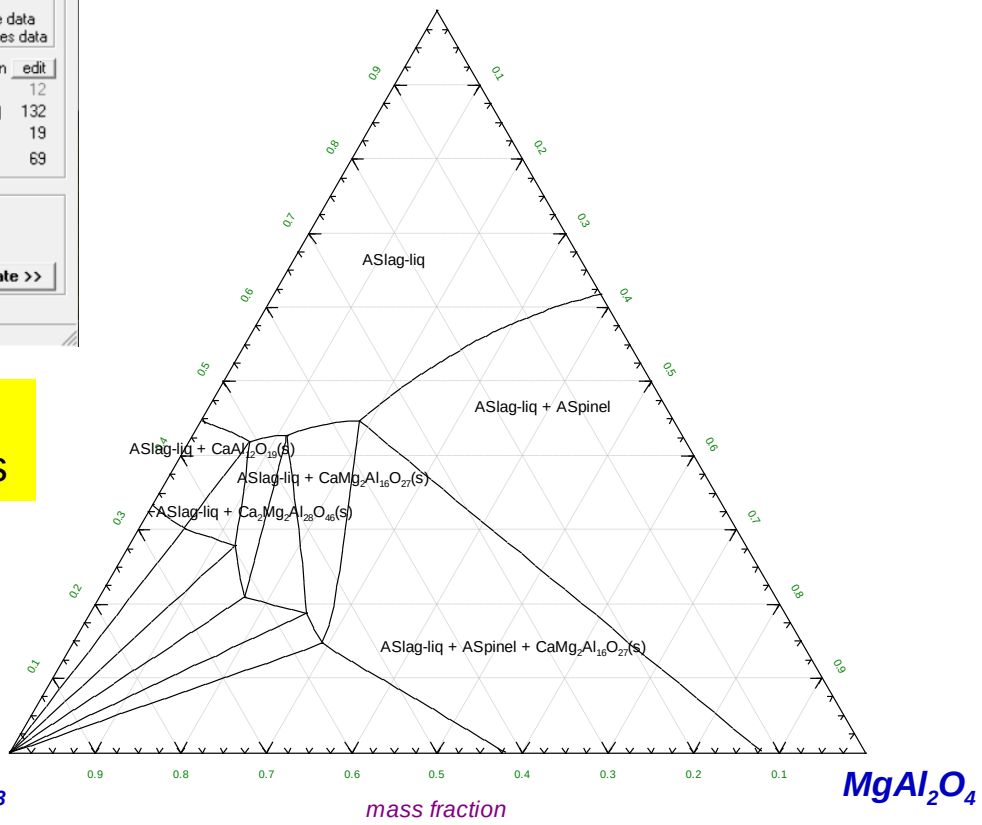


High Alumina (MgAl2O4-Al2O3)
Refractories dissolution into slags

$(CaO)_{0.5618}(SiO_2)_{0.3146}(SiO_2)_{0.1236}$ - $MgAl_2O_4$ - Al_2O_3

1600°C

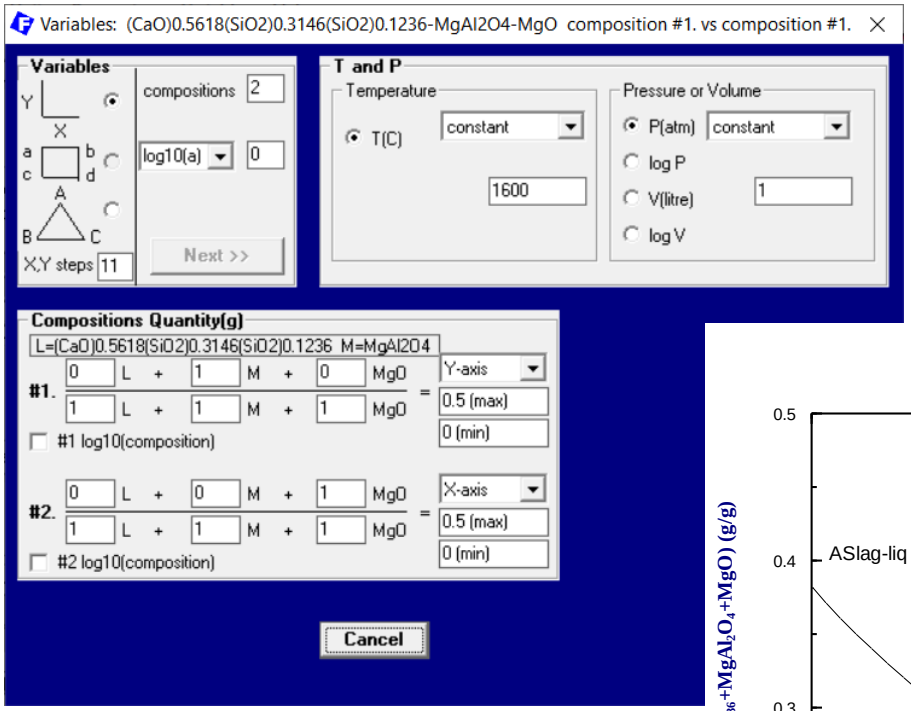
$(CaO)_{0.5618}(SiO_2)_{0.3146}(SiO_2)_{0.1236}$

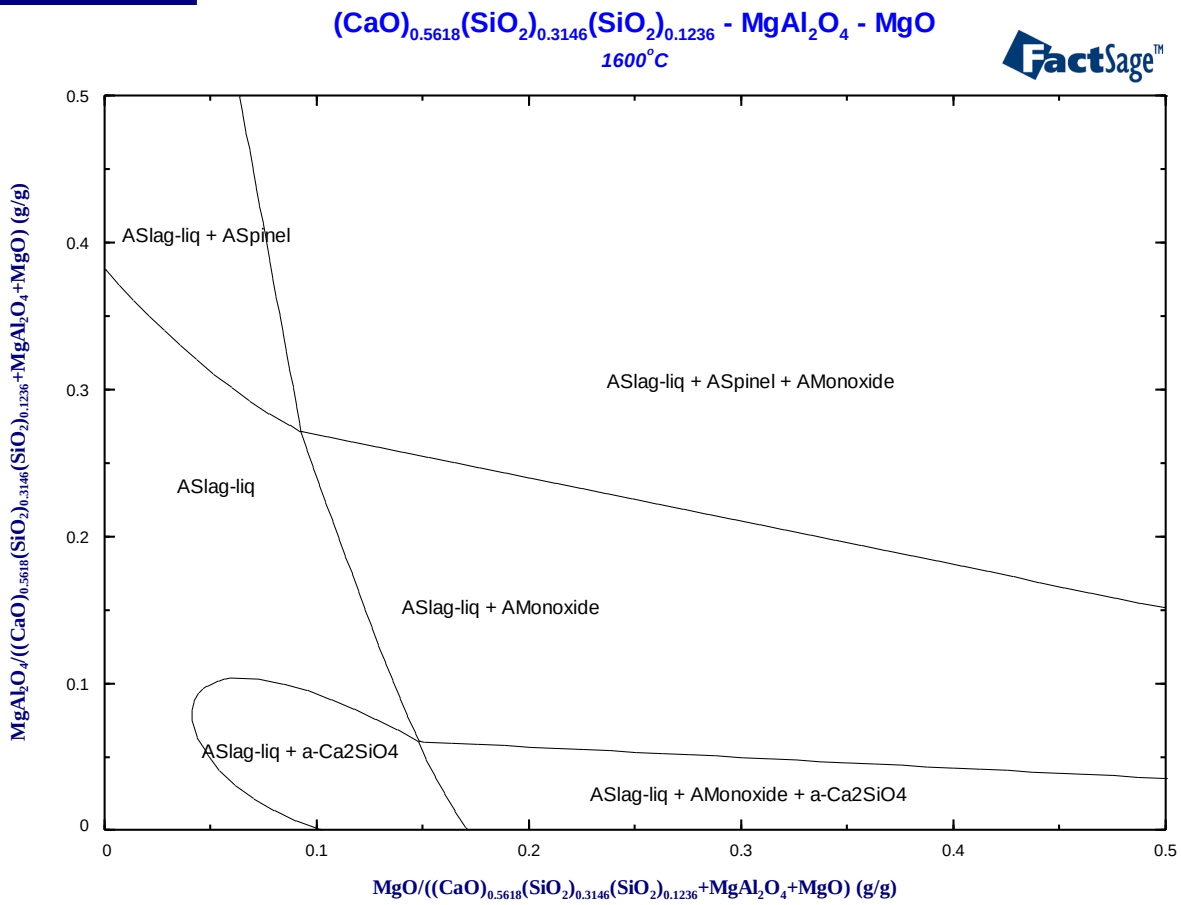


Al_2O_3 — $MgAl_2O_4$

mass fraction

CaO-Al2O2-SiO2 slag – MgAl2O4/MgO refractories



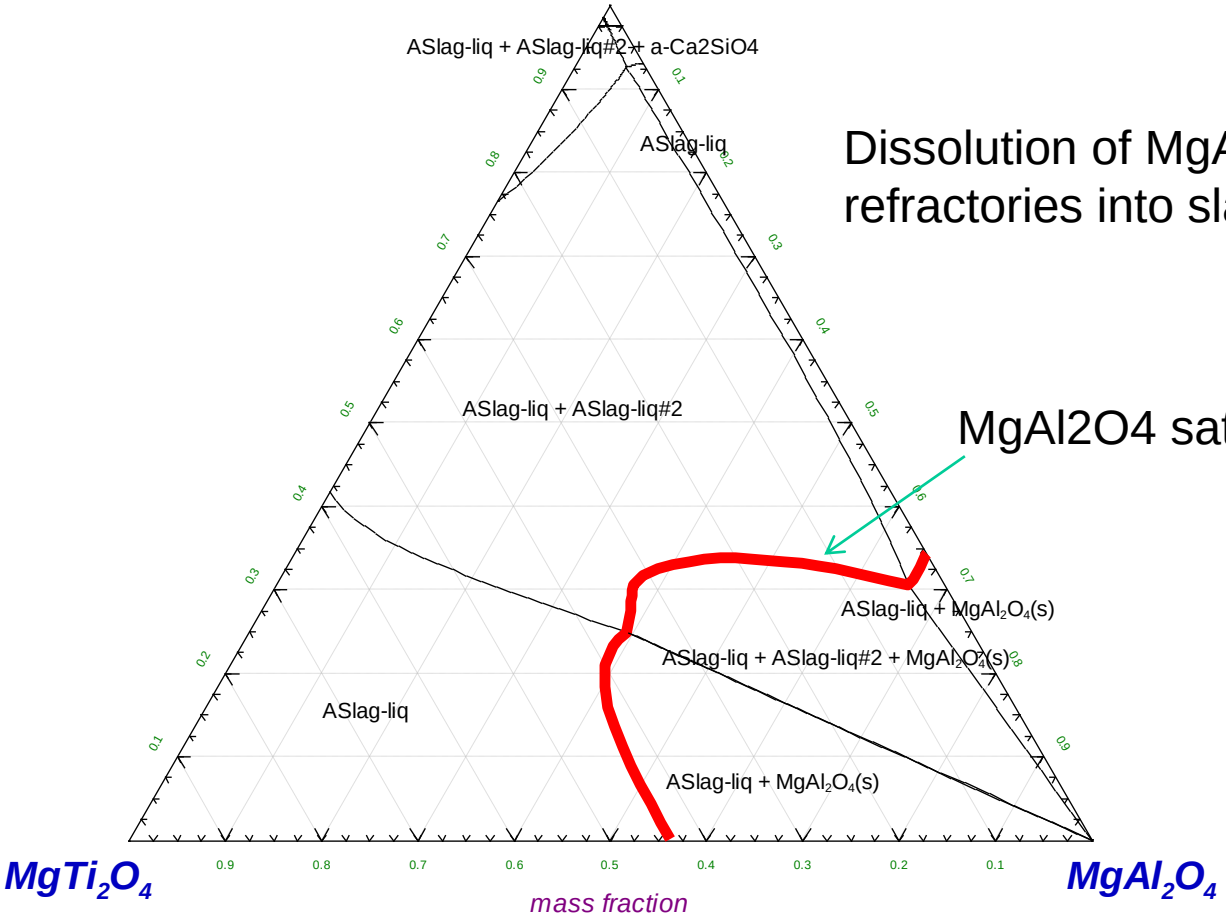


Phase diagram: Refractories design

$(CaO)_{0.535}(SiO_2)_{0.25}(Al_2O_3)_{0.05}(MgO)_{0.1}$ - $MgAl_2O_4$ - $MgTi_2O_4$ - Fe

1700°C, a(Fe(liq)) = 0.7943

$(CaO)_{0.535}(SiO_2)_{0.25}(Al_2O_3)_{0.05}(MgO)_{0.1}$

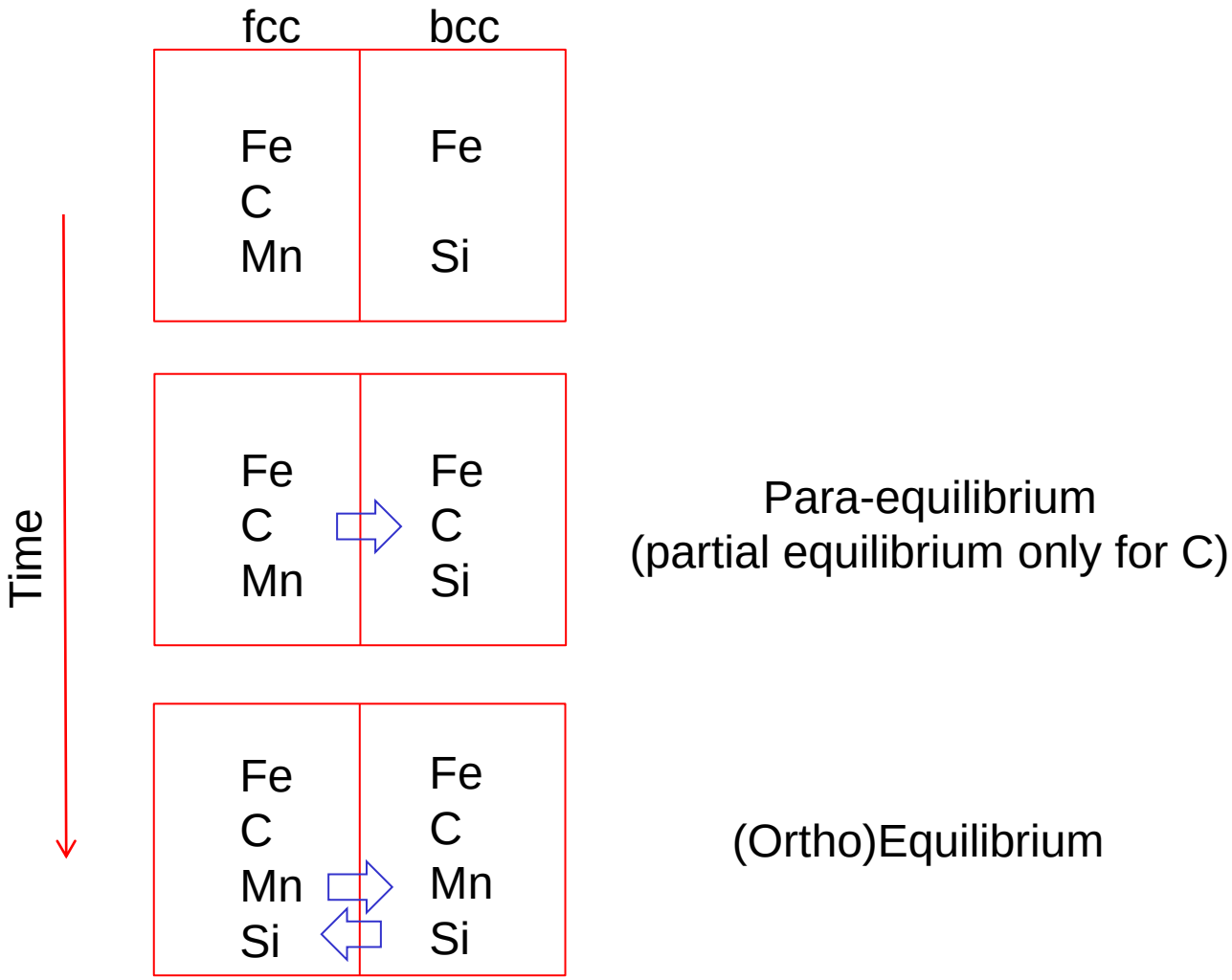


Dissolution of MgAl2O4/MgTi2O4 refractories into slag

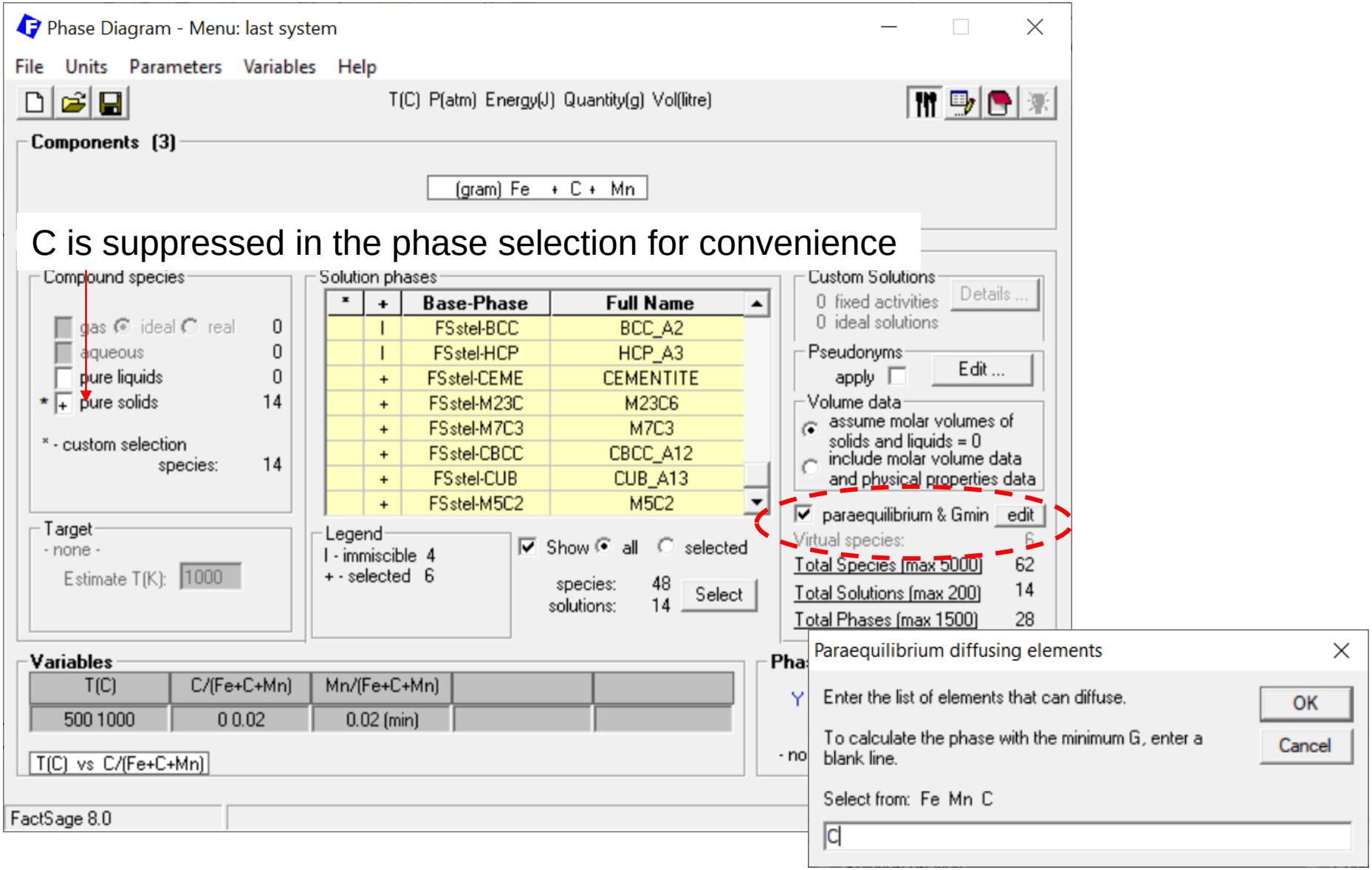
MgAl2O4 saturation line

Para-equilibrium (Partial equilibrium) vs Ortho-equilibrium (Fully equilibrium)

Diffusion of C is much faster than Mn or Si

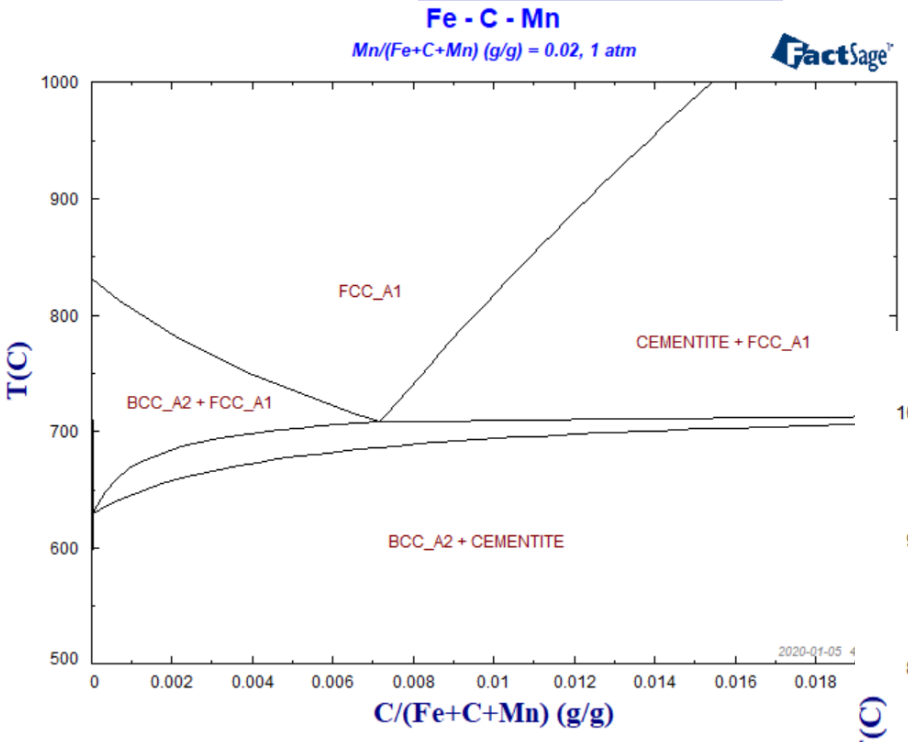


Para-equilibrium: Steel A3 temperature

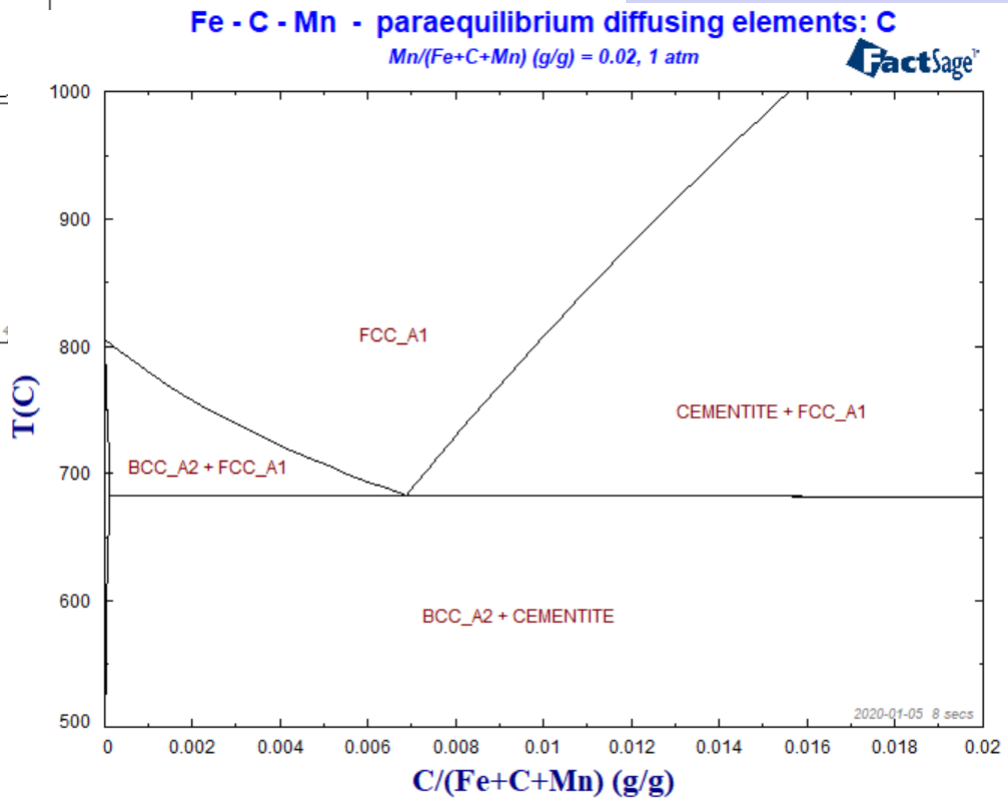


Para-equilibrium: Steel A3 temperature

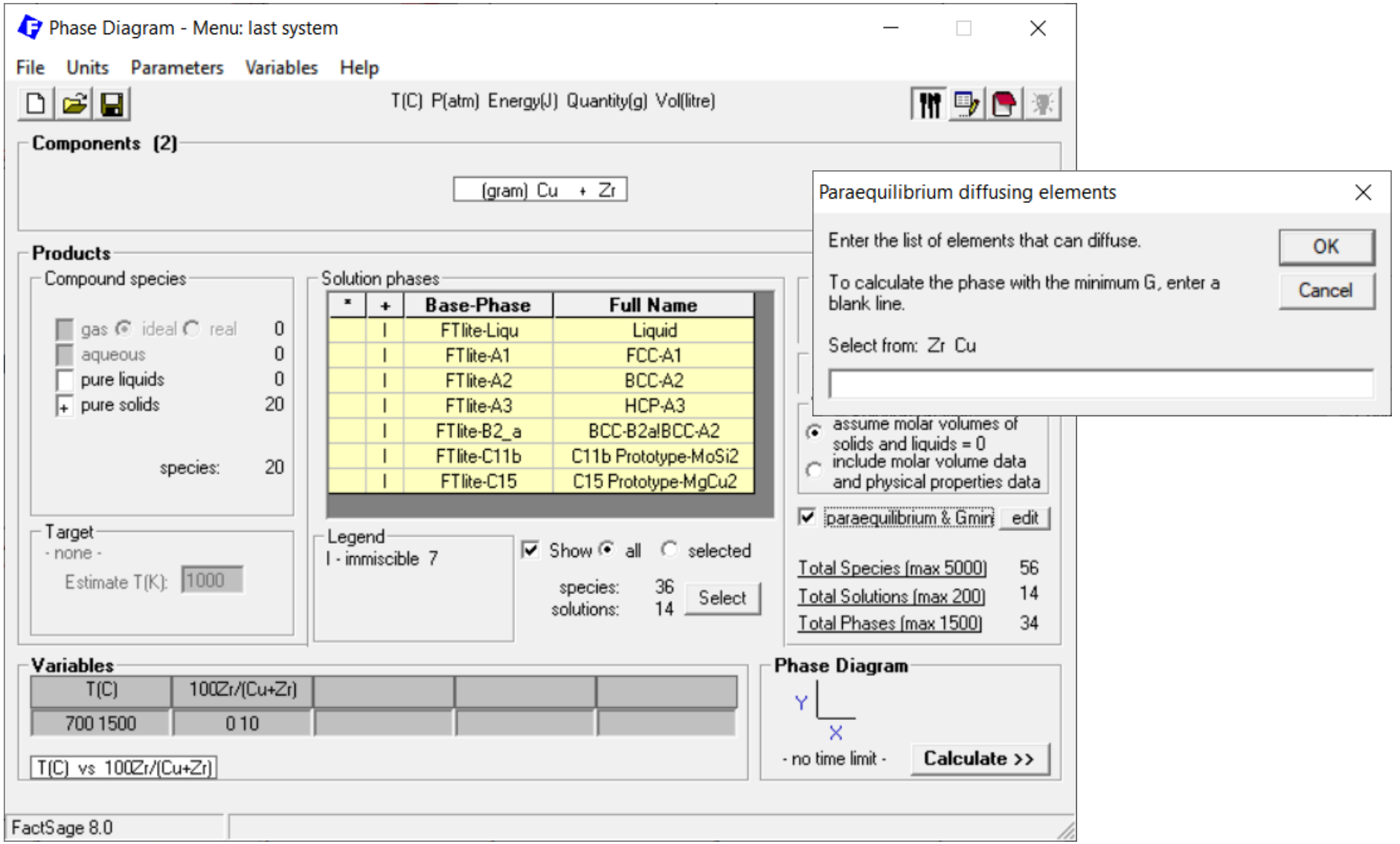
Full equilibrium



Para-equilibrium



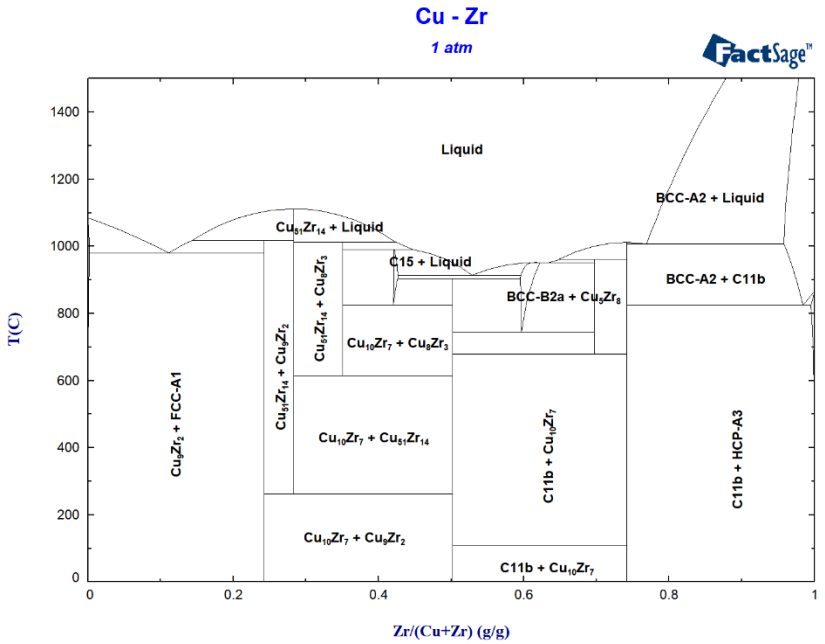
Para-equilibrium: Rapid solidification for amorphous metal



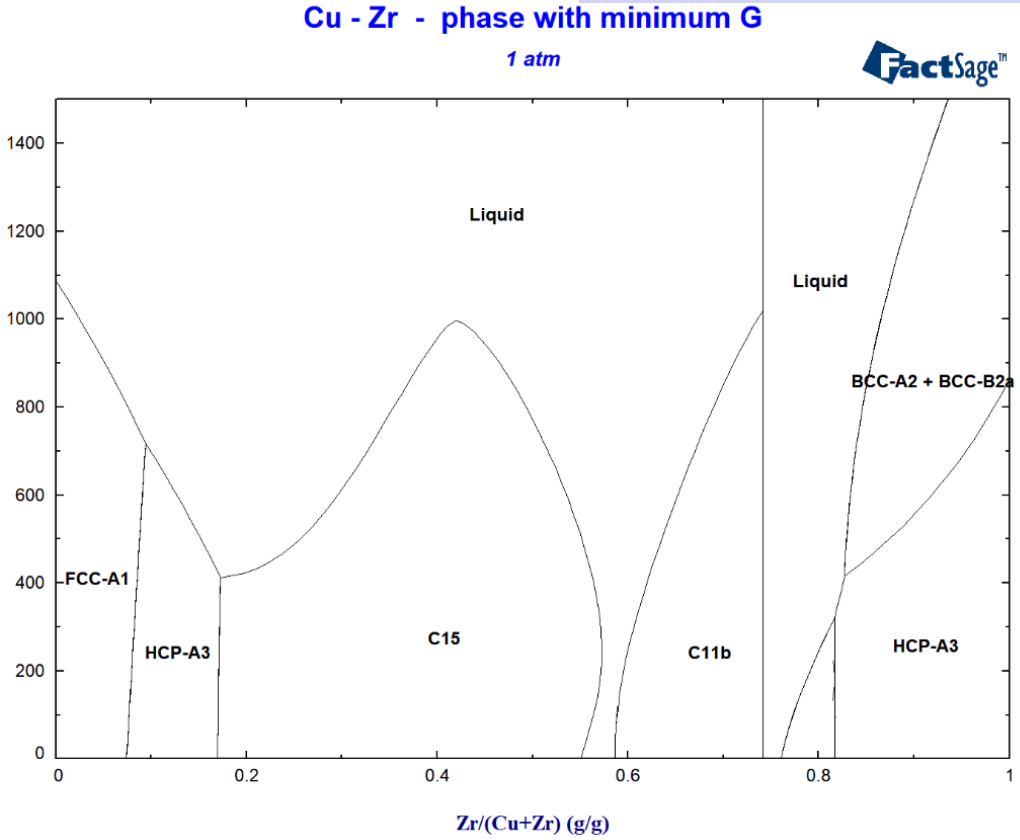
Blank → no diffusion of any element: this is what happens during rapid solidification

Para-equilibrium: Rapid solidification for amorphous metal

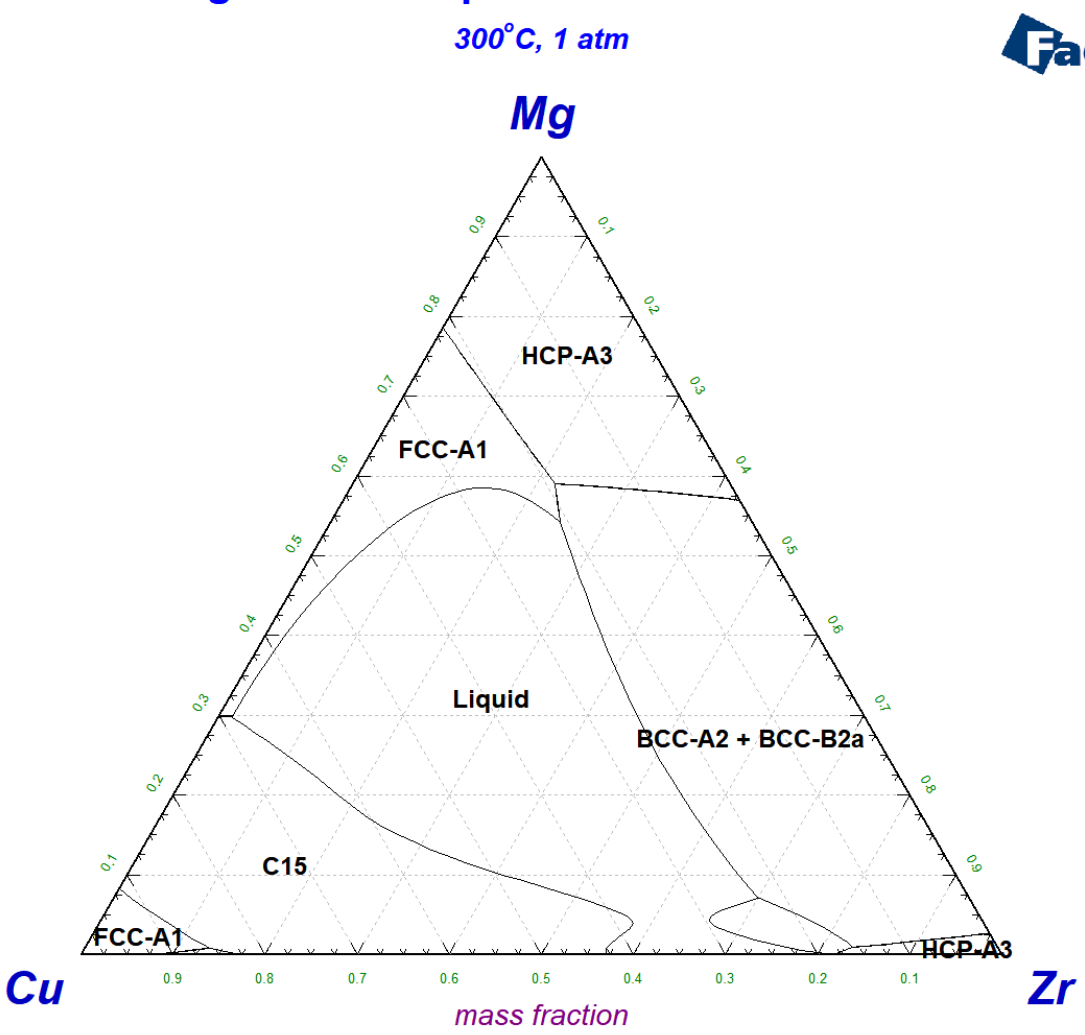
Full equilibrium



Paraequilibrium: Rapid solidification

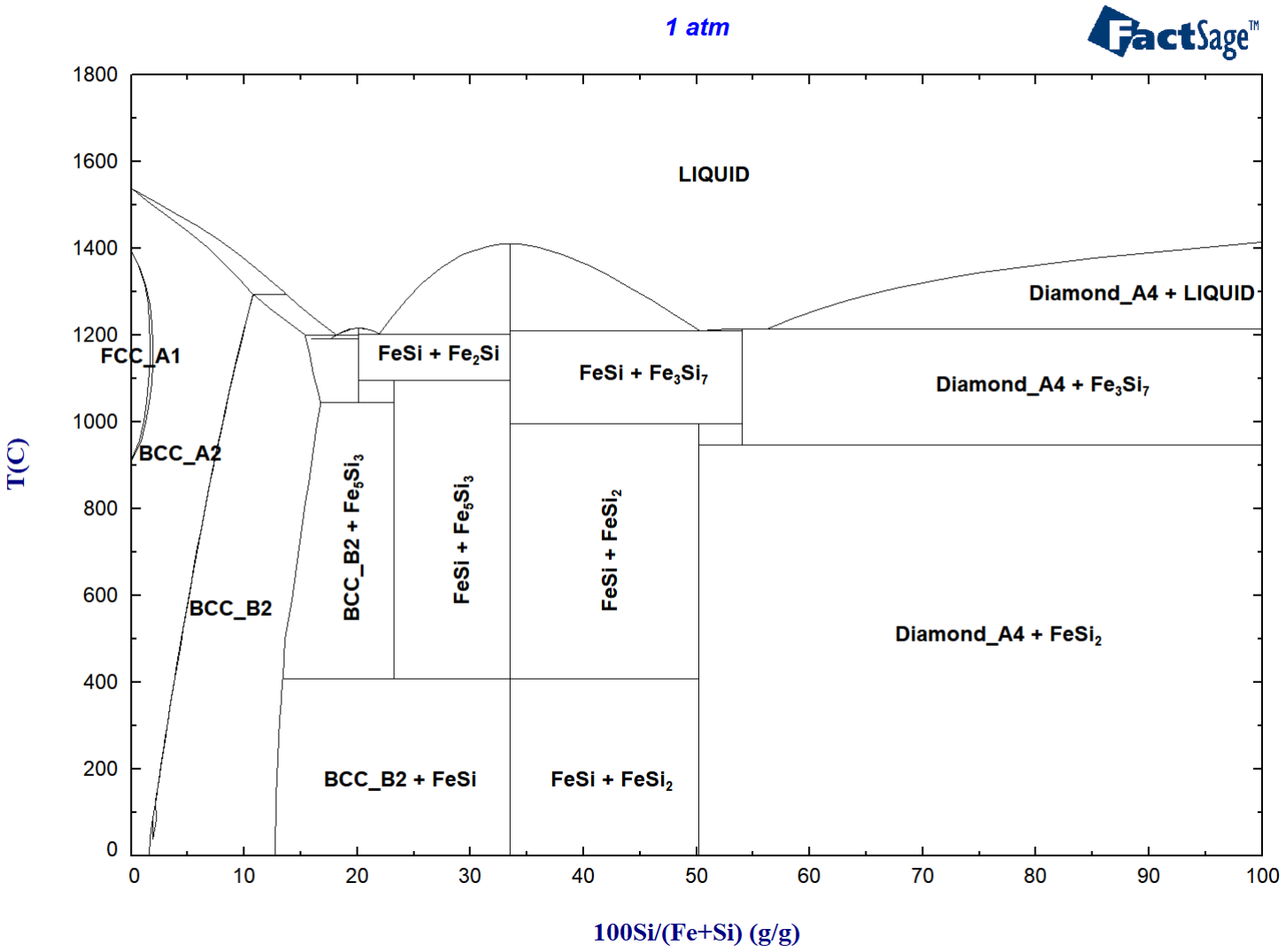


Para-equilibrium: Rapid solidification for amorphous metal



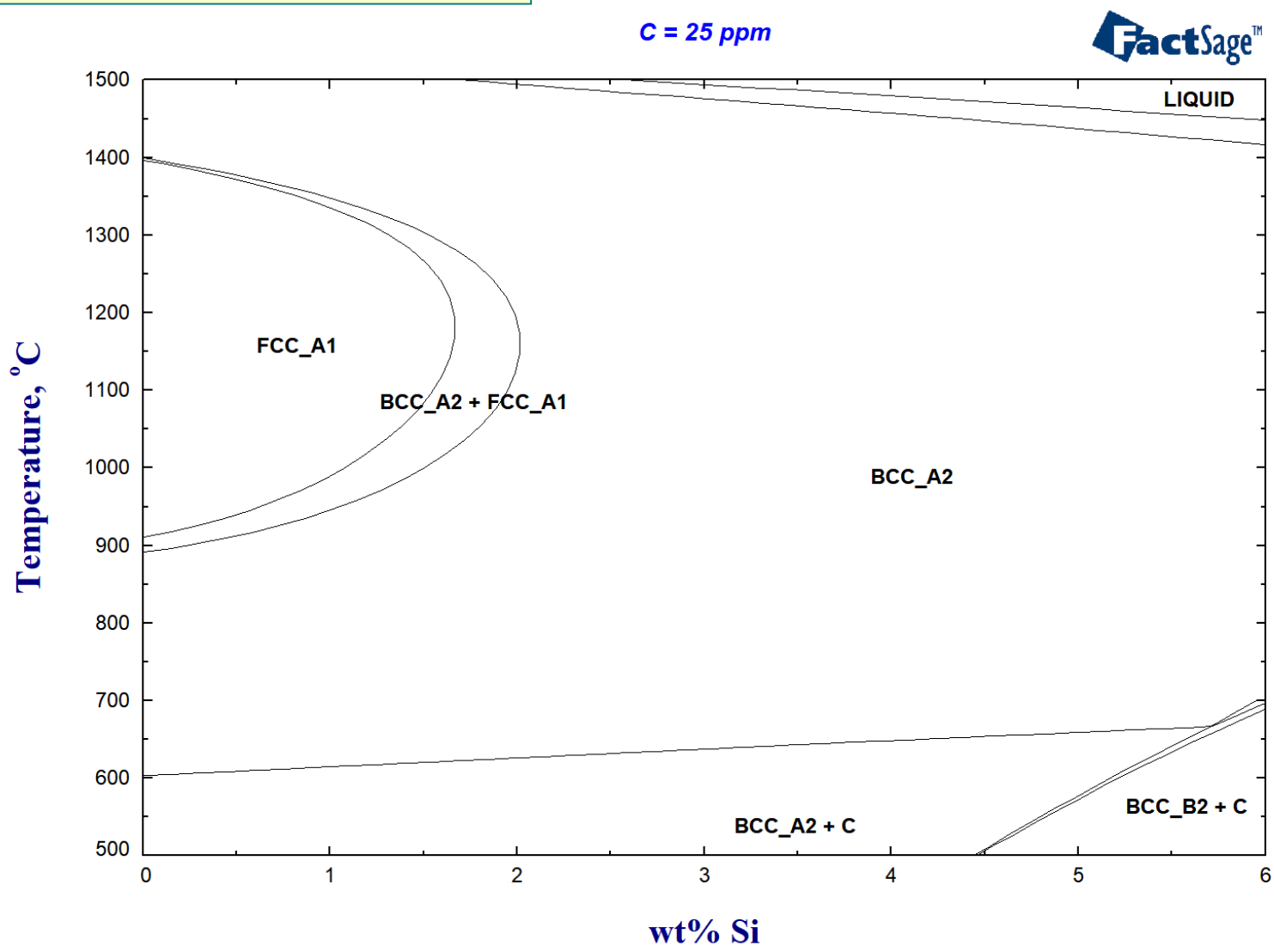
Alloy Design: Electric steel (Si-steel)

Phase diagram of Fe-Si system



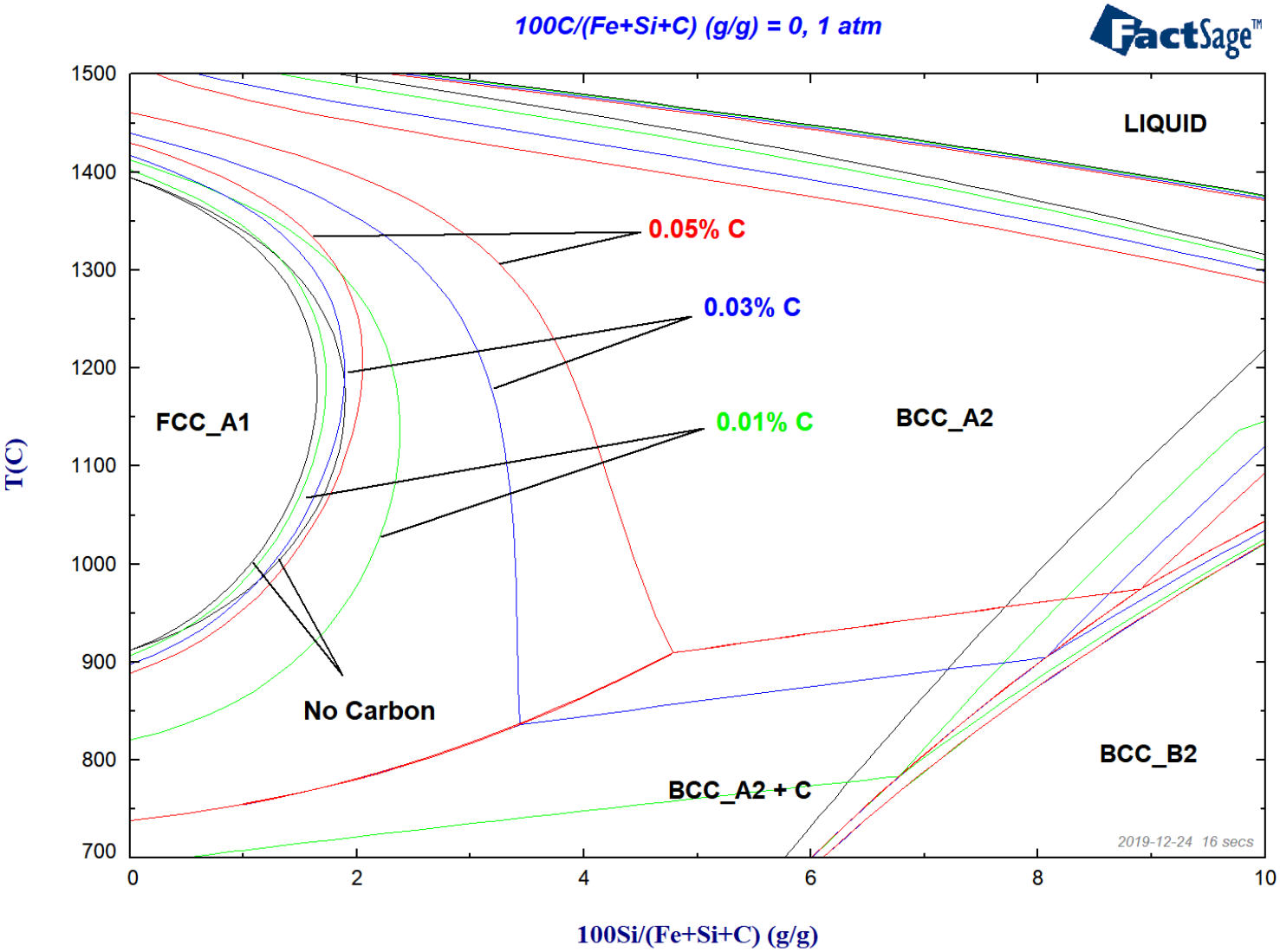
Alloy Design: Electric steel (Si-steel)

Alloy Design: Fe-Si + C



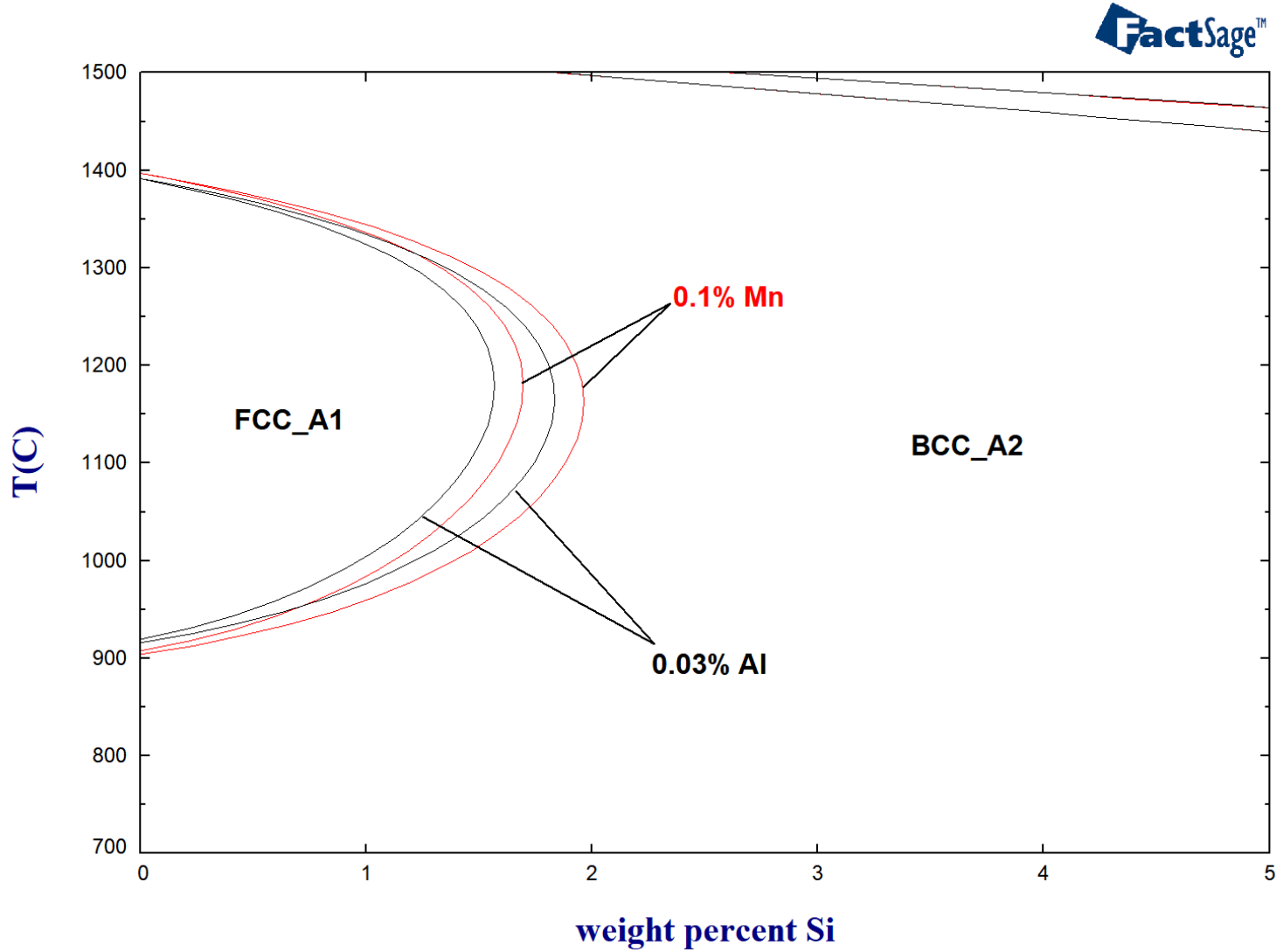
Alloy Design: Electric steel (Si-steel)

Alloy Design: Fe-Si + C

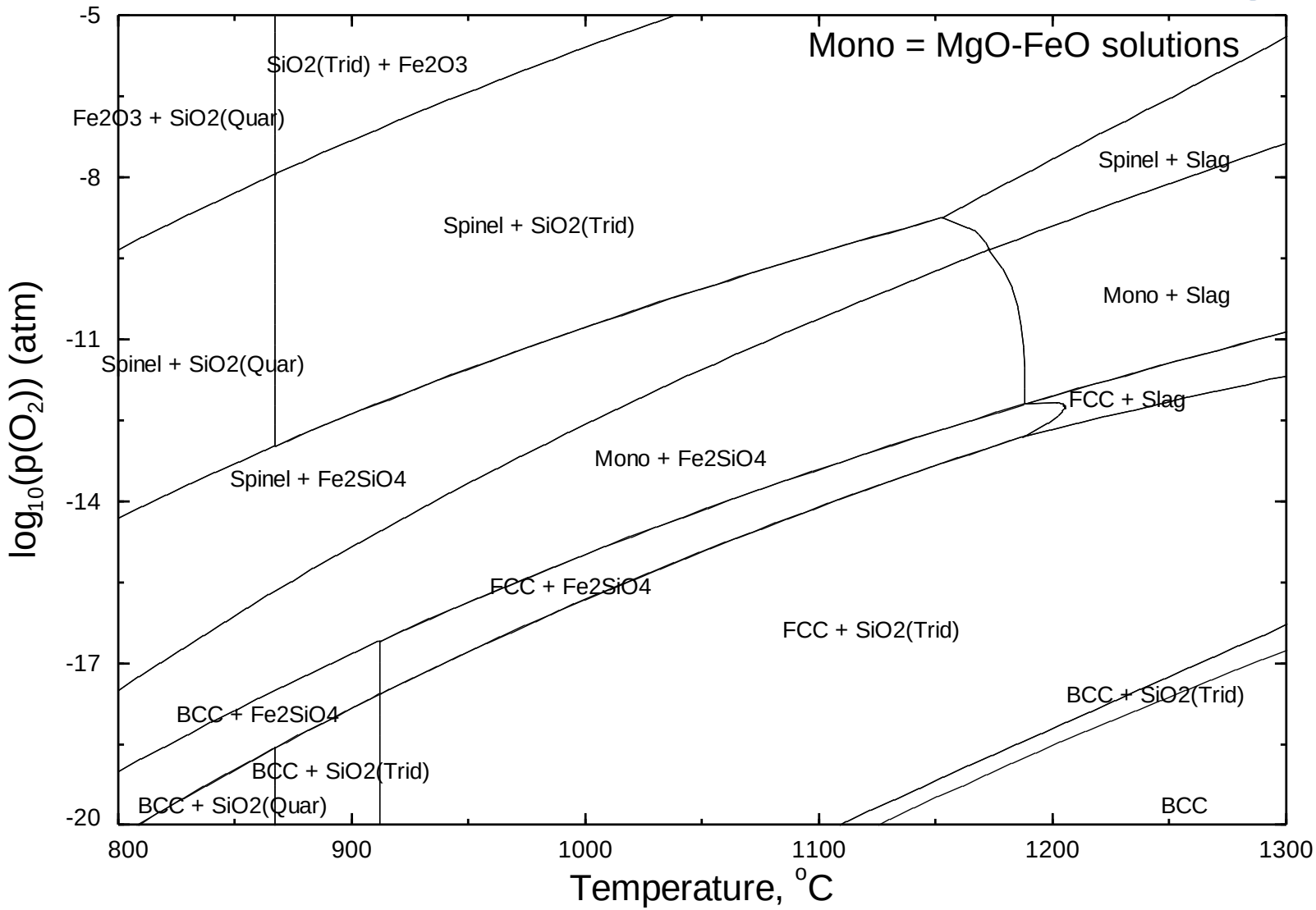


Alloy Design: Electric steel (Si-steel)

Alloy Design: Fe-Si + Al, Mn



Formation of base coating on the surface of a commercial Si steel



Thanks to
FactSage Steelmaking Consortium Members

Visit In-Ho Jung's research group website
http://in-ho-group.snu.ac.kr/