

# Application 4: Killing of steel in the ladle

Deoxidation of steel

Inclusion formation / composition in molten steels  
: Mn/Si/Ti steel

Inclusion stability diagram (phase diagram): Al/Ti steel

# Ex3-1. Deoxidation of steel (Ferromanganese)

Liquid Fe-1wt.%C-500 ppm O at 1600°C

**Data Search**

Databases - 2/19 compound databases, 2/19 solution databases

- Fact**: FactPS, FToxic, FTsalt, FTmisc, FTall, FTOxCN, FTfritz, FThelg, FTpulp, FTlite
- FactSage**: FSscop, FSlead, FSsite, FSstel, FSnobl, FSups, ELEM, FTdemo
- SGTE**: BINS, SGPS, SGTE, SGnobl, SGsold, SGnucl

compounds only, solutions only, no database

**Miscellaneous**: EXAM, SGTE#, SGTE+

Clear All, Select All, Add/Remove Data, RefreshDatabases

**F Menu - Equilib:**

File Units Parameters Help

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

**Reactants (3)**

(gram) 98.95 Fe + C + 0.05 O

**Products**

Compound species	Base-Phase	Full Name
gas	ideal	Fe-liq
aqueous		
pure liquids		
pure solids		
<input checked="" type="checkbox"/> suppress duplicates	<input type="button" value="apply"/>	
species:	3	

Solution species	Base-Phase	Full Name
FToxic-FeLQ		Fe-liq
FToxic-SLAGA		ASlag-liq all oxides + S
FToxic-SPINA		ASpinel
FToxic-MeO_A		AMonoxide

**Custom Solutions**: 0 fixed activities, 0 ideal solutions, 0 activity coefficients, Details...

**Pseudonyms**: apply, List...

include molar volumes

Total Species (max 1500) 18, Total Solutions (max 40) 5

**Final Conditions**: <A>, <B>, T(C), P(atm), Product H(J), 1600, 1, 10 steps, Table, 1 calculation

**Equilibrium**: normal, transitions only, open, Calculate >

FactSage 6.3

# Ex3-1. Deoxidation of steel (Ferromanganese)

F Results - Equilib 1600 C

Output Edit Show Pages

Save or Print T(C) P(atm) Energy(J) Mass(g) Vol(litre)

Plot Equilib Results file Stream File Recycle all streams ... Save stream file Stream file properties ... Summary of streams Directory (C:\FactSage\ ...) Format Fact-XML Fact-Optimal Fact-Function-Builder wt.% C 2 wt.% O Refresh ...

System component Mole fraction Mass fraction

Fe	0.95351	0.98950
O	1.6818E-03	5.0000E-04
C	4.4805E-02	1.0000E-02

+ 0 gram AMonoxide  
(1600 C, 1 atm, a=0.15453)  
( 95.355 wt.% FeO  
+ 4.6453 wt.% Fe2O3

+ 0 gram ASlag-liq#1  
(1600 C, 1 atm, a=0.10522)  
( 92.358 wt.% FeO  
+ 7.6419 wt.% Fe2O3

+ 0 gram ASlag-liq#2  
(1600 C, 1 atm, a=0.10522)  
( 92.358 wt.% FeO  
+ 7.6419 wt.% Fe2O3

FactSage 6.3

Save gas phase ...  
Save pure liquids ...  
Save aqueous ...  
Save pure solids ...  
Save solutions ALL solutions  
FTmisc-FeLQ Fe-liq  
FToxid-SLAGA#1 ASlag-liq  
FToxid-SLAGA#2 ASlag-liq  
FToxid-SPINA ASpinel  
FToxid-MeO\_A AMonoxide

Save as stream

100.00 gram Fe-liq  
(100.00 gram, 1.8583 mol)  
(1600 C, 1 atm, a=1.0000)  
( 98.950 wt.% Fe  
+ 1.0000 wt.% C  
+ 5.0000E-02 wt.% O

System component Mole fraction Mass fraction

Fe	0.95351	0.98950
O	1.6818E-03	5.0000E-04
C	4.4805E-02	1.0000E-02

# Ex3-1. Deoxidation of steel (Ferromanganese)

**F Reactants - Equilib**

File Edit Table Units Data Search Help

Add a new Reactant Ctrl+R (atm) Energy(J) Mass(g) Vol(litre)

Mixtures and Streams

- Import a mixture
- Import a stream (or single-line mixture)
- Ferromanganese All solutions stream
- liquidFe-C-O\_1600C All solutions stream
- Edit a mixture or stream
- Directory (C:\FactSage\ ...)

Re-order the reactants

Export list of reactants

Import list of reactants

Clear Example

**F Menu - Equilib: Deoxidation of steel (Ferromanganese)**

File Units Parameters Help

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

**Reactants (3)**

(gram) <100-A> [liquidFe-C-O\_1600C] + <0.65A> Mn + <0.35A> Fe

**Products**

Compound species	Solution species
gas <input checked="" type="radio"/> ideal <input type="radio"/> real 0	* + Base-Phase Full Name
aqueous 0	+ FTmisc-FeLQ Fe-liq
pure liquids 0	+ FTmisc-BCCS bcc
+ pure solids 7	+ FTmisc-FCCS fcc
<input checked="" type="checkbox"/> suppress duplicates <input type="button" value="apply"/>	I FT oxid-SLAGA ASlag-liq all oxides + S
species: 7	+ FToxid-SPINB BSpinel
	+ FToxid-MeO_B BMonoxyde
	+ FToxid-CORU M203(Corundum)
	+ FToxid-TSpi Tetragonal-Spinel

**Custom Solutions**

- 0 fixed activities
- 0 ideal solutions
- 0 activity coefficients

**Pseudonyms**

apply  List ...

include molar volumes

Total Species (max 1500) 70  
Total Solutions (max 40) 10

**Final Conditions**

<A>	<B>	T(C)	P(atm)	Product H(J)
0 10 0.05		1600	1	
10 steps	<input type="checkbox"/> Table	201 calculations		

**Equilibrium**

- normal
- normal + transitions
- transitions only
- open

**Calculate >>**

FactSage 6.3 Compound: 3/19 databases Solution: 3/19 databases

Next >>

FactSage 6.3 C:\FactSage\EquiEx3-1.DAT

# Ex3-1. Deoxidation of steel (Ferromanganese)

**F Results - Equilib A=0 (page 1/201)**

**Output Edit Show Pages**

**Save or Print**

**Plot**

**Equilib Results file**

**Stream File**

**Format**

**Fact-XML**

**Fact-Optimal**

**Fact-Function-Builder**

**Refresh ...**

**System component Mole fraction Mass**

- Fe 0.95351
- O 1.6818E-03
- C 4.4805E-02

+ 0 gram BCC\_A2  
 (1600 C, 1 atm, a=0.92889)  
 ( 0.69434 wt.% Fe1C3  
 + 99.306 wt.% Fe1Va3

+ 0 gram FCC\_A1  
 (1600 C, 1 atm, a=0.92679)  
 ( 2.1931 wt.% Fe1Cl  
 + 97.807 wt.% Fe1Val

+ 0 gram CUB\_A13  
 (1600 C, 1 atm, a=0.71912)  
 ( 0.20013 wt.% FeC

**T(C) P(atm) Energy(J) Mass(g) Vol(litre)**

**Plot Results ...**

**Repeat Plot - log10(gram) vs Alpha ...**

**A=1.1 | A=1.15 | A=1.2 | A=0.45 | A=0.55 | A=0.5 | A=0.4 | A=0.35 | A=0.3 | A=0.25 | A=0.2 | A=0.15 | A=0.1 | A=0.05 | A=0.02 | A=0.01**

**F Plot: log10(gram) vs Alpha**

**Axes Variables**

**Y-axis**: gram

**X-axis**: Alpha

**Graph**

**Species Selection - EQUILIB Results: log10(gram) vs Alpha**

#	Species	Mole (min)	Mole (max)	Fraction (min)	Fraction (max)	Activity (min)	Activity (max)
33	Fe0(MONO)	0	7.3571E-05	2.0296E-02	1.	2.9605E-02	0.154038
34	Mn0(MONO)	0	2.2465E-03	0	0.979704	0	0.979858
35	Fe1(misc)	1.7719	1.8345	0.901692	0.953513	0.899227	0.945375
36	C(FeLQ)	8.3259E-02	8.3259E-02	4.0924E-02	4.4805E-02	3.6592E-02	4.5856E-02
37	Mn(FeLQ)	0	0.115923	0	5.6978E-02	0	5.2637E-02
38	O(FeLQ)	6.8732E-04	3.1251E-03	3.3793E-04	1.6818E-03	3.1977E-06	1.5826E-05
39	Mn0(FeLQ)	0	1.3862E-04	0	6.8132E-05	0	6.7946E-05
<b>FToxic: SLAG</b>							
40	Fe0(SLAGA#1)	0	0	5.4309E-02	0.96411	3.7818E-02	0.19677
41	Fe2O3(SLAGA#1)	0	0	3.0027E-04	3.5890E-02	1.1103E-07	1.4877E-05
42	Mn0(SLAGA#1)	0	0	0	0.943529	0	0.657311
43	Mn2O3(SLAGA#1)	0	0	0	3.1769E-03	0	1.8248E-05
<b>FToxic: SLAG</b>							
44	Fe0(SLAGA#2)	0	0	5.4309E-02	0.96411	3.7818E-02	0.19677
45	Fe2O3(SLAGA#2)	0	0	3.0027E-04	3.5890E-02	1.1103E-07	1.4877E-05
46	Mn0(SLAGA#2)	0	0	0	0.943529	0	0.657311
47	Mn2O3(SLAGA#2)	0	0	0	3.1769E-03	0	1.8248E-05

**Clear**

**source**

**Mass**

**Order**

**Select Top**

**1 species selected**

**201 pages**

**Select ...**

**OK**

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

**Axes: log10(gram) vs Alpha**

**Y-variable**: log10(gram)

**X-variable**: Alpha

**Swap Axes**

**Y-axis**: log10(gram)

**X-axis**: Alpha

**maximum**: 1.3

**minimum**: -3

**tick every**: 0.1

**maximum**: 10

**minimum**: 0

**tick every**: 1

**Axes**

**Species**: log10(gram) vs Alpha

**1 selected**

**Select**

**Axes**

**Repeat**

**Plot >>**

**Labels**: size: 9 no: 4

**Display**: color, reactants, file name

**Reactants**: chemical, integer #, none

**Viewer**: full screen, Figure

**File name**: color, full screen, Figure

**FactSage 6.3**

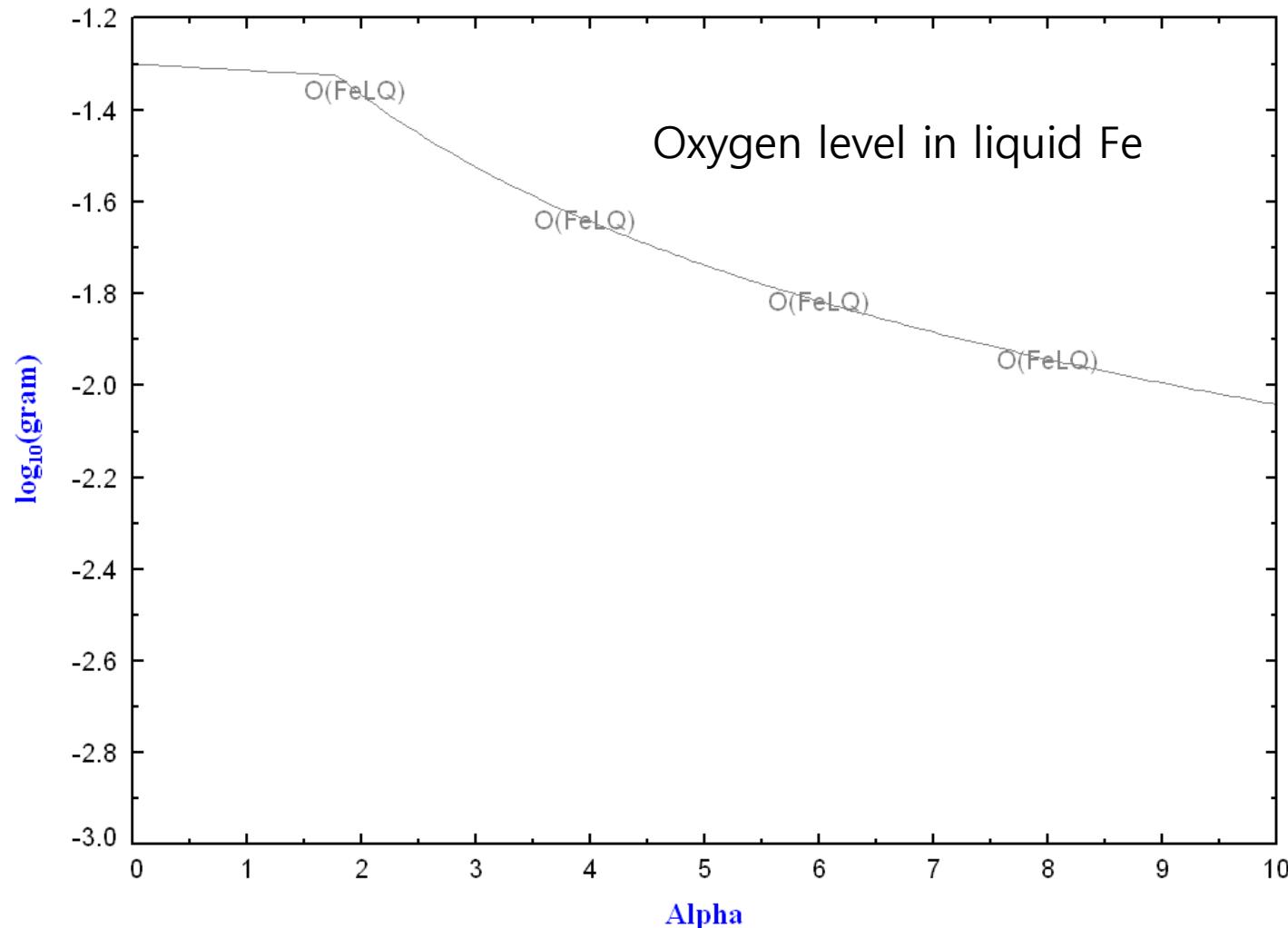
**C:\FactSage\Equi0.res**

**6Feb13**

**201 sets**

# Ex3-1. Deoxidation of steel (Ferromanganese)

<100-A> [liquidFe-C-O\_1600C] + <A> [Ferromanganese]

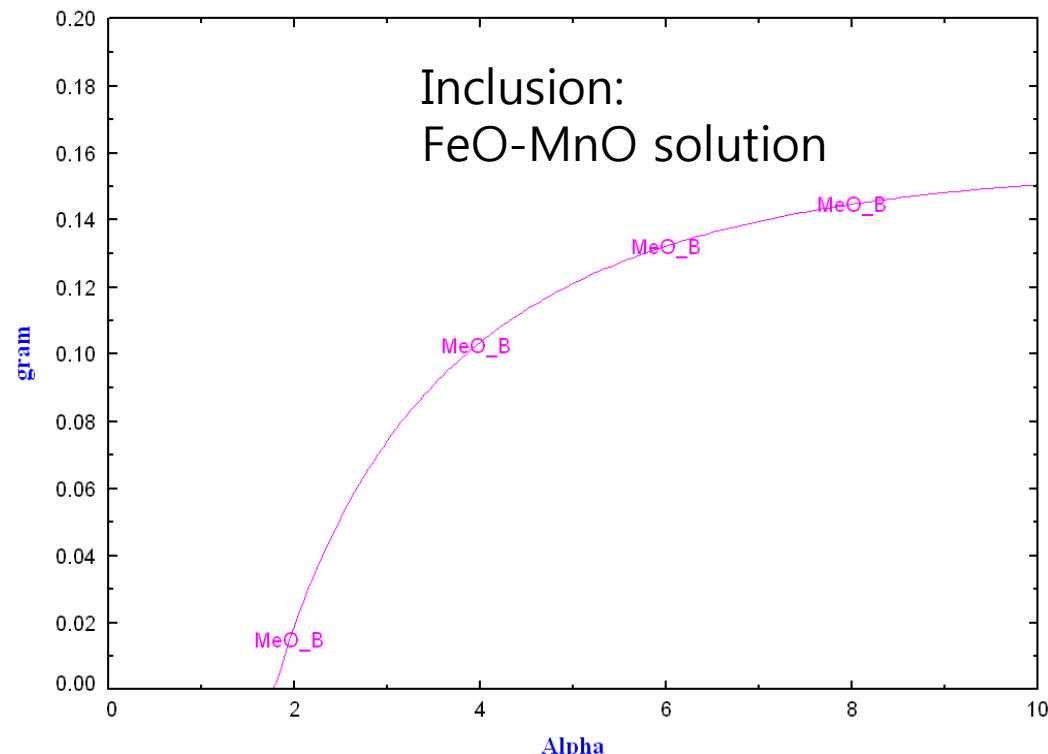


# Ex3-1. Deoxidation of steel (Ferromanganese)

**F Species Selection - EQUILIB Results: log10(gram) vs Alpha**

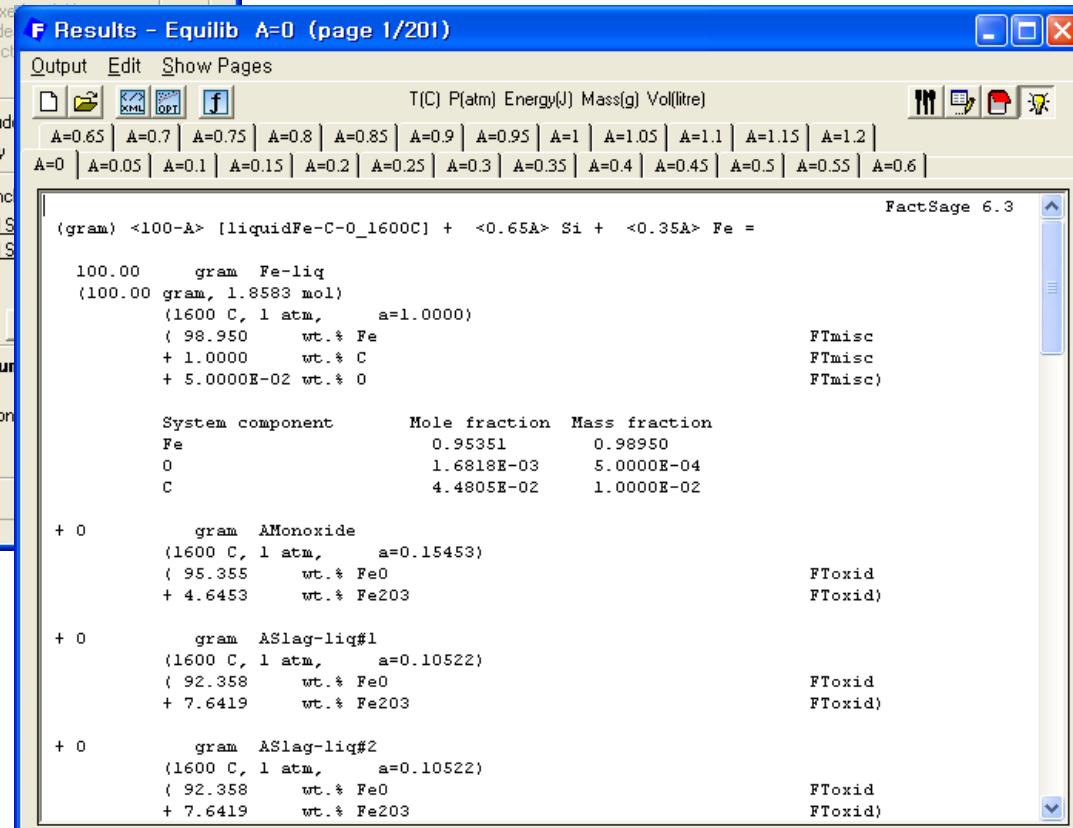
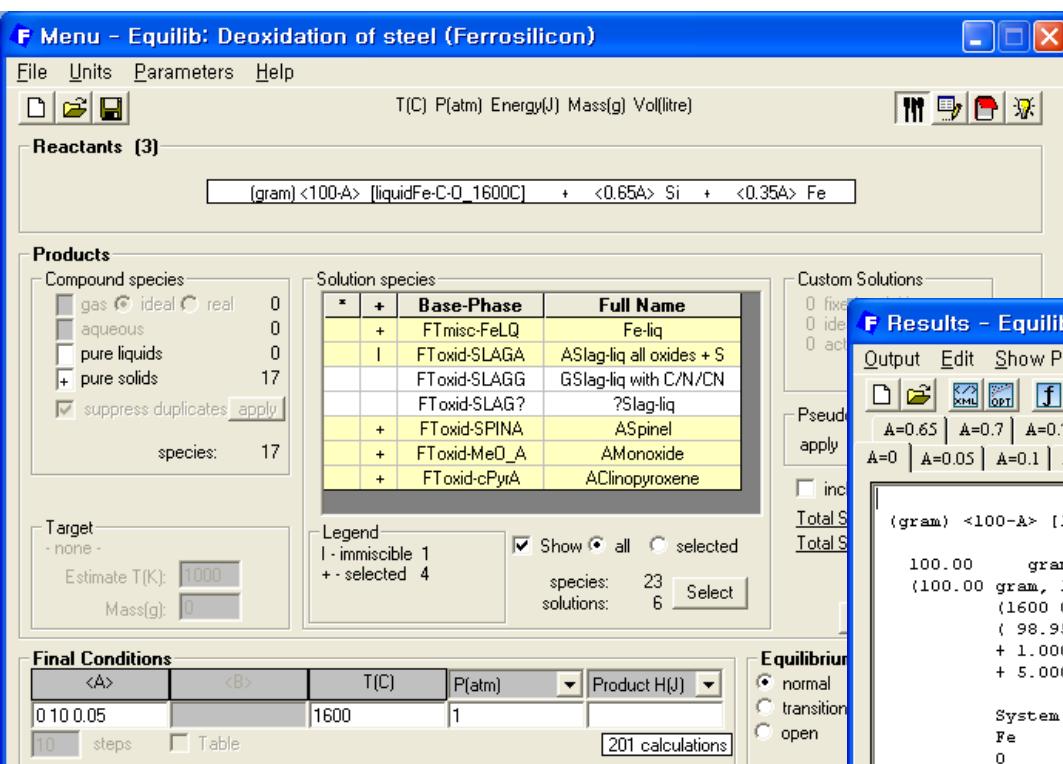
	#	Species	Mole (min)	Mole (max)	Fraction (min)	Fraction (max)	Activity (min)	Activity (max)
<b>FSstel: FCC1</b>								
1	Fe1C1(FCC1)	0	0	1.5462E-02	1.8119E-02	1.4903E-03	1.9635E-03	
2	Mn1C1(FCC1)	0	0	0	8.3613E-04	0	2.1103E-04	
3	Fe1V1a1(FCC1)	0	0	0.933237	0.981881	0.8649342	0.909331	
4	Mn1V1a1(FCC1)	0	0	0	5.0465E-02	0	4.3332E-02	
<b>FSstel: BCC1</b>								
5	Fe1C3(BCC1)	0	0	3.4204E-03	4.2319E-03	4.9121E-18	1.0164E-17	
6	Mn1C3(BCC1)	0	0	0	1.8222E-04	0	2.5896E-08	
7	Fe1V3(BCC1)	0	0	0.946	0.995768	0.872017	0.916769	
8	Mn1V3(BCC1)	0	0	0	5.0397E-02	0	4.5625E-02	
<b>FSstel: HCP1</b>								
9	Fe2C(HCP1)	0	0	1.3534E-02	1.5801E-02	5.3473E-04	7.4066E-04	
10	Mn2C(HCP1)	0	0	0	1.0915E-03	0	1.5515E-04	
11	Fe2V1a(HCP1)	0	0	0.451891	0.486466	0.35395	0.391212	
12	Mn2V1a(HCP1)	0	0	0	3.1216E-02	0	1.6295E-03	
<b>FSstel: CEME</b>								
13	Fe3C1(CEME)	0	0	0.908623	1.	3.9284E-02	5.7205E-02	
14	Mn3C1(CEME)	0	0	0	9.1377E-02	0	1.6972E-05	

<100-A> [liquidFe-C-O\_1600C] + <A> [Ferromanganese]



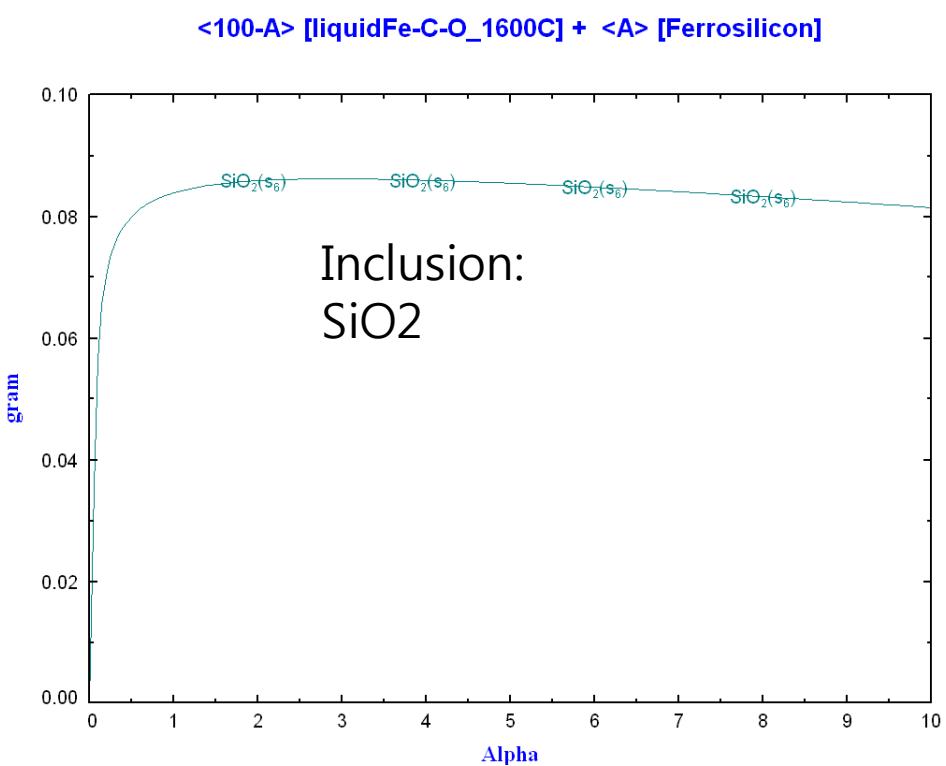
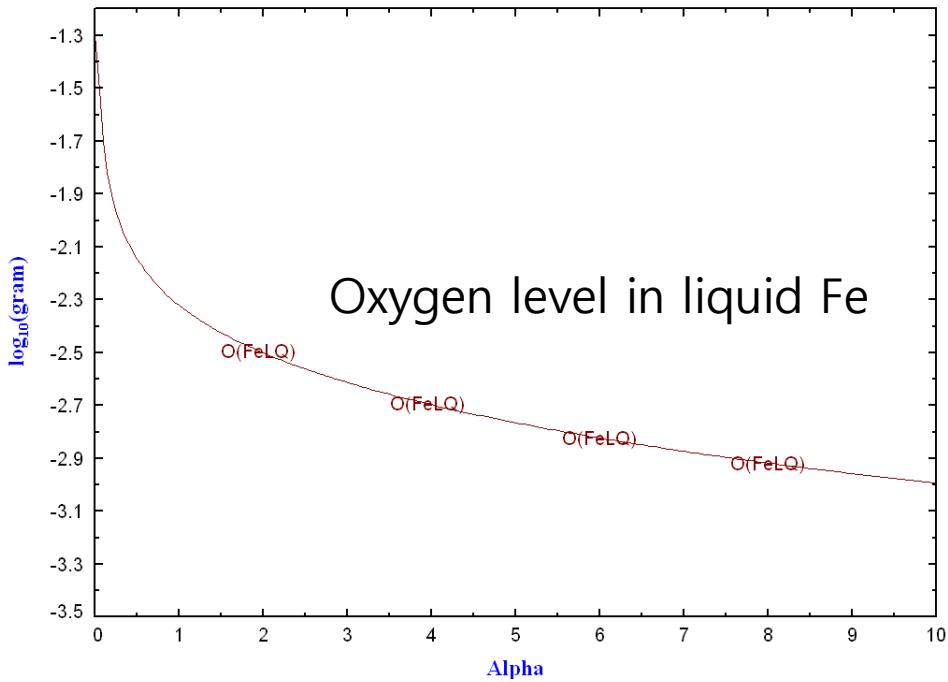
# Ex3-2. Deoxidation of steel (Ferrosilicon)

65%Si-35%Fe



# Ex3-2. Deoxidation of steel (Ferrosilicon)

<100-A> [liquidFe-C-O\_1600C] + <A> [Ferrosilicon]



# Ex3-3. Deoxidation of steel (Mn-Si)

50%Mn-50%Si

**F Menu - Equilib: Deoxidation of steel (Ferrosilicon)**

File Units Parameters Help

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

**Reactants (3)**

(gram) <100-A> [liquidFe-C-O\_1600C] + <0.5A> Mn + <0.5A> Si

**Products**

Compound species: 0  
 gas ideal real 0  
 aqueous 0  
 pure liquids 0  
 pure solids 23  
 suppress duplicates

species: 23

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

**Solution species**

*	+	Base-Phase	Full Name
+	+	FTmisc-FeLQ	Fe-liq
+	+	FTmisc-BCCS	bcc
+	+	FTmisc-FCCS	fcc
I	FToxic-SLAGA	ASlag-liq all oxides + S	
	FToxic-SLAGG	GSlag-liq with C/N/CN	
	FToxic-SLAG?	?Slag-liq	
+	FToxic-SPINB	BSpinel	
+	FToxic-MeO_B	BMonoxide	

**Legend**  
 I - immiscible 1  
 + - selected 12  
 species: 79  
 solutions: 14

**Final Conditions**

<A>	<B>	T(C)	P(atm)	Product H(J)
0 10 0.05		1600	1	

10 steps  Table

**Equilibrium**  
 normal  
 transition  
 open

**F Results - Equilib A=0 (page 1/201)**

Output Edit Show Pages

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

A=0.65 | A=0.7 | A=0.75 | A=0.8 | A=0.85 | A=0.9 | A=0.95 | A=1 | A=1.05 | A=1.1 | A=1.15 | A=1.2 |  
 A=0 | A=0.05 | A=0.1 | A=0.15 | A=0.2 | A=0.25 | A=0.3 | A=0.35 | A=0.4 | A=0.45 | A=0.5 | A=0.55 | A=0.6 |

**FactSage 6.3**

(gram) <100-A> [liquidFe-C-O\_1600C] + <0.5A> Mn + <0.5A> Si =

100.00 gram Fe-liq  
 (100.00 gram, 1.8583 mol)  
 (1600 C, 1 atm, a=1.0000)  
 { 98.950 wt.% Fe  
 + 1.0000 wt.% C  
 + 5.0000E-02 wt.% O

FTmisc  
 FTmisc  
 FTmisc

System component Mole fraction Mass fraction  
 Fe 0.95351 0.98950  
 O 1.6818E-03 5.0000E-04  
 C 4.4805E-02 1.0000E-02

+ 0 gram bcc  
 (1600 C, 1 atm, a=0.91677)  
 { 100.00 wt.% Fe:Va

FTmisc

+ 0 gram fcc  
 (1600 C, 1 atm, a=0.90933)  
 { 100.00 wt.% Fe:Va

FTmisc

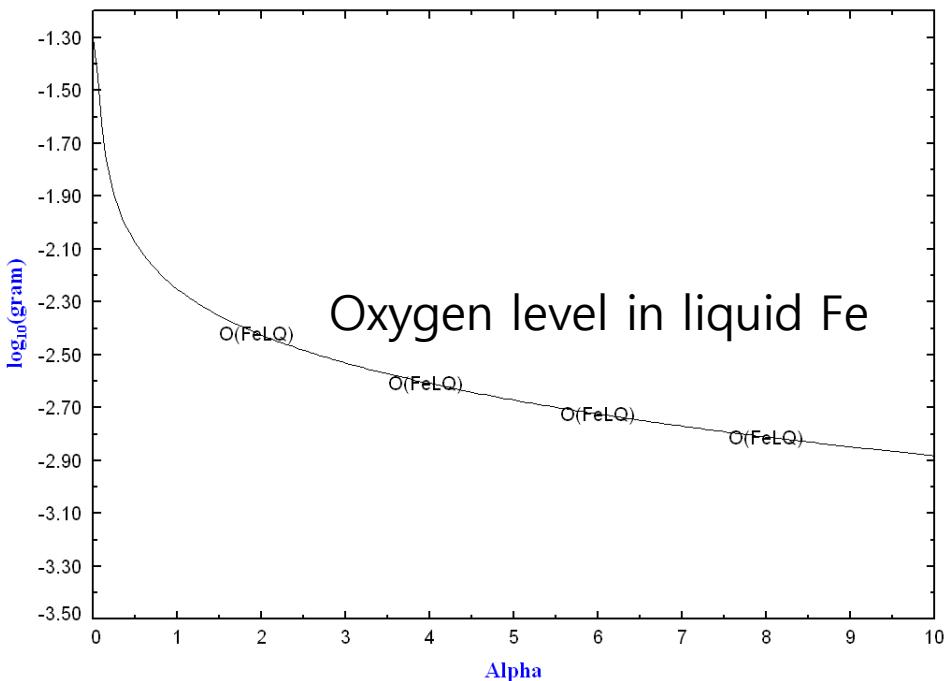
+ 0 gram BMonoxide  
 (1600 C, 1 atm, a=0.15453)  
 { 95.355 wt.% FeO  
 + 4.6453 wt.% Fe2O3

FToxic  
 FToxic

+ 0 gram ASlag-liq#1

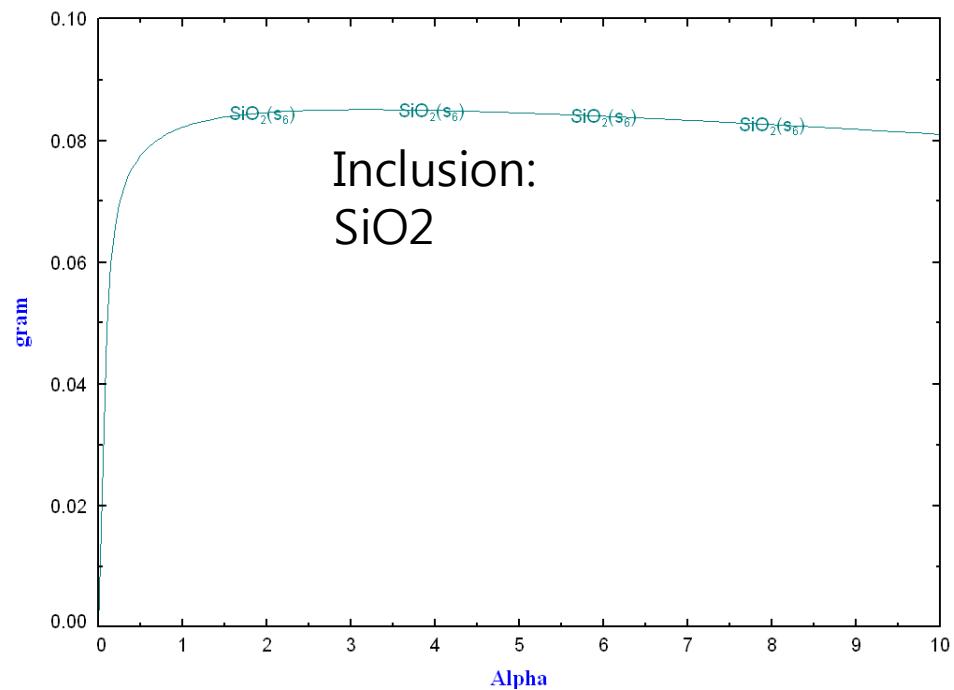
# Ex3-3. Deoxidation of steel (Mn-Si)

<100-A> [liquidFe-C-O\_1600C] + <0.5A> Mn + <0.5A> Si



Oxygen level in liquid Fe

<100-A> [liquidFe-C-O\_1600C] + <0.5A> Mn + <0.5A> Si



Inclusion:  
SiO<sub>2</sub>

# Ex3-4. Deoxidation of steel (Mn-Si-Al)

33.333%Mn-33.333%Si-33.333%Al

**F Menu - Equilib:**

File Units Parameters Help

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

**Reactants (4)**

[gram] <100-A> [liquidFe-C-O\_1600C] + <0.33333A> Mn + <0.33333A> Si + <0.33333A> Al

**Products**

Compound species: 0  
gas ideal real 0  
aqueous 0  
pure liquids 0  
pure solids 35  
 suppress duplicates apply  
species: 35

**Solution species**

*	+	Base-Phase	Full Name
+	+	FTmisc-FeLQ	Fe-liq
+	+	FTmisc-BCCS	bcc
+	+	FTmisc-FCCS	fcc
I	FToxic-SLAGA	ASlag-liq all oxides + S	
	FToxic-SLAGG	GSlag-liq with C/N/CN	
	FToxic-SLAG?	?Slag-liq	
I	FToxic-SPINA	ASpinel	
	FToxic-SPINB	BSpinel	

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

**Legend**  
I - immiscible 4  
+ - selected 12  
Show  all  selected  
species: 113  
solutions: 20 Select

**Final Conditions**

<A>	<B>	T(C)	P(atm)	Product H(J)
0 10 0.05		1600	1	201 calculations

FactSage 6.3

**F Results - Equilib A=0 (page 1/201)**

Output Edit Show Pages

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

A=0.65 | A=0.7 | A=0.75 | A=0.8 | A=0.85 | A=0.9 | A=0.95 | A=1 | A=1.05 | A=1.1 | A=1.15 | A=1.2 |  
A=0 | A=0.05 | A=0.1 | A=0.15 | A=0.2 | A=0.25 | A=0.3 | A=0.35 | A=0.4 | A=0.45 | A=0.5 | A=0.55 | A=0.6 |

FactSage 6.3

(gram) <100-A> [liquidFe-C-O\_1600C] + <0.33333A> Mn + <0.33333A> Si + <0.33333A> Al

100.00 gram Fe-liq  
(100.00 gram, 1.8583 mol)  
(1600 C, 1 atm, a=1.0000)  
( 98.950 wt.% Fe  
+ 1.0000 wt.% C  
+ 5.0000E-02 wt.% O

FTmisc  
FTmisc  
FTmisc

System component Mole fraction Mass fraction  
Fe 0.95351 0.98950  
O 1.6818E-03 5.0000E-04  
C 4.4805E-02 1.0000E-02

+ 0 gram bcc  
(1600 C, 1 atm, a=0.91677)  
( 100.00 wt.% Fe:Va

FTmisc

+ 0 gram fcc  
(1600 C, 1 atm, a=0.90933)  
( 100.00 wt.% Fe:Va

FTmisc

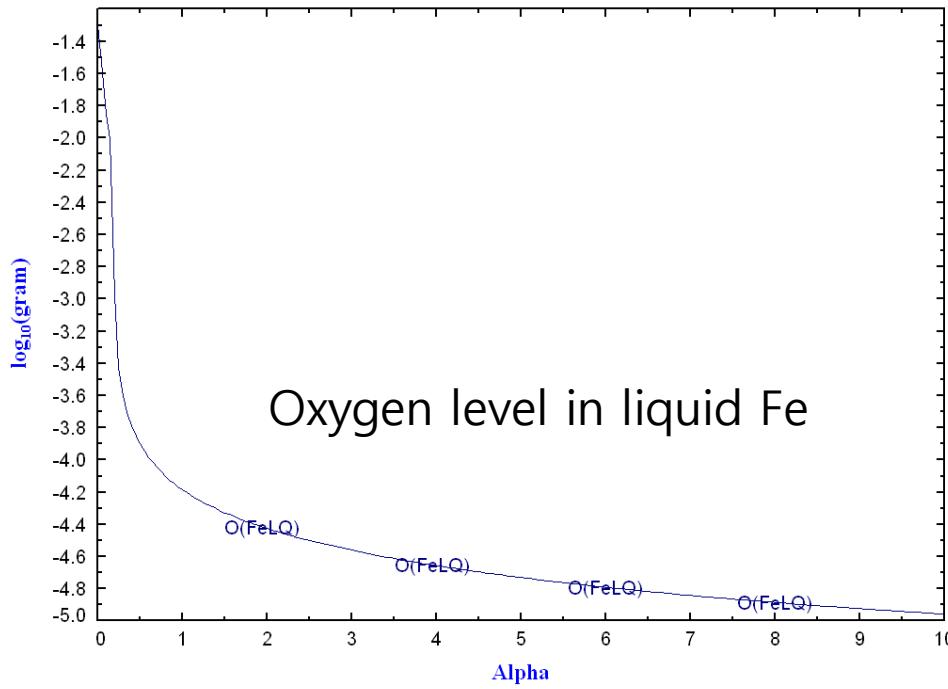
+ 0 gram AMonoxide  
(1600 C, 1 atm, a=0.15453)  
( 95.355 wt.% FeO  
+ 4.6453 wt.% Fe2O3

FToxic  
FToxic

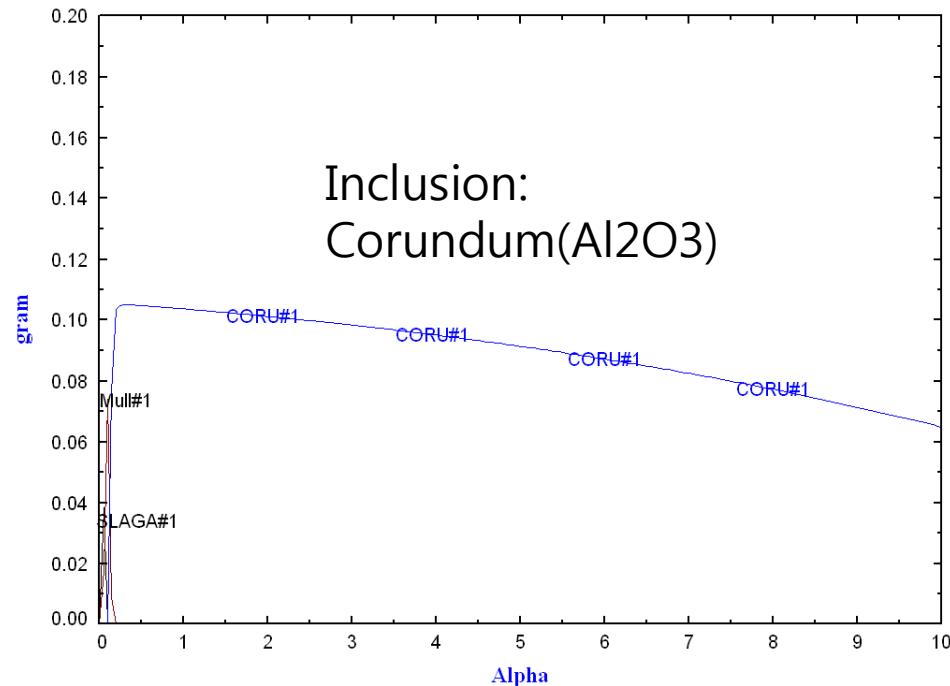
+ 0 gram ASlag-liq#1

# Ex3-4. Deoxidation of steel (Mn-Si-Al)

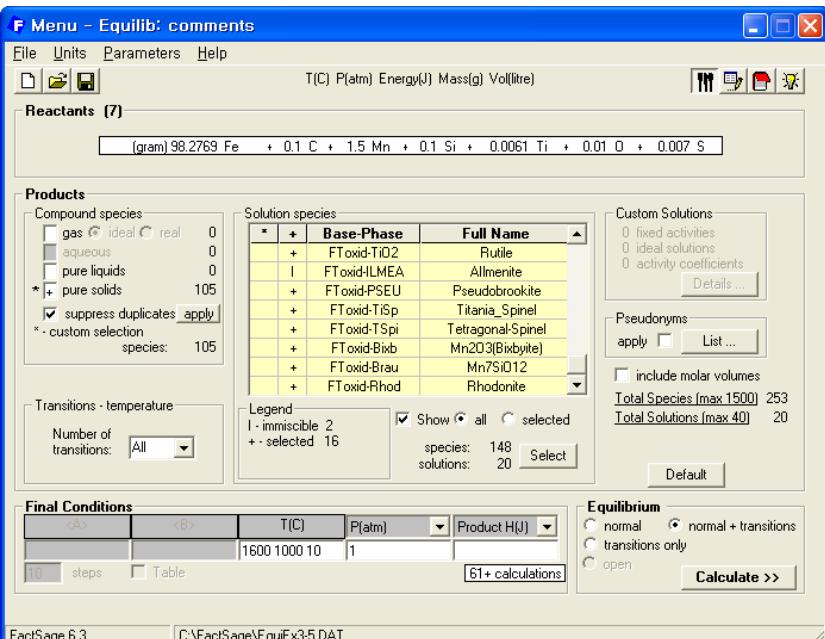
<100-A> [liquidFe-C-O\_1600C] + <0.3333A> Mn + <0.3333A> Si + <0.3333A> Al



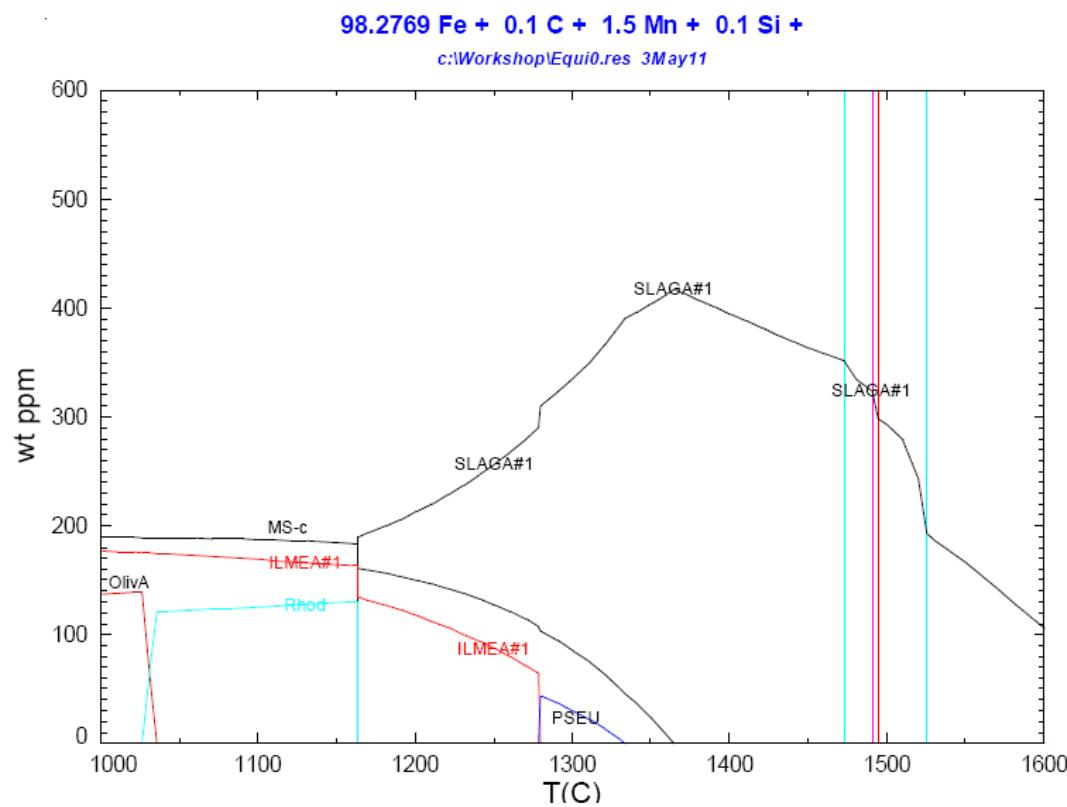
<100-A> [liquidFe-C-O\_1600C] + <0.3333A> Mn + <0.3333A> Si + <0.3333A> Al



# Ex3-5. Inclusion evolution with temperature: Mn/Si/Ti steel



- ← FToxic : oxide inclusions
- ← FTmisc: FeLq, MnS solid (MS\_c)
- ← FSStel: solid steel phases (fcc, bcc)



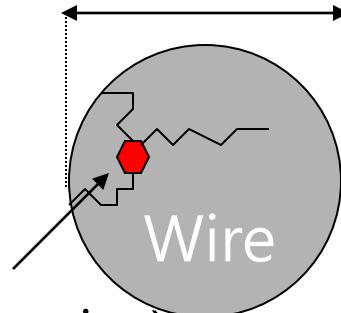
← Select all phases (pure solids and solutions) with amount > 0  
Or simply select all stable phases

# Application to Tire-Cord Steel (Mn/Si deoxidation)

Tire-Cord Steel

Inclusion (ex., alumina)

0.15~0.38mm diameter

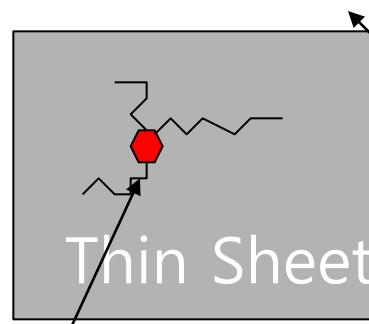


Crack Initiation

Fe-36%Ni Invar Steel

Inclusion (ex., alumina)

150 $\mu\text{m}$  thickness



Crack Initiation  
Surface Quality

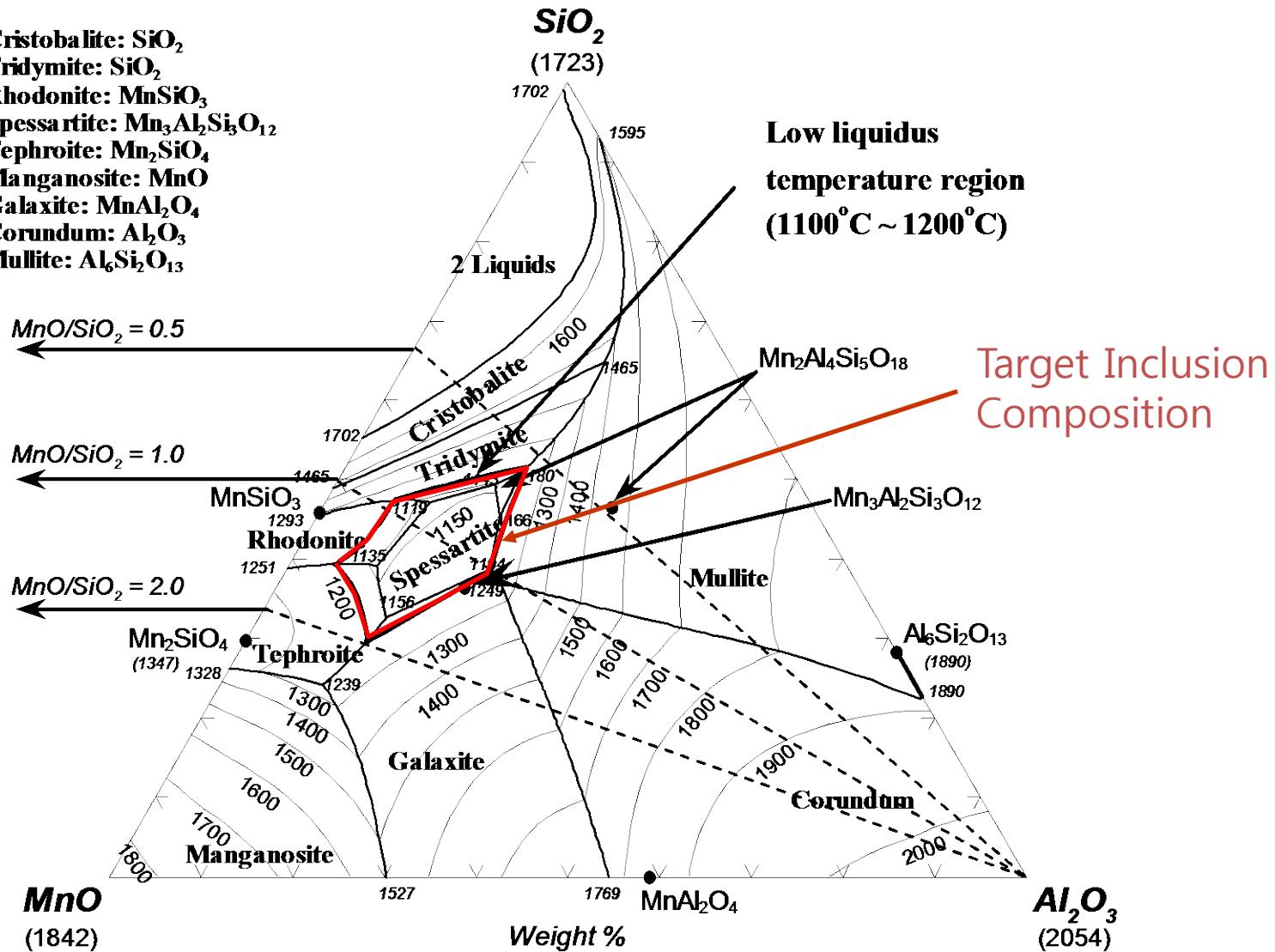
- Undeformable Inclusion should be removed
- Liquid phase is desirable at process temperature ( $\sim 1200^\circ\text{C}$ )



Mn/Si Deoxidation

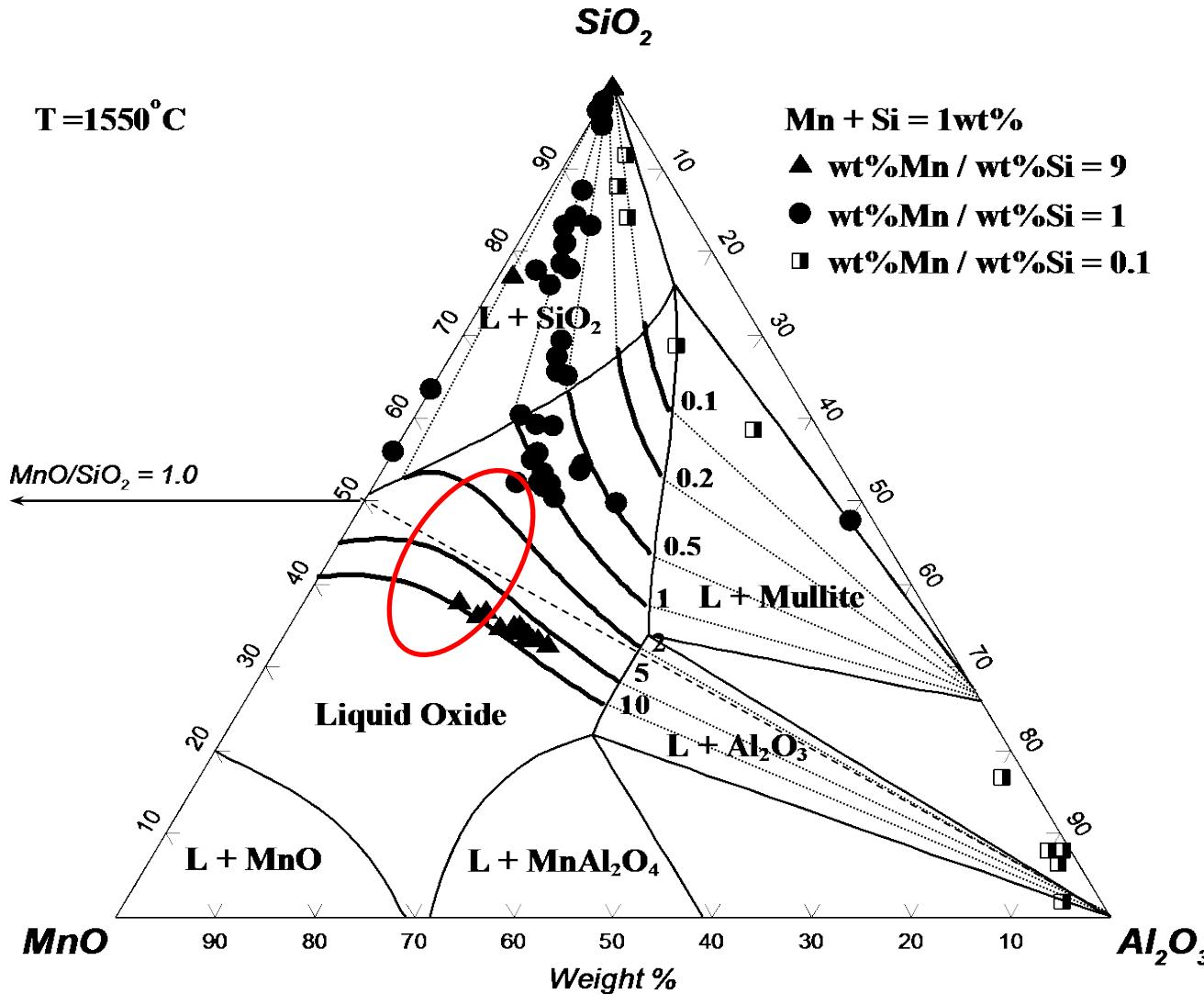
# MnO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> Phase Diagram

Cristobalite: SiO<sub>2</sub>  
 Tridymite: SiO<sub>2</sub>  
 Rhodonite: MnSiO<sub>3</sub>  
 Spessartite: Mn<sub>3</sub>Al<sub>2</sub>Si<sub>3</sub>O<sub>12</sub>  
 Tephroite: Mn<sub>2</sub>SiO<sub>4</sub>  
 Manganosite: MnO  
 Galaxite: MnAl<sub>2</sub>O<sub>4</sub>  
 Corundum: Al<sub>2</sub>O<sub>3</sub>  
 Mullite: Al<sub>6</sub>Si<sub>2</sub>O<sub>13</sub>



Jung et al., Metall. Mater. Trans. B, 2004, vol. 35B, pp. 259-268

# Inclusion composition with steel composition



Jung et al., Metall. Mater. Trans. B, 2004, vol. 35B, pp. 259-268  
Kang and Lee, ISIJ Inter., 2004.

# Ex3-6. Inclusion calculation in Mn/Si deoxidation

## Calculation of the inclusion trajectory using Equilib

The screenshot shows the FactSage 6.3 software interface for the 'Equilib' module. The window title is 'F Menu - Equilib: comments'. The menu bar includes File, Units, Parameters, and Help. The toolbar has icons for Open, Save, Print, and Calculate. The main area is divided into several sections:

- Reactants (5):** Shows the input composition: (gram) 98.995 Fe + 0.5 Mn + 0.5 Si + <A> Al + 0.007 O.
- Products:** A list of compound species:
  - gas (radio button selected)
  - ideal (radio button selected)
  - real (radio button)
  - aqueous (checkbox)
  - pure liquids (checkbox)
  - pure solids (checkbox)There are 69 species listed, with a checkbox for 'suppress duplicates' and an 'apply' button.
- Solution species:** A list of solution species with their base phases and full names:

Base-Phase	Full Name
I	FToxid-Mullite
I	FToxid-MulF
I	FToxid-CORU
+	FToxid-TSpi
+	FToxid-Bixb
+	FToxid-Brau
+	FToxid-Rhod
+	FToxid-AlSp
- Custom Solutions:** Options for fixed activities, ideal solutions, and activity coefficients, with a 'Details...' button.
- Pseudonyms:** Buttons for 'apply' and 'List...', and a checkbox for 'include molar volumes'.
- Total Species (max 1500):** 183  
**Total Solutions (max 40):** 19
- Final Conditions:** Set to <A> 0.005, <B> 0.0001, T(C) 1600, P(atm) 1, Product H(J) 51 calculations, 10 steps, Table checked.
- Equilibrium:** Options for normal, normal + transitions, transitions only, and open, with a 'Calculate >>' button.
- Status Bar:** FactSage 6.3, C:\FactSage\EquiEx3-6.DAT

The compositions of Mn and Si are set based on the target Mn/Si ratio and Mn+Si content. Oxygen content should be controlled reasonably. If O is too high, Mn and Si will be largely changed from original target composition after rxn with oxygen.

## Ex3-6. Inclusion calculation in Mn/Si deoxidation

F Results - Equilib A=0.001 (page 11/51)

Output Edit Show Pages

	T(C)	P(atm)	Energy(J)	Mass(g)	Vol(litre)			
A=0	A=1.00E-04	A=0.0002	A=0.0003	A=0.0004	A=0.0005	A=0.0006	A=0.0007	A=0.0008
A=0.0018	A=0.0019	A=0.002	A=0.0021	A=0.0022	A=0.0023	A=0.0024		
A=0.0009	-A=0.001	A=0.0011	A=0.0012	A=0.0013	A=0.0014	A=0.0015	A=0.0016	A=0.0017

(gram) 98.995 Fe + 0.5 Mn + 0.5 Si + <A> Al +

(gram) 0.007 O =

99.998 gram Fe-liq  
 (99.998 gram, 1.7998 mol)  
 (1600.00 C, 1 atm, a=1.0000)  
 ( 98.997 wt.% Fe  
 + 2.3649E-04 wt.% Al  
 + 0.49861 wt.% Mn  
 + 4.5663E-03 wt.% O  
 + 0.49882 wt.% Si  
 + 6.8340E-05 wt.% AlO  
 + 1.3779E-04 wt.% SiO  
 + 3.7851E-04 wt.% MnO  
 + 5.6476E-08 wt.% Al2O

FTmisc  
 FTmisc

System component	Mole fraction	Mass fraction
Fe	0.98492	0.98997
Mn	5.0455E-03	4.9890E-03
Si	9.8696E-03	4.9891E-03
Al	5.7541E-06	2.7944E-06
O	1.6415E-04	4.7271E-05

+ 5.3906E-03 gram ASlag-liq#1  
 (5.3906E-03 gram, 7.6111E-05 mol)  
 (1600.00 C, 1 atm, a=1.0000)  
 ( 25.257 wt.% Al2O3  
 + 43.746 wt.% SiO2  
 + 4.4146 wt.% FeO  
 + 1.2224E-03 wt.% Fe2O3  
 + 26.576 wt.% MnO  
 + 5.1664E-03 wt.% Mn2O3

FToxid  
 FToxid  
 FToxid  
 FToxid  
 FToxid  
 FToxid  
 FToxid

Site fraction of sublattice constituents:

Al	0.29850
Si	0.43869
Fe2+	3.7023E-02
Fe3+	9.2243E-06
Mn2+	0.22573
Mn3+	3.9435E-05
<hr/>	
O	1.0000

Mn + Si + Al + O → (Mn, Si, Al) oxide inclusion

After deoxidation, Mn ~ 0.5 and Si ~ 0.5

(Target steel composition: Mn/Si = 1 and Mn+Si = 1)

### → Extraction of slag composition

F Spreadsheet - Equilib T(C) = 1600, P(atm) = 1, Alpha = 0...

File Edit Show

Selected: 6/76 Spreadsheet Species Page 51 Refresh

	Code	Species	Data	Phase	T	V	Activity
+	44	AlO(FeLQ)	FTmisc	FTmisc-FeLQ			1.9788E-06
+	45	SiO(FeLQ)	FTmisc	FTmisc-FeLQ			1.2069E-06
+	46	MnO(FeLQ)	FTmisc	FTmisc-FeLQ			2.0599E-06
+	47	Al2O(FeLQ)	FTmisc	FTmisc-FeLQ			3.2461E-09
+	63	Al2O3(SLAGA)	FToxid	FToxid-SLAGA			0.2308
+	64	SiO2(SLAGA)	FToxid	FToxid-SLAGA			0.2550
+	65	FeO(SLAGA)	FToxid	FToxid-SLAGA			1.3509E-02
+	66	Fe2O3(SLAGA)	FToxid	FToxid-SLAGA			4.6227E-09
+	67	MnO(SLAGA)	FToxid	FToxid-SLAGA			1.9928E-02
+	68	Mn2O3(SLAGA)	FToxid	FToxid-SLAGA			1.4048E-09
+	123	FeO(MeO_A)	FToxid	FToxid-MeO_A			1.0181E-02
+	124	Fe2O3(MeO_A)	FToxid	FToxid-MeO_A			2.3568E-10
+	125	Al2O3(MeO_A)	FToxid	FToxid-MeO_A			6.9432E-03
+	126	MnO(MeO_A)	FToxid	FToxid-MeO_A			2.9716E-02
+	145	Fe1Fe1Si1O4(OlivA)	FToxid	FToxid-OlivA			5.4870E-05
+	146	Al2SiO5(Anorthite)	FToxid	FToxid-Anorthite			2.0227E-02

'+' denotes all the Species Properties as defined in the Spreadsheet Setup.

Select All Clear OK

# Ex3-6. Inclusion calculation in Mn/Si deoxidation

a) Select this

b) After select "Excel.." Click "Spreadsheet ..." Then go to next page

c) Click 'Spreadsheet setup'

The screenshot shows two windows of the FactSage software. The left window displays a list of chemical species and their compositions at 1710°C. The right window shows the software's output interface with various tabs like T, Fact, and FToxid. A yellow box highlights the 'Save or Print As...' option in the top menu. Another yellow box highlights the 'Excel' option in the 'Output' dialog that appears when this menu item is selected. A third yellow box highlights the 'Spreadsheet setup...' button in the same dialog. The main output area lists components like Mn<sub>solid\_gamma</sub>, Mn<sub>solid\_beta</sub>, Mn<sub>solid\_alpha</sub>, Ca<sub>2</sub>SiO<sub>4</sub>\_alpha, Ca<sub>2</sub>SiO<sub>4</sub>\_alpha-prime, and MnO<sub>solid</sub>.

# Ex3-6. Inclusion calculation in Mn/Si deoxidation

1) Click this area to change the data to be extracted

2) Then, click the "select" to choose wt% of what species

3) Select the species

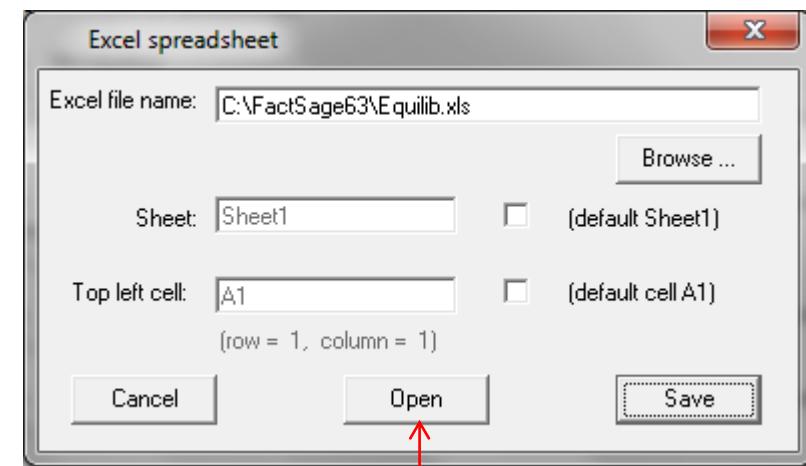
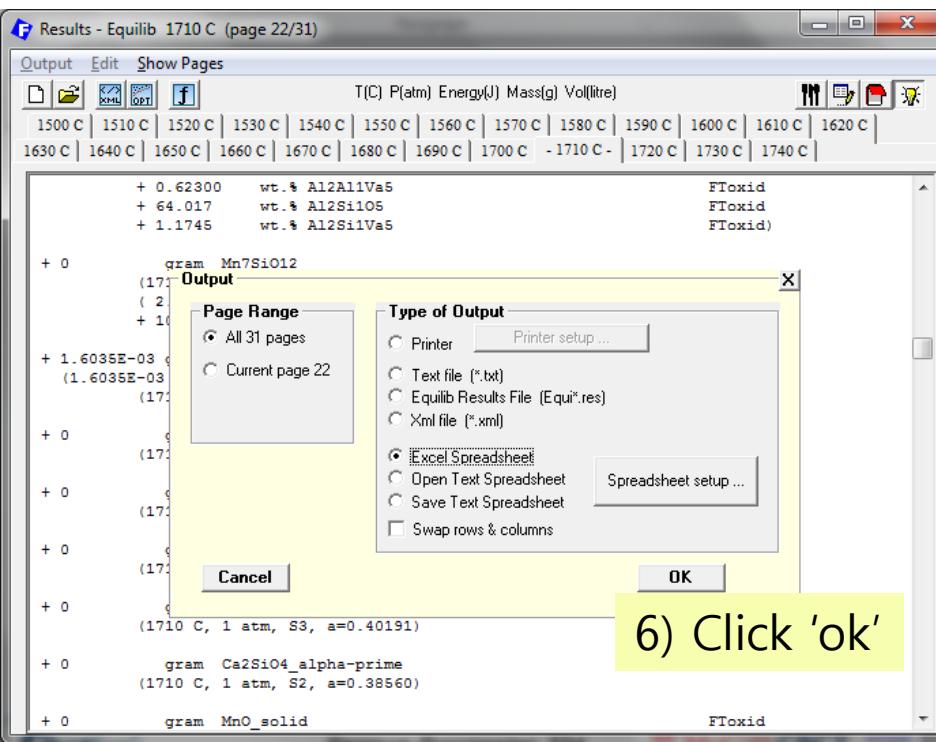
4) Click 'ok'

5) Click 'ok'

6) Click 'ok' for menu in the previous page

The screenshot shows the FactSage software interface for equilibrium calculations at 1710°C. A yellow box highlights the 'Output' tab where data like T(C), P(atm), Energy(J), Mass(g), and Vol(litre) are listed. Red arrows point from the numbered steps to specific controls: step 1 points to the 'Variable' dropdown in the 'System Properties' section; step 2 points to the 'Select...' button in the 'Species Properties' section; step 3 points to the 'Species' list in the 'Species Properties' dialog; step 4 points to the 'OK' button in the 'Species' dialog; step 5 points to the 'OK' button in the 'Spreadsheet Setup' dialog; and step 6 points to the 'OK' button in the 'Output' tab. A secondary window titled 'Spreadsheet - Equilib T(C) = 1500' shows a list of species and their properties, with red arrows indicating the selection of species like Mn3Si(s) and Mn5Si3(s).

# Ex3-6. Inclusion calculation in Mn/Si deoxidation



7) Click 'open' then you can see excel file containing all information.

# Ex3-6. Inclusion calculation in Mn/Si deoxidation

c:\Workshop\Equilib.xls - Equilib.xls

L18 F 25.4422

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Alpha	t%-Al2O3(SLAGA#)	Vt%-SiO2(SLAGA#)	Vt%-FeO(SLAGA#)	Vt%-Fe2O3(SLAGA#)	t%-MnO(SLAGA#)	%-Mn2O3(SLAGA%)	-Al2O3(SLAGA%)	%-SiO2(SLAGA%)	t%-FeO(SLAGA#)	t%-Fe2O3(SLAGA#)	Wt%-MnO(SLAGA#)	t%-Mn2O3(SLAGA#)	A corner	B corner	C corner	
2	0	0	99.590634	0.1269274	9.38178E-05	0.28145943	0.000884935	0	62.570747	6.6540505	0.005014931	30.767009	0.00317861	0.995906	0.004094	0	
3	0.0001	8.7711586	59.790802	5.559767	0.001167373	25.873633	0.003391942	0.88364011	97.580289	0.48783513	4.63662E-05	1.0475307	0.000659026	0.597909	0.31438	0.087712	
4	0.0002	11.759224	56.597871	5.3249481	0.001032080	26.31312	0.00380378	11.759224	56.597871	5.3249481	0.001032080	26.31312	0.00380378	0.565979	0.316429	0.117592	
5	0.0003	14.066974	54.208548	5.151598	0.001005925	26.567742	0.0044133219	14.066974	54.208548	5.151598	0.001005925	26.567742	0.0044133219	0.542085	0.317245	0.140667	
6	0.0004	16.049565	52.214521	5.0095657	0.001013321	26.720934	0.004400963	16.049565	52.214521	5.0095657	0.001013321	26.720934	0.004400963	0.522145	0.317359	0.160496	
7	0.0005	17.835339	50.467437	4.8866687	0.001036335	26.804901	0.004618552	17.835339	50.467437	4.8866687	0.001036335	26.804901	0.004618552	0.504674	0.316972	0.178353	
8	0.0006	19.486052	48.895636	4.7767601	0.001067679	26.835691	0.004793466	19.486052	48.895636	4.7767601	0.001067679	26.835691	0.004793466	0.488956	0.316183	0.194861	
9	0.0007	21.036027	47.458868	4.6763608	0.001103733	26.82271	0.004931303	21.036027	47.458868	4.6763608	0.001103733	26.82271	0.004931303	0.474589	0.315051	0.21036	
10	0.0008	22.506131	46.132115	4.583358	0.001142381	26.772216	0.005036713	22.506131	46.132115	4.583358	0.001142381	26.772216	0.005036713	0.461321	0.313618	0.225061	
11	0.0009	23.909924	44.898539	4.4964022	0.001182243	26.688838	0.005113818	23.909924	44.898539	4.4964022	0.001182243	26.688838	0.005113818	0.448985	0.311915	0.239099	
12	0.001	25.25674	43.745988	4.4145919	0.001222358	26.576291	0.005166381	25.25674	43.745988	4.4145919	0.001222358	26.576291	0.005166381	0.43746	0.309973	0.252567	
13	0.0011	26.553373	42.665141	4.3372955	0.001262035	26.477724	0.005402906	26.553373	42.665141	4.3372955	0.001262035	26.553373	0.005402906	0.40519186	0.307815	0.265534	
14	0.0012	27.805041	41.648467	4.2640469	0.001300776	26.2								0.005211418	0.416485	0.305465	0.27805
15	0.0013	29.015965	40.689634	4.1944816	0.001338226	26.0								0.00209911	0.406896	0.302944	0.29016
16	0.0014	30.189703	39.783161	4.1282982	0.001374146	25.8								0.015195882	0.397832	0.300271	0.301897
17	0.0015	31.329359	38.924207	4.0652354	0.001408385	25.6								0.006171568	0.389242	0.313294	
18	0.0016	32.437708	38.108454	4.0050587	0.001440861	25.								0.005138908	0.381088	0.294538	0.324377
19	0.0017	33.517264	37.332014	3.9475524	0.001471545	25.1								0.005099565	0.37332	0.291507	0.335173
20	0.0018	34.570329	36.591383	3.8925152	0.001500449	24.9								0.005064952	0.365914	0.288383	0.345703
21	0.0019	35.5599022	35.883392	3.8397581	0.001527614	24.6								0.005006259	0.358834	0.285176	0.35599
22	0.002	36.605295	35.205174	3.7891028	0.001553101	24.3								0.004954478	0.352052	0.281895	0.366053
23	0.0021	37.590952	34.554135	3.7403815	0.001576986	24.1								0.004900434	0.345541	0.278549	0.37591
24	0.0022	38.557655	33.927927	3.6934358	0.001599353	23.814537	0.004844809	38.557655	33.927927	3.6934358	0.001599353	23.814537	0.004844809	0.339279	0.275144	0.385577	
25	0.0023	38.958213	33.671179	3.6739139	0.0016082	23.690264	0.004821379	38.958213	33.671179	3.6739139	0.0016082	23.690264	0.004821379	0.336712	0.273706	0.389582	
26	0.0024	38.959257	33.66924	3.673336	0.001608031	23.691737	0.004821757	38.959257	33.66924	3.673336	0.001608031	23.691737	0.004821757	0.336692	0.273715	0.389593	
27	0.0025	38.96903	33.667301	3.6727582	0.001607862	23.693211	0.004822135	38.96903	33.667301	3.6727582	0.001607862	23.693211	0.004822135	0.336673	0.273724	0.389603	
28	0.0026	38.961344	33.665632	3.6721805	0.001607693	23.694683	0.004822514	38.961344	33.665632	3.6721805	0.001607693	23.694683	0.004822514	0.336654	0.273733	0.389613	
29	0.0027	38.962387	33.663423	3.6716029	0.001607524	23.696156	0.00482289	38.962387	33.663423	3.6716029	0.001607524	23.696156	0.004822892	0.3366615	0.273742	0.389624	
30	0.0028	38.96424	33.664194	3.6740254	0.001607355	23.697320	0.00482327	38.96424	33.664194	3.6740254	0.001607355	23.697320	0.00482327	0.336615	0.273751	0.389634	
31	0.0029	38.964474	33.665945	3.6704479	0.001607187	23.699102	0.004823648	38.964474	33.659545	3.6704479	0.001607187	23.699102	0.004823648	0.336595	0.27376	0.389645	
32	0.003	38.965518	33.657606	3.6698706	0.001607018	23.700574	0.004824207	38.965518	33.657606	3.6698706	0.001607018	23.700574	0.004824207	0.336576	0.273769	0.389655	
33	0.0031	38.966562	33.655667			23.702046	0.004824405							0.336557	0.273778	0.389666	
34	0.0032	38.967606	33.653728			23.703519	0.004824763							0.336537	0.273787	0.389676	
35	0.0033	39.008877	33.62625			23.692193	0.004822743							0.336263	0.273649	0.390089	
36	0.0034	39.790634	33.13269			23.441059	0.004775571							0.331327	0.270767	0.397906	
37	0.0035	39.791347	33.13292			23.440259	0.004775134							0.331329	0.270757	0.397913	
38	0.0036	39.79206	33.13315			23.439459	0.004774697							0.331332	0.270748	0.397921	
39	0.0037	39.792773	33.13338			23.438658	0.004774261							0.331334	0.270738	0.397928	
40	0.0038	39.793486	33.133611	3.628641 /	0.001623686	23.437858	0.004773824							0.331336	0.270729	0.397935	
41	0.0039	39.794199	33.133841	3.6285055	0.001623531	23.437058	0.004773388							0.331338	0.270727	0.397942	
42	0.004	39.794911	33.13407	3.6283639	0.001623376	23.436258	0.004772952							0.331341	0.270701	0.397949	
43	0.0041	39.795624	33.1343	3.6282223	0.001623221	23.435459	0.004772515	39.795624	33.1343	3.6282223	0.001623221	23.435459	0.004772515	0.331343	0.270701	0.397956	
44	0.0042	39.796336	33.134529	3.6280808	0.001623066	23.434659	0.004772079	39.796336	33.134529	3.6280808	0.001623066	23.434659	0.004772079	0.331345	0.270691	0.397963	
45	0.0043	39.797049	33.134758	3.6279392	0.00162291	23.433859	0.004771643	39.797049	33.134758	3.6279392	0.00162291	23.433859	0.004771643	0.331348	0.270682	0.39797	
46	0.0044	39.797761	33.134988	3.6277977	0.001622755	23.43306	0.004771207	39.797761	33.134988	3.6277977	0.001622755	23.43306	0.004771207	0.331345	0.270673	0.397978	
47	0.0045	40.292688	32.826409	3.604599	0.001633061	23.26993	0.004740786	40.292688	32.826409	3.604599	0.001633061	23.26993	0.004740786	0.328264	0.268809	0.402927	
48	0.0046	40.834298	32.491949	3.5794444	0.001644042	23.087958	0.004707142	40.834298	32.491949	3.5794444	0.001644042	23.087958	0.004707142	0.324919	0.266738	0.408343	

Composition from Slag #1

A corner = wt%SiO2/100

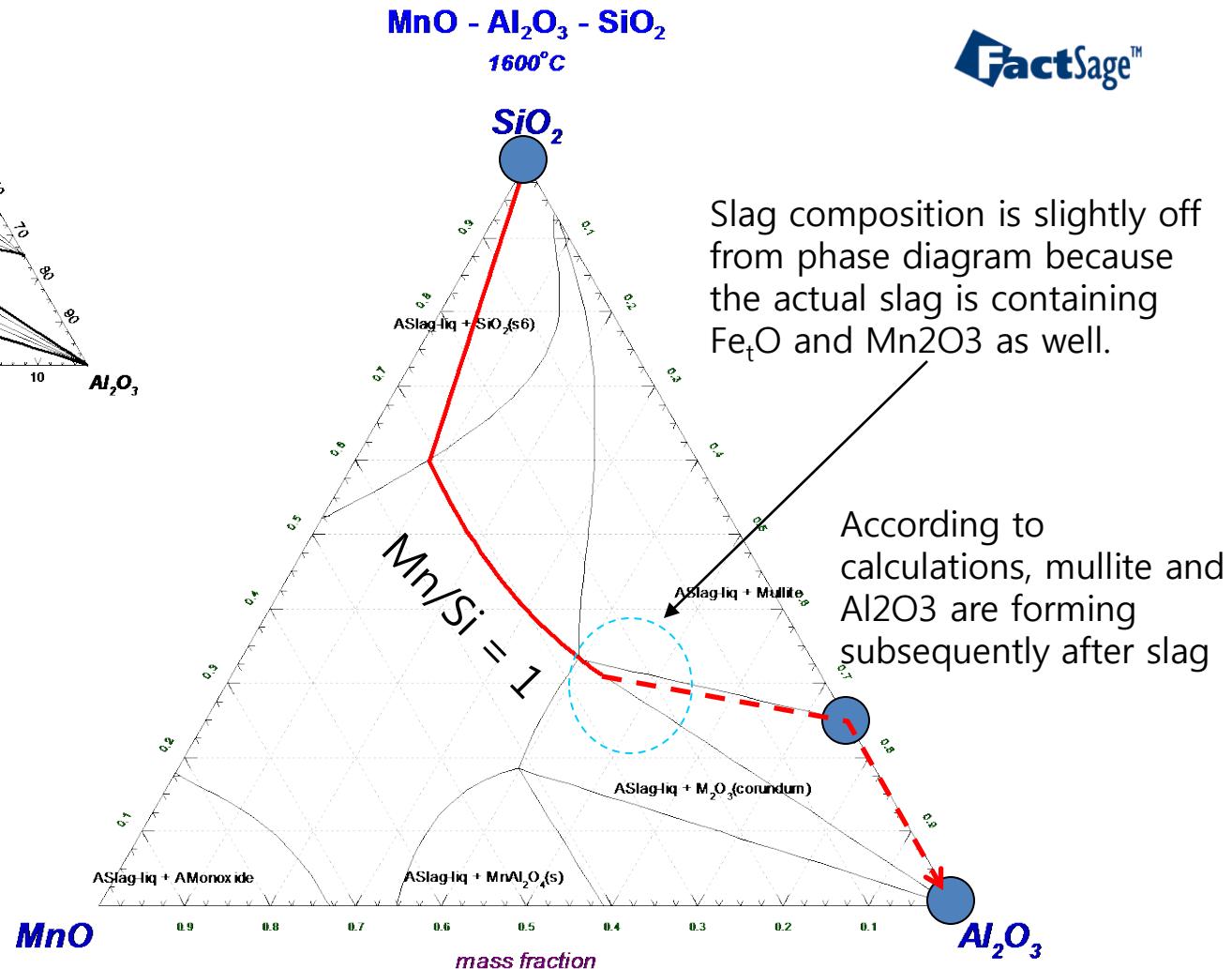
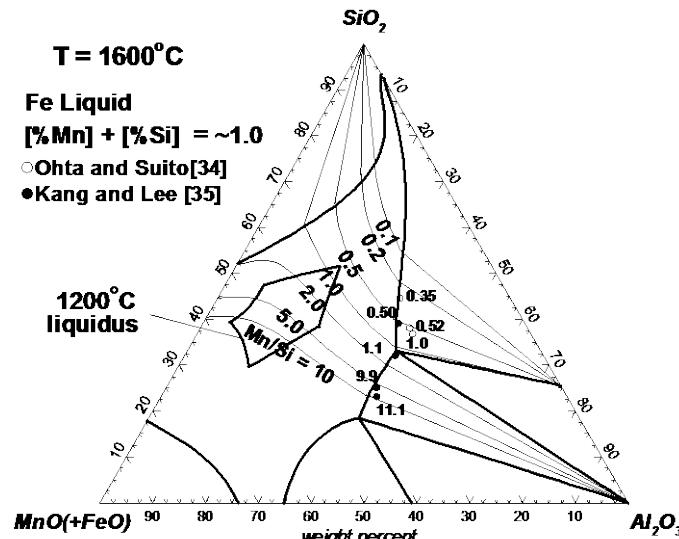
B corner = (wt%MnO+Mn2O3+FeO+Fe2O3)/100

C corner = wt%Al2O3/100

Slag #1 (stable slag)

Slag #2 (metastable or same as #1 except in case of stable miscibility gap)

# Ex3-6. Inclusion calculation in Mn/Si deoxidation



# Ex3-6. Inclusion calculation in Mn/Si deoxidation

**F Axes: weight % vs weight %**

Y-variable X-variable Swap Axes

Y-axis  
weight %  
maximum 100  
minimum 0  
tick every 5

X-axis  
weight %  
maximum 0.001  
minimum 0  
tick every 0.0001

Cancel Refresh OK

**F Species Selection - EQUILIB Results: weight % vs weight %**

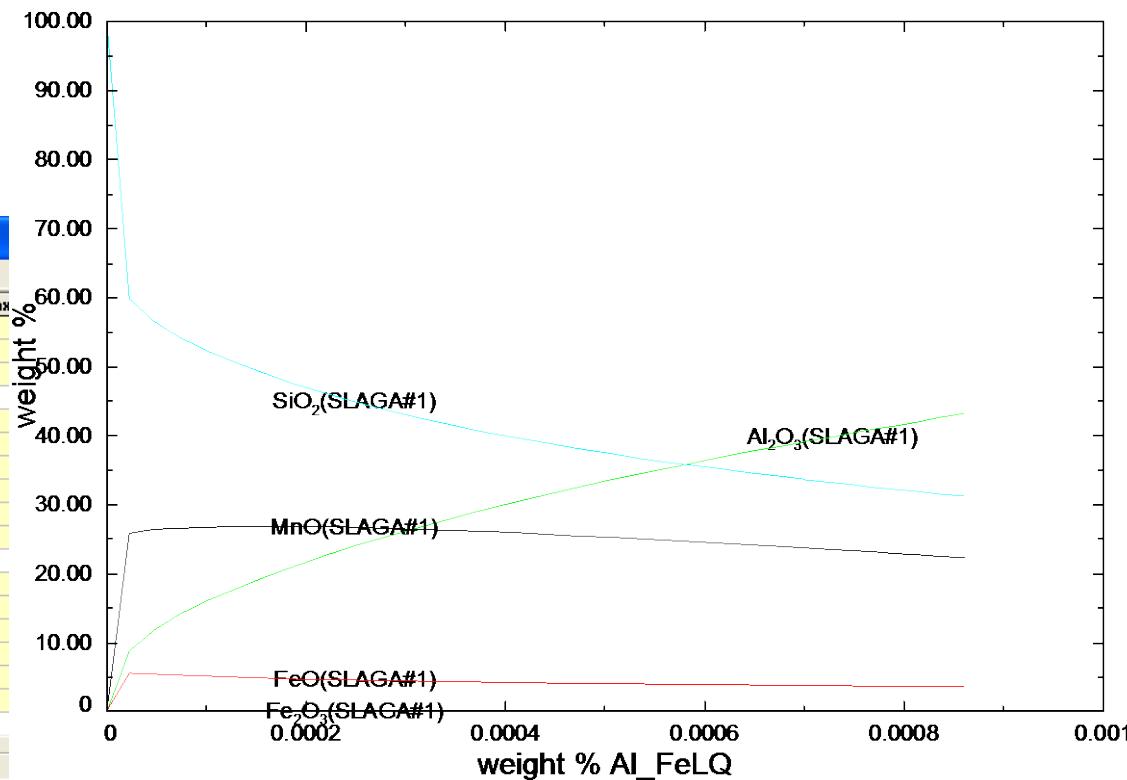
File Show Select

+	#	Species	Mole (min)	Mole (max)	Fraction (min)	Fraction (max)
+	15	SiO(FeLQ)	2.1732E-06	4.2194E-06	1.2075E-06	2.3442E-06
+	16	MnO(FeLQ)	3.7091E-06	7.2101E-06	2.0608E-06	4.0057E-06
+	17	Al2O(FeLQ)	0	5.8450E-09	0	3.2475E-09
<b>FToxic: SLAG</b>						
+	18	Al2O3(SLAGA#1)	0	2.8152E-05	0	0.324535
+	19	SiO2(SLAGA#1)	0	4.2063E-05	0.397325	0.996549
+	20	FeO(SLAGA#1)	0	3.8271E-06	1.0622E-03	5.0802E-02
+	21	Fe2O3(SLAGA#1)	0	7.4560E-10	3.5323E-07	8.1061E-06
+	22	MnO(SLAGA#1)	0	2.4992E-05	2.3855E-03	0.265522
+	23	Mn2O3(SLAGA#1)	0	2.2845E-09	3.3701E-06	2.3847E-05
<b>FToxic: SLAG</b>						
+	24	Al2O3(SLAGA#2)	0	0	0	0.324535
+	25	SiO2(SLAGA#2)	0	0	0.397325	0.981727
+	26	FeO(SLAGA#2)	0	0	4.1046E-03	5.9076E-02
+	27	Fe2O3(SLAGA#2)	0	0	1.7552E-07	2.0031E-05
+	28	MnO(SLAGA#2)	0	0	8.9265E-03	0.276648
+	29	Mn2O3(SLAGA#2)	0	0	2.5234E-06	2.3847E-05
<b>FToxic: SPIN</b>						

Y: weight % select species - use "+" column  
X: weight % enter one species # 10 Al(FeLQ)  
source [ ] [page] 51 pages Order [ ] mole [ ] gram [ ] integer # [ ] mass (max) [ ] fraction (max) [ ] activity (max)  
Select Top 15 [ ] b species selected Select ... OK  
Click on the '+' column to add or remove species.

Soluble Al vs. Inclusion composition

98.995 Fe + 0.5 Mn + 0.5 Si + <A> Al +  
c:\Workshop\Equi0.res 3May11



# **Application 5: Re-oxidation and inclusion modification in the tundish – Ca treatment**

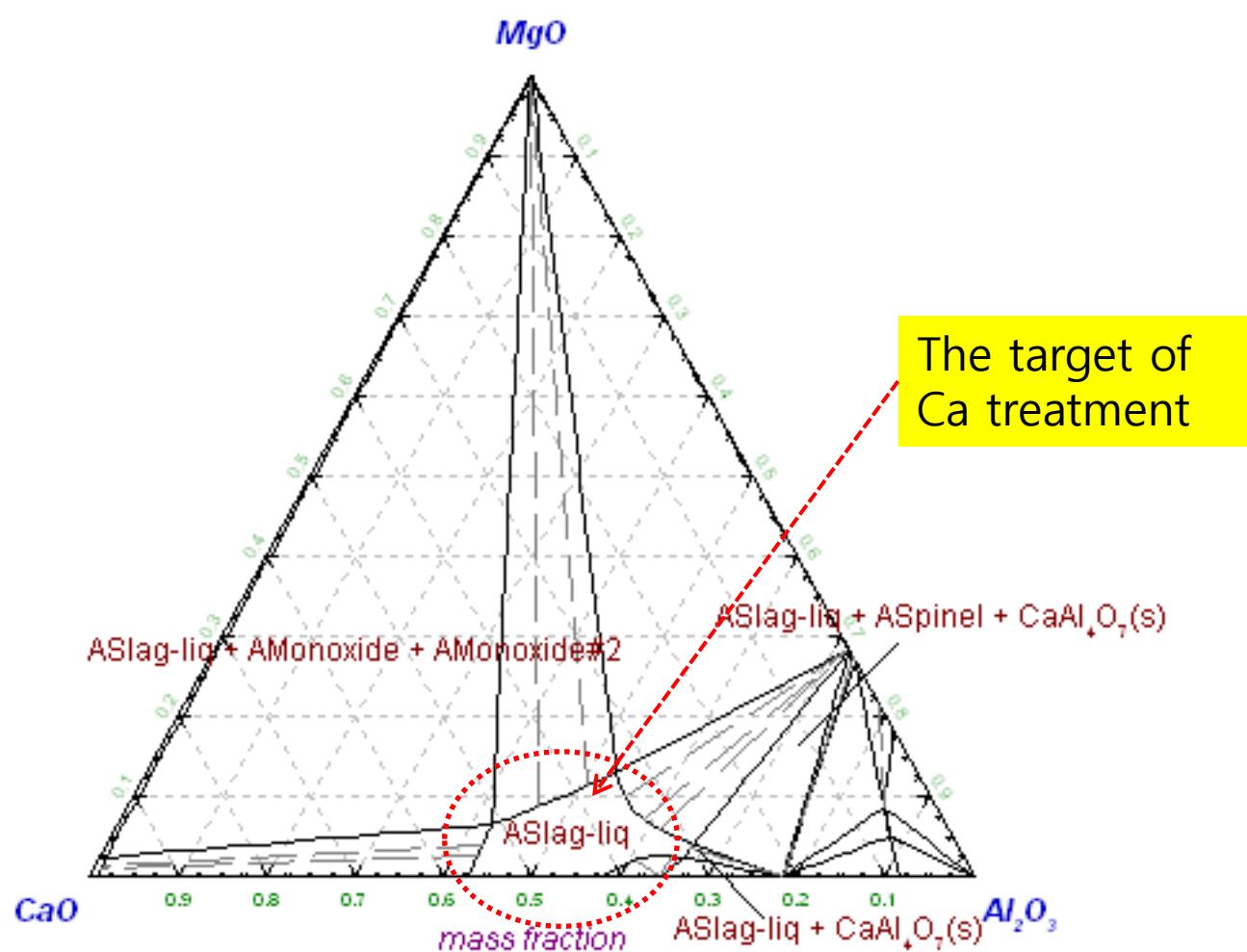
Junghwan Kim  
Email: junghwan.kim@mail.mcgill.ca

# Ex4-1. Reoxidation and inclusion modification in the tundish

MgO - CaO -  $\text{Al}_2\text{O}_3$

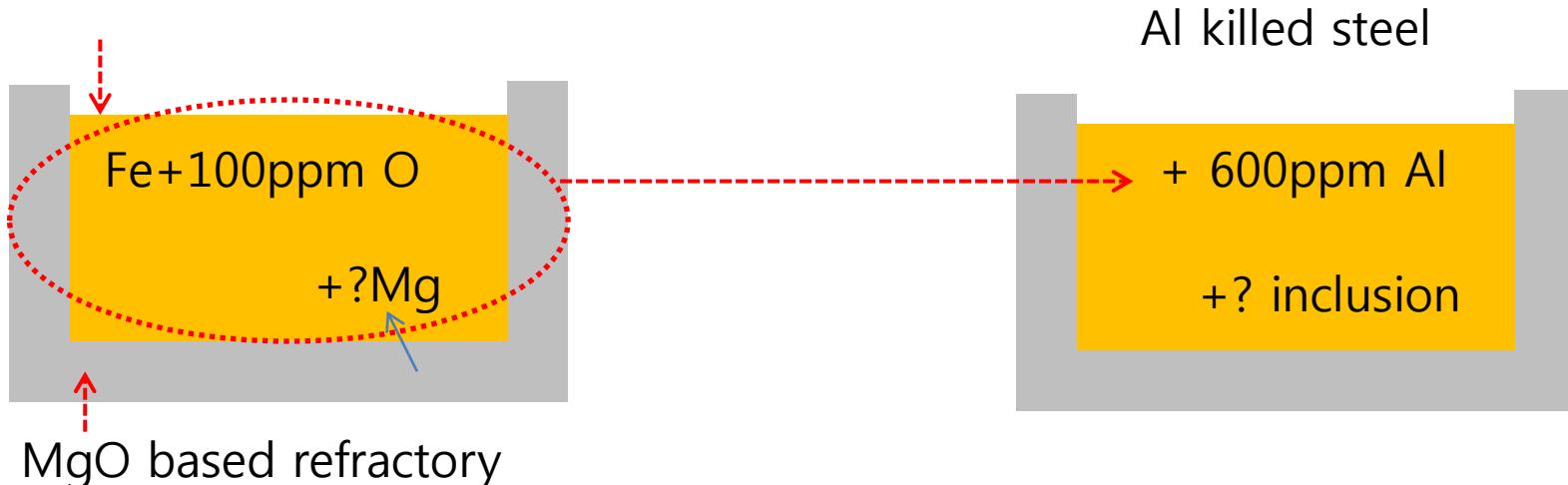
1550°C, 1 atm

FactSage™

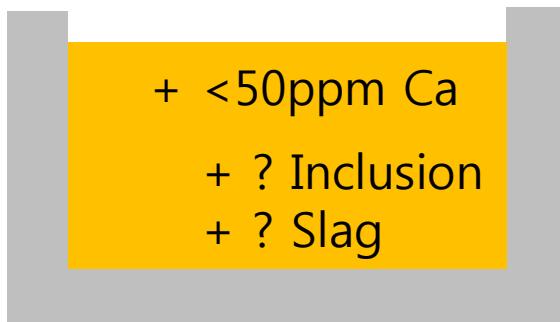


# Ex4-1. Reoxidation and inclusion modification in the tundish

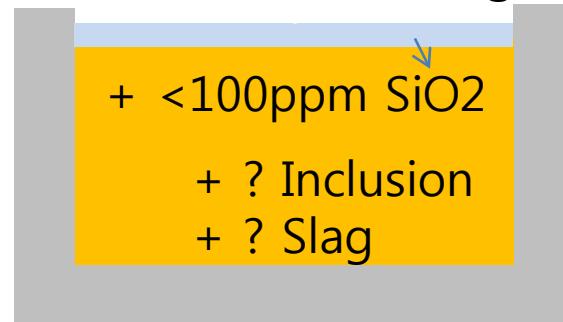
At 1550°C



Ca treatment: liquid slag

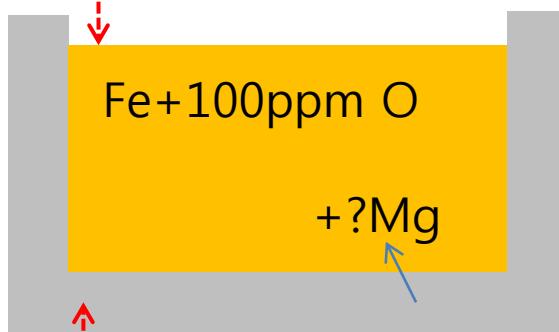


Reoxidation: assuming mainly due to  $\text{SiO}_2$  based slag

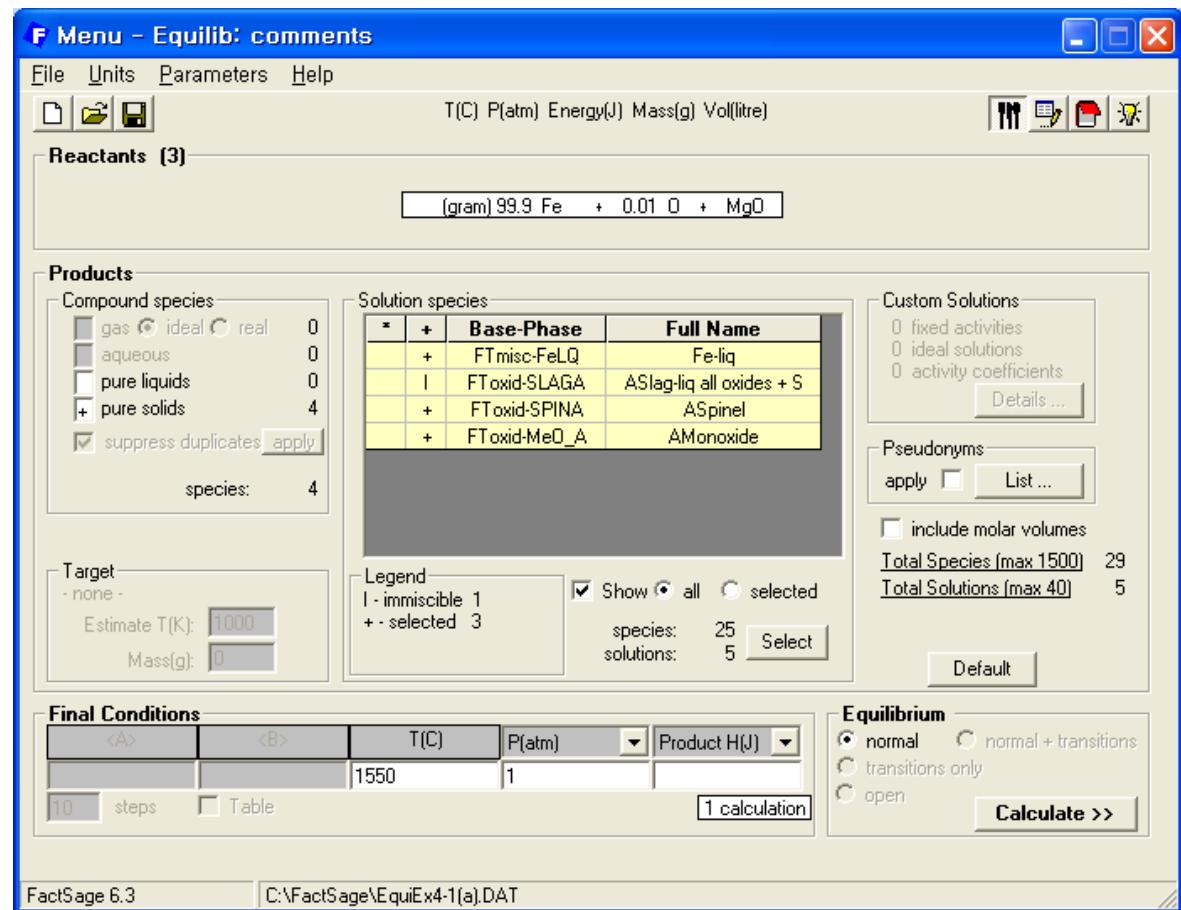


# Ex4-1. Reoxidation and inclusion modification in the tundish

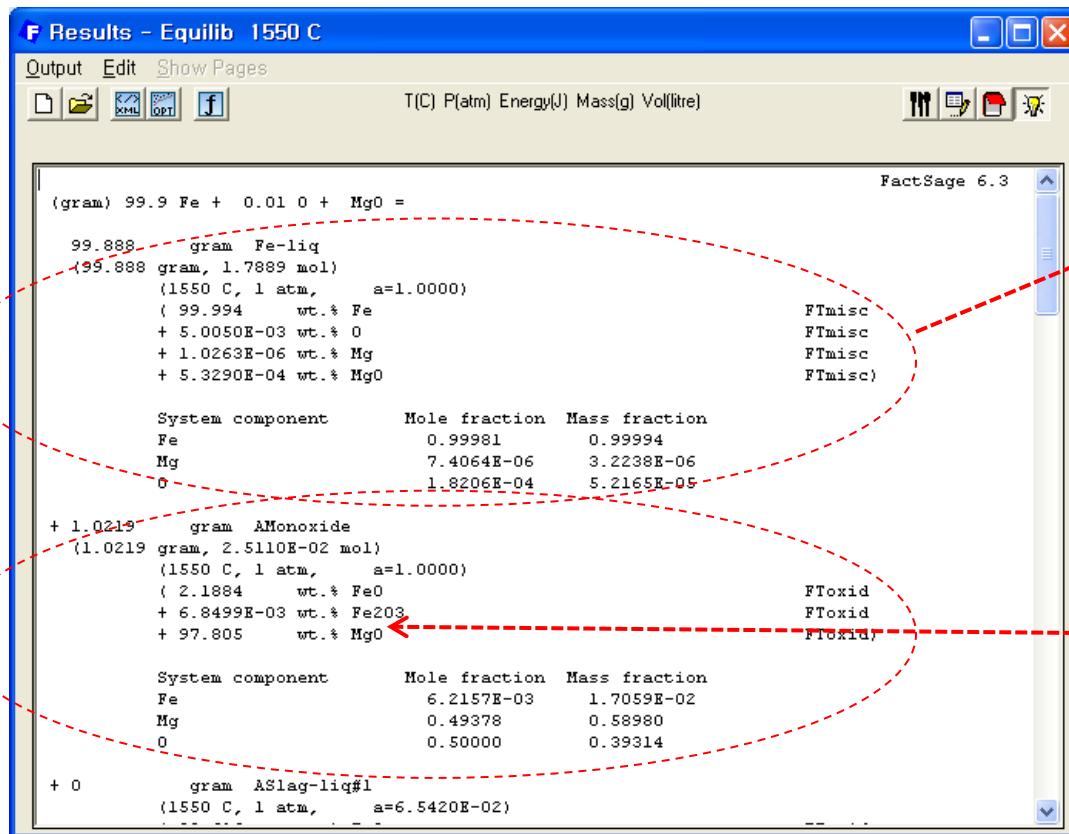
Al killed steel



MgO based refractory



# Ex4-1. Reoxidation and inclusion modification in the tundish



Only save liquid Fe as stream file for next step

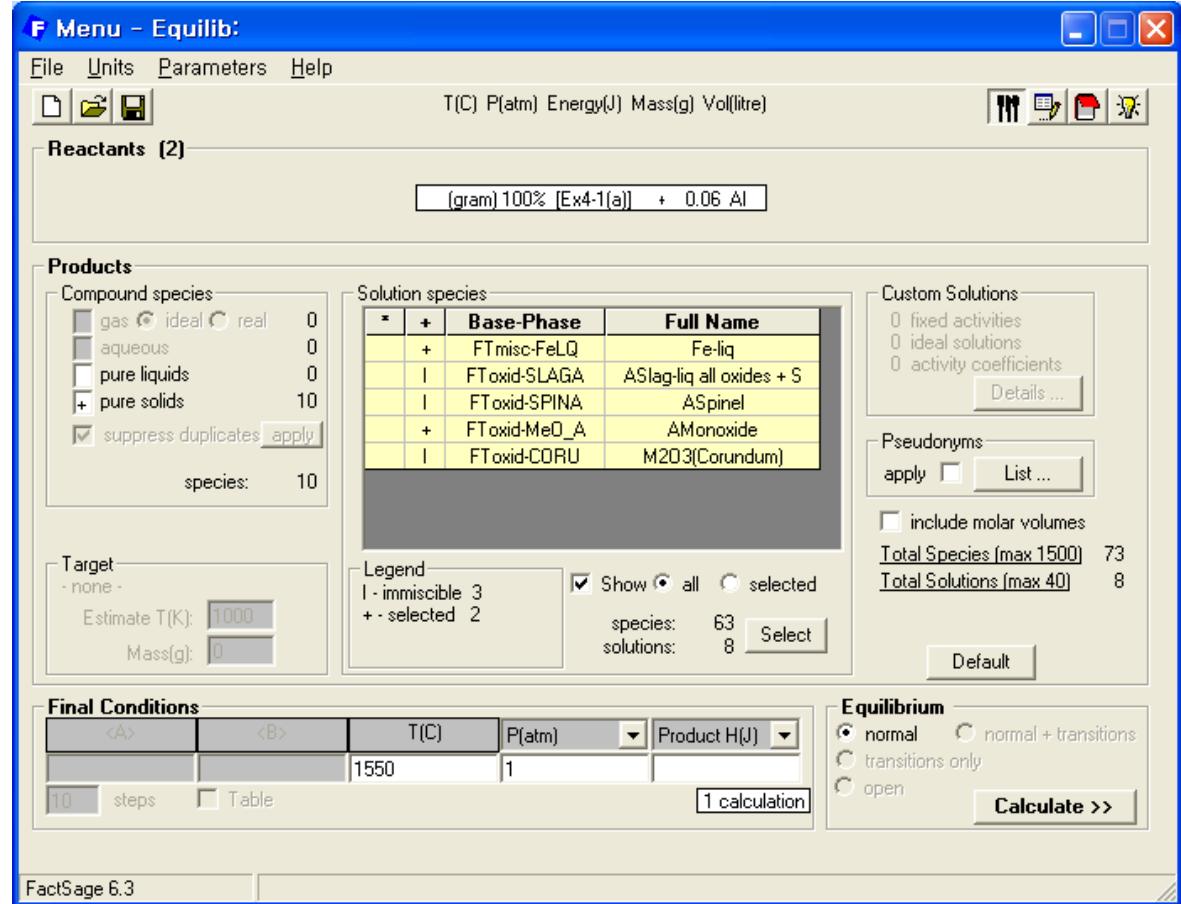
MgO based refractory

# Ex4-1. Reoxidation and inclusion modification in the tundish

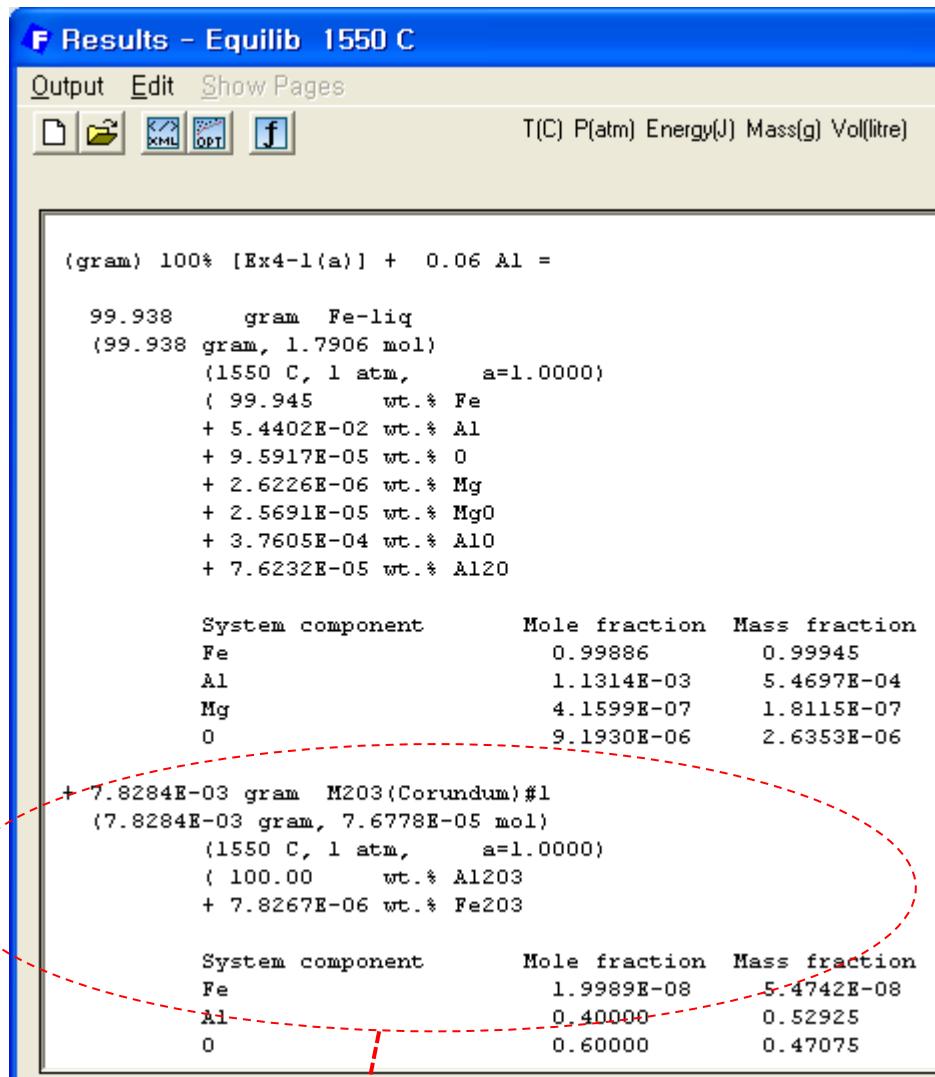
Al killed steel

+ 600ppm Al

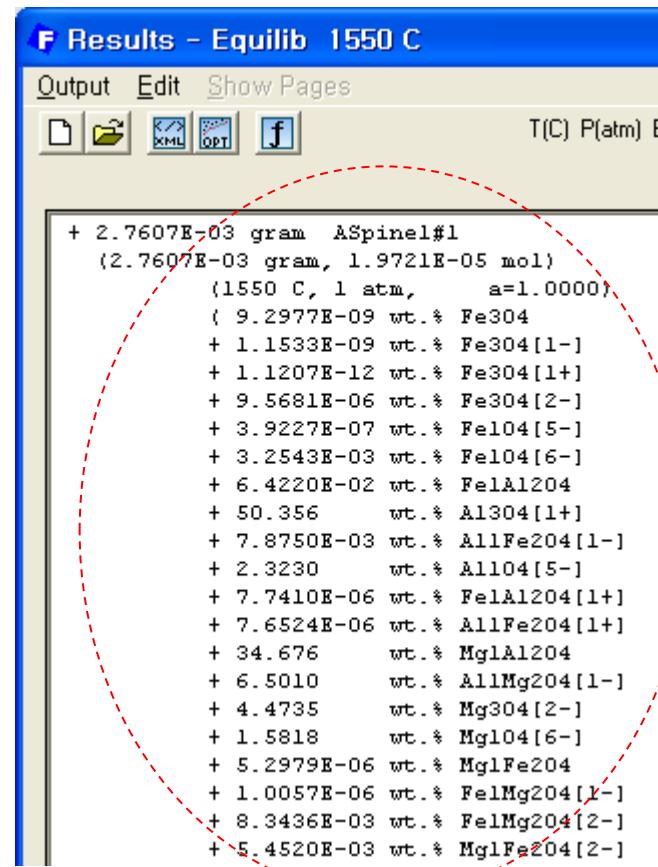
+? inclusion



# Ex4-1. Reoxidation and inclusion modification in the tundish



Alumina inclusion cause nozzle clogging



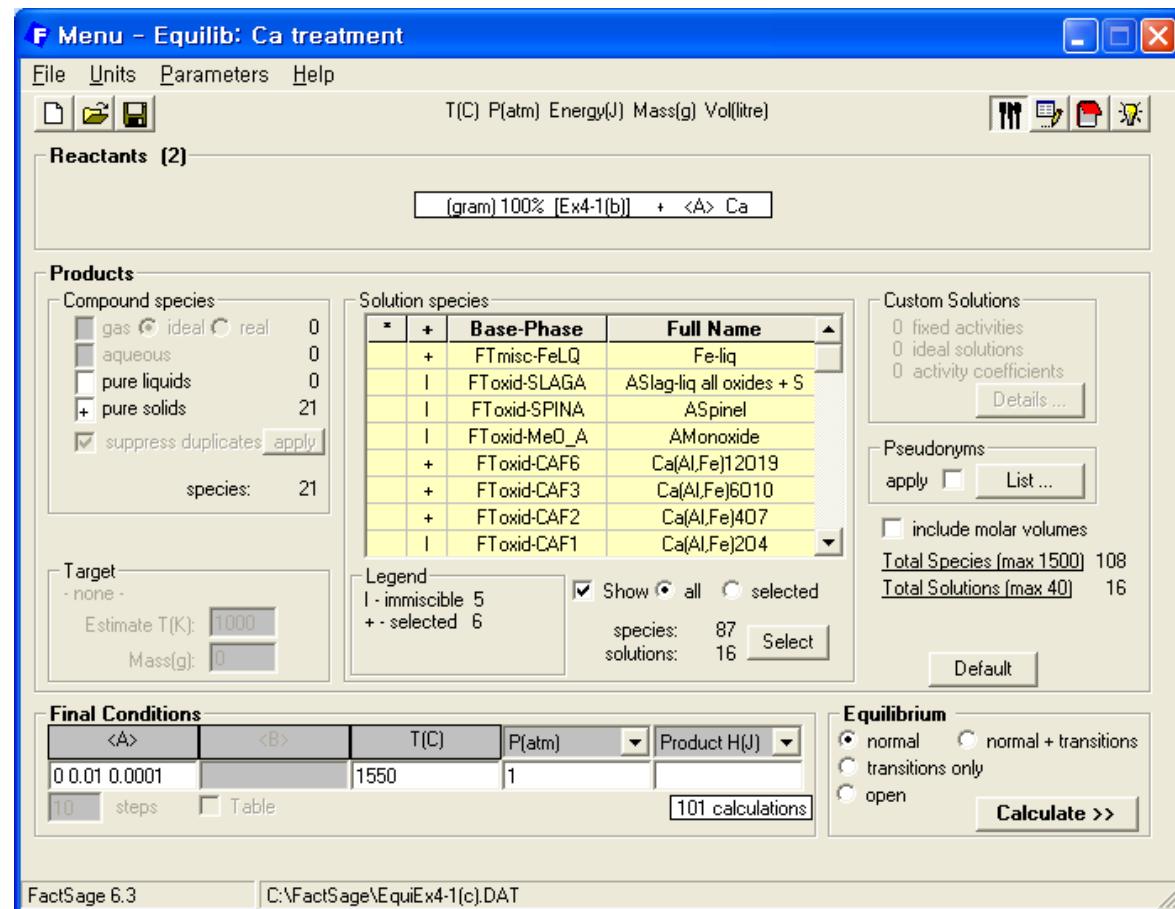
Formation of spinel phase

Save all phases as stream file for next step

# Ex4-1. Reoxidation and inclusion modification in the tundish

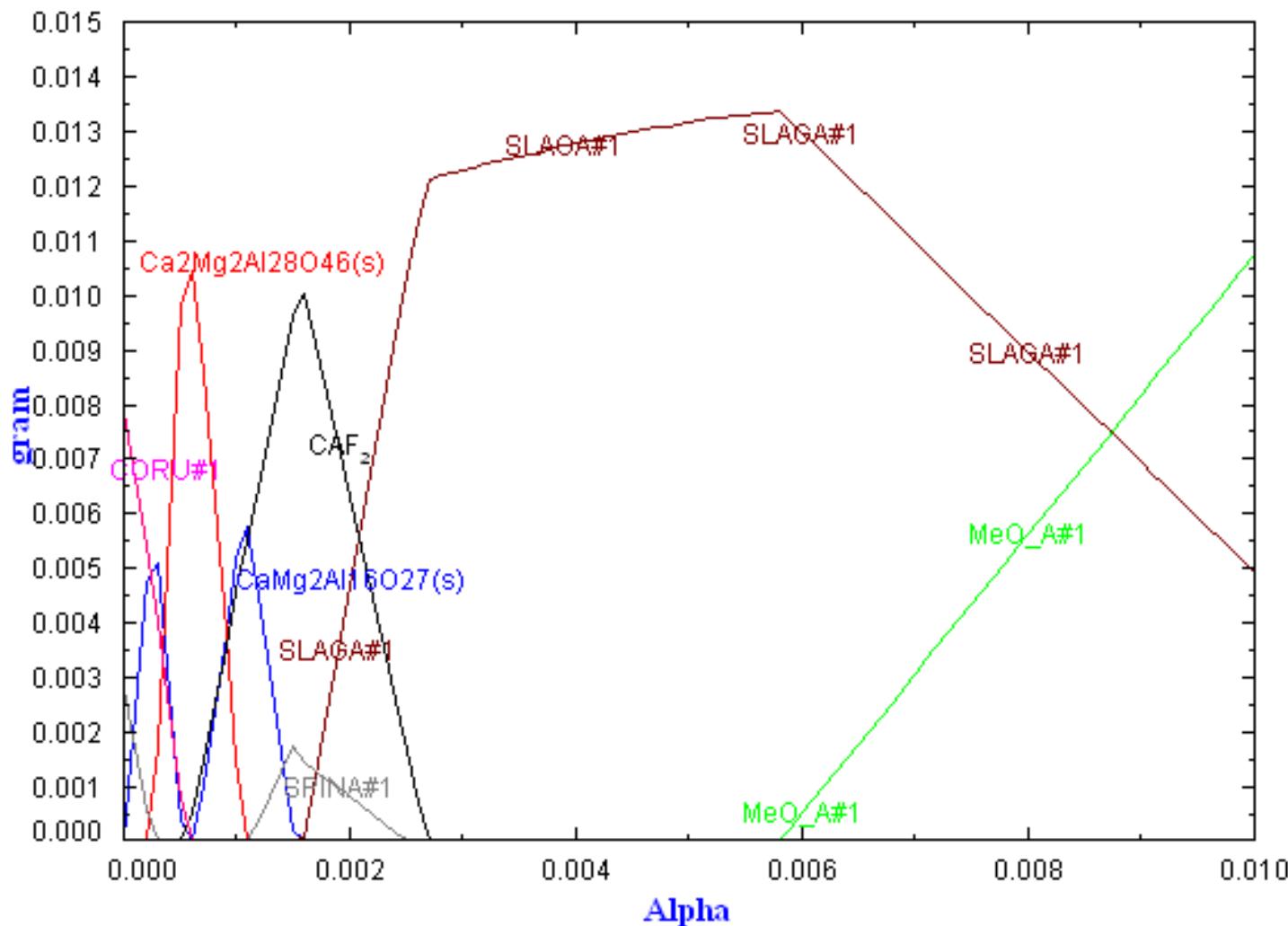
Ca treatment: liquid slag

- + <100ppm Ca
- + ? Inclusion
- + ? Slag



# Ex4-1. Reoxidation and inclusion modification in the tundish

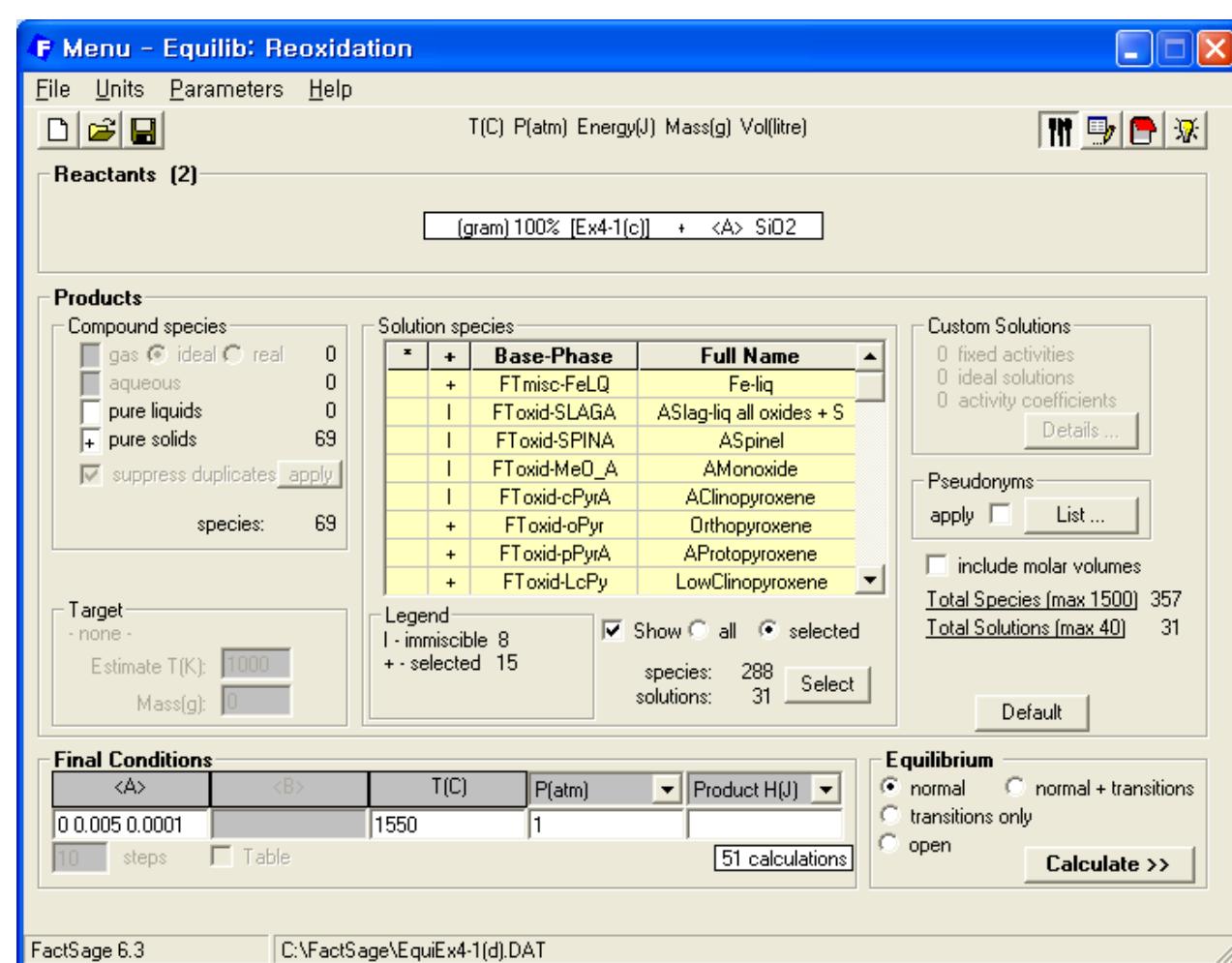
100% [Ex4-1(b)] + <A> Ca



# Ex4-1. Reoxidation and inclusion modification in the tundish

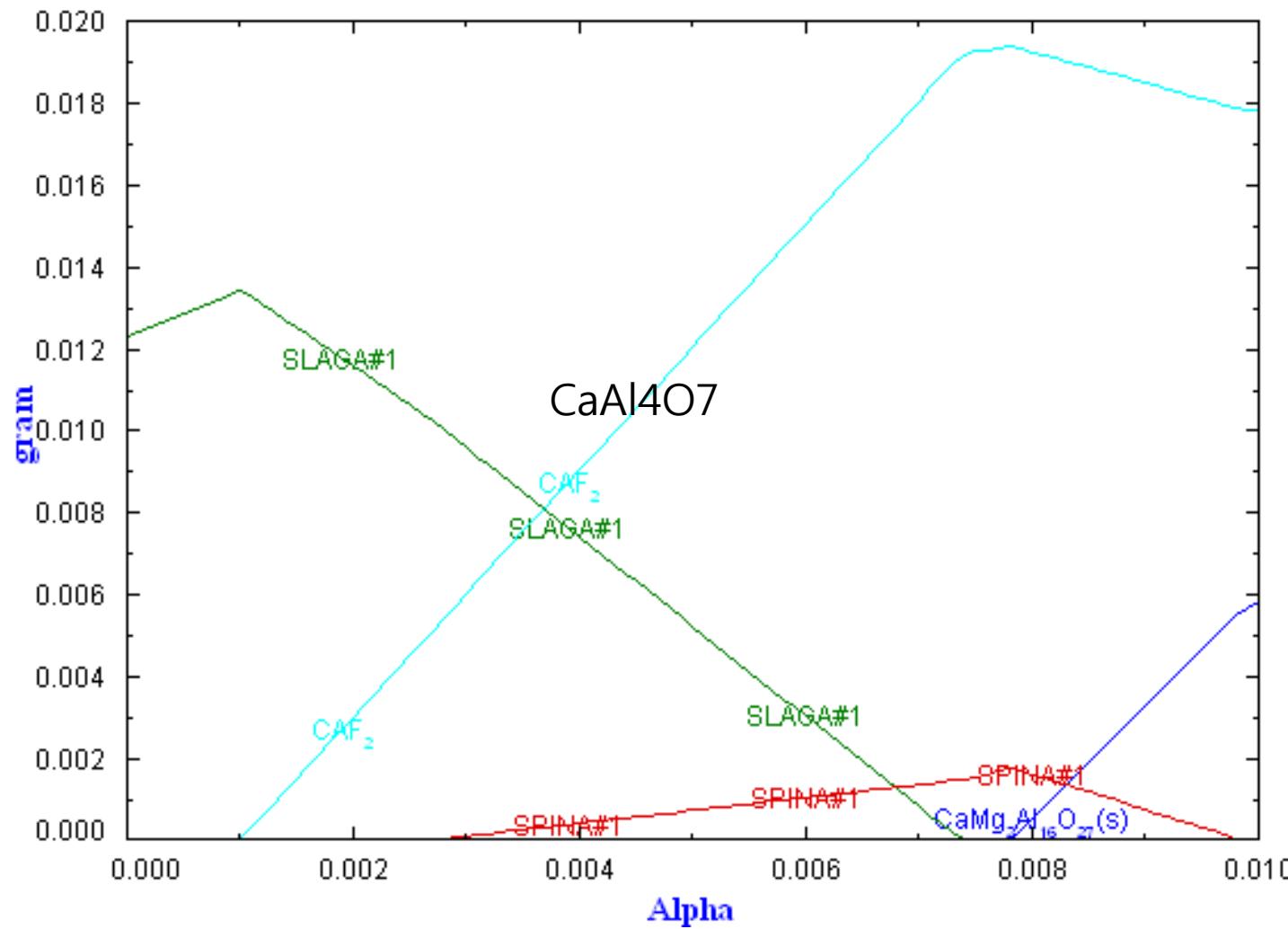
Reoxidation: assuming mainly due to SiO<sub>2</sub> based slag

+ <100ppm SiO<sub>2</sub>  
+ ? Inclusion  
+ ? Slag



# Ex4-1. Reoxidation and inclusion modification in the tundish

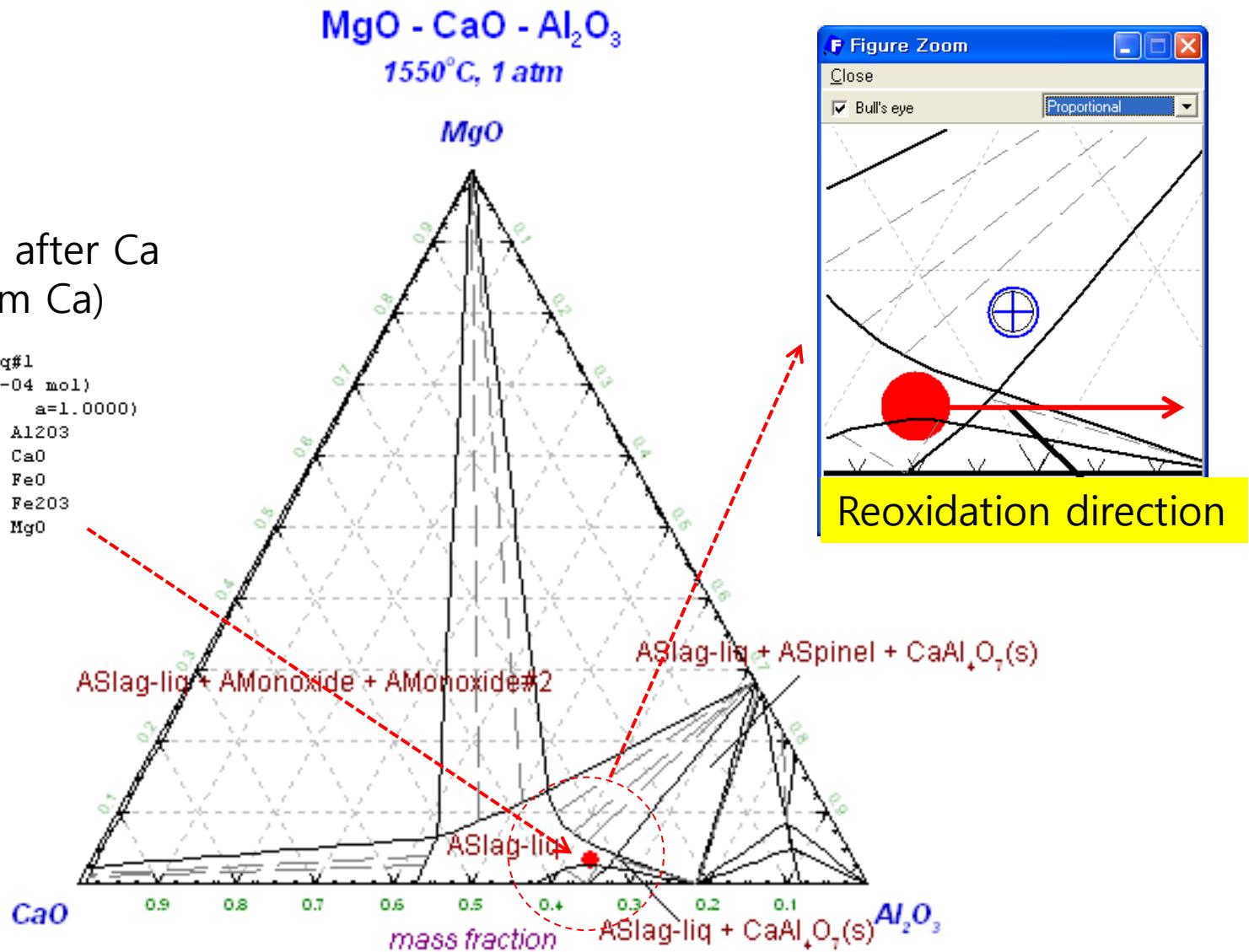
100% [Ex4-1(c)] + <A> SiO<sub>2</sub>



# Ex4-1. Reoxidation and inclusion modification in the tundish

Slag composition after Ca treatment (30 ppm Ca)

```
+ 1.2284E-02 gram ASlag-liq#1  
(1.2284E-02 gram, 1.5945E-04 mol)  
(1550 C, 1 atm, a=1.0000)  
+ 63.328    wt.% Al2O3  
+ 33.369    wt.% CaO  
+ 6.3444E-03 wt.% FeO  
+ 3.9494E-05 wt.% Fe2O3  
+ 3.2969    wt.% MgO
```



# Ex4-2. Reoxidation of Al killed Ti bearing steel

**Data Search**

Databases - 3/37 compound databases, 2/38 solution databases

**FactSGTE**

- FactIPS
- FToxid
- FTsalt
- FTmisc
- FThall
- FTOxCN
- FTfritz
- FTheulg
- FTpulp
- FTlite
- FSopp
- FSlead
- FSITE
- FSstel
- FSnobl
- FSnobl
- SGPS
- SGTE
- SGnobl
- SGsold
- SGnuc
- BINS
- CON1
- CON2
- BSIP

**Miscellaneous**

compounds only    solutions only    no database

Clear All    Select All    Add/Remove    RefreshData

**Other**

ELEM    TDnucl

**Information**

Options

Include

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

Default    Cancel    Summary

**Menu - Equilib: last system**

File    Units    Parameters    Help

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

**Reactants (8)**

(gram) 98.9475 Fe + 0.7 Mn + 0.03 Al + 0.2 Si + 0.0025 O + 0.015 N + 0.005 C + 0.1 Ti

**Products**

Compound species

<input type="radio"/> gas	<input checked="" type="radio"/> ideal	<input type="radio"/> real	56
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	0
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	0
<input checked="" type="checkbox"/> pure solids			123
* suppress duplicates <input type="button" value="apply"/>			
* custom selection			
species: 179			

Solution species

*	+	Base-Phase	Full Name
		FToxid-ILME?	?Ilmenite
	+	FToxid-PSEU	Pseudobrookite
	+	FToxid-TiSp	Titania_Spinel
	+	FToxid-TSp	Tetragonal-Spinel
	+	FToxid-Bixb	Mn <sub>2</sub> O <sub>3</sub> (Bixbyite)
	+	FToxid-Brau	Mn <sub>7</sub> SiO <sub>12</sub>
	+	FToxid-Rhod	Rhodonite
	+	FToxid-AlSp	Al-spinel

Custom Solutions

- fixed activities
- ideal solutions
- activity coefficients

Details ...

Pseudonyms

apply  List ...

include molar volumes

Total Species (max 1500) 318

Total Solutions (max 40) 21

Target

- none -

Estimate T(C): 1600

Mass(g): 0

Legend

I - immiscible 5  
+ - selected 11

Show  all  selected

species: 139

solutions: 21

Select

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
		1600	1	
10	steps	<input type="checkbox"/> Table		1 calculation

Equilibrium

normal     normal + transitions

transitions only

open

Calculate >>

FactSage 6.3

# Ex4-2. Reoxidation of Al killed Ti bearing steel

**Results - Equilib 1600 C**

**Output Edit Show Pages**

Save or Print Plot Equilib Results file Stream File Format Fact-XML Fact-Optimal Fact-Function-Builder Refresh ...

Recycle all streams ... Save stream file Stream file properties ... Summary of streams Directory (C:\Slag-Steel-Inclusions) ...

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

Fe (CO) 5 FactPS FactPS FactPS

Mn FTmisc FTmisc FTmisc

N FTmisc FTmisc FTmisc

O FTmisc FTmisc FTmisc

+ 0.20001 wt.% Si + 9.9530E-02 wt.% Ti + 4.9668E-04 wt.% AlO + 5.7546E-04 wt.% TiO + 3.3327E-06 wt.% SiO + 3.4562E-05 wt.% MnO + 4.6211E-05 wt.% Al2O + 1.9820E-05 wt.% Ti2O

System component Mole fraction Mass fraction Fe 0.98635 0.98951 Mn 7.0931E-03 7.0003E-03 Ti 1.1627E-03 9.9979E-04 Si 3.9642E-03 2.0001E-03 Al 5.7624E-04 2.7930E-04 O 2.2459E-05 6.4552E-06 N 5.9617E-04 1.5001E-04 C 2.3175E-04 5.0002E-05

+ 3.9506E-03 gram M2O3(Corundum)#1 (3.9506E-03 gram, 3.8637E-05 mol) (1600 C, 1 atm, a=1.0000) ( 99.036 wt.% Al2O3 + 2.8914E-05 wt.% Fe2O3 + 4.8020E-07 wt.% Mn2O3 + 0.96386 wt.% Ti2O3

System component Mole fraction Mass fraction Fe 7.4054E-08 2.0223E-07 Mn 1.2440E-09 3.3421E-09 Ti 2.7427E-03 6.4199E-03

FToxid FToxid FToxid

**Equilib 1600 C**

**dit Show Pages**

XMB OPT f T(C) P(atm) Energy(J) Mass(g) Vol(litre)

Fe (CO) 5 FactPS FactPS FactPS

+ 1.5906E-40 Fe (CO) 5

+ 2.8722E-45 N2O4

+ 3.6814E-55 N2O5

96 gram Fe-liq 996 gram, 1.7963 mol) (1600 C, 1 atm, a=1.0000) ( 98.951 wt.% Fe + 2.7583E-02 wt.% Al + 5.0002E-03 wt.% C + 0.70000 wt.% Mn + 1.5001E-02 wt.% N + 2.9406E-04 wt.% O + 0.20001 wt.% Si + 9.9530E-02 wt.% Ti + 4.9668E-04 wt.% AlO + 5.7546E-04 wt.% TiO + 3.3327E-06 wt.% SiO + 3.4562E-05 wt.% MnO + 4.6211E-05 wt.% Al2O + 1.9820E-05 wt.% Ti2O

System component Mole fraction Mass fraction Fe 0.98635 0.98951 Mn 7.0931E-03 7.0003E-03 Ti 1.1627E-03 9.9979E-04 Si 3.9642E-03 2.0001E-03 Al 5.7624E-04 2.7930E-04 O 2.2459E-05 6.4552E-06 N 5.9617E-04 1.5001E-04 C 2.3175E-04 5.0002E-05

+ 3.9506E-03 gram M2O3(Corundum)#1 (3.9506E-03 gram, 3.8637E-05 mol) (1600 C, 1 atm, a=1.0000) ( 99.036 wt.% Al2O3 + 2.8914E-05 wt.% Fe2O3 + 4.8020E-07 wt.% Mn2O3 + 0.96386 wt.% Ti2O3

System component Mole fraction Mass fraction Fe 7.4054E-08 2.0223E-07 Mn 1.2440E-09 3.3421E-09 Ti 2.7427E-03 6.4199E-03

FToxid FToxid FToxid

# Ex4-2. Reoxidation of Al killed Ti bearing steel

The screenshot shows the FactSage software interface. The main window has a menu bar with 'Output', 'Edit', and 'Show Pages'. A context menu is open over the 'Stream File' option, listing 'Recycle all streams ...', 'Save stream file', 'Stream file properties ...', 'Summary of streams', and 'Directory (C:\Slag-Steel-Inclusions)\ ...'. Below this, there's a table of system components and their mole and mass fractions. To the right, a 'Reactants - Equilib' dialog box is open, showing a table for entering reactant information.

System component	Mole fraction	Mass fraction
Fe	0.98635	0.98951
Mn	7.0931E-03	7.0003E-03
Ti	1.1627E-03	9.9979E-04
Si	3.9642E-03	2.0001E-03

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
100%	[Rc_Fe-liq]				2	
+ 100%	[Rc_M2O3(Corund)]				3	

**"Recycle all streams"**

- you don't have to save the stream one by one. But the results will be used only one time because it is not saved under special stream name.
- Convenient option when you want to do one calculation

Initial Conditions

System component	Mole fraction	Mass fraction
Fe	7.4054E-08	2.0223E-07
Mn	1.2440E-09	3.3421E-09
Ti	2.7427E-03	6.4199E-03

FactSage 6.3   Compound: 3/37 databases   Solution: 2/28 databases

Next >

## Ex4-2. Reoxidation of Al killed Ti bearing steel

Menu - Equilib: last system

File Units Parameters Help

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

Reactants (3)

(gram) 100% [Rc\_Fe-liq] + 100% [Rc\_M2O3(Corundum)] + <A> O<sub>2</sub>

Products

Compound species

- + gas  ideal  real 56
- aqueous 0
- pure liquids 0
- \* + pure solids 123

suppress duplicates

\* - custom selection species: 179

Solution species

*	+	Base-Phase	Full Name
*	+	FTmisc-FeLQ	Fe-liq
		FTmisc-BCCS	bcc
		FTmisc-FCCS	fcc
I	FToxic-SLAGA	ASlag-liq all oxides + S	
	FToxic-SLAGG	GSlag-liq with C/N/CN	
I	FToxic-SLAG?	?Slag-liq	
I	FToxic-SPINA	ASpinel	
	FToxic-SPINB	BSpinel	

Legend

I - immiscible 5  
+ - selected 11

Show  all  selected

species: 139 solutions: 21

Total Species (max 1500) 318  
Total Solutions (max 40) 21

Default

Final Conditions

<A>	<B>	T(C)	P(atm)	Product H(J)
0 0.05 0.001		1600	1	
10 steps	<input type="checkbox"/> Table	51 calculations		

Equilibrium

normal  normal + transitions  
 transitions only  open

FactSage 6.3

Addition of oxygen to simulation reoxidation phenomena.  
Real source of oxygen could be high SiO<sub>2</sub> slag or refractories

## Ex4-2. Reoxidation of Al killed Ti bearing steel

This calculation shows that mixed inclusion of  $\text{Al}_2\text{O}_3(s)$  and liquid ( $\text{Al}_2\text{O}_3\text{-TiO}_2\text{-Ti}_2\text{O}_3$ ) can be formed by the reoxidation of Al-killed Ti bearing steel.

→ Nozzle clogging.

100% [Rc\_Fe-liq] + 100% [Rc\_M2O3(Corundum)] + <A> O<sub>2</sub>

C:\Slag-Steel-Inclusions\Equi0.res 25Sep12

