

Ferrous Applications II

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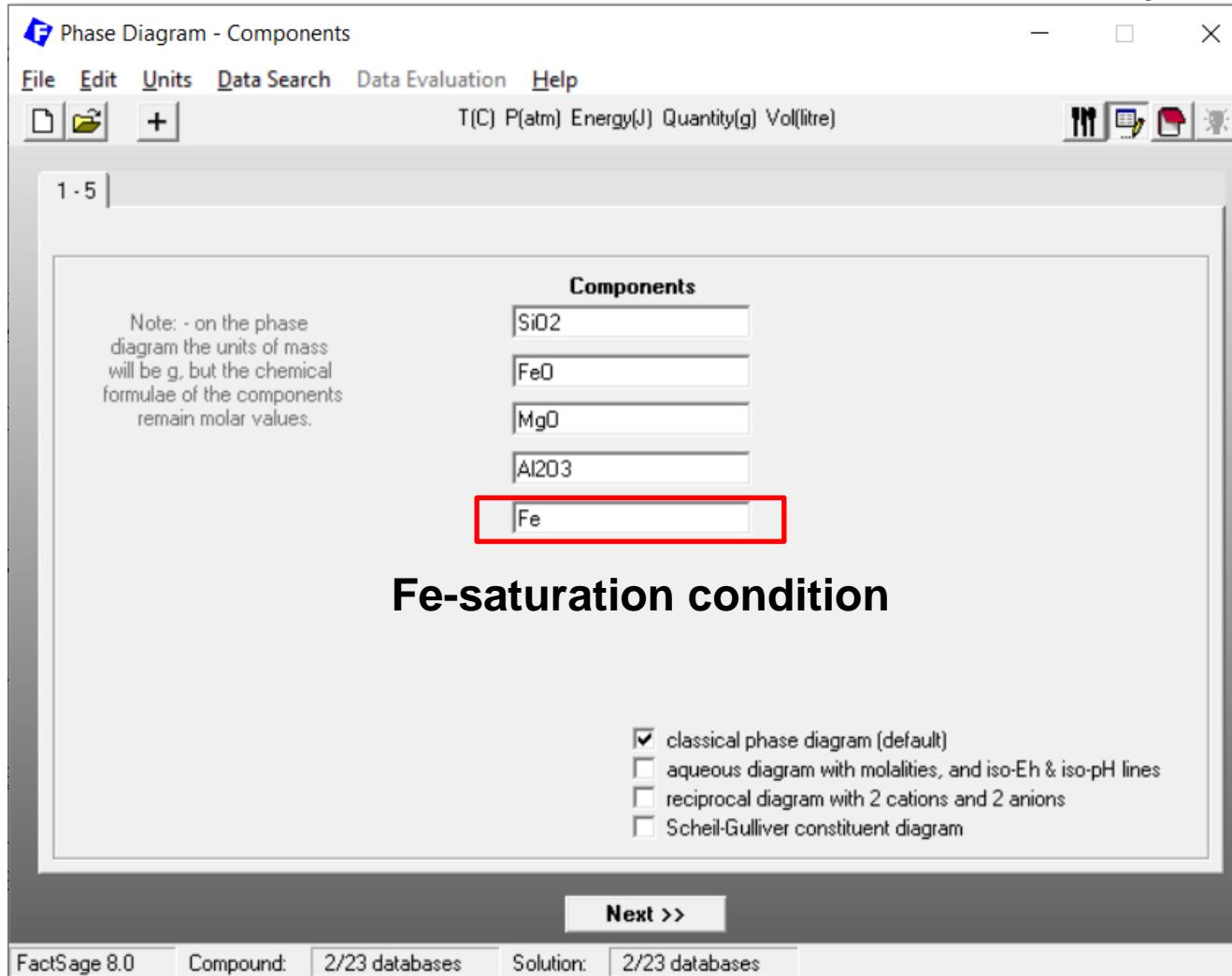
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The effect of SiO_2/MgO and FeO and Al_2O_3 in Slag on the liquidus temperature of the Slag

Phase Diagram / Equilib

Phase diagram of $\text{SiO}_2\text{-MgO-Al}_2\text{O}_3\text{-FeO-Fe}$

Actually, SiO_2/MgO of Laterite is almost same as that of the produced Slag
The main system of Slag is virtually $\text{SiO}_2\text{-MgO-Al}_2\text{O}_3\text{-FeO}$



Phase diagram of SiO_2 - MgO - Al_2O_3 - FeO - Fe

Selection - Phase Diagram - no results -

File Edit Show Sort

Selected: 41/97 **SOLID** Duplicates selected X denotes species excluded by default

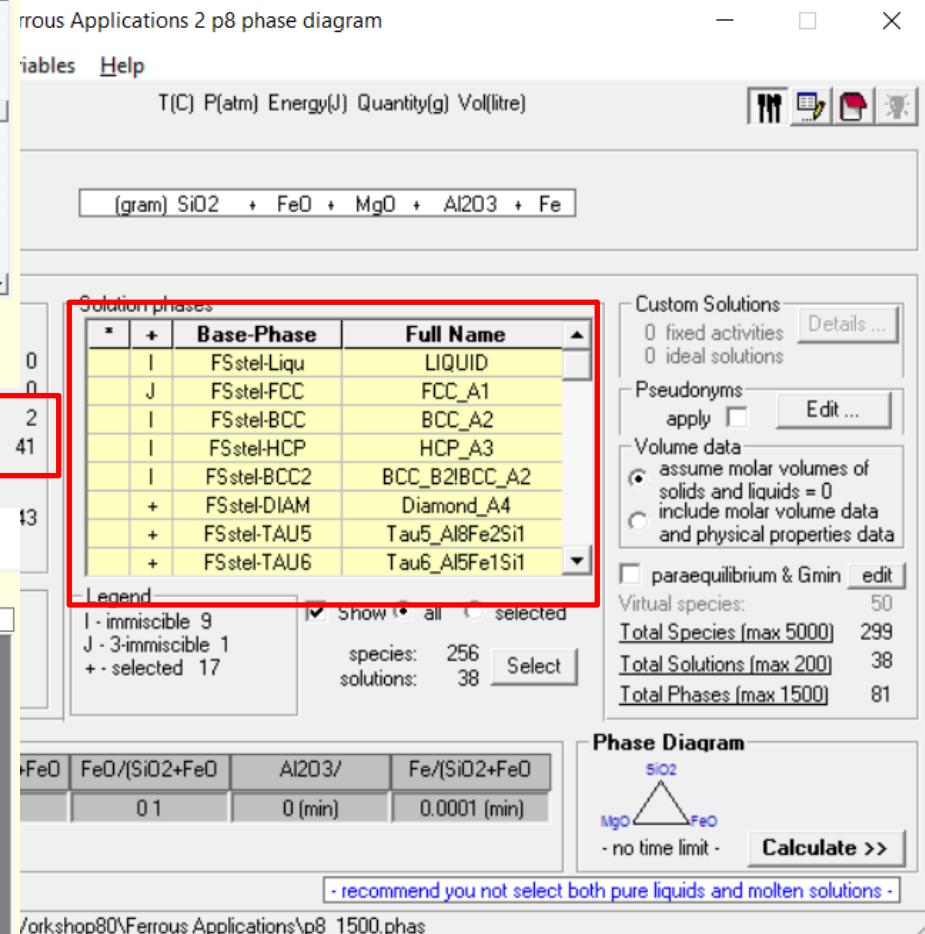
- no results -

+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
X	49	$\text{SiO}_2(\text{s}4)$	FSstel	Tridymite(h)	V				
X	50	$\text{SiO}_2(\text{s}5)$	FSstel	Cristobalite(l)	V				
X	51	$\text{SiO}_2(\text{s}6)$	FSstel	Cristobalite(h)	V				
X	52	$\text{SiO}_2(\text{s}7)$	FSstel	coesite	V				
X	53	$\text{SiO}_2(\text{s}8)$	FSstel	stishovite	V				
	54	$\text{Mg}_2\text{Si}(\text{s})$	FSstel	cF12-Fm(3)m	V				
+	55	$\text{Fe}(\text{s})$	FSstel	BCC_A2	o				
+	56	$\text{Fe}(\text{s}2)$	FSstel	FCC_A1	o				
X	57	$\text{FeO}(\text{s})$	FSstel	Wustite	V				
X	58	$\text{Fe}_2\text{O}_3(\text{s})$	FSstel	hematite	V				
X	59	$\text{Fe}_2\text{O}_3(\text{s}2)$	FSstel	High-Pressure-H	V				
X	60	$\text{Fe}_2\text{O}_3(\text{s}3)$	FSstel	High-Pressure-H	V				
X	61	$\text{Fe}_3\text{O}_4(\text{s})$	FSstel	Magnetite	V				
X	62	$\text{Fe}_3\text{O}_4(\text{s}2)$	FSstel	Magnetite	V				
..

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

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

Select pure solid and liquid of Fe for Fe-saturation condition



File Edit Show Sort

Selected: 1/12 **LIQUID** Duplicates selected X denotes species excluded by default

- no results -

+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
4	4	$\text{Mg}(\text{lq})$	FSstel	liquid	V				
X	5	$\text{MgO}(\text{lq})$	FSstel	liquid	V				
6	6	$\text{Al}(\text{lq})$	FSstel	liquid	V				
X	7	$\text{Al}_2\text{O}_3(\text{lq})$	FSstel	liquid	V				
8	8	$\text{Si}(\text{lq})$	FSstel	liquid	V				
X	9	$\text{SiO}_2(\text{lq})$	FSstel	liquid	V				
+	10	$\text{Fe}(\text{lq})$	FSstel	liquid	o				
11	11	$\text{FeO}(\text{lq})$	FSstel	liquid	V				
X	12	$\text{Fe}_3\text{O}_4(\text{lq})$	FSstel	liquid	V				
X	13	$\text{MgO}(\text{lq})$	FToxid	liquid	V				
X	14	$\text{Al}_2\text{O}_3(\text{lq})$	FToxid	liquid	V				
X	15	$\text{SiO}_2(\text{lq})$	FToxid	liquid	V				

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

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

Phase diagram of SiO₂-MgO-Al₂O₃-FeO-Fe

F Variables: SiO₂-FeO-MgO-Al₂O₃-Fe composition #1. vs composition #1.

Variables

compositions 4
 log10(a) 0
 Next >>

T and P

Temperature constant T(C) 1500
 Pressure or Volume P(atm) constant 1
 log P
 V(litre)
 log V

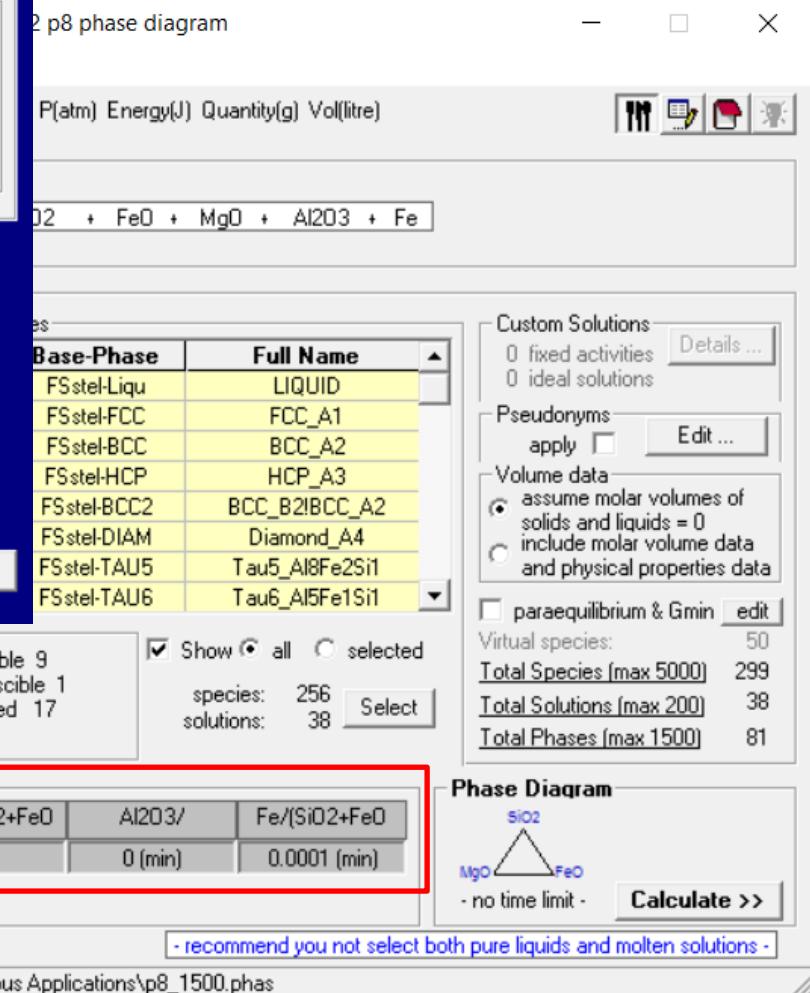
Compositions Quantity(g)

#1. 1 SiO₂ + 0 FeO + 0 MgO + 0 Al₂O₃ + 0 Fe = A-Corner
 1 (max)
 0 (min)

#1 SiO₂ + 1 FeO + 1 MgO + 0 Al₂O₃ + 0 Fe
 #4 log10(composition)

Composition # #1 max = 5

Cancel OK



Phase diagram of SiO₂-MgO-Al₂O₃-FeO-Fe

Variables: SiO₂-FeO-MgO-Al₂O₃-Fe composition #1. vs composition #1.

Variables

- compositions 4
- X** Y
- a b c d
- A B C
- X,Y steps 11

T and P

- Temperature constant T(C) 1500
- Pressure or Volume P(atm) constant 1
- log P
- V(litre)
- log V

Compositions Quantity(g)

#1. 1 SiO₂ + 0 FeO + 0 MgO + 0 Al₂O₃ + 0

#1. 1 SiO₂ + 1 FeO + 1 MgO + 0 Al₂O₃ + 0

#4 log10(composition)

Composition # **#1** max = 5

Cancel

Add small amount of Fe

**Ternary phase diagram
of FeO-MgO-SiO₂
at constant Al₂O₃
with Fe-saturation**

Variables

- compositions 4
- X** Y
- a b c d
- A B C
- X,Y steps 11

T and P

- Temperature constant T(C) 1500
- Pressure or Volume P(atm) constant 1
- log P
- V(litre)
- log V

Compositions Quantity(g)

#5. 0 SiO₂ + 0 FeO + 0 MgO + 0 Al₂O₃ + 1 Fe

#5. 1 SiO₂ + 1 FeO + 1 MgO + 0 Al₂O₃ + 0 Fe

#5 log10(composition)

Composition # **#5** max = 5

Constant
0.0001

Cancel **OK**

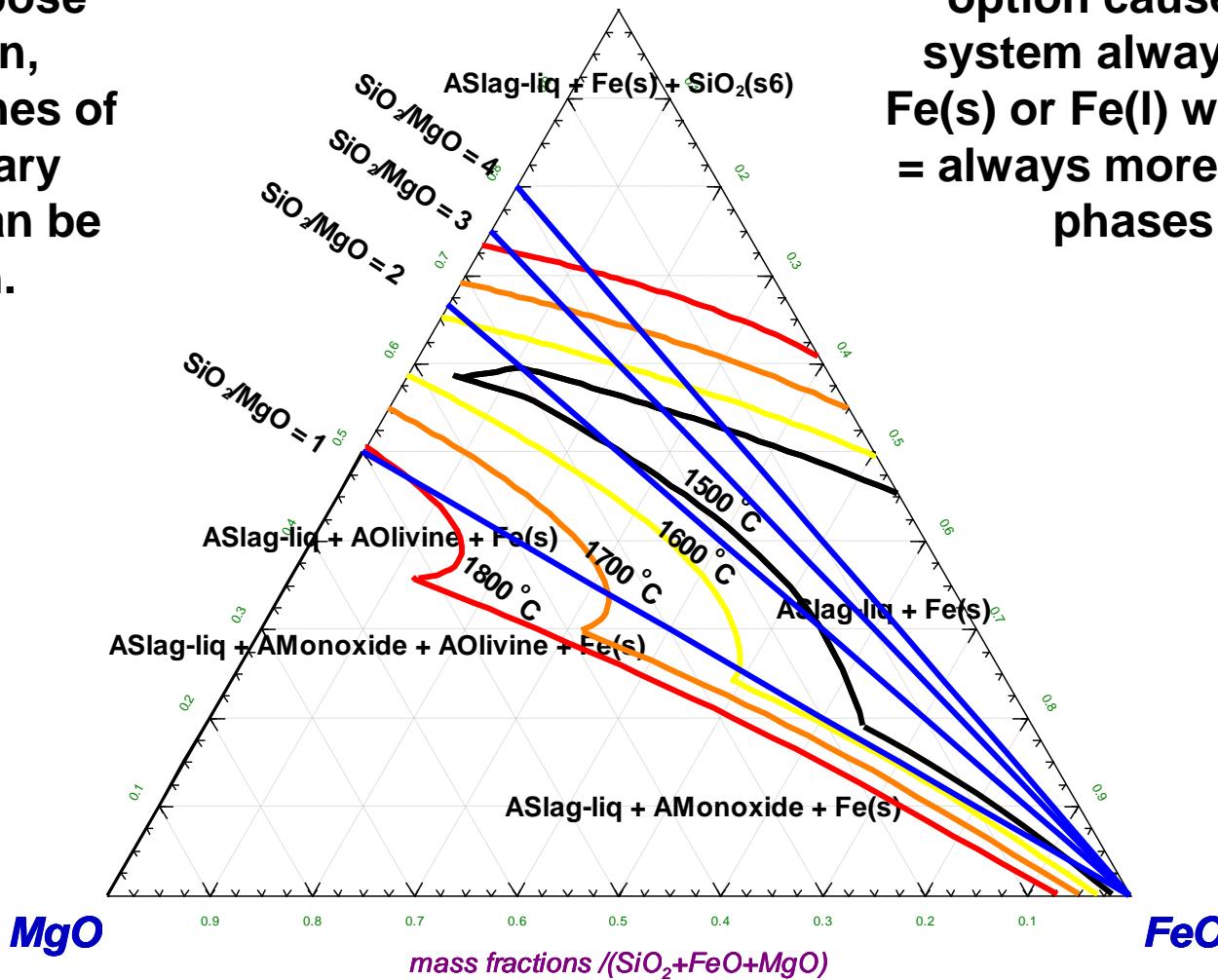
Phase diagram of SiO_2 - MgO - Al_2O_3 - FeO - Fe

Using
'superimpose'
function,
liquidus lines of
the ternary
system can be
drawn.

SiO_2 - FeO - MgO - Al_2O_3 - Fe

$$\text{Al}_2\text{O}_3/Z (\text{g/g}) = 0, \text{Fe}/Z (\text{g/g}) = 0.00001, \\ Z = (\text{SiO}_2 + \text{FeO} + \text{MgO}),$$

SiO_2

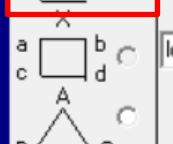


Impossible for 'O'
option cause the
system always has
Fe(s) or Fe(l) with slag
= always more than 2
phases

Phase diagram of SiO₂-MgO-Al₂O₃-FeO-Fe

Variables: SiO₂-FeO-MgO-Al₂O₃-Fe T(C) vs composition #1.

Variables

- Y X
- compositions 4
- a b c d
- log10(a) 0
- A 
- X,Y steps 11

T and P

Temperature

- T(C) Y-axis
- 1/TK
- Max: 2000
- Min: 1000

Pressure or Volume

- P(atm) constant
- log P
- V(litre) 1
- log V

Next >>

With change 0 to 8 wt% of Al₂O₃ at constant SiO₂/MgO=1 under Fe-saturation

Compositions Quantity(g)

#3. $1 \text{ SiO}_2 + 0 \text{ FeO} + -1 \text{ MgO} + 0 \text{ Al}_2\text{O}_3 + 0 \text{ Fe} = \text{constant}$

$1 \text{ SiO}_2 + 1 \text{ FeO} + 1 \text{ MgO} + 1 \text{ Al}_2\text{O}_3 + 1 \text{ Fe} = 0$

#3 log10(composition)

Composition # max = 4

-Al₂O₃-Fe T(C) vs composition #1.

T and P

Temperature

- T(C) Y-axis
- 1/TK
- Max: 2000
- Min: 1000

Pressure or Volume

- P(atm) constant
- log P
- V(litre) 1
- log V

#4. $0 \text{ SiO}_2 + 0 \text{ FeO} + 0 \text{ MgO} + 100 \text{ Al}_2\text{O}_3 + 0 \text{ Fe} = \text{constant}$

$1 \text{ SiO}_2 + 1 \text{ FeO} + 1 \text{ MgO} + 1 \text{ Al}_2\text{O}_3 + 1 \text{ Fe} = 5$

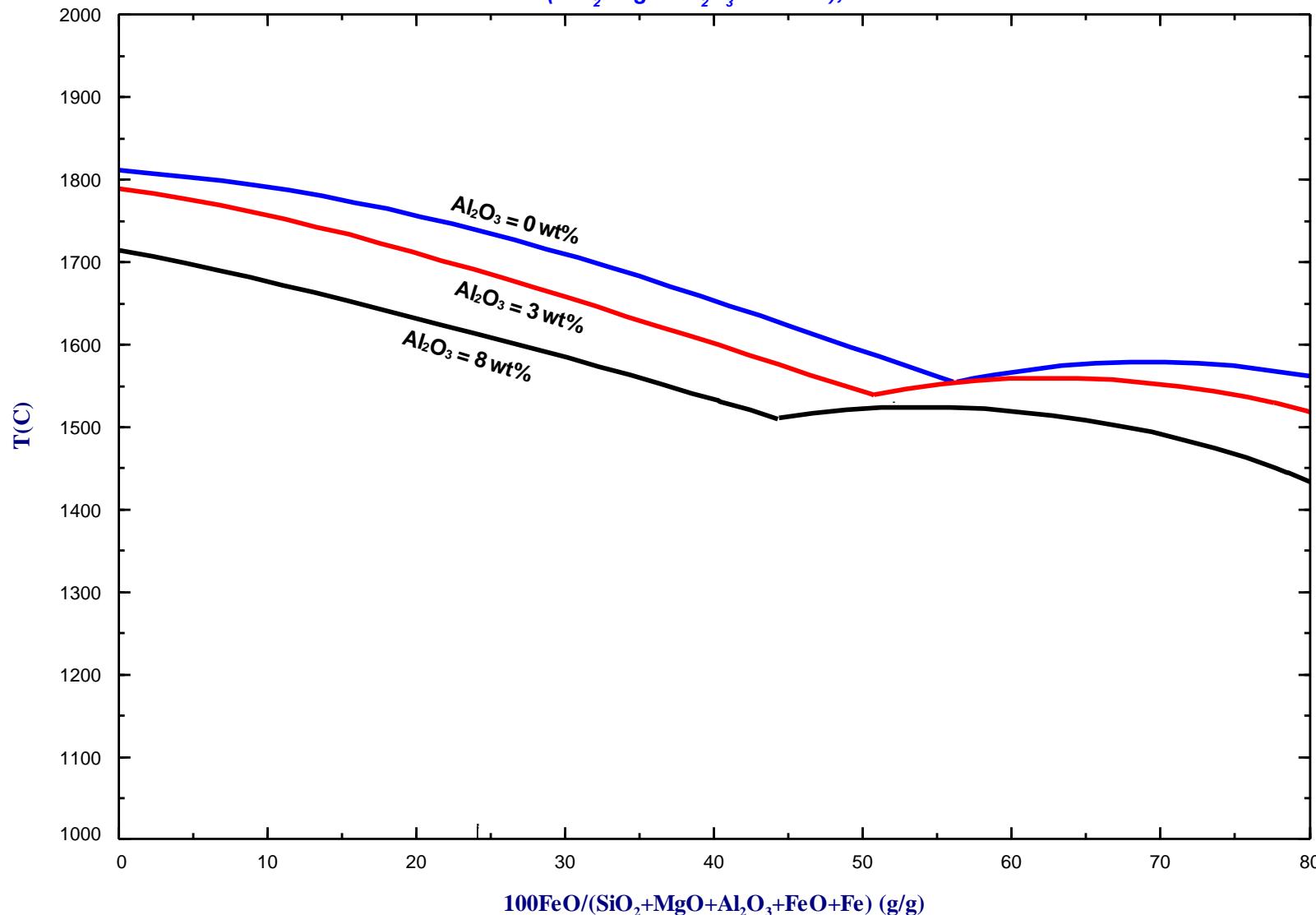
#4 log10(composition)

Composition # max = 4

Phase diagram of SiO_2 - MgO - Al_2O_3 - FeO - Fe

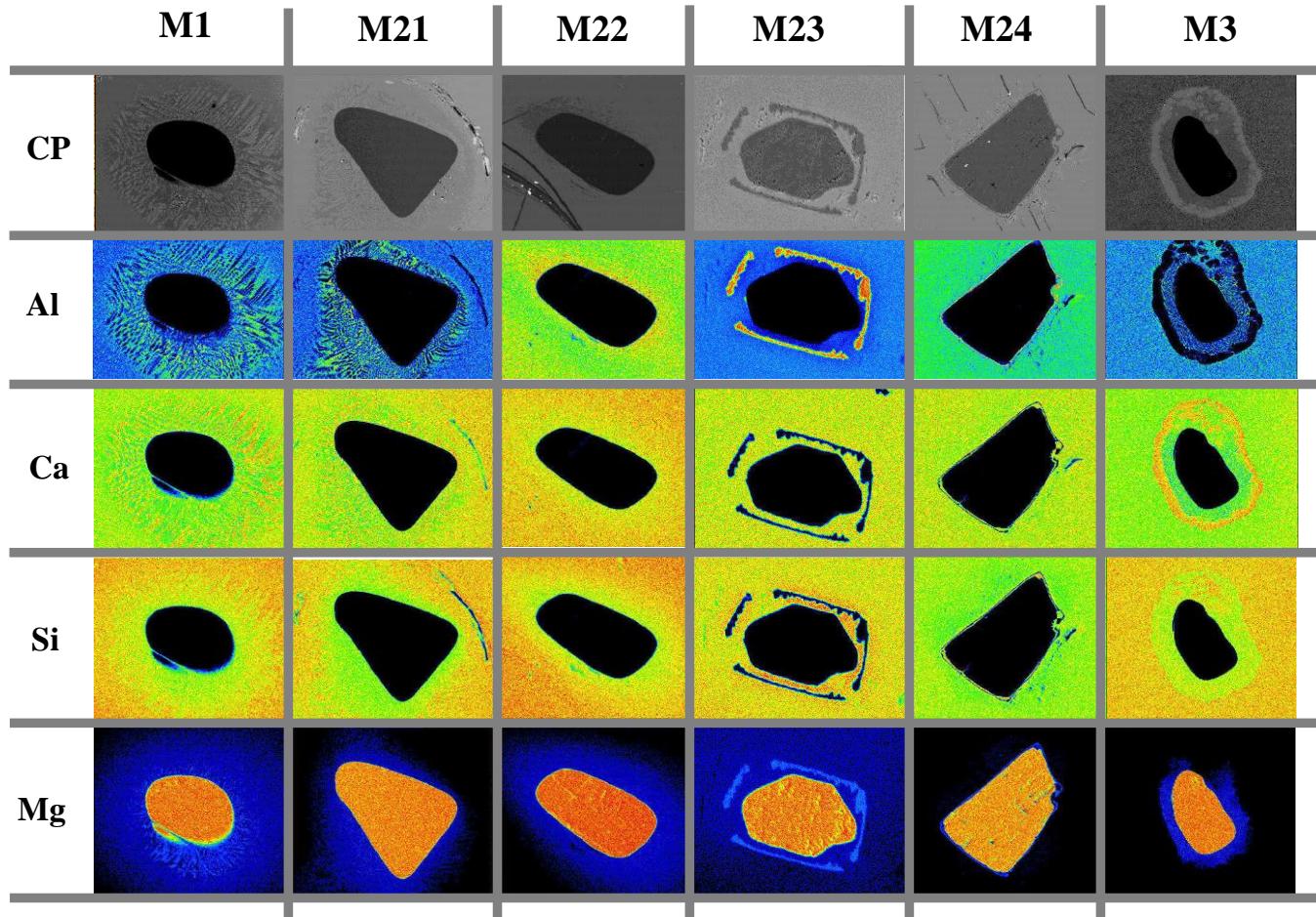
SiO_2 - MgO - Al_2O_3 - FeO - Fe

SiO_2 - $1\text{MgO}/Z \text{ (g/g)} = 0$, $100\text{Al}_2\text{O}_3/Z \text{ (g/g)} = 0$, $100\text{Fe}/Z \text{ (g/g)} = 1$,
 $Z = (\text{SiO}_2 + \text{MgO} + \text{Al}_2\text{O}_3 + \text{FeO} + \text{Fe})$, 1 atm



Dissolution of Inclusions into Molten Slags

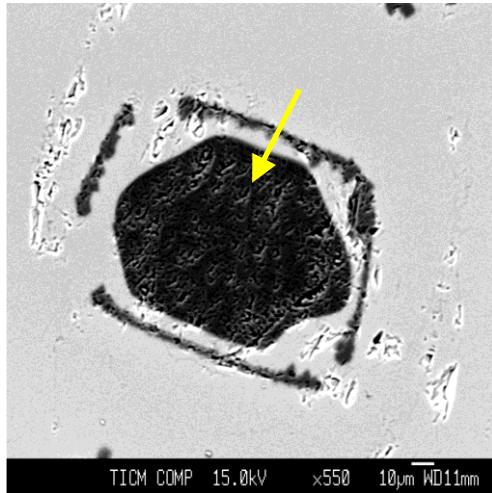
Phase diagram between slag and inclusion to understand the inclusion dissolution mechanism



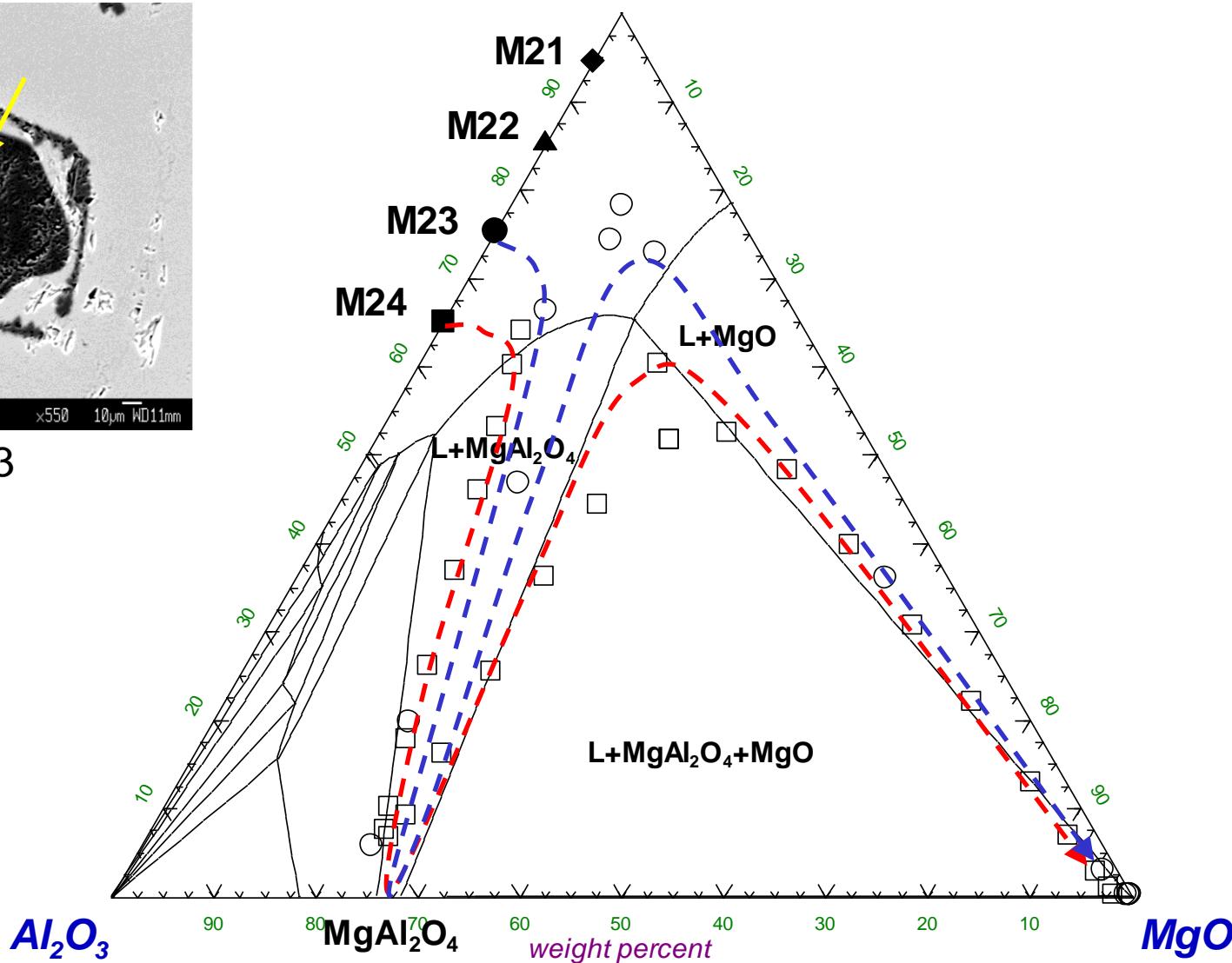
Park, Jung and Lee: ISIJ Inter. No. 11, 2006

Dissolution of Inclusions into Molten Slags

$$(CaO)_{0.525}(SiO_2)_{0.475}$$

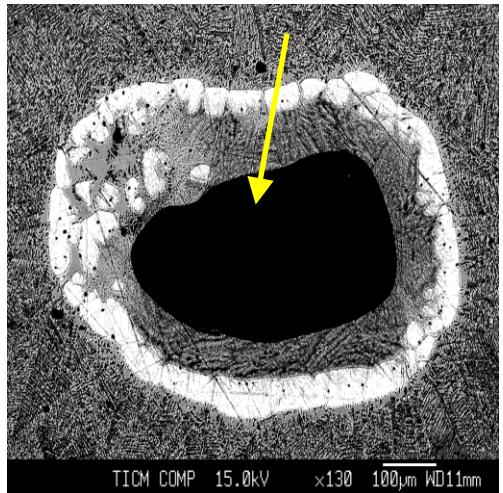


M23

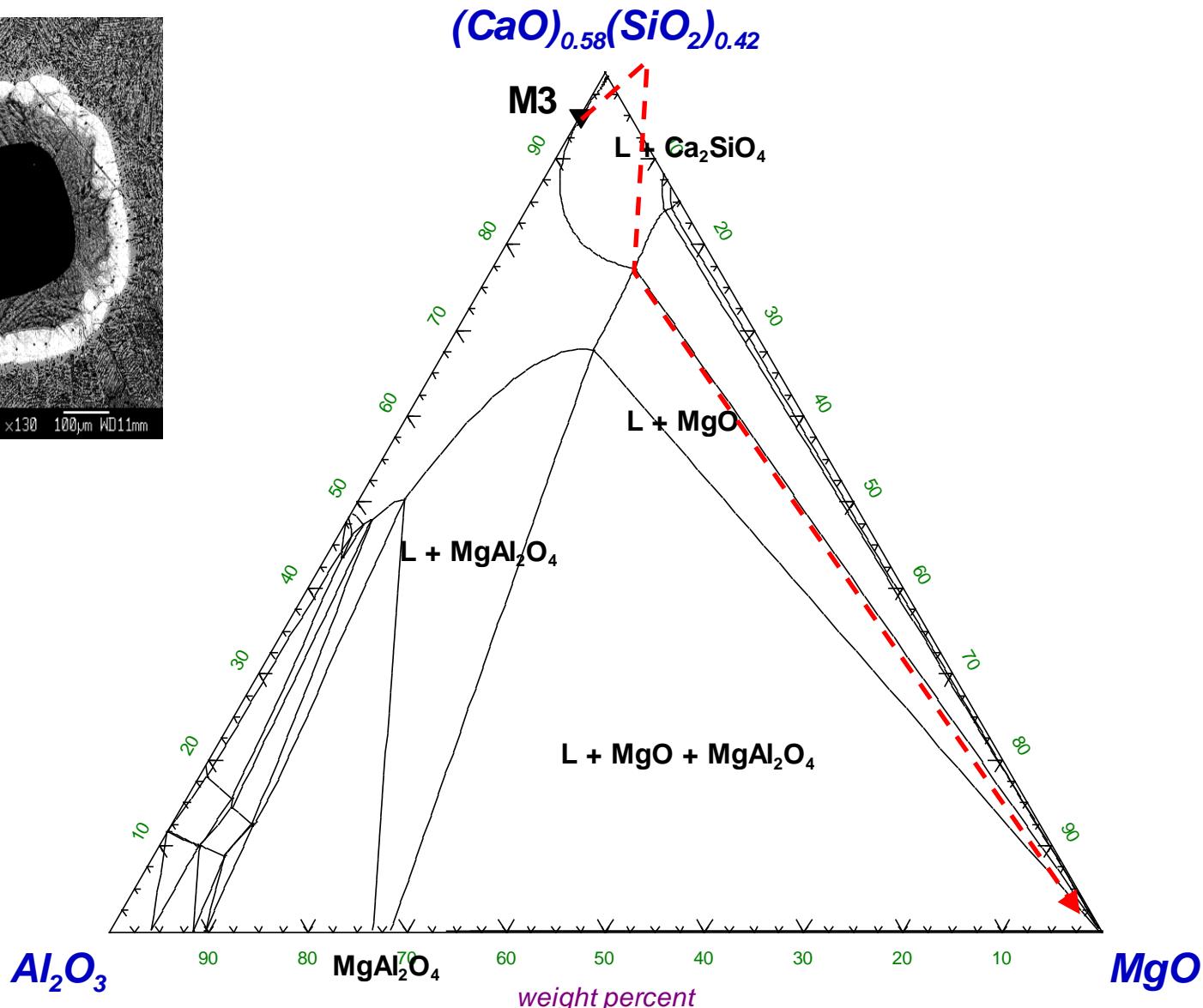


Park, Jung and Lee: ISIJ Inter. No. 11, 2006

Dissolution of Inclusions into Molten Slags



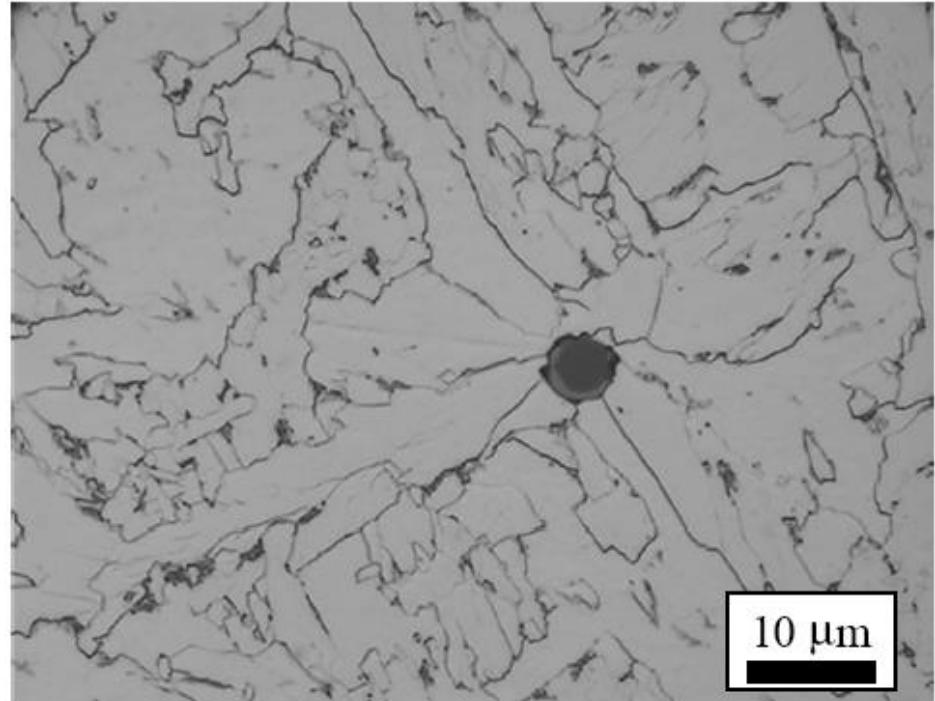
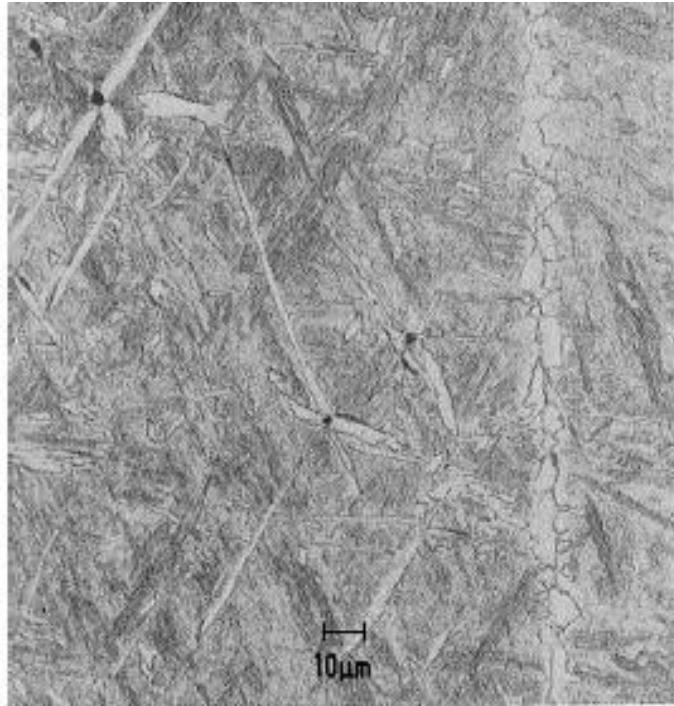
M3



Park, Jung and Lee: *ISIJ Inter.* No. 11, 2006

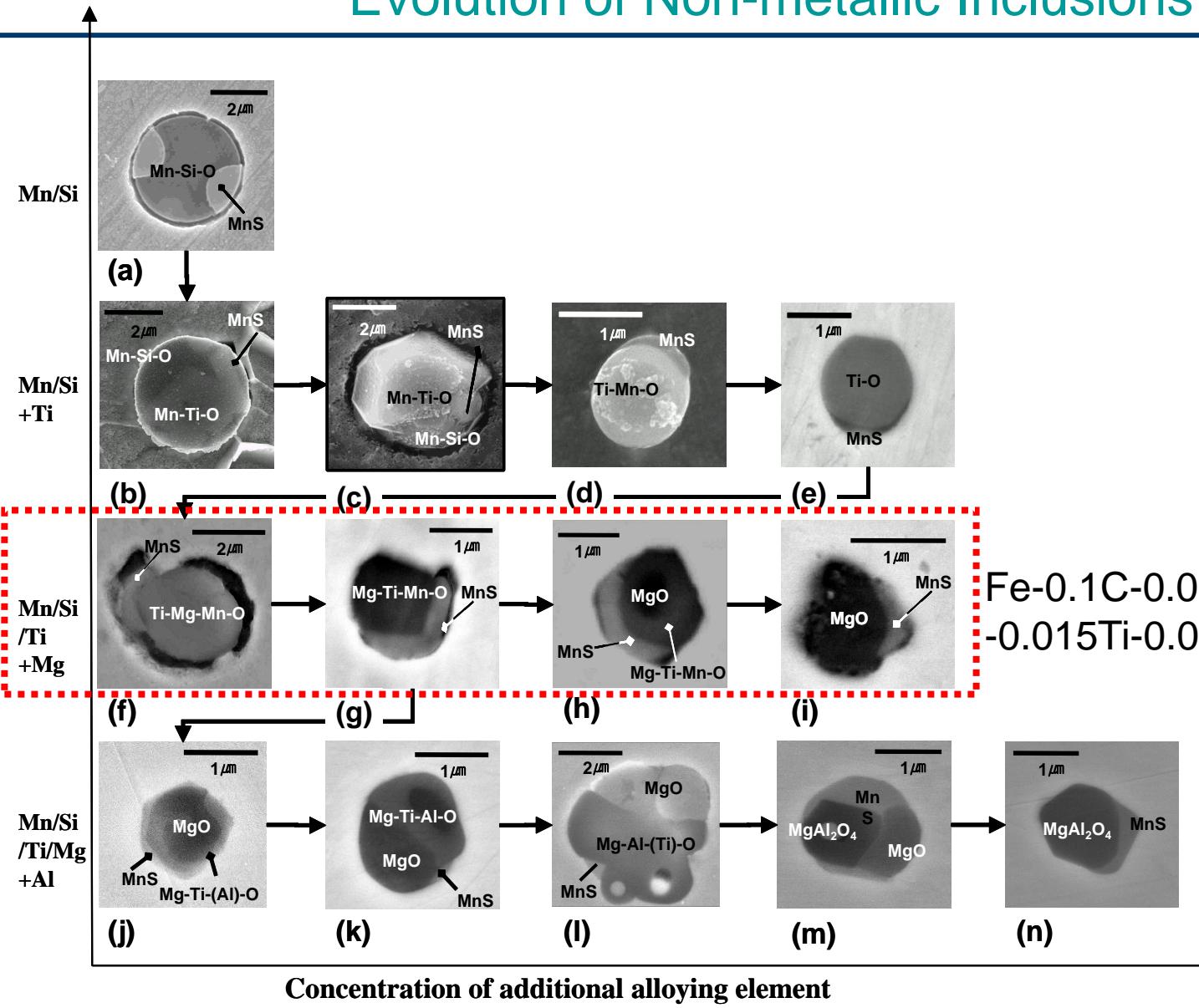
Applications to Oxide metallurgy (Inclusion control)

- Evolution of non-metallic inclusions: Formation of acicular ferrite -



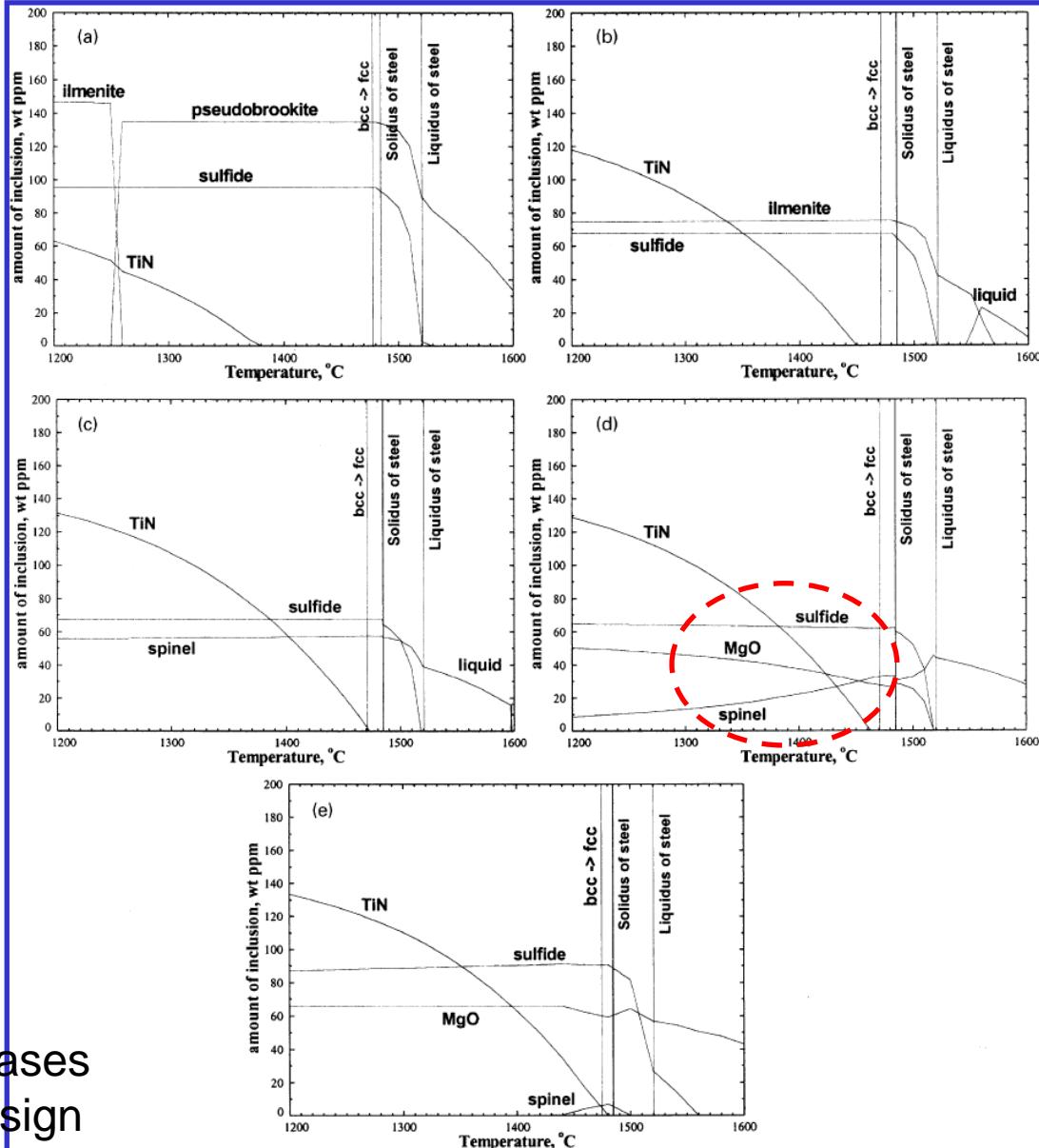
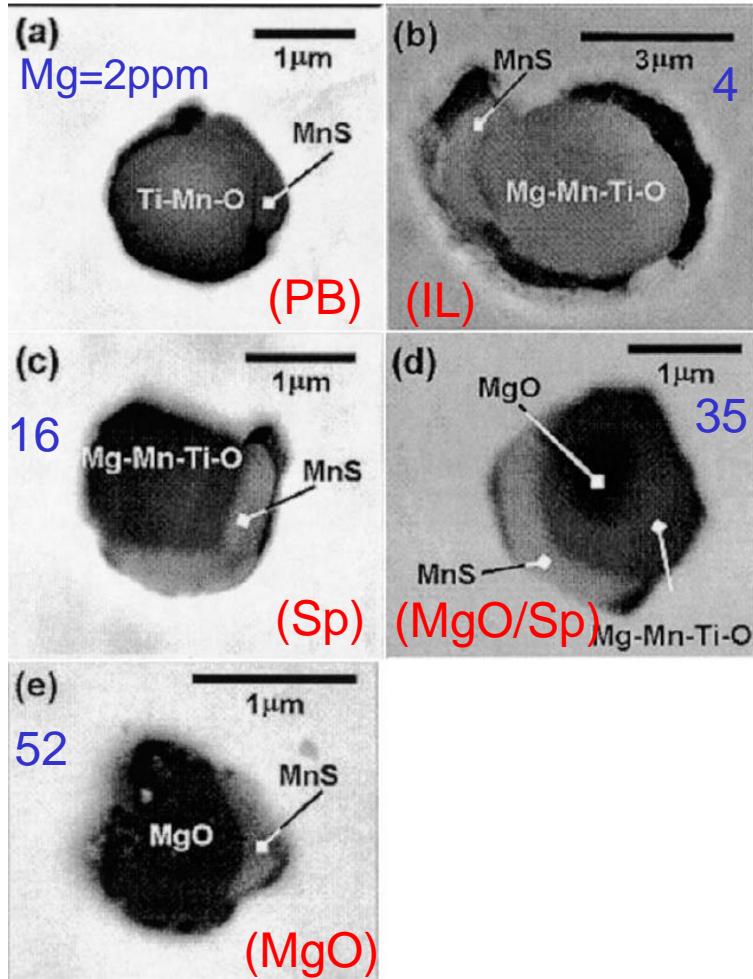
- Non-metallic inclusions: nucleation sites for acicular ferrite
- Acicular ferrite: enhances the strength of steel

Evolution of Non-metallic Inclusions



Morphologies of typical inclusions found in Fe-C-Mn-Si-O-S-Ti-Mg-Al-N

Evolution of Non-metallic Inclusions



Thermodynamic Calculations

- Accurate prediction of inclusions phases
- Application to high strength steel design

Inclusion evolution with temperature: Mn/Si/Ti steel

Equilib - Menu: Ferrous Applications II 17

File Units Parameters Help

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

Reactants (7)

(gram) 98.2769 Fe + 0.1 C + 1.5 Mn + 0.1 Si + 0.0061 Ti + 0.01 O + 0.007 S

Products

Compound species

	Base-Phase	Full Name
gas	I	FSstel-Liqu
ideal	J	FSstel-FCC
real	I	FSstel-BCC
aqueous	I	FSstel-HCP
pure liquids	+	FSstel-CEME
pure solids	+	FSstel-M23C
* solid selection	+	FSstel-M7C3
species:	+	FSstel-CBCC
114		CENTIMENTITE
		M23C6
		M7C3
		CBCC_A12

Custom Solutions
0 fixed activities
0 ideal solutions

Pseudonyms
apply Edit ...

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

paraequilibrium & Gmin edit

Virtual species: 182

Total Species (max 5000) 437

Total Solutions (max 200) 47

Total Phases (max 1500) 161

Number of transitions: All

Legend:
I - immiscible 8
J - 3-immiscible 1
+ selected 28

Show all selected

species: 323
solutions: 47 Select

Transitions - temperature

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		1600 1000 10	1	61+ calculations
10 steps	Table			

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

FactSage 8.0 F:\...\Ferrous_Applications_II_p17.equi

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

File Show Select

#	Species	Mole (min)	Mole (max)	Fraction (min)	Fraction (max)	Activity (min)	Activity (max)
FCC#1	FCC A1						
1	Fe	0	1.7517	0.976078	0.98397	0.940654	0.979686
2	Mn	0	2.6932E-02	1.3550E-02	1.5442E-02	1.1030E-02	1.3980E-02
3	O	0	6.5173E-08	1.0735E-12	3.0516E-07	1.1111E-12	2.9401E-07
4	S	0	1.5476E-04	4.2779E-07	8.6433E-05	2.3357E-11	2.2182E-08
5	Si	0	3.4536E-03	9.8553E-04	1.9292E-03	1.3657E-08	1.3694E-06
6	Ti	0	3.8713E-06	5.4859E-08	3.7450E-06	2.9596E-09	5.4271E-07
7	FeC	0	8.1847E-03	1.3904E-03	6.5086E-03	1.3473E-04	6.2172E-04
8	MnC	0	1.2578E-04	1.9473E-05	1.0297E-04	6.9153E-06	7.7598E-05
9	DC	0	3.0463E-10	5.0162E-15	4.5463E-10	8.1083E-16	6.7248E-11
10	SC	0	7.2300E-07	1.9889E-09	4.0390E-07	5.1891E-10	2.4673E-08
11	SiC	0				1.3249E-05	3.1196E-04
12	TiC	0					
FCC#2	FCC A1						
13	Fe	0				0.940654	0.979686
14	Mn	0				1.1030E-02	1.3980E-02
15	O	0				1.1111E-12	2.9401E-07

Select all stable phases

Select stable pure liquids

Select stable pure solids

Select stable solution phases

Clear

phase name [page] gram fraction (max) activity (max) ignore species and phase with zero mass

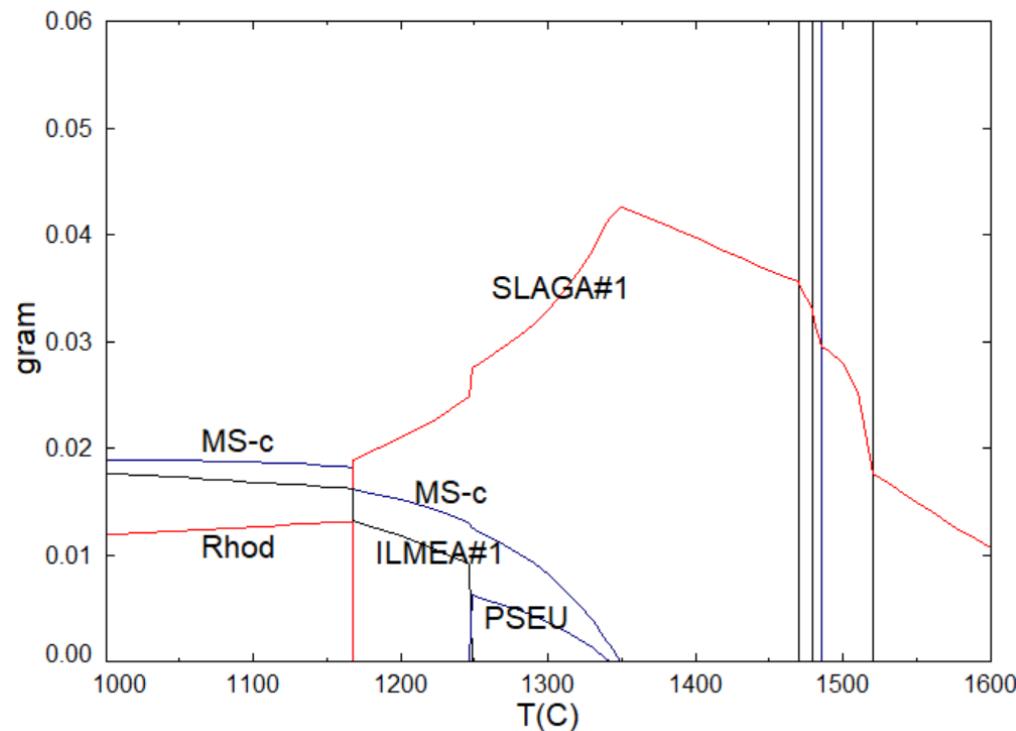
OK

Select ...

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

Select → “Select all stable phases”

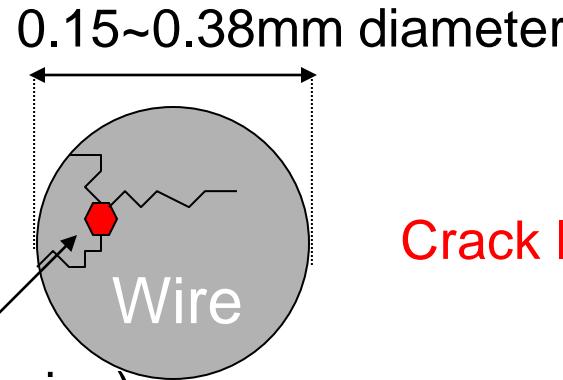
If inclusion evolution **in both liquid steel and solid steel** is needed, we recommend to use FToxid and FSStel database (if you want to use FTmisc-FeLq special caution is needed)



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

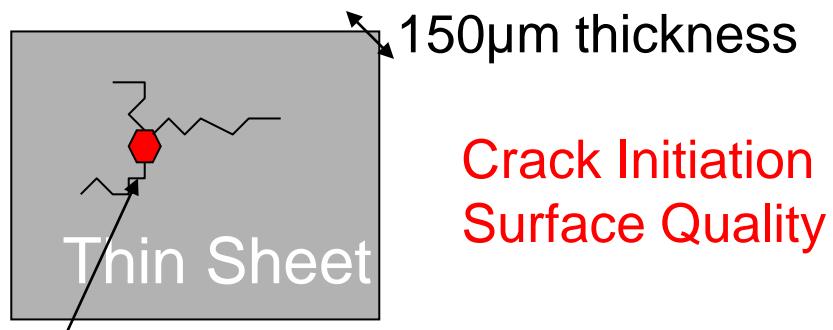
Tire-Cord Steel

Inclusion (ex., alumina)



Fe-36%Ni Invar Steel

Inclusion (ex., alumina)



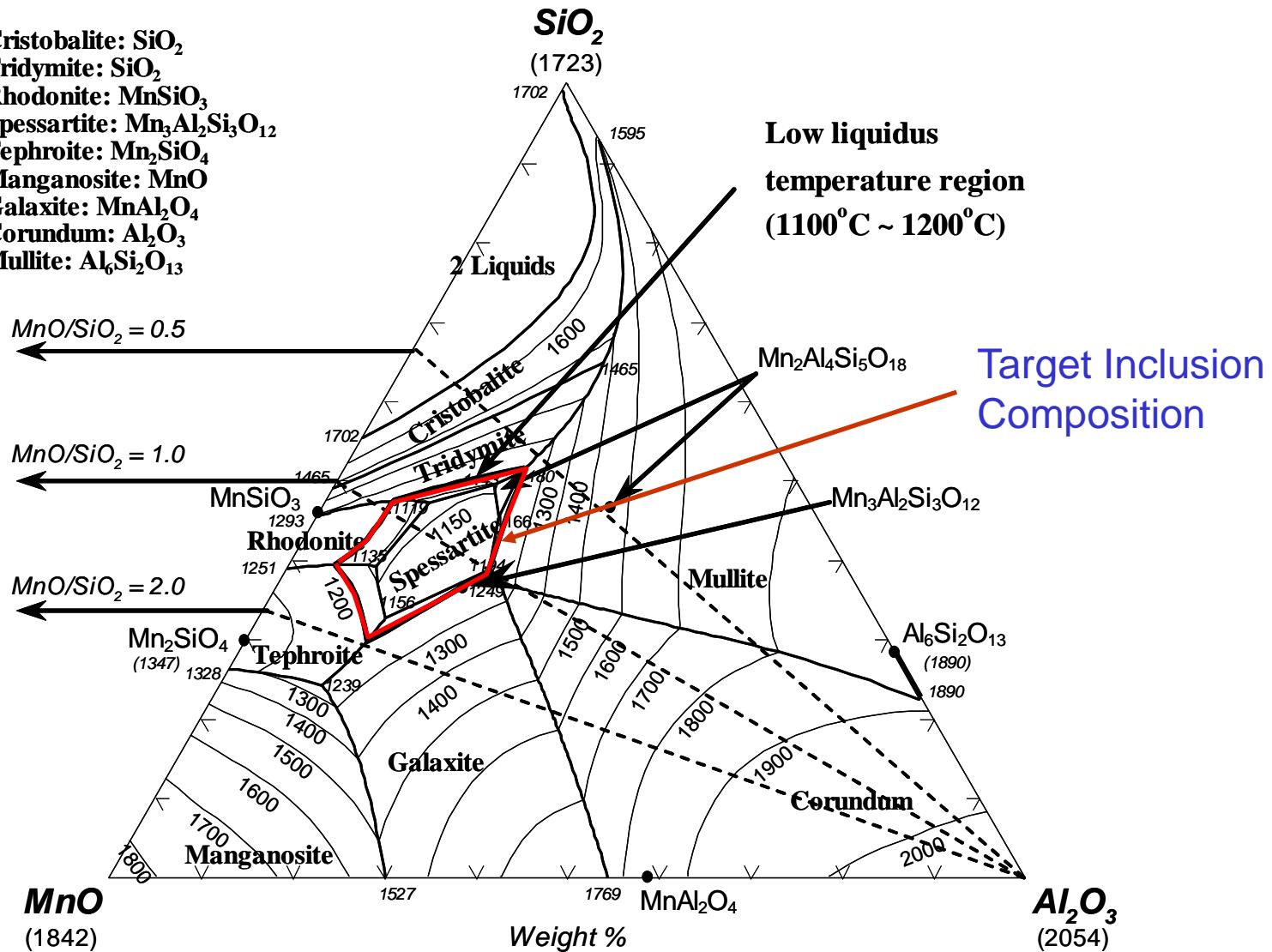
- Undeformable Inclusion should be removed
- Liquid phase is desirable at process temperature (~1200°C)



Mn/Si Deoxidation

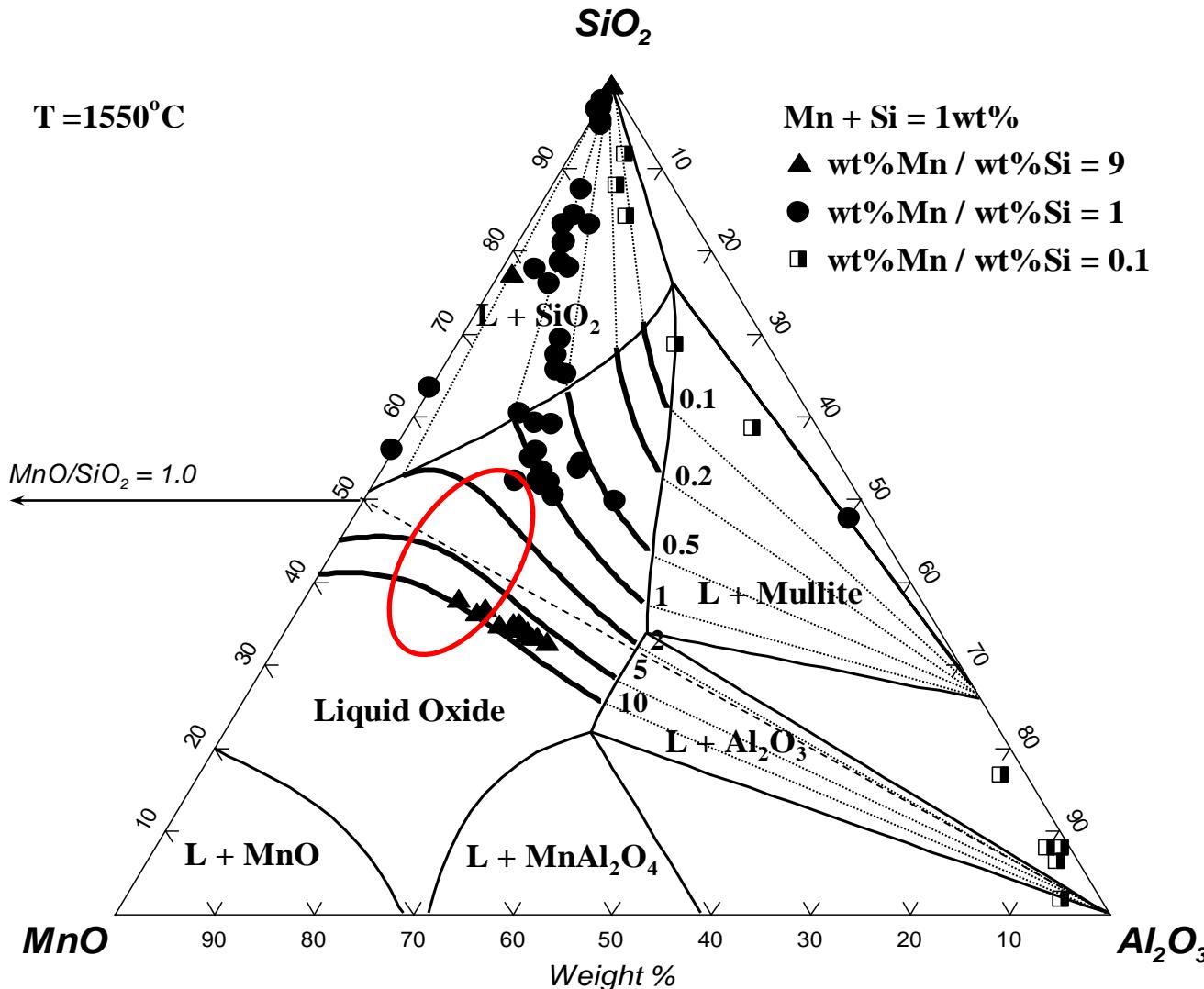
MnO-Al₂O₃-SiO₂ Phase Diagram

Cristobalite: SiO₂
 Tridymite: SiO₂
 Rhodonite: MnSiO₃
 Spessartite: Mn₃Al₂Si₃O₁₂
 Tephroite: Mn₂SiO₄
 Manganosite: MnO
 Galaxite: MnAl₂O₄
 Corundum: Al₂O₃
 Mullite: Al₆Si₂O₁₃



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.

Inclusion calculation in Mn/Si deoxidation

Phase Diagram - Menu: last system

File Units Parameters Variables Help

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

Components (3)

[gram] SiO₂ + Al₂O₃ + MnO

Products

- Compound species
- gas ideal real 0
- aqueous 0
- pure liquids 0
- * pure solids 32
- * - custom selection species: 32

Target - none - Estimate T(K): 1000

Variables

T(C)	SiO ₂ /	Al ₂ O ₃ /
1600	0.1	0.1

A = SiO₂, B = MnO, C = Al₂O₃

Solution phases

*	+	Base-Phase	Full Name
I		FToxid-SLAGA	A-Slag-liq all oxides + S
+		FToxid-SPINB	B-Spinel
+		FToxid-MeO_A	A-Monoxide
		FToxid-MeO_B	B-Monoxide
		FToxid-MeO_?	?-Monoxide
I		FToxid-N	
+		FToxid-CC	
+		FToxid-T	

Custom Solutions

- fixed activities
- ideal solutions

Pseudonyms apply Edit ...

Volume data assume molar volumes of solids and liquids = 1

Variables

compositions 2

Temperature constant 1600

Pressure or Volume P(atm) constant 1

Legend: 1 - immiscible 2 - selected 6

log10(a) 0

X, Y steps 11

Next >

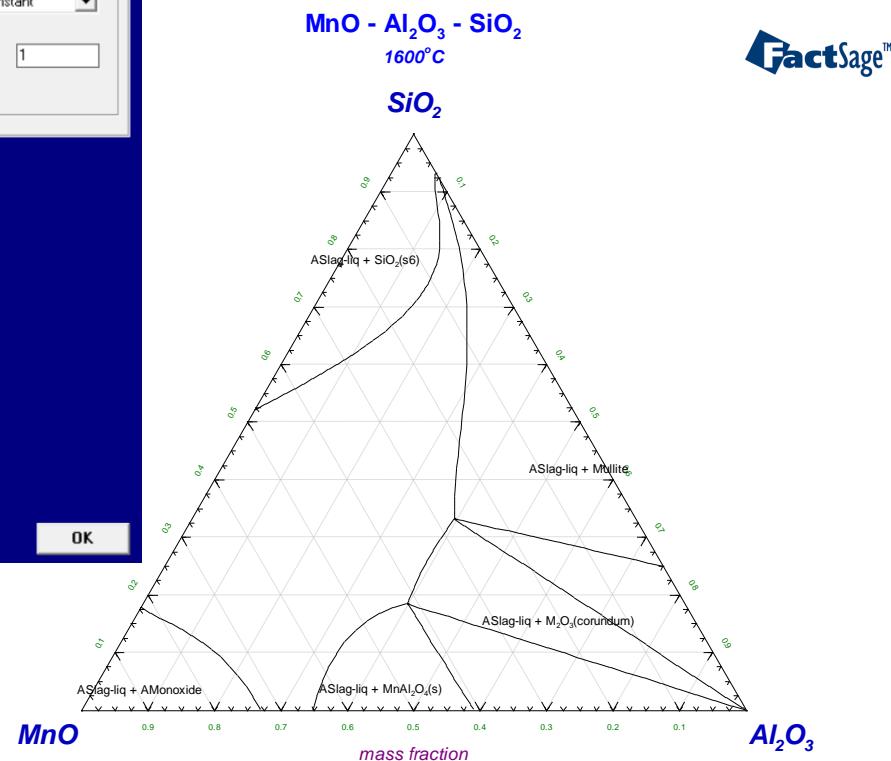
Compositions Quantity(g)

#1. 1 SiO₂ + 0 Al₂O₃ + 0 MnO = A-Corner
 1 SiO₂ + 1 Al₂O₃ + 1 MnO = 1 (max)
 0 (min)

#2. 0 SiO₂ + 1 Al₂O₃ + 0 MnO = C-Corner
 1 SiO₂ + 1 Al₂O₃ + 1 MnO = 1 (max)
 0 (min)

#3. 0 SiO₂ + 0 Al₂O₃ + 1 MnO = B-Corner
 1 SiO₂ + 1 Al₂O₃ + 1 MnO = 1 (max)
 0 (min)

Cancel OK



Inclusion calculation in Mn/Si deoxidation

Calculation of the inclusion trajectory using Equilib

Equilib - Menu: last system

File Units Parameters Help

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

Reactants (5)

(gram) 98.995 Fe + 0.5 Mn + 0.5 Si + <A> Al + 0.007 O

Products

Compound species

gas	ideal	real	0
aqueous			0
pure liquids			0
+ pure solids			33
species: 33			

Solution phases

*	+	Base-Phase	Full Name
+		FTmisc-FeLQ	Fe-liq
+		FTmisc-BCCS	bcc
+		FTmisc-FCCS	fcc
		FToxid-SLAGA	A-Slag-liq all oxides + S
		FToxid-SPINB	B-Spinel
+		FToxid-MeO_A	A-Monoxide
+		FToxid-cPyrA	A-Clinopyroxene
+		FToxid-OlivA	A-Olivine

Custom Solutions

0 fixed activities Details...
0 ideal solutions

Pseudonyms apply Edit...

Volume data

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

paraequilibrium & Gmin edit

Total Species (max 5000) 198
Total Solutions (max 200) 18
Total Phases (max 1500) 51

Target

- none -

Estimate T(K): 1000

Quantity(g): 0

Legend

I - immiscible 4
+ - selected 10

Show all selected

species: 165
solutions: 18 Select

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
0.0005 0.0001		1000	1	
10 steps	Table			51 calculations

Equilibrium

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

FactSage 8.0

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.

Inclusion calculation in Mn/Si deoxidation

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

Output Edit Show Pages Final Conditions

T(C) P(atm) Energy(J) Quantity(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-liqu
(99.998 gram, 1.7998 mol)
(1600 C, 1 atm, a=1.0000)
(98.997 wt.% Fe
+ 2.2191E-04 wt.% Al
+ 0.49858 wt.% Mn
+ 4.5488E-03 wt.% O
+ 0.49882 wt.% Si
+ 6.3879E-05 wt.% AlO
+ 1.3726E-04 wt.% SiO
+ 3.7704E-04 wt.% MnO
+ 4.9534E-08 wt.% Al2O)

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

Fe	1.7727	98.995	0.98492	0.98997
Mn	9.0805E-03	0.49886	5.0452E-03	4.9888E-03
Si	1.7763E-02	0.49890	9.8696E-03	4.9891E-03
Al	9.7117E-06	2.6204E-04	5.3960E-06	2.6204E-06
O	2.9422E-04	4.7073E-03	1.6347E-04	4.7074E-05

+ 5.4382E-03 gram Slag-lig#1
(5.4382E-03 gram, 7.6652E-05 mol)
+ 0 gram Slag-lig#2

(1600 C, 1 atm, a=1.0000)
(25.640 wt.% Al2O3
+ 43.413 wt.% SiO2
+ 3.9764 wt.% FeO
+ 1.1443E-03 wt.% Fe2O3
+ 26.966 wt.% MnO
+ 4.1969E-03 wt.% Mn2O3)

Site fraction of sublattice constituents:

Al	0.30279
Si	0.43499
Fe2+	3.3321E-02
Fe3+	8.6284E-06
Mn2+	0.22886
Mn3+	3.2009E-05



After deoxidation, Mn ~ 0.5 and Si ~ 0.5

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

→ Extraction of slag composition

Spreadsheets - Equilib Page 1/51 : T(C) = 1600, P(atm) = 1

File Edit Show Select Stable

Selected: 6/185 Spreadsheet Species

Page 1/51 : T(C) = 1600, P(atm) = 1

+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
46	Fe:Va(BCCS)	FTmisc	FTmisc-BCCS		0.9546		0.9546 [1]	0.9547 [27]	
47	Mn:Va(BCCS)	FTmisc	FTmisc-BCCS		4.2376E-03		4.2273E-03 [27]	4.2394E-03 [51]	
48	Fe:Va(FCCS)	FTmisc	FTmisc-FCCS		0.9469		0.9469 [1]	0.9470 [27]	
49	Mn:Va(FCCS)	FTmisc	FTmisc-FCCS		4.0246E-03		4.0148E-03 [27]	4.0263E-03 [51]	
+	50	Al2O3(SLAGA)	FToxid	FToxid-SLAGA#			0 [1]	0.2308 [51]	
+	51	SiO2(SLAGA)	FToxid	FToxid-SLAGA#		0.9628	0.2550 [51]	0.9628 [1]	
+	52	FeO(SLAGA)	FToxid	FToxid-SLAGA#		2.6267E-02	1.3509E-02 [51]	2.6267E-02 [1]	
+	53	Fe2O3(SLAGA)	FToxid	FToxid-SLAGA#		3.3986E-08	4.6227E-09 [51]	3.3986E-08 [1]	
+	54	MnO(SLAGA)	FToxid	FToxid-SLAGA#		3.6735E-02	1.9928E-02 [51]	3.6735E-02 [1]	
+	55	Mn2O3(SLAGA)	FToxid	FToxid-SLAGA#		1.0321E-08	1.4048E-09 [51]	1.0321E-08 [1]	
56	Fe3O4(SPINB)	FToxid	FToxid-SPINB#		2.0314E-09		1.4210E-10 [51]	2.0314E-09 [1]	
57	Fe3O4[1][SPINB]	FToxid	FToxid-SPINB#		3.1323E-10		3.1323E-10 [1]	1.1148E-07 [8]	
58	Fe3O4[1+][SPINB]	FToxid	FToxid-SPINB#		6.8466E-09		4.5641E-13 [51]	6.8466E-09 [1]	
59	Fe3O4[2-][SPINB]	FToxid	FToxid-SPINB#		3.3630E-11		3.3630E-11 [1]	1.2051E-05 [11]	
60	Fe1O4[5-][SPINB]	FToxid	FToxid-SPINB#		3.0706E-23		3.0706E-23 [1]	1.5756E-08 [12]	
61	Fe1O4[6-][SPINB]	FToxid	FToxid-SPINB#		3.2971E-24		3.2971E-24 [1]	1.9180E-06 [12]	
62	Fe1Al2O4(SPINB)	FToxid	FToxid-SPINB#		0 [1]		1.5976E-02 [28]		
63	Al3O4[1+][SPINB]	FToxid	FToxid-SPINB#		0 [1]		0.3866 [51]		

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

Select All Clear OK

Inclusion calculation in Mn/Si deoxidation

자동 저장 ○ 편집 □ ↻ 🔍 ⌂ 검색

Equilib.xls - 호환성 모드 - C:\Workshop80\Ferrous Applications\Equilib... 로그인

파일 흠 삽입 페이지 레이아웃 수식 데이터 검토 보기 도움말

W15

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	Alpha	Wt%-Al2O3(SLAGA#1)	Wt%-SiO2(SLAGA#1)	Wt%-FeO(SLAGA#1)	Wt%-Fe2O3(SLAGA#1)	Wt%-MnO(SLAGA#1)	Wt%-Mn2O3(SLAGA#1)	Wt%-Al2O3(SLAGA#2)	Wt%-SiO2(SLAGA#2)	Wt%-FeO(SLAGA#2)	Wt%-Fe2O3(SLAGA#2)	Wt%-MnO(SLAGA#2)	Wt%-Mn2O3(SLAGA#2)	A corner	B corner	C corner
2	0	0	99.590634	0.1269274	9.38178E-05	0.28145942	0.000884936	0	62.570747	6.6540508	0.005014931	30.767009	0.00317861	0.99591	0.00409	0
3	0.0001	8.7792688	59.689018	5.3548953	0.001087166	26.17281	0.00292115	0.90530635	97.519694	0.4731067	4.64102E-05	1.101222	0.000623975	0.59689	0.31532	0.08779
4	0.0002	11.776833	56.5178	5.0792122	0.000952035	26.621992	0.003211165	11.776833	56.5178	5.0792122	0.000952035	26.621992	0.003211165	0.56518	0.31705	0.11777
5	0.0003	14.104421	54.13043	4.8765629	0.000924089	26.884209	0.003453587	14.104421	54.13043	4.8765629	0.000924089	26.884209	0.003453587	0.5413	0.31765	0.14104
6	0.0004	16.115769	52.12597	4.7091915	0.000930548	27.044486	0.003653455	16.115769	52.12597	4.7091915	0.000930548	27.044486	0.003653455	0.52126	0.31758	0.16116
7	0.0005	17.938484	50.358053	4.5625986	0.000953004	27.136094	0.003816174	17.938484	50.358053	4.5625986	0.000953004	27.136094	0.003816174	0.50358	0.31703	0.17938
8	0.0006	19.633667	48.756118	4.4296695	0.0009843	27.175616	0.003945834	19.633667	48.756118	4.4296695	0.0009843	27.175616	0.003945834	0.48756	0.3161	0.19634
9	0.0007	21.234874	47.280873	4.3064771	0.001020872	27.172709	0.004045789	21.234874	47.280873	4.3064771	0.001020872	27.172709	0.004045789	0.47281	0.31484	0.21235
10	0.0008	22.762045	45.908307	4.1907137	0.001060611	27.133755	0.004119056	22.762045	45.908307	4.1907137	0.001060611	27.133755	0.004119056	0.45908	0.3133	0.22762
11	0.0009	24.227658	44.622638	4.0809764	0.001102103	27.063457	0.004168505	24.227658	44.622638	4.0809764	0.001102103	27.063458	0.004168505	0.44623	0.3115	0.24228
12	0.001	25.639853	43.412797	3.9763934	0.001144321	26.965515	0.004166924	25.639853	43.412797	3.9763934	0.001144321	26.965515	0.004166934	0.43413	0.30947	0.2564
13	0.0011	27.004183	42.270514	3.8764115	0.001186484	26.843	0.004186484	27.004183	42.270514	3.8764115	0.001186484	27.004183	0.004207056	0.42271	0.30725	0.27004
14	0.0012	28.324636	41.18924	3.7806664	0.001227993	26.707C	0.004227993	28.324636	41.18924	3.7806664	0.001227993	28.324636	0.004201469	0.41189	0.30486	0.28235
15	0.0013	29.604261	40.163517	3.6889036	0.001268339	26.537	0.004268339	29.604261	40.163517	3.6889036	0.001268339	29.604261	0.004182606	0.40164	0.30232	0.29604
16	0.0014	30.845546	39.188614	3.6009286	0.001307333	26.356	0.004307333	30.845546	39.188614	3.6009286	0.001307333	30.845546	0.004151527	0.39189	0.29966	0.30846
17	0.0015	32.050641	38.260325	3.516577	0.001344458	26.166	0.004344458	32.050641	38.260325	3.516577	0.001344458	32.050641	0.004113759	0.3826	0.29689	0.32051
18	0.0016	33.221495	37.374844	3.4356982	0.001379968	25.962	0.004379968	33.221495	37.374844	3.4356982	0.001379968	33.221495	0.004067552	0.37375	0.29404	0.33221
19	0.0017	34.359918	36.5287	3.3581458	0.001413399	25.747	0.004413399	34.359918	36.5287	3.3581458	0.001413399	34.359918	0.0040151618	0.36529	0.29111	0.3436
20	0.0018	35.467624	35.718717	3.2837738	0.001444829	25.524	0.00444829	35.467624	35.718717	3.2837738	0.001444829	35.467624	0.003959273	0.35719	0.28814	0.35468
21	0.0019	36.546246	34.941984	3.212436	0.001474255	25.29:	0.004474255	36.546246	34.941984	3.212436	0.001474255	36.546246	0.00388963	0.34942	0.28512	0.36546
22	0.002	37.59734	34.195842	3.1439854	0.001501703	25.0574*	0.00450574*	37.59734	34.195842	3.1439854	0.001501703	37.59734	0.00383762	0.34196	0.28207	0.35797
23	0.0021	38.622386	33.477858	3.0782765	0.001527226	24.816178	0.004774015	38.622386	33.477858	3.0782765	0.001527226	38.622386	0.003774015	0.33478	0.279	0.38622
24	0.0022	39.622789	32.785816	3.0151654	0.001550888	24.570969	0.004709449	39.622789	32.785816	3.0151654	0.001550888	39.622789	0.003709449	0.32786	0.27591	0.39623
25	0.0023	40.599785	32.1177	2.954512	0.001572768	24.322696	0.003664444	40.599785	32.1177	2.954512	0.001572768	40.599785	0.003644444	0.32118	0.27282	0.406
26	0.0024	41.554894	31.471674	2.8961804	0.001592947	24.072079	0.003579405	41.554894	31.471674	2.8961804	0.001592947	41.554894	0.003579405	0.31472	0.26973	0.41555
27	0.0025	42.489017	30.846074	2.8400399	0.0016111515	23.819743	0.003514678	42.489017	30.846074	2.8400399	0.0016111515	42.489017	0.003514678	0.30846	0.26665	0.42489
28	0.0026	43.403342	30.239387	2.7859654	0.001628557	23.566227	0.003450526	43.403342	30.239387	2.7859654	0.001628557	43.403342	0.003450526	0.30239	0.26357	0.43403
29	0.0027	43.641561	30.081907	2.7718137	0.001632672	23.499652	0.003433744	43.641561	30.081907	2.7718137	0.001632672	43.641561	0.003433744	0.30082	0.26277	0.43642
30	0.0028	43.641639	30.081465	2.7715307	0.001632482	23.500299	0.003433782	43.641639	30.081465	2.7715307	0.001632482	43.641639	0.003433782	0.30081	0.26277	0.43642
31	0.0029	43.641716	30.081023	2.7715378	0.001632391	23.500947	0.003433821	43.641716	30.081023	2.7715378	0.001632391	43.641716	0.003433821	0.30081	0.26277	0.43642
32	0.003	43.641793	30.080581	2.7715378	0.001632391	23.501595	0.003433859	43.641793	30.080581	2.7715378	0.001632391	43.641793	0.003433859	0.30081	0.26278	0.43642
33	0.0031	43.641871	30.080139	2.7689864	0.001630771	23.502242	0.003433897	43.641871	30.080139	2.7689864	0.001630771	43.641871	0.003433897	0.3008	0.26278	0.43642
34	0.0032	43.641948	30.079697	2.7689864	0.001630771	23.50289	0.003433935	43.641948	30.079697	2.7689864	0.001630771	43.641948	0.003433935	0.3008	0.26278	0.43642
35	0.0033	43.642025	30.079255	2.7689864	0.001630771	23.503537	0.003433973	43.642025	30.079255	2.7689864	0.001630771	43.642025	0.003433973	0.30079	0.26279	0.43642
36	0.0034	43.642102	30.078813	2.7689864	0.001630771	23.504185	0.003434011	43.642102	30.078813	2.7689864	0.001630771	43.642102	0.003434011	0.30078	0.26279	0.43642
37	0.0035	43.64218	30.078372	2.7689864	0.001630771	23.504832	0.003434049	43.64218	30.078372	2.7689864	0.001630771	43.64218	0.003434049	0.30078	0.26279	0.43642
38	0.0036	43.642257	30.07793	2.7689864	0.001630771	23.505548	0.003434087	43.642257	30.07793	2.7689864	0.001630771	43.642257	0.003434087	0.30078	0.2628	0.43642
39	0.0037	43.642334	30.077488	2.7689864	0.001630771	23.506127	0.003434125	43.642334	30.077488	2.7689864	0.001630771	43.642334	0.003434125	0.30077	0.2628	0.43642
40	0.0038	43.642411	30.077046	2.7689864	0.001630771	23.506774	0.003434163	43.642411	30.077046	2.7689864	0.001630771	43.642411	0.003434163	0.30077	0.26281	0.43642
41	0.0039	43.642499	30.076604	2.7689864	0.001630771	23.507421	0.003434201	43.642499	30.076604	2.7689864	0.001630771	43.642499	0.003434201	0.30077	0.26281	0.43642

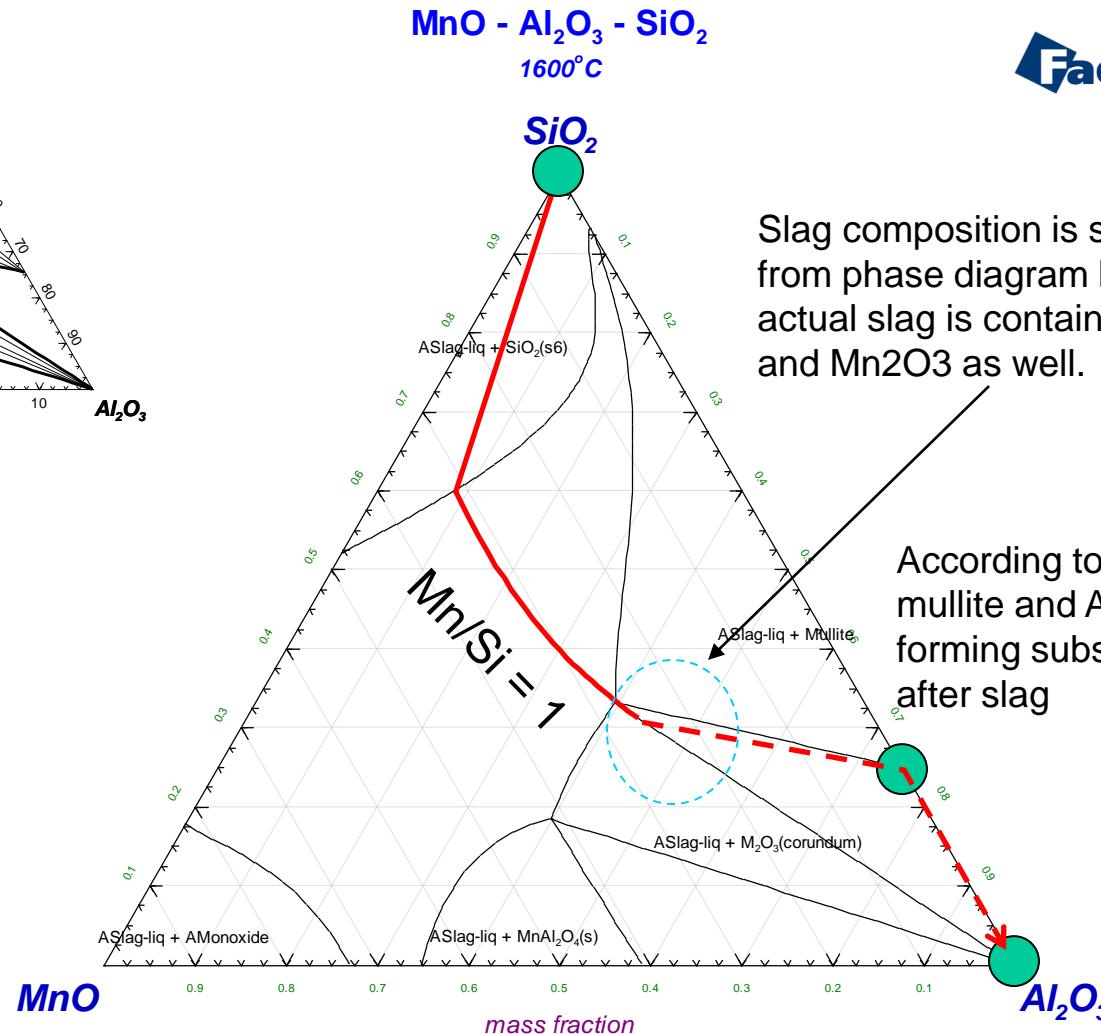
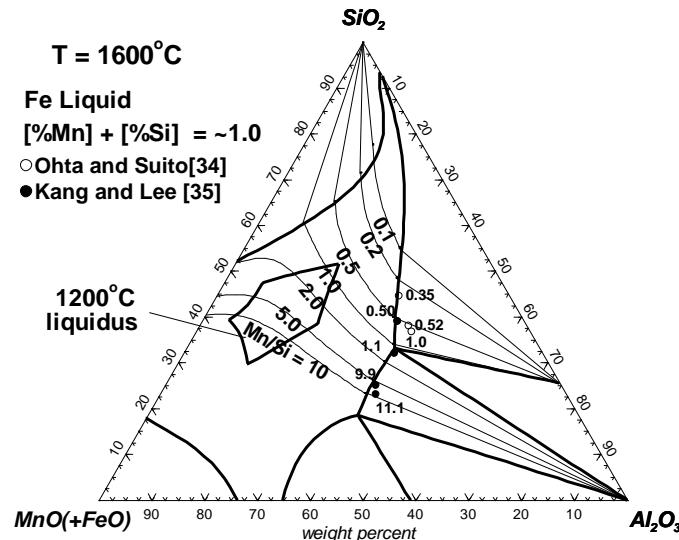
Composition from Slag #1
A corner = wt%SiO2/100
B corner = (wt%MnO+Mn2O3+FeO+Fe2O3)/100
C corner = wt%Al2O3/100

Slag #1
(stable slag)

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

Sheet1

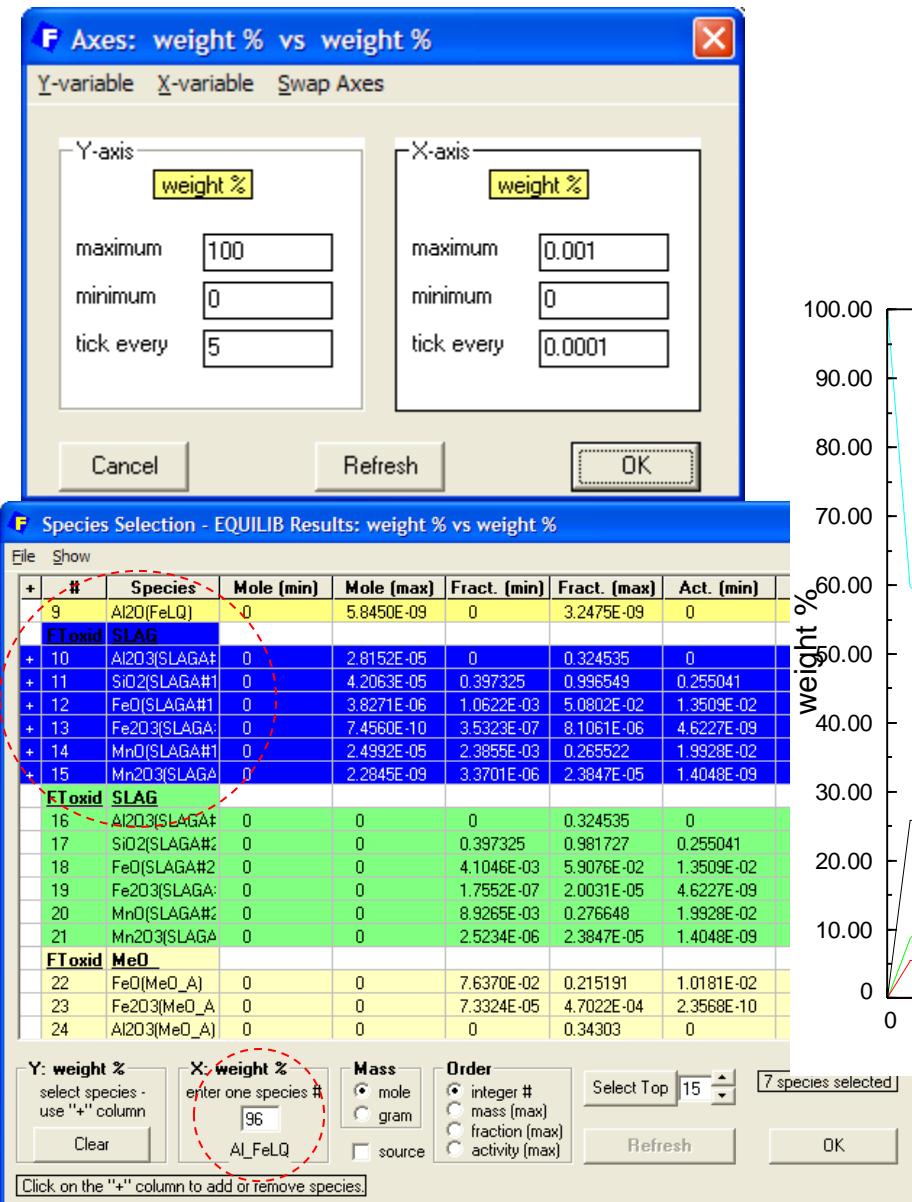
Inclusion calculation in Mn/Si deoxidation



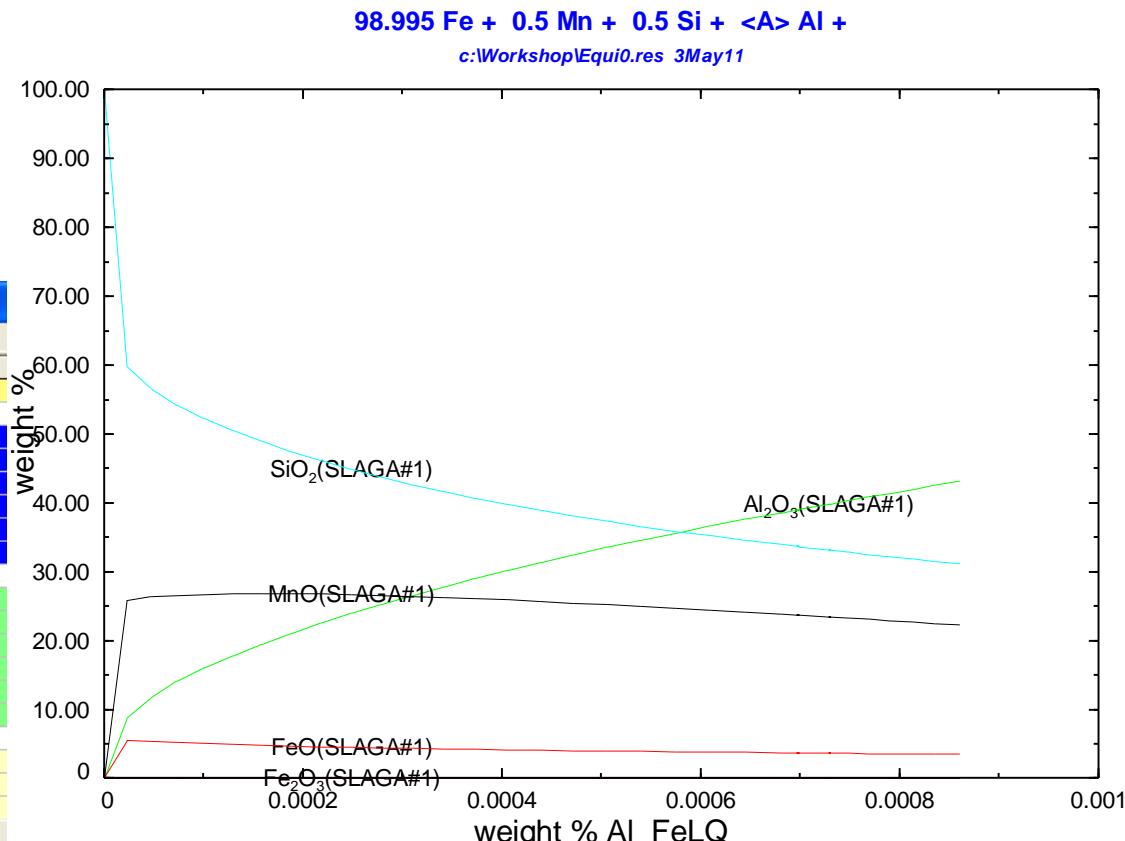
Slag composition is slightly off from phase diagram because the actual slag is containing Fe_3O_4 and Mn_2O_3 as well.

According to calculations, mullite and Al_2O_3 are forming subsequently after slag

Inclusion calculation in Mn/Si deoxidation



Soluble Al vs. Inclusion composition



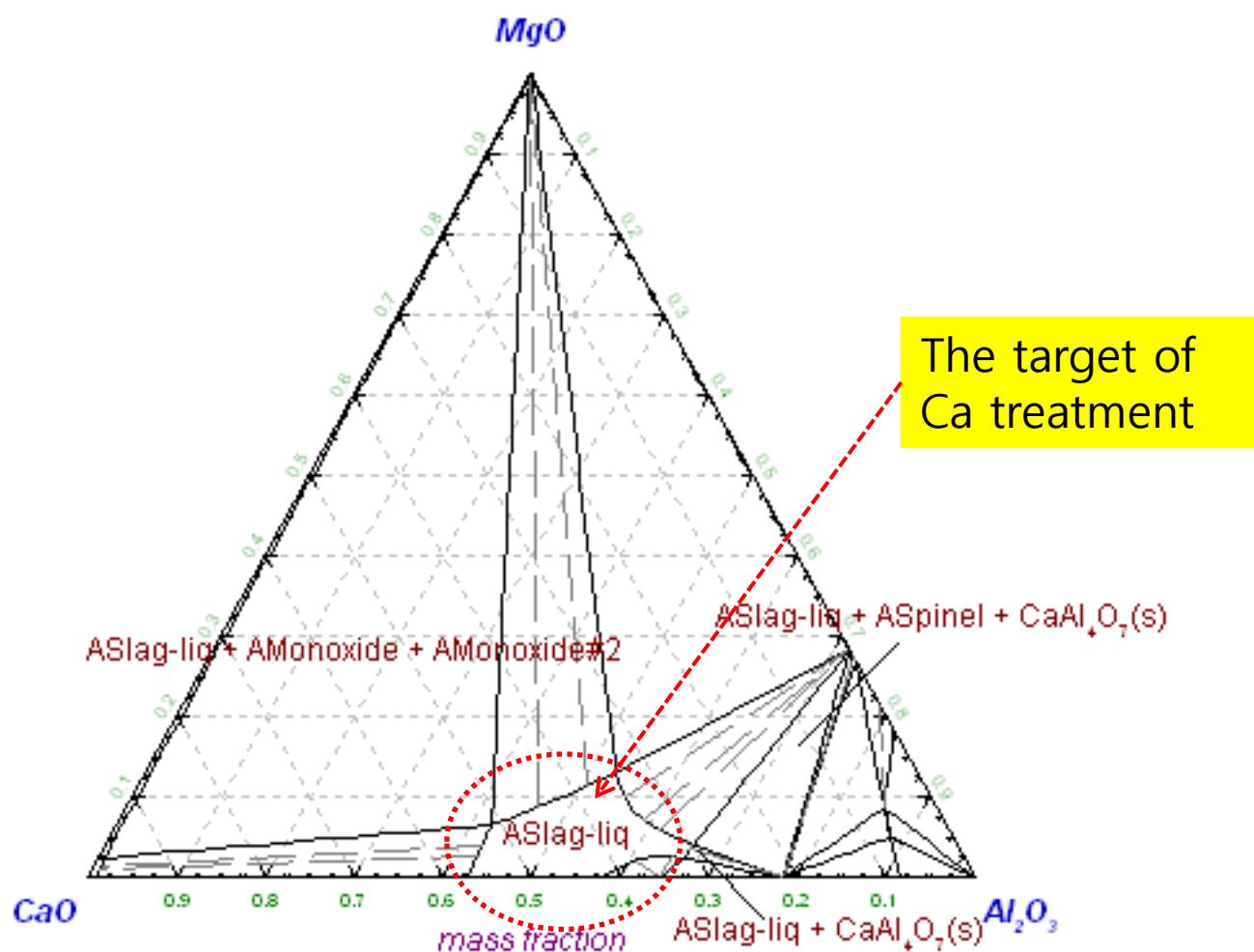
Re-oxidation and inclusion modification in the tundish – Ca-treated steel

Reoxidation and inclusion modification in the tundish

MgO - CaO - Al_2O_3

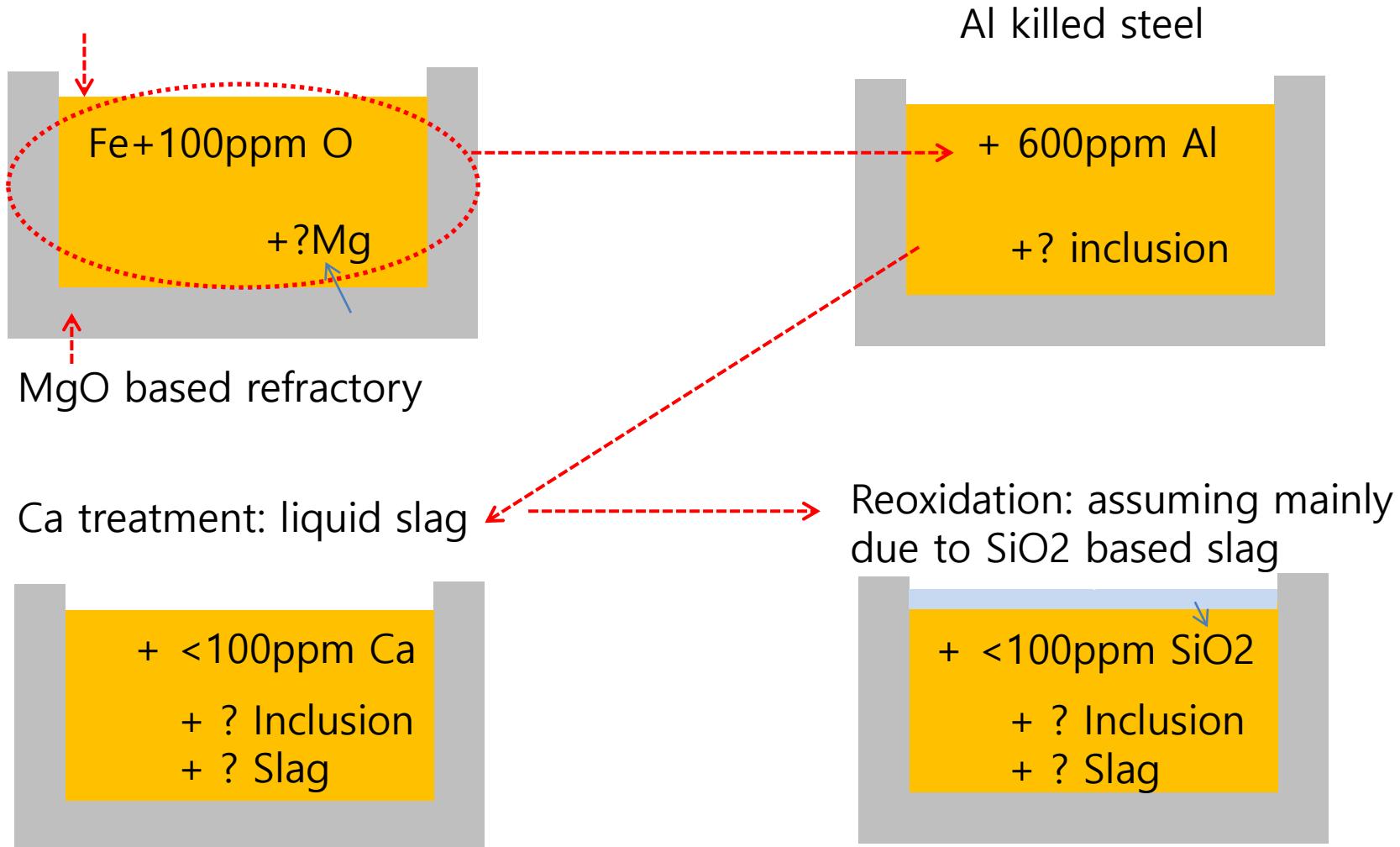
1550°C, 1 atm

FactSage™



Reoxidation and inclusion modification in the tundish

At 1550°C



Reoxidation and inclusion modification in the tundish

Al killed steel

Fe+100ppm O

+?Mg

MgO based refractory

Databases: FACTPS + FTOxid + FTMisc

Equilib - Menu: last system

File Units Parameters Help

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

Reactants (3)

(gram) 99.09 Fe + 0.01 O + MgO

Products

Compound species

gas ideal real 8
aqueous 0
pure liquids 0
* pure solids 7

* - custom selection
species: 15

Target

- none -

Estimate T(K): 1000

Quantity(g): 0

Solution phases

*	+	Base-Phase	Full Name
*	+	FTmisc-FeLQ	Fe-liq
I		FToxid-SLAGA	A-Slag-liq all oxides + S
*	+	FToxid-SPINA	A-Spinel
*	+	FToxid-MeO_A	A-Monoxide

Legend

I - immiscible 1

+ - selected 3

Show all selected

species: 25

solutions: 5

Custom Solutions

0 fixed activities

0 ideal solutions

Pseudonyms

apply Edit ...

Volume data

assume molar volumes of
solids and liquids = 0

include molar volume data
and physical properties data

paraequilibrium & Gmin edit

Virtual species:

Total Species (max 5000) 40

Total Solutions (max 200) 5

Total Phases (max 1500) 13

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		1550	1	
10 steps	<input type="checkbox"/> Table			1 calculation

Equilibrium

normal normal + transitions

transitions only open

- no time limit -

Calculate >

FactSage 8.0

Reoxidation and inclusion modification in the tundish

Equilib - Results 1550 C

Output Edit Show Pages Final Conditions

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

(gram) 99.09 Fe + 0.01 O + MgO =

0 mol gas_ideal
(1550 C, 1 atm, a=8.7885E-05)
(4.4878E-05 Mg
+ 4.2996E-05 Fe
+ 1.0485E-08 FeO
+ 4.4275E-10 MgO
+ 2.0110E-10 O
+ 1.7956E-12 O2
+ 3.8285E-13 Mg2
+ 5.3278E-26 O3)

+ 99.078 gram Fe-liq
(99.078 gram, 1.7744 mol)
(1550 C, 1 atm, a=1.0000)
(99.994 wt.% Fe
+ 5.0250E-03 wt.% O
+ 1.0221E-06 wt.% Mg
+ 5.3287E-04 wt.% MgO)

System component Amount/mol Amount/gmol Mole fraction Mass fraction
Fe 1.7741 99.072 0.99981 0.99994
Mg 1.3141E-05 3.1939E-04 7.4059E-06 3.2236E-06
O 3.2428E-04 5.1883E-03 1.8276E-04 5.2366E-05

+ 1.0220 gram Monoxide
(1.0220 gram, 2.5111E-02 mol)
(1550 C, 1 atm, a=1.0000)
(2.1972 wt.% FeO
+ 6.8918E-03 wt.% Fe2O3
+ 97.796 wt.% MgO)

Final Conditions <A> T(C) P(atm) Product H(J) 1 calculation Calculate >

FactSage 8.0

Only save liquid Fe
as stream file for next step
Stream name: "Ex4-1(a)"

MgO based
refractory

Reoxidation and inclusion modification in the tundish

Al killed steel

+ 600ppm Al

+? inclusion

Equilib - Menu:

File Units Parameters Help

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

Reactants (2)

(gram) 100% [Ex4-1(a)] + 0.06 Al

Products

Compound species

<input type="radio"/> gas	<input checked="" type="radio"/> ideal	<input type="radio"/> real	15
<input type="radio"/> aqueous			0
<input type="radio"/> pure liquids			0
<input checked="" type="radio"/> pure solids			14
* - custom selection			
species: 29			

Solution phases

*	+	Base-Phase	Full Name
	+	FTmisc-FeLQ	Fe-liq
I		FToxid-SLAGA	A-Slag-liq all oxides + S
I		FToxid-SPINA	A-Spinel
	+	FToxid-MeO_A	A-Monoxide
I		FToxid-CORU	M203(Corundum)

Custom Solutions

0 fixed activities Details ...
0 ideal solutions

Pseudonyms

apply Edit ...

Volume data

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

paraequilibrium & Gmin edit

Virtual species: 12
Total Species (max 5000) 92
Total Solutions (max 200) 8
Total Phases (max 1500) 23

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		1550	1	
10	steps	<input type="checkbox"/> Table		1 calculation

Equilibrium

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

FactSage 8.0

Reoxidation and inclusion modification in the tundish

F Equilib - Results 1550 C

Output Edit Show Pages Final Conditions

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

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	1.7741	99.072	0.99985	0.99945
Al	2.0267E-03	5.4684E-02	1.1411E-03	5.5165E-04
Mg	7.3947E-07	1.7973E-05	4.1634E-07	1.8131E-07
O	1.6331E-05	2.6129E-04	9.1949E-06	2.6359E-06

+ 7.8073E-03 gram M₂O₃(Corundum)#1
(7.8073E-03 gram, 7.6571E-05 mol)
+ 0 gram M₂O₃(Corundum)#2
(1550 C, 1 atm, a=1.0000)
(100.000 wt.% Al₂O₃
+ 7.7599E-06 wt.% Fe₂O₃)

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	7.5877E-12	4.2374E-10	1.9819E-08	5.4274E-08
Al	1.5314E-04	4.1320E-03	0.40000	0.52925
O	2.2971E-04	3.6753E-03	0.60000	0.47075

+ 2.7380E-03 gram Spinel#1
(2.7380E-03 gram, 1.9559E-05 mol)
+ 0 gram Spinel#2
(1550 C, 1 atm, a=1.0000)
(9.1657E-09 wt.% Fe₃O₄
+ 1.1370E-09 wt.% Fe₃O₄[1-]
+ 1.1017E-12 wt.% Fe
+ 9.4593E-06 wt.% Fe
+ 3.8893E-07 wt.% Fe

Only 55 ppm soluble Al
Only 2.6 ppm soluble O

Alumina inclusion which can cause later nozzle clogging

Formation of spinel inclusion which is bad for steel quality

Stream name: "Ex4-1(b)"

Save all phases as stream file for next step

(assumption: all inclusions stay without any floatation removal)

Reoxidation and inclusion modification in the tundish

Ca treatment: liquid slag

+ <100ppm Ca
+ ? Inclusion
+ ? Slag

Equilib - Menu: last system

Units Parameters Help

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

Reactants (2)

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

Products

Compound species

- gas (radio button selected) ideal real 18
- aqueous 0
- pure liquids 0
- pure solids 31

* - custom selection species: 49

Solution phases

*	+	Base-Phase	Full Name
+		FTmisc-FeLQ	Fe-liq
I		FToxid-SLAGA	A-Slag-liq all oxides + S
I		FToxid-SPINA	A-Spinel
I		FToxid-MeO_A	A-Monoxide
+		FToxid-CAF6	Ca(Al,Fe)12019
+		FToxid-CAF3	Ca(Al,Fe)6010
+		FToxid-CAF2	Ca(Al,Fe)407
I		FToxid-CAF1	Ca(Al,Fe)204

Custom Solutions

- 0 fixed activities
- 0 ideal solutions

Pseudonyms

- apply Edit ...

Volume data

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

paraequilibrium & Gmin edit

Virtual species: 20

Total Species (max 5000) 136

Total Solutions (max 200) 16

Total Phases (max 1500) 48

Legend

- I - immiscible 5
- + - selected 6

Show all selected

species: 87

solutions: 16

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
0 0.01 0.0001		1550	1	
10 steps	<input type="checkbox"/> Table			101+ calculations

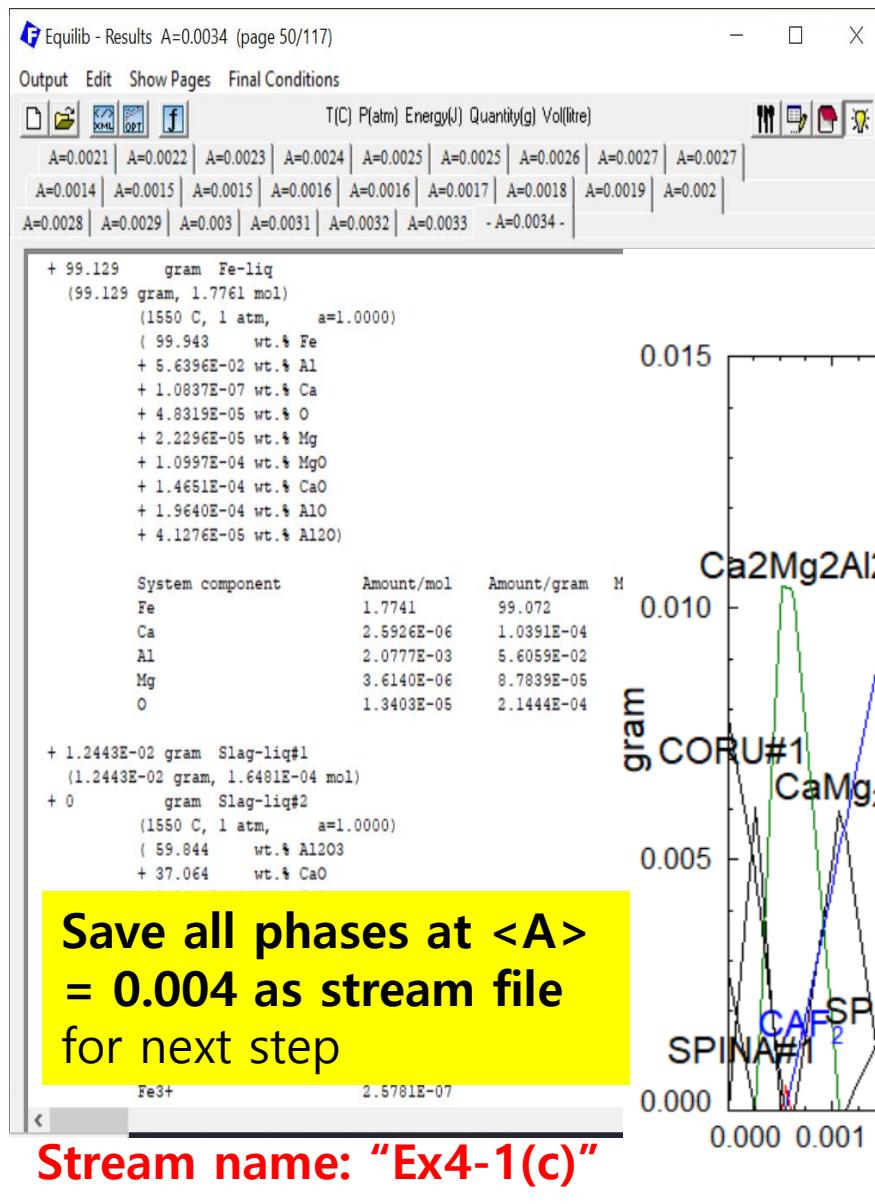
Equilibrium

- normal
- normal + transitions
- transitions only
- open

- no time limit -

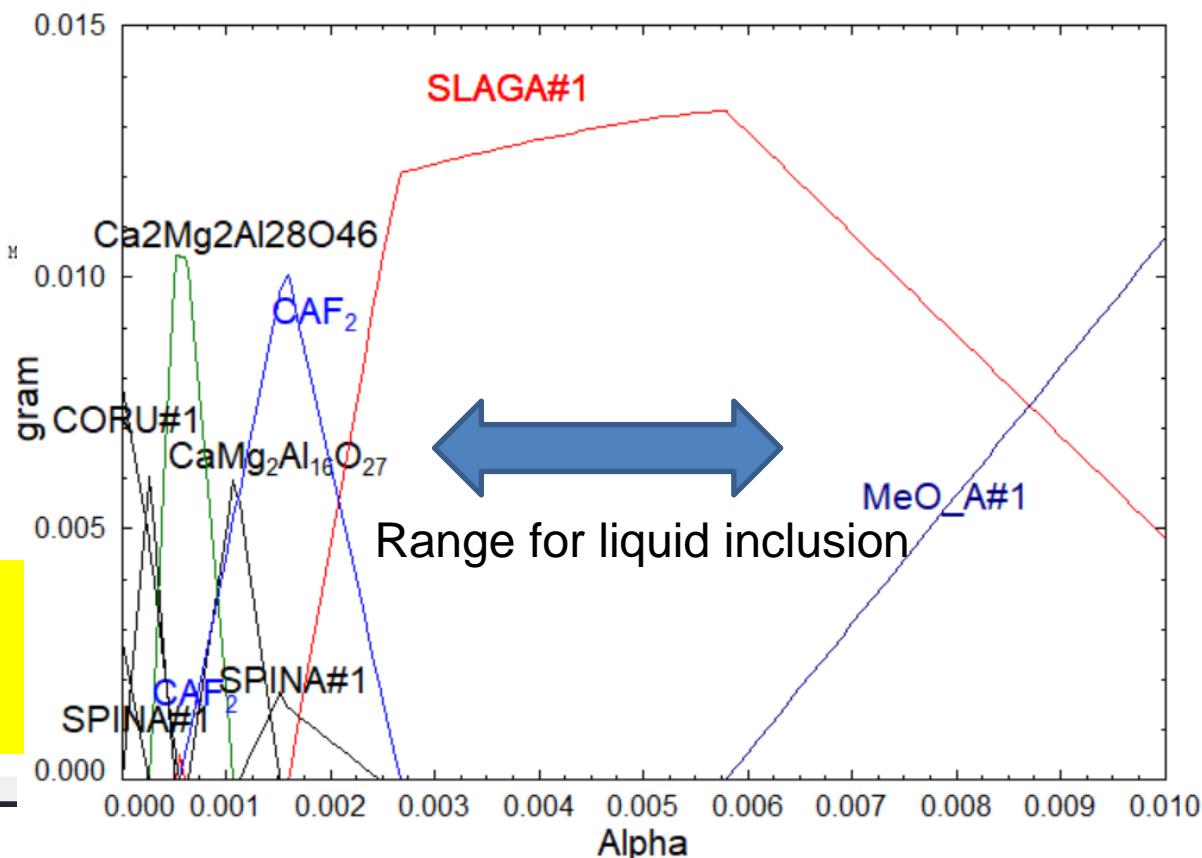
FactSage 8.0

Reoxidation and inclusion modification in the tundish



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

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Reoxidation and inclusion modification in the tundish

Reoxidation: assuming mainly due to SiO₂ based slag

+ <100ppm SiO₂
+ ? Inclusion
+ ? Slag

Equilib - Menu:

File Units Parameters Help

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

Reactants (2)

(gram) 100% [Ex4-1(c)] + <A> SiO₂

Products

Compound species

- + gas ideal real 23
- aqueous 0
- pure liquids 0
- * + pure solids 88

* - custom selection species: 111

Target

- none -

Estimate T(K): 1000

Quantity(g): 0

Solution phases

*	+	Base-Phase	Full Name
+		FTmisc-FeLQ	Fe-liq
I		FToxid-SLAGA	A-Slag-liq all oxides + S
I		FToxid-SPINA	A-Spinel
I		FToxid-MeO_A	A-Monoxide
I		FToxid-cPyrA	A-Clinopyroxene
+		FToxid-oPyrA	A-Orthopyroxene
+		FToxid-pPyrA	A-Protopyroxene
+		FToxid-LcPy	LowClinopyroxene

Legend

- I - immiscible 8
- + - selected 16

Show all selected

species: 306

solutions: 32

Select

Custom Solutions

- 0 fixed activities
- 0 ideal solutions

Pseudonyms

apply Edit ...

Volume data

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

paraequilibrium & Gmin edit

Virtual species: 30

Total Species (max 5000) 417

Total Solutions (max 200) 32

Total Phases (max 1500) 121

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
0 0.01 0.0001		1550	1	
10 steps	<input type="checkbox"/> Table	101 calculations		

Equilibrium

normal normal + transitions

transitions only open

- no time limit -

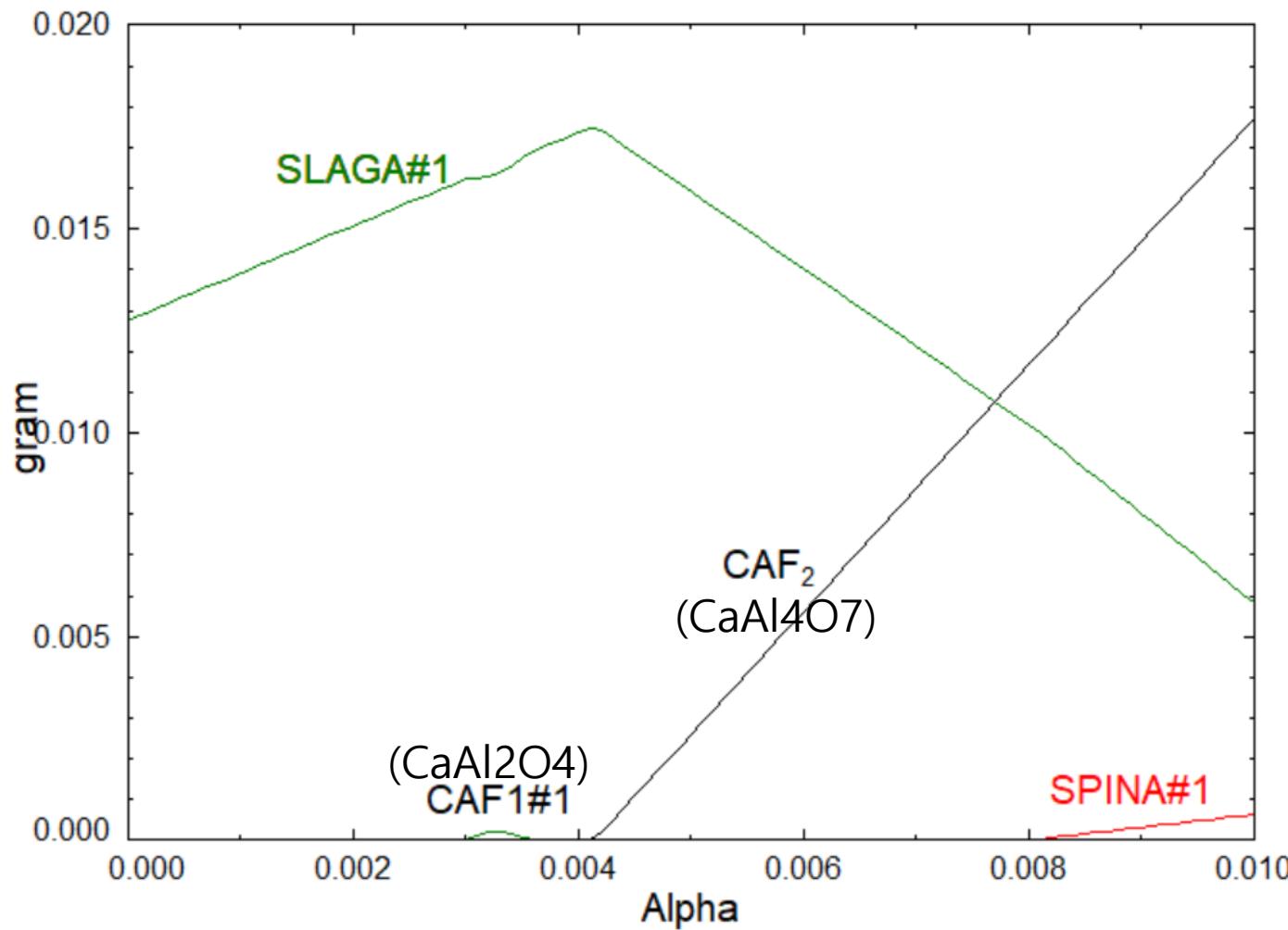
Calculate >

FactSage 8.0

Reoxidation and inclusion modification in the tundish

100% [Ex4-1(c)] + <A> SiO₂

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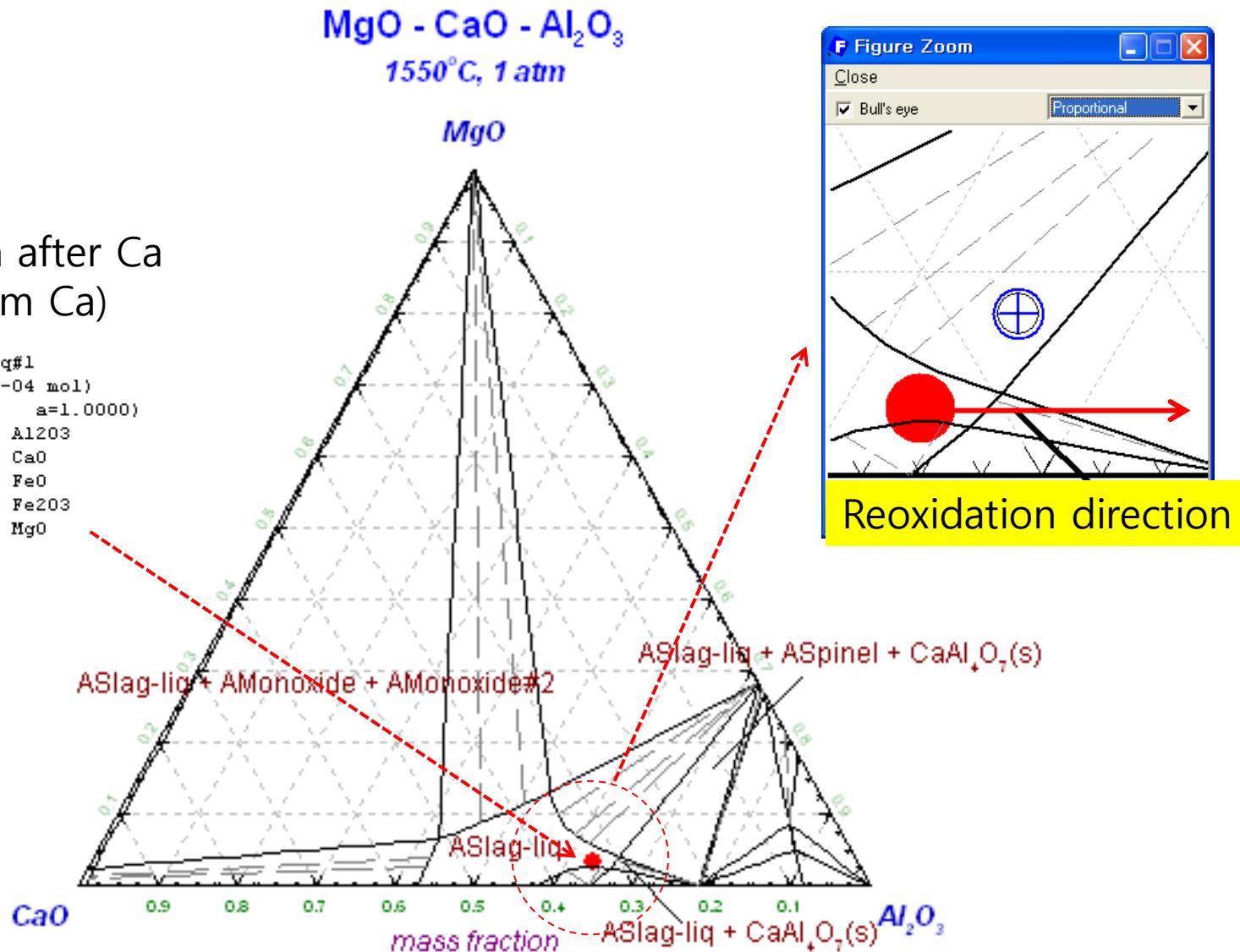


In this condition,
SiO₂ is reduced by Al during the reoxidation

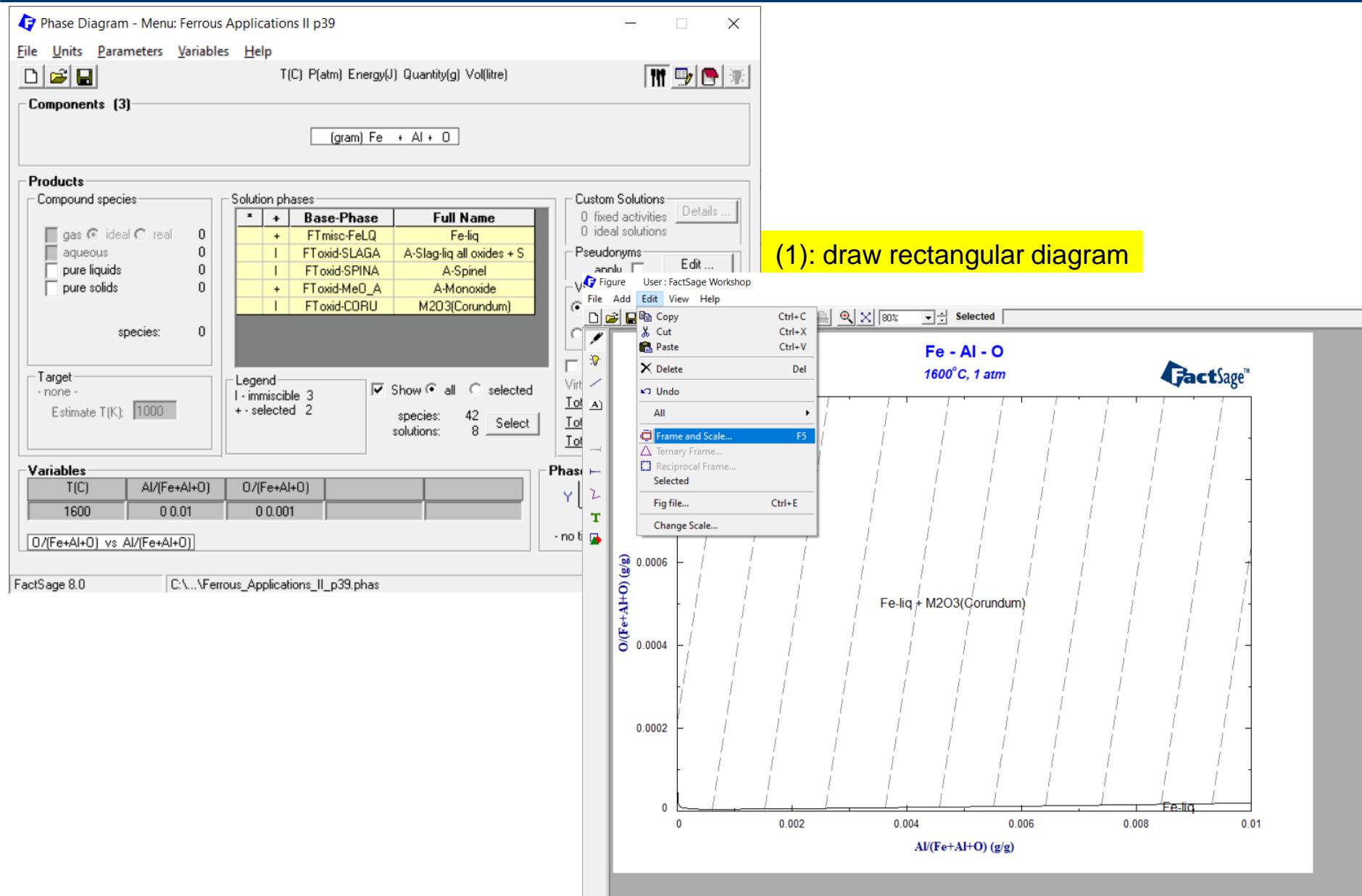
Reoxidation and inclusion modification in the tundish

Slag composition after Ca treatment (30 ppm Ca)

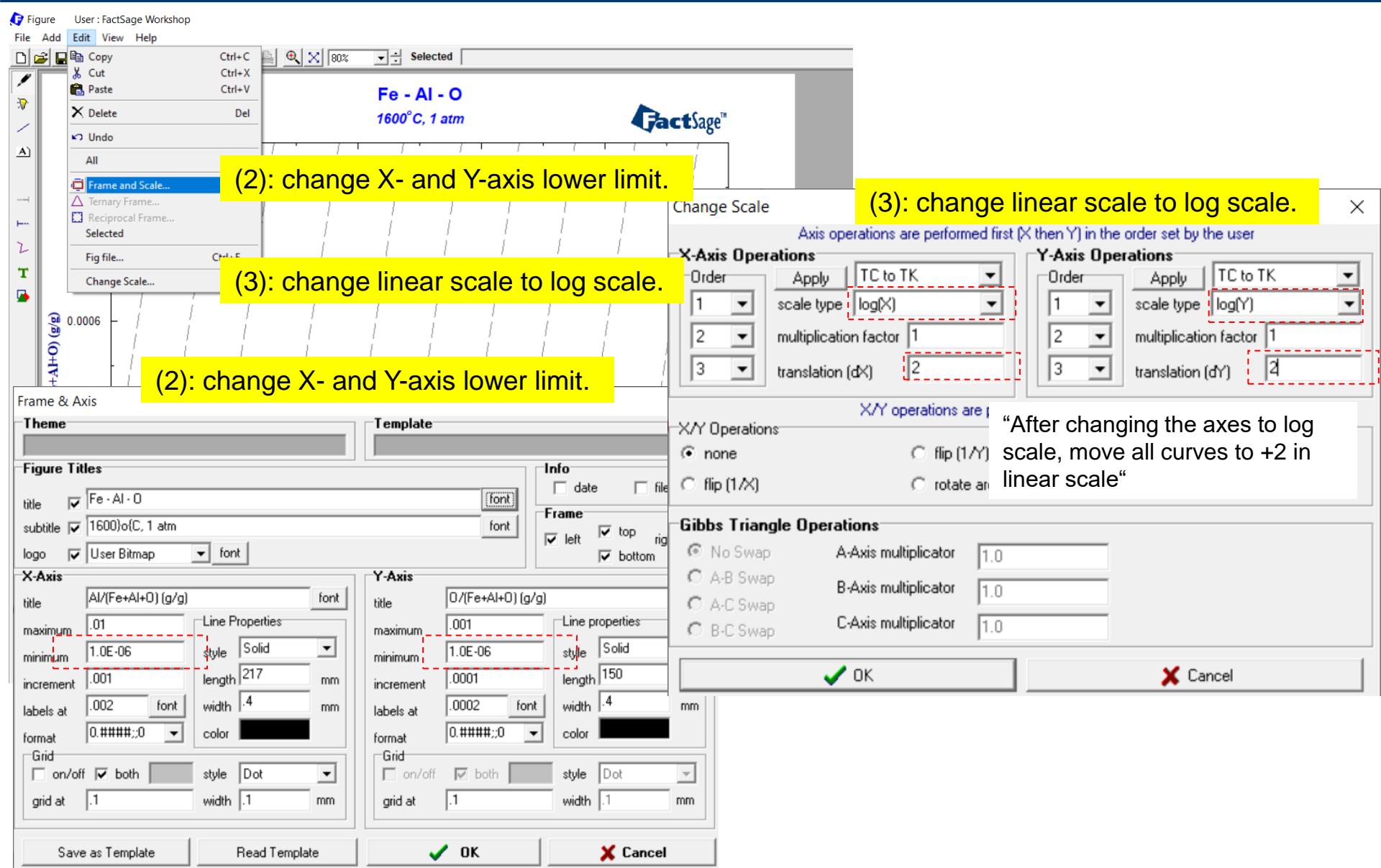
```
+ 1.2284E-02 gram ASlag-liq#1
(1.2284E-02 gram, 1.5945E-04 mol)
(1550 C, 1 atm, a=1.0000)
( 63.328    wt.% Al2O3
+ 33.369    wt.% CaO
+ 6.3444E-03 wt.% FeO
+ 3.9494E-05 wt.% Fe2O3
+ 3.2969    wt.% MgO
```



Inclusion diagram: Fe-Al-O, Al deoxidation

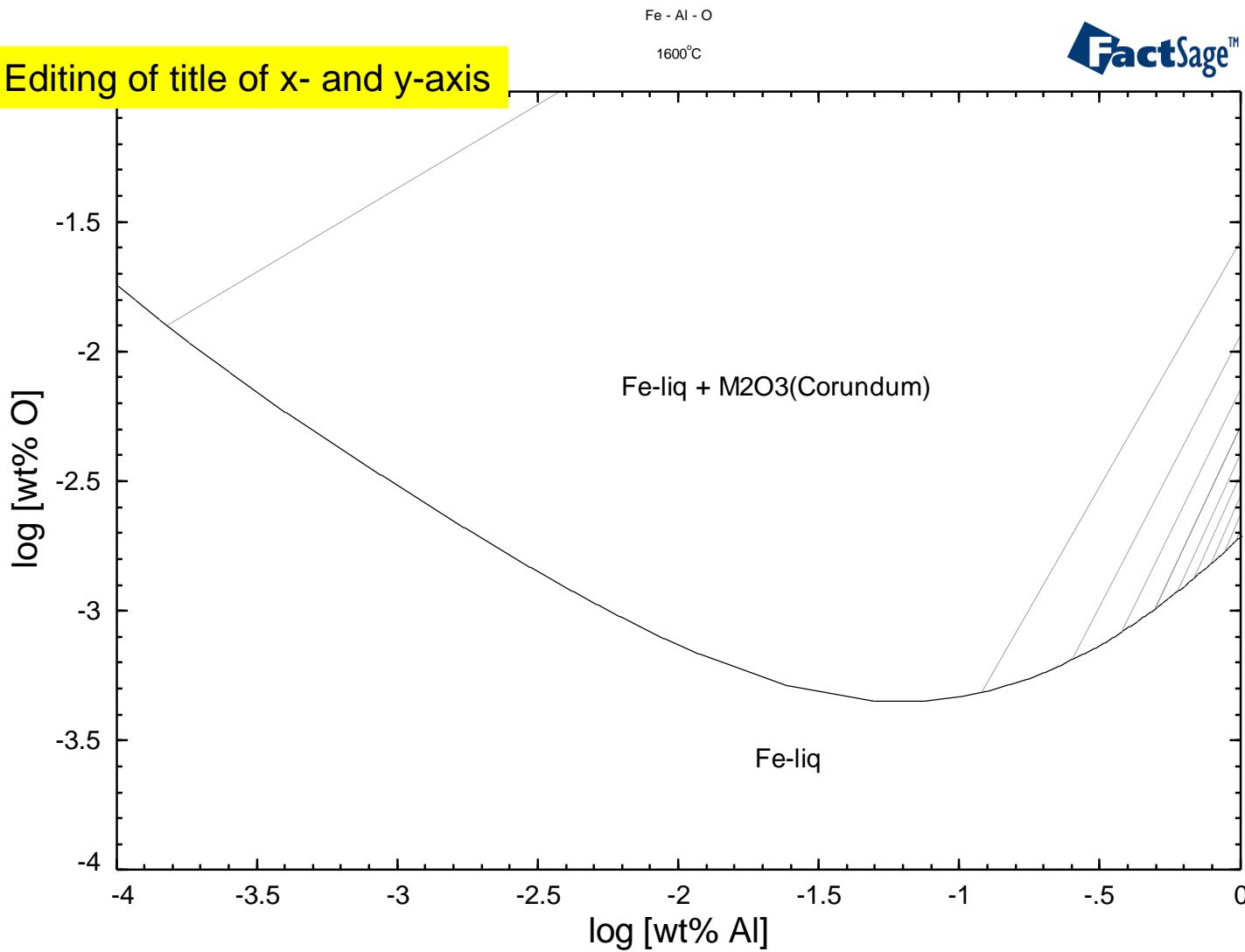


Inclusion diagram: Fe-Al-O, Al deoxidation



Inclusion diagram: Fe-Al-O, Al deoxidation

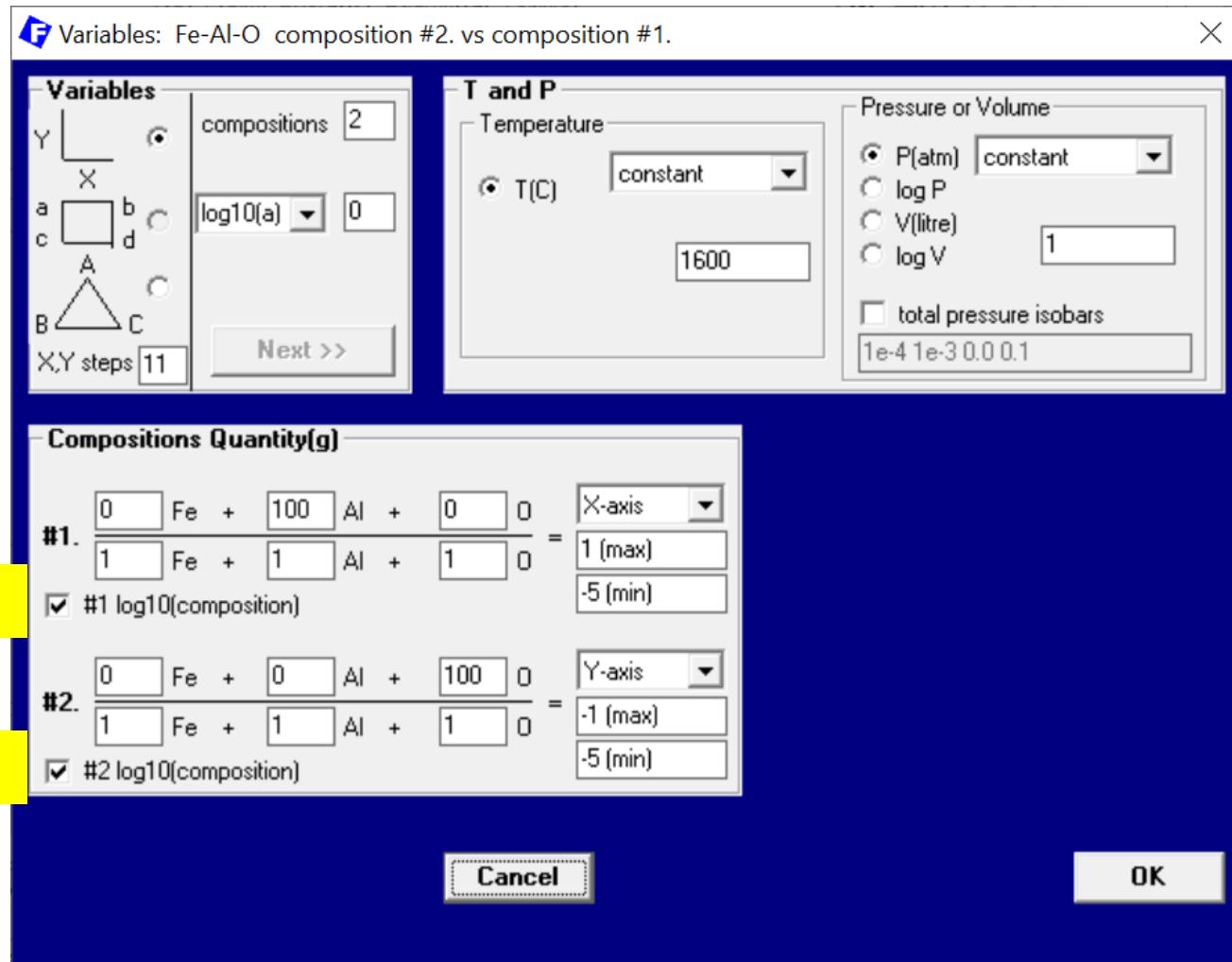
(4) Editing of title of x- and y-axis



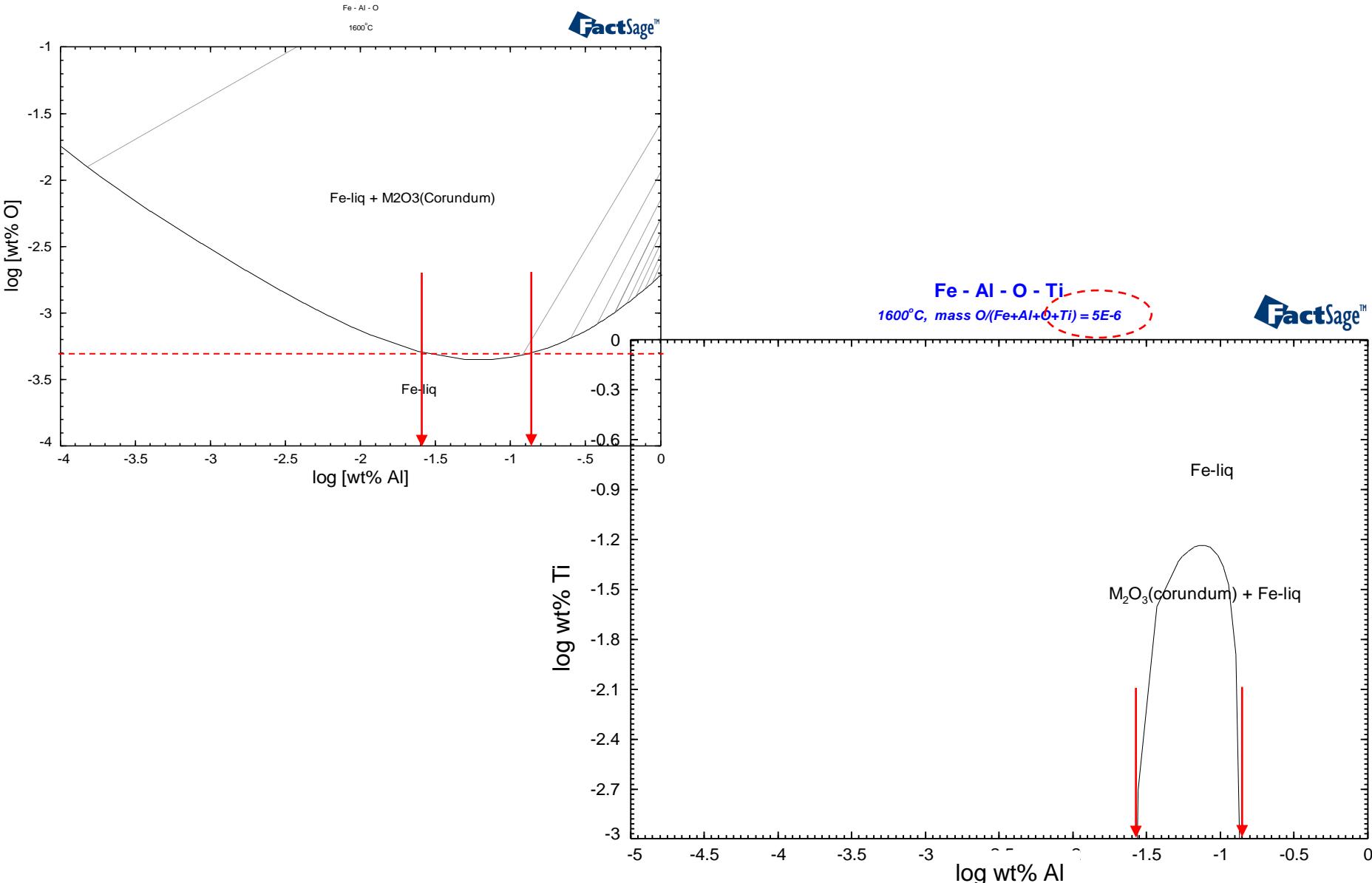
Inclusion diagram: Fe-Al-O, Al deoxidation

New way to set the axis in log scale

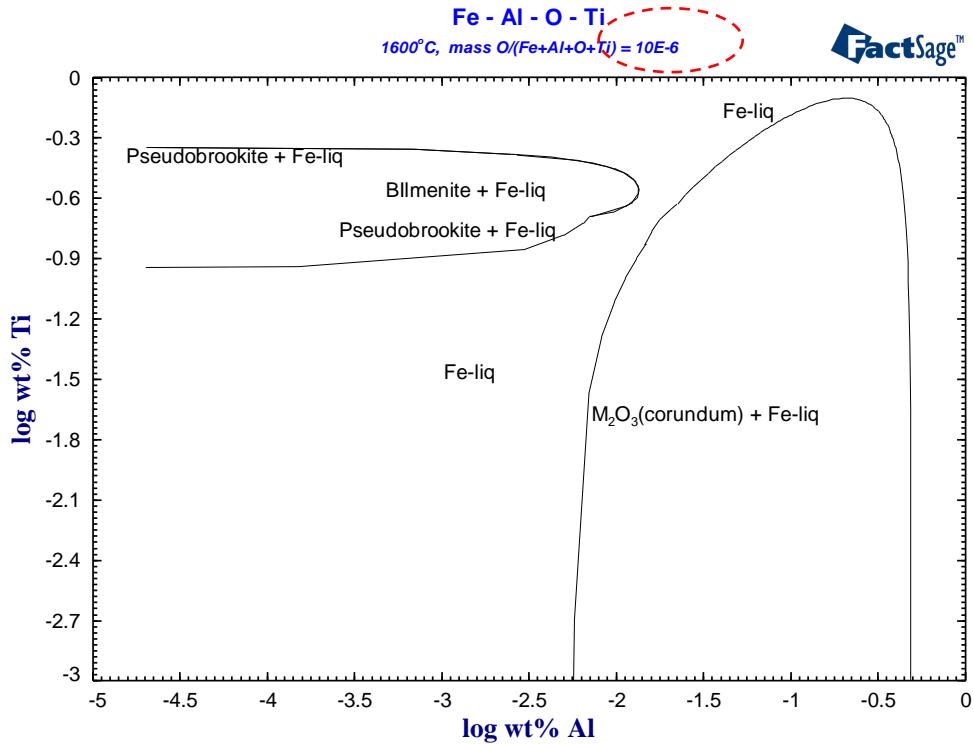
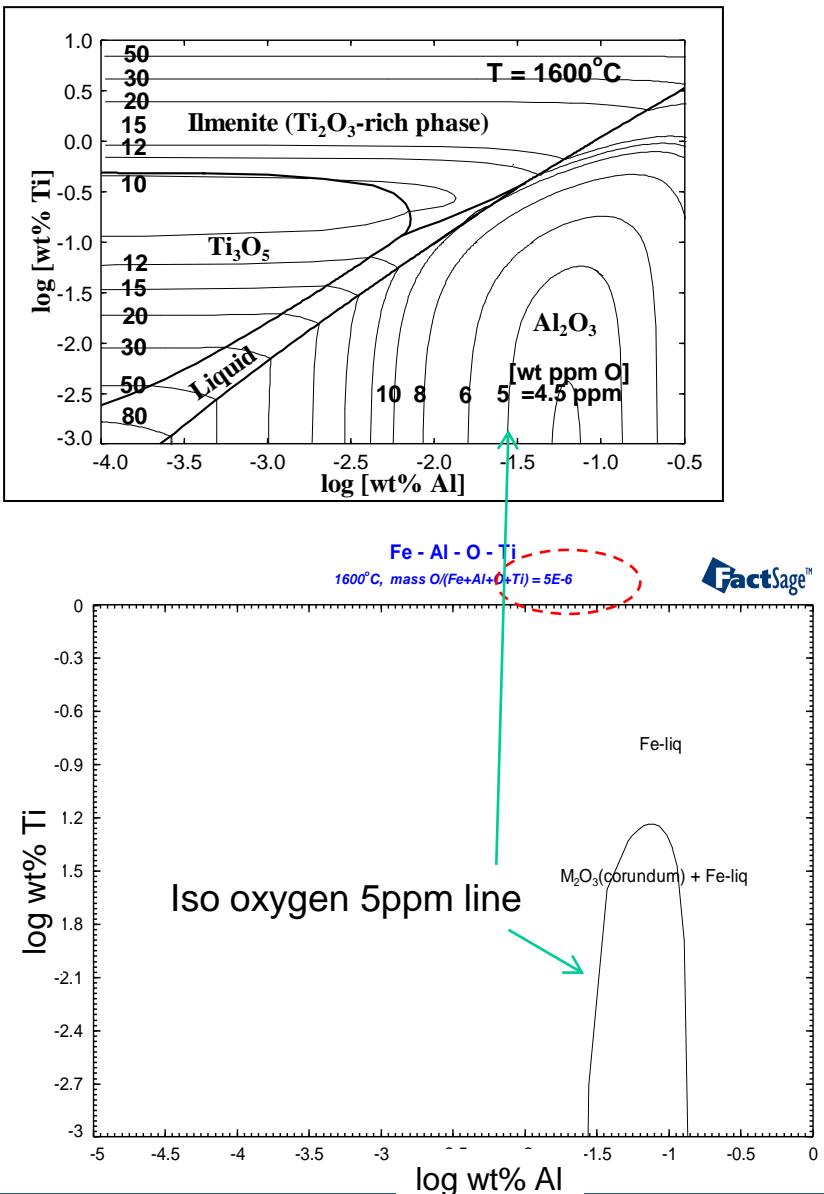
→ log – log diagram or log – linear scale diagram can be calculated now



Inclusion diagram: Fe-Al-Ti-O, Al/Ti deoxidation



Inclusion diagram: Fe-Al-Ti-O, Al/Ti deoxidation



- 1) Change oxygen content and calculate similar diagram
- 2) Superimpose all the diagram together
- 3) Calculate the phase boundaries from Equilib (or simply connect boundaries in the calculated diagram)

Inclusion after Mn/Si deoxidation

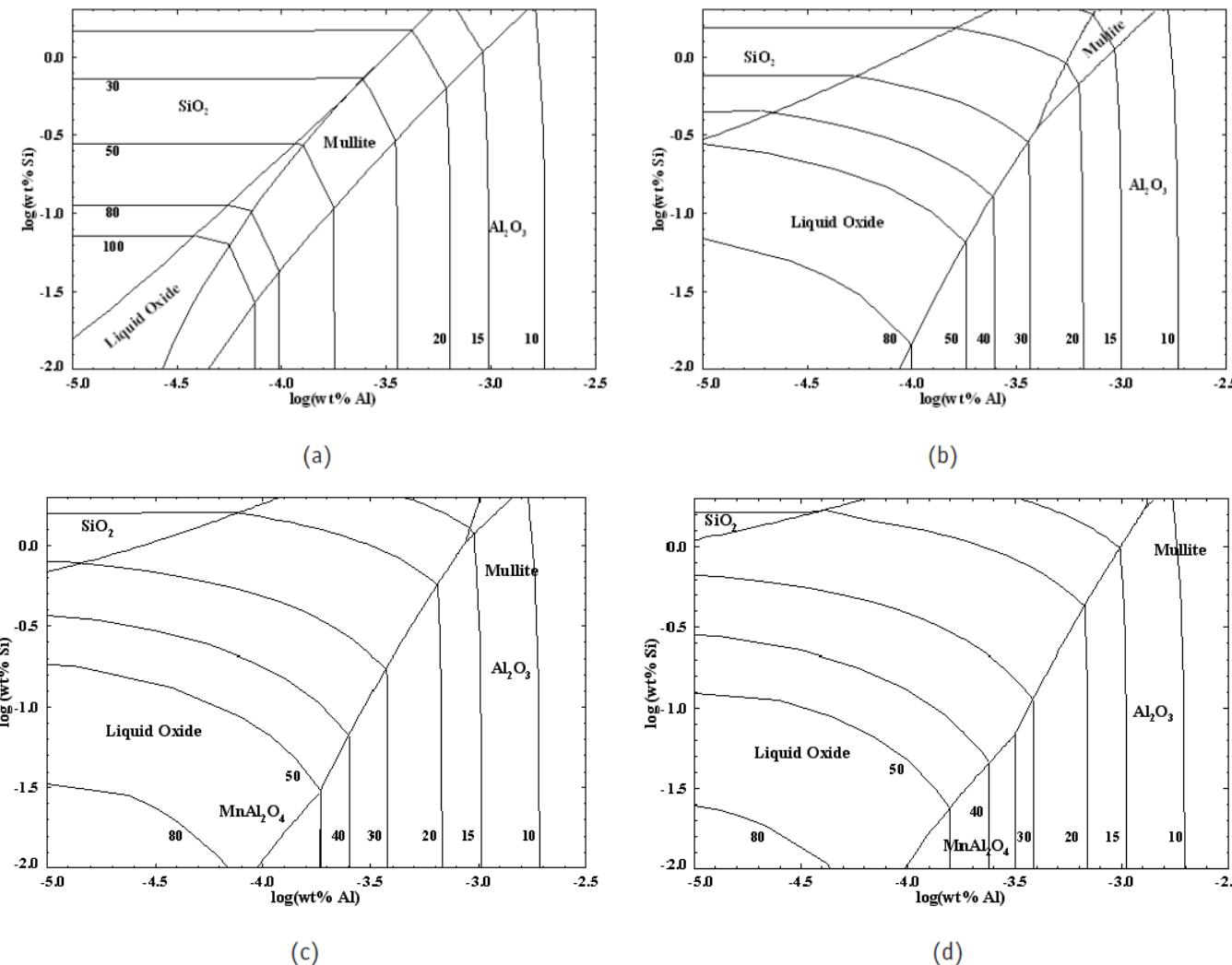


Figure 11: Calculated inclusion stability diagrams in the Fe-Mn-Si-Al-O system at 1550°C for (a) mass% Mn = 0, (b) mass% Mn = 0.5, (c) mass% Mn = 1.0 and (d) mass% Mn = 1.5. Numbers adjacent to each line represent equilibrium oxygen contents (in ppm) in liquid steel [23].

AI killed Ti bearing steel

Data Search

Databases - 3/26 compound databases, 2/26 solution databases

Fact **FactSage™ SGTE**

	compounds only	solutions only	no data
<input checked="" type="checkbox"/> FactPS	<input type="checkbox"/> FSscopp	<input type="checkbox"/> BINS	
<input checked="" type="checkbox"/> FToxid	<input type="checkbox"/> FSlead	<input type="checkbox"/> SGPS	
<input type="checkbox"/> FTsalt	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGTE	
<input checked="" type="checkbox"/> FTmisc	<input type="checkbox"/> FSups	<input type="checkbox"/> SGsold	
<input type="checkbox"/> FThall			
<input type="checkbox"/> FTOxCN			
<input type="checkbox"/> FTfitz			
<input type="checkbox"/> FThelp	<input checked="" type="checkbox"/> ELEM	<input type="checkbox"/> SGnobl	
<input type="checkbox"/> FTpulp	<input type="checkbox"/> FTdemo	<input type="checkbox"/> SpMCBN	
<input type="checkbox"/> FTlite	<input type="checkbox"/> FTnucl	<input type="checkbox"/> TDmeph	
		<input type="checkbox"/> TDnucl	

Other

Add/Remove
 RefreshData
 Clear All

Private Databases

EXAM SGTEa SGTEb

Equilib - Menu: Ferrous Applications II 46

File Units Parameters Help

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

- gas ideal real 57
- aqueous 0
- pure liquids 0
- pure solids 107

* - custom selection species: 164

Solution phases

*	+	Base-Phase	Full Name
*	+	FToxid-ILMEB	B-Ilmenite
		FToxid-ILME?	?-Ilmenite
*	+	FToxid-PSEU	Pseudobrookite
	+	FToxid-TiSp	Titania_Spinel
*	+	FToxid-TSpi	Tetragonal-Spinel
	+	FToxid-Bixb	Mn2O3(Bixbyite)
*	+	FToxid-Brau	Braunite_Mn7SiO12
	+	FToxid-Rhod	Rhodonite

Legend

- I - immiscible 5
- + - selected 13

Show all selected
 species: 207
 solutions: 23 Select

Information

Options - search for product species

Include compounds

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

Default

Custom Solutions

- 0 fixed activities
- 0 ideal solutions

Pseudonyms

apply Edit ...

Volume data

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

paraequilibrium & Gmin edit

Virtual species: 56

Total Species (max 5000) 371

Total Solutions (max 200) 23

Total Phases (max 1500) 131

Final Conditions

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

Equilibrium

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

FactSage 8.0 C:\Workshop80\Ferro\Ferrous_Applications_II_46.equi

AI killed Ti bearing steel

F Equilib - Results 1600 C

Output Edit Show Pages Final Conditions

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

+ 1.5906E-40 Fe (CO) 5
+ 2.8722E-45 N2O4
+ 3.6814E-55 N2O5)

+ 99.996 gram Fe-liq
(99.996 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.% Al2O
+ 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	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	1.7718	98.947	0.98635	0.98951
Mn	1.2742E-02	0.70000	7.0931E-03	7.0003E-03
Ti	2.0886E-03	9.9975E-02	1.1627E-03	9.9979E-04
Si	7.1211E-03	0.20000	3.9642E-03	2.0001E-03
Al	1.0351E-03	2.7929E-02	5.7624E-04	2.7930E-04
O	4.0345E-05	6.4549E-04	2.2459E-05	6.4552E-06
N	1.0709E-03	1.5000E-02	5.9617E-04	1.5001E-04
C	4.1630E-04	5.0000E-03	2.3175E-04	5.0002E-05

+ 3.9506E-03 gram M2O3(Corundum)#1
(3.9506E-03 gram, 3.8637E-05 mol)
+ 0 gram M2O3(Corundum)#2
(1600 C, 1 atm, a=1.0000)
(99.036 wt.% Al2O3

Reoxidation of Al killed Ti bearing steel

The screenshot shows two windows of the FactSage software interface. The top window is titled 'Equilib - Results 1600 C' and has a menu bar with 'Output', 'Edit', 'Show Pages', and 'Final Conditions'. The 'Output' menu is open, showing options like 'Save or Print As ...', 'Repeat Save', 'Plot', 'Equilib Results file', 'Stream File' (which is highlighted), 'Format', 'Fact-XML', 'Fact-Optimal', 'Fact-Function-Builder', 'Refresh ...', and 'Swap loops ...'. Below this is a table of element amounts:

	Amount/mol	Amount/gram
Fe	1.7718	98.947
Mn	1.2742E-02	0.70000
Ti	2.0886E-03	9.9975E-02
Si	7.1211E-03	0.20000
Al	1.0351E-03	2.7929E-02
O	4.0345E-05	6.4549E-04
N	1.0709E-03	1.5000E-02
C	4.1630E-04	5.0000E-03

Below the table, there are several lines of calculation output:

```
+ 3.9506E-03 gram M2O3(Corundum)#1  
(3.9506E-03 gram, 3.8637E-05 mol)  
+ 0 gram M2O3(Corundum)#2  
(1600 C, 1 atm, a=1.0000)  
( 99.036 wt.% Al2O3  
+ 2.8914E-05 wt.% Fe2O3
```

The bottom window is titled 'Equilib - Reactants' and shows a table of species and their properties:

Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
100%	[Rc_A-Monoxide]				2	
+	100%	[Rc_Fe-liq]			3	
+	100%	[Rc_M2O3(Corundum)]			4	
+	100%	[Rc_SOLID]			5	

A yellow box highlights the text "Recycle all streams" in the left-hand window.

“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

Next >>

Reoxidation of Al killed Ti bearing steel

Equilib - Menu: last system

File Units Parameters Help

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

Reactants (3)

(gram) 100% [Rc_Fe-liq] + 100% [Rc_M2O3(Corundum)] + <A> O₂

Products

Compound species

- + gas ideal real 57
- aqueous 0
- pure liquids 0
- * + pure solids 107

* - custom selection species: 164

Target

- none -

Estimate T(K): 1000

Quantity(g): 0

Solution phases

*	+	Base-Phase	Full Name
	+	FTmisc-FeLQ	Fe-liq
		FTmisc-BCCS	bcc
		FTmisc-FCCS	fcc
I		FToxid-SLAGA	A-Slag-liq all o
		FToxid-SLAG?	?-Slag-liq
I		FToxid-SPINB	B-Spinel
+		FToxid-MeO_A	A-Monoxide
		FToxid-MeO_B	B-Monoxide

Legend

- I - immiscible 5
- + - selected 11

Show all selected

species: 203

solutions: 21

Select

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

paraequilibrium & Gmin edit

Virtual species: 56

Total Species (max 5000) 367

Total Solutions (max 200) 21

Total Phases (max 1500) 129

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
0.005 0.001		1600	1	
10 steps	<input type="checkbox"/> Table			51 calculations

Equilibrium

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

FactSage 8.0 C:\Workshop80\Ferro\Ferrous_Applications_II_46.equi

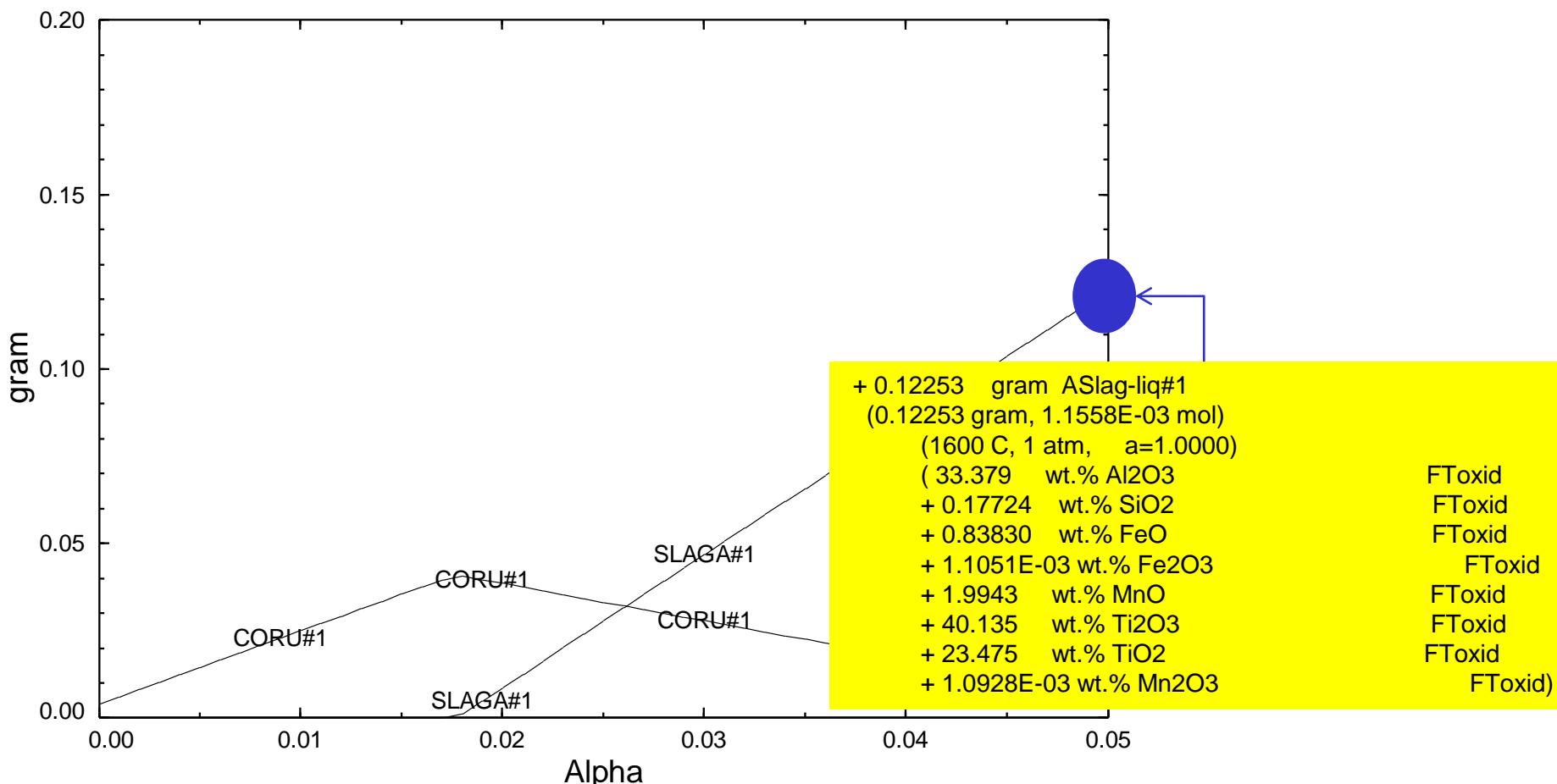
Addition of oxygen to simulation reoxidation phenomena.
Real source of oxygen could be high SiO₂ slag or refractories

Reoxidation of Al killed Ti bearing steel

This calculation shows that mixed inclusion of $\text{Al}_2\text{O}_3(\text{s})$ 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> O₂

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



TiN formation in Al killed and Ti bearing steel

Original steel composition at 1600C: high N and high Ti → may form TiN

(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

F Equilib - Menu: last system

File Units Parameters Help

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

Reactants (2)

(gram) 100% [Rc_Fe-liq] + 100% [Rc_M2O3(Corundum)]

Products

Compound species

[+]	gas	<input checked="" type="radio"/> ideal	<input type="radio"/> real	57
[+]	aqueous	0		
[+]	pure liquids	0		
* [+]	pure solids	107		
* - custom selection	species:	164		

Target

- none -

Estimate T(K): 1000

Quantity(g): 0

Solution phases

*	+	Base-Phase	Full Name
*	+	FTmisc-FeLQ	Fe-liq
*	+	FTmisc-BCCS	bcc
*	+	FTmisc-FCCS	fcc
I	FToxic-SLAGA	A-Slag-liq all oxides + S	
I	FToxic-SLAG?	?-Slag-liq	
I	FToxic-SPINB	B-Spinel	
*	+	FToxic-MeO_A	A-Monoxide
*	+	FToxic-MeO_B	B-Monoxide

Legend

I - immiscible 5
+ - selected 13

Show all selected

species: 207

solutions: 23

Custom Solutions

0 fixed activities

0 ideal solutions

Pseudonyms

apply Edit ...

Volume data

assume molar volumes of solids and liquids = 0

include molar volume data and physical properties data

paraequilibrium & Gmin edit

Total Species (max 5000) 371

Total Solutions (max 200) 23

Total Phases (max 1500) 131

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		1600 1500 10	1	
10	steps	<input type="checkbox"/> Table		11 calculations

Equilibrium

normal

normal + transitions

transitions only

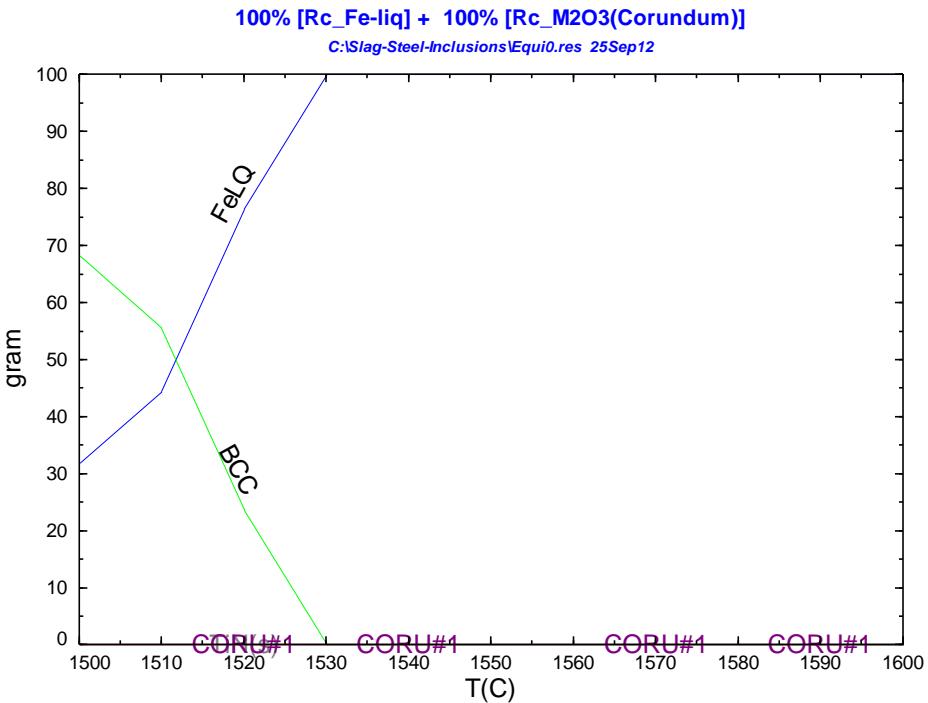
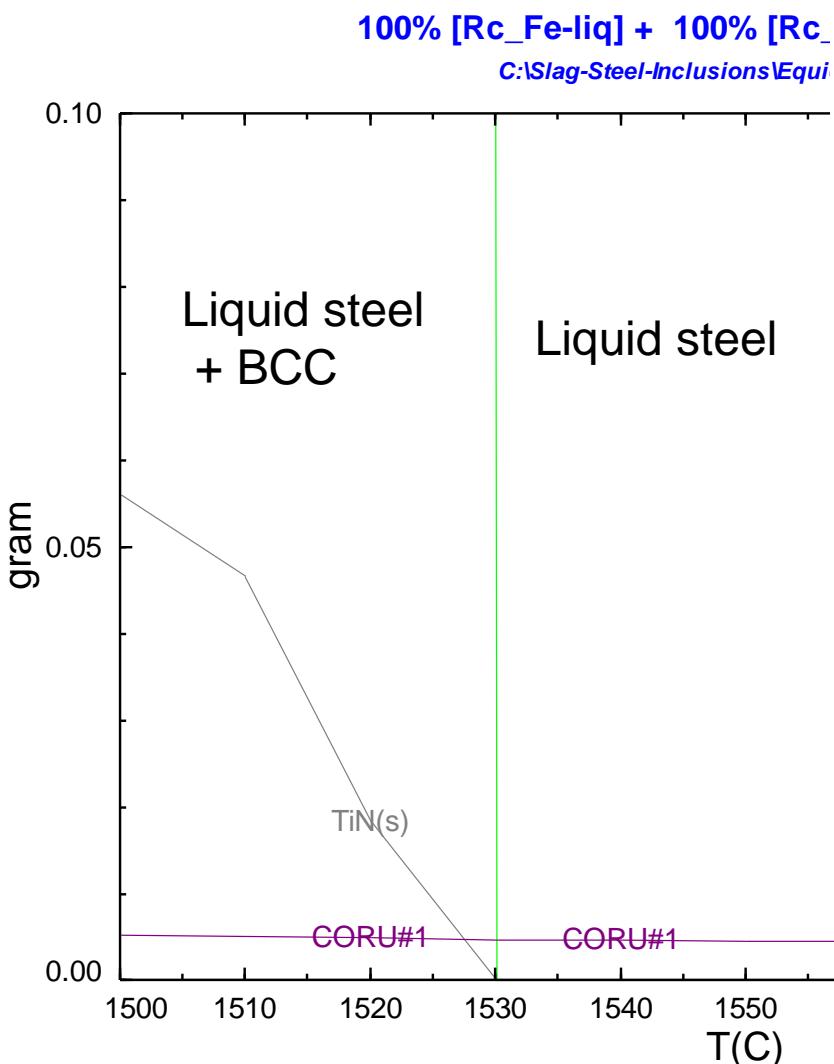
open

- no time limit -

Calculate >>

FactSage 8.0 C:\Workshop80\Ferro\Ferrous_Applications_II_46.equi

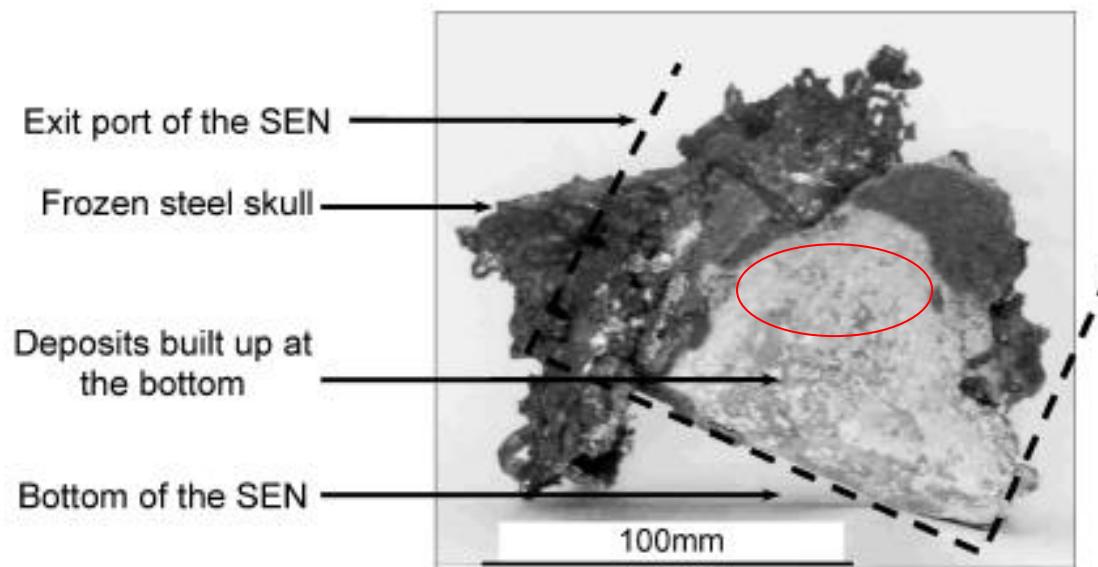
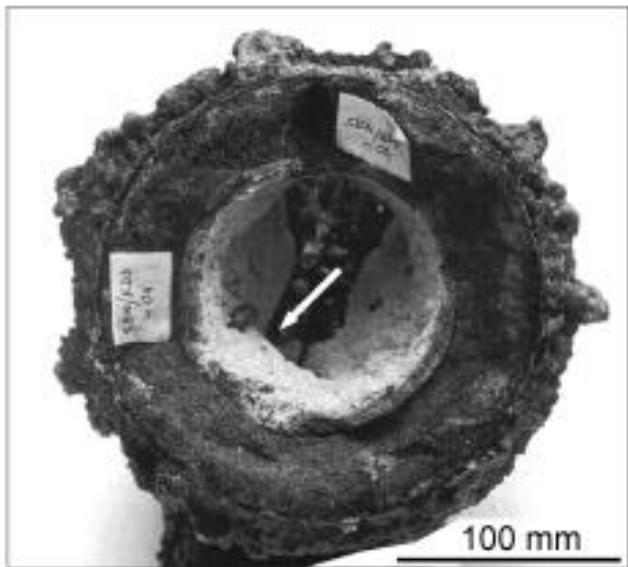
TiN formation in Al killed and Ti bearing steel



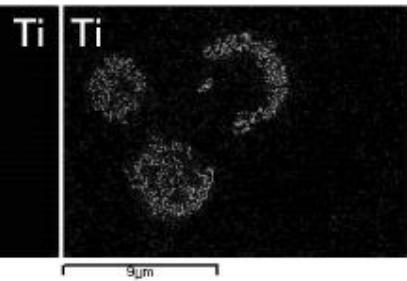
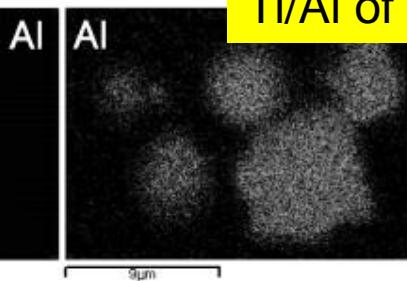
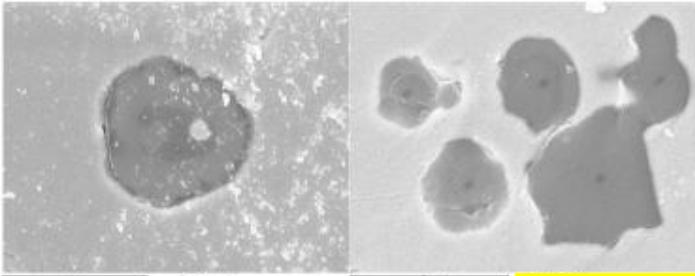
During the solidification,
a large amount of TiN can be formed.

Nozzle Clogging in Ti-bearing Al-killed steel

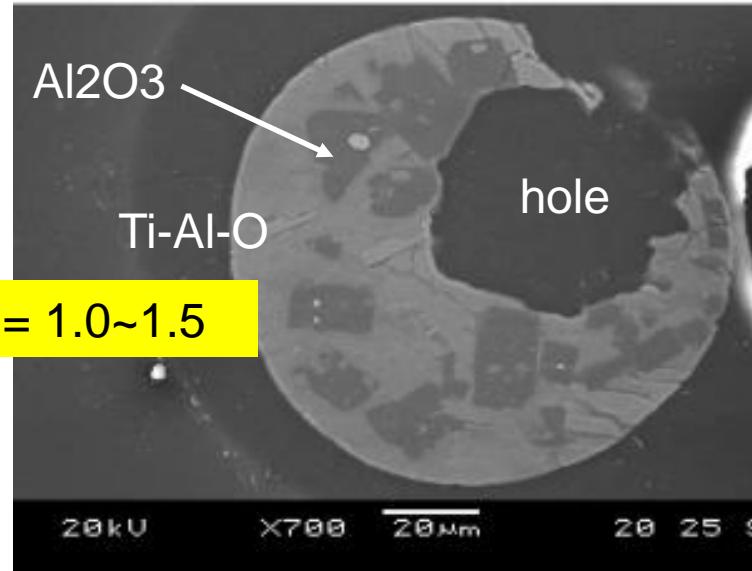
- Kawashima *et al.*, CAMP-ISIJ (1991)
 - Liquid Al-Ti-O (reoxidation) attached to Al_2O_3 inclusions
- Basu *et al.* ISIJ Int. (2004)
 - Significant difference of nozzle clogging of Ti-bearing steel from and Ti-free steel is the existence of the Al-Ti-O inclusions covering Al_2O_3 core oxides.
 - Reoxidation in tundish (high SiO_2 slags) causes the nozzle clogging.



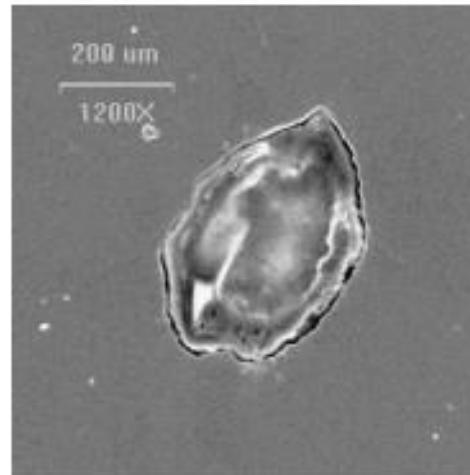
Inclusions generated by Reoxidation process



Reoxidation in Tundish
(high SiO₂ slags)
Park et al. (2004)

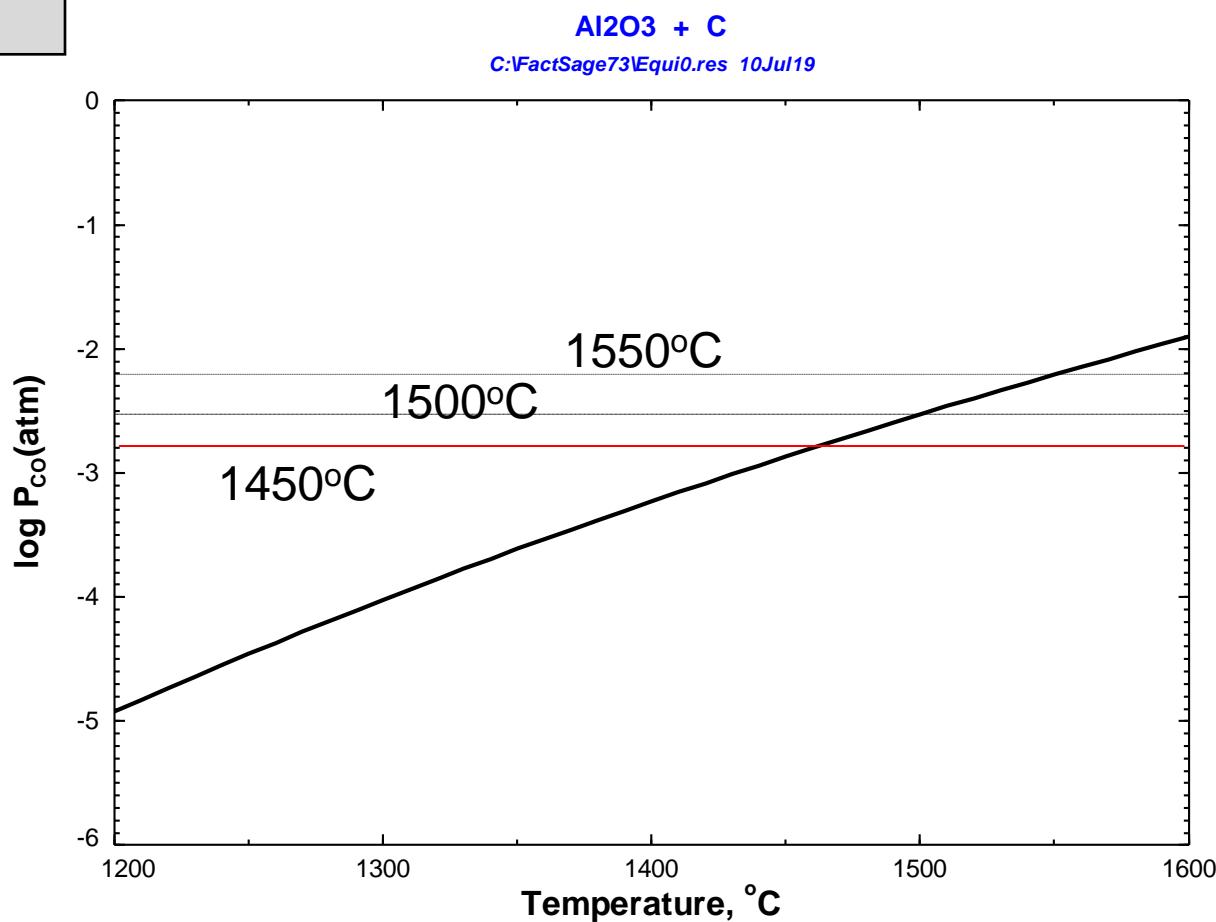
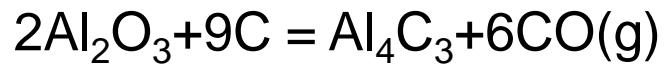
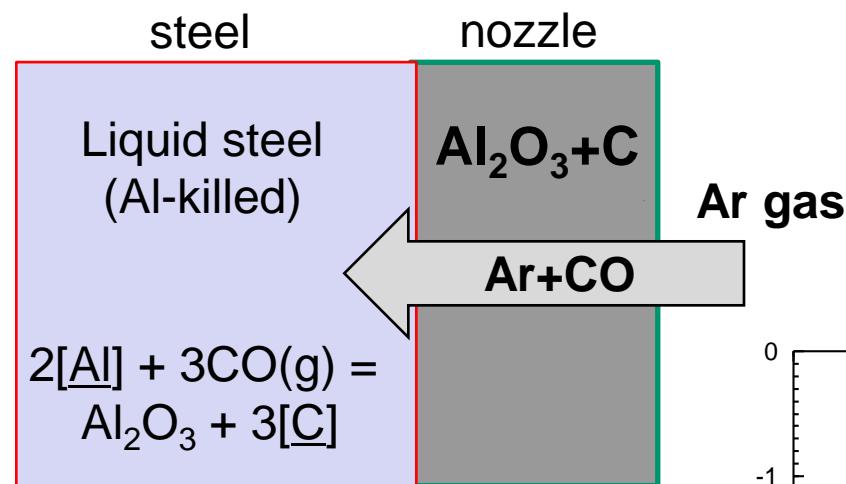


RH process after Ti addition (POSCO)
Doo et al. (2007)

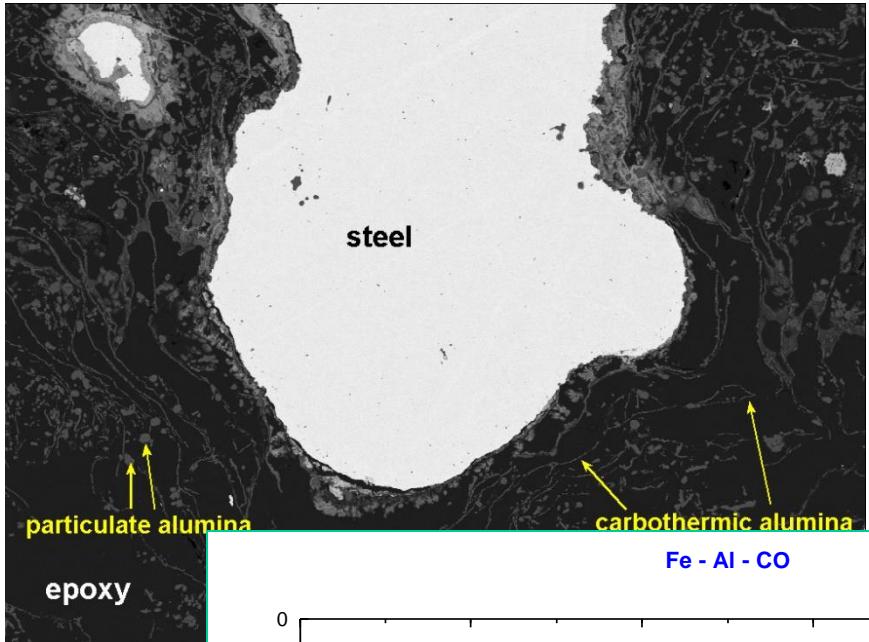


Reoxidation in Tundish
Basu et al. (2004)

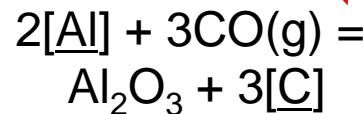
Reoxidation of steel by CO gas



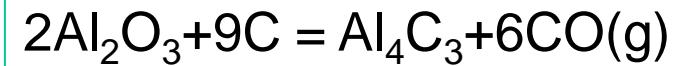
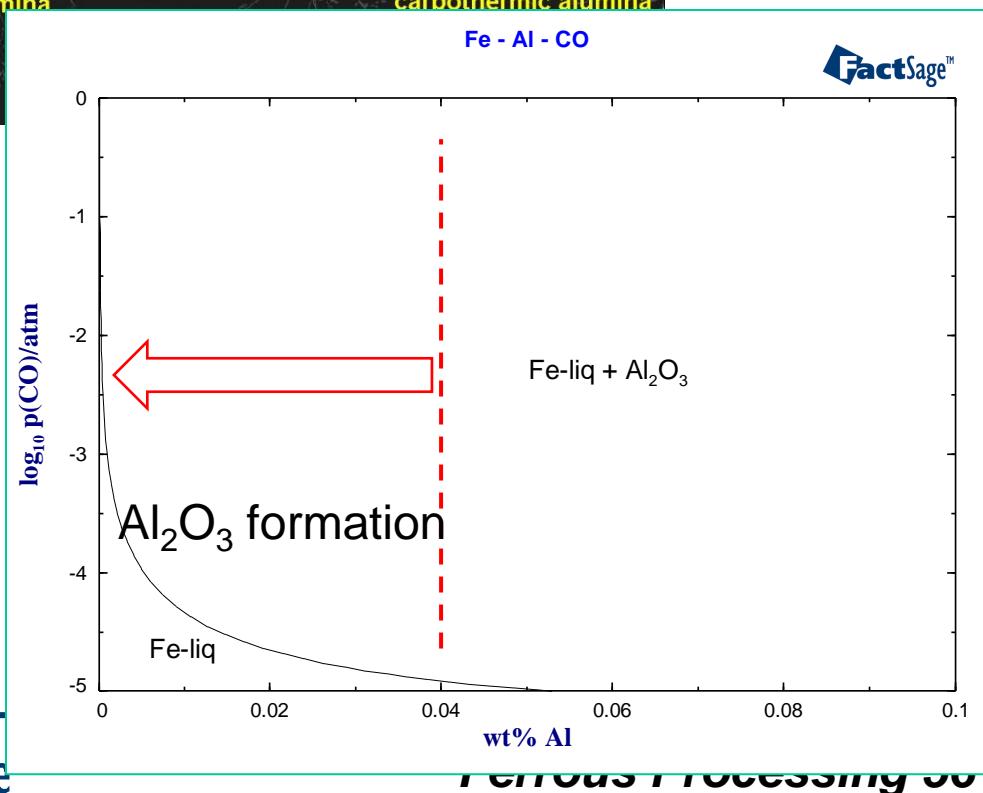
Reoxidation of steel by CO gas



Liquid steel
(Al-killed)



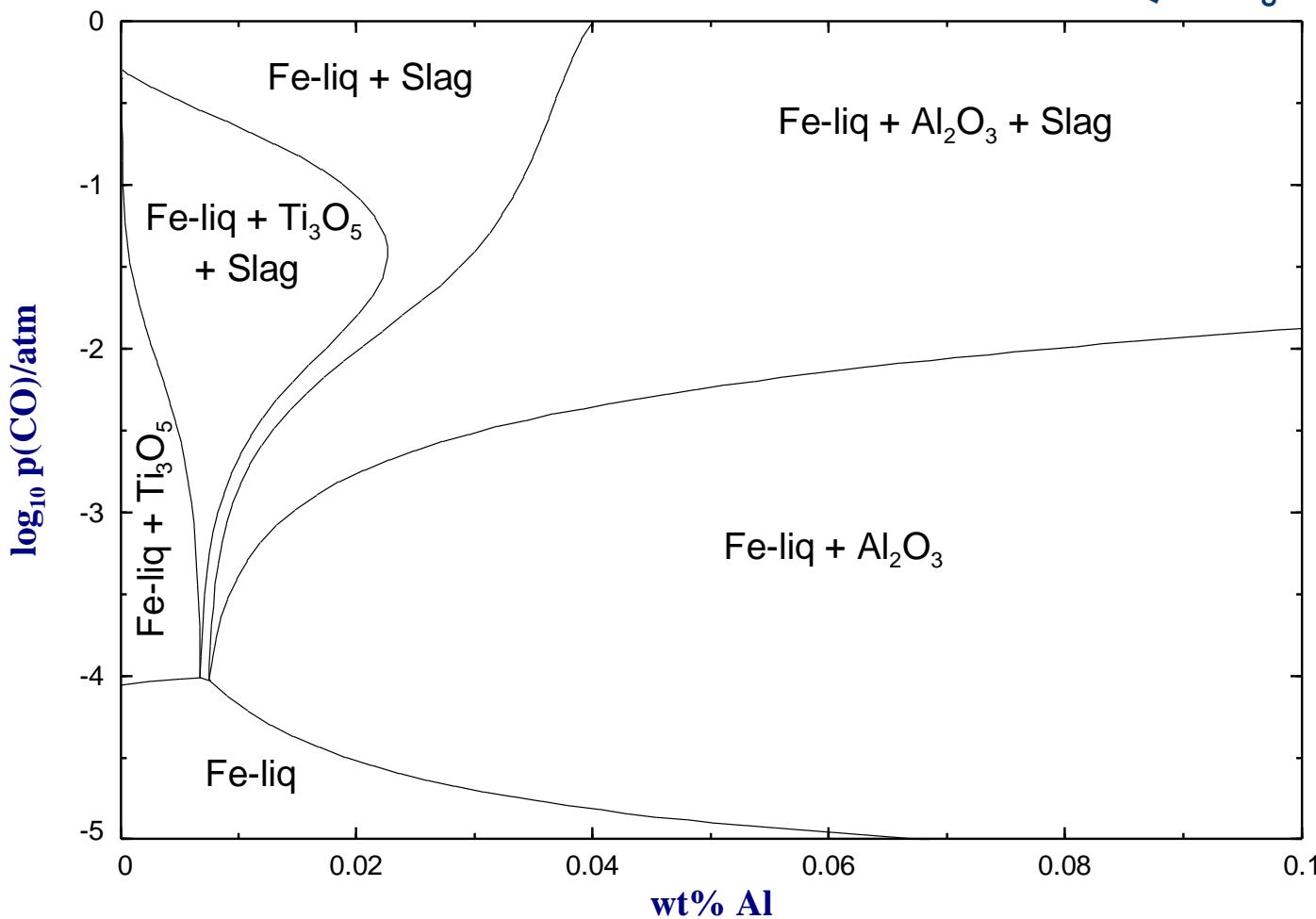
Ar gas



Reoxidation of steel by CO gas

Fe - Al - Ti - CO

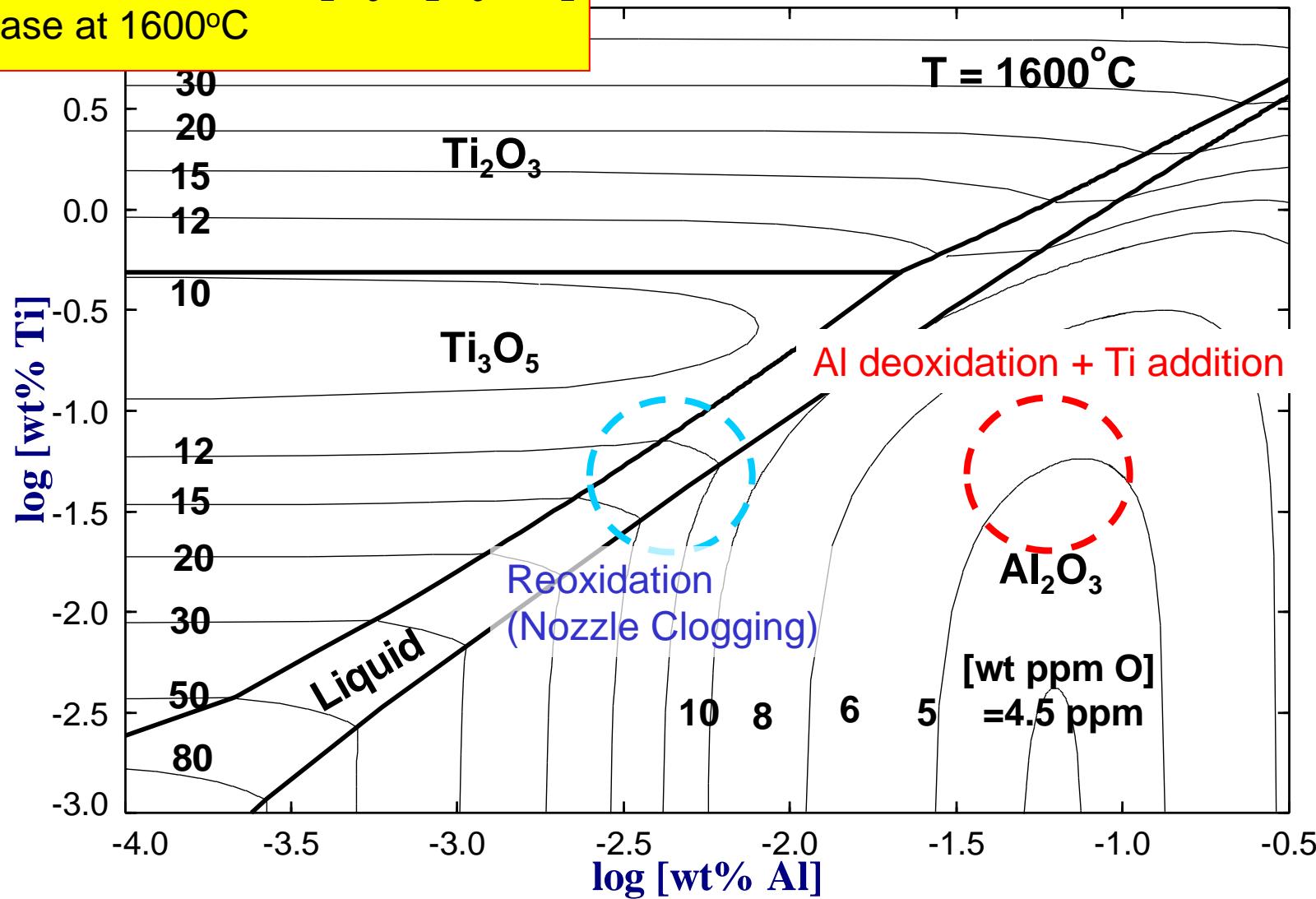
Ti = 1000 ppm, 1550°C



Reoxidation of steel by CO gas through ceramic nozzle to form slag(Al-Ti-O) and Al_2O_3

Newly calculated Inclusion diagram of Fe-Al-Ti-O system

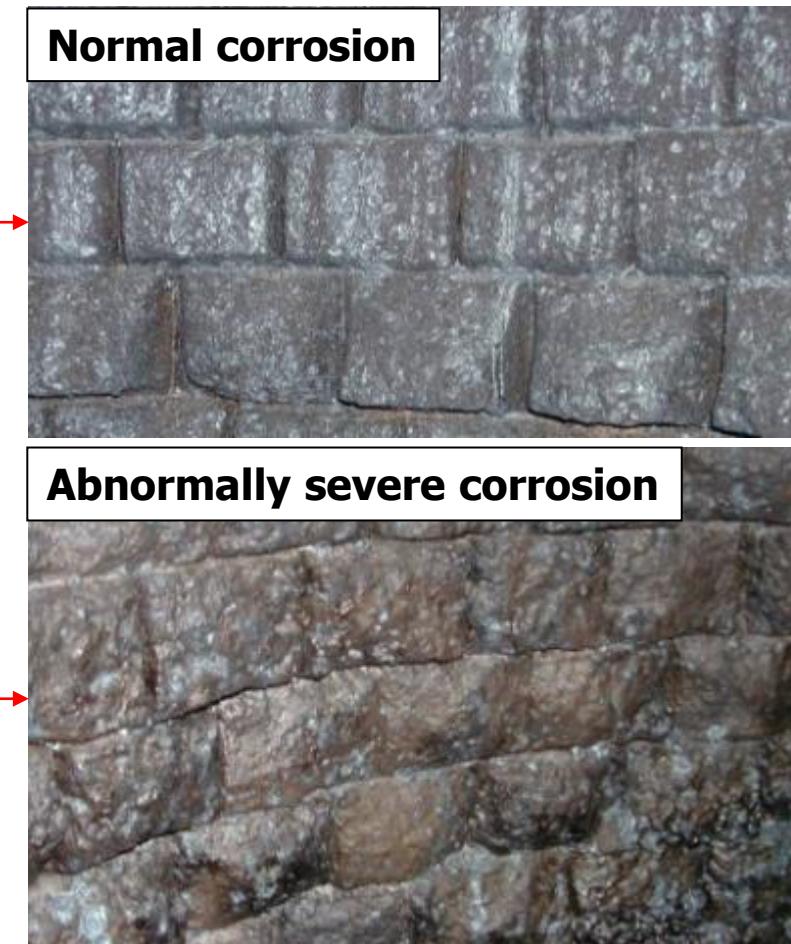
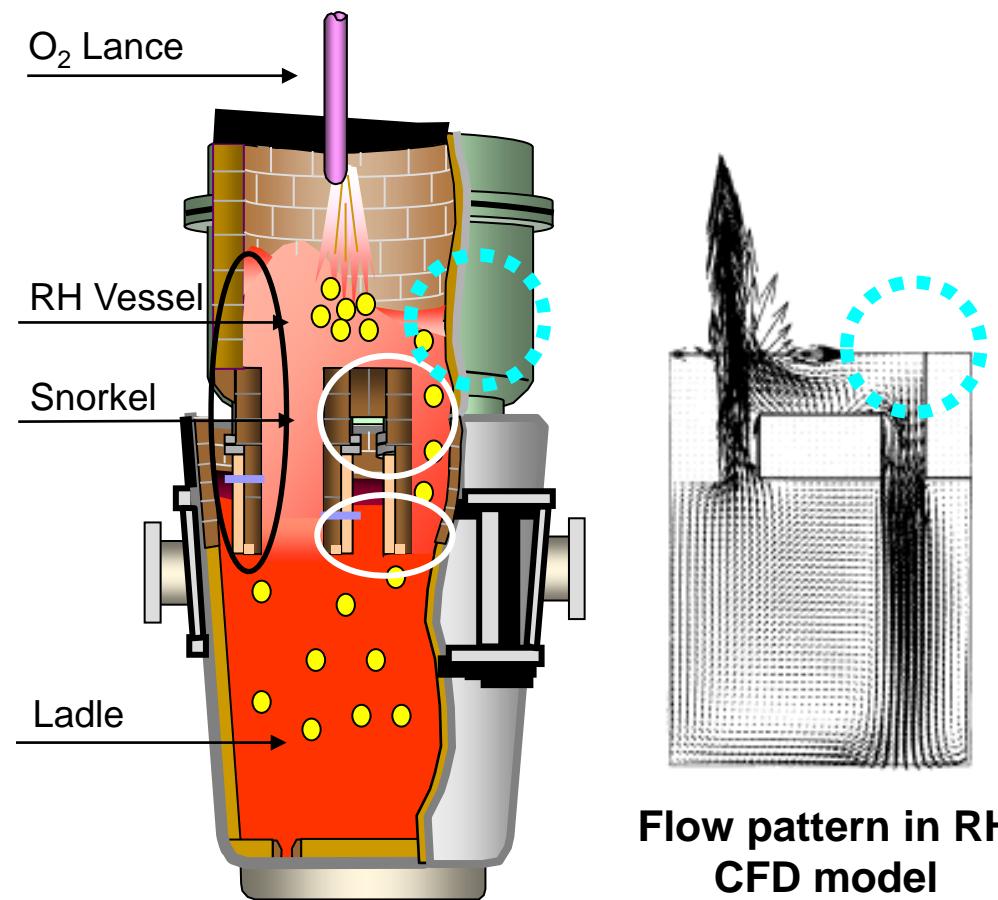
Existence of Liquid $\text{Al}_2\text{O}_3\text{-Ti}_2\text{O}_3\text{-TiO}_2$ phase at 1600°C



RH Vessel Refractory

RH OB

- *High amount of oxygen blowing*
- *Increase of Ferro-alloy (Al, Si, Mn, etc) addition*
→ *More severe local corrosion of RH vessel refractory*



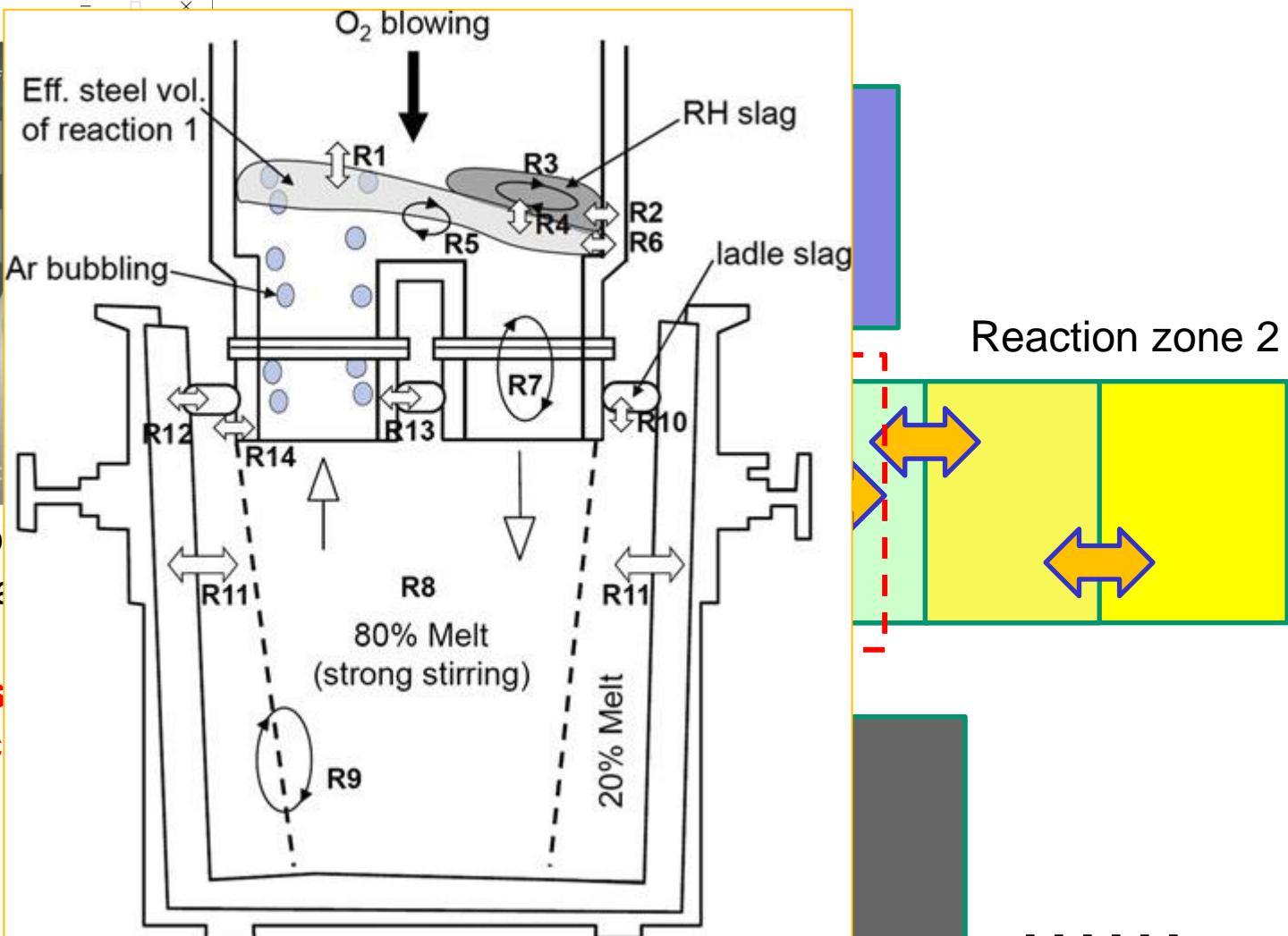
Flow pattern in RH
CFD model

Concept for RH process simulation modeling



Quite enough thermo
(gas, molten steel, slag)

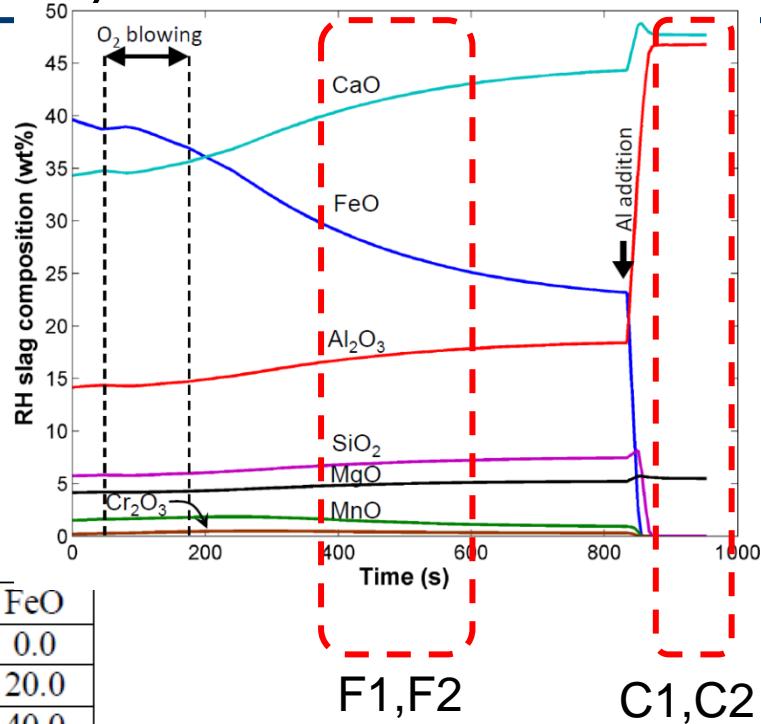
**Write kinetic process
input/output to Excel**



Heat & Mass balance ..

RH Vessel Refractory

Predicted slag composition in RH vessel from RH process simulation →



Experimental and calculation conditions

Table 1: Composition of the synthetic slags (wt%).

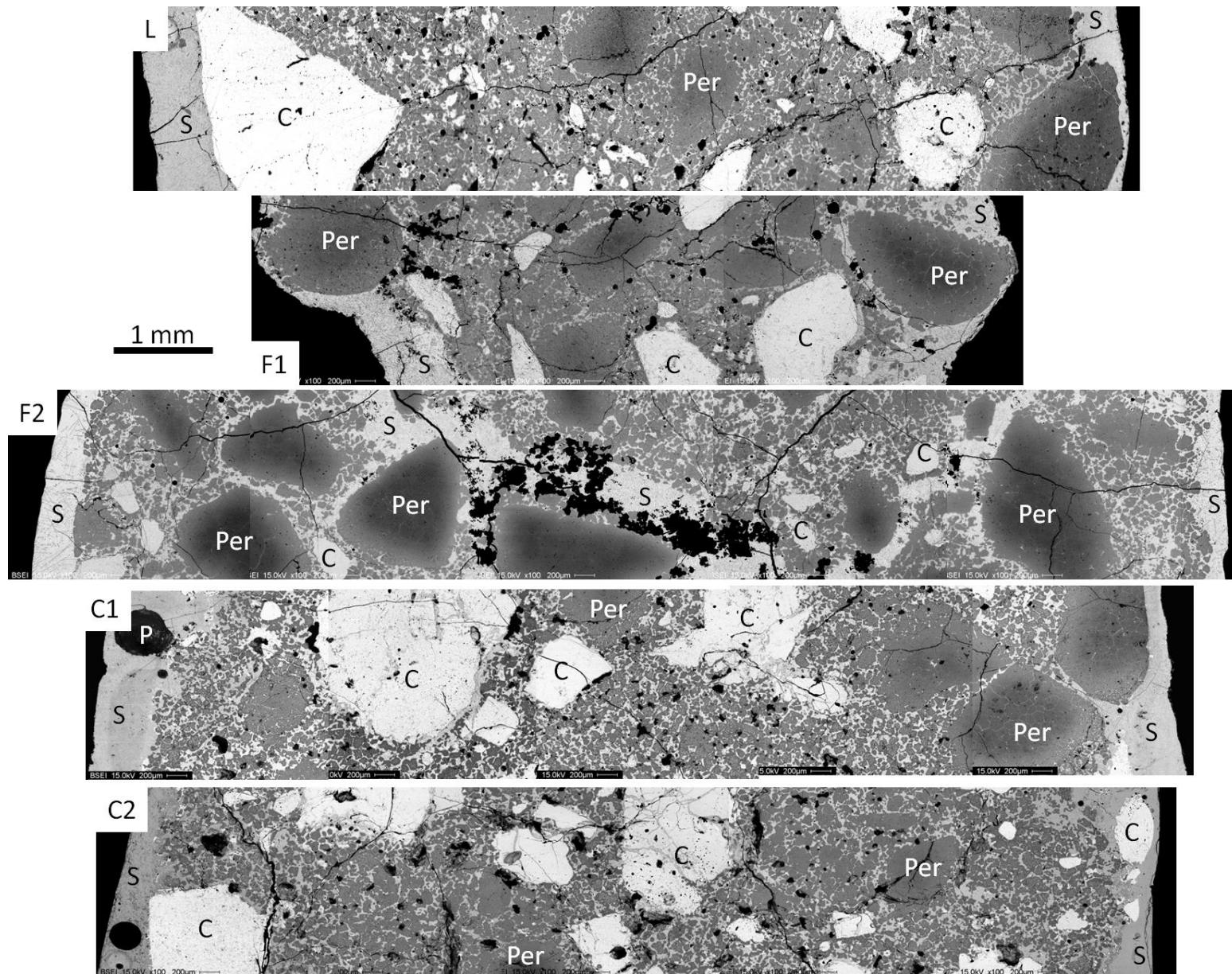
Slag	Symbol	MgO	Al ₂ O ₃	SiO ₂	CaO	FeO
Ladle slag	L	5.3	27.7	10.7	56.3	0.0
FeO-rich slag 1	F1	4.2	22.2	8.6	45.0	20.0
FeO-rich slag 2	F2	3.2	16.6	6.4	33.8	40.0
CaO-Al ₂ O ₃ slag 1	C1	0.0	45.0	0.0	55.0	0.0
CaO-Al ₂ O ₃ slag 2	C2	0.0	60.0	0.0	40.0	0.0

Table 2: Overall composition and apparent porosity of the investigated refractories.

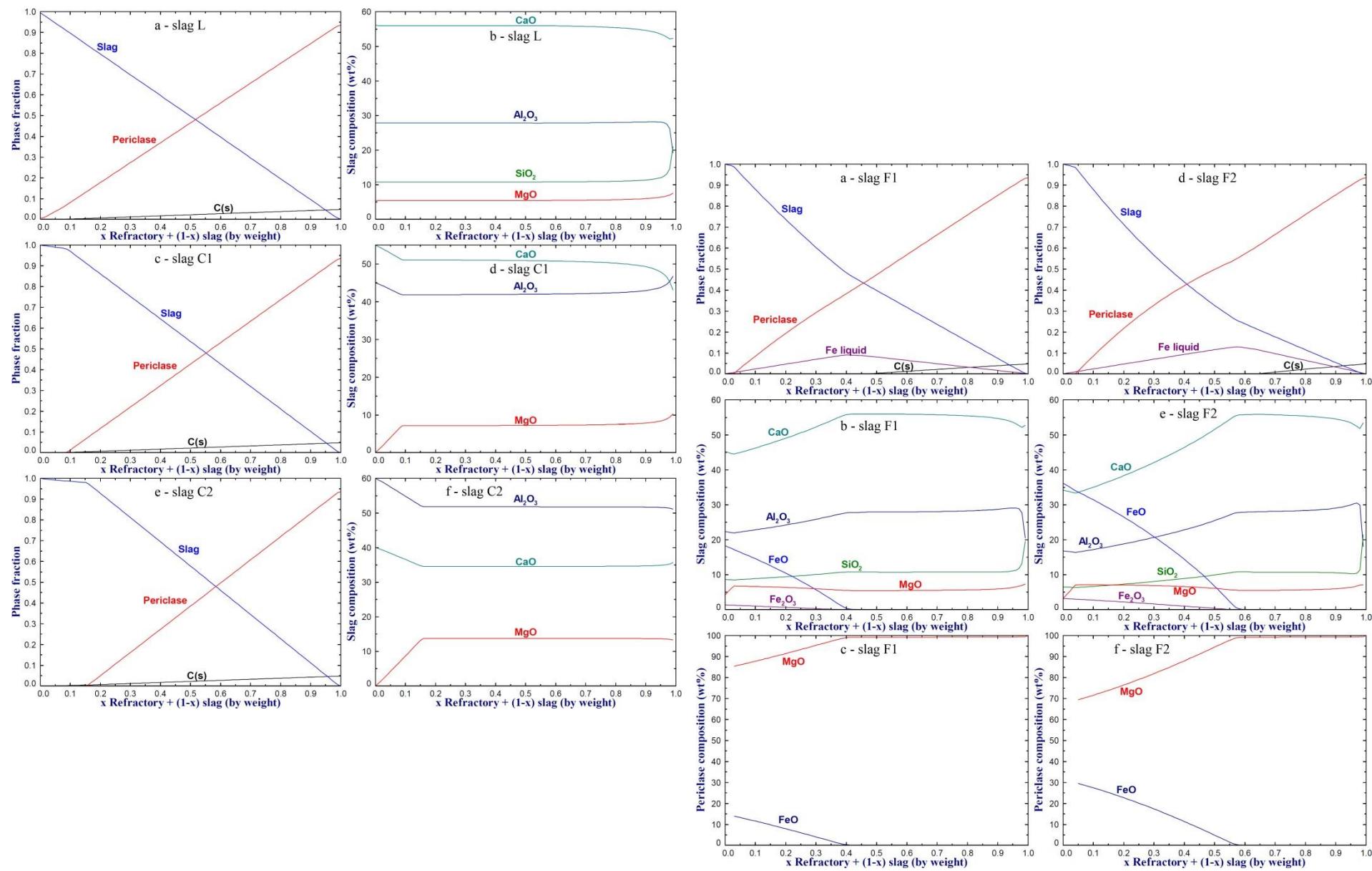
Refractory	Overall composition (wt%)						Apparent porosity (%)	
	MgO	Cr ₂ O ₃	CaO	SiO ₂	Al ₂ O ₃	FeO _t		
Magnesia-chromite	55.8	22.9		2.1	8.2	11.0	16~17	
Magnesia-carbon	90.3		0.8	2.2	6.8		5.1	11~13

M.-K. Cho, M.-A. Van Ende, T.-H. Eun and I.-H. Jung, "Investigation of slag-refractory interactions for the Ruhrstahl Heraeus (RH) vacuum degassing process in steelmaking", J. Eur. Ceram. Soc., 2012, 32, 1503-1517.

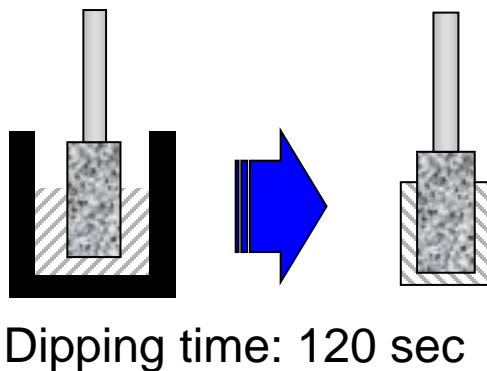
Refractory Finger tests at 1600°C



Thermodynamic Calculations: Refractories – Slag Interactions



Ladle Glaze formation

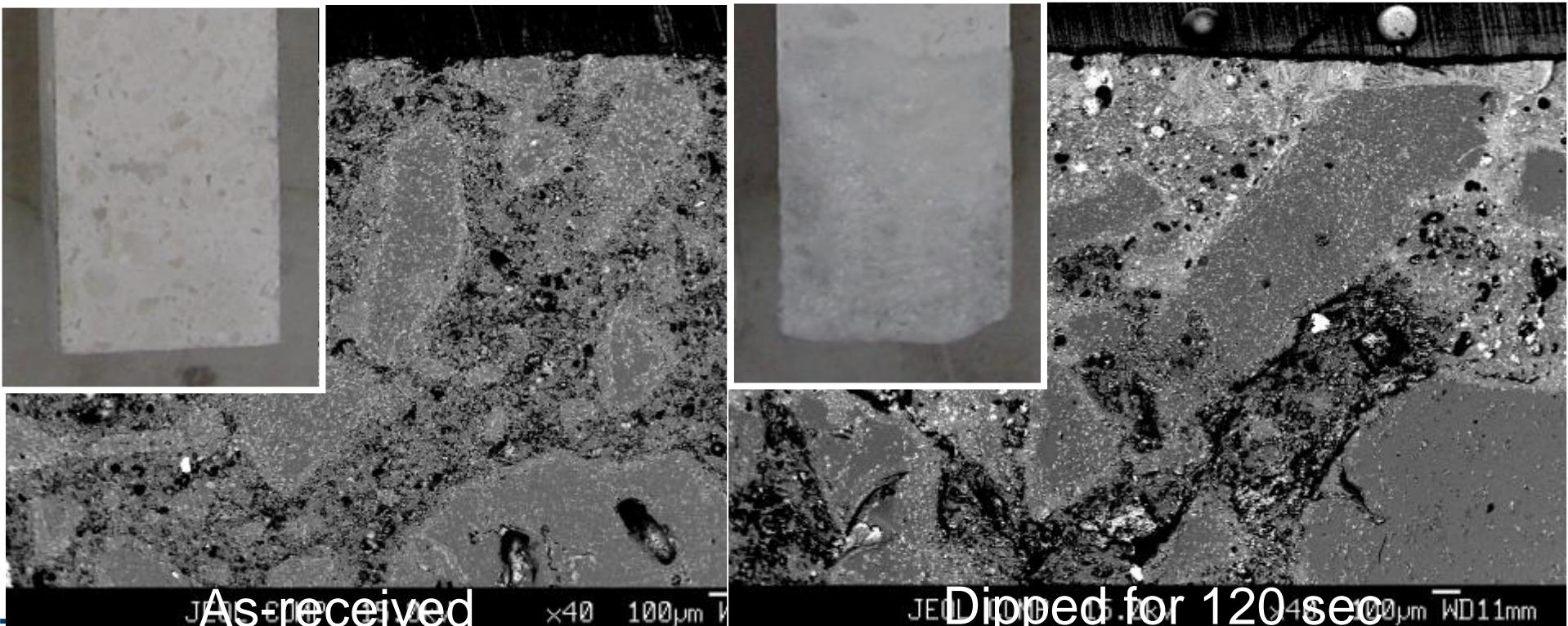


Refractory composition (wt.%)

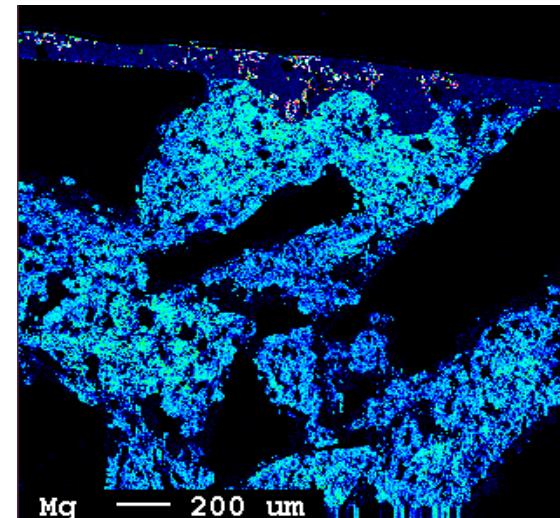
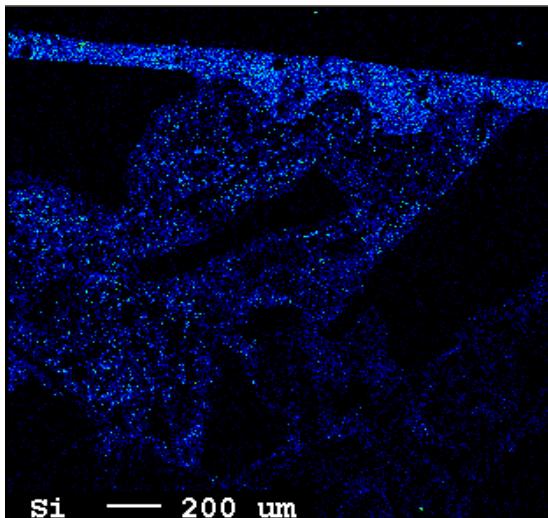
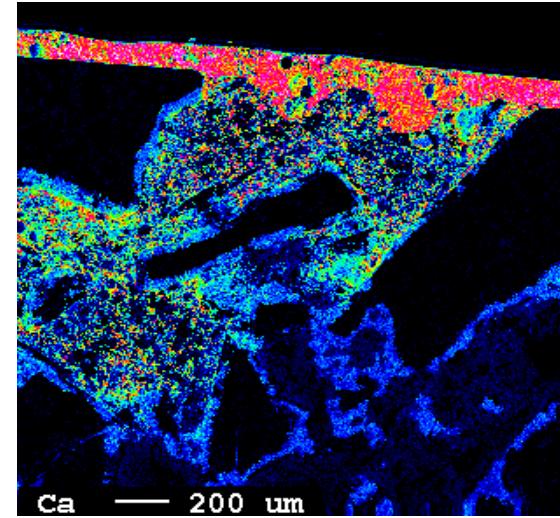
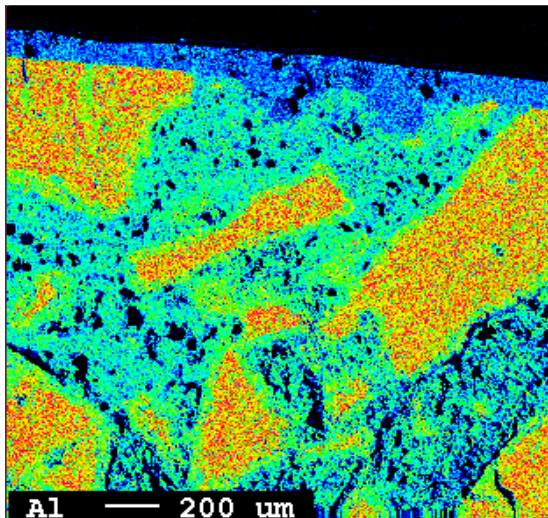
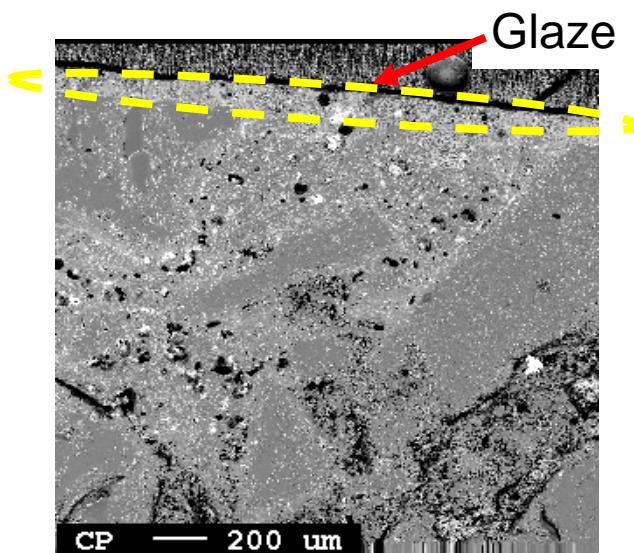
CaO	SiO ₂	Al ₂ O ₃	MgO
2.35	0.76	88.06	8.35

Slag composition (wt.%)

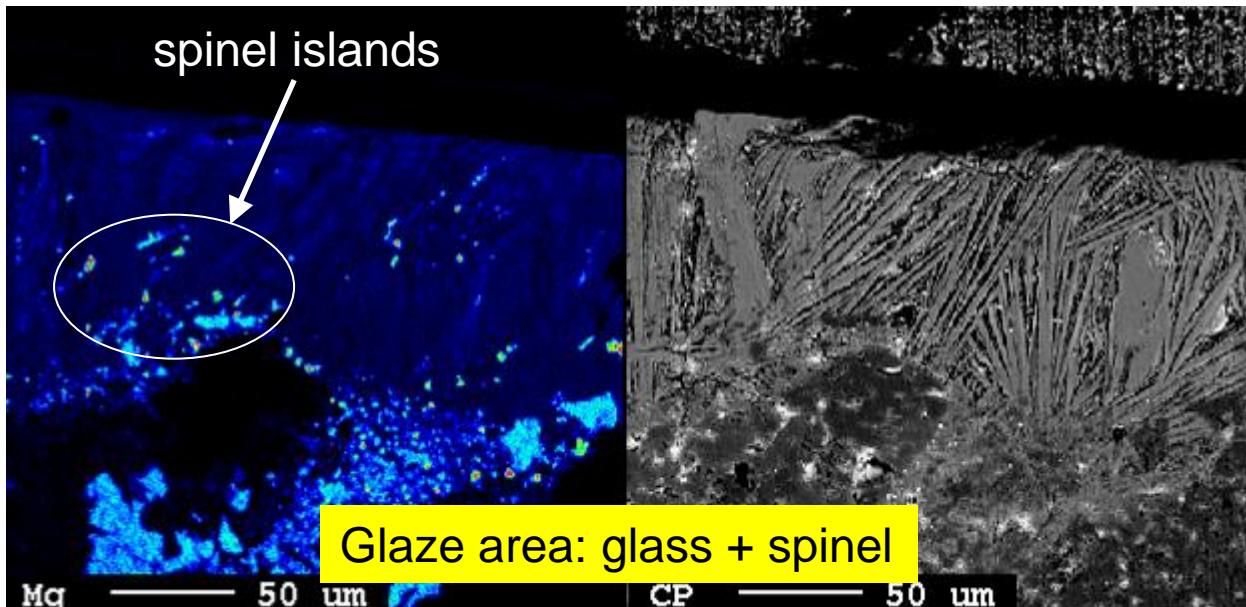
CaO	SiO ₂	Al ₂ O ₃	MgO
54.06	10.47	26.24	9.23



Glazed Refractory

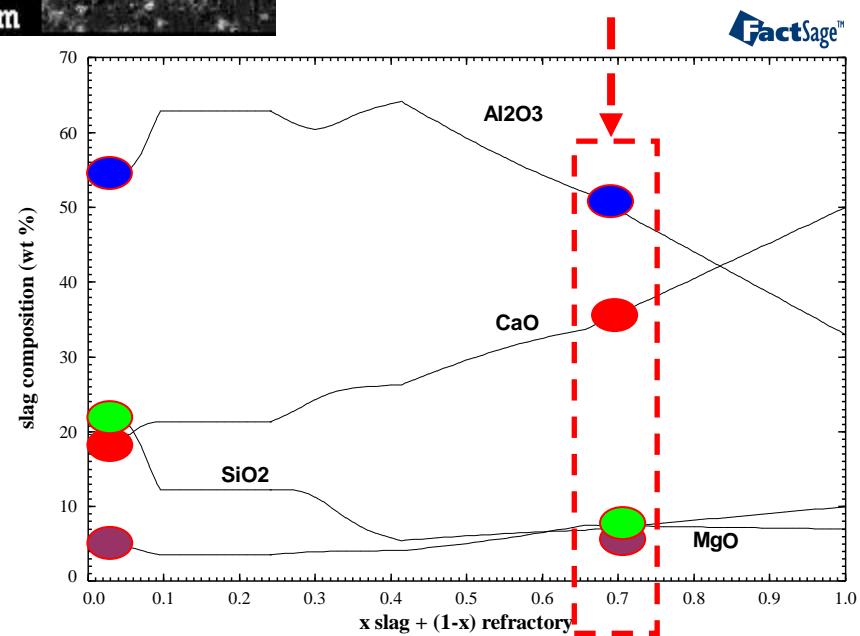
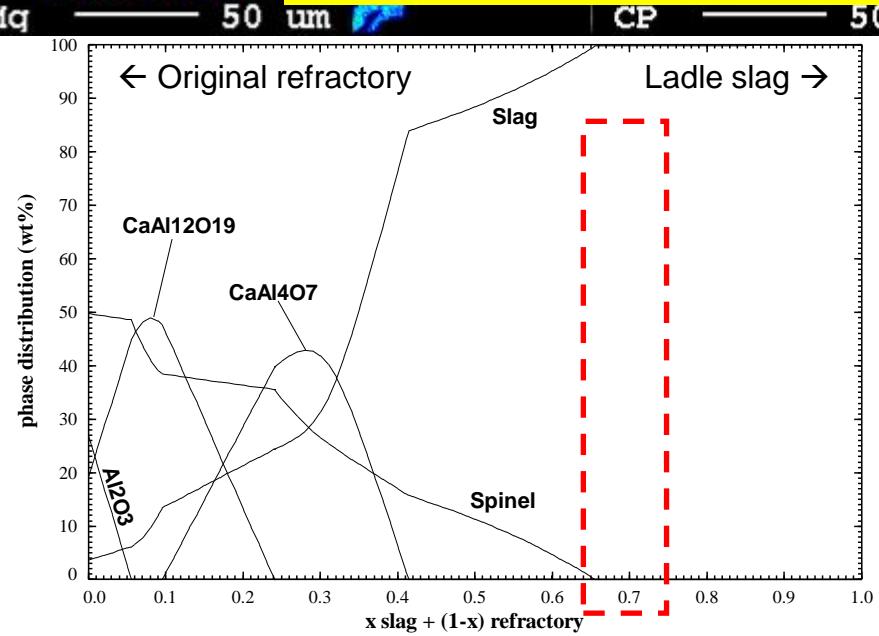


Glaze (Reaction product of slag and refractory)



Glaze composition (glass)

CaO	SiO ₂	Al ₂ O ₃	MgO
35.8	6.6	51.1	6.5



Equilibrium stability calculations with temperature: refractories

Equilibrium stability of 20MgO-78Al₂O₃-2CaO refractories

Equilib - Menu: last system

File Units Parameters Help

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

Reactants (3)

(gram) 2 CaO + <A> MgO + <98-A> Al₂O₃

Products

Compound species

<input type="checkbox"/> gas	<input checked="" type="radio"/> ideal	<input type="radio"/> real
0		
<input type="checkbox"/> aqueous		
0		
<input type="checkbox"/> pure liquids		
0		
<input type="checkbox"/> + pure solids		
13		

species: 13

Solution phases

*	+	Base-Phase	Full Name
	I	FToxid-SLAGA	A-Slag-liq all oxides + S
	+	FToxid-SPINA	A-Spinel
	I	FToxid-MeO_A	A-Monoxide

Custom Solutions

0 fixed activities

0 ideal solutions

Pseudonyms

apply

Volume data

assume molar volumes of
solids and liquids = 0

include molar volume data
and physical properties data

paraequilibrium & Gmin

Virtual species: 6

Total Species (max 5000) 31

Total Solutions (max 200) 5

Total Phases (max 1500) 18

Transitions - temperature

Number of transitions: All

Legend

I - immiscible 2
+ - selected 1

Show all selected

species: 18

solutions: 5

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
20		1200 1800 50	1	
10 steps	<input type="checkbox"/> Table	13+ calculations		

Equilibrium

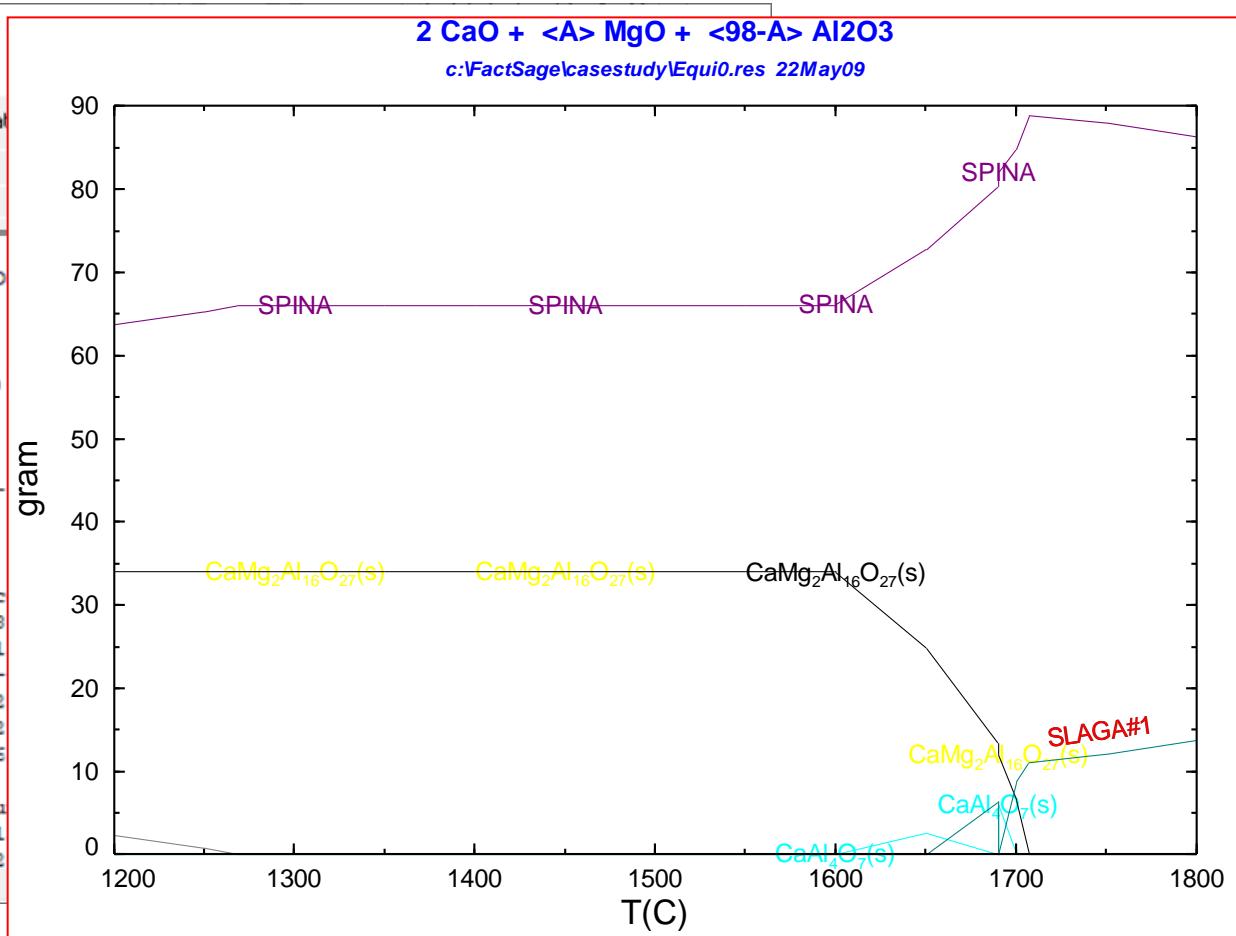
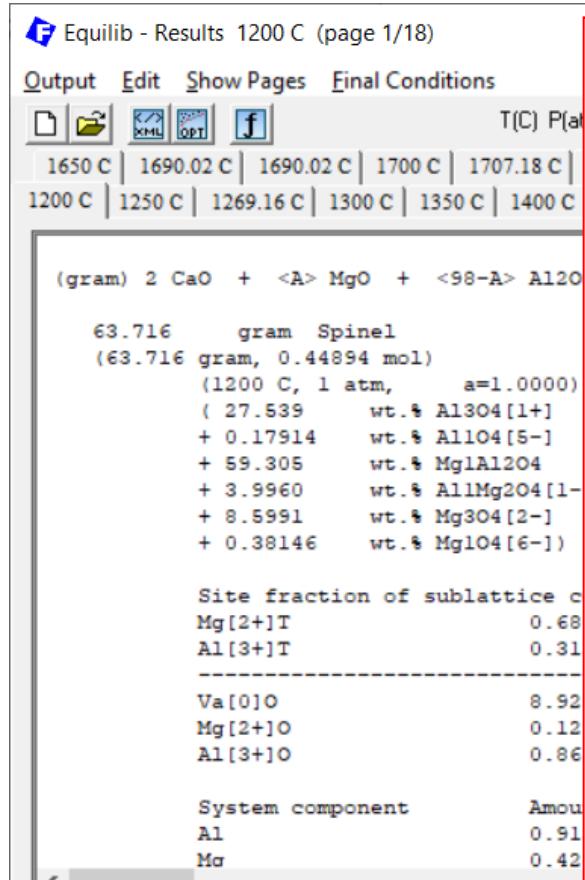
normal normal + transitions

transitions only open

- no time limit -

FactSage 8.0

Equilibrium stability calculations with temperature: refractories



The refractory is mechanically unstable above 1600°C:

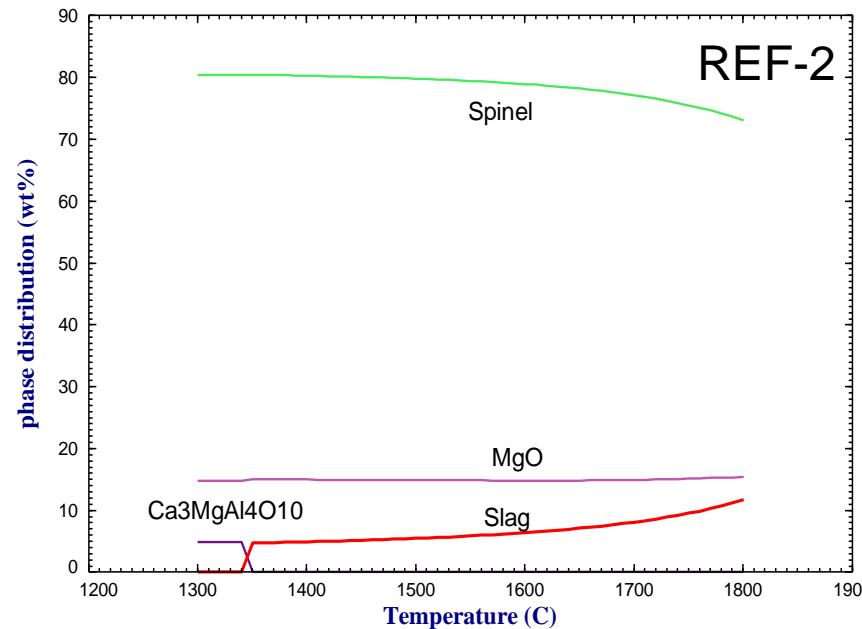
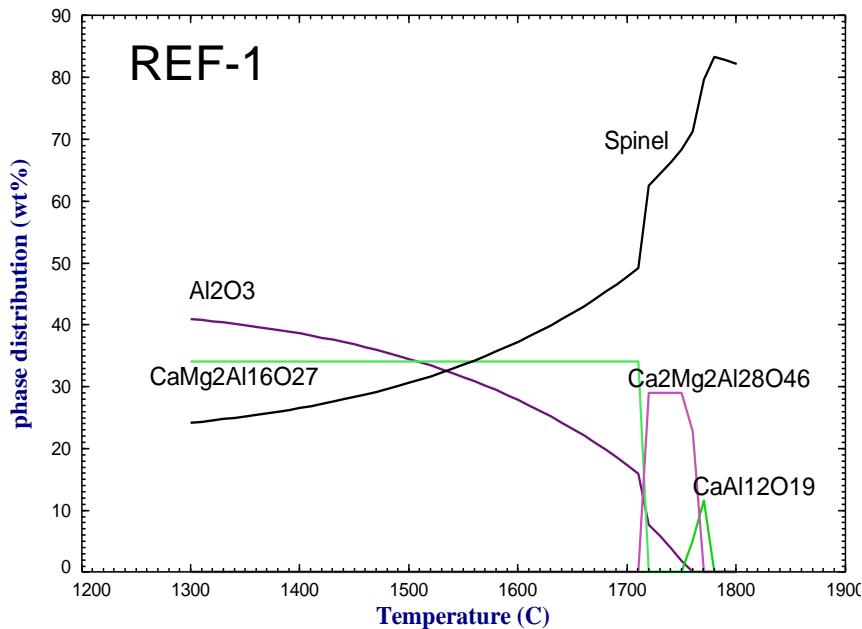
- considerable volume change due to the significant change in phase distribution

The refractory cannot be used above 1690°C:

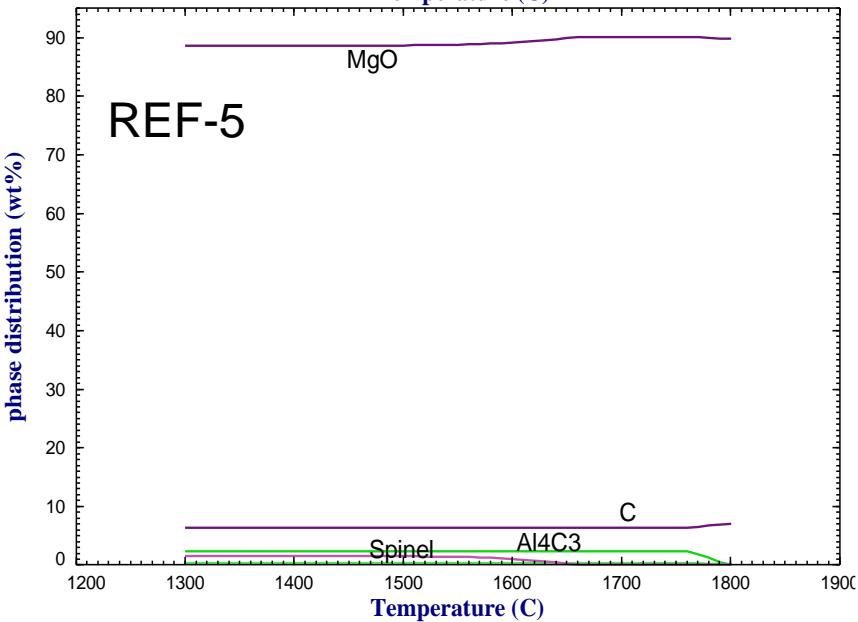
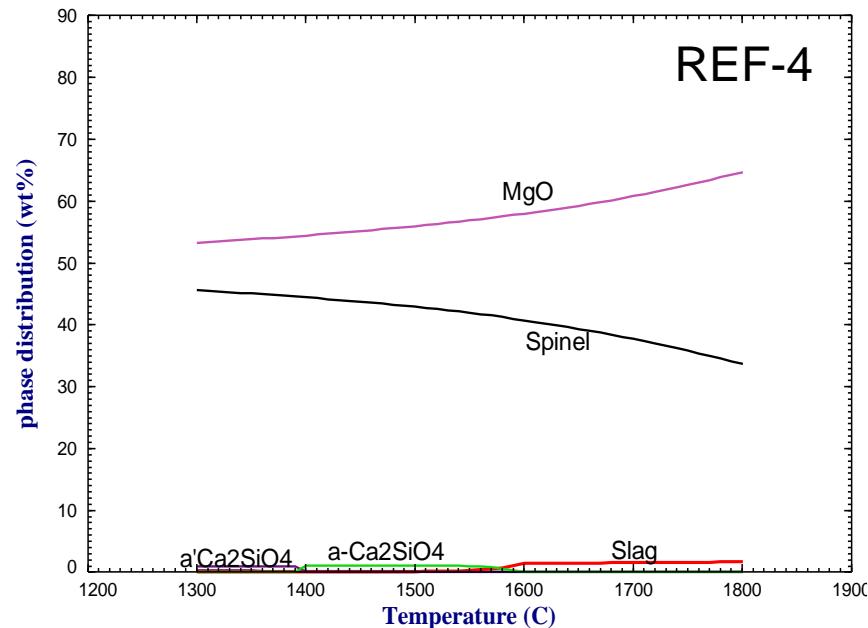
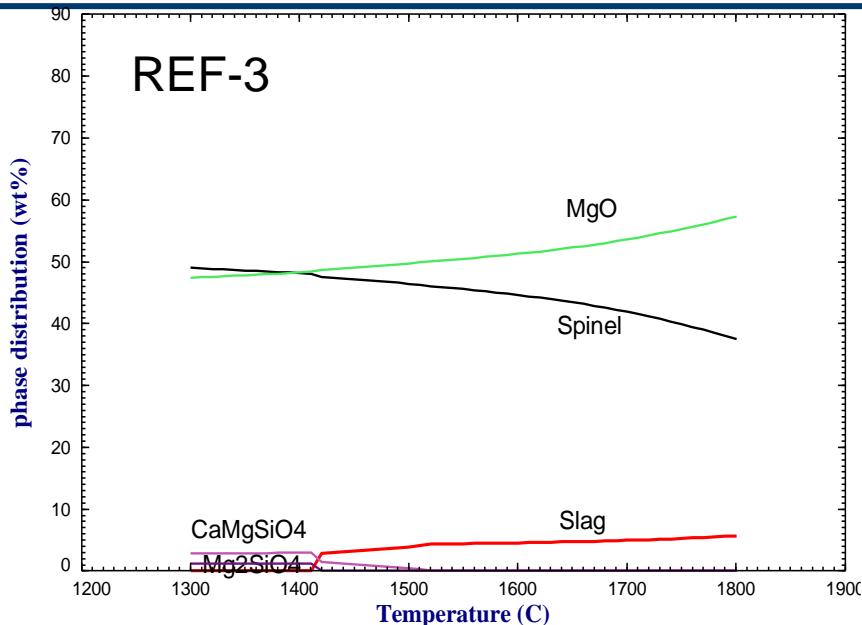
- significant amount of liquid phase formation

Thermal Stability test of Refractories

wt%	REF-1	2	3	4	5	6
Al_2O_3	88	60	11	4	0.5	0.5
MgO	9	38	58	61	89	75
CaO	2	2	0.9	0.7		
Cr_2O_3			20	29		
Fe_2O_3			8.8	4.8		
SiO_2			1.6	0.4	0.5	1.2
C					7	17
Al					2	4



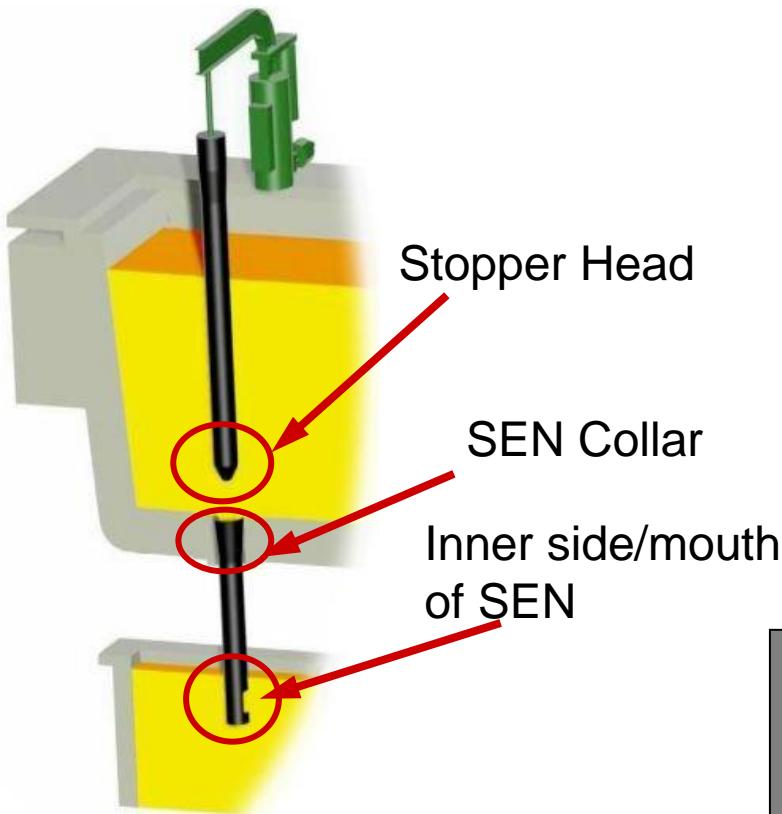
Thermal Stability test of Refractories



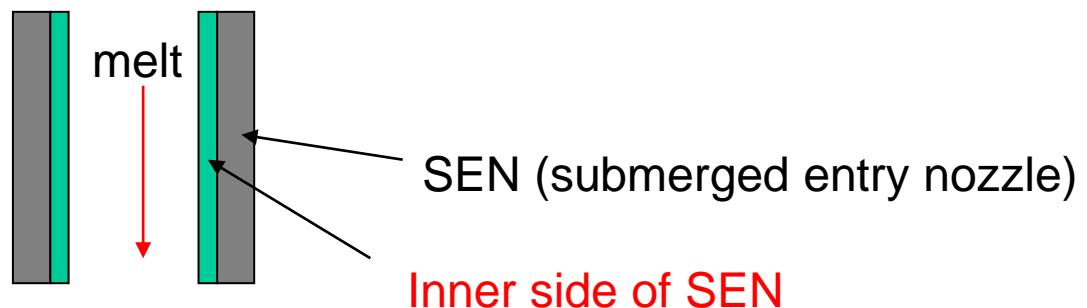
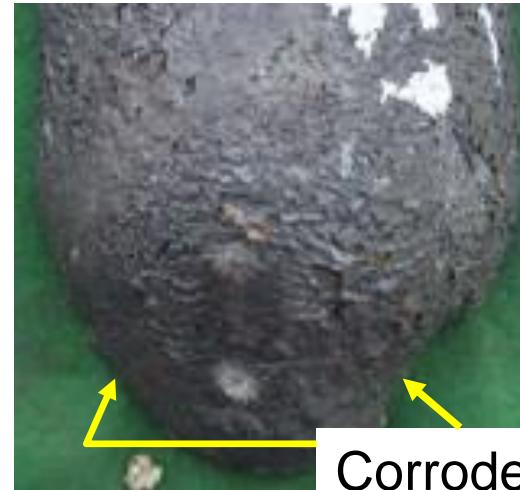
Depending on the refractory compositions, the refractory components can vary drastically.

- Formation of liquid
 - Stability of refractory ↓
- Change in MgO/Spinel fraction
 - Mechanical wear resistance
 - Volume change

Refractory – Liquid Inclusion Interactions



Stopper ($\text{Al}_2\text{O}_3\text{-C}$)



M.-K. Cho and I.-H. Jung, "Corrosion of nozzle refractories by liquid inclusion in high oxygen steels", *ISIJ Inter.* 2012, vol. 52, pp. 1289-1296.

Refractory – Liquid Inclusion Interactions

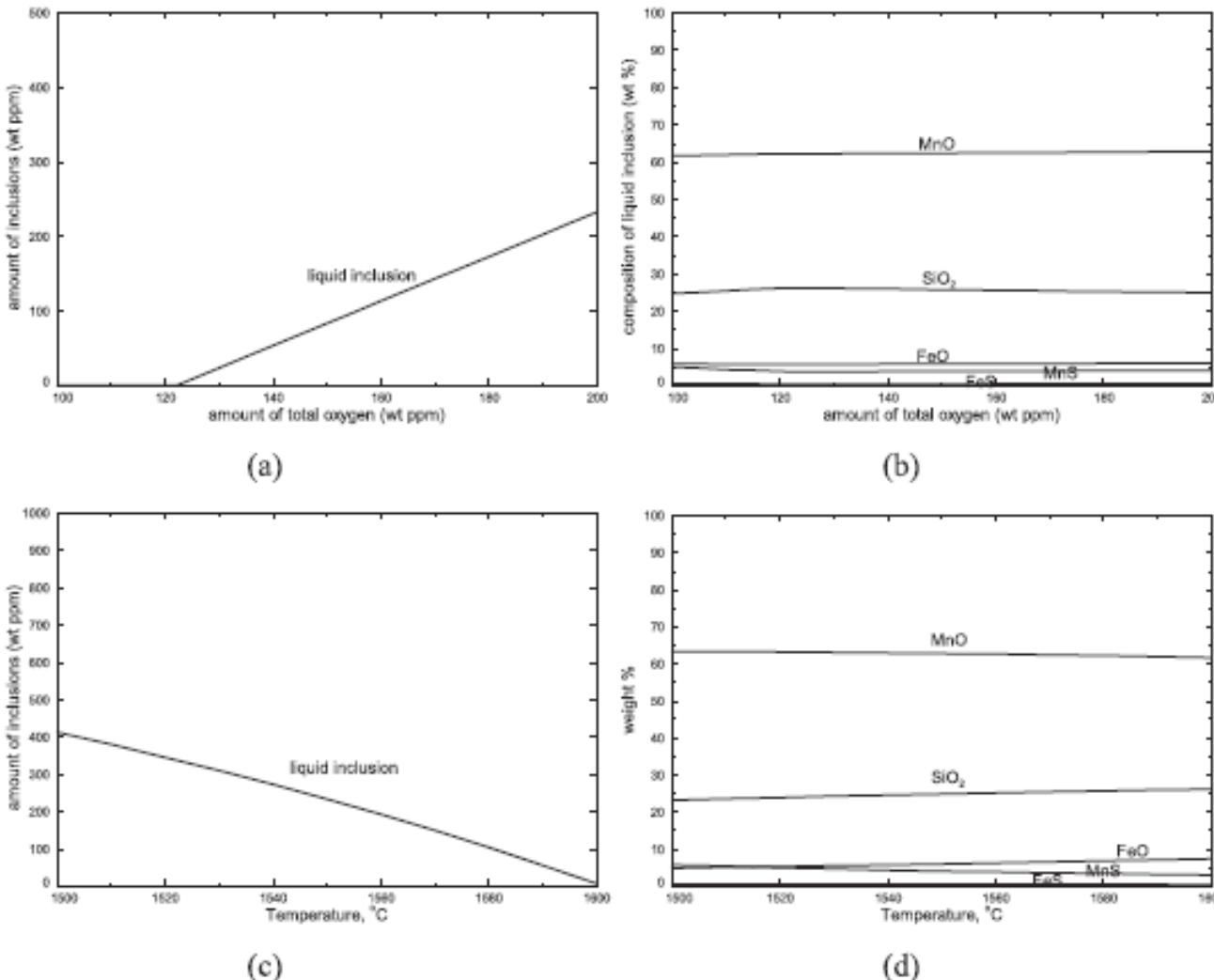


Fig. 2. Calculated inclusions formed in high oxygen steel (Fe-0.08C-1.2Mn-0.3S-0.01Si-O-minor P, Bi, etc. in wt%) during continuous casting process. (a) and (b): amount and composition of liquid inclusion varied with total oxygen content in steel at 1550°C, (c) and (d) amount and composition of liquid inclusion in molten steel containing 200 wt ppm oxygen varied with temperature.

Refractory – Liquid Inclusion Interactions

Table 1. Chemical compositions of the refractories investigated in the present study.

wt%	Al ₂ O ₃ -C	Al ₂ O ₃ -AlN-C	Spinel-L-C	Spinel-H-C	ZrO ₂ -C
Al ₂ O ₃	95	54	70	62	
MgO			26	25	
ZrO ₂					85*
C	3	15	4	13	13
SiC	2				2
AlN		30			
etc.		1			

* CaO stabilized ZrO₂.

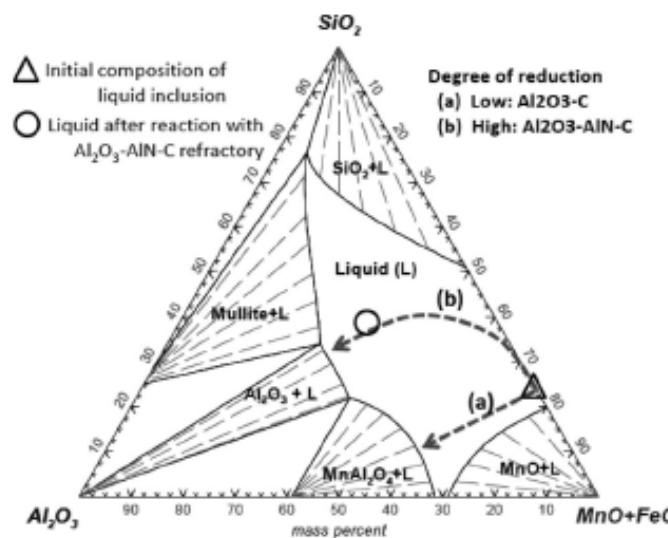


Fig. 8. Variation of liquid inclusion composition depending on the degree of reduction by carbon contained in refractory.

Please see the details in the ISIJ paper

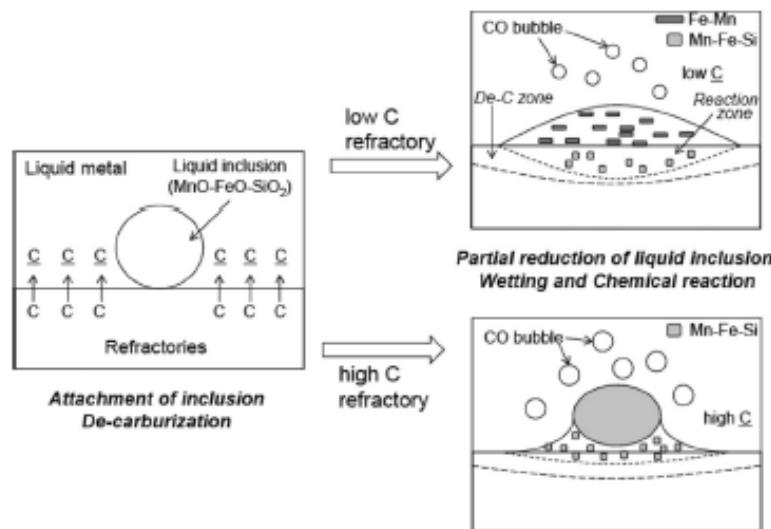


Fig. 9. Refractory corrosion mechanism by liquid inclusion in high oxygen steels.

Refractory – Liquid Inclusion Interactions

Relative Stability of the refractories against liquid MnO-SiO₂ type inclusion

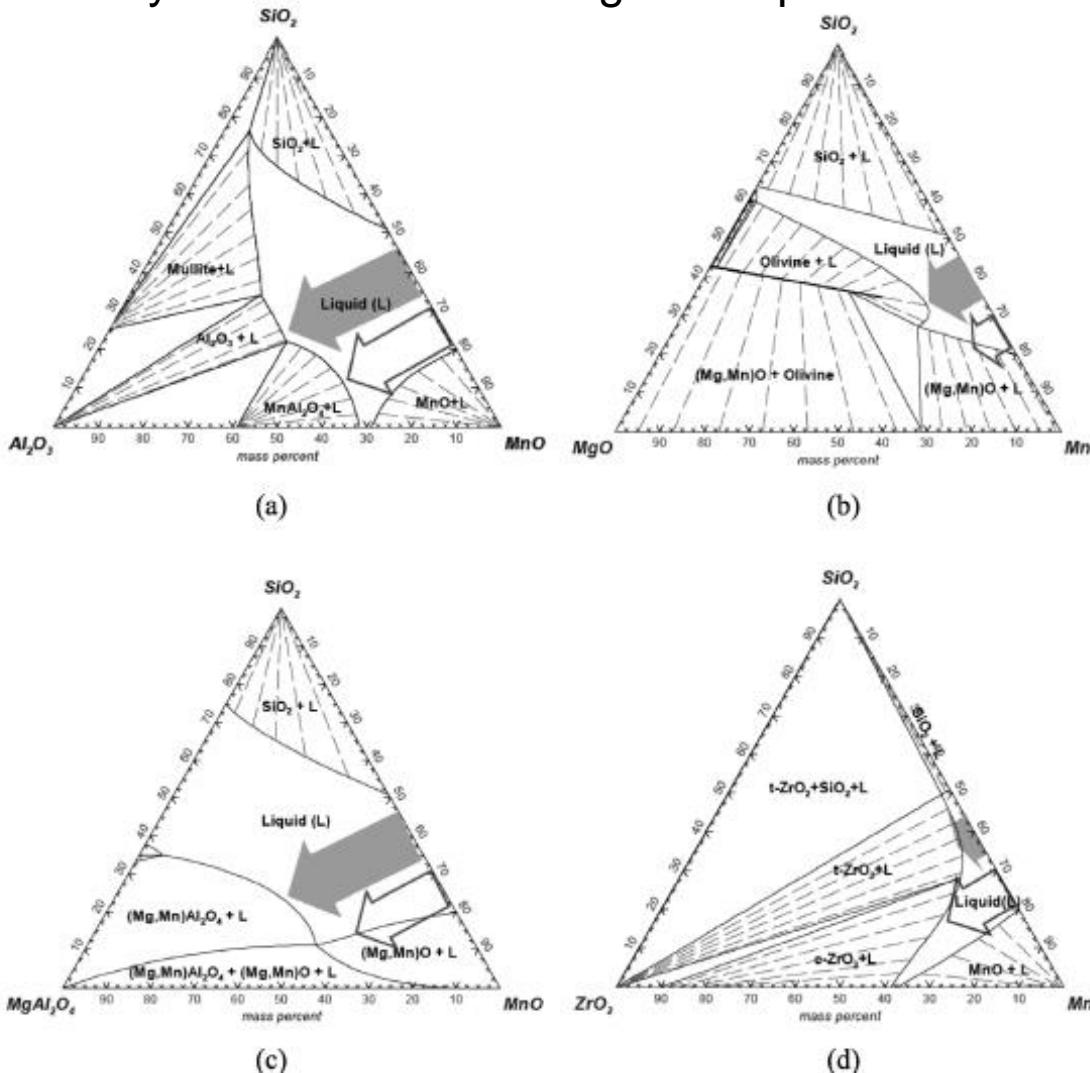


Fig. 10. Thermodynamic stability of the refractory components against liquid inclusion (MnO-SiO₂) at 1550°C. The arrows (gray arrow represents high degree of reduction, and empty arrow represents low degree of reduction) in phase diagrams represent the possible amount of dissolution of each refractory component.

Refractory-Steel Interaction

Equilib - Menu: last system

File Units Parameters Help

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

Reactants (5)

(gram) 95 Fe + 4 Mn + Si + <100-100A> MgO + <100A> Al2O3

Products

Compound species

<input type="checkbox"/> gas	<input checked="" type="radio"/> ideal	<input type="radio"/> real	0	
<input type="checkbox"/> aqueous	0			
<input type="checkbox"/> pure liquids	0			
* <input type="checkbox"/> pure solids	68			
* - custom selection		species:		68

Target

- none -

Estimate T(K): 1000

Quantity(g): 0

Solution phases

*	+	Base-Phase	Full Name
	+	FTmisc-FeLQ	Fe-liq
	+	FTmisc-BCCS	bcc
	+	FTmisc-FCCS	fcc
	FToxid-SLAGA	A-Slag-liq all oxides + S	
	FToxid-SPINB	B-Spinel	
+	FToxid-MeO_A	A-Monoxide	
	FToxid-MeO_B	B-Monoxide	
	FToxid-MeO_?	?-Monoxide	

Legend

I - immiscible 4
+ - selected 14

Show all selected

species: 281 solutions: 22

Custom Solutions

0 fixed activities
0 ideal solutions

Pseudonyms

apply

Volume data

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

paraequilibrium & Grmin

Virtual species: 42

Total Species (max 5000) 349

Total Solutions (max 200) 22

Total Phases (max 1500) 90

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
0 1 0.01		1600	1	
10 steps	<input type="checkbox"/> Table	101 calculations		

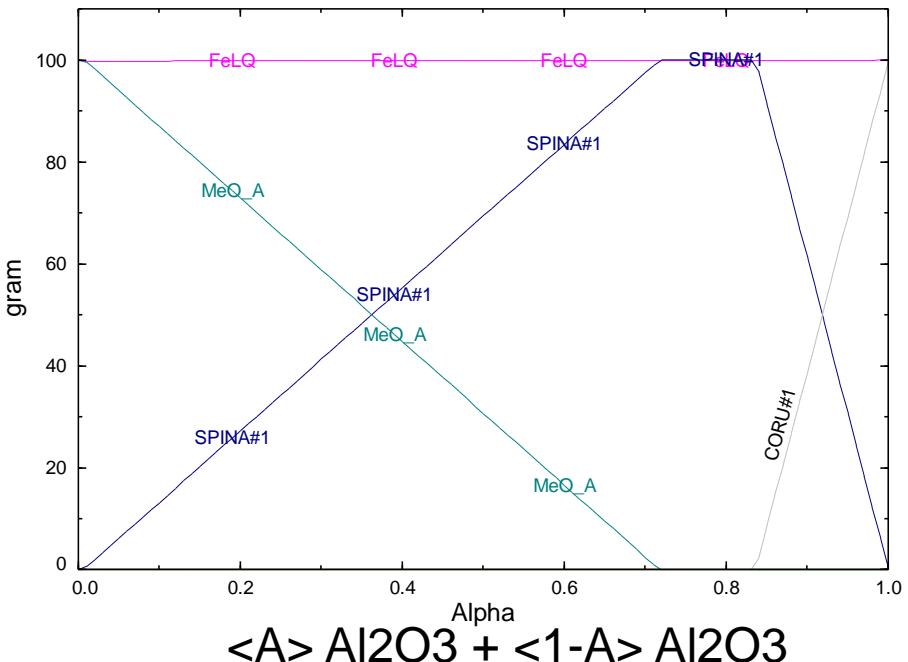
Equilibrium

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

FactSage 8.0

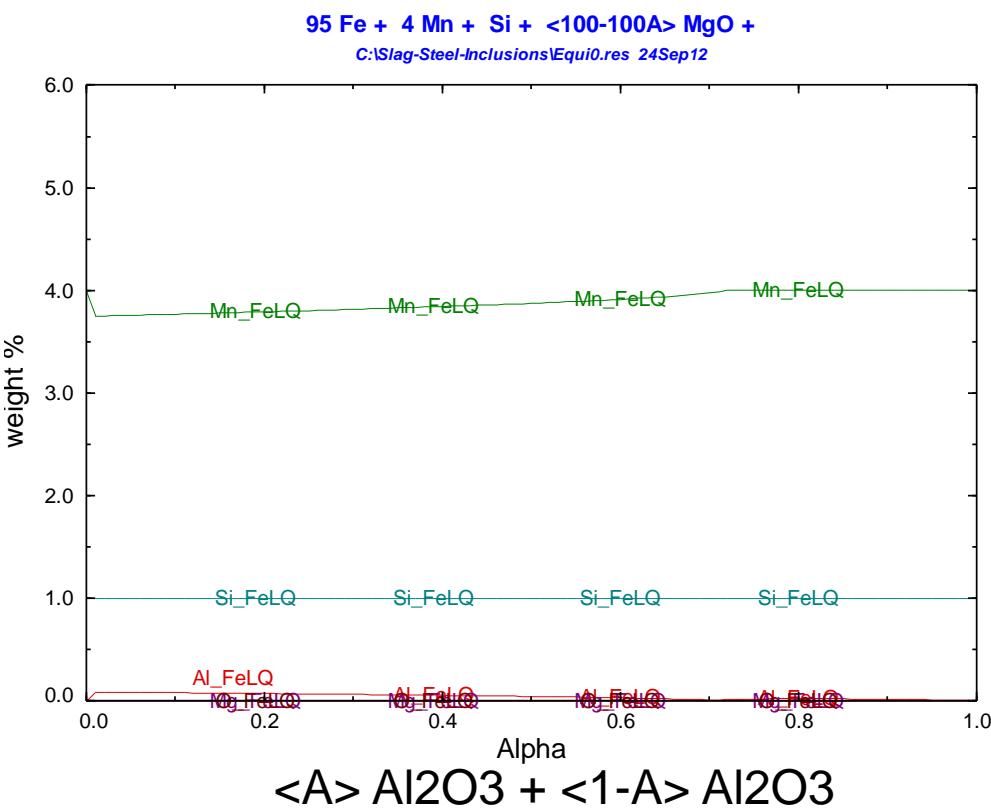
Refractory-Steel Interaction

95 Fe + 4 Mn + Si + <100-100A> MgO +
C:\Slag-Steel-Inclusions\Equi0.res 24Sep12



← Change in the amount of phases

Change in steel composition →

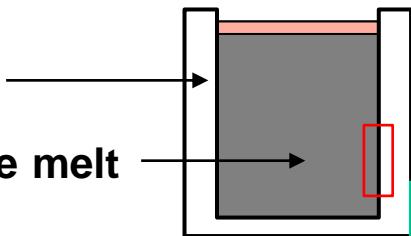


High Mn-Fe melt storage for TWIP Steel production

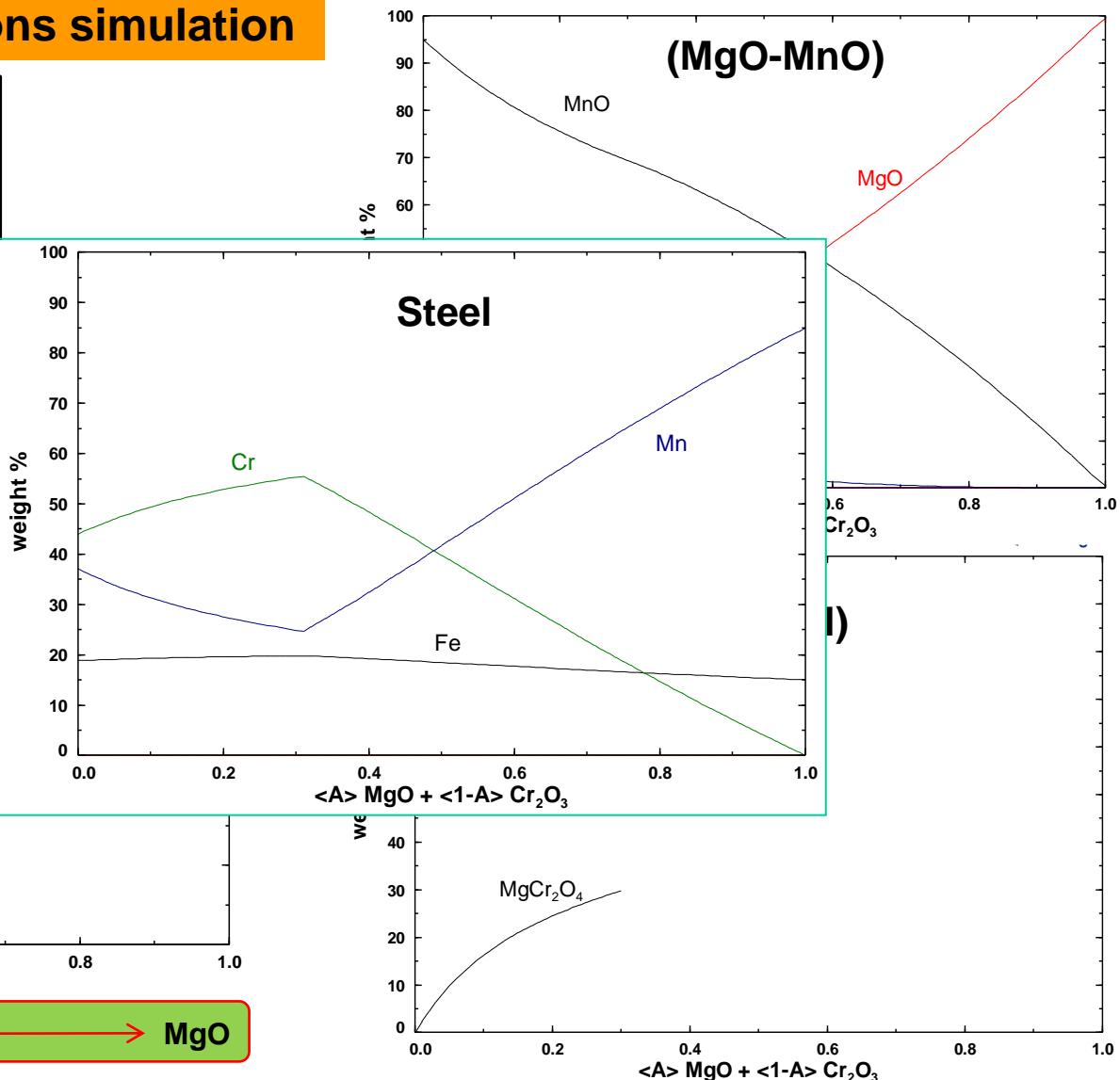
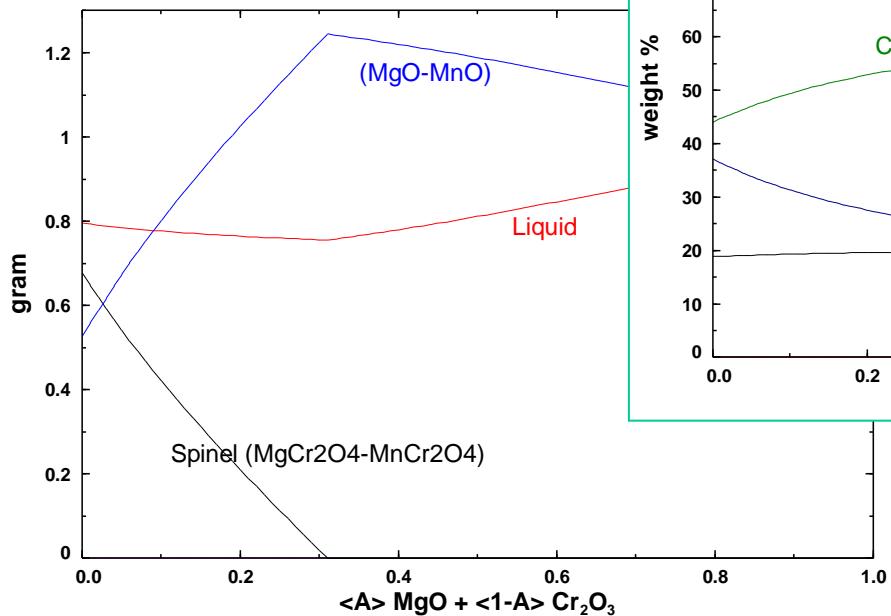
Melt / refractory reactions simulation

Refractories

85%Mn-15%Fe melt

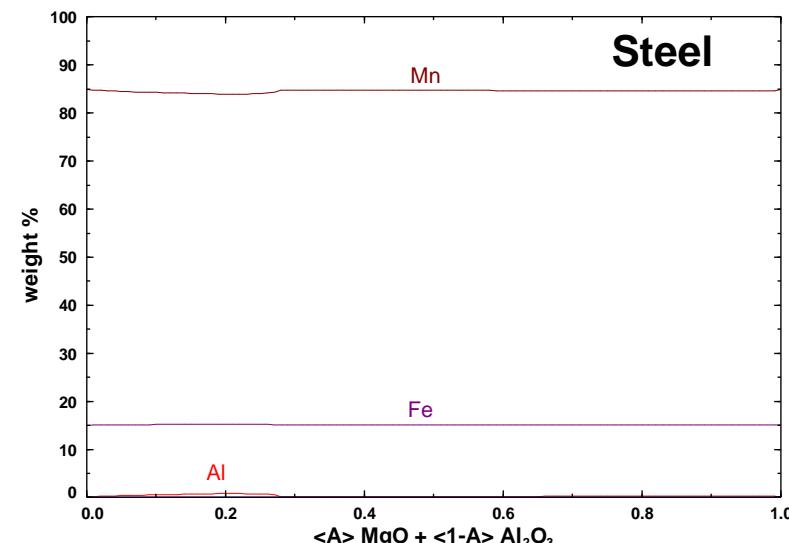
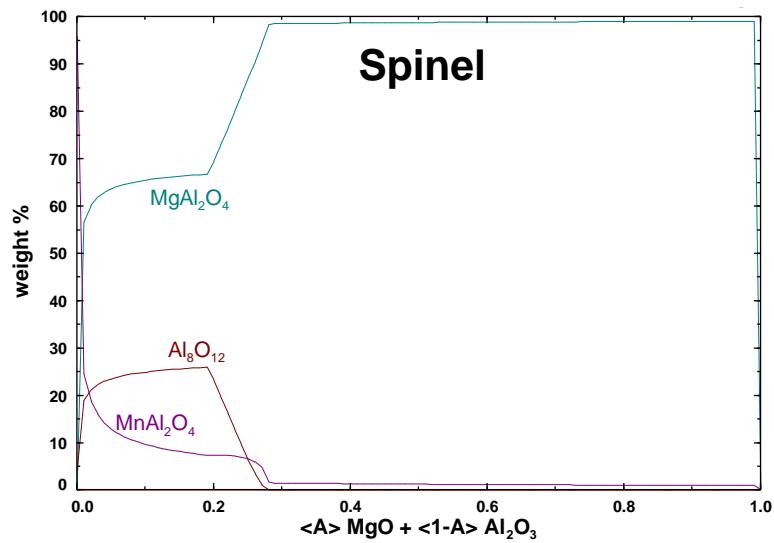
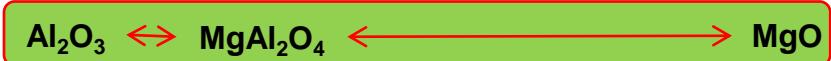
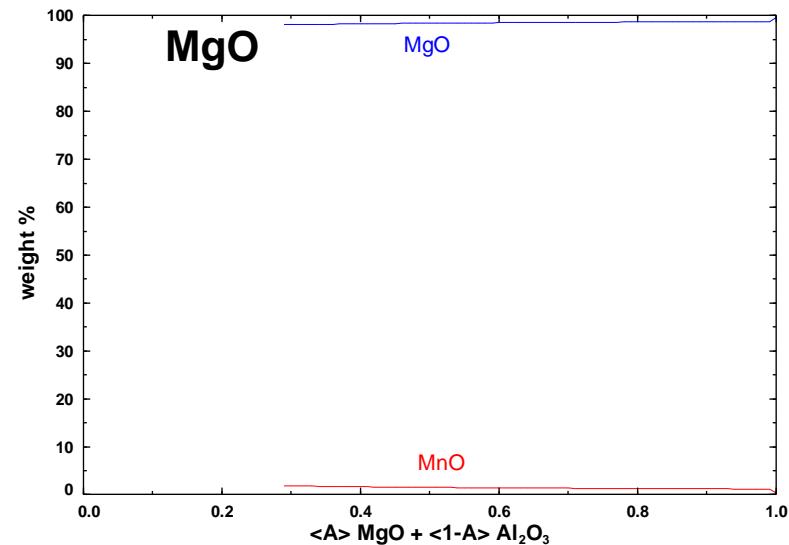
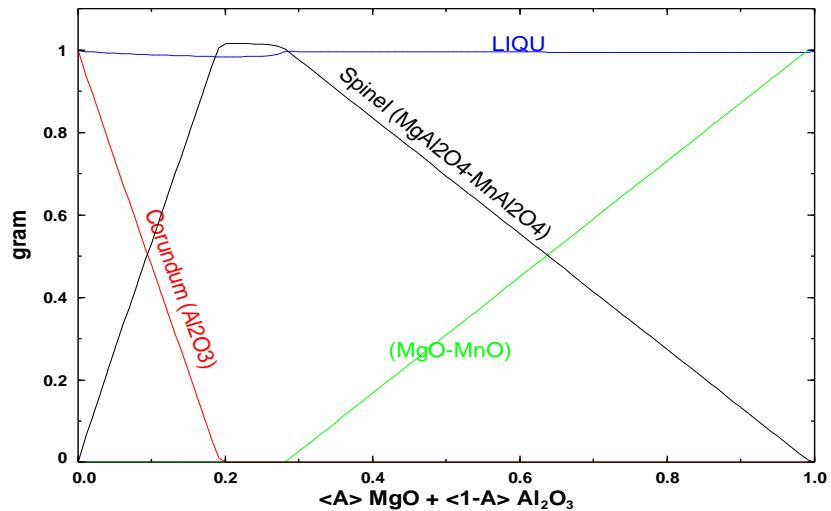


1g Mn-Fe melt + 1g refractor



High Mn-Fe melt storage for TWIP Steel production

1g Mn-Fe melt + 1g refractory ($\text{MgO}-\text{Al}_2\text{O}_3$)

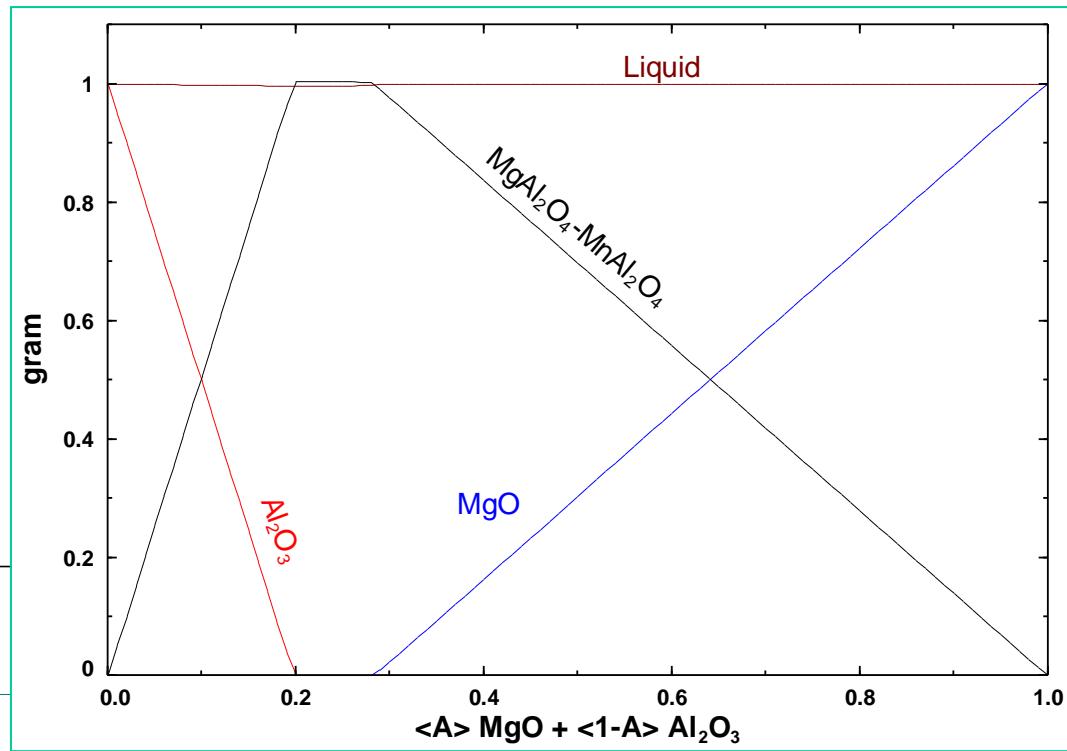
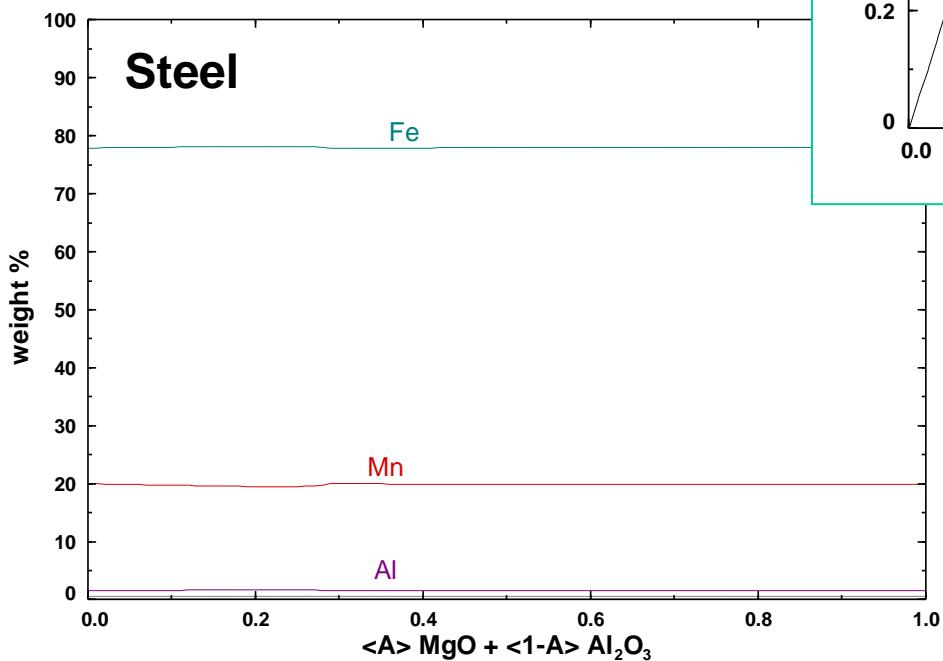
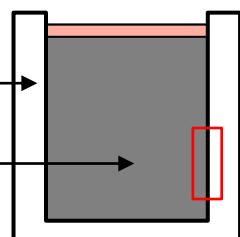


Refractory for TWIP steel: Fe-20%Mn-1.5%Al-0.6%C

T = 1500°C

Refractories

Twip steel



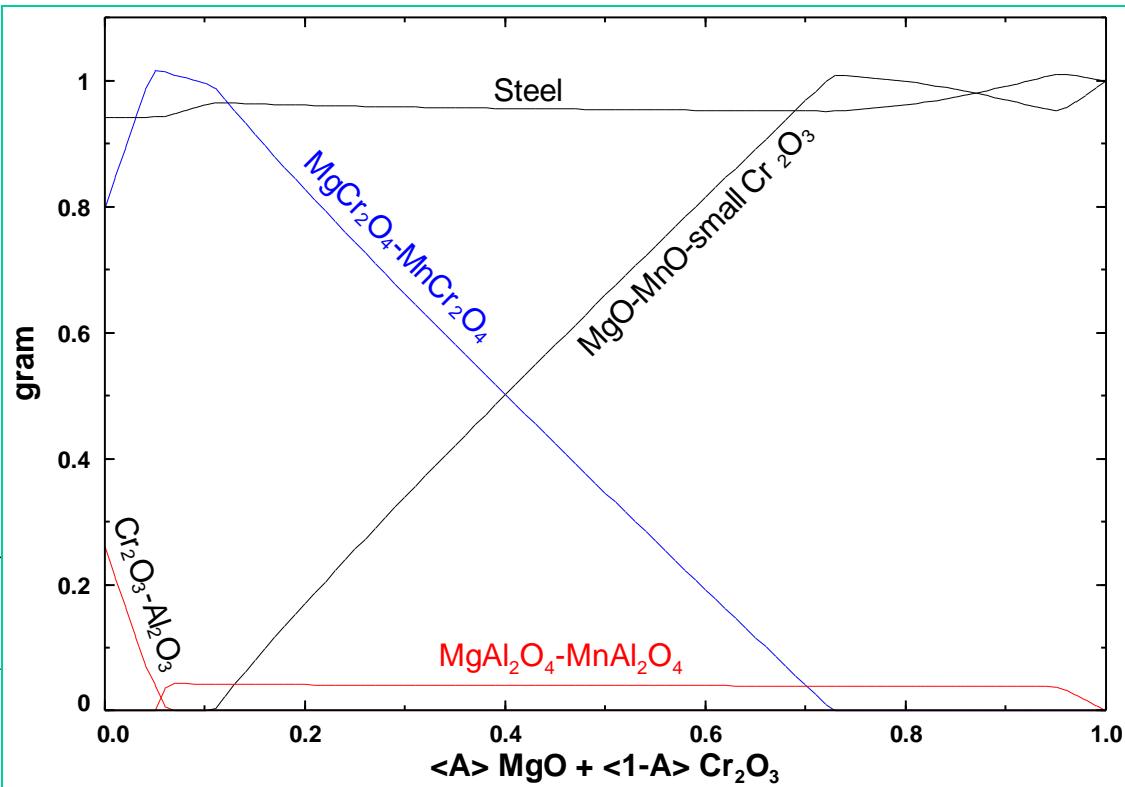
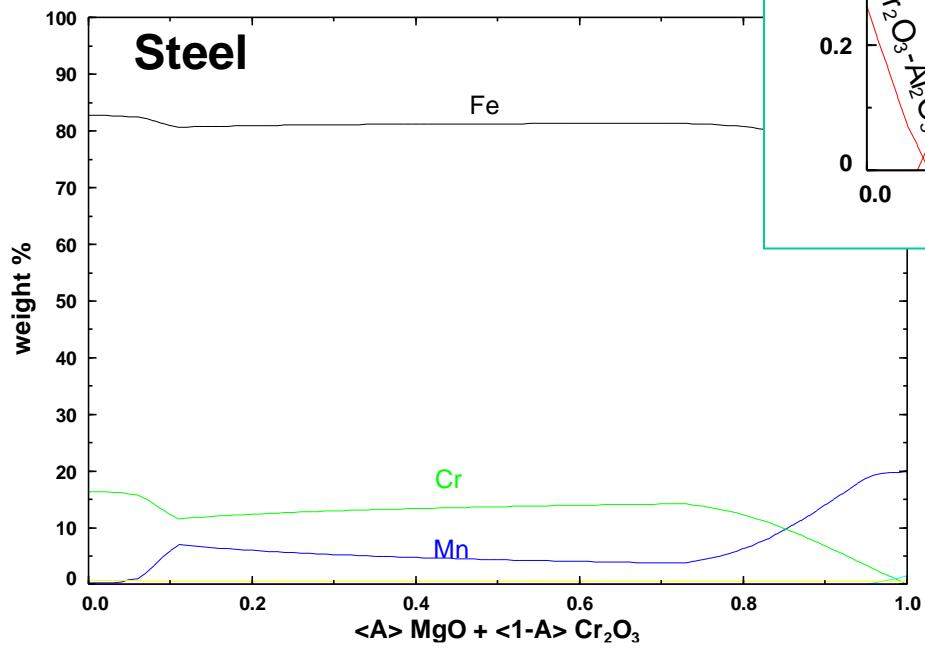
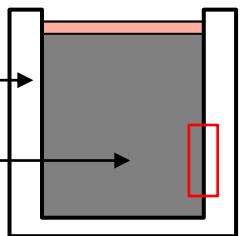
MgO-Al₂O₃ type: Very stable refractory

Refractory for TWIP steel: Fe-20%Mn-1.5%Al-0.6%C

$T = 1500^\circ\text{C}$

Refractories

Twip steel



MgO-Cr₂O₃ type: less stable
 → Cr pickup
 → Al loss

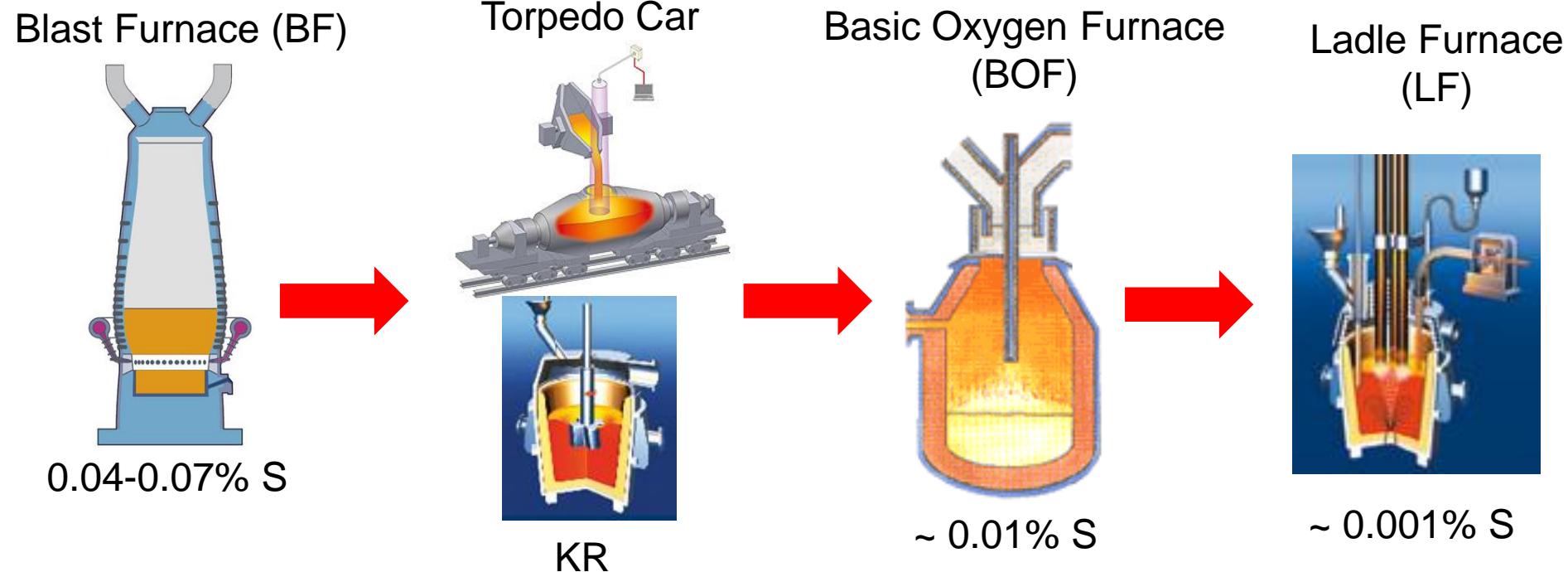
Desulphurization

Desulphurization of Hot Metal in the De-S station,
Desulphurization of steel during Ladle treatment
and calculating Sulphide Capacity

More examples can be found in:
http://in-ho-group.snu.ac.kr/?page_id=398

Desulphurization of Hot Metal

- The hot metal tapped out of the blast furnace typically contains 0.04-0.07% S.
- To reduce the amount of sulphur in the hot metal between the blast furnace and the oxygen converter, desulphurization is usually performed at a De-S station such as KR using flux (CaO, CaC₂, Mg, ...)
- In the secondary steelmaking (recently in LF unit), de-S can occur between slag (CaO-rich) and steel due to strong agitation.



Desulphurization of Hot Metal

The following reactions have been proposed to reduce the sulphur content in hot metal:



In the following pages, it will be shown how FactSage could be used to calculate the efficiency of each desulphurizing agent.

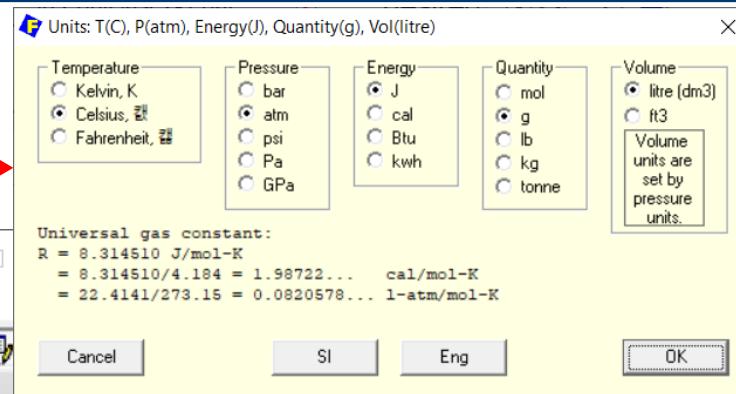
It will then be shown how the exact amount of desulphurizing agent can be selected to achieve the desired sulphur content.

Desulphurization of Hot Metal using Mg

1. Double-click on units...

This example can be found
in EquiCase2-1.dat

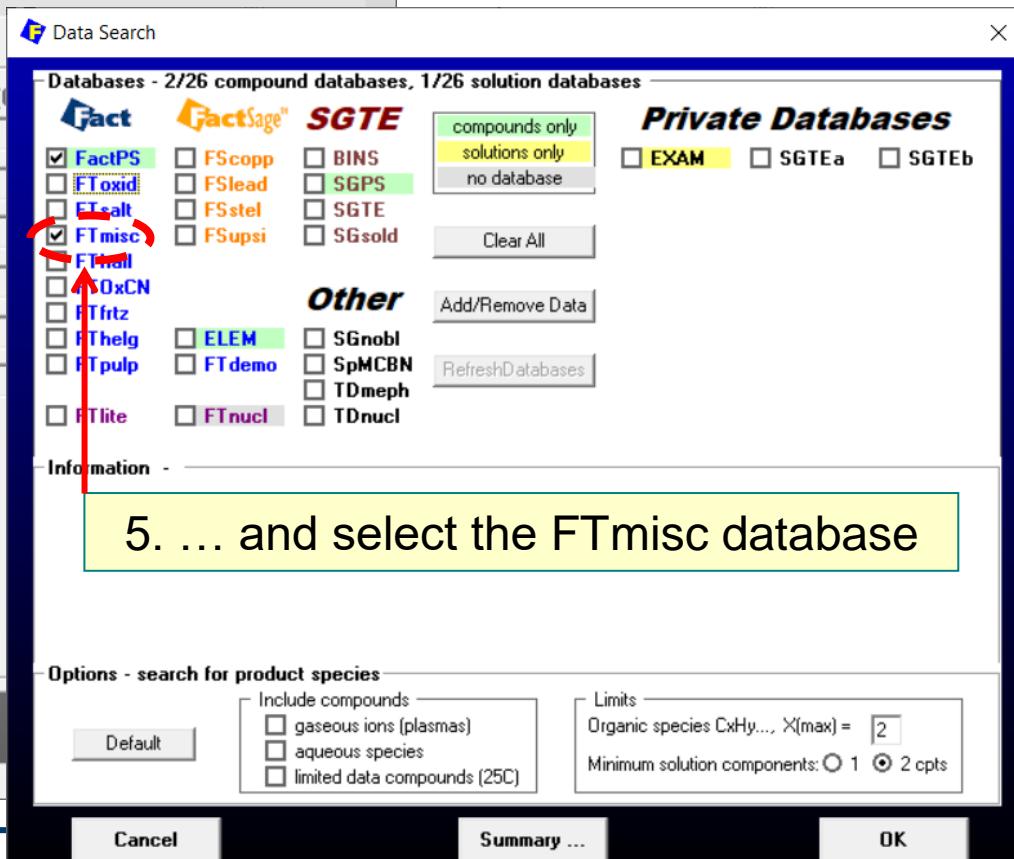
2. ... to select the
desired units



4. Click on "Data Search"...

Quantity(g)	Species	Phase
94.335	Fe	
+ 4.5	C	
+ 0.5	Si	
+ 0.6	Mn	
+ 0.065	S	
+ <A>	Mg	

3. Enter the hot metal composition
and put <A> for the
desulphurizing agent amount



6. Click "Next"

→ Next >

FactSage 8.0 Compound: 2/26 databases Solution: 1/26 databases

Desulphurization of Hot Metal using Mg

1. Right-click on “pure solids”

The screenshot shows the FactSage software interface for thermodynamic calculations. On the left, the 'Reactants' section shows a composition of (gram) 94.335 Fe + 4.5. The 'Products' section includes a 'pure solids' entry with a value of 40. The 'Target' section has 'none' selected. In the 'Final Conditions' section, the temperature is set to 1600 K. The 'Equilibrium' options are set to 'normal'.

The right side of the screen shows a 'Selection - Equilib' window. It displays a table of species with their codes, names, data sources (FactPS or FTmisc), and phases. The table highlights several rows in red, indicating 'Duplicates'. The table includes columns for Species, Data, Phase, T, V, Activity, Minimum, and Maximum.

	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
X	78	'Fe7S8'(s)	FactPS	pyrrhotite-4					
X	79	Fe9S10(s)	FactPS	pyrrhotite-5					
X	80	Fe10S11(s)	FactPS	pyrrhotite-1					
X	81	Fe11S12(s)	FactPS	pyrrhotite-6					
+	82	S(s)	FTmisc	Orthorhombic					
+	83	S(s2)	FTmisc	Monoclinic					
+	84	MnS(s)	FTmisc	Alabandite					
+	85	MnS2(s)	FTmisc	Hauerite					
+	86	FeS(s)	FTmisc	Pyrrhotite-2					
+	87	FeS2(s)	FTmisc	Pyrite					
+	88	'Fe7S8'(s)	FTmisc	pyrrhotite-4					
+	89	Fe9S10(s)	FTmisc	pyrrhotite-5					
+	90	Fe10S11(s)	FTmisc	pyrrhotite-1	0				
+	91	Fe11S12(s)	FTmisc	pyrrhotite-6C	0				

Selected: 40/52 SOLID Duplicates selected. X denotes species excluded by default
- no results -

2. The selection contains data from both FTmisc and FactPS. Some of the data is overlapping (highlighted in red as “Duplicates”)

Desulphurization of Hot Metal using Mg

1. Left-click to select the liquid steel solution phase

The screenshot shows the FactSage software interface for equilibrium calculations. A red arrow points from the text "1. Left-click to select the liquid steel solution phase" to the "Solution phases" table. The table lists various phases, and the "Fe-liq" row is highlighted in yellow, indicating it is selected. Another red arrow points from the text "2. If you don't see the available solution phase, click 'show all'" to the "Show" dropdown menu in the "Legend" section, which is set to "all". A third red arrow points from the text "3. Enter the desired equilibrium temperature." to the "Estimate T(K)" input field, which contains the value "1000". A fourth red arrow points from the text "4. We will vary the amount of desulphurizing agent from 0 to 1 g in steps of 0.01g" to the "Final Conditions" table. The table shows the composition of the system: <A> 0.1 0.01, 1400, T(C) 1400, P(atm) 1, Product H(J) 101 calculations. A fifth red arrow points from the text "5. Press 'Calculate'" to the "Calculate >>" button in the bottom right corner.

Equilib - Menu: last system

File Units Parameters Help

Reactants (6)

(gram) 94.335 Fe + 4.5 C + 0.5 Si + 0.6 Mn + 0.065 S + <A> Mg

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- * pure solids 40

* - custom selection species: 40

Solution phases

*	Base-Phase	Full Name
+	FTmisc-FeLQ	Fe-liq
	FTmisc-MATT	Matte
	FTmisc-FeS_	FeS-liq
	FTmisc-MAT2C	C-liq(Matte/Metal)
	FTmisc-PYRRC	C-Pyrrhotite
	FTmisc-BCCS	bcc
	FTmisc-FCCS	fcc
	FTmisc-MS-c	MeS_cubic

Custom Solutions

- 0 fixed activities
- 0 ideal solutions

Pseudonyms

- apply Edit ...

Volume data

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

paraequilibrium & Gmin edit

Virtual species: 0

Total Species (max 5000) 46

Total Solutions (max 200) 1

Total Phases (max 1500) 41

Target

- none -

Estimate T(K): 1000

Quantity(g): 0

Legend

+ selected 1

Show all selected

species: 6

solutions: 1 Select

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
0 1 0.01	1400	1		101 calculations
10 steps	<input type="checkbox"/> Table			

FactSage 8.0

Equilibrium

- normal
- normal + transitions
- transitions only
- open

- no time limit -

Calculate >>

3. Enter the desired equilibrium temperature.

4. We will vary the amount of desulphurizing agent from 0 to 1 g in steps of 0.01g

2. If you don't see the available solution phase, click "show all"

5. Press "Calculate"

Desulphurization of Hot Metal using Mg

Now we want to see how the amount of sulphur in the hot metal decreased with the addition of magnesium.

1. Press “Output”
→ “Plot” → “Plot Results...”

The screenshot shows the FactSage 8.0 software interface. A red box highlights the "Output" menu item. A blue box highlights the "Plot Results..." button in the "Plot" dropdown menu. A green box highlights the "Axes" button in the "Plot Results..." dialog box. A yellow box contains the text "3. This window will pop-up".

Output Edit Show Pages Final Conditions

Save or Print As ... Repeat Save Plot > Plot Results ...

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

A=0.17 | A=0.18 | A=0.19 | A=0.2 | A=0.21 | A=0.22 | A=0.23 | A=0.24 |
A=0.09 | A=0.1 | A=0.11 | A=0.12 |

Equilib Results file Stream File Format Fact-XML Fact-Optimal Fact-Function-Build Refresh ... Swap loops ... system Fe Mn S Si C + 0 gram (1400 0) Axes 0 selected Axes Spec Cancel Refresh OK

Results Processor: C:\Workshop80\Ferro\Equi0.res

File Help

94.335 Fe + 4.5 C + 0.5 Si + 0.6 Mn +

Axes	Variables	Minimum	Maximum
	activity	0	12.202
	mole	0	
	mole fract. soln. species	0	
	gram	0	
	weight % soln. species	0	

Axes: log10(weight % soln. species) vs Alpha

Y-variable X-variable Swap Axes

Y-axis: log10(weight % soln. species)
maximum: 0
minimum: -10
tick every: 1

X-axis: Alpha
maximum: 1
minimum: 0
tick every: 0.1

ass fraction
0.94335
6.0000E-03
6.5000E-04
5.0000E-03
4.5000E-02

FactSage 8.0 | C:\Workshop80\Ferro\Equi0.res | 22Dec19 | 101 sets

2. Press “Axes”

3. This window will
pop-up

Desulphurization of Hot Metal using Mg

1. Press “Y-variable”

Axes: $\log_{10}(\text{weight \% soln. species})$ vs Alpha

Y-variable X-variable Swap Axes

2. Select “weight %” in
“ $\log_{10}(Y)$ ” scale

- activity
- mole
- mole fract. soln. species
- gram
- weight % soln. species**
- Alpha
- T(C)
- P(atm)
- Cp(J/K)
- G(J)
- Vol(litre)
- H(J)
- V(litre)
- S(J/K)
- page -
- Y**
- $\log_{10}(Y)$**
- In(Y)
- exp(Y)
- 1/Y
- phase distribution

weight % soln. species

sum 0

sum -10

very 1

Alpha

maximum 1

minimum 0

tick every 0.1

del

Refresh

OK

3. Select the maximum, minimum and increment value for the graph

4. In the same way,
select Alpha as the X-variable

Desulphurization of Hot Metal using Mg

Now we can see that the axes have been selected. We just need to choose sulphur as the species.

1. Press “Select” species

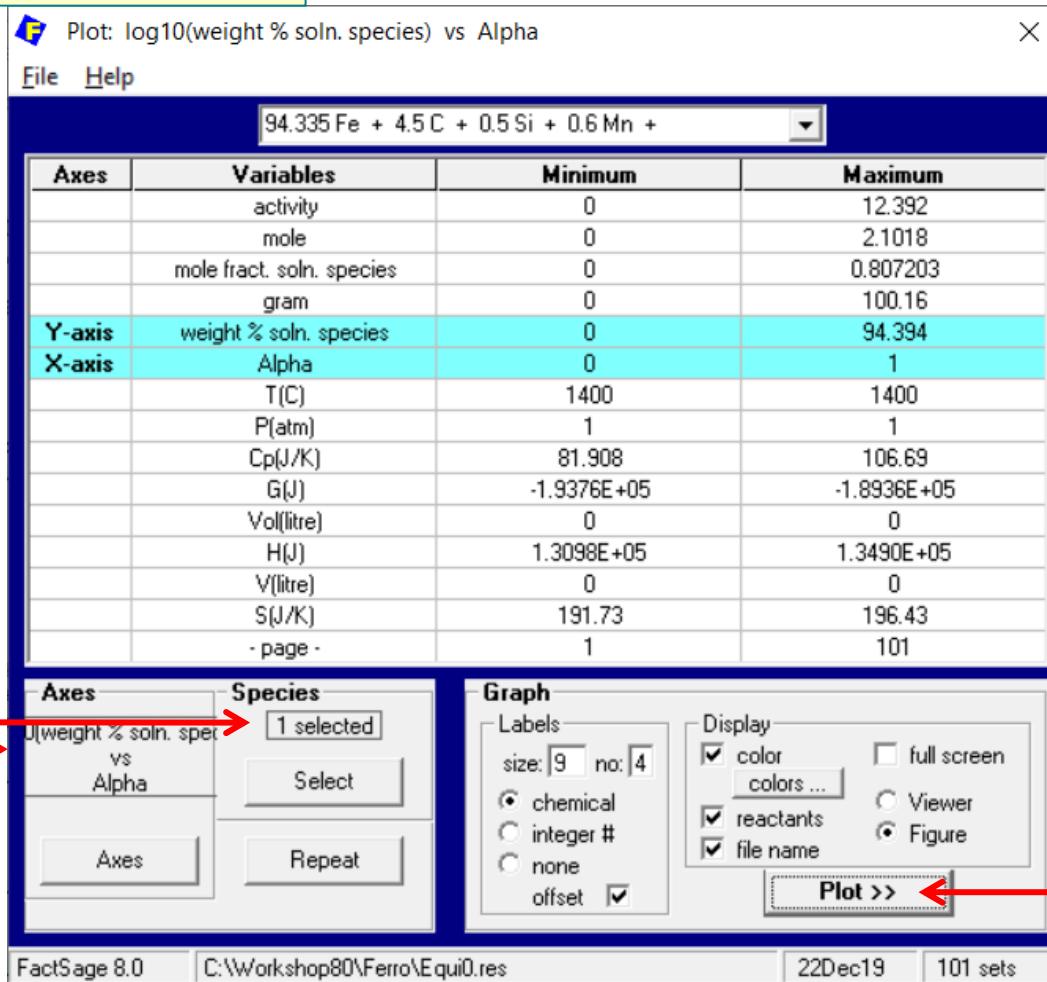
2. Select S(FeLQ) – sulphur in the liquid steel solution.

3. Press “OK”

The screenshot shows the FactSage 8.0 software interface for selecting species. On the left, a small window titled "Plot: log10(weight % soln. species) vs Alpha" has its Y-axis set to "weight % soln. species" and X-axis to "Alpha". A red arrow points from this window to the "Y-axis" and "X-axis" buttons in the main "Plot Species Selection" dialog. The main dialog lists various species with their properties: FeLQ, Fe, C, Mn, S, Si, Mg, and several pure solids like C, Mg, MgC₂, etc. The "S" row is highlighted with a yellow background. A red arrow points to the "Select" button at the bottom of the left window. Another red arrow points to the "OK" button at the bottom right of the main dialog. The "OK" button has a red box around it and a red arrow pointing to the text "3. Press ‘OK’". The status bar at the bottom shows "FactSage 8.0" and "C:\Workshop80\Ferro".

Desulphurization of Hot Metal using Mg

1. Now we can see that both the axes and the species have been selected.



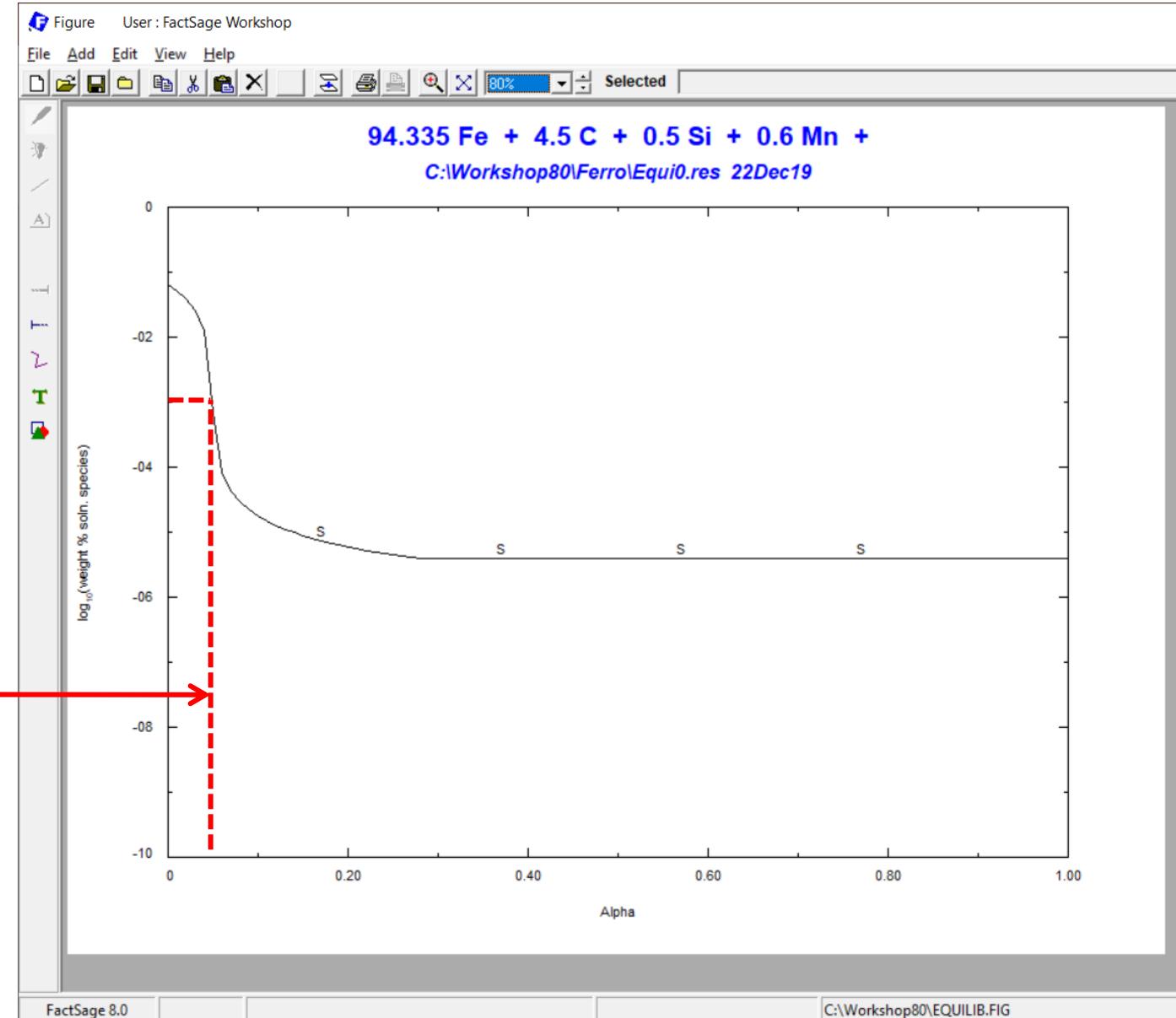
2. The “Plot” button is now activated. Click it!

Desulphurization of Hot Metal using Mg

1. It can be seen that after the addition of 0.1g Mg, the desulphurization is not so effective.

2. If our target was 0.001% S, we can read off the graph that this sulphur level will be achieved after adding approximately 0.05g Mg.

3. However, there is a better way.



Desulphurization of Hot Metal using Mg: Composition target

1. Right-click on the Ftmisc-FeLQ selection

2. Click on “composition target”

3. This window will pop-up

The screenshot shows the FactSage software interface for equilibrium calculations. A context menu is open over a selection labeled 'Ftmisc-FeLQ'. The menu items include:

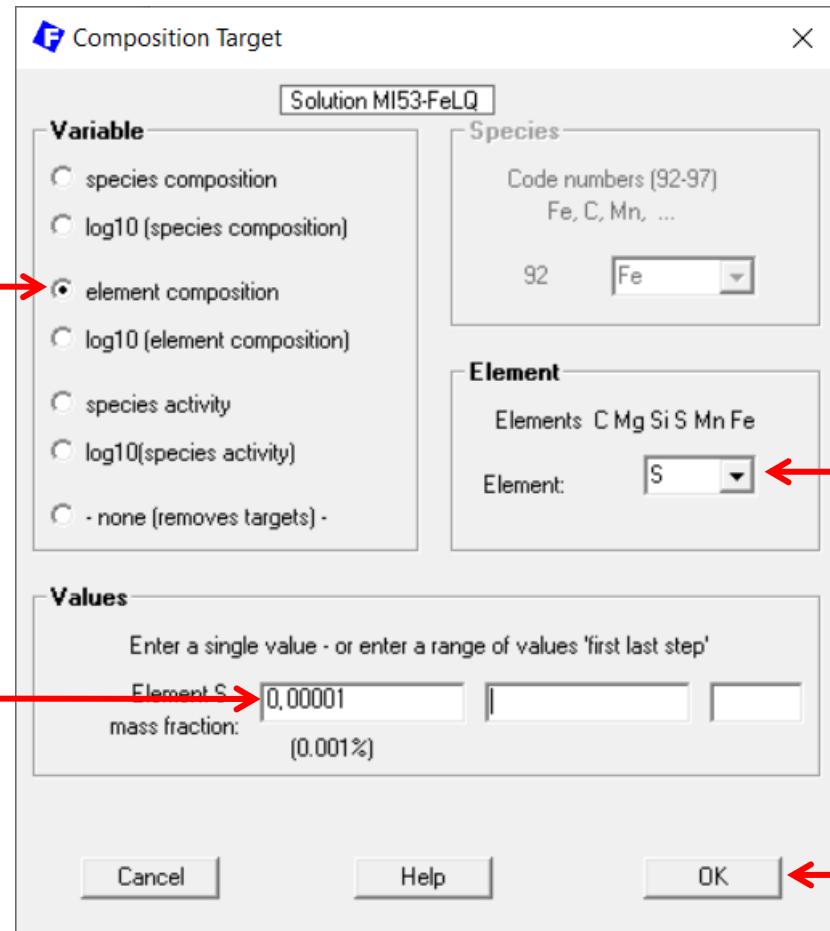
- clear
- all end-members
- * - custom select end-members
- m - merge dilute solution from
- solution properties
- + - single phase
- I - possible 2-phase immiscibility
- J - possible 3-phase immiscibility
- standard stable phase
- ! - dormant (metastable) phase
- F - formation target phase
- P - precipitate target phase
- C - composition target ... **(highlighted with a red arrow)**
- L - cooling calculation ...

The 'Composition Target' dialog box is displayed, titled 'Solution MI53-FeLQ'. It contains the following fields:

- Variable:**
 - species composition
 - log10 (species composition)
 - element composition
 - log10 (element composition)
 - species activity
 - log10(species activity)
 - none (removes targets) -
- Species:** Code numbers (92-97)
Fe, C, Mn, ...
92 Fe
- Element:** Elements C Mg Si S Mn Fe
Element: C
- Values:** Enter a single value - or enter a range of values 'first last step'
- none -

Buttons at the bottom include Cancel, Help, and OK.

Desulphurization of Hot Metal using Mg: Composition target



1. Select “element composition”

2. Choose element S

3. Enter the desired value (here – 0.001%)

4. Press “OK”

Desulphurization of Hot Metal using Mg: Composition target

1. Now “C” indicates that we have selected a composition target for this calculation

Equilib - Menu: last system

File Units Parameters Help

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

Reactants (6)

(gram) 94.335 Fe + 4.5 C + 0.5 Si + 0.6 Mn + 0.065 S + <A> Mg

Products

Compound species

gas	ideal	real	0
aqueous			0
pure liquids			0
* pure solids			40
* - custom selection			
species: 40			

Solution phases

*	Base-Phase	Full Name
C	FTmisc-FeLQ	Fe-liq
	FTmisc-MATT	Matte
	FTmisc-FeS_	FeS-liq
	FTmisc-MAT2C	C-Liq(Matte/Metal)
	FTmisc-PYRRC	C-Pyrhotite
	FTmisc-BCCS	bcc
	FTmisc-FCCS	fcc
	FTmisc-MS-c	MeS_c

Custom Solutions

0 fixed activities Details ...
0 ideal solutions

Pseudonyms apply Edit ...

Volume data assume molar volumes of solids and liquids = 0

Composition target Element S - FTmisc-FeLQ
Estimate ALPHA: 0.5
Quantity(g): 0

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		1400	1	
10 steps	Table			1 calculation

Equilibrium

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

FactSage 8.0

2. We must leave the <A> field blank, because <A> is what we want to calculate.

3. Press “Calculate”. Note that only one calculation will be performed.

Desulphurization of Hot Metal using Mg: Composition target

1. The $\langle A \rangle$ value for reducing sulphur content to 0.001% is 0.0494g.

Equilib - Results 1400 C, A=0.0494

Output Edit Show Pages Final Conditions

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

(gram) 94.335 Fe + 4.5 C + 0.5 Si + 0.6 Mn +

(gram) 0.065 S + $\langle A \rangle$ Mg =

99.937 gram Fe-liqu
(99.937 gram, 2.0927 mol)
(1400 C, 1 atm, a=1.0000)
(94.395 wt.% Fe
+ 4.5028 wt.% C
+ 0.60038 wt.% Mn
+ 1.0000E-03 wt.% S ←
+ 0.50032 wt.% Si
+ 8.9384E-04 wt.% Mg)

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

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	1.6892	94.335	0.80721	0.94395
Mn	1.0921E-02	0.60000	5.2188E-03	6.0000E-03
S	3.1167E-05	9.9937E-04	1.4893E-05	1.0000E-05
Si	1.7803E-02	0.50000	8.5071E-03	5.0032E-03
Mg	3.6753E-05	8.9328E-04	1.7562E-05	8.9384E-06
C	0.37467	4.5000	0.17904	4.5028E-02

+ 0.11251 gram MgS_solid
(0.11251 gram, 1.9960E-03 mol)
(1400 C, 1 atm, S1, a=1.0000)

+ 0 gram C_Graphite
(1400 C, 1 atm, S1, a=0.81691)

2. The mass fraction of S is exactly what we want it to be.

Desulphurization of Hot Metal using CaC₂

In the same manner, we can calculate the desulphurization ability of CaC₂



Equilib - Reactants

File Edit Table Units Data Search Data Evaluation Help

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

1 - 6 |

Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
94.335	Fe				1	
+ 4.5	C				1	
+ 0.5	Si				1	
+ 0.6	Mn				1	
+ 0.065	S				1	
+ <A>	CaC ₂				1	

We will keep the same hot metal composition, the only thing we will change is the desulphurizing agent

Initial Conditions

Next >>

FactSage 8.0 Compound: 2/26 databases Solution: 1/26 databases

Desulphurization of Hot Metal using CaC₂

The same conditions are selected

Equilib - Menu: comments

File Units Parameters Help

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

Reactants (6)

(gram) 94.335 Fe + 4.5 C + 0.5 Si + 0.6 Mn + 0.065 S + <A> CaC₂

Products

Compound species

<input type="checkbox"/> gas	<input checked="" type="radio"/> ideal	<input type="radio"/> real	0
<input type="checkbox"/> aqueous			0
<input type="checkbox"/> pure liquids			0
* <input checked="" type="checkbox"/> pure solids			43
* - custom selection		species:	43

Target

- none -

Estimate ALPHA: 0.5

Quantity(g): 0

Solution phases

*	+	Base-Phase	Full Name
*	+	FTmisc-FeLQ	Fe-liq
		FTmisc-MATT	Matte
		FTmisc-FeS_	FeS-liq
		FTmisc-MAT2C	C-Liq(Matte/Metal)
		FTmisc-PYRRC	C-Pyrrhotite
		FTmisc-BCCS	bcc
		FTmisc-FCCS	fcc
		FTmisc-MS-c	MeS_cubic

Legend

+ - selected 1

Show all selected

species: 6

solutions: 1

Select

Custom Solutions

0 fixed activities

0 ideal solutions

Pseudonyms

apply Edit ...

Volume data

assume molar volumes of
solids and liquids = 0

include molar volume data
and physical properties data

paraequilibrium & Gmin edit

Total Species (max 5000) 49

Total Solutions (max 200) 1

Total Phases (max 1500) 44

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
0 1 0.01		1400	1	
10 steps	<input type="checkbox"/> Table	101 calculations		

Equilibrium

normal normal + transitions

transitions only open

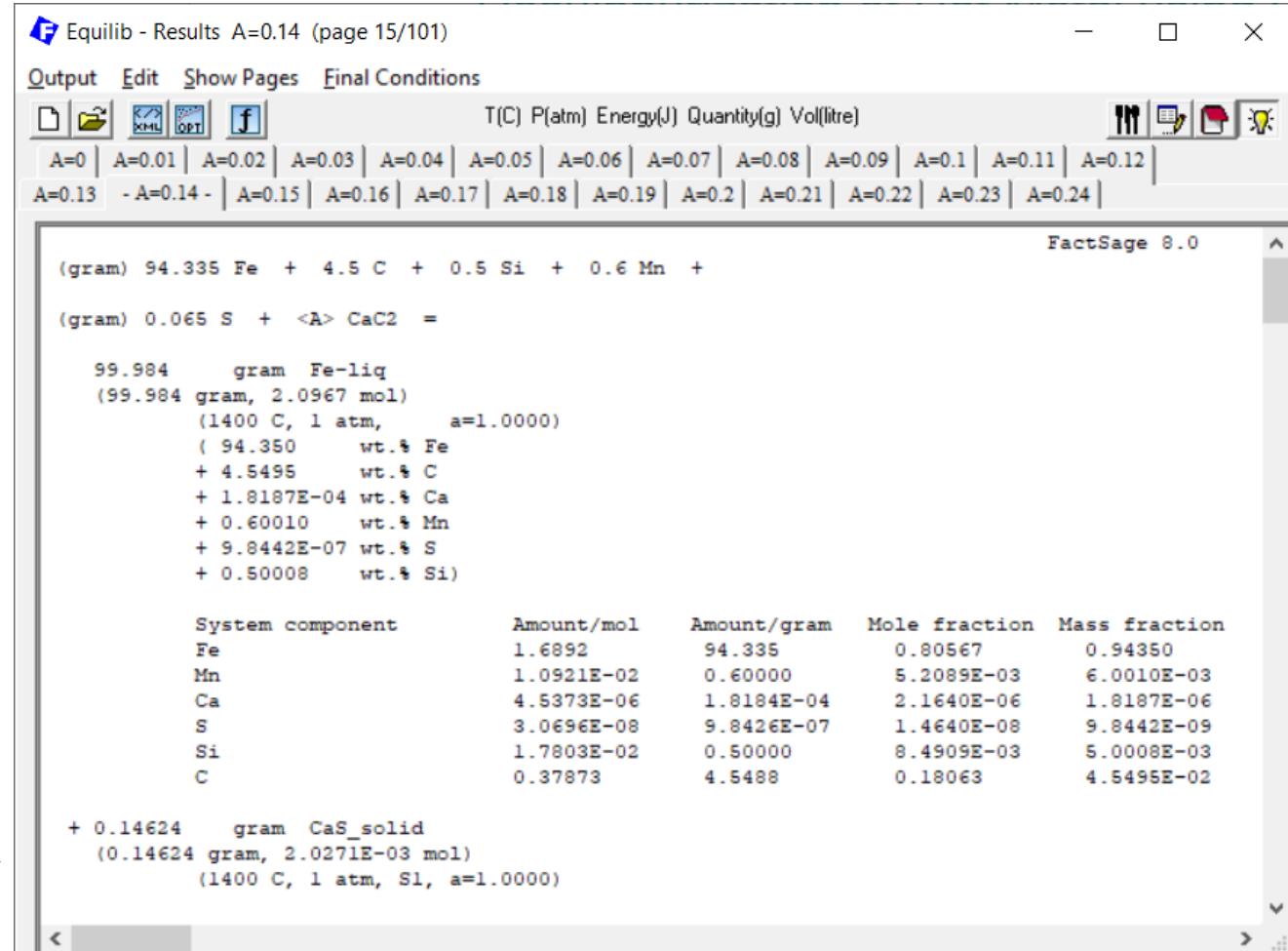
- no time limit -

Calculate >

FactSage 8.0 C:\Workshop80\Ferro\Ferrous_Applications_II_p91.equi

Desulphurization of Hot Metal using CaC₂

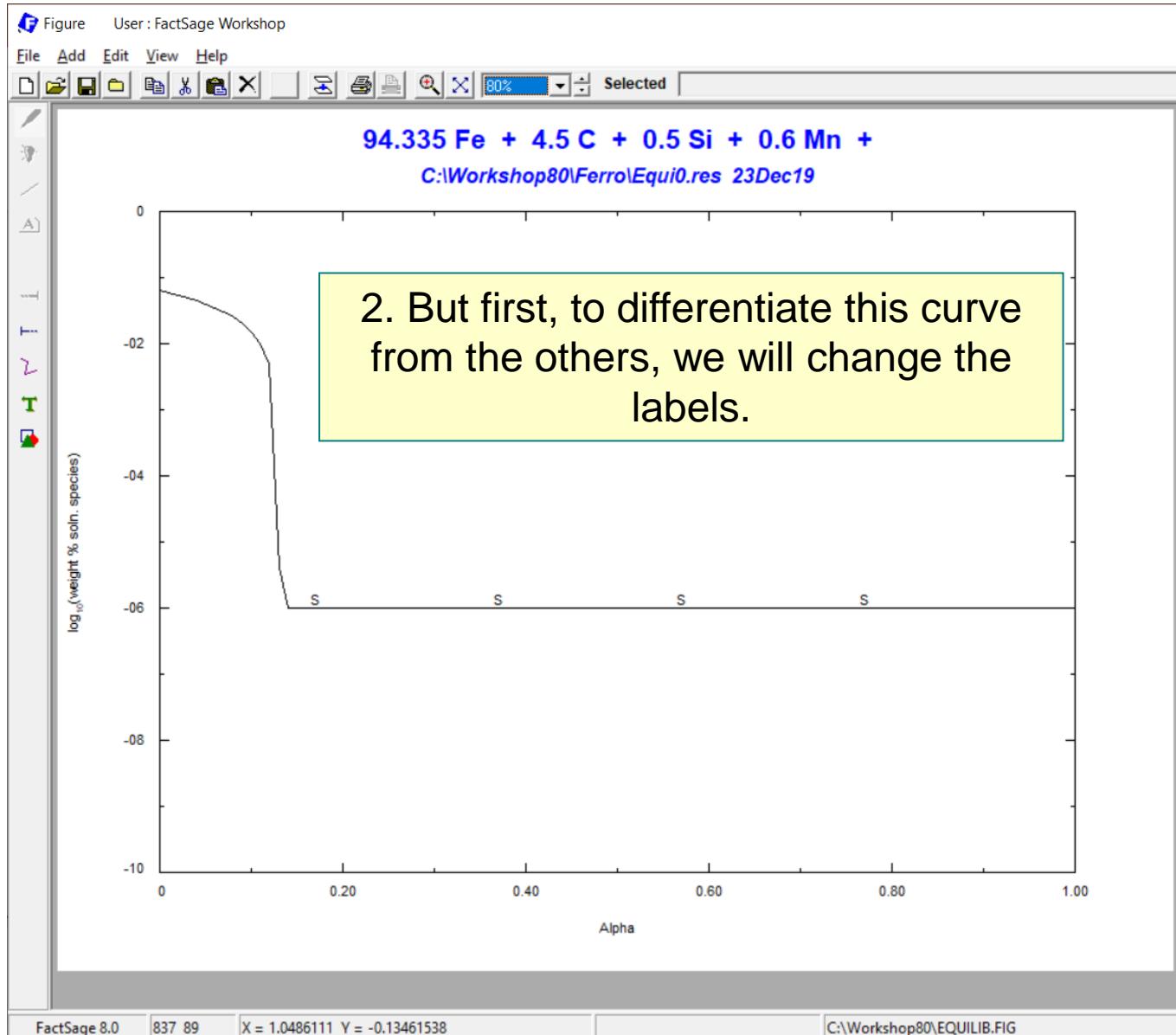
After addition of 0.14g of CaC₂, the amount of S in the hot metal becomes so small, that the reaction does not proceed and CaC₂ is precipitated as a solid phase.



Desulphurization of Hot Metal using CaC₂

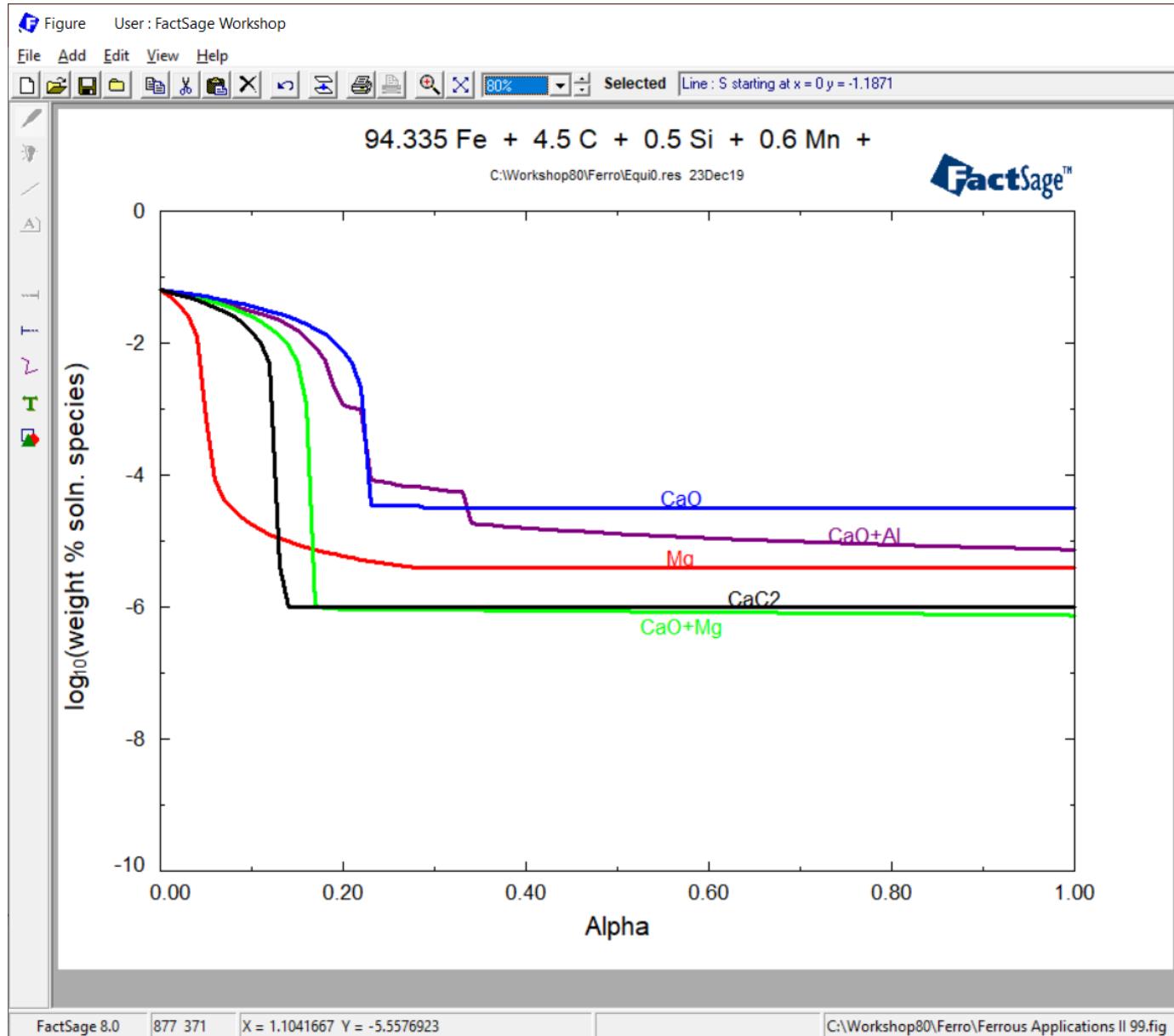
This can also be seen on the graph – after $\langle A \rangle = 0.14$, the sulphur level remains constant.

1. In order to compare this graph with the graph for Mg desulphurization, we should save this figure.



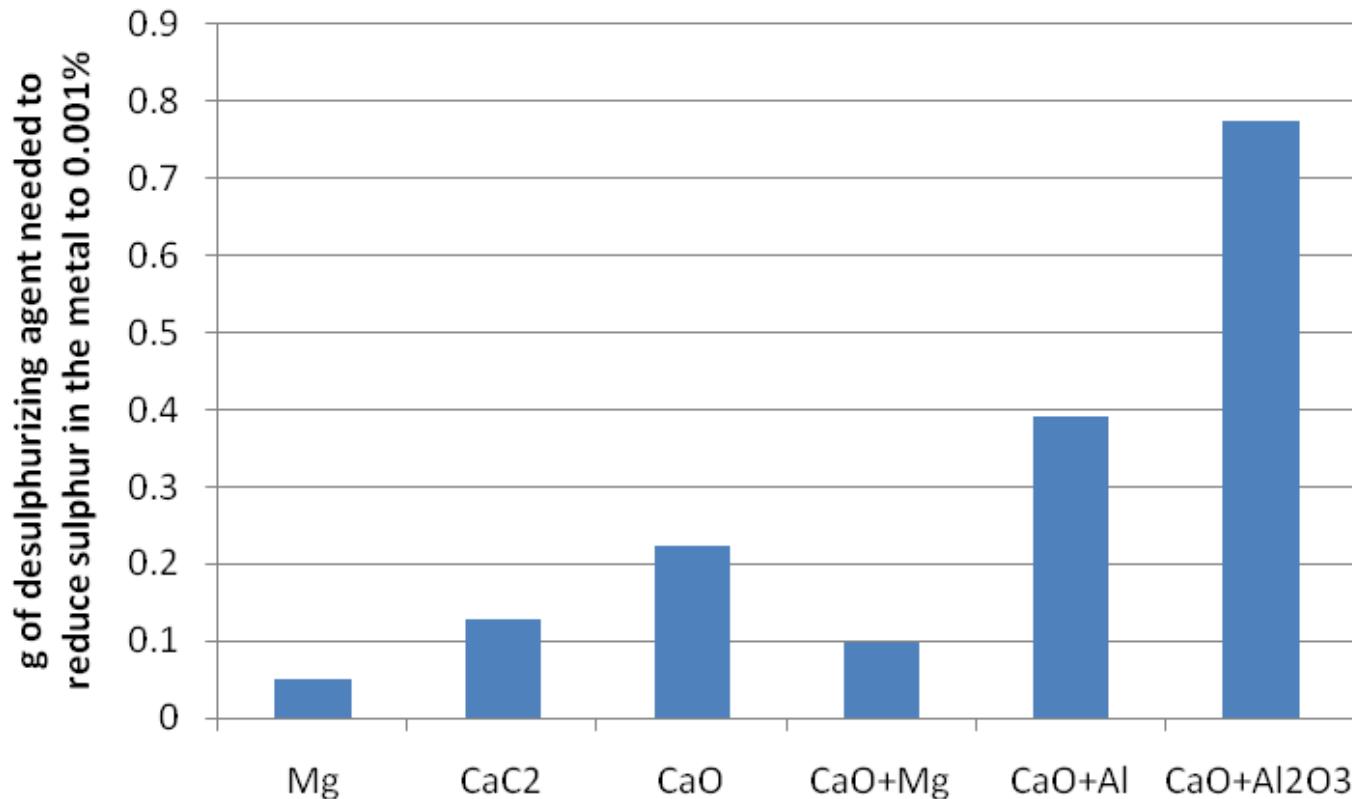
Desulphurization of Hot Metal

It can now readily be seen that Mg and CaO+Mg are the most effective hot metal desulphurizing agents.



Desulphurization of Hot Metal

It is also convenient to compare the amounts obtained using “Composition Target”



Desulphurization of Steel using Slag

We will now apply the same calculations for the desulphurization of steel in the ladle.

The starting steel contains 0.01% S and it needs to be reduced down to 0.001% S

We will also assume that a slag is present in the ladle. It consists of 40% CaO, 40% Al₂O₃, 10% MgO and 10% SiO₂. The ratio of slag to metal is 1/10

Desulphurization of Steel using Slag

We will now apply the same calculations for the desulphurization of steel in the ladle.

The starting steel contains 0.01% S and it needs to be reduced down to 0.001% S

We will also assume that a slag is present in the ladle. It consists of 40% CaO, 40% Al₂O₃, 10% MgO and 10% SiO₂. The ratio of slag to metal is 1/10

Desulphurization of Steel using Slag

1. Enter the metal and slag composition

This example can be found
in EquiCase2-7.dat

Equi - Reactants

File Edit Table Units Data Search Data Eval T(C) P(atm)

1 - 9

Quantity(g) Species

99.84 Fe

+ 0.05 C

+ 0.1 Mn

+ 0.01 S

+ 4 CaO

+ 4 Al2O3

+ 1 SiO2

+ 1 MgO

+ <A> Mg

Data Search

Databases - 3/23 compound databases, 27/23 solution databases

Fact FactSage™ SGTE Private Databases

FactPS FScoopp BINS EXAM

FToxid FSlead SGPS SGTEa

FTsalt FSstel SGTEb

FTmisc FSupsip SGsold

FTball ELEM Add/Remove Data

FTOxCN FTdemo RefreshDatabases

FTfritz FTlite FTnucl

FThelg FTpulp TDmeph

FTpulp FTlite TDnucl

Other

SGnobl SpMCBN

SpMCBN TDmeph

TDmeph TDnucl

Information

Options - search for product species

Include compounds

gaseous ions (plasmas)

aqueous species

limited data compounds (25C)

Limits

Organic species CxHy..., X(max) =

Minimum solution components: 1 2 cpts

Cancel Summary ... OK

FactSage 8.0 Compound: 3/23 databases

Desulphurization of Steel using Slag

2. Select liquid steel and SlagA as the solutions

The screenshot shows the Equilib software interface. In the 'Reactants' section, the input is: (gram) 99.84 Fe + 0.05 C + 0.1 Mn + 0.01 S + 4 CaO + 4 Al2O3 + SiO2 + MgO + <A> Mg. In the 'Products' section, under 'Compound species', there are checkboxes for gas (ideal), aqueous, pure liquids, and pure solids. Below these are sections for custom selection and target conditions (Estimate T(K): 1000, Quantity(g): 0). In the 'Solution phases' table, the first row is selected, showing 'FTmisc-FeLQ' as the base phase and 'Fe-liq' as the full name. A red arrow points from the text '3. Note that the slag phase is selected with possible immiscibility' to this row. In the 'Equilibrium' section, the 'normal' option is selected. A red arrow points from the text '1. Enter the <A> and Temperature' to the '<A>' field in the 'Final Conditions' table, which contains '0 1 0.01'. Another red arrow points from the text '4. Press "Calculate"' to the 'Calculate >>' button.

1. Enter the <A> and Temperature

2. Select liquid steel and SlagA as the solutions

3. Note that the slag phase is selected with possible immiscibility

4. Press "Calculate"

Desulphurization of Steel using Slag

Results show a slag phase and a metal phase

Solid periclase (MgO) appears as $\langle A \rangle$ is increased

We can plot the results in the same way as was done for the hot metal desulphurization in the previous slides

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

Output Edit Show Pages Final Conditions

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

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

FactSage 8.0

```
(gram) 99.84 Fe + 0.05 C + 0.1 Mn + 0.01 S +
(gram) 4 CaO + 4 Al2O3 + SiO2 + MgO +
(gram) <A> Mg =
99.975 gram Fe-liq
(99.975 gram, 1.7938 mol)
(1600 C, 1 atm, a=1.0000)
( 99.844 wt.% Fe
+ 7.0615E-04 wt.% Al
+ 5.0012E-02 wt.% C
+ 2.0657E-08 wt.% Ca
+ 8.9110E-02 wt.% Mn
+ 1.2958E-03 wt.% O
+ 6.0873E-03 wt.% S
+ 6.8675E-03 wt.% Si
+ 1.1721E-05 wt.% Mg
+ 1.0673E-03 wt.% MgO
+ 4.2280E-04 wt.% CaO
+ 5.4841E-05 wt.% AlO
+ 4.9590E-07 wt.% SiO
```

Final Conditions

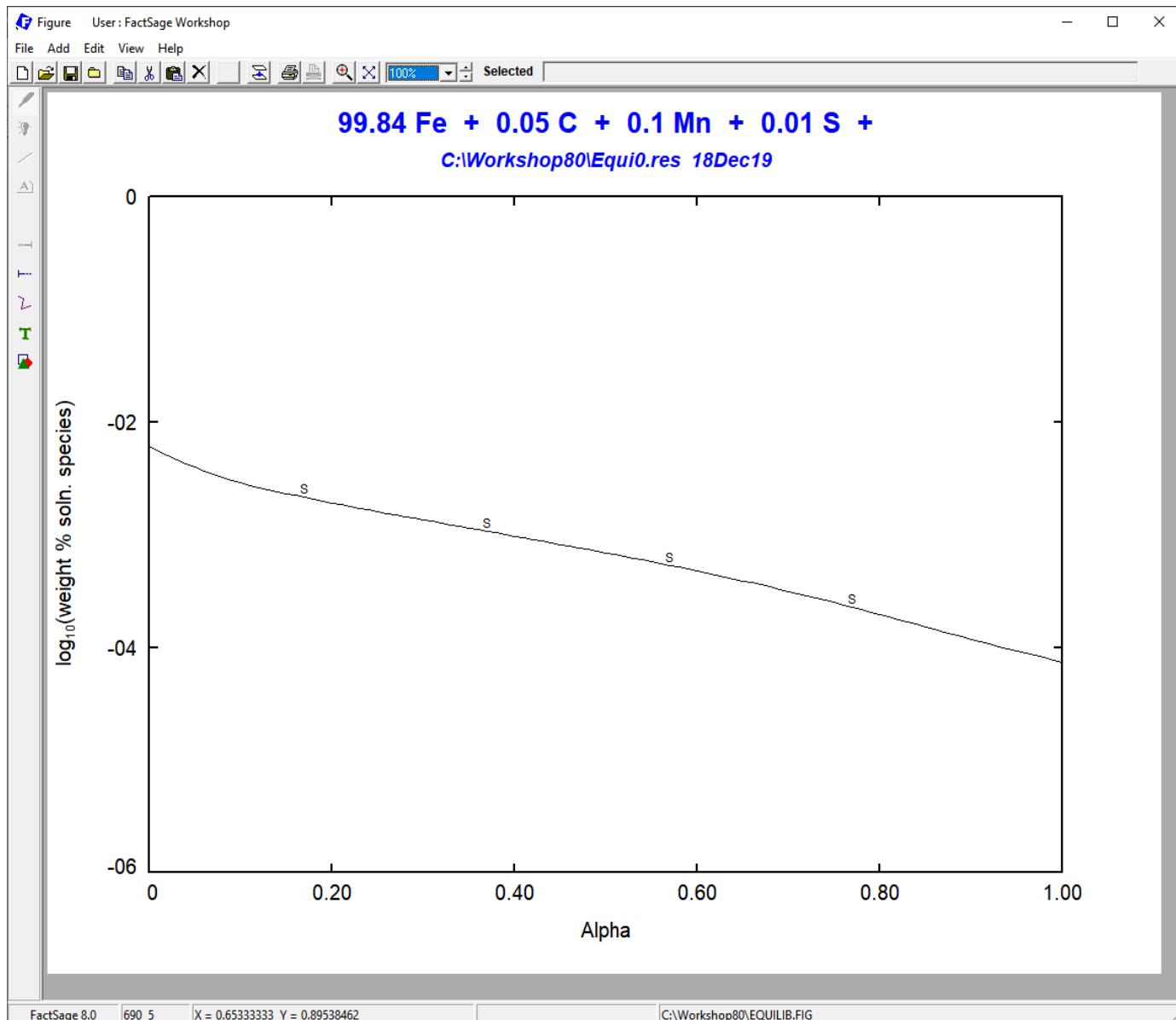
$\langle A \rangle$	$\langle B \rangle$	T(C)	P(atm)	Product H(J)
01 0.01		1600	1	

101 calculations

Calculate >>

Desulphurization of Steel using Mg

A constant decrease in metal sulphur content is observed



Desulphurization of Steel using Mg

Another useful way to visualize these results, is the sulphur partition coefficient:

$$L_s = (S_{\text{in slag}}) / (S_{\text{in metal}})$$

1. Press "Output" →
"Save or Print As"

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

Output Edit Show Pages Final Conditions

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

A=0.13 | A=0.14 | A=0.15 | A=0.16 | A=0.17 | A=0.18 | A=0.19 | A=0.20 | A=0.21 | A=0.22 | A=0.23 | A=0.24 |
A=0 | A=0.01 | A=0.02 | A=0.03 | A=0.04 | A=0.05 | A=0.06 | A=0.07 | A=0.08 | A=0.09 | A=0.1 | A=0.11 | A=0.12 |

(gram) 99.84 Fe + 0.05 C + 0.1 Mn + 0.01 S +

(gram) 4 CaO + 4 Al2O3 + SiO2 + MgO +

(gram) <A> Mg

Output

Page Range Type of Out

99.975
(99.975)

Output

Page Range

All 101 pages

Current page 1

Type of Output

Printer

Text file (*.txt)

Equilib Results File (Equi*.res)

Xml file (*.xml)

Excel Spreadsheet

Open Text Spreadsheet

Save Text Spreadsheet

Swap rows & columns

Cancel OK

FactSage 8.0

2. Select "Open Text Spreadsheet"

3. Press "Spreadsheet Setup"

Desulphurization of Steel using Mg

1. Select “Alpha” as the property column

The screenshot shows the FactSage 8.0 software interface with the following details:

- Top Bar:** T(C) P(atm) Energy(J) Quantity(g) Vol(litre)
- Chemical Equations:**
 - (gram) 99.84 Fe + 0.06 C + 0.1 Mn + 0.01 S +
 - (gram) 4 CaO + 4 Al₂O₃ + SiO₂ + MgO +
- FactSage 8.0** label in the top right corner.
- Spreadsheet Setup Dialog:**
 - System Properties:** Property columns 1. Column: -1. Variable: Alpha.
 - Species Properties:** Columns per species 1. Order: order props. Column: -1. Variable: Wt%.
- Species Dialog:** Species: 0. Buttons: Select..., Cancel, Default, OK.
- Bottom Bar:** <A> T(C) P(atm) Product H(J) 101 calculations X

2. Select “wt%” as the Species properties

3. Select the desired species

Desulphurization of Steel using Mg

1. Select sulphur from liquid steel and all elements from the slag

The screenshot shows a software window titled "Spreadsheet - Equilib Page 101/101 : T(C) = 1600, P(atm) = 1, Alpha = 1". The window includes a menu bar with File, Edit, Show, and Select Stable, and a toolbar with buttons for Selected: 2/200, Spreadsheet Species, and a page navigation section. The main area displays a table of species properties. A red arrow points down to the "Activity" column header. Another red arrow points up to the "OK" button at the bottom right of the window.

	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
403	SiO ₂ (SLAGA)	FToxid	FToxid-SLAGA#				1.0243E-05	1.0243E-05 [101]	5.4302E-04 [1]
404	CaO(SLAGA)	FToxid	FToxid-SLAGA#				0.1194	4.2993E-02 [1]	0.1194 [101]
405	FeO(SLAGA)	FToxid	FToxid-SLAGA#				8.8671E-05	8.8671E-05 [101]	5.6044E-03 [1]
406	Fe2O ₃ (SLAGA)	FToxid	FToxid-SLAGA#				1.3084E-15	1.3084E-15 [101]	3.2612E-10 [1]
407	MgO(SLAGA)	FToxid	FToxid-SLAGA#				0.1494	0.1226 [1]	0.1494 [10]
408	MnO(SLAGA)	FToxid	FToxid-SLAGA#				2.5909E-05	2.5909E-05 [101]	1.5016E-03 [1]
409	Mn ₂ O ₃ (SLAGA)	FToxid	FToxid-SLAGA#				1.5600E-17	1.5600E-17 [101]	3.2695E-12 [1]
410	Al ₂ S ₃ (SLAGA)	FToxid	FToxid-SLAGA#				1.9141E-18	1.9141E-18 [101]	4.3621E-17 [16]
411	Si ₂ S(LAGA)	FToxid	FToxid-SLAGA#				1.9401E-16	1.9401E-16 [101]	2.7858E-14 [8]
412	CaS(SLAGA)	FToxid	FToxid-SLAGA#				5.9758E-02	2.6124E-02 [1]	6.1767E-02 [76]
413	FeS(SLAGA)	FToxid	FToxid-SLAGA#				9.5623E-06	9.5623E-06 [101]	7.3403E-04 [1]
414	Fe ₂ S ₃ (SLAGA)	FToxid	FToxid-SLAGA#				3.8240E-28	3.8240E-28 [101]	1.7076E-22 [1]
415	MgS(SLAGA)	FToxid	FToxid-SLAGA#				4.6821E-04	4.6652E-04 [1]	9.0589E-04 [21]
416	MnS(SLAGA)	FToxid	FToxid-SLAGA#				4.2284E-06	4.2284E-06 [101]	2.9763E-04 [1]
417	Mn ₂ S ₃ (SLAGA)	FToxid	FToxid-SLAGA#				7.2816E-19	7.2816E-19 [101]	2.7340E-13 [1]
	956	Solution	FTmisc	FTmisc-FelQ			1.000	1.000	1.000
	964	Solution	FToxid	FToxid-SLAGA#			1.000	1.000	1.000
	964	Solution	FToxid	FToxid-SLAGA#			1.000	1.000	1.000
	1007	All Elements	FTmisc	FTmisc-FelQ					
+	1015	All Elements	FToxid	FToxid-SLAGA#					

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

Buttons: Select All, Clear, OK

2. Press "OK"

Desulphurization of Steel using Mg

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

Output Edit Show Pages Final Conditions

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

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

(gram) 99.84 Fe + 0.05 C + 0.1 Mn + 0.01 S +

(gram) 4 CaO + 4 Al2O3 + SiO2 + MgO +

Spreadsheet Setup

System Properties

Property columns 1

Column:	-1-
Variable:	Alpha

Species Properties

Columns per species 1

order species order props.

Column:	-1-
Variable:	Wt%

Species

Columns: 3

Select ...

Cancel

Default

OK

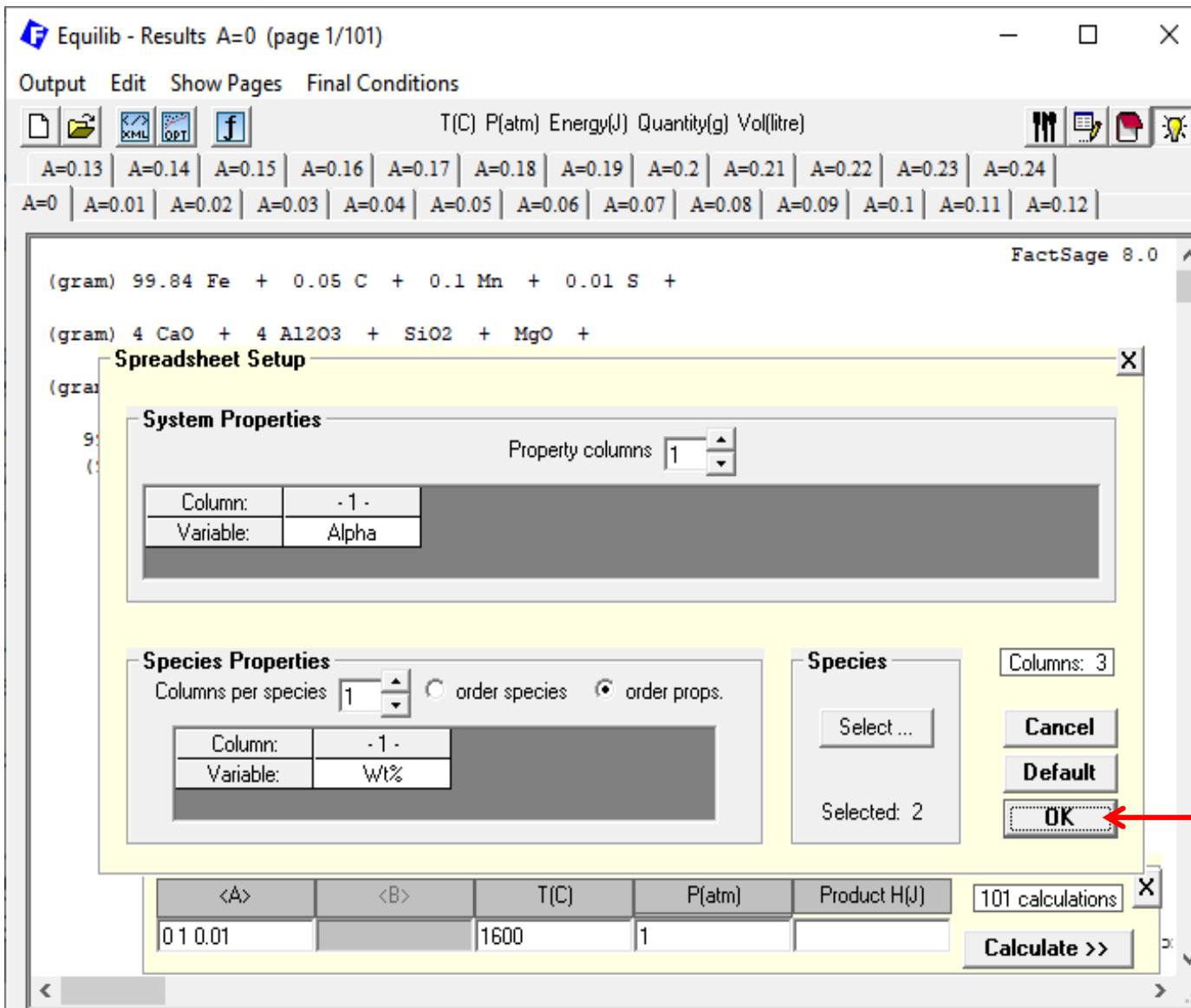
Selected: 2

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

01 0.01		1600	1	
---------	--	------	---	--

101 calculations

Calculate >>



1. Press “OK” on this window and the next one

Desulphurization of Steel using Mg

1. A spreadsheet with the composition of slag and metal at each <Alpha> value will appear.

2. It is convenient to copy the whole table and paste it in Excel.

Equilib Results

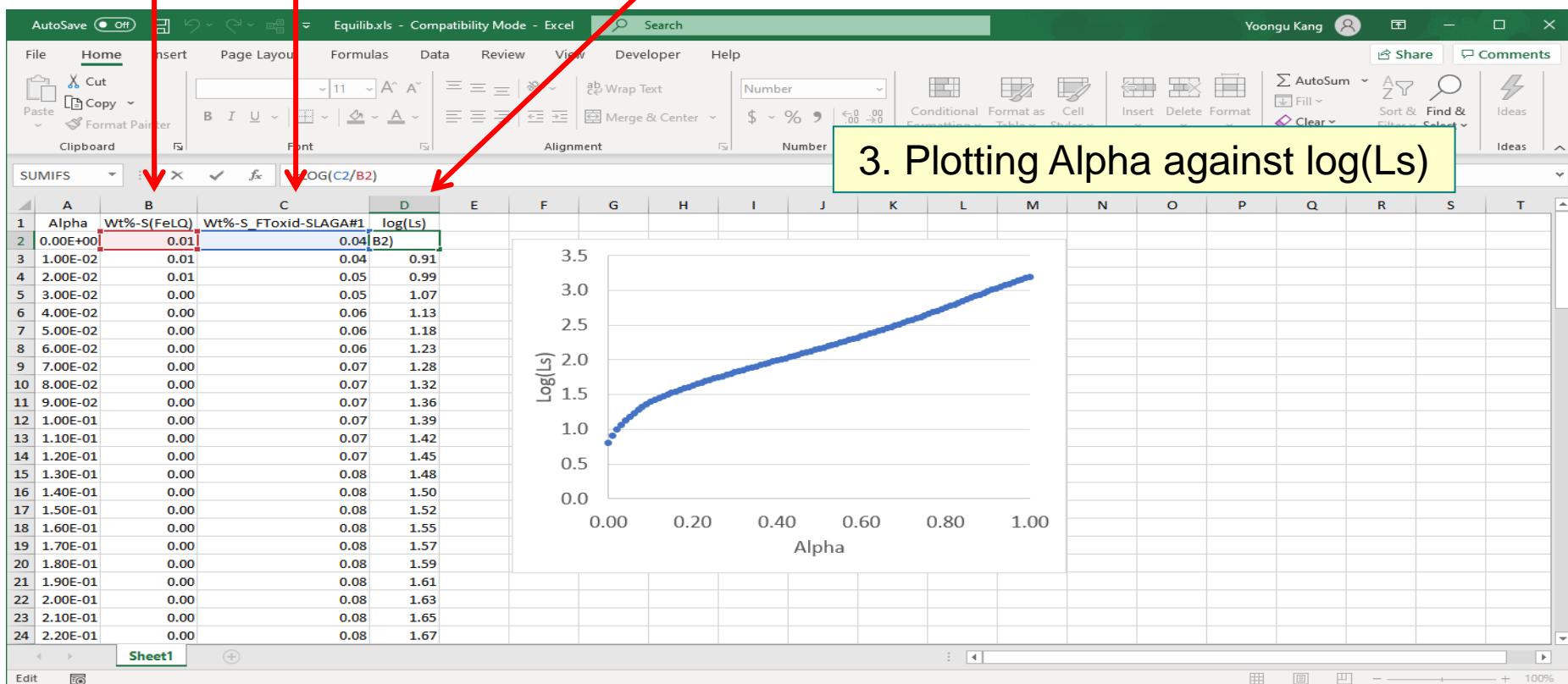
File Edit Swap rows and columns

Alpha	Wt%-S(FeLQ)	Wt%-Fe_FToxid-SLAGA#1	Wt%-Mn_FToxid-SLAGA#1	Wt%-Ca_FToxid-SLAGA#1	Wt%-S_FToxid-SLAGA#1	Wt%-Si_FToxid-SLAGA#1	Wt%-Al_FToxid-SLAGA#1	Wt%-Mg_FTox
0.000000E+00	6.0872865E-03	2.0547678E-01	1.0870141E-01	2.8513378E+01	3.9044801E-02	4.5942107E+00	2.1109887E+01	6.008795
1.000000E-02	5.5225548E-03	1.6564708E-01	8.8667249E-02	2.8510641E+01	4.4667417E-02	4.5581833E+00	2.1105213E+01	6.107786
2.000000E-02	5.0337812E-03	1.3913174E-01	7.4715083E-02	2.8504557E+01	4.9527274E-02	4.5157601E+00	2.1097873E+01	6.206024
3.000000E-02	4.6167677E-03	1.2065334E-01	6.4657395E-02	2.8496514E+01	5.3667022E-02	4.4693002E+00	2.1089018E+01	6.303784
4.000000E-02	4.2585811E-03	1.0711369E-01	5.7090835E-02	2.8487309E+01	5.7216547E-02	4.4202732E+00	2.1079294E+01	6.401224
5.000000E-02	3.9470613E-03	9.6751746E-02	5.1175530E-02	2.8477384E+01	6.0297849E-02	4.3695512E+00	2.1069051E+01	6.498433
6.000000E-02	3.6726691E-03	8.8536064E-02	4.6402166E-02	2.8466994E+01	6.3006610E-02	4.3176633E+00	2.1058484E+01	6.595464
7.000000E-02	3.4282375E-03	8.1834264E-02	4.2450319E-02	2.8456290E+01	6.5414709E-02	4.2649440E+00	2.1047707E+01	6.692345
8.000000E-02	3.2083949E-03	7.6240456E-02	3.9110084E-02	2.8445368E+01	6.7576026E-02	4.2116136E+00	2.1036788E+01	6.789098
9.000000E-02	3.0141722E-03	7.1490402E-02	3.6277282E-02	2.8441841E+01	6.9499072E-02	4.1589003E+00	2.1031348E+01	6.871593
1.000000E-01	2.8712463E-03	6.7434155E-02	3.4058621E-02	2.8490517E+01	7.1041455E-02	4.1131828E+00	2.1064473E+01	6.856172
1.100000E-01	2.7408098E-03	6.3883364E-02	3.2101881E-02	2.8539279E+01	7.2464348E-02	4.0670142E+00	2.1097652E+01	6.840637
1.200000E-01	2.6209568E-03	6.0739609E-02	3.0357977E-02	2.8588138E+01	7.3786197E-02	4.0204494E+00	2.1130891E+01	6.825014
1.300000E-01	2.5101776E-03	5.7929062E-02	2.8789783E-02	2.8637101E+01	7.5021608E-02	3.9735304E+00	2.1164190E+01	6.809320
1.400000E-01	2.4072591E-03	5.5395195E-02	2.7368663E-02	2.8686175E+01	7.6182305E-02	3.9262900E+00	2.1197550E+01	6.793570
1.500000E-01	2.3112135E-03	5.3093943E-02	2.6072142E-02	2.8735364E+01	7.7277833E-02	3.8787543E+00	2.1230973E+01	6.777776
1.600000E-01	2.2212269E-03	5.0990405E-02	2.4882312E-02	2.8784673E+01	7.8316045E-02	3.8309447E+00	2.1264456E+01	6.761945
1.700000E-01	2.1366218E-03	4.9056552E-02	2.3784707E-02	2.8834103E+01	7.9303478E-02	3.7828785E+00	2.1297998E+01	6.746087
1.800000E-01	2.0568285E-03	4.7269589E-02	2.2767501E-02	2.8883659E+01	8.0245624E-02	3.7345702E+00	2.1331599E+01	6.730205
1.900000E-01	1.9813636E-03	4.5610765E-02	2.1820916E-02	2.8933341E+01	8.1147135E-02	3.6860323E+00	2.1365257E+01	6.714306
2.000000E-01	1.9098140E-03	4.4064505E-02	2.0936793E-02	2.8983153E+01	8.2011988E-02	3.6372753E+00	2.1398970E+01	6.698393
2.100000E-01	1.8418238E-03	4.2617746E-02	2.0108258E-02	2.9033096E+01	8.2843605E-02	3.5883085E+00	2.1432736E+01	6.682468
2.200000E-01	1.7770845E-03	4.1259446E-02	1.9329477E-02	2.9083171E+01	8.3644951E-02	3.5391399E+00	2.1466554E+01	6.666535
2.300000E-01	1.7153267E-03	3.9980196E-02	1.8595457E-02	2.9133381E+01	8.4418610E-02	3.489770E+00	2.1500421E+01	6.650596

Desulphurization of Steel using Mg

1. All unnecessary columns were deleted keeping only the sulphur content in the steel and the slag.

2. The last column was used to calculate the sulphur partition coefficient L_s .



Calculating Slag Sulphide Capacity

A good way of comparing the ability of a slag to absorb sulphur is the sulphide capacity calculated in the following manner:

$$C_S = (S_{\text{in slag}}) * (P_{O_2} / P_{S_2})^{1/2}$$

In the following slides, the sulphide capacity of four different slags will be calculated

Steelmaking Slag Parameters	BOF Slag		Ladle Furnace Slag	
	Type 1	Type 2	Type 1	Type 2
	Low-P Hot Metal	High-P Hot Metal	Al-Killed Steel	Si-Killed Steel
CaO	44.0	54.0	53.0	55.0
MgO	9.0	1.0	9.0	9.0
SiO ₂	13.0	14.0	5.0	20.0
Al ₂ O ₃	1.8	1.0	30.0	12.0
Fe (total)	18.0	19.0	1.0	1.0
MnO	4.5	0.5	1.0	0.6
S	0.07	0.06	0.50	0.50
P ₂ O ₅	2.00	3.50	0.05	0.05
TiO ₂	1.0	<0.5	<0.5	<0.5
Slag Basicity (CaO / SiO ₂)	3.4	3.9	10.6	2.8
Slag Basicity (CaO + MgO) / (SiO ₂ + Al ₂ O ₃)	3.6	3.7	1.8	2.0

Calculating Slag Sulphide Capacity

1. Enter the amount and species for the first slag

This example can be found in EquiCase2-13.dat

The screenshot shows the FactSage software interface. On the left, the 'Equilib - Reactants' window displays a table of reactant amounts and species. A red arrow points from the 'Quantity(g)' column to the 'Species' column. The table includes rows for CaO, MgO, SiO₂, Al₂O₃, Fe, MnO, S, P₂O₅, and TiO₂. On the right, a 'Data Search' dialog box is open, showing a list of databases. A red arrow points to the 'FactPS' and 'Ftoxic' checkboxes, which are selected. Other databases listed include FTsalt, FTmisc, FThall, FTOxCN, FTfrtz, FThelg, FTpulp, FTlite, FSopp, FSlead, FSstel, FSups, BINS, SGPS, SGTE, SGsold, ELEM, SGnobl, SpMCBN, TDmeph, and FTnucl.

1. Enter the amount and species for the first slag

2. Select FactPS and Ftoxic databases

File Edit Table Units Data Search Data Evaluation T(C) P(atm)

Quantity(g) Species

44	CaO
9	MgO
13	SiO ₂
1.8	Al ₂ O ₃
18	Fe
4.5	MnO
0.07	S
2	P ₂ O ₅
1	TiO ₂

Databases - 2/23 compound databases, 1/23 solution databases

Fact **FactSage™ SGTE** **Private Databases**

FactPS FSopp BINS EXAM
 Ftoxic FSlead SGPS SGTEa
 FTsalt FSstel SGTE SGTEb
 FTmisc FSups SGsold
 FThall
 FTOxCN
 FTfrtz
 FThelg
 FTpulp
 FTlite
 ELEM
 FTdemo
 FTnucl
 SGnobl
 SpMCBN
 TDmeph
 TDnucl

compounds only
solutions only
no database

Clear All Add/Remove Data RefreshDatabases

Information - Click on a box to include (or exclude) a database in the data search. Normally databases are 'coupled' - that is both the compound and solution database (when available) will be selected. To 'uncouple' a database click-mouse-right-button

2. Select FactPS and Ftoxic databases

Options - search for product species

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

Limits -
Organic species CxHy... X(max) =
Minimum solution components: 1 2 cpts

Cancel Summary ... OK

FactSage 8.0 Compound: 3/23 databases Sol

Calculating Slag Sulphide Capacity

1. Select gas and SlagA as possible products

Equilib - Menu: last system

File Units Parameters Help

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

Reactants (9)

(gram) 44 CaO + 9 MgO + 13 SO₂ + 1.8 Al₂O₃ + 18 Fe + 4.5 MnO + 0.07 S + 2 P₂O₅ + TiO₂

Products

Compound species

+ gas	<input checked="" type="radio"/>	ideal	<input type="radio"/>	real	59
aqueous	<input type="checkbox"/>	0			
pure liquids	<input type="checkbox"/>	0			
pure solids	<input type="checkbox"/>	0			

species: 59

Solution phases

*	Base-Phase	Full Name
I	FToxid-SLAGA	A-Slag-liq all oxides + S

Custom Solutions

0 fixed activities Details ...
0 ideal solutions

Pseudonyms apply Edit ...

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

paraequilibrium & Gmin edit

Virtual species: 352

Total Species (max 5000) 103
Total Solutions (max 200) 2
Total Phases (max 1500) 3

Target - none -

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

Legend I - immiscible 1
Show all selected
species: 44
solutions: 2 Select

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
1580	1620	20	1	3 calculations
10 steps	<input type="checkbox"/> Table			

Equilibrium

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

3. Press "Calculate"

FactSage 8.0

2. We will calculate the sulphide capacity at three temperatures: 1580, 1600 and 1620°C

Calculating Slag Sulphide Capacity

It is now possible to calculate the sulphide capacity using these results.

In the next slides, two ways of calculating sulphide capacity will be demonstrated.

Equilib - Results 1580 C (page 1/3)

Output Edit Show Pages Final Conditions

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

1580 C | 1600 C | 1620 C

FactSage 8.0

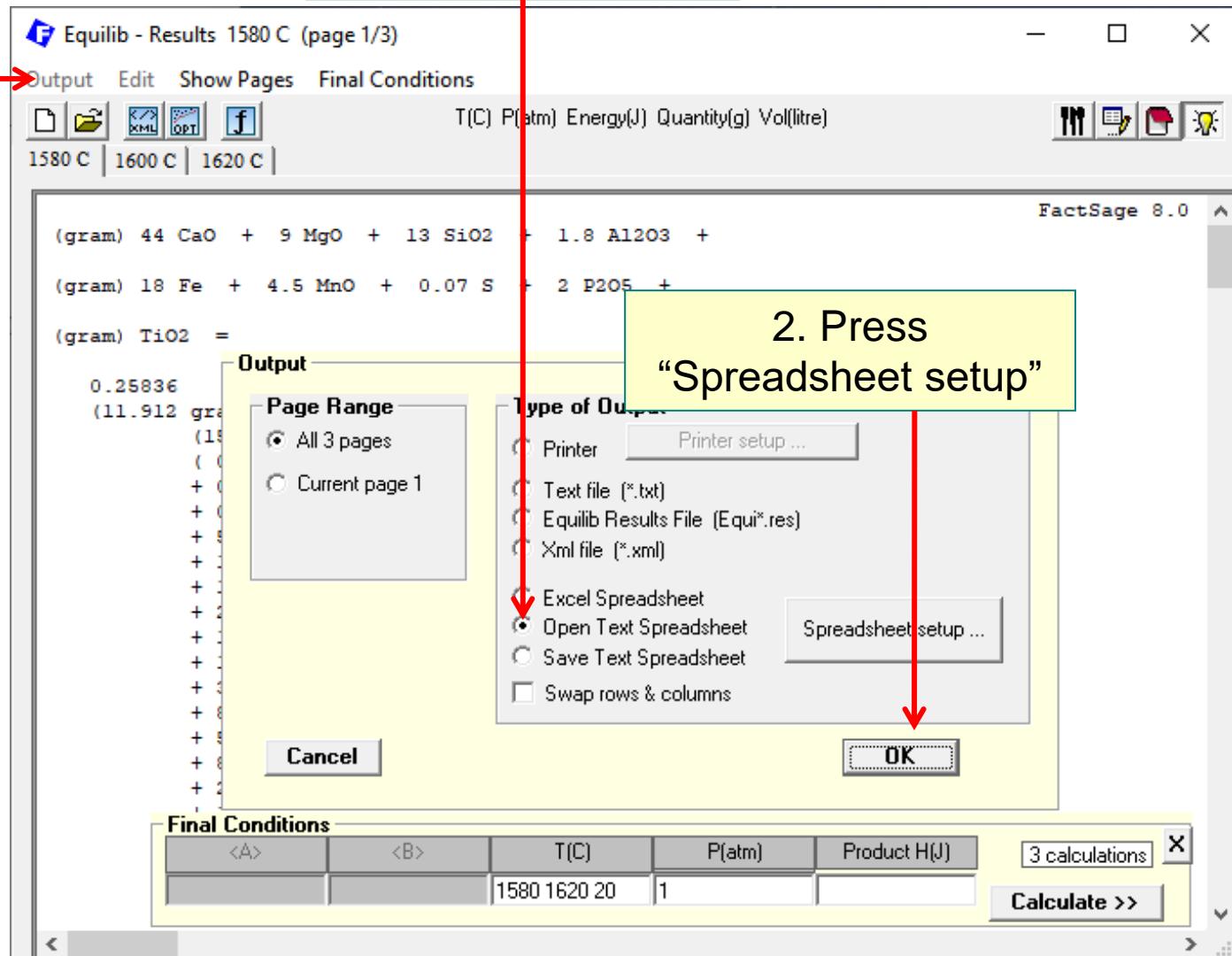
```
(gram) 44 CaO + 9 MgO + 13 SiO2 + 1.8 Al2O3 +
(gram) 18 Fe + 4.5 MnO + 0.07 S + 2 P2O5 +
(gram) TiO2 =
0.25836 mol gas_ideal
(11.912 gram, 0.25836 mol, 39.287 litre, 3.0322E-04 gram.cm-3)
(1580 C, 1 atm, a=1.0000)
( 0.41969 Fe
+ 0.31259 Mg
+ 0.21176 Mn
+ 5.4274E-02 P2
+ 1.5083E-03 Ca
+ 1.2401E-04 P4
+ 2.9676E-05 P
+ 1.7819E-05 Mg2
+ 1.0388E-05 SiO
+ 3.8851E-07 PO
+ 8.5797E-08 Al
+ 5.5088E-08 FeO
+ 8.0970E-09 Si
+ 2.0679E-09 Ca2
+ 1.0252E-09 V2O5
Final Conditions
<A> <B> T(C) P(atm) Product H(J)
1580 1620 20 1
3 calculations
Calculate >
```

Calculating Slag Sulphide Capacity

The first way is to use Excel

1. Save the results in a text spreadsheet

Press “Output”
→ “Save or Print As”



Calculating Slag Sulphide Capacity

F Equilib - Results 1580 C (page 1/3)

Output Edit Show Pages Final Conditions

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

1580 C | 1600 C | 1620 C

FactSage 8.0

1. Set T(C) as the system property

(grz) 2 + 1.8 Al₂O₃ +

(grz) S + 2 P₂O₅ +

Spreadsheet Setup

System Properties

Property columns 1

Column: -

Variable: T(C)

Species Properties

Columns per species 2

order species order props.

Column: -1- -2-

Variable: Wt% a

Species

Columns: 1

Select ...

Cancel

Default

OK

Selected: 0

2. We need wt%S and the activity of O₂ and S₂ in the gas, so select "wt%" and "a" as the species properties.

3. Select the species

P(atm)

Calculate >>

www.factsage.com

Calculating Slag Sulphide Capacity

1. Select O₂(g), S₂(g) and All Elements in SlagA

3/3 : T(C) = 1620, P(atm) = 1

File Edit Show Select Stable

Selected: 4/87 Spreadsheet Species

Page 3/3 : T(C) = 1620 [min = 1580 at page 1; max = 1620 at page 3], P(atm) = 1

+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
	1	O(g)	FactPS	gas			1.6997E-13	1.6997E-13 [1]	5.7303E-13 [3]
+	2	O ₂ (g)	FactPS	gas			7.4406E-19	7.4406E-19 [1]	4.2019E-18 [3]
	3	O ₃ (g)	FactPS	gas			1.6600E-35	1.6600E-35 [1]	2.7199E-34 [3]
	4	Mg(g)	FactPS	gas			0.3126	0.3126 [1]	0.3139 [3]
	22	P0(g)	FactPS	gas			8.1052E-07	3.8851E-07 [1]	8.1052E-07 [3]
	23	P0 ₂ (g)	FactPS	gas			3.1717E-11	9.5129E-12 [1]	3.1717E-11 [3]
	24	P2O ₅ (g)	FactPS	gas			1.1650E-28	8.3620E-30 [1]	1.1650E-28 [3]
	25	(P2O ₃) ₂ (g)	FactPS	gas			8.1479E-22	1.2887E-22 [1]	8.1479E-22 [3]
	26	(P2O ₅) ₂ (g)	FactPS	gas			1.1847E-55	1.4682E-57 [1]	1.1847E-55 [3]
	27	S(g)	FactPS	gas			3.8457E-12	1.3485E-12 [1]	3.8457E-12 [3]
+	28	S ₂ (g)	FactPS	gas			6.1835E-18	1.3827E-18 [1]	6.1835E-18 [3]
	29	S ₃ (g)	FactPS	gas			7.1013E-29	8.0337E-30 [1]	7.1013E-29 [3]
	30	S ₄ (g)	FactPS	gas			2.4192E-39	1.3890E-40 [1]	2.4192E-39 [3]
	31	S ₅ (g)	FactPS	gas			6.6612E-51	2.0529E-52 [1]	6.6612E-51 [3]
	32	S ₆ (g)	FactPS	gas			8.5441E-61	1.3578E-62 [1]	8.5441E-61 [3]
	33	S ₇ (g)	FactPS	gas			8.5252E-71	6.7937E-73 [1]	8.5252E-71 [3]
	1194	Solution	FToxid	FToxid-SLAGA#			1.000	1.000	1.000
	1247	All Elements		GAS					
+	1251	All Elements	FToxid	FToxid-SLAGA#					
+	1251	All Elements	FToxid	FToxid-SLAGA#					

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

Select All Clear OK

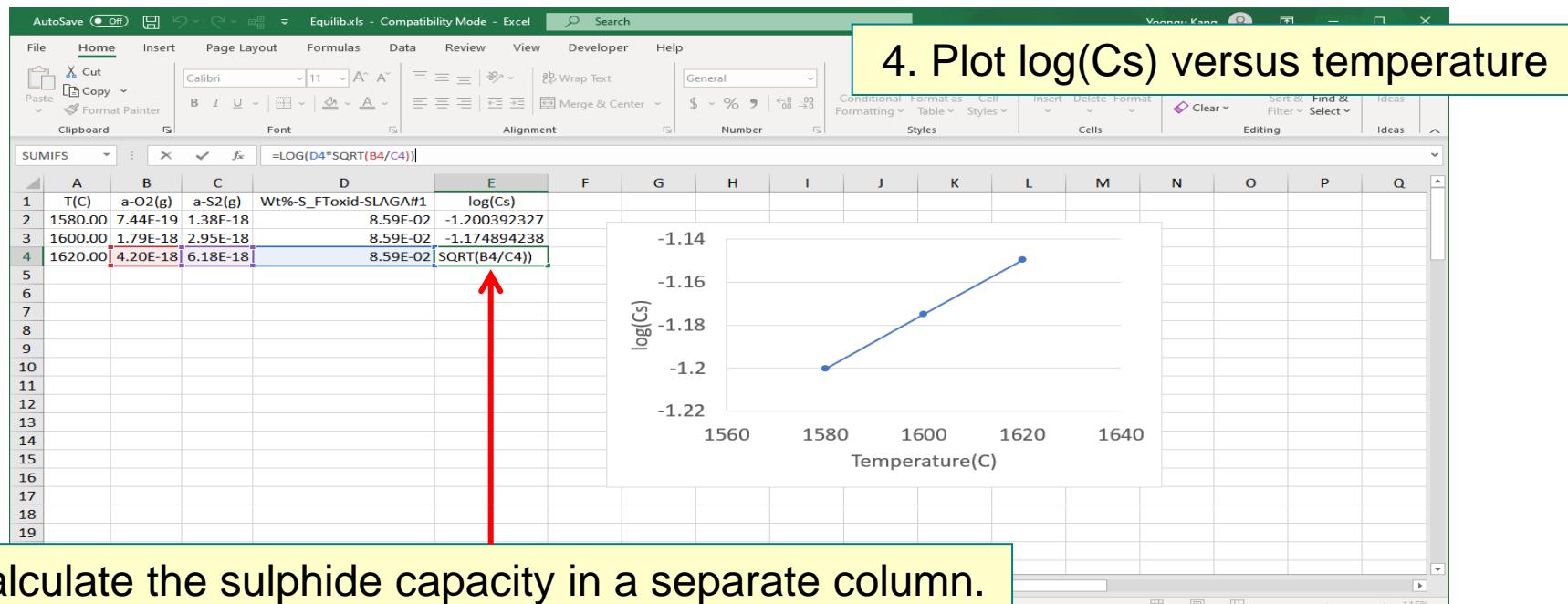
2. Press “OK” on all three screens

Calculating Slag Sulphide Capacity

1. All the needed results (and even more) appear in the spreadsheet.

T(C)	Wt%O2(g)	Wt%S2(g)	a-O2(g)	a-S2(g)	Wt%Fe_FToxic-SLAGA#1	Wt%Mn_FToxic-SLAGA#1	Wt%Ti_FToxic-SLAGA#1	Wt%Ca_FToxic-SLAGA#1	Wt%S_FToxic-SLAGA#1
1.580000E+03	5.1637146E-17	1.9231229E-16	7.4406462E-19	1.3826999E-18	1.4663848E+01	5.8864892E-01	7.3577311E-01	3.8585457E+01	8.5934254E-02
1.600000E+03	1.2396872E-16	4.1051196E-16	1.7854731E-18	2.9501184E-18	1.4653391E+01	6.0921013E-01	7.3574367E-01	3.8582714E+01	8.5930795E-02
1.620000E+03	2.9188401E-16	8.6085431E-16	4.2018929E-18	6.1835344E-18	1.4642836E+01	6.2987870E-01	7.3571473E-01	3.8579942E+01	8.5927386E-02

2. Copy the results in Excel and delete the unnecessary columns



3. Calculate the sulphide capacity in a separate column.

Calculating Slag Sulphide Capacity

Another way to plot the sulphide capacity is to use the function builder tool coupled with Fact-XML

The screenshot shows the FactSage 8.0 software interface. The main window title is "Equilib - Results 1580 C (page 1/3)". The menu bar includes "Output", "Edit", "Show Pages", and "Final Conditions". A context menu is open over a list of chemical species and their properties. The "Fact-Function-Builder" option is highlighted in blue. A red arrow points from a callout box to the "Edit/create functions ..." option in the expanded "Fact-Function-Builder" submenu. The submenu also contains "Select function group(s)", "Always calculate function groups(s) - (nothing selected)", "Refresh Results ...", "Edit function group", "Rename function group", "Delete function group", and "Summary of function groups ...". At the bottom of the software window, there is a "Final Conditions" table with columns for T(C), P(atm), Product H(J), and a "Calculate >>" button.

1. Press “Edit/Create functions” under the Fact-Function-Builder Menu

Output Edit Show Pages Final Conditions

Save or Print As ... Repeat Open Spreadsheet Plot Equilib Results file Stream File Format Fact-XML Fact-Optimal Fact-Function-Builder Refresh ... Swap loops ...

+ 2.9676E-05
+ 1.7819E-05
+ 1.0388E-05
+ 3.8851E-07
+ 8.5797E-08
+ 5.5088E-08
+ 8.0970E-09
+ 2.0679E-09
+ 1.1225E-09

Final Conditions

<A>		T(C)	P(atm)	Product H(J)	3 calculations
		1580	1620	20	1

Calculate >>

Calculating Slag Sulphide Capacity

1. We need to select wt%S as one variable

2. Select “Amount/Composition” under “Variable selection”

4. Right-click on S(total) in slag and add it to variables list

The screenshot shows the FactSage Function Builder window. The 'Variables List' on the left contains letters A through J. The 'Functions' section has a text input f1= and a preview button. The 'Variable selection' dropdown is set to 'Amount/Composition'. A red arrow points from the text '2. Select “Amount/Composition” under “Variable selection”' to this dropdown. In the 'Species/phases' table, the row for 'S (total)' in 'Slag-liq#1' is selected, highlighted with a blue border. A context menu is open over this row, with the option 'Add to variables list' highlighted. A red arrow points from the text '4. Right-click on S(total) in slag and add it to variables list' to this menu item. At the bottom of the table, there are radio buttons for selecting units: mol, mol fract., gram, Wt. fract., Wt. %, kg, and lb. A red arrow points from the text '3. Select “wt%”' to the 'Wt. %' radio button, which is currently selected.

	Species	Phase	Data	Amount/Co...	MIN	MAX	Pseudonym
Mn (total)	Slag-liq#1		5.886E-01	1.949E-09	1.466E+01		
Ti (total)	Slag-liq#1		7.358E-01	1.949E-09	1.466E+01		
Ca (total)	Slag-liq#1		3.859E+01	1.949E-09	3.859E+01		
S (total)	Slag-liq#1		3E-02	1.949E-09	3.859E+01		
P (total)	Slag-liq#1		7E-07	1.949E-09	3.859E+01		
Si (total)	Slag-liq#1		7.460E+00	1.949E-09	3.859E+01		
Al (total)	Slag-liq#1		1.170E+00	1.949E-09	3.859E+01		
Mg (total)	Slag-liq#1		4.253E+00	1.949E-09	3.859E+01		
O (total)	Slag-liq#1		3.246E+01	1.949E-09	3.859E+01		
Al2O3	Slag-liq#2	FToxid	0.000E+00	0.000E+00	0.000E+00		
SiO2	Slag-liq#2	FToxid	0.000E+00	0.000E+00	0.000E+00		
CaO	Slag-liq#2	FToxid	0.000E+00	0.000E+00	0.000E+00		

3. Select “wt%”

Calculating Slag Sulphide Capacity

1. The amount of S now appears in the variables list.

2. Right-click on the variable and rename it to “wtS”

3. Partial pressure and activity of a gas is the same thing, so we need to select activity of O₂ and S₂ in the gas as the two other variables.

The screenshot shows the FactSage Function Builder interface. In the top left, there's a 'Variables List' window with items A through J. Item A is selected and has a context menu open with options: Delete, Rename, Ask for value (once), Ask for value (every page), Set as constant, and Use value from one page only. A red arrow points from the 'Rename' option to a 'Name' dialog box. This dialog box has a text input field containing 'wtS' and two buttons: 'OK' and 'Cancel'. A red arrow also points from the 'OK' button to the 'wtS' input field. Below these windows is a large table titled 'Species/phases:' with columns for Species, Phase, Data, Amount/Co..., MIN, MAX, and Pseudonym. The table lists various elements and compounds: Mn (total), Ti (total), Ca (total), S (total), P (total), Si (total), Al (total), Mg (total), O (total), Al2O3, SiO2, and C. The row for S (total) is highlighted with a blue background. At the bottom of the table, there are radio buttons for selecting units: mol, mol fract., gram, Wt. fract., Wt. %, kg, and lb. A 'Close' button is located at the bottom right of the main window.

Species	Phase	Data	Amount/Co...	MIN	MAX	Pseudonym
Mn (total)	Slag-liq#1	5.886E-01	1.949E-09	1.466E+01		
Ti (total)	Slag-liq#1	7.358E-01	1.949E-09	1.466E+01		
Ca (total)	Slag-liq#1	3.859E+01	1.949E-09	3.859E+01		
S (total)	Slag-liq#1	8.593E-02	1.949E-09	3.859E+01		
P (total)	Slag-liq#1	5.257E-07	1.949E-09	3.859E+01		
Si (total)	Slag-liq#1	7.460E+00	1.949E-09	3.859E+01		
Al (total)	Slag-liq#1	1.170E+00	1.949E-09	3.859E+01		
Mg (total)	Slag-liq#1	4.253E+00	1.949E-09	3.859E+01		
O (total)	Slag-liq#1	3.246E+01	1.949E-09	3.859E+01		
Al2O3	FToxid	0.000E+00	0.000E+00	0.000E+00		
SiO2	FToxid	0.000E+00	0.000E+00	0.000E+00		
C	FToxid	0.000E+00	0.000E+00	0.000E+00		

Calculating Slag Sulphide Capacity

Function Builder

File Help

Variables List

wtS : Amount/Composition (S (total))/Slag-liq#1) wt.%
aO2 : Activity (O2/Gas)
aS2 : Activity (S2/Gas)
G
I
J
K
L

Functions

f1 = Preview results

Operations: * + - / () ^ abs, ln, log, exp, cos, sin, tg, arcsin, arccos, arctg or arctan, sgn or sign, sqrt

Variable selection

Activity

Selection

Species/phases:

	Species	Phase	Data	Activity	MIN	MAX	Pseudonym
1	P0	Gas	FactPS	3.885E-07	3.885E-07	8.105E-07	
2	P02	Gas	FactPS	9.513E-12	9.513E-12	3.172E-11	
3	P205	Gas	FactPS	8.362E-30	8.362E-30	1.165E-28	
4	(P203)2	Gas	FactPS	1.289E-22	1.289E-22	8.148E-22	
5	(P205)2	Gas	FactPS	1.468E-57	1.468E-57	1.185E-55	
6	S	Gas	FactPS	1.349E-12	1.349E-12	3.846E-12	
7	S2	Gas	FactPS	1.383E-18	1.383E-18	6.184E-18	
8	S3	Gas	FactPS	8.034E-30	8.034E-30	7.101E-29	
9	S4	Gas	FactPS	1.389E-40	1.389E-40	2.419E-39	
10	S5	Gas	FactPS	2.053E-52	2.053E-52	6.661E-51	
11	S6	Gas	FactPS	1.358E-62	1.358E-62	8.544E-61	
12	S7	Gas	FactPS	0.7045E-72	0.7045E-72	0.5055E-71	

mol mol fract. gram Wt. fract. Wt. % kg lb

Close

3. Rename the variables to aO2 and aS2 accordingly

1. Select "Activity" under "Variable Selection"

2. Right-click on the O2 and S2 and add them to the variable list

Calculating Slag Sulphide Capacity

1. Enter the function for $\log(C_s)$

Functions

$f1 = \log(wtS * \sqrt{aO2/aS2})$

Operations: * + - / () ^ abs, ln, log, exp, cos, sin, tg, arcsin, arccos, arctg or arctan, sgn or sign, sq

Variable selection

Activity

Selection

Species/phases:

	Species	Phase	Data	Activity	MIN	MAX	Pseudonym
PO	Gas	FactPS	3.885E-07	3.885E-07	8.105E-07		
PO2	Gas	FactPS	9.513E-12	9.513E-12	3.172E-11		
P2O5	Gas	FactPS	8.362E-30	8.362E-30	1.165E-28		
(P2O3)2	Gas	FactPS	1.289E-22	1.289E-22	8.148E-22		
(P2O5)2	Gas	FactPS	1.468E-57	1.468E-57	1.185E-55		
S	Gas	FactPS	1.349E-12	1.349E-12	3.846E-12		
S2	Gas	FactPS	1.383E-18	1.383E-18	6.184E-18		
S3	Gas	FactPS	8.034E-30	8.034E-30	7.101E-29		
S4	Gas	FactPS	1.389E-40	1.389E-40	2.419E-39		
S5	Gas	FactPS	2.053E-52	2.053E-52	6.661E-51		
S6	Gas	FactPS	1.358E-62	1.358E-62	8.544E-61		
S7	Gas	FactPS	0.704E-72	0.704E-72	0.505E-71		

Close

3. Note that the results are the same as for the Excel calculation

Calculating Slag Sulphide Capacity

1. Save the function as "Sulphide_Capacity"

The screenshot shows the FactSage Function Builder interface. A red arrow points from the text "1. Save the function as 'Sulphide_Capacity'" to the "Name" input field in a modal dialog. Another red arrow points from the "OK" button in the same dialog to the "File" menu where the function is being saved. The "File" menu has a dropdown option "Save current functions group" which is highlighted. The "Preview results" window on the right shows the calculated values for the function $f1 = \log(wtS * \sqrt{aO2/aS2})$ across three pages.

Function Builder

File Help

Save current functions group

Open > (g-liqu#1) wt.%

Rename >

Delete >

clear

Preview results Copy to clipboard

Name

Please enter a name for this system :

Sulphide_Capacity

OK Cancel

Selection

Species/phases:

	Species	Phase	Data	Activity	MIN	MAX	Pseudonym
1	PO	Gas	FactPS	3.885E-07	3.885E-07	8.105E-07	
2	PO2	Gas	FactPS	9.513E-12	9.513E-12	3.172E-11	
3	P2O5	Gas	FactPS	8.362E-30	8.362E-30	1.165E-28	
4	(P2O3)2	Gas	FactPS	1.289E-22	1.289E-22	8.148E-22	
5	(P2O5)2	Gas	FactPS	1.468E-57	1.468E-57	1.185E-55	
6	S	Gas	FactPS	1.349E-12	1.349E-12	3.846E-12	
7	S2	Gas	FactPS	1.383E-18	1.383E-18	6.184E-18	
8	S3	Gas	FactPS	8.034E-30	8.034E-30	7.101E-29	
9	S4	Gas	FactPS	1.389E-40	1.389E-40	2.419E-39	
10	S5	Gas	FactPS	2.053E-52	2.053E-52	6.661E-51	
11	S6	Gas	FactPS	1.358E-62	1.358E-62	8.544E-61	
12	S7	Gas	FactPS	0.7045E-72	0.7045E-72	0.5055E-71	

Close

2. Close the window

Calculating Slag Sulphide Capacity

The screenshot shows the FactSage software interface. On the left, the 'Fact-Function-Builder' menu is open under the 'Output' tab. A red arrow points from the text '2. Check "Always calculate function groups"' to the 'Always calculate function groups(s) [3.]' option in the dropdown menu. Another red arrow points from the text '3. Click "Refresh Results ..."' to the 'Refresh Results ...' button. A yellow box highlights the 'Sulphide_Capacity' function group in the list. On the right, the 'Final Conditions' window is visible, showing temperature (T(C)) set to 1580, 1620, 20, and pressure (P(atm)) set to 1.

1. Go back to the “Results” window, and select the “Sulphide_Capacity” function group

2. Check “Always calculate function groups”

3. Click “Refresh Results ...”

Calculating Slag Sulphide Capacity

1. A separate “Functions” tab will appear with the results of the calculations

F Equilib - Results Functions

Output Edit Show Pages Final Conditions

Functions | 1580 C | 1600 C | 1620 C |

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

Group Name : 3. Sulphide_Capacity
wtS : Amount/Composition (S (total)/Slag-liq#1)) wt.%
aO2 : Activity (O2/Gas)
aS2 : Activity (S2/Gas)

Page f1 = log(wtS*SQRT(aO2/aS2))

1 -1.200392
2 -1.174894
3 -1.149764

2. Each tab will have the information on the function along with the calculated equilibrium.

F Equilib - Results 1580 C (page 1/2)

Output Edit Show Pages Final Conditions

Functions | 1580 C | 1600 C | 1620 C |

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

Group Name : 3. Sulphide_Capacity
wtS : 0.8593426E-01 : Amount/Composition (S (total)/Slag-liq#1)) wt.%
aO2 : 0.7440646E-18 : Activity (O2/Gas)
aS2 : 0.1382700E-17 : Activity (S2/Gas)

Page f1 = log(wt...
1 -1.200392

(gram) 44 CaO + 9 MgO + 13 SiO2 + 1.8 Al2O3 + FactSage 8.0
(gram) 18 Fe + 4.5 MnO + 0.07 S + 2 P2O5 +
(gram) TiO2 =
0.25836 mol gas_ideal
(11.912 gram, 0.25836 mol, 39.287 litre, 3.0322E-04 gram.cm-3)

Calculating Slag Sulphide Capacity

1. In order to plot the sulphide capacity as a function of temperature, press the XML button

Equilib - Results Functions

Output Edit Show Pages Final Conditions

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

Functions 1580 C | 1600 C | 1620 C

Group wtS
aO2
aS2

File Units Tools Graph Help

XML Viewer - [C:\WORKSHOP80\Xml_out.xml]

Graph Setup...

Fact Format ItemMessage Format Tree

Page 1 1580 C
2 1600 C
3 1620 C

Page 1 2 3

Page 1 2 3

Page 1 2 3

Graph - Setup

Saved graphs... Function Builder

Variables

wtS : Amount/Col
aO2 : Activity (O₂)
aS2 : Activity (S₂/Gas)
G
I
J

Import

1 - Fe-N_Sievert
2 - SiO₂-MnO₂-S_capacity
3 - Sulphide_Capacity

Figure Settings
Font size : 10

Y-Axis

Functions ▾ Y + variable

f1 = log(wtS*sqrt(aO2/aS2))

MIN MAX STEP Label every

-1.21 -1.13 0.01 0.0079999

Temperature ▾ X + variable

f =

MIN MAX STEP Label every

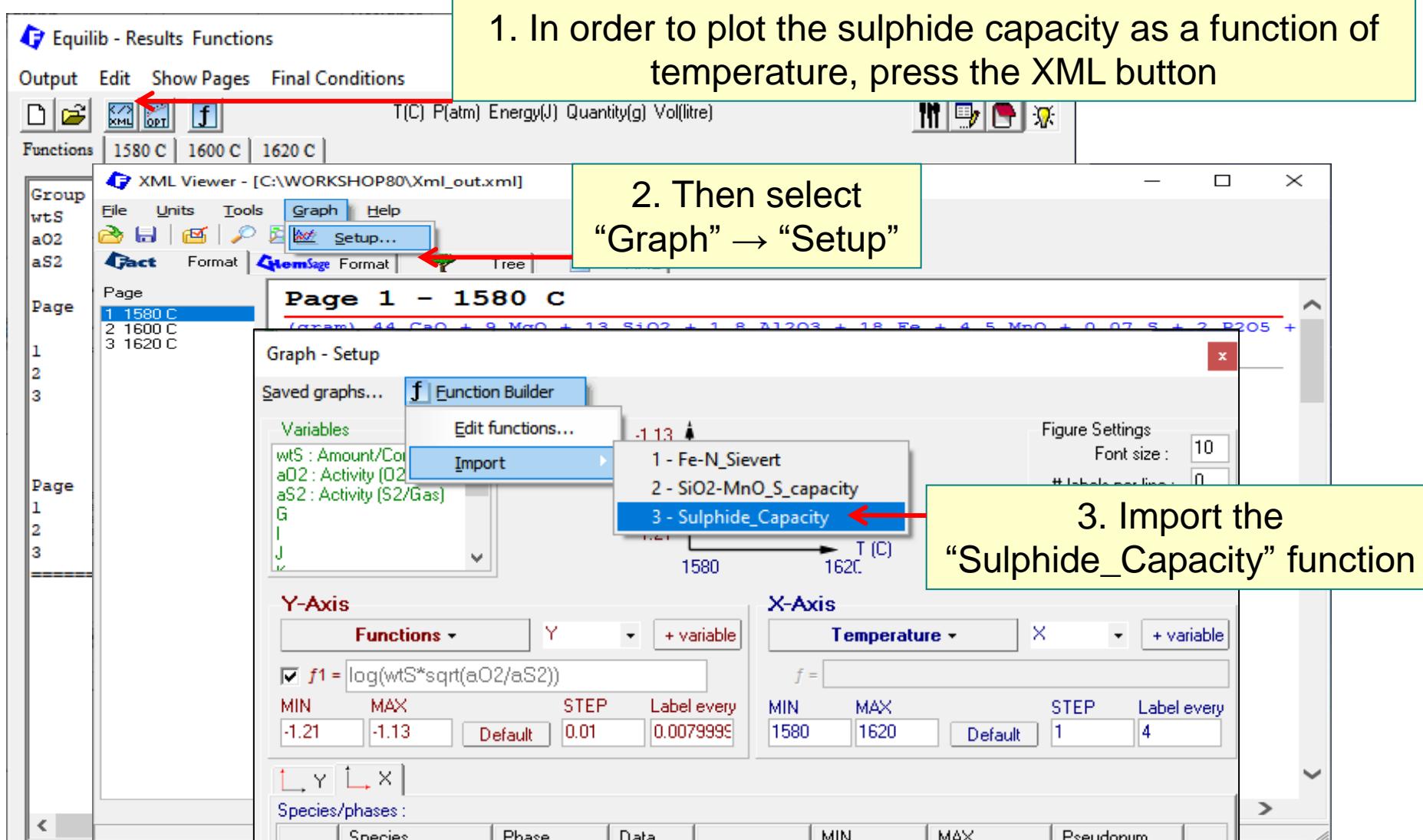
1580 1620 1 4

Species/phases :

Snecies Phase Data MIN MAX Pseudonum

2. Then select “Graph” → “Setup”

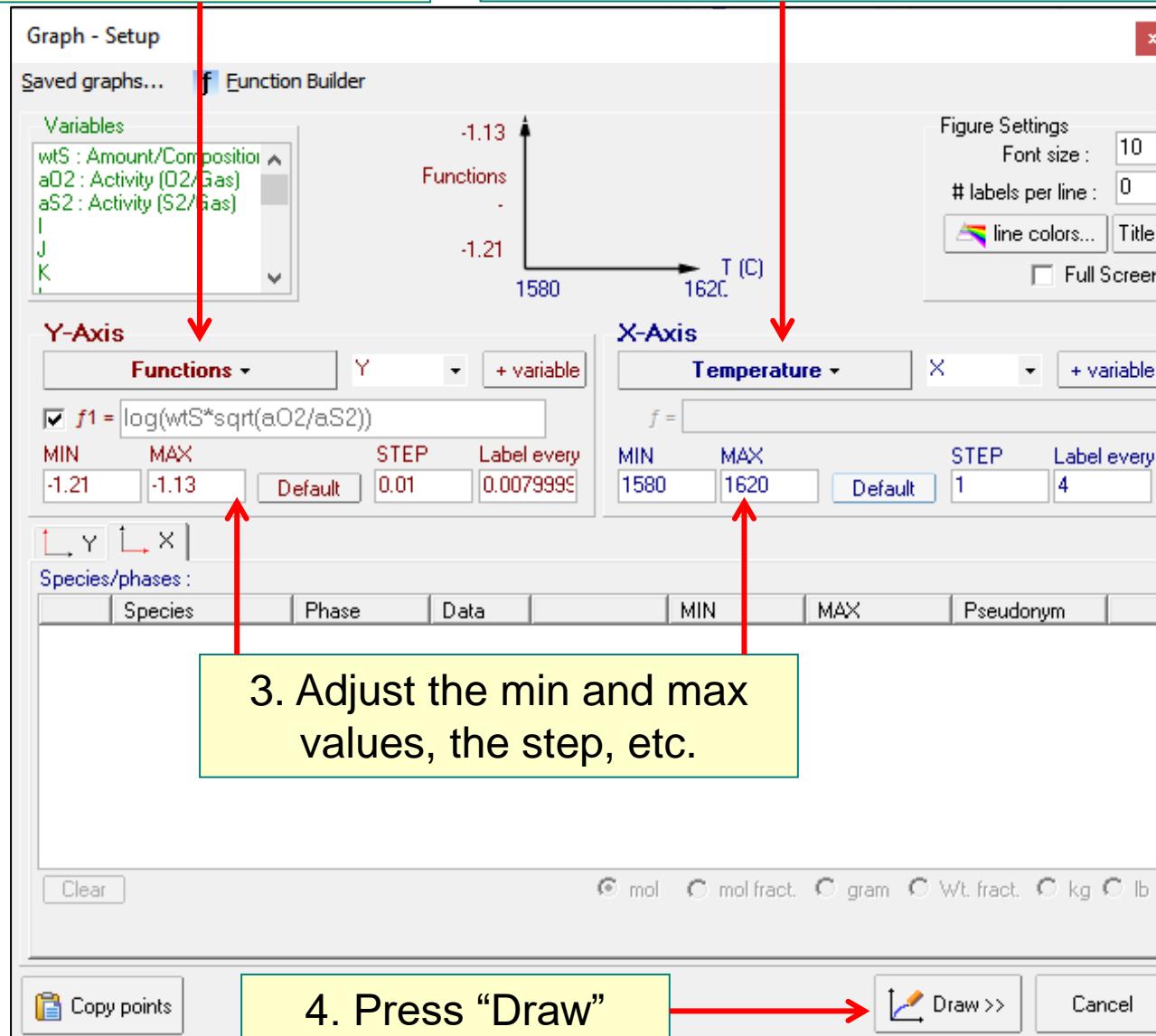
3. Import the “Sulphide_Capacity” function



Calculating Slag Sulphide Capacity

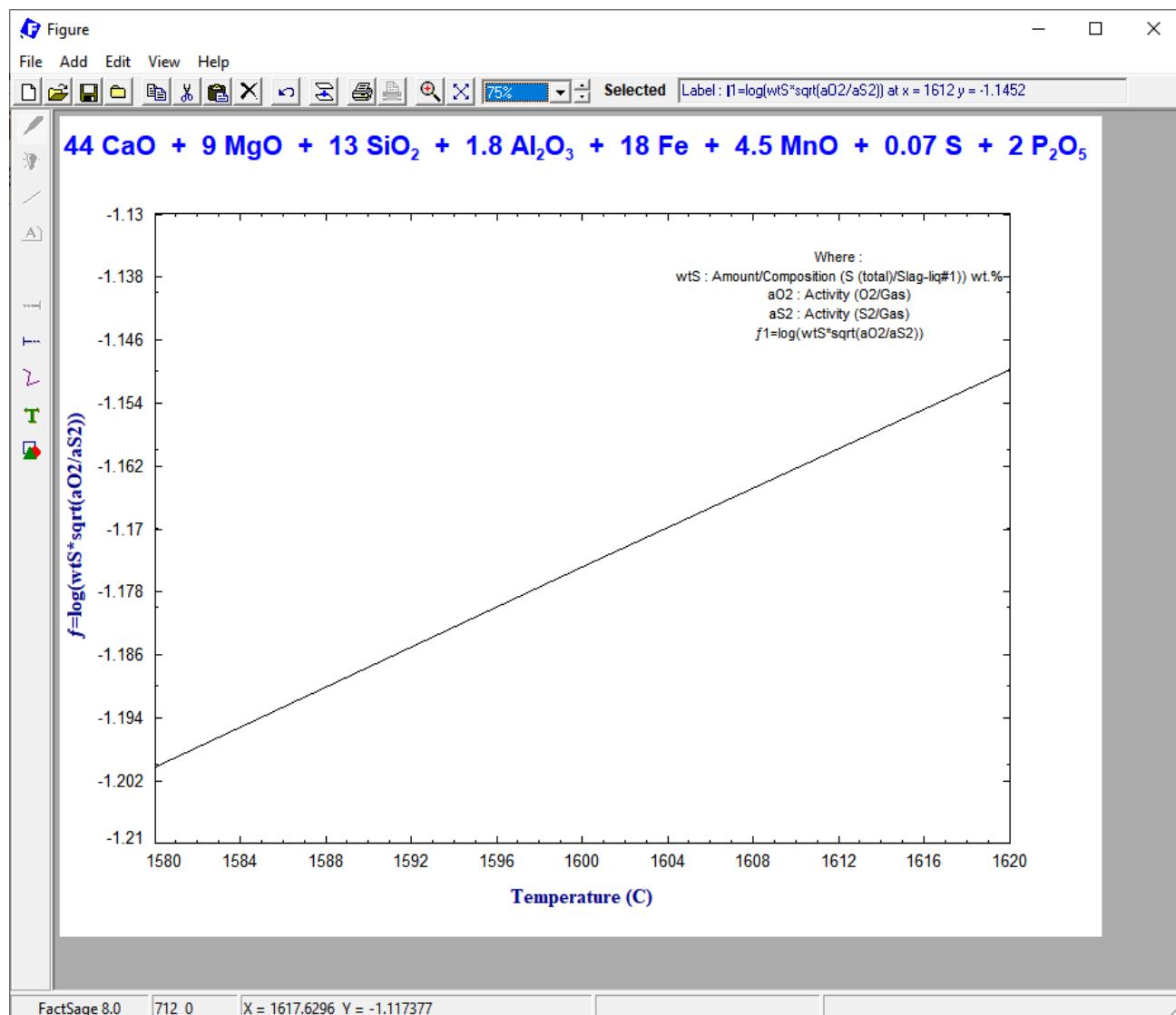
1. Select “Functions” as the Y-Axis

2. Select “Temperature” as the X-axis



Calculating Slag Sulphide Capacity

The figure is then obtained



Slag cooling and heating (Enthalpy diagram)

- When slag forms from pure oxides, a certain amount of heat (enthalpy) is needed.
- When slag is cooled down, a certain amount of heat should be extracted.
- FactSage Phase diagram: [Enthalpy diagram](#)

Heat required to form and increase temperature of slag

ΔH = H_{final} – H_{initial}
So initial conditions(phase,T,P) should be defined

FactSage™ SGTE

Databases - 2/23 compound databases, 1/23 solution databases

FactPS FToxid FSopp FSlead FSstel FSupsig SGPS SGTE SGsold

FTsalt FTmisc FTall FTOxCN FTfritz FThelg FTpulp FTlite

ELEM SGnobl SpMCBN TDmeph TDnucl

Other

Add/Remove Data RefreshDatabases

Clear All

ilib - Reactants

File Table Units Data Search Data Evaluation Help

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

Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
<A>	MgO	solid-FactPS Periclase	25	1.0	1	FactPS
+ <1-A-B>	FeO	solid-FactPS Wustite	25	1.0	1	FactPS
+ 	SiO ₂	solid-1-FactPS Quartz	25	1.0	1	FactPS

FactSage can used two variables, <A> and
<A> can be really varied and should be constant

Initial condition

Pure FeO(s) is not in FToxid compound database
(Strictly speaking, FeO is non-stoichiometric compound so it is in MeO solution)

The hydrostatic pressure above the phase.
aqueous stream this is the sum of the
pressures of the species in that stream.

Initial Conditions

Next >>

FactSage 8.0 Compound: 2/23 databases Solution: 1/23 databases

Heat required to form slag and increase the temperature of slag

Equilib - Menu:

File Units Parameters Help

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

Reactants (3)

(gram) <A> MgO	+ <1-A-B> FeO	+ SiO ₂
(25C,s-FactPS,#1)	(25C,s-FactPS,#1)	(25C,s1-FactPS,#1)

Products

Compound species

gas	ideal real	0
aqueous	0	0
pure liquids	0	0
* pure solids	37	37

* - custom selection species: 37

Solution phases

*	+	Base-Phase	Full Name
	+	FToxid-SLAGA	A-Slag-liq all oxides + S
	+	FToxid-SPINA	A-Spinel
	+	FToxid-MeO_A	A-Monoxide
		FToxid-cPyrA	A-Clinopyroxene
		FToxid-oPyrA	A-Orthopyroxene
		FToxid-pPyrA	A-Protopyroxene
	+	FToxid-OlivA	A-Olivine

Custom Solutions

- 0 fixed activities
- 0 ideal solutions

Target

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

Legend

- I - immiscible 1
- + - selected 3

Show all selected

species: 27 solutions: 5

Final Conditions

<A>		T(C)	P(atm)	Delta H(J)
0 0.5 0.	0.3	1600	1	

10 steps

Final condition

Equilib - Results A=0 (page 1/2)

Output Edit Show Pages Final Conditions

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

A=0 | A=0.5

$\Delta H = H_{\text{final}} - H_{\text{initial}}$

This is the heat we add to increase the temperature up to 1600°C.

That is, $\Delta H = H_{\text{slag at } 1600^\circ\text{C}} - H_{\text{initial oxides at } 25^\circ\text{C}}$

DELTA H (J)

1.02861E+03	-3.03364E+03	0.00000E+00	1.93428E+00	3.31068E-01
-------------	--------------	-------------	-------------	-------------

H (J) G (J) V (litre) S (J/K) Cp (J/K)

-5.30858E+03	-1.04054E+04	0.00000E+00	2.72097E+00	1.03703E+00
--------------	--------------	-------------	-------------	-------------

Slag-liq#1 Fe_bcc Final

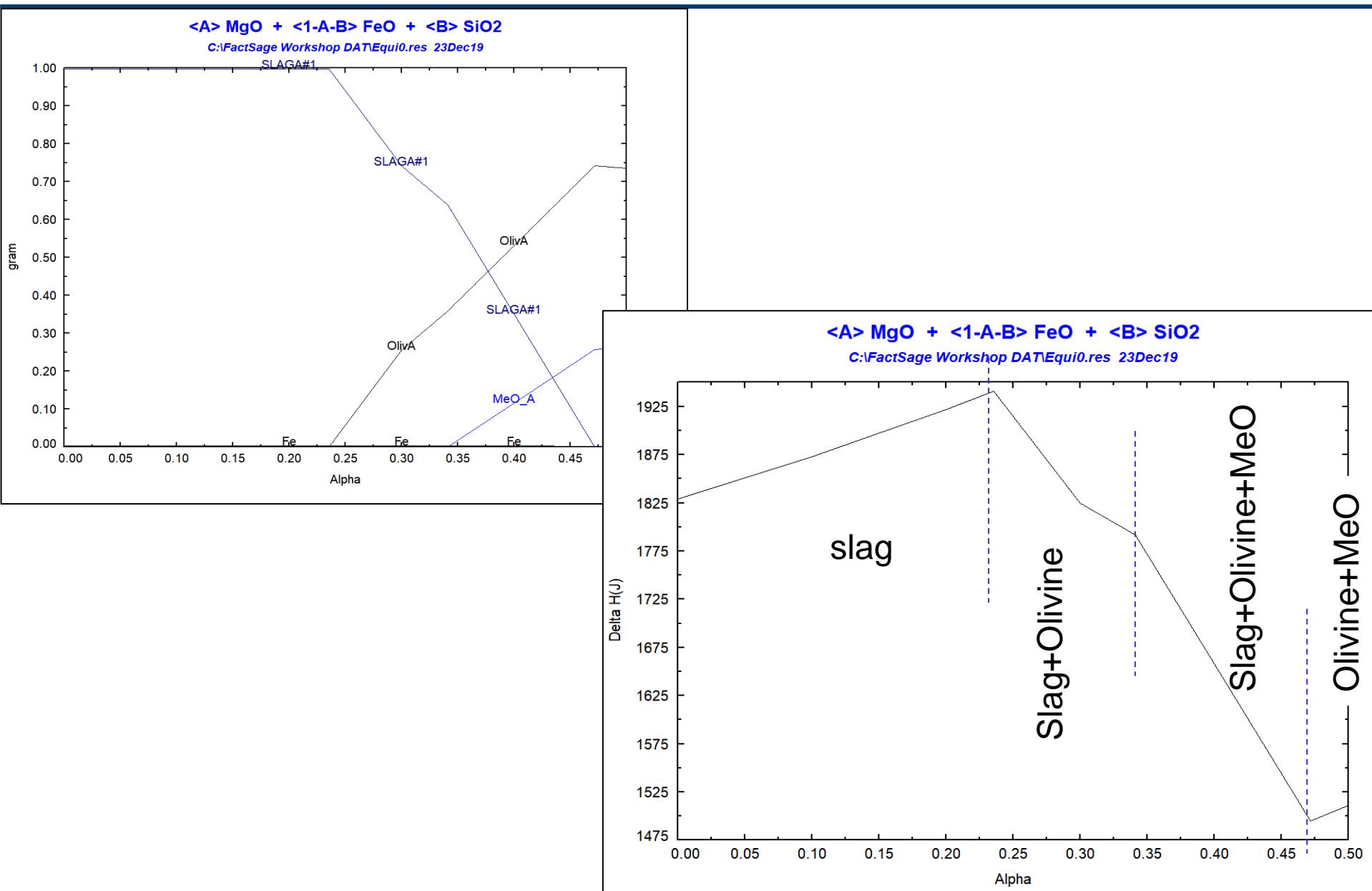
Total ma

0 0.5 0.	0.3	1600	1
----------	-----	------	---

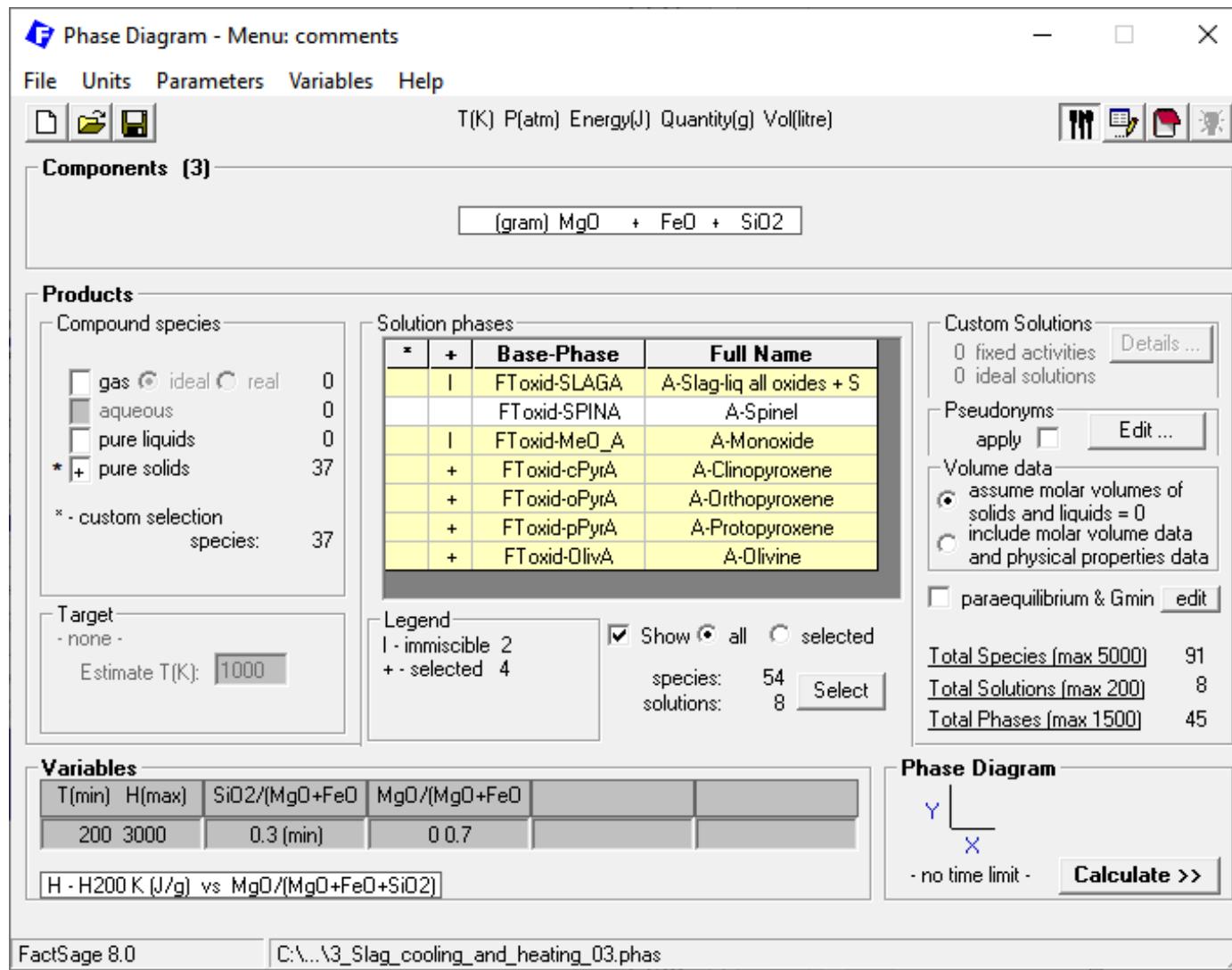
Calculate >>

This is the enthalpy of the final products at 1600°C

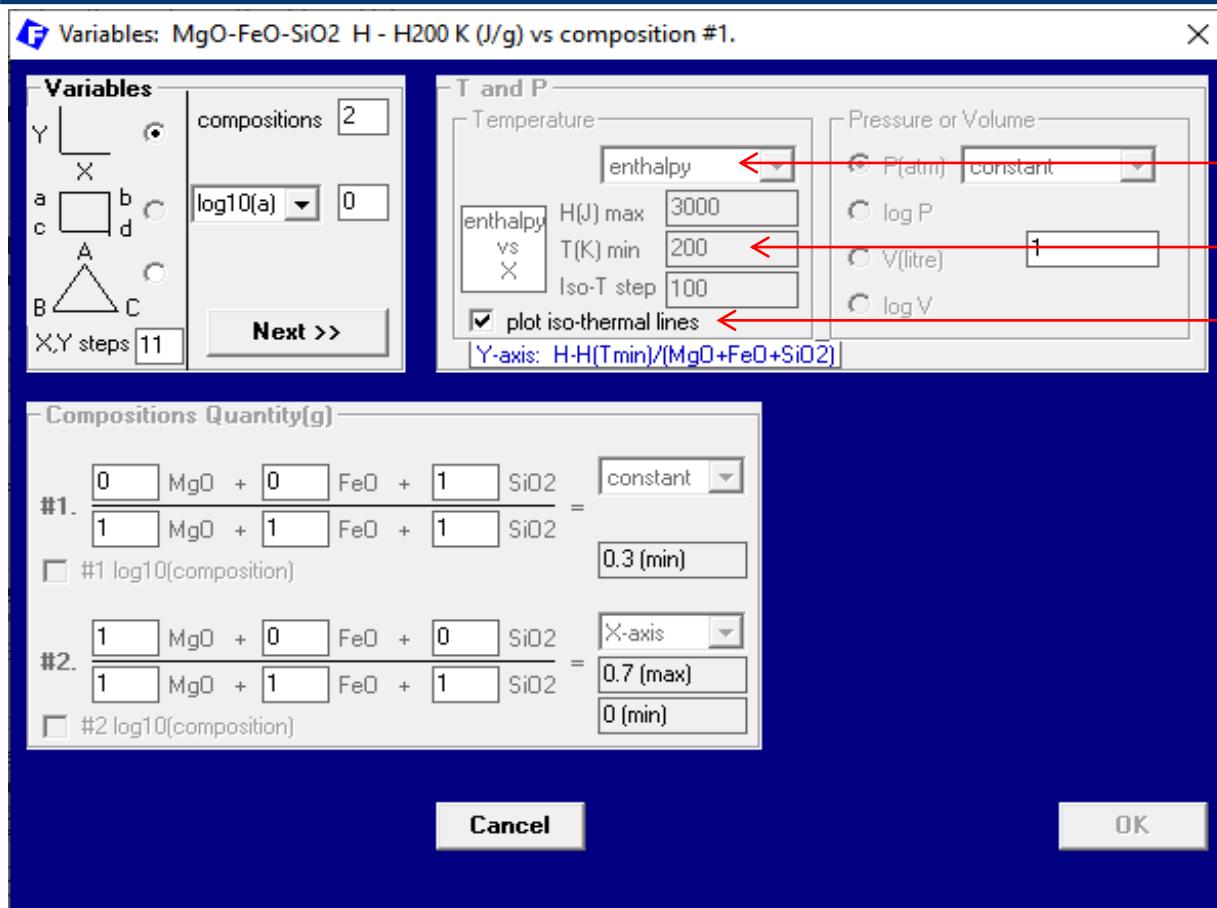
Heat required to form slag and increase the temperature of slag



Enthalpy diagram: phase change with ΔH



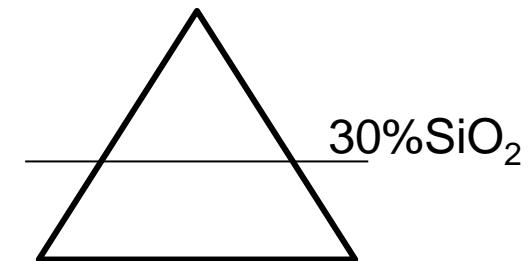
Enthalpy diagram: phase change with ΔH



Enthalpy diagram option

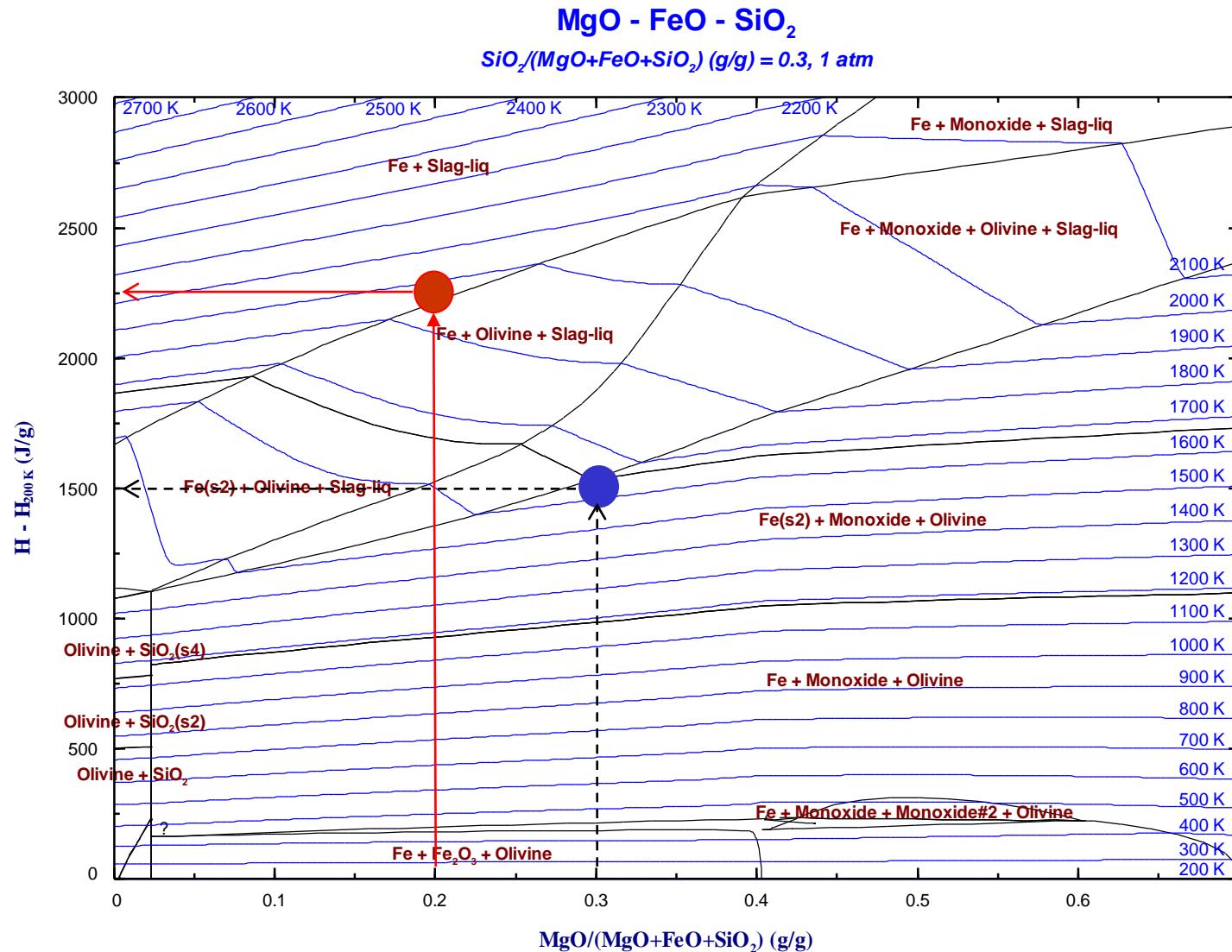
T_{initial}

Iso-Temperature



- Only X-Y type diagram allowed.
- Y axis should be Enthalpy (H-H_{Tmin}).
- H_{initial} (H_{Tmin}) is the enthalpy of products stable at T_{min}. For example, Fe₂SiO₄ (fayalite_olivine) and SiO₂ are stable at 0% MgO and 30% SiO₂ instead of FeO and SiO₂.

Enthalpy diagram: phase change with ΔH

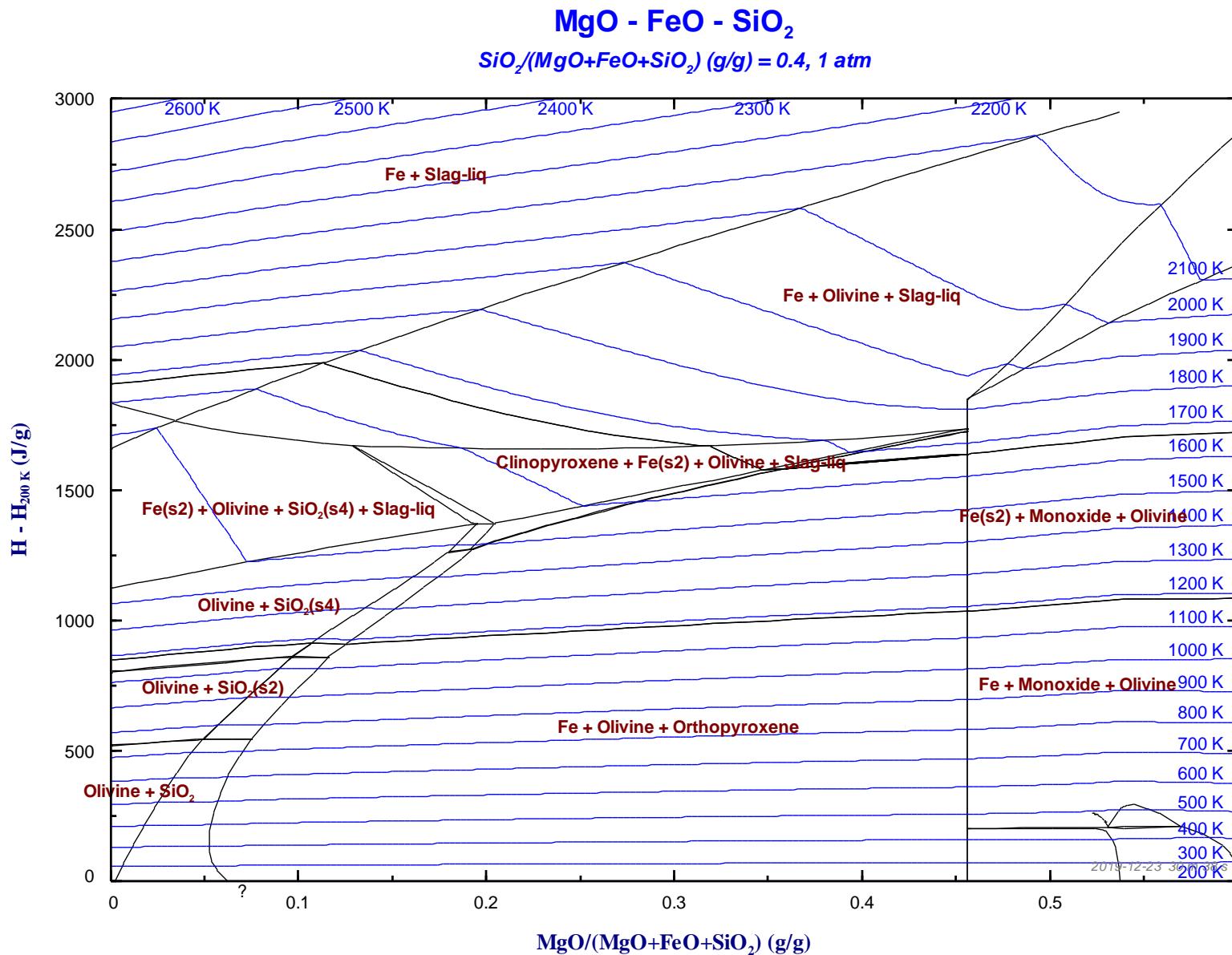


If we heat the mixture of (Monoxide + olivine) at 30 wt % MgO and 30 wt % SiO₂ from 25 °C by 1500 J/g, the mixture becomes mixture of (liquid slag + olivine) at about 1425 °C.



- If we increase the temperature of the mixture of (Monoxide + olivine) at 20 wt % MgO and 30 wt % SiO₂ from 25 °C to 1625 °C, liquid slag is forming and the amount of heat required for this is about 2250 J/g.

Enthalpy diagram: phase change with ΔH



Application: Addition of new compound and solution (user defined) in calculations

MnCr₂O₄-MnAl₂O₄ ideal solid solution

- New stainless steel production: high Mn stainless steel 400 grade. High MnO formation in AOD / VOD refining process
- MnCr₂O₄-MnAl₂O₄ inclusion formation in Mn and Cr containing steels

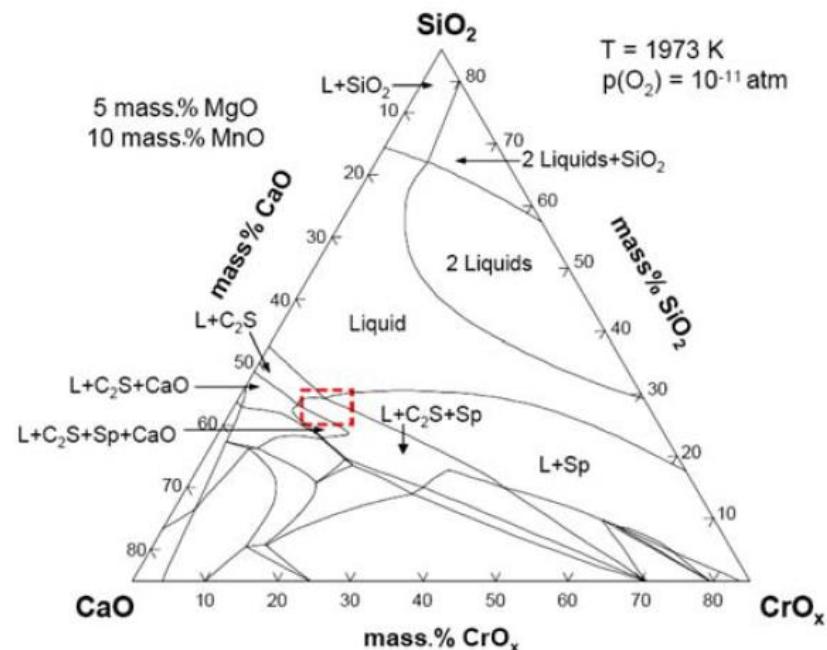
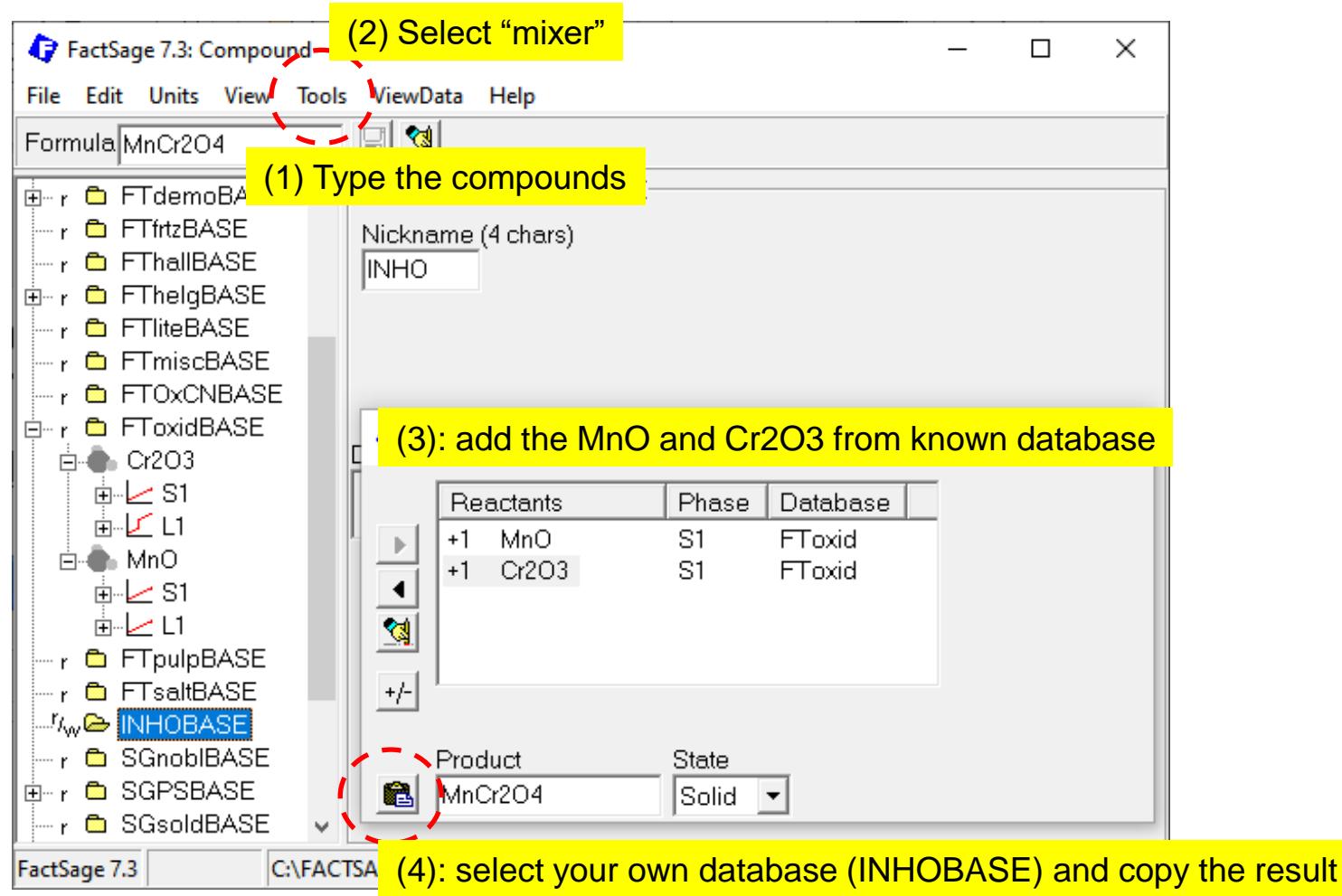


Fig. 1. Computed phase diagram of the CaO-SiO₂-CrO_x-5 mass.%MgO-10 mass.%MnO system at 1973 K under the oxygen partial pressure, $p(O_2) = 10^{-11}$ atm.

User Compound Database

Creating user compound database: MnCr₂O₄ from MnO and Cr₂O₃



User Compound Database

Energy: Joules Pressure: atm MnCr2O4

File Edit Units View Tools ViewData Help

Formula MnCr2O4

S1 properties
 Heat of form. + Entropy

Form. of S1

ΔH_{298} (Joules)	S_{298} (J/(mol K))
-1511177.5333252	147.058391929535

Phase Name Reference no. Density g/cc

5.28404

MnCr2O4 tree view:

- r FTOxCNBASE
- r FToxidBASE
 - Cr2O3
 - S1
 - L1
 - MnO
 - S1
 - L1
- r FTpulpBASE
- r FTsaltBASE
- r INHOBASE
- r/w MnCr2O4
 - S1
 - Cp 298
 - Cp 2115
 - Cp 2500
 - Cp 3000
- r SGnoblBASE
- r SGPSBASE
- r SGsoldBASE

FactSage 7.3 C:\FACTSAGE72\FACTDATA\User\INHO.CDB (v5.0) 1 compounds read/write

Before ΔH^f and ΔS^f

$$G^o(\text{cubic-MnCr}_2\text{O}_4) = G^o(\text{MnO}) + G^o(\text{Cr}_2\text{O}_3) + \Delta H^f - T\Delta S^f$$

$$\Delta H^f = -51 \text{ kJ/mol}, \Delta S = 0 \text{ J/mol-K}$$

Energy: Joules Pressure: atm MnCr2O4

File Edit Units View Tools ViewData Help

Formula MnCr2O4

S1 properties
 Heat of form. + Entropy

Form. of S1

ΔH_{298} (Joules)	S_{298} (J/(mol K))
-1560021.23212144	155.865854066175

Phase Name Reference no. Density g/cc

5.28404

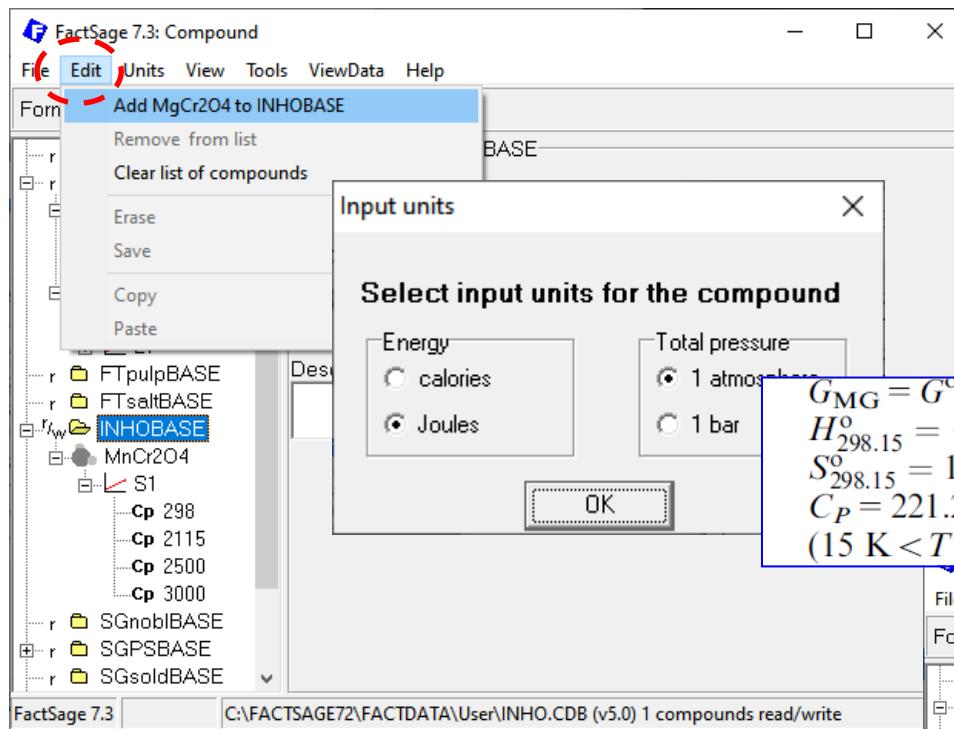
MnCr2O4 tree view:

- r FTOxCNBASE
- r FToxidBASE
 - Cr2O3
 - S1
 - L1
 - MnO
 - S1
 - L1
- r FTpulpBASE
- r FTsaltBASE
- r INHOBASE
- r/w MnCr2O4
 - S1
 - Cp 298
 - Cp 2115
 - Cp 2500
 - Cp 3000
- r SGnoblBASE
- r SGPSBASE
- r SGsoldBASE

FactSage 7.3 Modified C:\FACTSAGE72\FACTDATA\User\INHO.CDB (v5.0) 1 compounds read/write

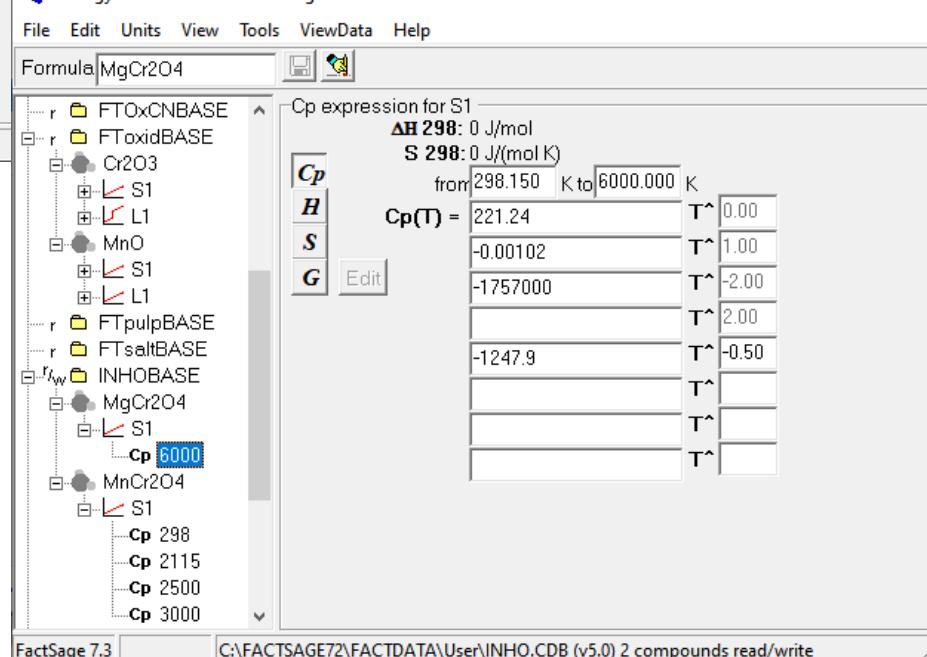
after ΔH^f and ΔS^f

User Compound Database



Creating user compound database: MgCr₂O₄ from H₂₉₈, S₂₉₈ and Cp

$$G_{\text{MG}} = G^{\circ}(\text{MgCr}_2\text{O}_4)^{+}: \\ H_{298.15}^{\circ} = -1769907.76 \\ S_{298.15}^{\circ} = 118.300 \\ C_P = 221.24 - 0.001020T - 1.757(10^6)T^{-2} - 1247.9T^{-0.5} \\ (15 \text{ K} < T < 3000 \text{ K})$$



Add ΔH_{298} , S_{298} and C_p , respectively →

Ideal Solution between compounds

Selection - Phase Diagram - no results -

File Edit Show Sort

Selected: 84/131 SOLID Duplicates selected X denotes species excluded by default

- no results -

	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
+	150	(Ca ₂ Cr ₃)Cr ₁₀₀ O ₂₀ (s)	FToxid	solid	o				
+	151	(CaCr)Si ₄ O ₁₀ (s)	FToxid	solid	o				
+	152	Ca ₃ Cr ₂ Si ₃ O ₁₂ (s)	FToxid	Uvarovite	V				
+	153	MnO(s)	FToxid	solid	V				
+	154	MnO ₂ (s)	FToxid	Pyrolusite	V				
+	155	Mn ₂ O ₃ (s)	FToxid	Bixbyite-LT(orthc)	V				
+	156	Mn ₂ O ₃ (s2)	FToxid	Bixbyite-HT(cubi)	o				
+	157	Mg ₆ Mn ₈ O ₈ (s)	FToxid	solid	V				
+	158	MnSiO ₃ (s)	FToxid	Rhodonite	V				
+	159	Mn ₂ SiO ₄ (s)	FToxid	Tephrorite	V				
+	160	CaMn ₃ O ₄ (s)	FToxid	solid	V				
+	161	Ca ₂ MnO ₄ (s)	FToxid	solid	V				
+	162	CaMn ₂ O ₄ (s)	FToxid	solid	o				
+	163	Ca ₃ Mn ₂ O ₇ (s)	FToxid	solid	V				
+	164	CaMn ₃ O ₆ (s)	FToxid	solid	o				
+	165	Ca ₂ Mn ₃ O ₈ (s)	FToxid	solid	V				
+	166	Ca ₄ Mn ₃ O ₁₀ (s)	FToxid	Ca ₄ Mn ₃ O ₁₀	V				
+	167	CaMn ₄ O ₉ (s)	FToxid	solid	o				
+	168	LaMn ₇ O ₁₂ (s)	FToxid	solid	o				
+	169 #1	MgCr ₂ O ₄ (s)	INHO	S1	o				
+	170 #1	MnCr ₂ O ₄ (s)	INHO	S1	V				

permit selection of 'X' species Help Suppress Duplicates Edit priority list:

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

MnCr₂O₄-MgCr₂O₄ ideal sol'n: (Mg,Mn)Cr₂O₄

→ Both MnCr₂O₄ and MgCr₂O₄ are selected as ideal solution #1 with 0 activity coefficients

Variables: O₂-CaO-SiO₂-Cr₂O₃-MnO-MgO composition #1. vs composition #1.

Variables

compositions 4

a b c d
 log₁₀(a) 1
 A  Next >

T and P

Temperature T(C) constant 1700

Pressure or Volume P(atm) constant 1
 log P
 V(litre) 1
 log V

Chemical Potentials

#1 log₁₀(p/atm) constant 0.1
 O₂ gas-FactPS -11

Compositions Quantity(g)

#4. 0 CaO + 0 SiO₂ + 0 Cr₂O₃ + 1 MnO + 0 MgO = Constant
 1 CaO + 1 SiO₂ + 1 Cr₂O₃ + 1 MnO + 1 MgO 0.1
 #4 log₁₀(composition)
 Composition # #4 max = 5

Cancel OK

Application: Addition of new component in slag

V₂O₃ into molten slag for V distribution calculations
(Henrian Solution)

New component in slag: Henrian activity coefficient

Equilib - Menu: last system

File Units Parameters Help

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

Reactants (6)

(gram) 0.5 CaO + 0.3 SiO₂ + 0.19 Al₂O₃ + 0.01 V₂O₃ + 0.95 Fe + 0.05 Al

Products

Compound species

gas	ideal	real	0
aqueous			0
pure liquids			0
+ pure solids			48
species:			48

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

Solution phases

*	+	Base-Phase	Full Name
*	+	FTmisc-FelQ	Fel-liquid
I		FToxid-SLAGA	A-Slag-liq all oxides + S
		FToxid-SPINA	A-Spinel
		FToxid-MeO_A	A-Monoxide
		FToxid-pPyA	A-Clinopyroxene
		FToxid-WOLLA	A-Wollastonite
		FToxid-bC2SA	A-a'(Ca,Si,Ba)2SiO4
		FToxid-aC2SA	A-a'(Ca,Si)2SiO4

Custom Solutions

- 0 fixed activities
- 0 ideal solutions

Pseudonyms

- apply
- Edit ...

Volume data

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

paraequilibrium & Gmin

Legend

- I - immiscible 1
- + selected 1

Show all selected

species: 22 Select

solutions: 3

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		1600	1	

10 steps Table

Equilib - Results 1600 C

Output Edit Show Pages Final Conditions

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

FactSage 8.0

(gram) 0.5 CaO + 0.3 SiO₂ + 0.19 Al₂O₃ + 0.01 V₂O₃ + 0.95 Fe + 0.05 Al =

1.0070 gram Slag-liq#1
(1.0070 gram, 1.5414E-02 mol)
+ 0 gram Slag-liq#2
(1600 C, 1 atm, a=1.0000)
(28.169 wt.% Al₂O₃
+ 22.163 wt.% SiO₂
+ 49.654 wt.% CaO
+ 1.4222E-02 wt.% FeO
+ 2.5953E-05 wt.% Fe₂O₃)

Site fraction of sublattice constituents:

Element	Site fraction
Al	0.30577
Si	0.20412
Ca	0.49000
Fe ²⁺	1.0955E-04
Fe ³⁺	1.7987E-07
O	1.0000

System component

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Fe	1.9966E-06	1.1150E-04	4.6554E-05	1.1073E-04
Ca	8.9162E-03	0.35734	0.20789	0.35487
Si	3.7143E-03	0.10432	8.6603E-02	0.10360
Al	5.5638E-03	0.15012	0.12973	0.14908
O	2.4693E-02	0.39507	0.57573	0.39234

+ 0.99304 gram Fe-liquid
(0.99304 gram, 1.8438E-02 mol)
(1600 C, 1 atm, a=1.0000)
(95.654 wt.% Fe
+ 4.3769E-02 wt.% Al
+ 5.4492E-07 wt.% Ca
+ 8.4224E-05 wt.% O
+ 3.6164 wt.% Si
+ 0.68441 wt.% V
+ 2.9689E-04 wt.% Al₂O
+ 3.3267E-04 wt.% Al₂O
+ 3.8423E-05 wt.% SiO
+ 9.1228E-05 wt.% VO
+ 7.2552E-05 wt.% Al₂O
+ 5.4408E-05 wt.% V₂O)

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		1600	1	

Calculate >>

V₂O₃ containing slag // Liquid Fe-Al steel

→ All V go to liquid Fe ??
(because no V oxide in slag yet)

New component in slag: Henrian activity coefficient

Data Search

Databases - 3/27 compound databases, 2/26 solution databases

Fact	FactSage™	SGTE
<input checked="" type="checkbox"/> FacIPS	<input type="checkbox"/> FScoop	<input type="checkbox"/> BINS
<input checked="" type="checkbox"/> FToxid	<input type="checkbox"/> FSlead	<input type="checkbox"/> SIGPS
<input checked="" type="checkbox"/> FTsalt	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGTE
<input checked="" type="checkbox"/> FTmisc	<input type="checkbox"/> FSups	<input type="checkbox"/> SGTEa
<input type="checkbox"/> FTall	<input type="checkbox"/> SGold	<input type="checkbox"/> SGTEb
<input type="checkbox"/> FTOxCN	<input type="checkbox"/> ELEM	<input type="checkbox"/> Other
<input type="checkbox"/> FTInz	<input type="checkbox"/> SGmobi	<input type="checkbox"/> Add/Remove Data
<input type="checkbox"/> FTulg	<input type="checkbox"/> SpMCBN	<input type="checkbox"/> RefreshDatabases
<input type="checkbox"/> FTite	<input type="checkbox"/> TDneph	<input type="checkbox"/> TDnucl
<input type="checkbox"/> FTnucl	<input type="checkbox"/> TDnucl	

Information

Equilib - Menu: last system

File Units Parameters Help

Reactants [6]

(gram) 0.5 CaO + 0.3 SiO₂ + 0.19 Al₂O₃ 0.01 V₂O₃

Products

Compound species

- gas ideal real 0
- aqueous pure liquids pure solids 80
- * - custom selection species: 81

Target

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

Solution phases

*	+	Base-Phase	Full Name
*	+	FTmisc-FeLQ	Fe-liq
#1	I	FToxid-SLAGA	A-Slag-liq all oxides + S
		FToxid-SPINA	A-Spinel
		FToxid-MeO_A	A-Monoxide
		FToxid-cPyrA	A-Clinopyroxene
		FToxid-WOLLA	A-Wollastonite
		FToxid-bC2SA	A-a-(Ca,Sr,Ba)SiO ₄
		FToxid-aC2SA	A-a-(Ca,Sr)SiO ₄

Legend

- I - immiscible 1
- + - selected 1

Show all selected

species: 22 solutions: 3 Select

Final Conditions

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

recommend you not select both pure liquids and molten solutions

FactSage 8.0

Selection - Equilib - no results

File Edit Show Sort

Selected: 1/17 LIQUID Duplicates selected X denotes species excluded by default

- no results -

*	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
24	Alliq	FacIPS	liquid		V				
X 25	Al2O3(liq)	FacIPS	liquid		V				
26	Si(liq)	FacIPS	liquid		V				
X 27	SiO2(liq)	FacIPS	liquid		V				
28	Ca(liq)	FacIPS	liquid		V				
X 29	CaO(liq)	FacIPS	liquid		V				
30	V(liq)	FacIPS	liquid		V				
31	VO(liq)	FacIPS	liquid		V				
+	32 #1 V2O3(liq)	FacIPS	Liquid_1_Vanadi	V					
33	V2O4(liq)	FacIPS	Liquid_1_Vanadi	V					
34	V2O5(liq)	FacIPS	liquid		V				
35	Fe(liq)	FacIPS	liquid		V				
36	FeO(liq)	FacIPS	liquid		V				
X 37	Fe3O4(liq)	FacIPS	liquid		V				
38	Al2O3(liq)	FToxid	liquid		V				
39	SiO2(liq)	FToxid	liquid		V				
40	CaO(liq)	FToxid	liquid		V				

Setting activity coefficient
of V₂O₃ in slag

32 V₂O₃(liq) dissolved in Ideal Solution #1

32 V₂O₃(liq) - Henrian activity coefficient, gamma
 $\log_{10}(\text{gamma}) = A/\text{TK} + B$

A = 1000

B = -3.5

New mixing particles P = 2 (P > 0)

#1 Ideal Solution name: Ideal-1 (max 10 chars)

For ideal behaviour A = 0, B = 0, P = 1.

Click on [Help] for an explanation of P.

Click on [Cancel] to remove this species from the ideal solution.

Cancel Help OK

New component in slag: Henrian activity coefficient

Equilib - Menu: last system

File Units Parameters Help

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

Reactants (6)

(gram) 0.5 CaO + 0.3 SiO₂ + 0.19 Al₂O₃ + 0.01 V₂O₃ + 0.95 Fe + 0.05 Al

Products

Solution FToxid-SLAGA

- clear
- all end-members
- * - custom select end-members
- m - merge dilute solution from
- solution properties
- + - single phase
- I - possible 2-phase immiscibility
- J - possible 3-phase immiscibility
- standard stable phase
- I - dormant (metastable) phase
- F - formation target phase
- P - precipitate target phase
- C - composition target ...
- L - cooling calculation ...

Help ...

Solution phases

	Base-Phase	Full Name
+	FTmisc-FeLQ	Fe-liq
#1	FToxid-SLAGA	A-Slag-liq all oxides + S
	FToxid-SLAGA	spinel
		oxynio
		pyroxene
		perovskite
		astenite
	FToxid-bC2SA	A-a'(Ca,Sr,Ba)2SiO ₄
	FToxid-aC2SA	A-a-(Ca,Sr)2SiO ₄

Dilute Solution # 1 - Ideal-1

Remove dilute components

Legend

- immiscible 1
- + - selected 1

Show all selected

species: 22 Select

solutions: 3

Custom Solutions

- 0 fixed activities
- 1 ideal solutions

Details ...

Pseudonyms

apply Edit ...

Volume data

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

paraequilibrium & Gmin edit

Total Species (max 5000) 103

Total Solutions (max 200) 4

Total Phases (max 1500) 84

Equilibrium

normal normal + transitions

transitions only open

- no time limit -

- recommend you not select both pure liquids and molten solutions -

FactSage 8.0

New component in slag: Henrian activity coefficient

32 V₂O₃(liq) dissolved in Ideal Solution #1

32 V₂O₃(liq) - Henrian activity coefficient, gamma
 $\log_{10}(\text{gamma}) = A/\text{TK} + B$

A =

B =

New mixing particles P = (P > 0)

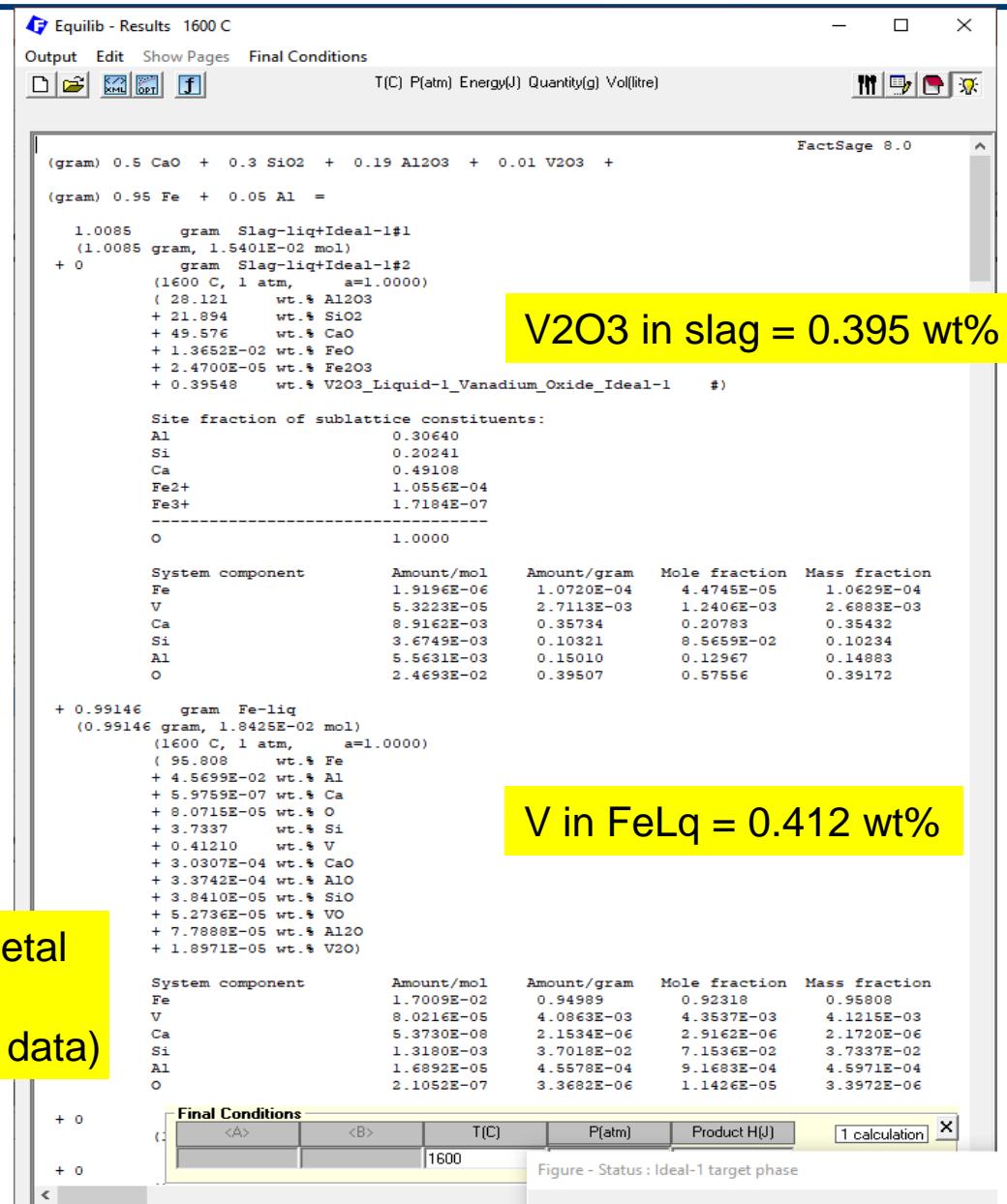
#1 Ideal Solution name: (max 10 chars)

For ideal behaviour A = 0, B = 0, P = 1.

Click on [Help] for an explanation of P.

Click on [Cancel] to remove this species from the ideal solution.

Cancel **Help** **OK**



The distribution of V between slag and metal can be varied depending on the activity coefficient. (evaluated from experimental data)

Vanadium Partition Coefficient In
Steel/Slag Melts based on literature data
(BOF condition)

FINAL REPORT for MIME572

By Jonathan Spring
Undergraduate student
McGill University

More details can be found in:
http://in-ho-group.snu.ac.kr/?page_id=398

Background

- Partition coefficients used to purify/quantity solute concentration in steel/slag
- Partition coefficient, $L_v = (\text{wt\% V}) / [\text{wt\% V}]$
- No known expression to predict vanadium distribution coefficient

Henry's Law

- We are dealing with dilute solutions
 - $(V_2O_3) \sim 3 \text{ wt\%}$
- $2 \underline{V} + 3 \underline{O} = V_2O_3$
- $K_{eq} = A_{V2O_3} / (A_V^2 * A_O^3)$
- Activity = $Y_{V2O_3} X_{V2O_3}$
- $\log_{10}(Y_{V2O_3}) = A/T + B$

Literature Search

- Found ~ 20 articles with data on vanadium partition coefficients in slag/steel melts
- 3 of those contained tables of raw data with slag compositions (Zhang, Shin and Inoue) and 2 were performed at similar temperatures (Shin and Inoue). These 2 were used initially.
- Shin's article dealt with slag containing Al₂O₃. His experiments were performed without proper control of the oxygen partial pressure and the partition coefficients for V he found were drastically different than in Inoue's article. His results are therefore unreliable. Furthermore, the initial V partition coefficient model had trouble fitting Shin's data. It was decided after my presentation to redo the model using only Inoue's data.
- Total data points: 63

- 1550 °C: 15 data points
- 1600 °C: 28 data points
- 1650 °C: 18 data points
- Slag
 - $x \text{ SiO}_2$
 - $x \text{ CaO}$
 - $x \text{ FeO}$
 - $x \text{ Fe}_2\text{O}_3$
 - $x \text{ MgO}$
- L_v for each data point

V distribution coefficient between steel and slag

Data from Inoue's Article

T (C)	Slag (wt%)						Lv
	(CaO)	(SiO ₂)	(FeO)	(Fe ₂ O ₃)	(MgO)	(V)	
1650	27	28	21	2	19	1	410.1
1650	19	22	36	4	16	1	751.4
1650	29	15	36	6	10	1	1087.6
1650	8	13	52	4	22	1	850.6
1650	25	7	47	11	8	2	1510.0
1650	17	3	58	12	7	2	1439.3
1650	1	4	71	6	16	1	1142.9
1650	1	15	50	3	29	1	705.9
1650	19	28	29	2	20	1	522.1
1650	28	22	30	4	13	1	761.7
1650	37	14	31	8	8	2	1174.2
1650	21	13	46	6	11	2	937.9
1650	31	7	40	13	7	2	1495.1
1650	0	1	82	6	8	2	1006.2
1650	1	7	71	5	14	1	900.7

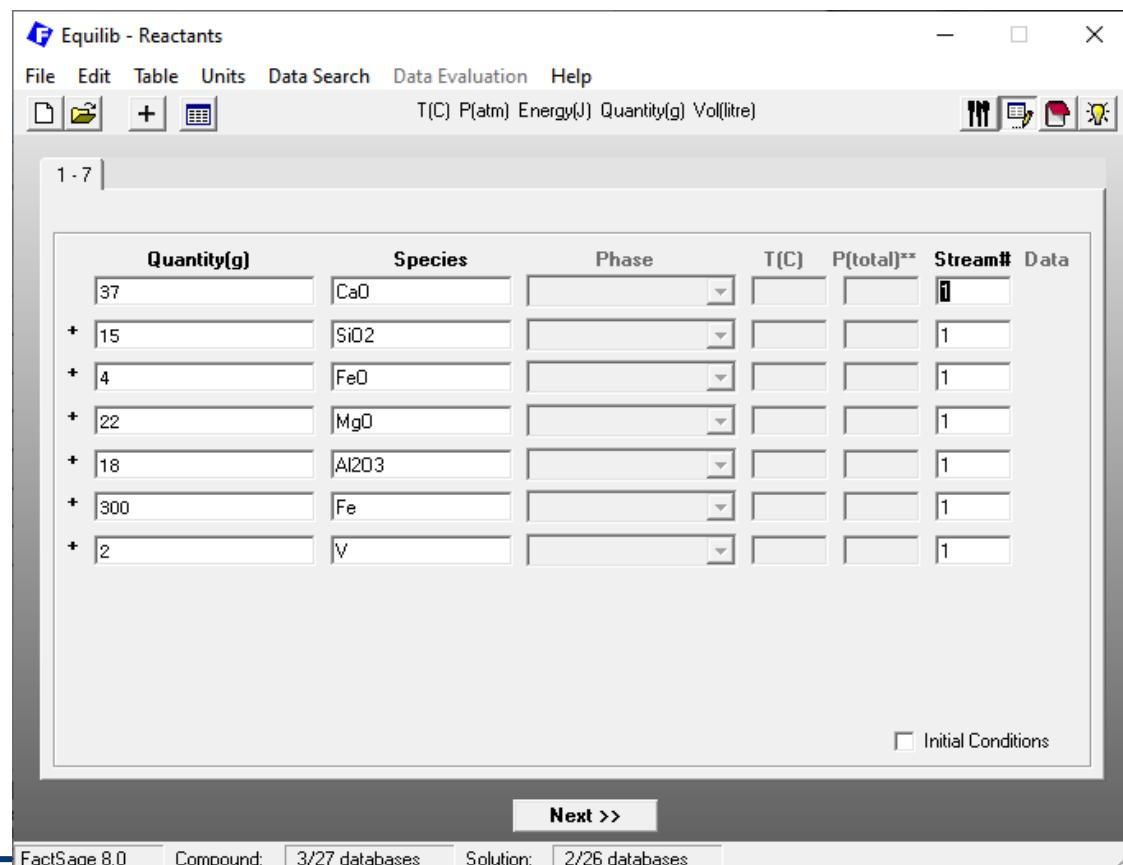
The amount of V in the slag was not considered. The same fixed amount of V was used for all equilibrium calculations and the subsequent calculation of Lv.

Ref: R. Inoue and H. Suito, Trans. ISIJ, vol. 22, p 705 (1982).

V distribution coefficient between steel and slag

- Databases: FToxic, Ftmisc (FeLQ), FactPS
- Equilibrium
 - x SiO₂
 - x CaO
 - x FeO
 - x Fe₂O₃
 - x MgO
 - 300 g Fe
 - 2 g V

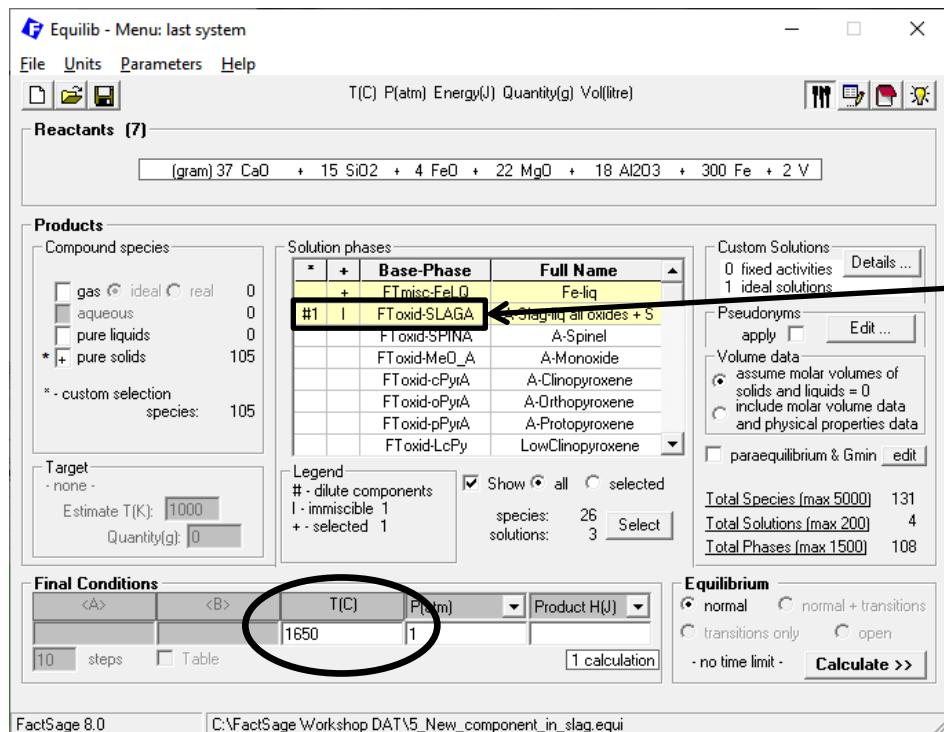
100 g



3:1 metal to slag ratio

V distribution coefficient between steel and slag

- Assume V in slag exists as V_2O_3



Selection - Equilib - no results -

Selected: 105/186 SOLID Duplicates selected denotes species excluded by default

- no results -

+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
X	115	Ca2Al2SiO7(s)	FactPS	Gehlenite		V			
X	116	Ca3Al2SiO12(s)	FactPS	Grossularite		V			
+	117	V(s)	FactPS	solid		V			
+	118	V(%)	FactPS	solid		V			
	119 #1	V2O3(s)	FactPS	Solid_II		V			
	120	V2O4(s)	FactPS	Solid_I		V			
+	121	V2O4(s2)	FactPS	Solid_II		V			
+	122	V2O5(s)	FactPS	solid		V			
+	123	V3O5(s)	FactPS	solid		o			
+	124	V4O7(s)	FactPS	solid		o			
+	125	(MgO)(V2O5)(s)	FactPS	solid		o			
+	126	(MgO)(2V2O5)(s)	FactPS	solid		o			
+	127	Si2V(s)	FactPS	Si2V		o			
+	128	Si3V5(s)	FactPS	solid		o			
+	129	(CaO)(V2O5)(s)	FactPS	solid		o			
+	130	(CaO)2(V2O5)(s)	FactPS	solid		o			
+	131	(CaO)3(V2O5)(s)	FactPS	solid		o			
+	132	Fe(s)	FactPS	bcc		V			
+	133	Fe(s2)	FactPS	fcc		V			
+	134	FeO(s)	FactPS	Wustite		V			
X	135	Fe2O3(s)	FactPS	hematite		V			

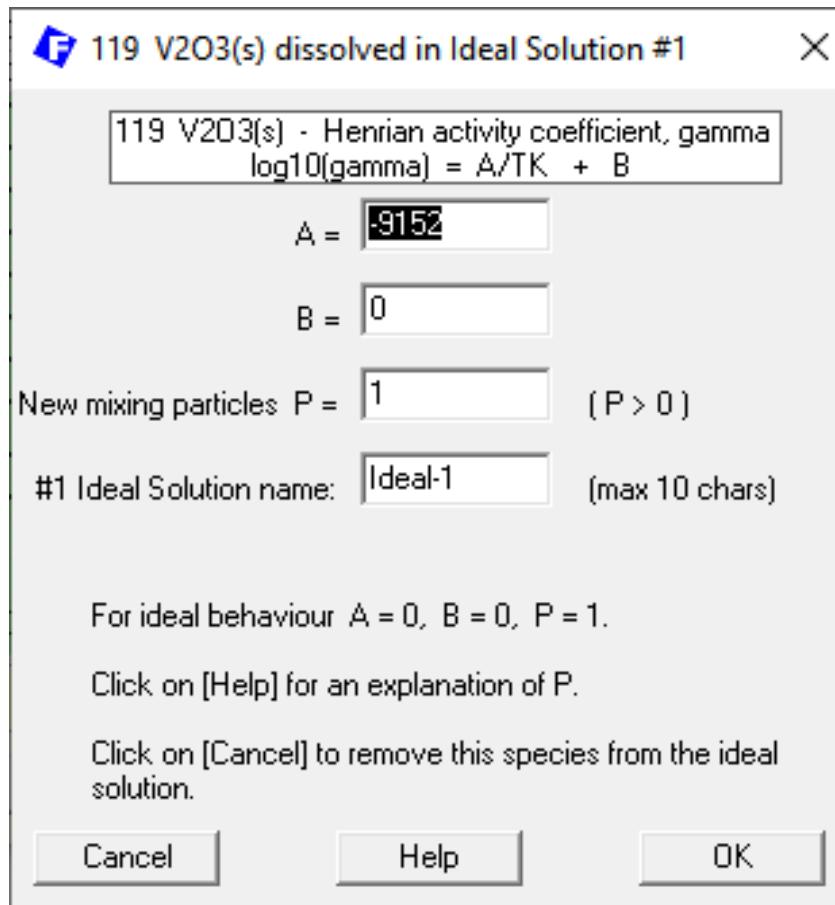
permit selection of X species Help Suppress Duplicates Edit priority list ...

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

Solid V₂O₃ was considered because solid V₂O₃ is stable at these temperatures.

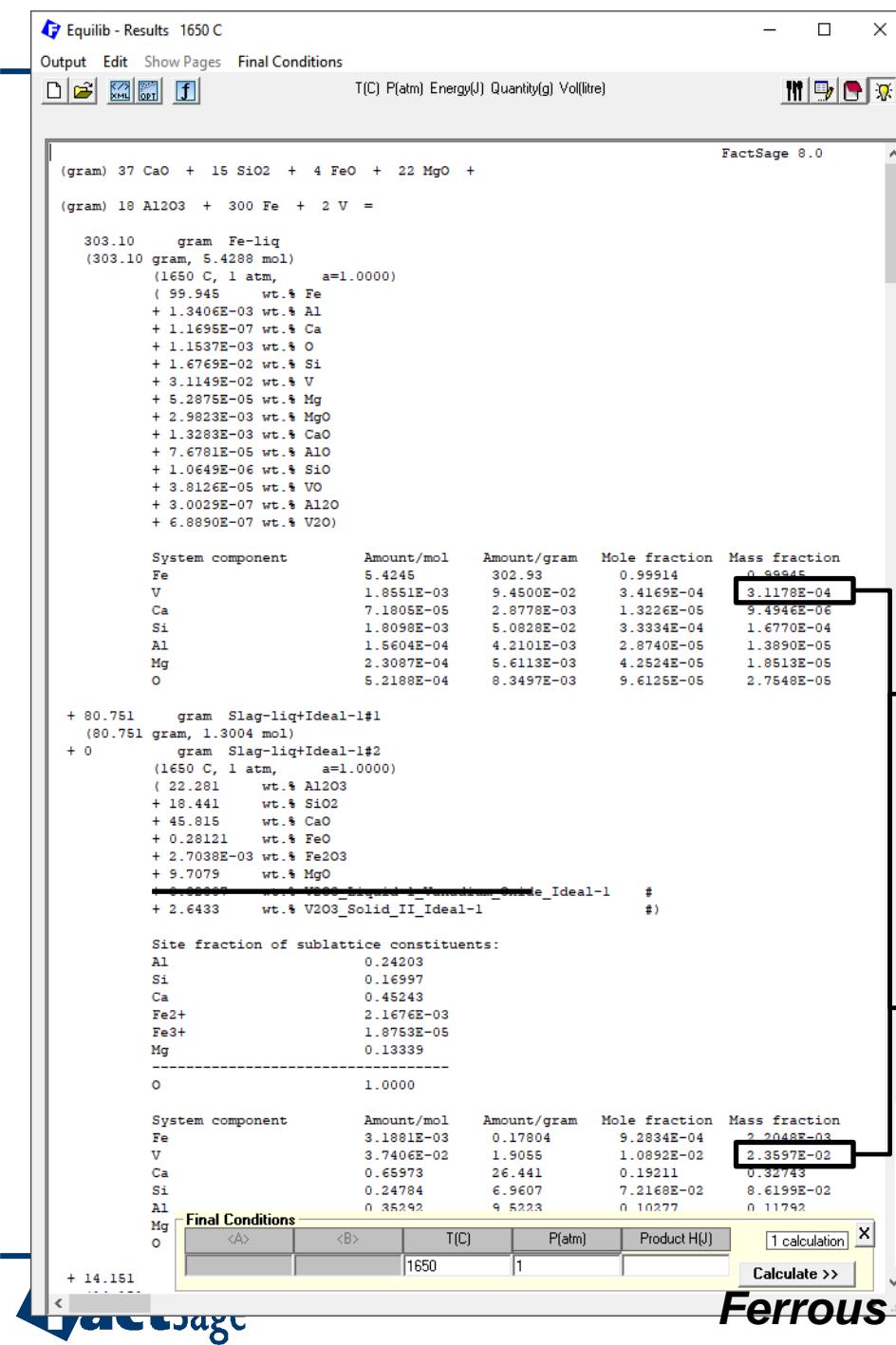
V distribution coefficient between steel and slag

- Change “A” value, “B” assumed to be 0



- Calculate equilibrium
- Calculate L_v
- Compare to measured L_v
- Go back and try new “A” value
- Trial and error
- More negative “A” value creates a smaller L_v

$$L_v = \frac{Wt\% V}{[Wt\% V]}$$



Slag (wt%)						Lv
T (C)	(CaO)	(SiO ₂)	(Fe ₂ O ₃)	(MgO)	(FeO)	
1650	37	15	18	22	4	12.6

V distribution coefficient between steel and slag

“A” Value to Activity Coefficient

T (C)	Slag (wt%)							Lv	A	Y
	(CaO)	(SiO ₂)	(FeO)	(Fe ₂ O ₃)	(MgO)	(V)				
1650	27	28	21	2	19	1	410.1	-1025	0.29	
1650	19	22	36	4	16	1	751.4	-1200	0.24	
1650	29	15	36	6	10	1	1087.6	-2175	0.07	
1650	8	13	52	4	22	1	850.6	-1100	0.27	
1650	25	7	47	11	8	2	1510.0	-2750	0.04	
1650	17	3	58	12	7	2	1439.3	-2300	0.06	
1650	1	4	71	6	16	1	1142.9	-1300	0.21	
1650	1	15	50	3	29	1	705.9	-750	0.41	
1650	19	28	29	2	20	1	522.1	-1000	0.30	
1650	28	22	30	4	13	1	761.7	-1475	0.17	

$$\log_{10}(Y_{V_2O_3}) = A/T + B$$

$$\log_{10}(Y_{V_2O_3}) = -1025/1923$$

$$Y_{V_2O_3} = 10^{-1025/1923}$$

$$Y_{V_2O_3} = 0.293$$

A more negative “A” value indicates a smaller activity coefficient.

V distribution coefficient between steel and slag

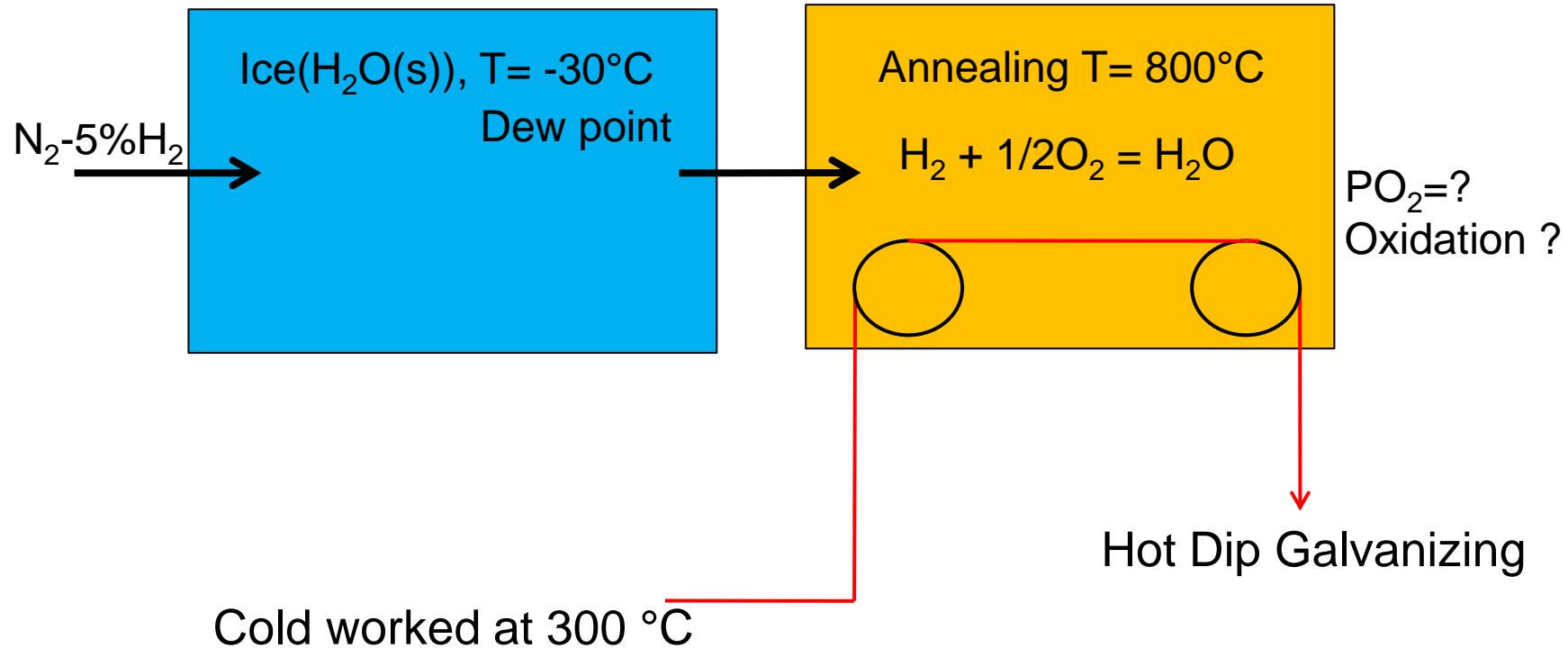
- The regression using slag basicity, $A = a\text{CaO}/\text{SiO}_2 + b\text{MgO}/\text{SiO}_2 + c(\text{FeO} + \text{Fe}_2\text{O}_3)$, was discarded because the fit was not as good as for the regression using each slag component.
- The regression using each slag component was poor nonetheless. Another regression, using all slag components and the slag temperature, was introduced.
- Option #1
$$A = a\text{CaO} + b\text{SiO}_2 + c(\text{FeO} + \text{Fe}_2\text{O}_3) + d\text{MgO}$$
- Option #2 (Option #1 including temperature)
$$A = aT(K) + b\text{CaO} + c\text{SiO}_2 + d(\text{FeO} + \text{Fe}_2\text{O}_3) + e\text{MgO}$$
- Option #3 (Option #2 including Constant)
$$A = aT(K) + b\text{CaO} + c\text{SiO}_2 + d(\text{FeO} + \text{Fe}_2\text{O}_3) + e\text{MgO} + \text{Constant}$$

- Regression #3 is best
 - Slope of Measured vs Predicted “A” and Measured vs Predicted Lv is closest to 1
 - Smaller residuals
 - Residuals are randomly distributed
- $A = -7 * \text{Temperature (K)} - 51 * \text{wt\% CaO} + 133 * \text{wt\% SiO}_2 + 31 * (\text{wt\% FeO} + \text{wt\% Fe}_2\text{O}_3) - 37 * \text{wt\% MgO} + 10,100$
- Need to test against more data!

Zn Galvanizing process

Reduction furnace: selective oxidation
Galva-Annealing: Zn melting and oxidation

Oxygen partial pressure control using Dew-point control



N2-H2 gas with -30C dew point

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

The screenshot shows the FactSage 8.0 software interface. On the left, the 'Equilib - Reactants' window displays the input quantities: 95 g N2, 5 g H2, and 1 g H2O. The 'Equilib - Menu: com' window shows the selected parameters: T(C) and P(total)**. In the center, the 'Reactants (3)' section lists the input components: (gram) 95 N2 + 5 H2 + H2O. The 'Products' section includes a dropdown menu where 'real' is selected instead of 'ideal'. The 'Solution phases' section is currently empty. On the right, various settings are shown, including 'Custom Solutions' (fixed activities, ideal solutions), 'Pseudonyms' (apply, edit), 'Volume data' (assume molar volumes of solids and liquids = 0, include molar volume data and physical properties data), and 'Equilibrium' options (normal, normal + transitions, transitions only, open). The bottom status bar indicates FactSage 8.0 and the file path C:\FactSage Workshop DAT\7_Zn_Galvanizing_process.equi.

N2-H2 gas with -30C dew point

Mixtures - Results -30 C

Output Edit Show Pages Final Conditions

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

FactSage 8.0

T = -30.00 C
P = 1 bar
V = 82.660 dm³

STREAM CONSTITUENTS

	AMOUNT/gram
N2	9.5000E+01
H2	5.0000E+00
H2O	1.0000E+00

PHASE: gas_real

	EQUIL AMOUNT mol	MOLE FRACTION	FUGACITY bar
N2	2.5651E+00	6.2423E-01	6.2457E-01
NH3	1.5419E+00	3.7522E-01	3.6993E-01
H2	1.9275E-03	4.6908E-04	4.7153E-04
H2O	3.1735E-04	7.7229E-05	7.4573E-05
N2H4	1.1022E-38	2.6822E-39	2.65557E-39
N2H5OH	8.5004E-39	2.0686E-39	2.0481E-39
H	5.1408E-46	1.2510E-46	1.2386E-46
NH2	4.1917E-46	1.0201E-46	1.0100E-46
HNNH	7.8817E-55	1.9180E-55	1.8990E-55
OH	9.6807E-60	2.3558E-60	2.3325E-60
NO	2.2037E-69	5.3627E-70	5.3575E-70
N2O	3.0469E-72	7.4148E-73	7.3453E-73
TOTAL:	4.1092E+00	1.0000E+00	1.0000E+00

System component

	Amount/mol	Amount/gram	Mole fraction	Mass fraction
O	3.1735E-04	5.0774E-03	2.8078E-05	5.1744E-05
N	6.6721	93.454	0.59032	0.95239
H				

Final Conditions

(NH4) ₂ O_liquid	<A>		T(C)	P(bar)	Product H(J)	1 calculation
NH4OH_liquid			-30	1		Calculate >>
NH4OH_solid						

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

N2-H2 gas with -30C dew point

Creating stream file

Output Edit Show

Save or Print As ...

Repeat Save

Plot

Equilib Results file

Stream File

Format

Fact-XML

Fact-Optimal

Fact-Function-Builder

Refresh ...

Swap loops ...

H₂O

N₂H₄

N₂H₅OH

H

NH₂

HNNH

OH

NO

N₂O

TOTAL:

System component

O

N

H

Final Conditions

(NH₄)₂O₂ liquid

NH₄OH liquid

NH₄OH solid

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

Recycle all streams ...

Save stream file

Stream file properties ...

Summary of streams

Directory (C:\FactSage Workshop DAT) ...

EQUIL AMOUNT MOLE FRACTION FUGACITY

mol bar

	EQUIL AMOUNT	MOLE FRACTION	FUGACITY
V	2.5651E+00	6.2423E-01	6.2457E-01
V	1.5419E+00	3.7522E-01	3.6993E-01
V	1.9275E-03	4.6908E-04	4.7153E-04
V	3.1735E-04	7.7229E-05	7.4573E-05
V	1.1022E-38	2.6822E-39	2.6555E-39
V	8.5004E-39	2.0686E-39	2.0328E-39
V	5.1408E-46	1.2510E-46	1.2252E-46
V	4.1917E-46	1.0201E-46	9.9453E-47
V	7.8817E-55	1.9180E-55	1.8922E-55
V	9.6807E-60	2.3558E-60	2.3300E-60
V	2.2037E-69	5.3627E-70	5.2369E-70
V	3.0469E-72	7.4148E-73	7.2890E-73
	4.1092E+00	1.0000E+00	9.9999E+00
System component	Amount/mol	Amount/gram	
O	3.1735E-04	5.0774E-03	5.0774E-03
N	6.6721	93.454	93.454

Save File C:\FactSage Workshop DAT\gas-30C.mixt

Saving file gas-30C.mixt

Enter one line of comments

Gas-30C

OK Cancel

1 calculation

Calculate >

N₂-H₂ gas with -30°C dew point → 800°C

Equilib - Menu:

Reactants (1)

(gram) 100% [gas-30C]

Products

Compound species

- + gas (ideal) real 29
- aqueous 0
- + pure liquids 8
- + pure solids 8

species: 45

Target: none

Estimate T(K): 1000

Quantity(g): 0

Final Conditions

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

10 steps Table

Mixtures - Results 800 C

Output Edit Show Pages Final Conditions

Legend Show all selected

species: 0 solutions: 0

Final partial pressure of oxygen

EQUIL AMOUNT MOLE FRACTION FUGACITY

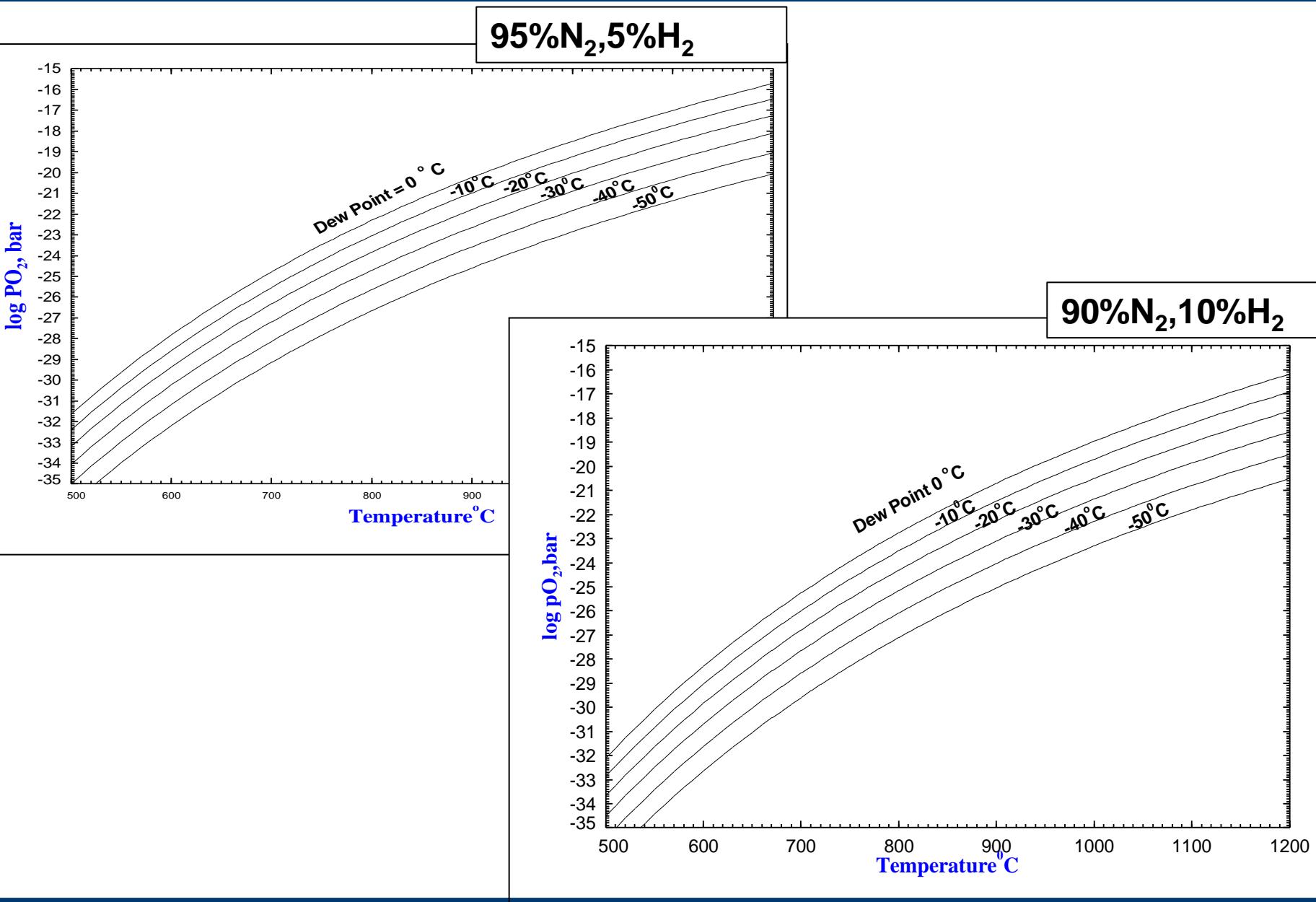
PHASE: gas_ideal	mol		
N ₂	3.3358E+00	5.9034E-01	5.9034E-01
H ₂	2.3141E+00	4.0953E-01	4.0953E-01
NH ₃	4.2239E-04	7.4750E-05	7.4750E-05
H ₂ O	3.1735E-04	5.6162E-05	5.6162E-05
H	5.0862E-08	9.0010E-09	9.0010E-09
NH ₂	1.2010E-11	2.1254E-12	2.1254E-12
OH	2.7091E-14	4.7943E-15	4.7943E-15
HNNH	8.8329E-17	1.5632E-17	1.5632E-17
NO	7.2047E-17	1.2750E-17	1.2750E-17
N ₂ H ₄	2.1778E-17	3.8540E-18	3.8540E-18
NH	1.4548E-17	2.5746E-18	2.5746E-18
N	6.3961E-20	1.1319E-20	1.1319E-20
HNO	1.3579E-20	2.4030E-21	2.4030E-21
N ₂ O	4.0409E-21	7.1512E-22	7.1512E-22
O	6.4478E-22	1.1411E-22	1.1411E-22
N ₃	1.3642E-23	2.4142E-24	2.4142E-24
HOOH	1.8966E-25	3.3565E-26	3.3565E-26
O ₂	4.7088E-26	8.3331E-27	8.3331E-27
N ₂ H ₅ OH	2.5192E-27	4.4582E-28	4.4582E-28
HOO	1.0721E-28	1.8973E-29	1.8973E-29
HONO (g2)	8.7194E-29	1.5431E-29	1.5431E-29
HONO (g)	6.7653E-29	1.1972E-29	1.1972E-29
NO ₂	4.6738E-31	8.2712E-32	8.2712E-32
HONO ₂	1.1815E-43	2.0908E-44	2.0908E-44
O ₃	1.2124E-49	2.1455E-50	2.1455E-50
NO ₃	1.3873E-50	2.4551E-51	2.4551E-51
N ₂ O ₃	2.6505E-53	4.7048E-54	4.7048E-54
N ₂ O ₄			
TOTAL:			
System			
O			
N			

Final Conditions

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

Calculate >>

Dew points – PO_2/T Relationship



Phase diagram PO_2 – T: Oxidation of Fe-1%Mn-1%Si

Data Search

Databases - 3/27 compound databases, 2/26 solution databases

Fact **FactSage™** **SGTE** **Private Databases**

Phase Diagram - Menu: last system

File Units Parameters Variables Help

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

Components (4)

(gram) O_2 + Fe + Mn + Si

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- * pure solids 51

* - custom selection species: 51

Solution phases

*	+	Base-Phase	Full Name
*	I	FSstel-Liqu	LIQUID
J		FSstel-FCC	FCC_A1
I		FSstel-BCC	BCC_A2
I		FSstel-HCP	HCP_A3
+		FSstel-CBCC	CBCC_A12
+		FSstel-CUB	CUB_A13
+		FSstel-M3Si	Me3Si1
+		FSstel-M1Si	Me1Si1

Custom Solutions

- 0 fixed activities
- 0 ideal solutions

Pseudonyms

- apply Edit ...

Volume data

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

paraequilibrium & Gmin edit

Total Species (max 5000) 187
 Total Solutions (max 200) 29
 Total Phases (max 1500) 80

Options - search for product spec

Include cor

- gaseo
- aquo
- limited

Default

Cancel

Variables

T(C)	log10(p(O_2))	Mn/(Fe+Mn+Si)	Si/(Fe+Mn+Si)
500 1000	-40 -20	0.01 (min)	0.01 (min)

log10 p(O_2)/atm vs T(C)

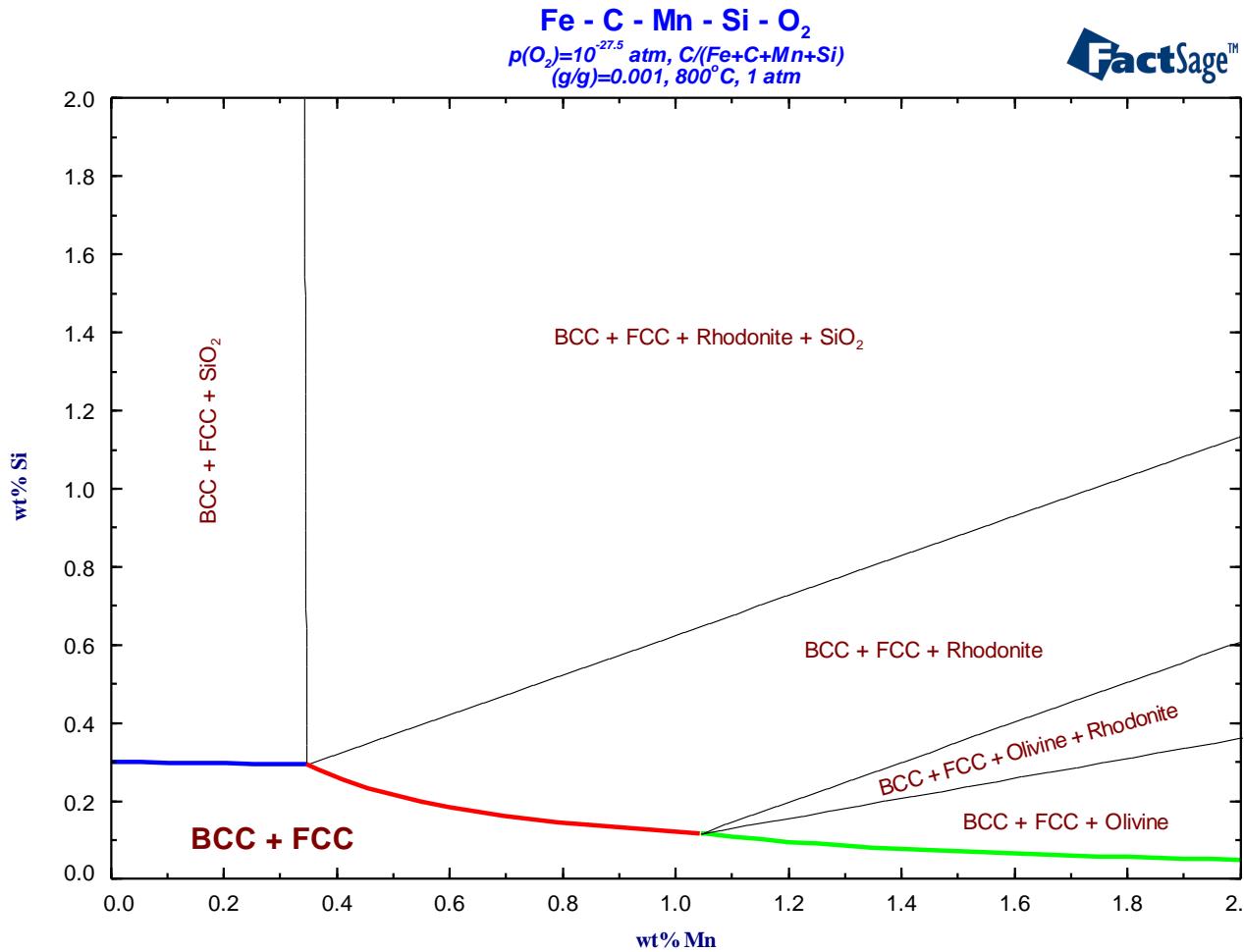
Phase Diagram

Y X

- no time limit - Calculate >

FactSage 8.0

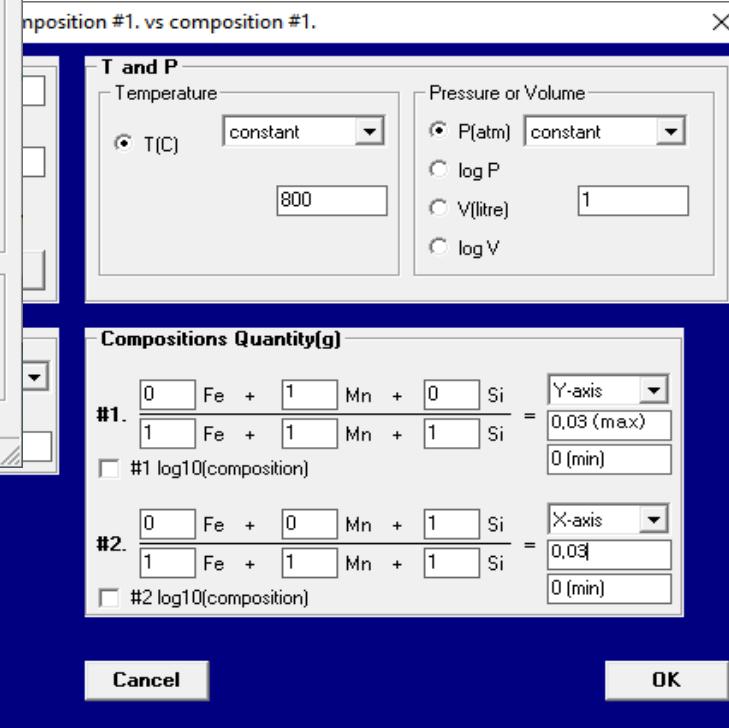
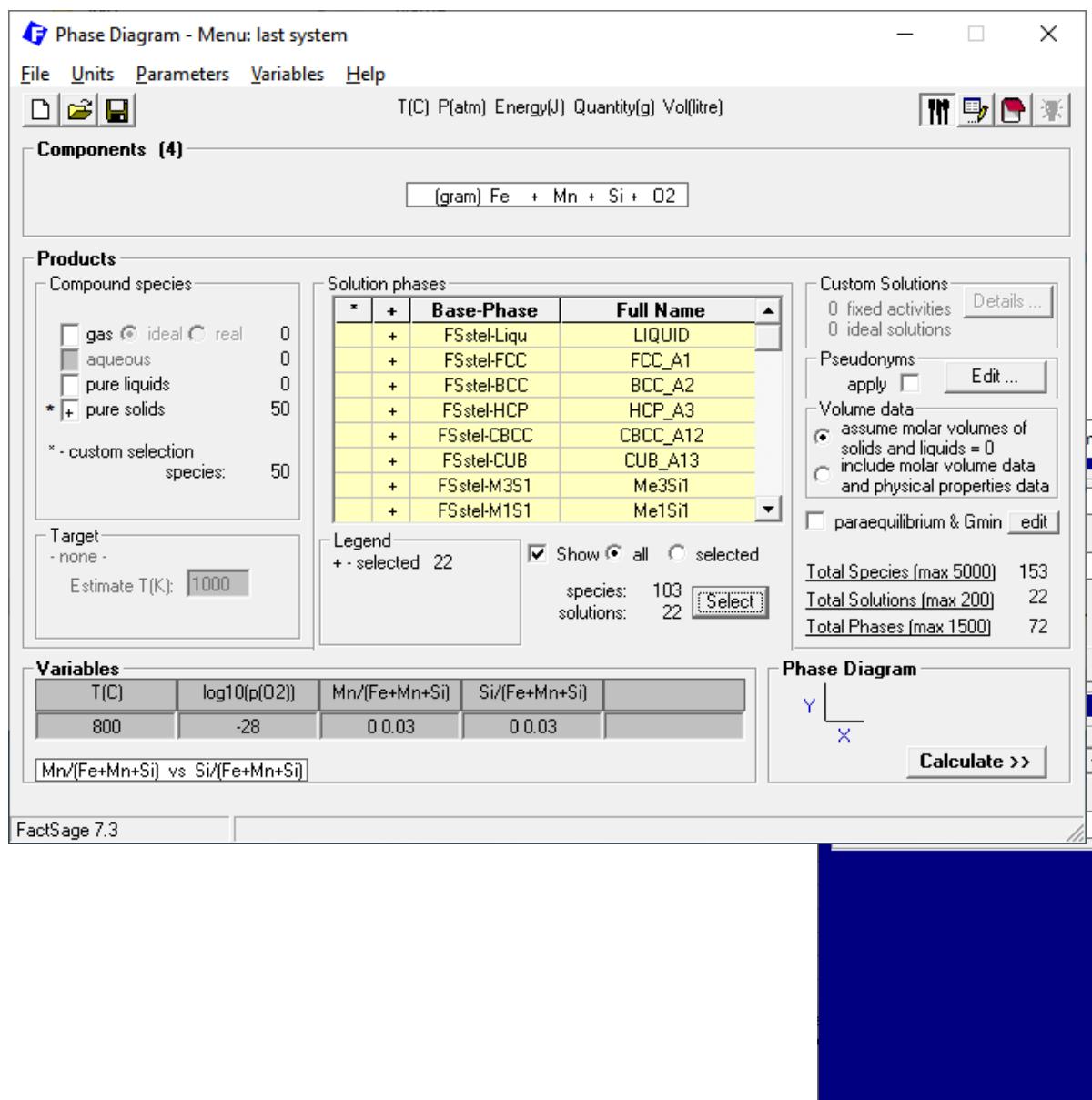
Primary oxide formation diagram



Drawing of the diagram:

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

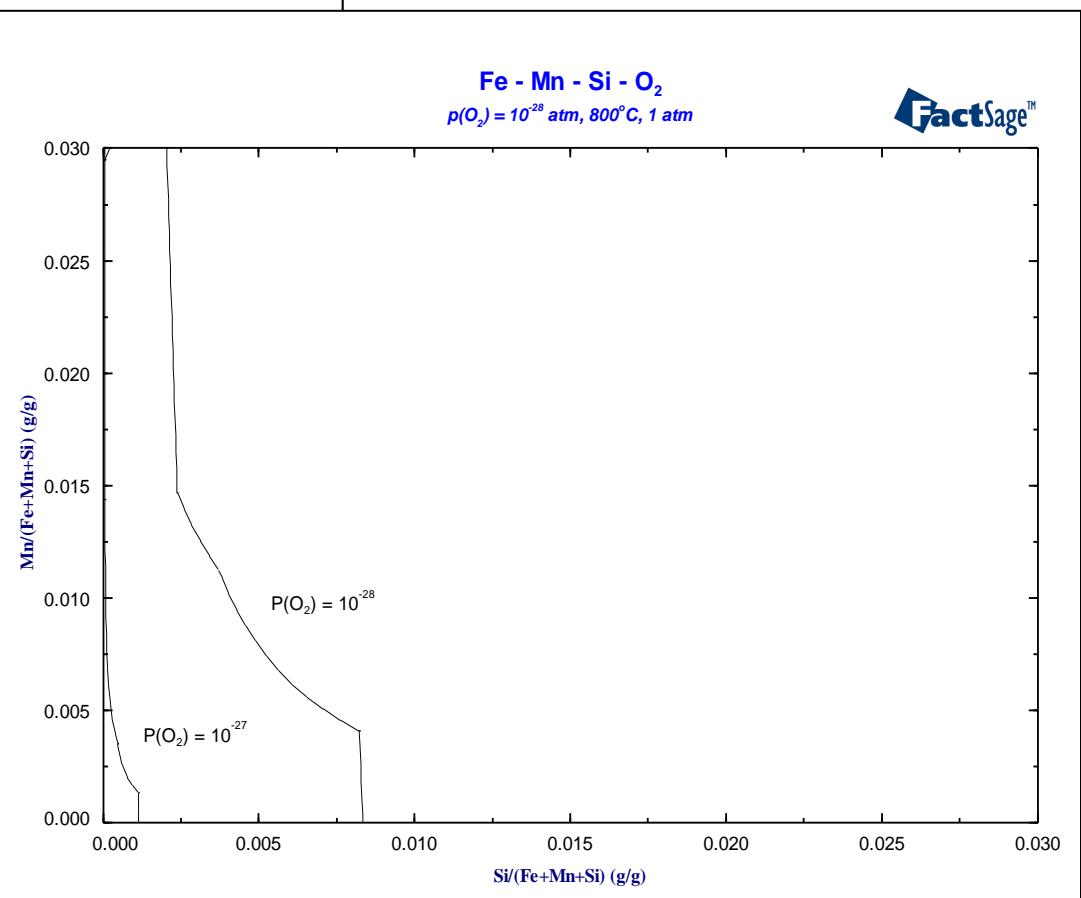
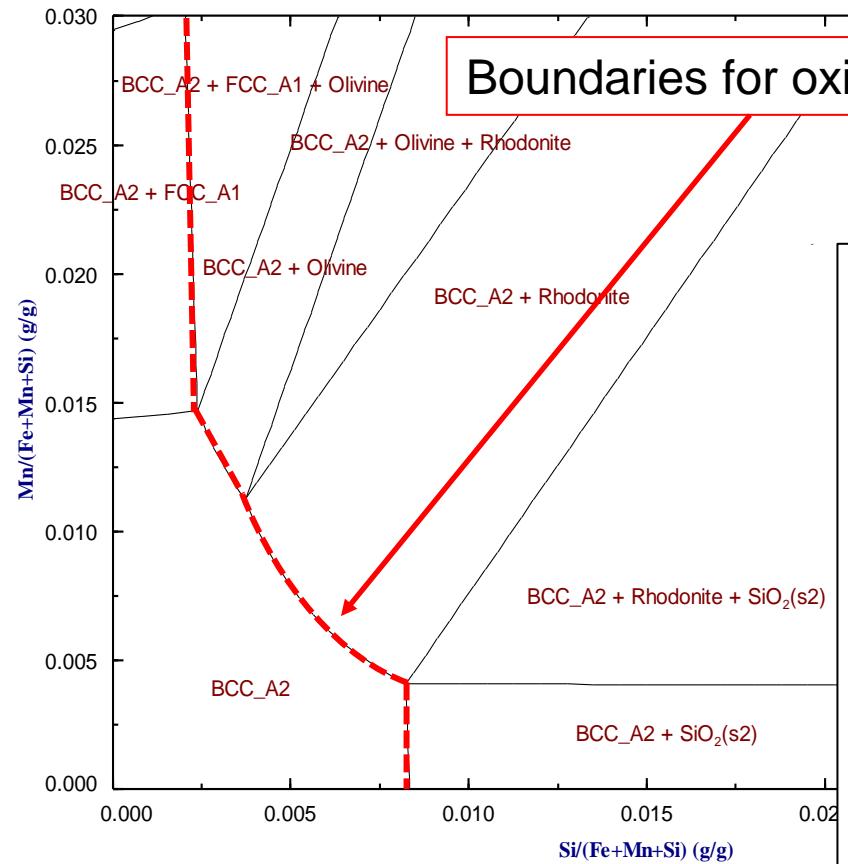
Fe-Mn-Si at $\text{PO}_2=10^{-28}\text{atm}$, $T=800^\circ\text{C}$



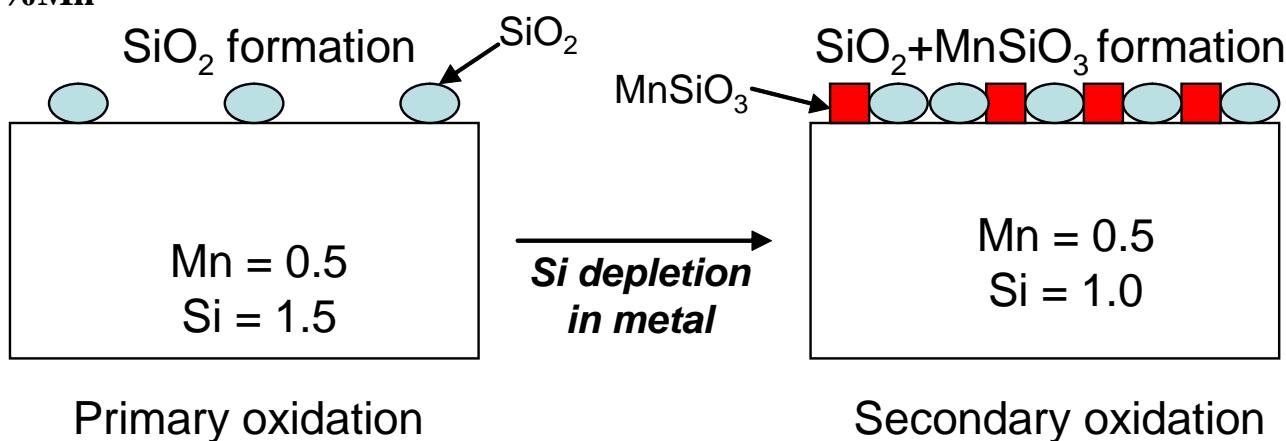
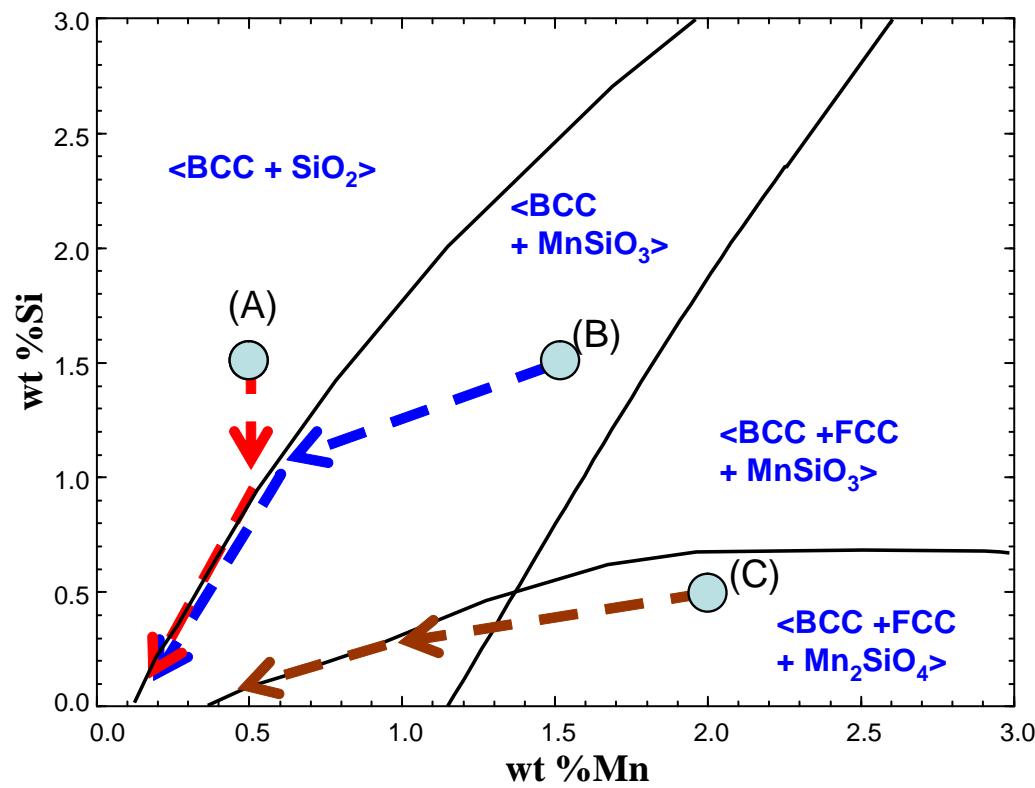


FactSage™

Boundaries for oxide phase

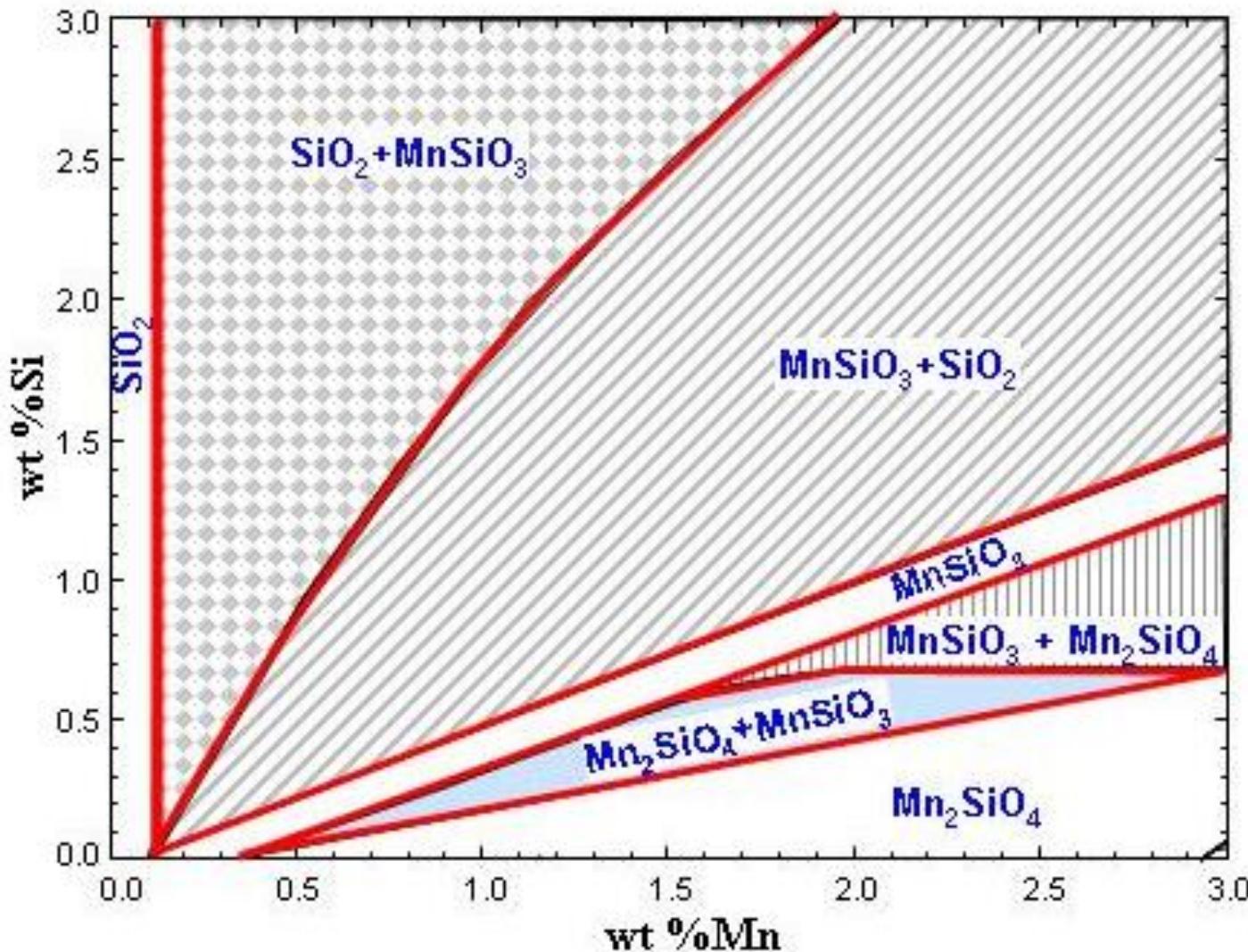


Primary and Secondary Oxidations

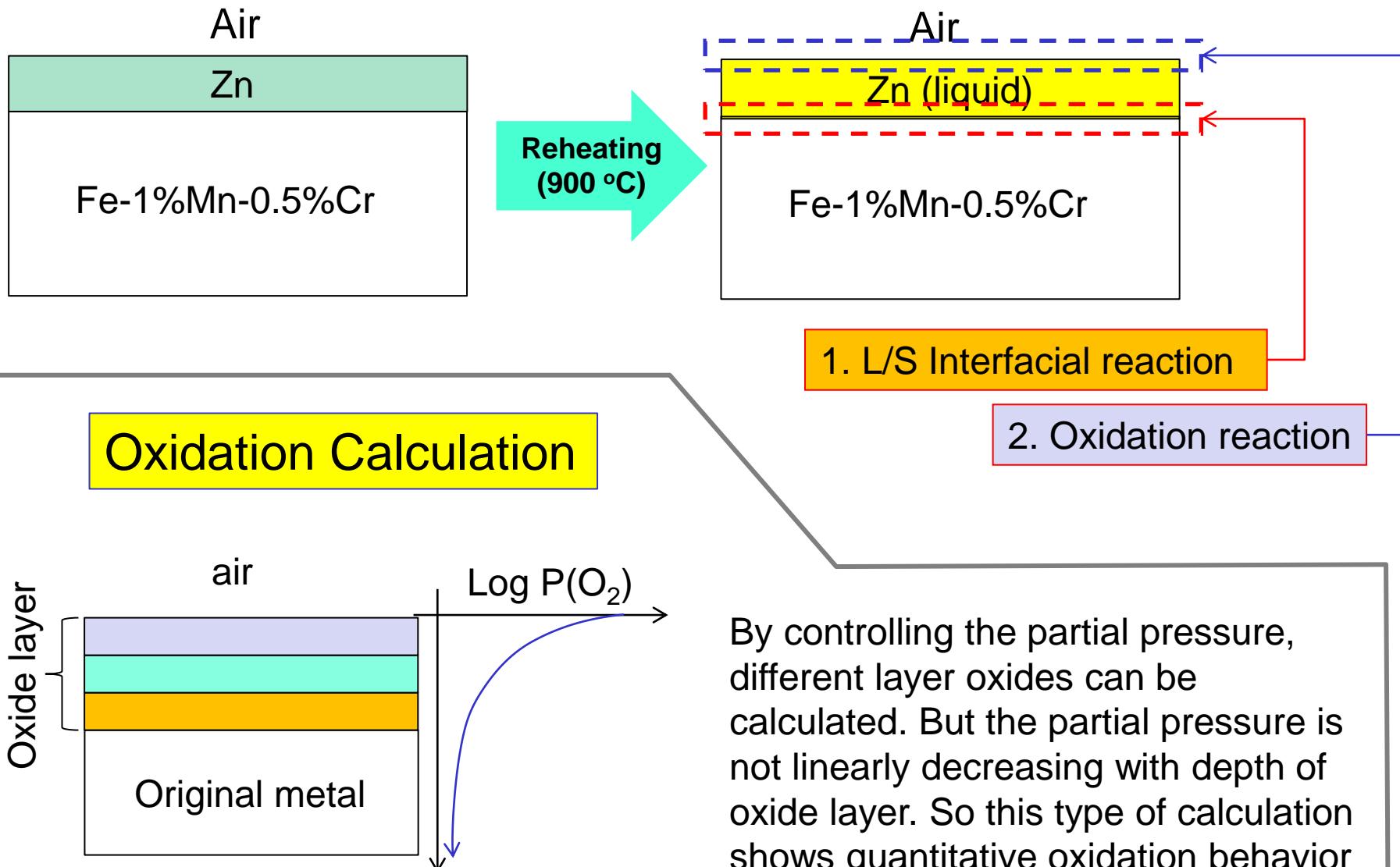


Oxidation phase diagram

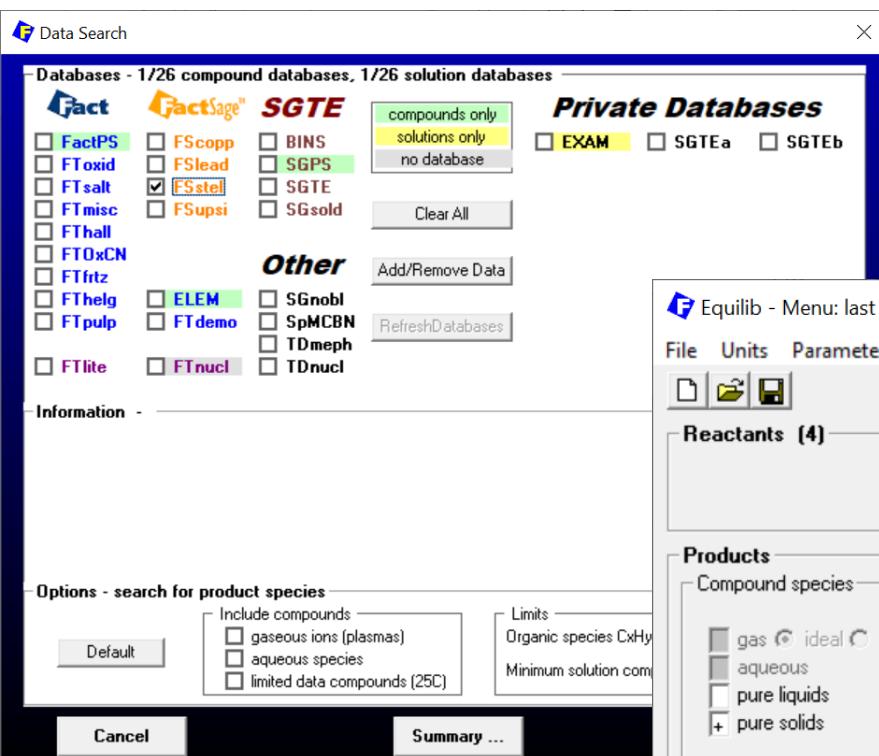
Oxidation phase diagram of the Fe-0.002%C-Mn-Si steel at 800°C



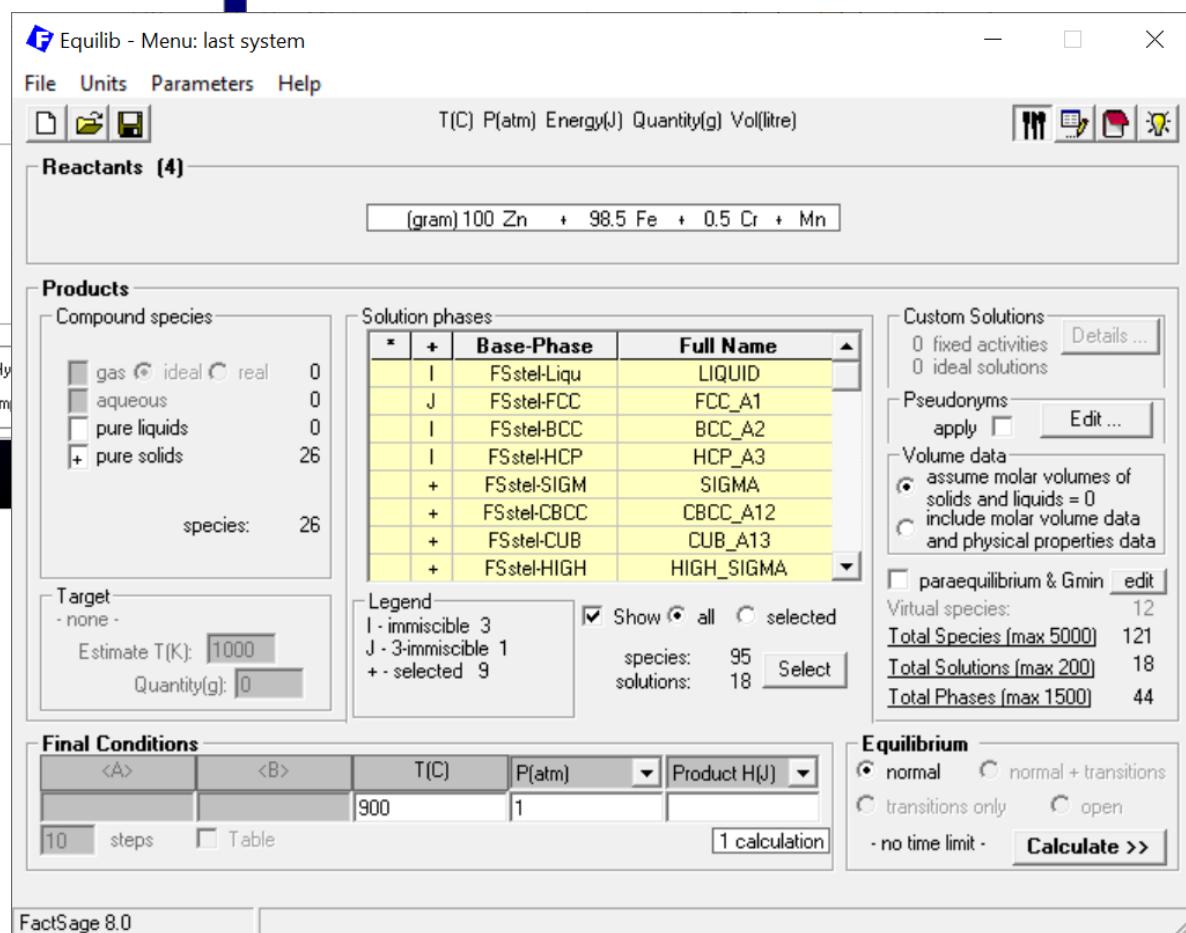
Remelting and oxidation of Zn galvanized steel



Interface reaction between liquid Zn and steel



FSStel database contains reasonable Zn bath data for Zn-galvanizing (Zn-Al-Fe-Mg-Si).



Oxidation of liquid Zn

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

FactSage 8.0 Software Interface:

- Databases:** FactPS, FactToxic, FactSalt, FactMisc, FactHall, FactOxCN, FactFitz, FactThelg, FactPulp, FactLite, FactSopp, FactLead, FactStel, FactSGPS, FactSGTE, FactSGold.
- Other:** ELEM, SGnobl, SpMCBN, TDmeph, TDnucl.
- Information:** Options - search for product species (Include compounds, gaseous ions, aqueous species, limited data compounds).
- Reactants:** (2) [gram] 100% [liquidZn-afterRxn] + 0 02
- Products:** Co (1) species: 1, 0, 0, 41, 42. Target: none. Estimate T(K): 1000, Quantity(g): 0.
- Solution phases:** Base-Phase: I (FSstel-Liquid), J (FSstel-FCC), L (FSstel-BCC), S (FSstel-Supercooled liquid), FS (FSstel-Subcooled liquid), FSs (FSstel-Solid), FSs (FSstel-Subsolidus), FSs (FSstel-Solid solution), FSs (FSstel-Subsolidus solution).
- Final Conditions:** <A>, , T(C): 900, 10 steps, Table.
- Legend:** I - immiscible, J - 3-immiscible, + - selected: 16.
- Fixed Partial Pressure (2-b):** Enter the value of $\log_{10}(p)$ (or for a range of values enter 'first last step') for 2 O₂(g). Value entered: -30 0 0.5. OK and Cancel buttons.

Oxidation of liquid Zn

Equilib - Results a=1.00E-30 (page 1/61)

Output Edit Show Pages Final Conditions



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

a=1.00E-21 | a=3.16E-21 | a=1.00E-20 | a=3.16E-20 | a=1.00E-19 | a=3.16E-19 | a=1.00E-18 |
 a=3.16E-26 | a=1.00E-25 | a=3.16E-25 | a=1.00E-24 | a=3.16E-24 | a=1.00E-23 | a=3.16E-23 | a=1.00E-22 |
 a=1.00E-30 | a=3.16E-30 | a=1.00E-29 | a=3.16E-29 | a=1.00E-28 | a=3.16E-28 | a=1.00E-27 | a=3.16E-27 | a=

(gram) 100% [liquidZn-afterRxn] + 0 O2 =

+ 1.4817E-10 O2

BCC_A2#1, selected as a dormant (metastable) phase, has an activity > 1
 BCC_A2#2, selected as a dormant (metastable) phase, has an activity > 1

0 mol gas_ideal
 (900 C, 1 atm, a=1.0000E-30)
 (1.0000E-30 O2)

+ 50.439 gram LIQUID#1
 (50.439 gram, 0.78598 mol)
 + 0 gram LIQUID#2
 (900 C, 1 atm, a=1.0000)
 (0.41922 wt.% Cr)
 + 9.6155 wt.% Fe
 + 0.68502 wt.% Mn
 + 2.9376E-10 wt.% O
 + 89.280 wt.% Zn)

System component Amount/mol
 Zn 0.68878
 Fe 8.6847E-02
 Mn 6.2892E-03
 Cr 4.0666E-03
 O 9.2611E-12

+ 0 gram BCC_A2#1
 + 0 gram BCC_A2#2
 (900 C, 1 atm, a=1.0000)
 (0.19293 wt.% Cr)
 + 62.617 wt.% Fe
 + 0.43760 wt.% Mn

Plot Species Selection - Equilib Results:

	#	Species	Gas	Phase
1	02		Liquid	Liquid
2	Cr			
3	Fe			
4	Mn			
5	Zn			
Liquid# 2				
6	Cr			
7	Fe			
8	Mn			
9	Zn			
A1#1		FCC-A1		
10	Cr			
11	Fe-gamma			
12	Mn			
13	Zn			

Setting X-axis

Y: gram
select species - use "+" column
Clear

X: log10(activity)
enter one species #

Display
 source
 phase
 name
 [page]
61 pages

Mass
 mole
 gram

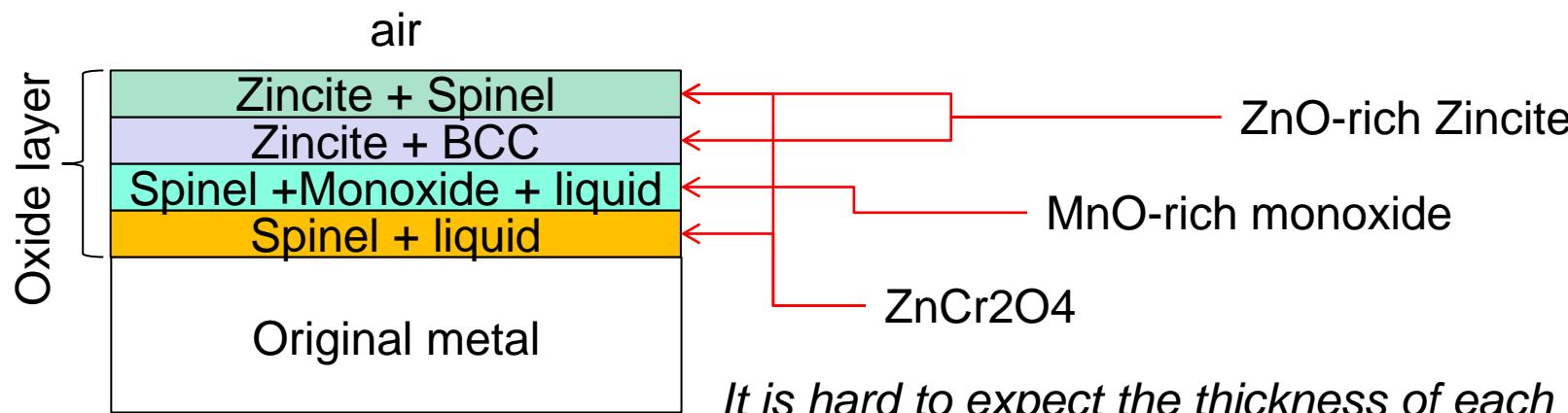
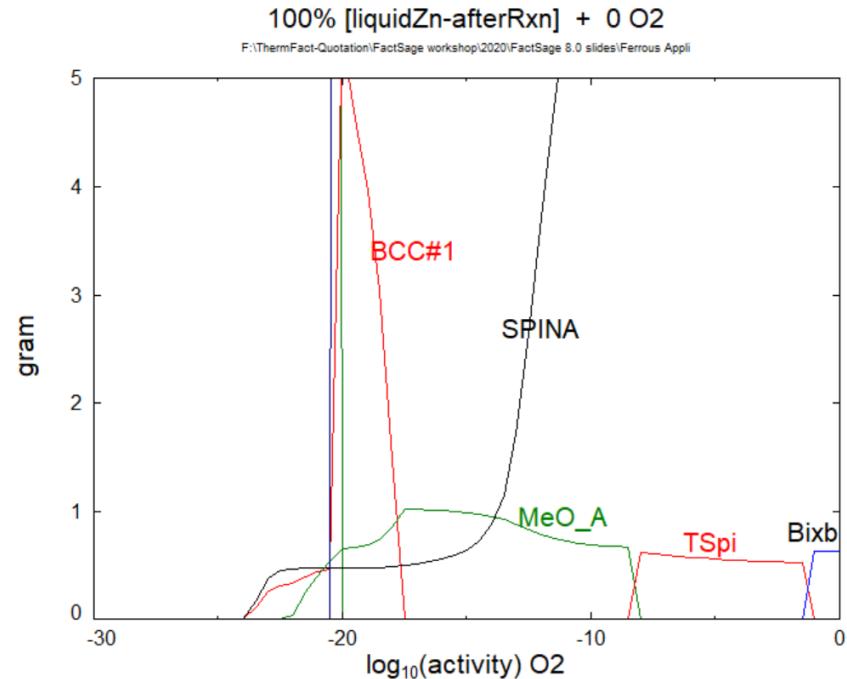
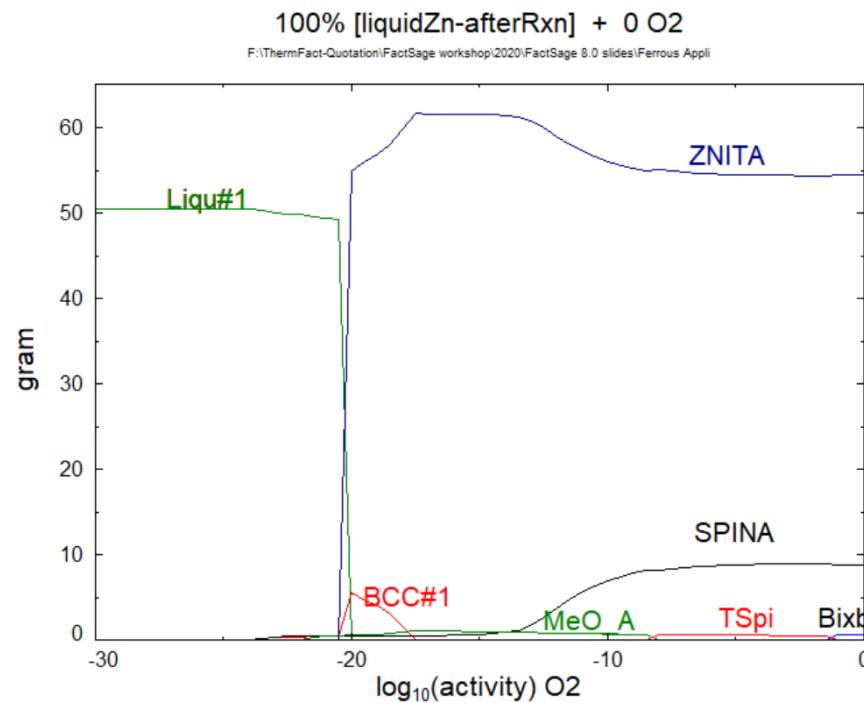
Order
 integer #
 mass (max)
 fraction (max)
 activity (max)

Select Top 15
0 species selected

ignore species and phases with zero mass
Select ...

OK

Oxidation of liquid Zn



It is hard to expect the thickness of each layer

Carburization and Decarburization of Steel

Equilib - Reactants

File Edit Table Data Search Data Evaluation Help

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

1 - 6

Quantity(g)	Species	Phase
99.62	Fe	
+ 0,08	C	
+ 0,2	Mn	
+ 0,1	Si	
+ <1-A> mol	CO	
+ <A> mol	CO ₂	

Next >

FactSage 7.3 Compound: 2/24 databases Solution: 1/25 databases

CO / CO₂ is variable

Equilib - Menu: comments

File Units Parameters Help

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

Reactants (6)

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

Products

Compound species

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

* - custom selection species: 24

Target - none -

Estimate T(K): 1000

Quantity(g): 0

Solution phases

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

Legend + - selected 2

Show all selected

species: 16 solutions: 2 Select

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

Pseudonyms apply Edit ...

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

paraequilibrium & Gmin edit

Total Species (max 5000) 40

Total Solutions (max 200) 2

Total Phases (max 1500) 3

Final Conditions

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

Equilibrium

normal normal + transitions
 transitions only open

Calculate >

FactSage 7.3 C:\...\Equi11_Carburization_and_Decarburization_of_Steel.DAT

Carburization and Decarburization of Steel

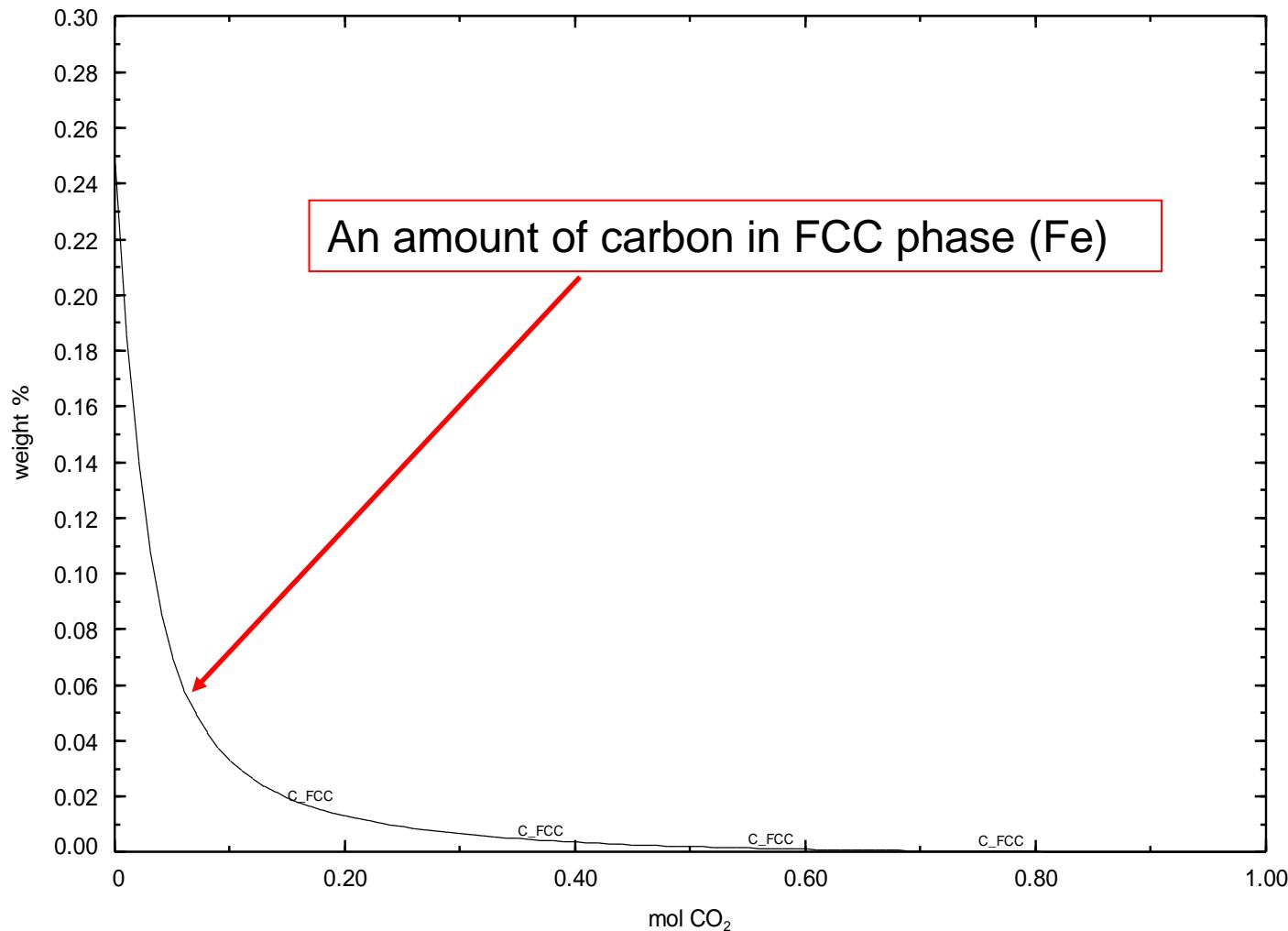
The screenshot shows the FactSage 7.3 interface with the following details:

- Top Bar:** Equilib - Results A=0 (page 1/101), Output, Edit, Show Pages, Final Conditions.
- Left Sidebar:** Save or Print, Plot, Equilib Results file, Stream File, Format, Fact-XML, Fact-Optimal, Fact-Function-Builder, Refresh ..., Swap loops ...
- Central Area:**
 - Plot Results Dialog:** T(C) P(atm) Energy(J) Quantity(g) Vol(litre). Buttons: Print, Copy, Paste, Cut, Undo, Redo.
 - FactSage 7.3 Version:** FactSage 7.3
 - Chemical Reaction:** + 0.2 Mn + 0.1 Si +
 - Plot Species Selection Dialog:** Shows a table of species with columns: #, Species, Mole (min), Mole (max), Fraction (min), Fraction (max), Activity (min), Activity (max). Species listed include FCC, BCC, Fe_GAS, Mn_GAS, SL_GAS, O_GAS, C_GAS, Fe_FCC, Mn_FCC, SL_FCC, O_FCC, C_FCC, Fe_BCC, Mn_BCC, SL_BCC, O_BCC, C_BCC.
- Bottom Area:**
 - Plot Configuration Dialog:** Axes: gram vs Alpha. Y-axis: gram, X-axis: Alpha. Settings: maximum 0.3, minimum 0, tick every 0.01.
 - Graph Options:** Axes: gram vs Alpha, Species: 0 selected, Graph: Labels size: 9 no: 4, Display: color, reactants, file name, full screen, Viewer, Figure.
 - Status Bar:** FactSage 7.3, C:\FactSage73\Equi0.res, 26Dec19, 101 sets.

Carburization and Decarburization of Steel

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

C:\FactSage73\Equi0.res 26Dec19



Carburization and Decarburization: Composition target

Equilib - Menu: comments

File Units Parameters Help

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

Reactants (6)

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

Products

Compound species: 24

* gas ideal real 24
aqueous 0
pure liquids 0

Solution FSstel-FCC

- clear
- all end-members
- * - custom select end-members
- m - merge dilute solution from
- solution properties

- + - single phase
- I - possible 2-phase immiscibility
- J - possible 3-phase immiscibility
- standard stable phase
- ! - dormant (metastable) phase
- F - formation target phase
- P - precipitate target phase
- C - composition target ...
- L - cooling calculation ...

Help ...

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

Base-Phase Full Name

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

Custom Solutions
0 fixed activities
0 ideal solutions

Composition Target

Solution ST53-FCC

Variable

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

Species

Code numbers (161-168)
Fe, Mn, O, ...

161 Fe

Element

Elements C O Si Mn Fe

Element: C

Values

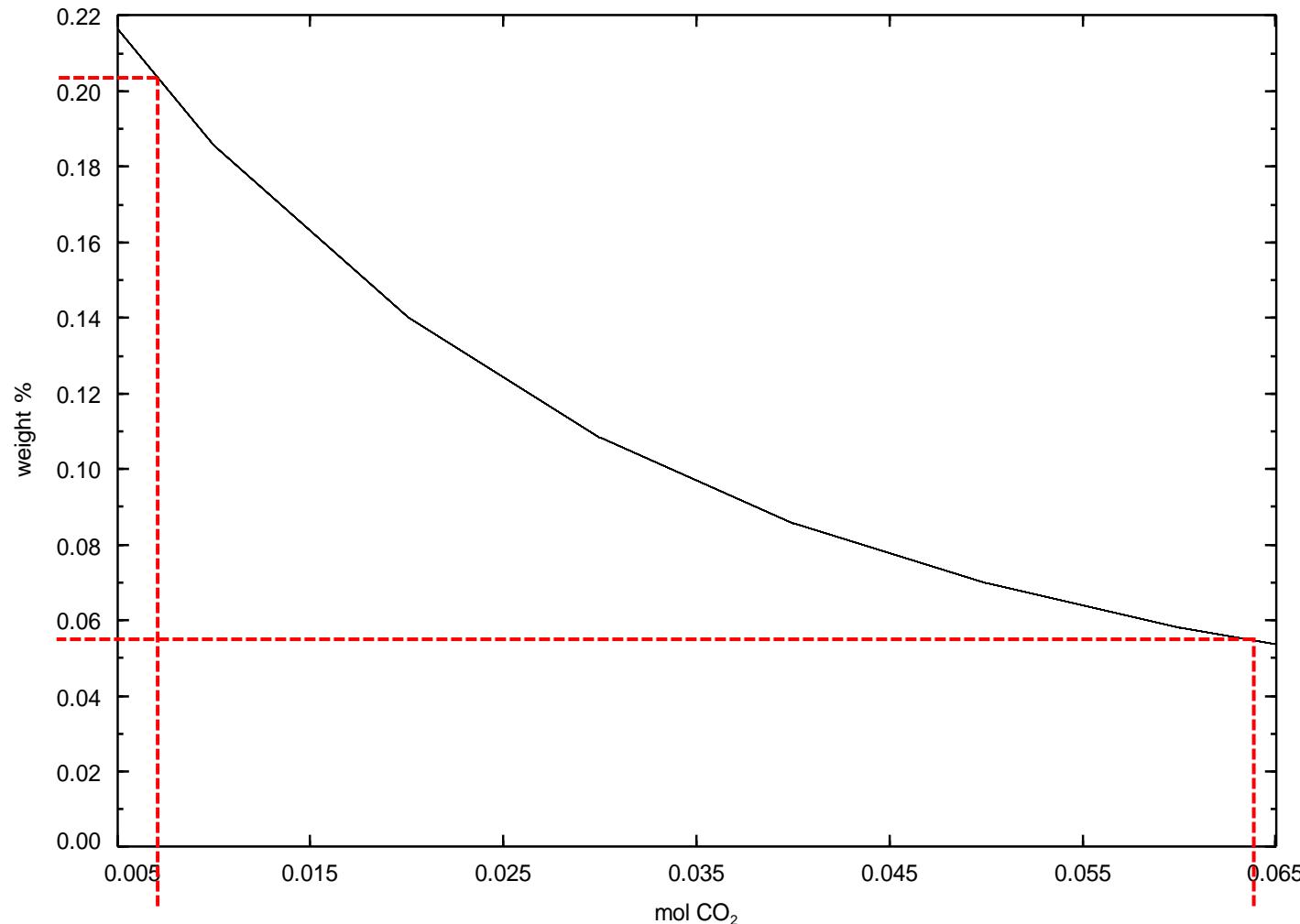
Enter a single value - or enter a range of values 'first last step'

Element C: 0,0005, 0,002, 0,0001
mass fraction: (0.05%), (0.2%)

Cancel Help OK

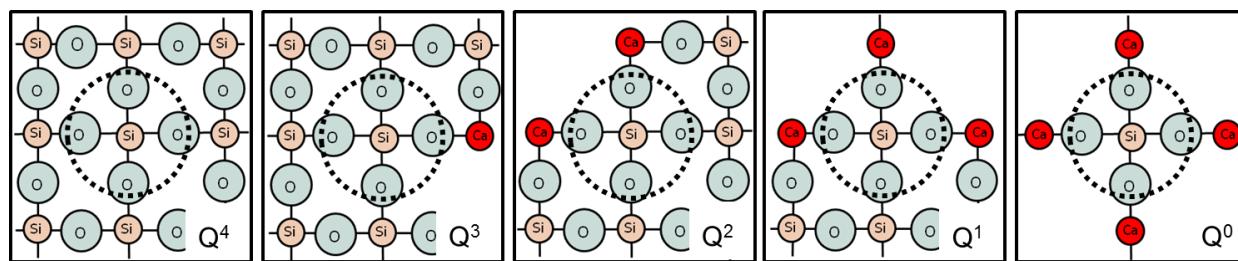
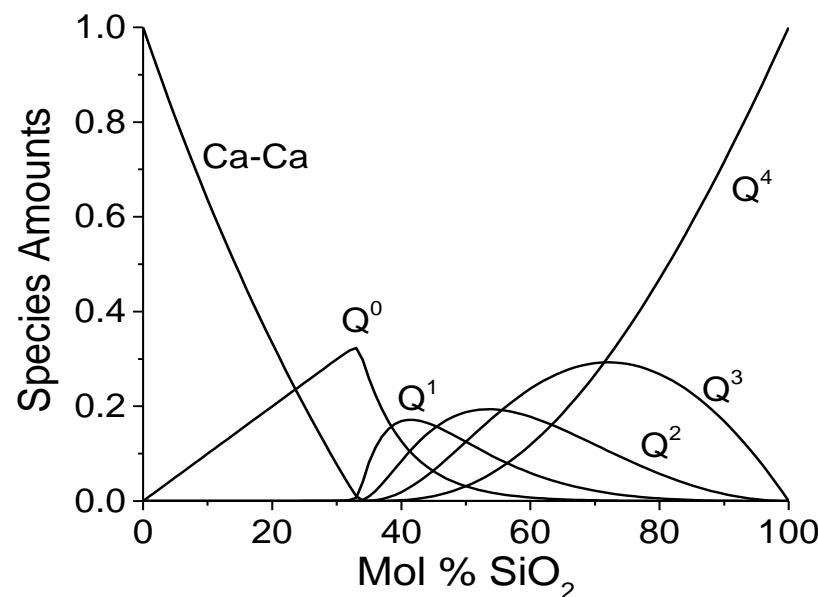
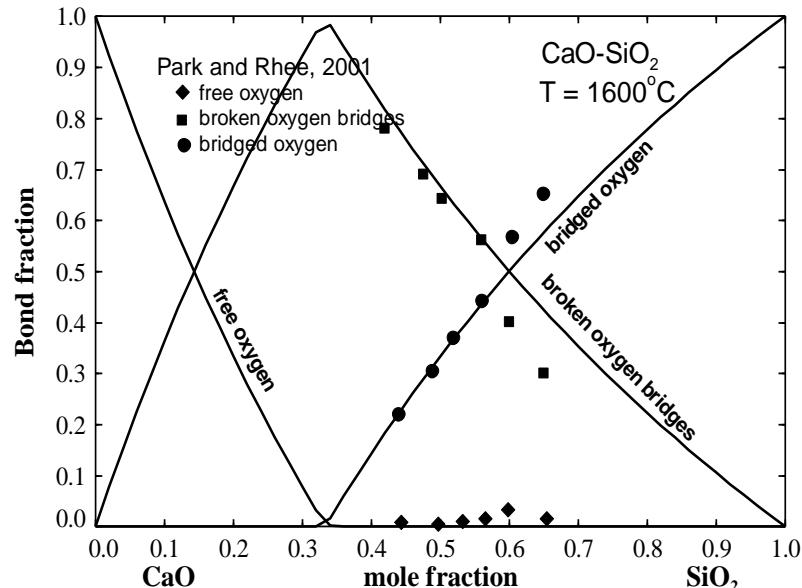
Carburization and Decarburization: Composition target

99.62 Fe + 0.08 C + 0.2 Mn + 0.1 Si +
C:\FactSage73\Equi0.res 26Dec19



Structure of silicate slag

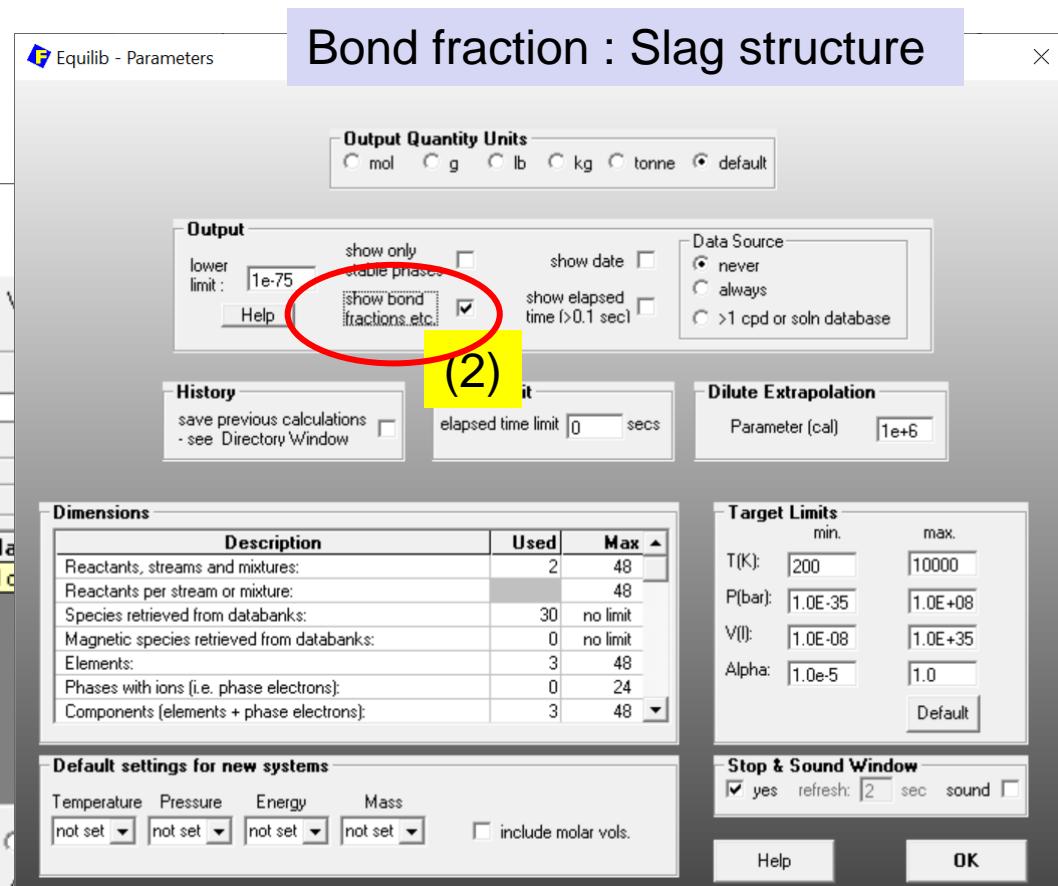
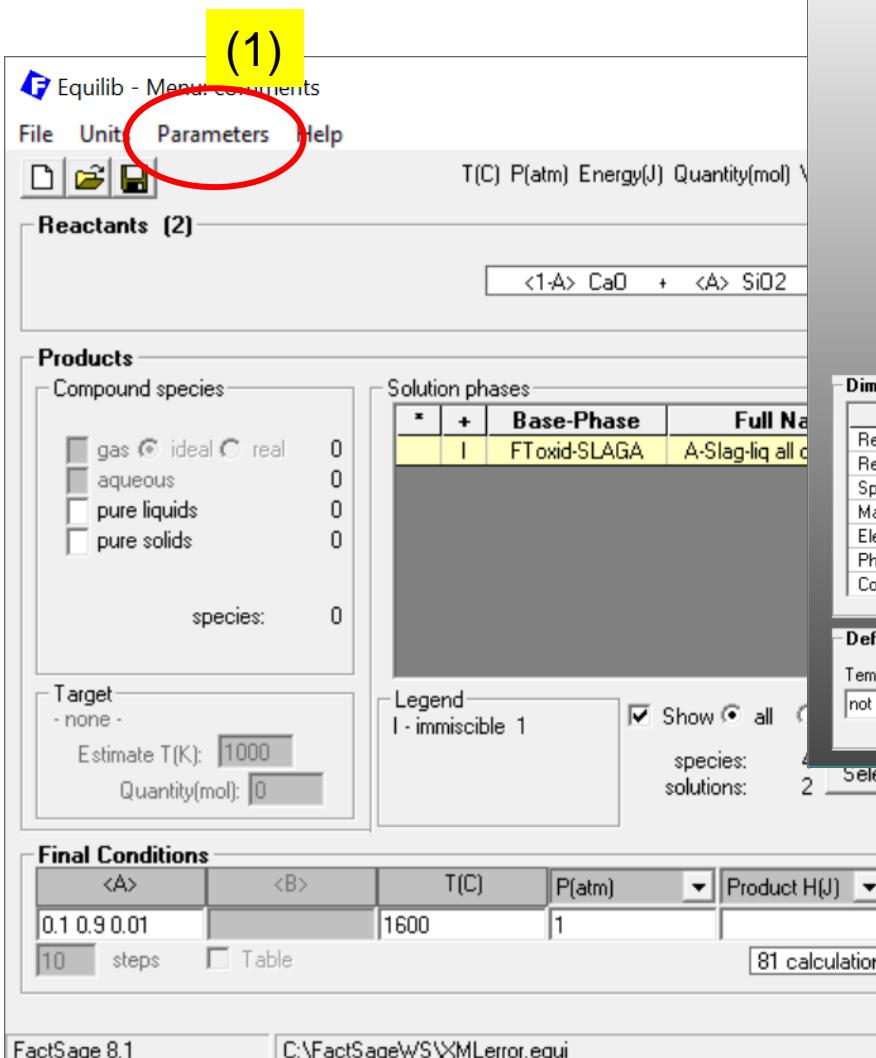
Modified Quasichemical Model: $O^{2-} + O^0 = 2O^-$



See the following paper for the calculation of Q species from bond fraction:

ERIC THIBODEAU, AIMEN E. GHERIBI, and IN-HO JUNG: METALLURGICAL AND MATERIALS TRANSACTIONS B vol. 47B, 2016, p. 1147

Structure of molten slag



Structure of molten slag

Equilib - Results A=0.1 (page 11/101)

Output Edit Show Pages Final Conditions

A=0.13 | A=0.14 | A=0.15 | A=0.16 | A=0.17 | A=0.18 | A=0.19 | A=0.20 | A=0.21 | A=0.22 | A=0.23 | A=0.24 |
A=0 | A=0.01 | A=0.02 | A=0.03 | A=0.04 | A=0.05 | A=0.06 | A=0.07 | A=0.08 | A=0.09 | A=0.1 | A=0.11 | A=0.12 |

<1-A> CaO + <A> SiO₂ =

1.0000 mol Slag-liq#1
(56.478 gram, 1.0000 mol)
+ 0 mol Slag-liq#2
(1600 C, 1 atm, a=1.0000)
(0.10000 SiO₂
+ 0.90000 CaO)

Site fraction of sublattice constituents:

Si	0.10000
Ca	0.90000
O	1.0000

Mole fraction of quadruplets:

Si-Si-O-O	1.3397E-05
Ca-Ca-O-O	0.63638
Si-Ca-O-O	0.36361
Total amount/mol	0

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

Ca	0.90000	36.070	0.42857	0.63866
Si	0.10000	2.8085	4.7619E-02	4.9728E-02
O	1.1000	17.599	0.52381	0.31161

where "A" on the reactant side is 0.10000

Cut-off limit for phase activities = 1.00E-75

Bond fraction : Slag structure

Si-Si-O-O : O⁰ (bridged oxygen)

Ca-Ca-O-O: O²⁻ (free oxygen)

Si-Ca-O-O: O⁻ (broken oxygen)

Structure of molten slag

The figure shows the Equilibrium software interface. The top left displays the XML output for various compositions (A=0.23, A=0.24, A=0.1, A=0.11, A=0.12). The top right shows the XML file path: C:\Users\...S\XML_out.xml. The bottom right shows the Graph setup window for Page 1, where the Y-axis is set to 'Bond Fractions'. The bottom center shows a list of species/phases: Si-Si-0-0, Ca-Ca-0-0, Si-Ca-0-0, Ca-Ca-0-0, Si-Ca-0-0, Ca-Ca-0-0, and Si-Ca-0-0.

(1) Run XML output

(2)

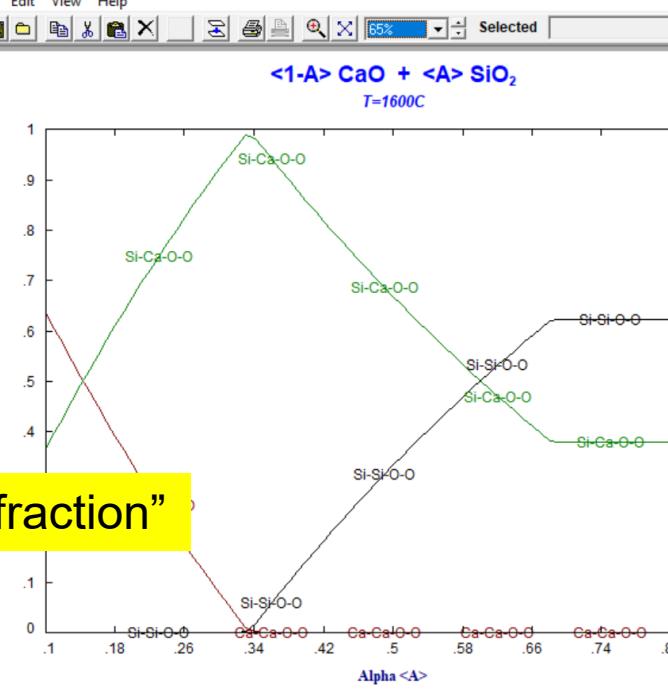
(3) Select

(4)

Final results

Figure

File Add Edit View Help



bond fraction”

MIN MAX Pseudonym

1.340E-05	9.939E-01	
1.605E-07	6.364E-01	
6.089E-03	9.872E-01	
1.605E-07	6.364E-01	
6.089E-03	9.872E-01	
1.605E-07	6.364E-01	
6.089E-03	9.872E-01	

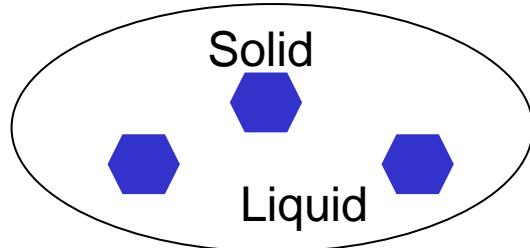
(5)

ol fract. C gram C Wt. fract. kg C lb



Draw >> Cancel

Viscosity Calculation: S+L mixtures (Einstein-Roscoe Eq.)



Viscosity of liquid slag can be calculated from “Viscosity” module from slag composition calculated from “Equilib” (Step-2)

Einstein-Roscoe Equation (one of the most well-accepted equation of viscosity for solid+liquid mixture)

$$\text{Viscosity}_{(\text{solid+liquid mixture})} \approx \text{Viscosity}_{(\text{liquid})} \cdot (1 - \text{solid fraction})^{-2.5}$$

Original Einstein-Roscoe equation use ‘volume fraction of solid’ instead of ‘solid fraction’ and correction term for morphology, but all these values are not very well-known for general solids, we can simply use the solid fraction (wt fraction) for this equation as approximation.

This value can be calculated using “Equilib” module at given system composition and temperature (Step-1).

Viscosity Calculations “Step-1”: Composition of liquid slag

Equilib - Menu: last system

File Units Parameters Help

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

Reactants (4)

(gram) 40 CaO + 10 MgO + 15 Al₂O₃ + 35 SiO₂

Products

Compound species

gas	ideal	real	0
aqueous	0	0	0
pure liquids	0	0	0
+ pure solids	50	50	50
species:	50		

Target: none

Estimate T(K): 1000

Quantity(g): 0

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
		1500	1400	10

10 steps Table 11 calculations

FactSage 7.3

Equilib - Results 1500 C (page 1/11)

Output Edit Show Pages Final Conditions

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

1500 C | 1490 C | 1480 C | 1470 C | 1460 C | 1450 C | 1440 C | 1430 C | 1420 C | 1410 C | 1400 C

(gram) 40 CaO + 10 MgO + 15 Al₂O₃ + 35 SiO₂ =

100.00 gram Slag-liq#1
(100.00 gram, 1.6910 mol)

+ 0 Spreadsheet Setup

System Properties

Property columns: 1

Column: -1 - Variable: T(C)

Species Properties

Columns per species: 2

order species: order props.

Column: -1 - -2 - Variable: Wt% g

Species

Columns: 9

Select... Cancel Default

Spreadsheet - Equilib Page 1/11 : T(C) = 1500, P(atm) = 1

File Edit Show

Selected: 4/137 Spreadsheet Species 1 Pages: 1 - 11 [page]

Page 1/11 : T(C) = 1500 [min = 1400 at page 11; max = 1500 at page 1], P(atm) = 1

+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
49	Ca3MgSi2O8(s)	FToxid	Merwinite	V	0.4383		0.4383 [1]	0.9184 [11]	
50	CaAl2SiO6(s)	FToxid	Ca-Tschermak	V	3.6329E-02		3.6329E-02 [1]	5.5510E-02 [9]	
51	CaAl2Si2O8(s)	FToxid	Hexagonal	T	o	1.7499E-07	1.7499E-07 [1]	4.5369E-07 [10]	
52	CaAl2Si2O8(s2)	FToxid	Anorthite	V	1.0647E-02		1.0647E-02 [1]	1.8093E-02 [9]	
53	Ca2Al2SiO7(s)	FToxid	Gehlenite	V	0.3592		0.3592 [1]	0.5650 [8]	
54	Ca3Al2Si3O12(s)	FToxid	Grossularite	V	2.9049E-04		2.9049E-04 [1]	8.3434E-04 [10]	
+ 0	gram a-(Ca,Mg,O)								
+ 55	Al2O3(SLAGA)	FToxid	FToxid-SLAGA#		1.0579E-02		7.1259E-03 [11]	1.0678E-02 [8]	
+ 56	SiO2(SLAGA)	FToxid	FToxid-SLAGA#		1.3952E-02		1.3422E-02 [8]	1.5124E-02 [11]	
+ 57	CaO(SLAGA)	FToxid	FToxid-SLAGA#		5.8151E-03		3.2050E-03 [11]	5.8151E-03 [1]	
+ 58	MgO(SLAGA)	FToxid	FToxid-SLAGA#		3.6617E-02		3.3706E-02 [8]	3.9552E-02 [11]	
+ 59	Al3O4[1+](SPINA)	FToxid	FToxid-SPINA		6.6803E-02		6.6803E-02 [1]	0.1082 [9]	
+ 60	Al10Al2O4(SPINA)	FToxid	FToxid-SPINA		2.4777E-08		1.5121E-09 [11]	2.4777E-08 [11]	
+ 61	Mg1Al2O4(SPINA)	FToxid	FToxid-SPINA		0.2186		0.2186 [1]	0.3749 [11]	
+ 62	Al11Mg2O4[1](SPINA)	FToxid	FToxid-SPINA		1.5367E-02		1.5367E-02 [1]	2.5878E-02 [9]	
+ 63	Mg3O4[2](SPINA)	FToxid	FToxid-SPINA		3.3358E-03		3.3358E-03 [1]	5.2168E-03 [9]	
+ 64	Mg1O4[6](SPINA)	FToxid	FToxid-SPINA		1.8434E-11		7.2979E-13 [11]	1.8434E-11 [1]	
+ 65	CaO(MeO_A)	FToxid	FToxid-MeO_A#		4.4352E-02		3.3739E-02 [11]	4.4352E-02 [1]	
+ 66	MgO(MeO_A)	FToxid	FToxid-MeO_A#		0.3182		0.3182 [1]	0.4592 [11]	

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

Select All Clear OK

Viscosity Calculations “Step-2”: Viscosity of liquid slag

Viscosity of liquid oxide “Melts” database is for liquid slag

File Edit Units Options Help

Calculate >>

Database : Melts

Glasses

Include/Remove Fluoride Components

Clear ALL

OPT

Enter the amounts of the constituents in the rows below. Then press on Calculate to show the viscosity.

	A SiO ₂ [g]	B Al ₂ O ₃ [g]	C CaO [g]	D MgO [g]	Z ZnF ₂ [g]	AA Temperature [°C]	AB visc[poise]	AC	AD
1									
2	35	15	40	10		1500.00	2.571	Melts	
3	35	15	40	10		1490.00	2.725	Melts	
4	35	15	40	10		1480.00	2.890	Melts	
5	35	15	40	10		1470.00	3.068	Melts	
6	35	15	40	10		1460.00	3.259	Melts	
7	35	15	40	10		1450.00	3.464	Melts	
8	35	15	40	10		1440.00	3.685	Melts	
9	35	15	40	10		1430.00	3.923	Melts	
10	32.971	13.594	37.333	9.5973		1420.00	4.122	Melts	
11	271	775	707	033					
12	26.358	9.9068	29.133	8.1082		1410.00	4.246	Melts	
13	269	833	419	062					
14									
15									
16	Composition of liquid slag from Equilib								
17									
18									
19									
20									
21									
22									

Take these results for next step

Composition of liquid slag from Equilib

Viscosity Calculations “Step-3”: Liquid + Solid mixture

	C	D	E	F	G	H	I	J	K	L
1	Wt%-SiO2(SLAGA#1)	Wt%-CaO(SLAGA#1)	Wt%-MgO(SLAGA#1)	g-xid-SLAGA#1	amount of solids	viscosity of liquid	solid+liquid			
2	35	40	10	100	0	2.366	2.366			
3	35	40	10	100	0	2.503	2.503			
4	35	40	10	100	0	2.649	2.649			
5	35	40	10	100	0	2.805	2.805			
6	35	40	10	100	0	2.972	2.972			
7	35	40	10	100	0	3.152	3.152			
8	35	40	10	100	0	3.345	3.345			
9	35	40	10	100	0	3.553	3.553			
10	35.264514	39.930352	10.264831	93.496742	6.503258	3.744	4.429397			
11	35.858294	39.633643	11.030572	73.506394	26.493606	3.897	8.412355			
12	36.252378	38.793831	12.32313	46.07094	53.92906	4.042	28.05619			
13										
14										
15										
16										
17										
18										
19										
20										
21										
22										
23										
24										
25										

Einstein-Roscoe
Eq.

Amount
of slag

Step-2

Amount of solids
(100-amount of liquid)

Thanks to FactSage Steelmaking Consortium Members

posco

 **TATA STEEL**

voestalpine



 **HYUNDAI
STEEL**

 **NIPPON STEEL**


DOOSAN

Doosan Heavy Industries
& Construction

SéAH Besteel


JFE

RioTinto


SCHOTT
glass made of ideas


RHI MAGNESITA

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