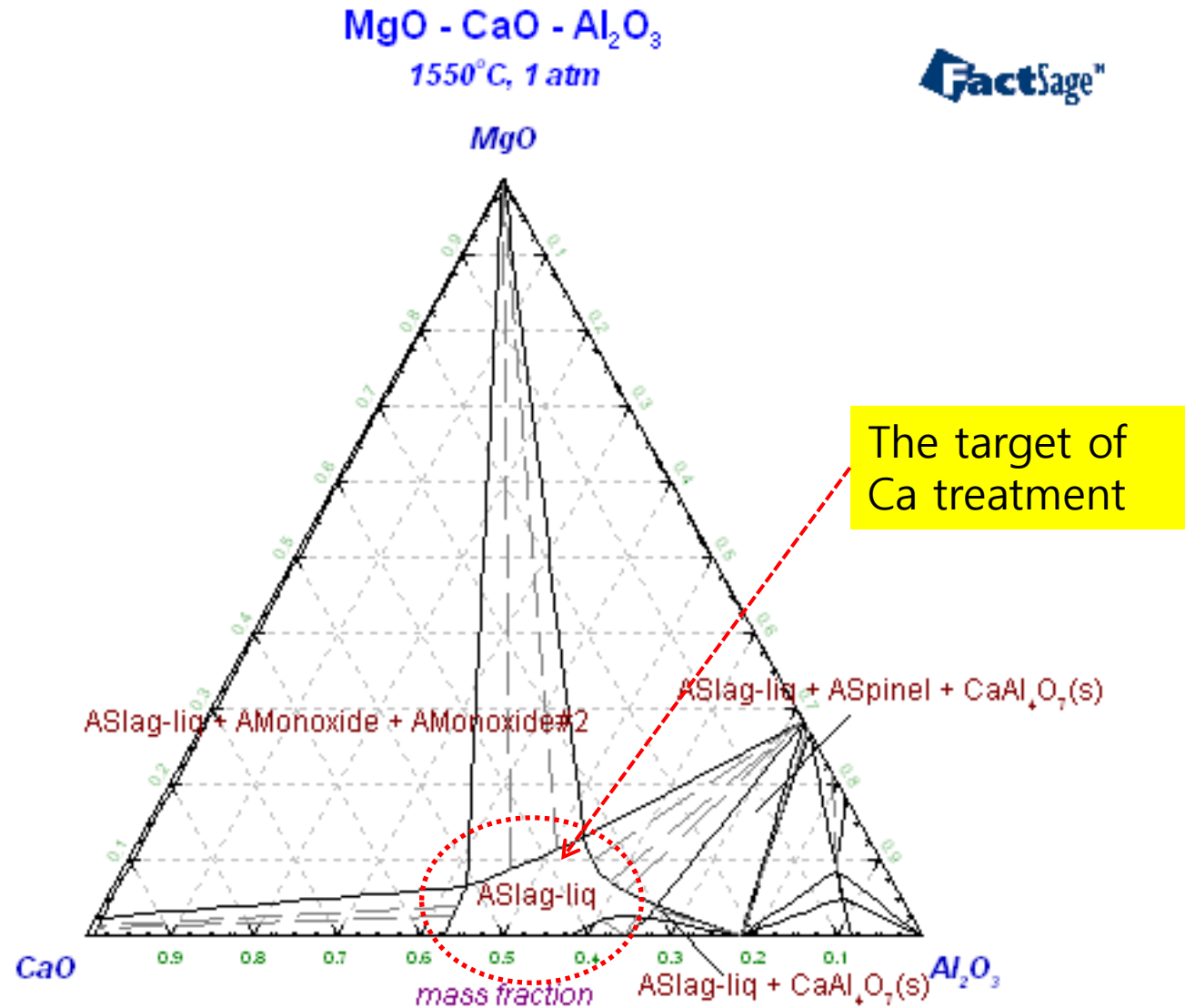


Application 5: **Re-oxidation and inclusion modification in the tundish – Ca treatment**

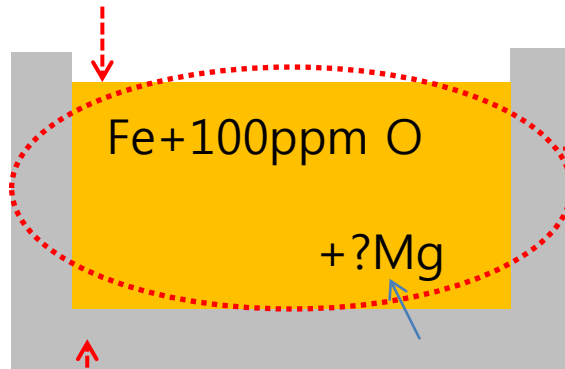
Junghwan Kim
Email: junghwan.kim@mail.mcgill.ca

Ex4-1. Reoxidation and inclusion modification in the tundish



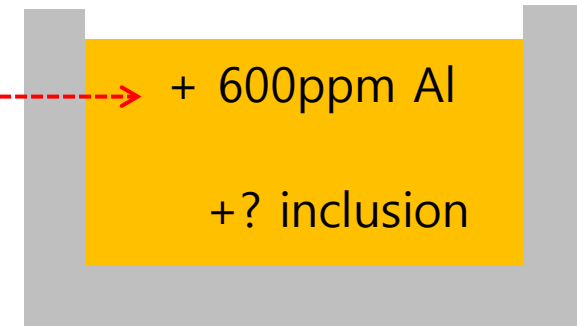
Ex4-1. Reoxidation and inclusion modification in the tundish

At 1550°C

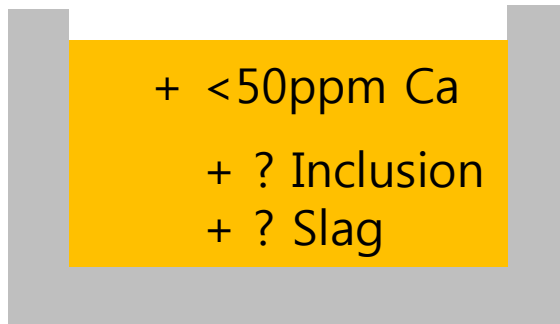


MgO based refractory

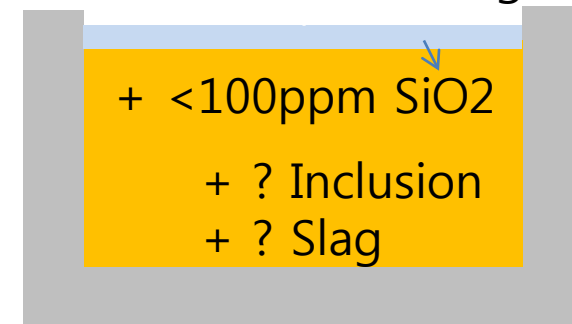
Al killed steel



Ca treatment: liquid slag

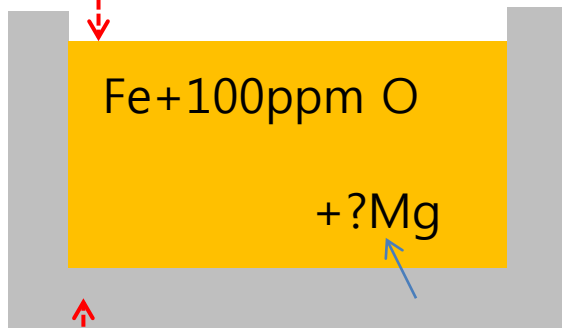


Reoxidation: assuming mainly due to SiO₂ based slag



Ex4-1. Reoxidation and inclusion modification in the tundish

Al killed steel



MgO based refractory

F Menu - Equilib: comments

File Units Parameters Help

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

Reactants (3)

(gram) 99.9 Fe + 0.01 O + MgO

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- pure solids 4
- suppress duplicates

species: 4

Target

- none -

Estimate T(K):

Mass(g):

Solution species

| * | + | Base-Phase | Full Name |
|---|---|--------------|--------------------------|
| | + | FTmisc-FeLQ | Fe-liq |
| | | FToxid-SLAGA | ASlag-liq all oxides + S |
| | + | FToxid-SPINA | ASpinel |
| | + | FToxid-MeO_A | AMonoxide |

Legend

| - immiscible 1

+ - selected 3

Show all selected

species: 25

solutions: 5

Custom Solutions

- fixed activities
- ideal solutions
- activity coefficients

Pseudonyms

apply

include molar volumes

Total Species (max 1500) 29

Total Solutions (max 40) 5

Final Conditions

| <A> | | T(C) | P(atm) | Product H(J) |
|-----|-----|------|--------|--------------|
| | | 1550 | 1 | |

10 steps Table

Equilibrium

- normal normal + transitions
- transitions only
- open

FactSage 6.3 C:\FactSage\EquiEx4-1(a).DAT

Ex4-1. Reoxidation and inclusion modification in the tundish

Results - Equilib 1550 C

Output Edit Show Pages

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

FactSage 6.3

(gram) 99.9 Fe + 0.01 O + MgO =

99.888 gram Fe-liq
(199.888 gram, 1.7889 mol)
(1550 C, 1 atm, a=1.0000)
(99.994 wt.% Fe FTmisc
+ 5.0050E-03 wt.% O FTmisc
+ 1.0263E-06 wt.% Mg FTmisc
+ 5.3290E-04 wt.% MgO FTmisc)

| System component | Mole fraction | Mass fraction |
|------------------|---------------|---------------|
| Fe | 0.99981 | 0.99994 |
| Mg | 7.4064E-06 | 3.2238E-06 |
| O | 1.8206E-04 | 5.2165E-05 |

+ 1.0219 gram AMonoxide
(1.0219 gram, 2.5110E-02 mol)
(1550 C, 1 atm, a=1.0000)
(2.1884 wt.% FeO FToxid
+ 6.8499E-03 wt.% Fe2O3 FToxid
+ 97.805 wt.% MgO FToxid)

| System component | Mole fraction | Mass fraction |
|------------------|---------------|---------------|
| Fe | 6.2157E-03 | 1.7059E-02 |
| Mg | 0.49378 | 0.58980 |
| O | 0.50000 | 0.39314 |

+ 0 gram ASlag-liq#1
(1550 C, 1 atm, a=6.5420E-02)

Only save liquid Fe
as stream file for next step

MgO based
refractory

Ex4-1. Reoxidation and inclusion modification in the tundish

Al killed steel

+ 600ppm Al

+? inclusion

The screenshot shows the FactSage 6.3 Equilib: software interface. The window title is "F Menu - Equilib:". The menu bar includes "File", "Units", "Parameters", and "Help". The main area is divided into several sections:

- Reactants (2):** A text box contains "(gram) 100% [Ex4-1(a)] + 0.06 Al".
- Products:**
 - Compound species:** Radio buttons for "gas", "ideal", "real", "aqueous", "pure liquids", and "pure solids" (checked). A "suppress duplicates" checkbox is also checked. The "species:" count is 10.
 - Solution species:** A table with columns "Base-Phase" and "Full Name".

| * | + | Base-Phase | Full Name |
|---|---|--------------|--------------------------|
| | + | FTmisc-FeLQ | Fe-liq |
| | | FToxid-SLAGA | ASlag-liq all oxides + S |
| | | FToxid-SPINA | ASpinel |
| | + | FToxid-MeO_A | AMonoxide |
| | | FToxid-CORU | M2O3(Corundum) |
 - Legend:** "I - immiscible 3", "+ - selected 2".
 - Show:** "all" (selected) or "selected".
 - species:** 63, **solutions:** 8.
- Final Conditions:** A table with columns "<A>", "", "T(C)", "P(atm)", and "Product H(J)".

| <A> | | T(C) | P(atm) | Product H(J) |
|-----|-----|------|--------|--------------|
| | | 1550 | 1 | |
- Equilibrium:** Radio buttons for "normal" (selected), "normal + transitions", "transitions only", and "open".

Buttons for "Calculate >>", "Default", "List ...", and "Details ..." are visible. The bottom status bar shows "FactSage 6.3".

Ex4-1. Reoxidation and inclusion modification in the tundish

```
F Results - Equilib 1550 C
Output Edit Show Pages
T(C) P(atm) Energy(J) Mass(g) Vol(litre)

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

99.938 gram Fe-liq
(99.938 gram, 1.7906 mol)
(1550 C, 1 atm, a=1.0000)
( 99.945 wt.% Fe
+ 5.4402E-02 wt.% Al
+ 9.5917E-05 wt.% O
+ 2.6226E-06 wt.% Mg
+ 2.5691E-05 wt.% MgO
+ 3.7605E-04 wt.% AlO
+ 7.6232E-05 wt.% Al2O

System component      Mole fraction      Mass fraction
Fe                    0.99886            0.99945
Al                    1.1314E-03         5.4697E-04
Mg                    4.1599E-07         1.8115E-07
O                     9.1930E-06         2.6353E-06

+ 7.8284E-03 gram M2O3(Corundum)#1
(7.8284E-03 gram, 7.6778E-05 mol)
(1550 C, 1 atm, a=1.0000)
( 100.00 wt.% Al2O3
+ 7.8267E-06 wt.% Fe2O3

System component      Mole fraction      Mass fraction
Fe                    1.9989E-08         5.4742E-08
Al                    0.40000            0.52925
O                     0.60000            0.47075
```

Alumina inclusion cause nozzle clogging

```
F Results - Equilib 1550 C
Output Edit Show Pages
T(C) P(atm) E

+ 2.7607E-03 gram ASpinel#1
(2.7607E-03 gram, 1.9721E-05 mol)
(1550 C, 1 atm, a=1.0000)
( 9.2977E-09 wt.% Fe3O4
+ 1.1533E-09 wt.% Fe3O4[1-]
+ 1.1207E-12 wt.% Fe3O4[1+]
+ 9.5681E-06 wt.% Fe3O4[2-]
+ 3.9227E-07 wt.% Fe1O4[5-]
+ 3.2543E-03 wt.% Fe1O4[6-]
+ 6.4220E-02 wt.% FeAl2O4
+ 50.356 wt.% Al3O4[1+]
+ 7.8750E-03 wt.% Al1Fe2O4[1-]
+ 2.3230 wt.% Al1O4[5-]
+ 7.7410E-06 wt.% FeAl2O4[1+]
+ 7.6524E-06 wt.% Al1Fe2O4[1+]
+ 34.676 wt.% MgAl2O4
+ 6.5010 wt.% Al1Mg2O4[1-]
+ 4.4735 wt.% Mg3O4[2-]
+ 1.5818 wt.% Mg1O4[6-]
+ 5.2979E-06 wt.% Mg1Fe2O4
+ 1.0057E-06 wt.% Fe1Mg2O4[1-]
+ 8.3436E-03 wt.% Fe1Mg2O4[2-]
+ 5.4520E-03 wt.% Mg1Fe2O4[2-]
```

Formation of spinel phase

Save all phases as stream file for next step

Ex4-1. Reoxidation and inclusion modification in the tundish

Ca treatment: liquid slag

+ <100ppm Ca
+ ? Inclusion
+ ? Slag

The screenshot shows the FactSage Equilib: Ca treatment software interface. The window title is "F Menu - Equilib: Ca treatment". The interface includes a menu bar (File, Units, Parameters, Help), a toolbar, and several main sections:

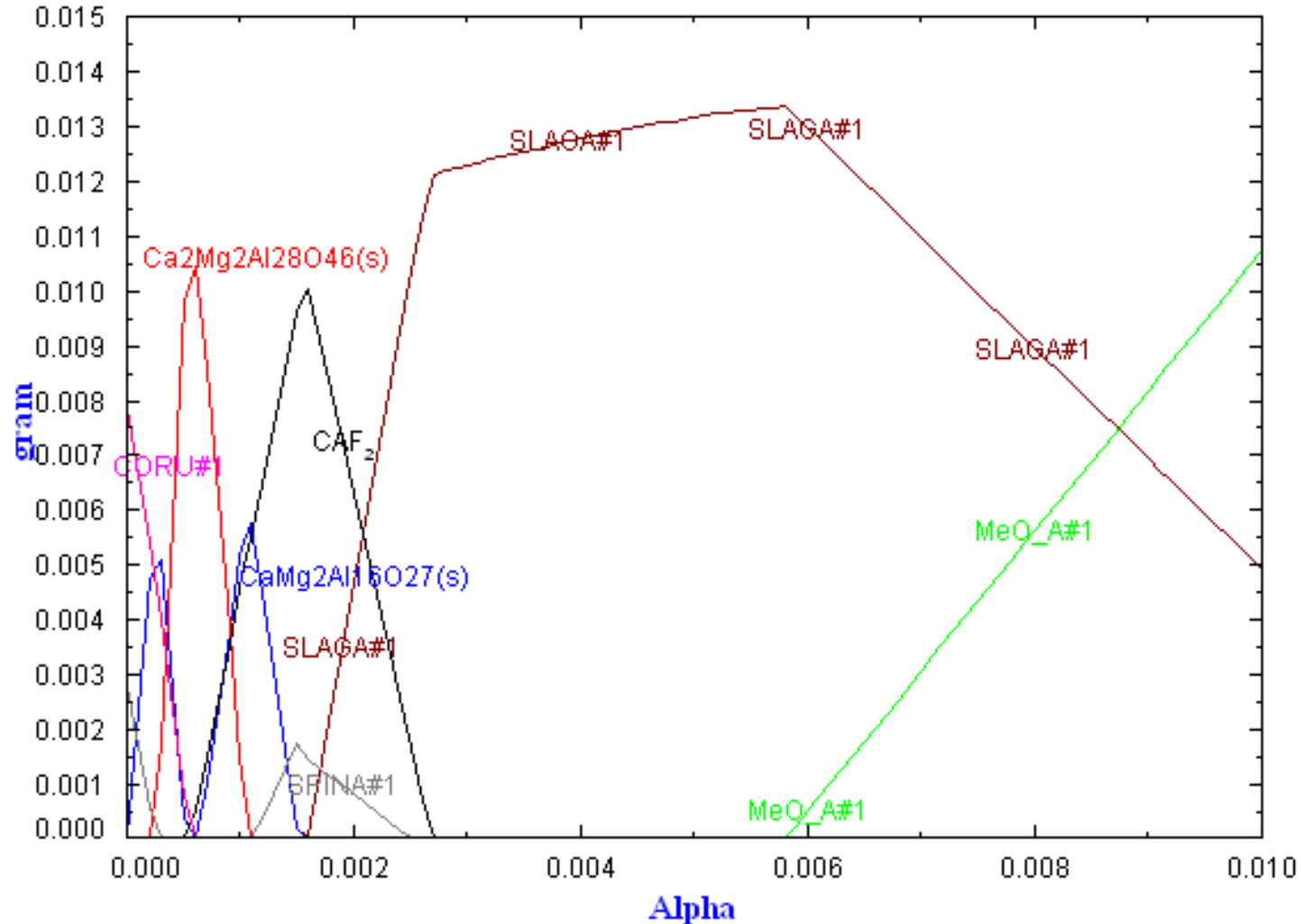
- Reactants (2):** A text box contains "[gram] 100% [Ex4-1(b)] + <A> Ca".
- Products:**
 - Compound species:** Radio buttons for gas, ideal (selected), and real. Checkboxes for aqueous, pure liquids, pure solids (checked), and suppress duplicates (checked). A button labeled "apply" is next to "suppress duplicates". The text "species: 21" is displayed.
 - Target:** A dropdown menu shows "- none -". Input fields for "Estimate T(K):" (value: 1000) and "Mass(g):" (value: 0) are present.
 - Solution species:** A table with columns for Base-Phase and Full Name. The table contains the following entries:

| * | + | Base-Phase | Full Name |
|---|---|--------------|--------------------------|
| | + | FTmisc-FeLQ | Fe-liq |
| | | FToxid-SLAGA | ASlag-liq all oxides + S |
| | | FToxid-SPINA | ASpinel |
| | | FToxid-MeO_A | AMonoxide |
| | + | FToxid-CAF6 | Ca(Al,Fe)12O19 |
| | + | FToxid-CAF3 | Ca(Al,Fe)6O10 |
| | + | FToxid-CAF2 | Ca(Al,Fe)4O7 |
| | | FToxid-CAF1 | Ca(Al,Fe)2O4 |
 - Legend:** Shows "I - immiscible 5" and "+ - selected 6". A "Show" dropdown is set to "all". The text "species: 87" and "solutions: 16" is displayed, along with a "Select" button.
 - Custom Solutions:** Radio buttons for fixed activities, ideal solutions, and activity coefficients. A "Details ..." button is present.
 - Pseudonyms:** An "apply" checkbox and a "List ..." button.
 - Summary:** "include molar volumes" checkbox is unchecked. "Total Species (max 1500)" is 108 and "Total Solutions (max 40)" is 16. A "Default" button is at the bottom.
- Final Conditions:** A table with columns for <A>, , T(C), P(atm), and Product H(J). The values are 0, 0.01, 0.0001, 1550, and 1. A "steps" dropdown is set to 10. A "Table" checkbox is unchecked. A "101 calculations" button is present.
- Equilibrium:** Radio buttons for normal (selected), normal + transitions, transitions only, and open. A "Calculate >>" button is at the bottom.

The status bar at the bottom shows "FactSage 6.3" and the file path "C:\FactSage\EquiEx4-1(c).DAT".

Ex4-1. Reoxidation and inclusion modification in the tundish

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



Ex4-1. Reoxidation and inclusion modification in the tundish

Reoxidation: assuming mainly due to SiO₂ based slag

+ <100ppm SiO₂
+ ? Inclusion
+ ? Slag

F Menu - Equilib: Reoxidation

File Units Parameters Help

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

Reactants (2)

(gram) 100% [Ex4-1(c)] + <A> SiO₂

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- pure solids 69

suppress duplicates apply

species: 69

Target

- none -

Estimate T(K): 1000

Mass(g): 0

Solution species

| * | + | Base-Phase | Full Name |
|---|---|--------------|--------------------------|
| | + | FTmisc-FeLQ | Fe-liq |
| | | FToxid-SLAGA | ASlag-liq all oxides + S |
| | | FToxid-SPINA | ASpinel |
| | | FToxid-MeO_A | AMonoxide |
| | | FToxid-cPyrA | AClinopyroxene |
| | + | FToxid-oPyr | Orthopyroxene |
| | + | FToxid-pPyrA | AProtopyroxene |
| | + | FToxid-LcPy | LowClinopyroxene |

Legend

- | - immiscible 8
- + - selected 15

Show all selected

species: 288

solutions: 31

Custom Solutions

- fixed activities
- ideal solutions
- activity coefficients

Details ...

Pseudonyms

apply List ...

include molar volumes

Total Species (max 1500) 357

Total Solutions (max 40) 31

Default

Final Conditions

| <A> | | T(C) | P(atm) | Product H(J) |
|-----|-------|--------|--------|--------------|
| 0 | 0.005 | 0.0001 | 1550 | 1 |

10 steps Table

51 calculations

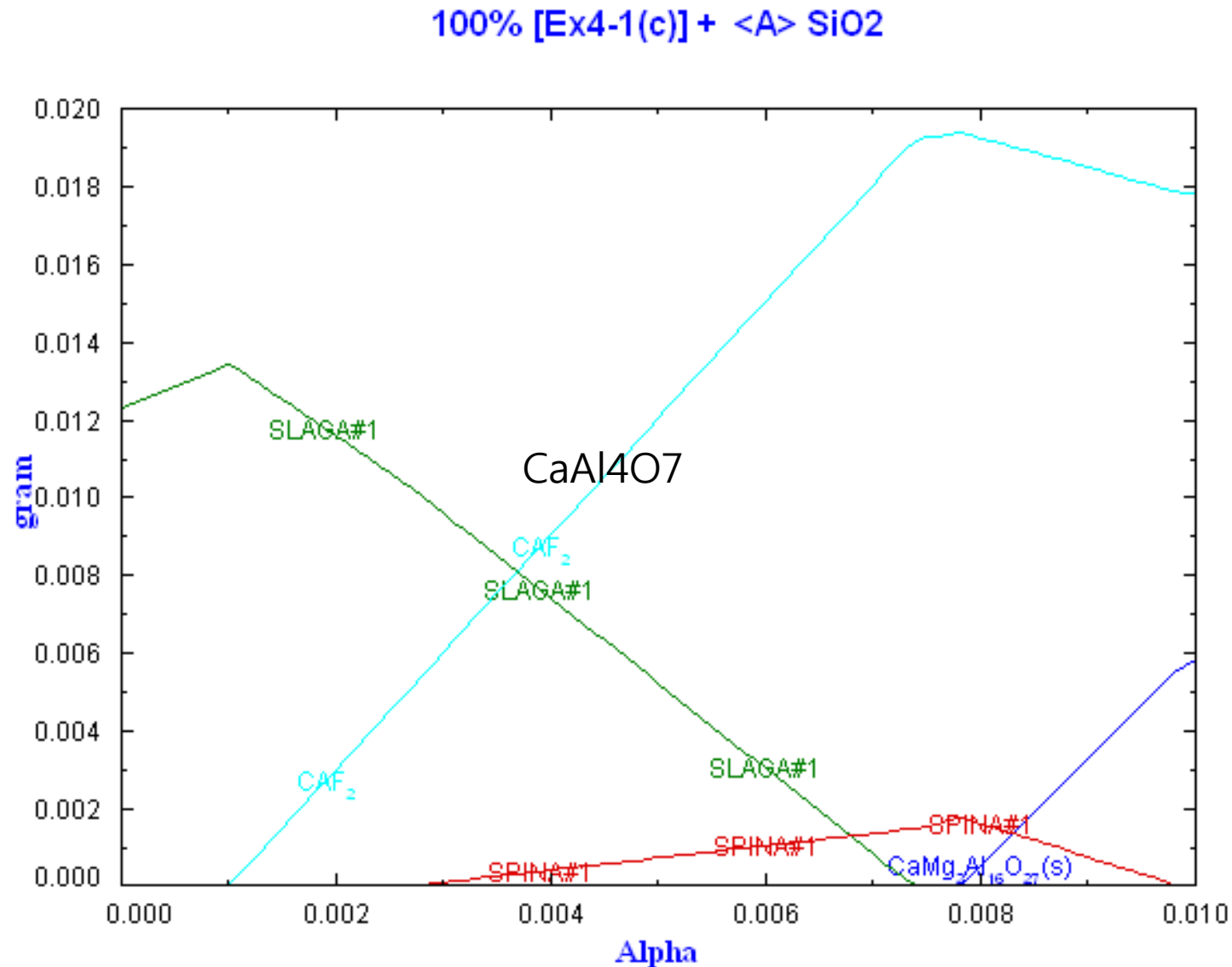
Equilibrium

- normal normal + transitions
- transitions only
- open

Calculate >>

FactSage 6.3 C:\FactSage\EquiEx4-1(d).DAT

Ex4-1. Reoxidation and inclusion modification in the tundish

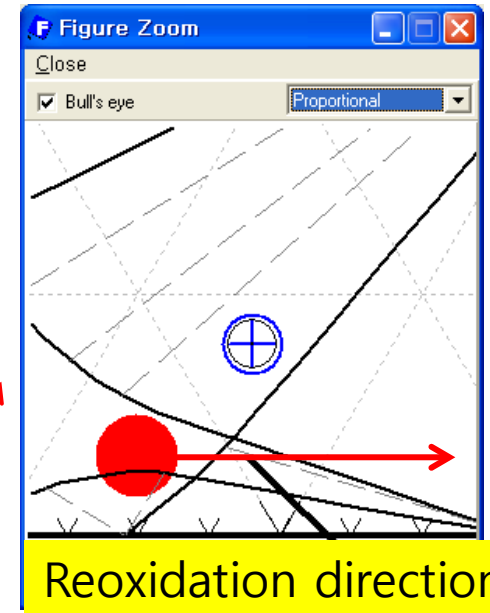
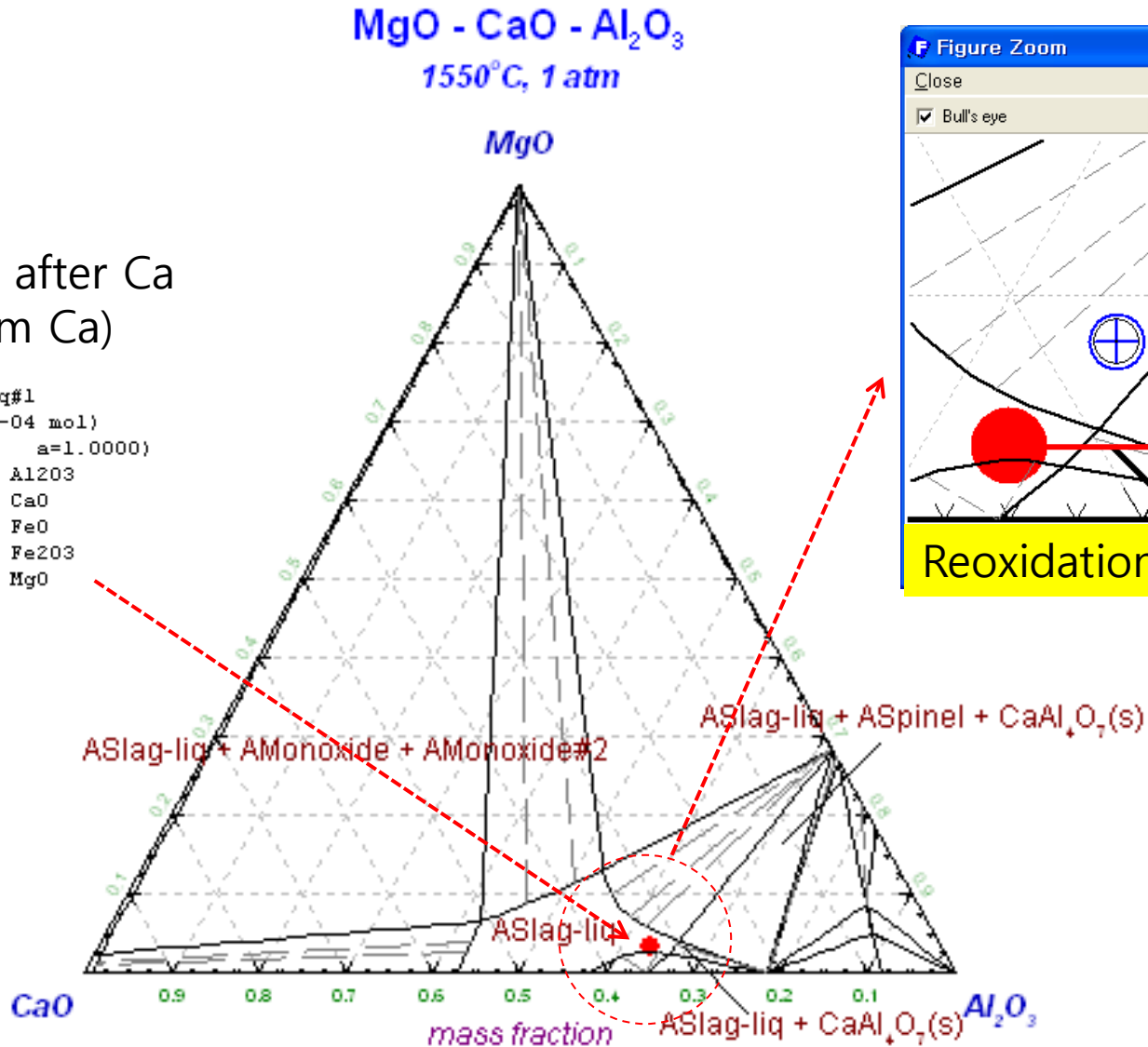


Ex4-1. Reoxidation and inclusion modification in the tundish

Slag composition after Ca treatment (30 ppm Ca)

```

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



Ex4-2. Reoxidation of Al killed Ti bearing steel

Data Search

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

Miscellaneous

FactPS FSopp BINS compounds only

FToxid FSlead SGPS solutions only

FTsalt FSlite SGTE no datab

FTmisc FSstel SGnobl Clear A

FTball FSnobl SGSold Select A

FToxCN FSupsi SGnucl Add/Remov

FTfritz RefreshData

FThelg ELEM **Other**

FTpulp FTdemo TDnucl

FTlite

Information

Options

Default

Include

gaseous ions (plasmas)

aqueous species

limited data compounds (25C)

Cancel Summ

Menu - Equilib: last system

File Units Parameters Help

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

Reactants (8)

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

Products

Compound species

gas ideal real 56

aqueous 0

pure liquids 0

pure solids 123

suppress duplicates apply

* - custom selection

species: 179

Solution species

| * | + | Base-Phase | Full Name |
|---|---|--------------|-------------------|
| | | FToxid-ILME? | ?Ilmenite |
| | + | FToxid-PSEU | Pseudobrookite |
| | + | FToxid-TiSp | Titania_Spinel |
| | + | FToxid-TSpi | Tetragonal-Spinel |
| | + | FToxid-Bixb | Mn2O3(Bixbyite) |
| | + | FToxid-Brau | Mn7SiO12 |
| | + | FToxid-Rhod | Rhodonite |
| | + | FToxid-AlSp | Al-spinel |

Legend

! - immiscible 5

+ - selected 11

Show all selected

species: 139

solutions: 21

Select

Custom Solutions

fixed activities

ideal solutions

activity coefficients

Details ...

Pseudonyms

apply List ...

include molar volumes

Total Species (max 1500) 318

Total Solutions (max 40) 21

Default

Final Conditions

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

10 steps Table

1 calculation

Equilibrium

normal normal + transitions

transitions only

open

Calculate >>

FactSage 6.3

Ex4-2. Reoxidation of Al killed Ti bearing steel

Results - Equilib 1600 C

Output Edit Show Pages

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

Plot

Equilib Results file

Stream File

Format

Fact-XML

Fact-Optimal

Fact-Function-Builder

Refresh ...

Fe (CO)5

Mn

N

O

+ 0.20001 wt.% Si

+ 9.9530E-02 wt.% Ti

+ 4.9668E-04 wt.% AlO

+ 5.7546E-04 wt.% TiO

+ 3.3327E-06 wt.% SiO

+ 3.4562E-05 wt.% MnO

+ 4.6211E-05 wt.% Al2O

+ 1.9820E-05 wt.% Ti2O

FactPS

FactPS

FactPS

FTmisc

FTmisc

FTmisc

FTmisc

FTmisc

FTmisc

FTmisc

FTmisc

FTmisc

FTmisc

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

Reactants - Equilib

File Edit Table Units Data Search Help

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

1 - 2

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

Initial Conditions

Next >>

FactSage 6.3 Compound: 3/37 databases Solution: 2/38 databases

“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

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

Ex4-2. Reoxidation of Al killed Ti bearing steel

Menu - Equilib: last system

File Units Parameters Help

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

Reactants (3)

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

Products

Compound species

- gas ideal real 56
- aqueous 0
- pure liquids 0
- pure solids 123
- suppress duplicates apply
- species: 179

Solution species

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

Legend

- I - immiscible 5
- + - selected 11

Target

Estimate T(C): 1600

Mass(g): 0

Final Conditions

| <A> | | T(C) | P(atm) | Product H(J) |
|-----|------|-------|--------|--------------|
| 0 | 0.05 | 0.001 | 1600 | 1 |

Equilibrium

- normal normal + transitions
- transitions only
- open

Calculate >>

FactSage 6.3

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

