

Case 2: Desulphurization

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

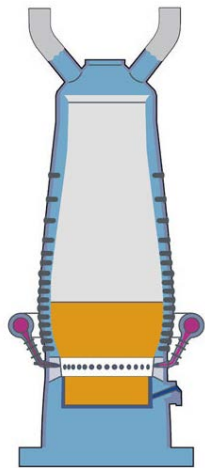
Desulphurization of Hot Metal

The hot metal tapped out of the blast furnace typically contains 0.04-0.07% S.

The oxygen converter must be charged with metal having 0.01-0.001% 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

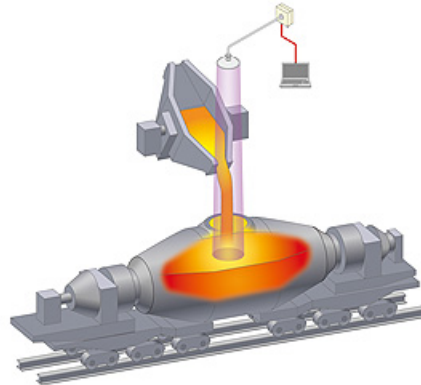
Blast Furnace (BF)



0.04-0.07% S



Torpedo Car



Basic Oxygen Furnace (BOF)



0.01-0.001% S

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.

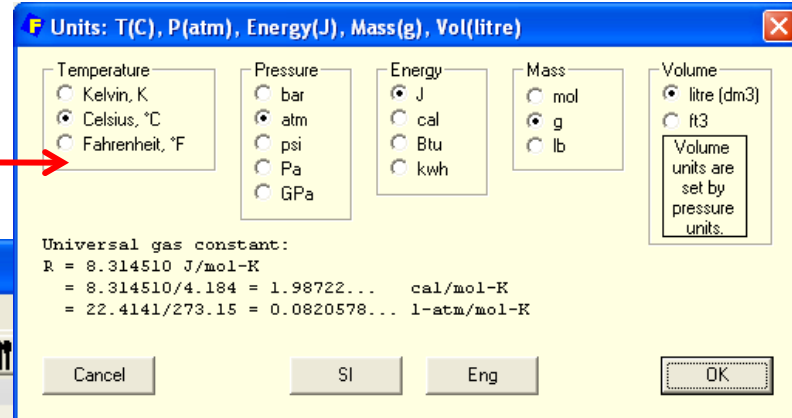
It will then be shown how the exact amount of desulphurizing agent can be selected to achieve the desired sulphur content.

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

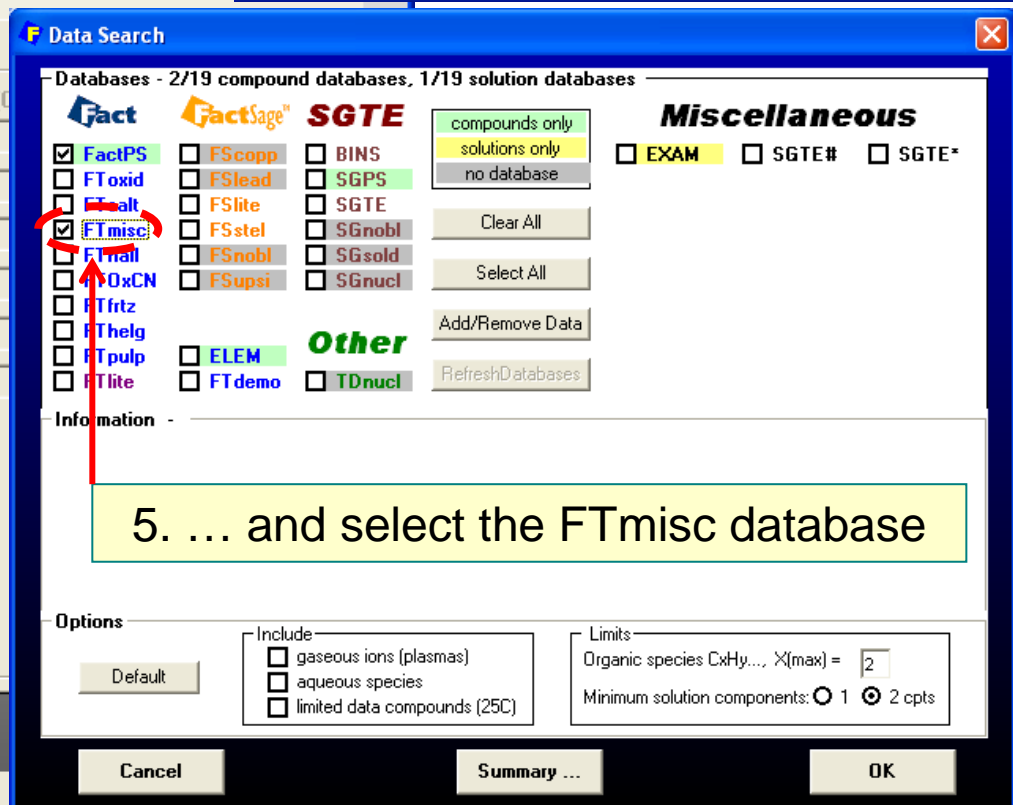


4. Click on "Data Search"...

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

6. Click "Next"

Next >>



5. ... and select the FTmisc database

Desulphurization of Hot Metal using Mg

1. Right-click on “pure solids”

F Selection - Equilib - no results -

File Edit Show Sort

Selected: 53/53 **SOLID** Duplicates selected.

- no results -

| | Code | Species | Data | Phase | T | V | Activity | Minimum | Maximum |
|---|------|------------|--------|----------------|---|---|----------|---------|---------|
| + | 40 | S(s) | FTmisc | orthorhombic | | o | | | |
| + | 41 | S(s2) | FTmisc | monoclinic | | o | | | |
| + | 42 | MnS(s) | FTmisc | alabandite | | | | | |
| + | 43 | MnS2(s) | FTmisc | hauerite | | | | | |
| + | 44 | FeS(s) | FTmisc | pyrrhotite-2c | | o | | | |
| + | 45 | FeS2(s) | FTmisc | pyrite | | | | | |
| + | 46 | Fe7S8(s) | FTmisc | pyrrhotite-4c | | o | | | |
| + | 47 | Fe9S10(s) | FTmisc | pyrrhotite-5c | | o | | | |
| + | 48 | Fe10S11(s) | FTmisc | pyrrhotite-11c | | o | | | |
| + | 49 | Fe11S12(s) | FTmisc | pyrrhotite-6c | | o | | | |
| + | 50 | C(s) | FactPS | graphite | | V | | | |
| + | 51 | Cr(s) | FactPS | diamond | | V | | | |

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

species: 0 solutions: 0 Select Default

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

3. We need to select each phase only once, so we will have to “suppress duplicates”

Desulphurization of Hot Metal using Mg

1. Left-click on “suppress duplicates”

The screenshot shows the FactSage 6.3 interface. In the 'Reactants' section, the input is '(gram) 94.335 Fe + 4.5 C + 0.5 Si + ...'. In the 'Products' section, under 'Compound species', the 'suppress duplicates' checkbox is checked, and the 'apply' button is highlighted with a red arrow. The 'Solution species' table is visible, listing various databases like FTmisc-FeLQ, FTmisc-MATT, etc. The 'Duplicate Compounds' dialog box is open, showing instructions on how to handle duplicate compounds and a list of databases in the priority list: FTmisc, FactPS.

| * | + | Base-Phase |
|---|---|--------------|
| | | FTmisc-FeLQ |
| | | FTmisc-MATT |
| | | FTmisc-FeS_ |
| | | FTmisc-MAT2C |
| | | FTmisc-PYRRC |
| | | FTmisc-BCCS |
| | | FTmisc-FCCS |
| | | FTmisc-MS-c |

Duplicate Compounds

When you click (mouse left button) on a "gas", "liquid", "aqueous" or "solid" compound check box, then all the compounds in that group are selected.

To avoid selecting duplicate compounds, you can specify a database priority list - the most important database is first and the least important is last. For duplicate compounds in a given group, only those compounds from the most important database will be selected. Not all the databases need to be entered - for example if only one database is specified, then duplicate compounds from the other databases will only be suppressed for those compounds found in this one database.

Note: a compound is considered a duplicate if a pure substance in another database has the same chemical formula in the same phase (solid, liquid or gas) - no distinction is made for allotropes and isomers. For example, Fe(s1) in databank A is duplicate of Fe(s1), Fe(s2) and Fe(s3) (but not Fe(g)) in databank B.

Enter the compound database priority list (most important first) fro

FTmisc FactPS

species: 0
solutions: 0

OK Cancel

3. Press “OK”

2. Then enter the database names in the order they should be prioritized. Here, FTmisc was given advantage over FactPS

4. Press “apply” – now the number of solids selected should be inferior to that selected in the beginning.

Desulphurization of Hot Metal using Mg

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

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

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

5. Press "Calculate"

F Menu - Equilib: Hot Metal desulphurization

File Units Parameters Help

T(C) P(atm) Energy(J) Mass(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 41
 suppress duplicates apply
* - custom selection species: 41

Solution species

| * | + | Base-Phase | Full Name |
|---|---|---------------|-------------------|
| | | FTmisc-FeLQ | Fe-liq |
| | | FTmisc-MATT | Matte |
| | | FTmisc-FeS_ | FeS-liq |
| | | FTmisc-MAT2C | CLiq(Matte/Metal) |
| | | FTmisc-PYRRRC | CPyrrhotite |
| | | FTmisc-BCCS | bcc |
| | | FTmisc-FCCS | fcc |
| | | FTmisc-MS-c | MeS_cubic |

Legend
- selected 1 Show all selected
species: 6 solutions: 1 Select

Custom Solutions
 fixed activities
 ideal solutions
 activity coefficients
Details ...

Pseudonyms
apply List ...

include molar volumes
Total Species (max 1500) 47
Total Solutions (max 40) 1
Default

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

Final Conditions

| <A> | | T(C) | P(atm) | Product H(J) |
|-----|-----|------|--------|--------------|
| 0 | 1 | 0.01 | 1400 | 1 |

10 steps Table 101 calculations

Equilibrium
 normal normal + transitions
 transitions only
 open
Calculate >>

FactSage 6.3 C:\FactSage\EquiCase2-1.DAT

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 6.3 interface. The main window is titled "F Results - Equilib A=0 (page 1/101)". A red arrow points from the "Plot Results ..." option in the "Output" menu to the "Results Processor" dialog box. The "Results Processor" dialog box shows the chemical formula "94.335 Fe + 4.5 C + 0.5 Si + 0.6 Mn +". Below this is a table with columns "Axes", "Variables", "Minimum", and "Maximum".

| Axes | Variables | Minimum | Maximum |
|------|-------------|---------|---------|
| | activity | 0 | 1.40E7 |
| | mole | 0 | |
| | mole fract. | 0 | |
| | gram | 0 | |
| | weight % | 0 | |
| | Alpha | | |
| | T(C) | | |
| | P(atm) | | |
| | Cp(J) | | |
| | G(J) | | |
| | Vol(litre) | | |
| | H(J) | | |
| | V(litre) | | |
| | S(J) | | |

At the bottom of the "Results Processor" dialog box, there are "Axes" and "Species" sections, each with "0 selected" and a "Select" button. A red arrow points from the "Axes" button to the "Axes: log10(weight %) vs Alpha" dialog box. This dialog box has "Y-variable" set to "log10(weight %)" and "X-variable" set to "Alpha". It also has input fields for "maximum", "minimum", and "tick every" for both axes.

3. This window will pop-up

2. Press “Axes”

Desulphurization of Hot Metal using Mg

1. Press "Y-variable"

2. Select "weight %" in "log10(Y)" scale

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

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

The screenshot shows the 'F Axes: log10(weight %) vs Alpha' dialog box in FactSage. The Y-axis is labeled 'log10(weight %)' and the X-axis is labeled 'Alpha'. The Y-axis settings are: maximum 0, minimum -10, and tick every 1. The X-axis settings are: maximum 1, minimum 0, and tick every 0.1. The dialog box has 'Cancel', 'Refresh', and 'OK' buttons. A list of variables is visible on the left, with 'weight %' and 'log10(Y)' selected.

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

Species Selection - EQUILIB Results: log10(weight %) vs Alpha

| # | Species | Mole (min) | Mole (max) | Fraction (min) | Fraction (max) | Activity (min) | Activity (max) |
|--------------------|----------|------------|------------|----------------|----------------|----------------|----------------|
| FTmisc FeLQ | | | | | | | |
| 1 | Fe(FeLQ) | 1.6892 | 1.6892 | 0.803704 | 0.807203 | 0.665194 | 0.666553 |
| 2 | C(FeLQ) | 0.374666 | 0.374666 | 0.178259 | 0.179035 | 0.81025 | 0.82257 |
| 3 | Mn(FeLQ) | 1.0921E-02 | 1.0921E-02 | 5.1962E-03 | 5.2188E-03 | 2.8496E-03 | 2.8714E-03 |
| + | 4 | S(FeLQ) | 1.2586E-07 | 2.0271E-03 | 5.9881E-08 | 9.6777E-04 | 1.2102E-08 |
| 5 | Si(FeLQ) | 1.7803E-02 | 1.7803E-02 | 8.4702E-03 | 8.5071E-03 | 4.4017E-05 | 4.6983E-05 |
| 6 | Mg(FeLQ) | 0 | 9.1863E-03 | 0 | 4.3706E-03 | 0 | 12.392 |
| Pure Solids | | | | | | | |
| 7 | S(s) | 0 | 0 | 0 | 0 | 1.8311E-10 | 2.9442E-06 |
| 8 | S(s2) | 0 | 0 | 0 | 0 | 2.1093E-10 | 3.3916E-06 |
| 9 | MnS(s) | 0 | 0 | 0 | 0 | 6.4071E-06 | 0.102265 |
| 10 | MnS2(s) | 0 | 0 | 0 | 0 | 5.7599E-16 | 1.4782E-07 |
| 11 | FeS(s) | 0 | 0 | 0 | 0 | 1.7623E-07 | 2.8343E-03 |
| 12 | FeS2(s) | 0 | 0 | 0 | 0 | 1.0575E-17 | 2.7347E-09 |
| 13 | Fe7S8(s) | 0 | 0 | 0 | 0 | 5.6383E-53 | 2.5234E-19 |

Species Selection - EQUILIB Results: log10(weight %) vs Alpha

Species: 0 selected

OK

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

3. Press "OK"

Desulphurization of Hot Metal using Mg

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

Plot: log10(weight %) vs Alpha

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

| Axes | Variables | Minimum | Maximum |
|--------|-------------|-------------|-------------|
| | activity | 0 | 1.4057 |
| | mole | 0 | 2.1317 |
| | mole fract. | 0 | 0.807194 |
| | gram | 0 | 100.89 |
| Y-axis | weight % | 0 | 94.394 |
| X-axis | Alpha | 0 | 1. |
| | T(C) | 1400. | 1400. |
| | P(atm) | 1. | 1. |
| | Cp(J) | 82.101 | 83.482 |
| | G(J) | -1.9454E+05 | -1.8967E+05 |
| | Vol(litre) | 0 | 0 |
| | H(J) | 1.3232E+05 | 1.3673E+05 |
| | V(litre) | 0 | 0 |
| | S(J) | 192.73 | 197.99 |
| | - page - | 1. | 101. |

log10(weight %) vs Alpha

Species: 1 selected

Graph: Labels size: 9 no: 4

Display: color full screen reactants Viewer file name Figure

Plot >>

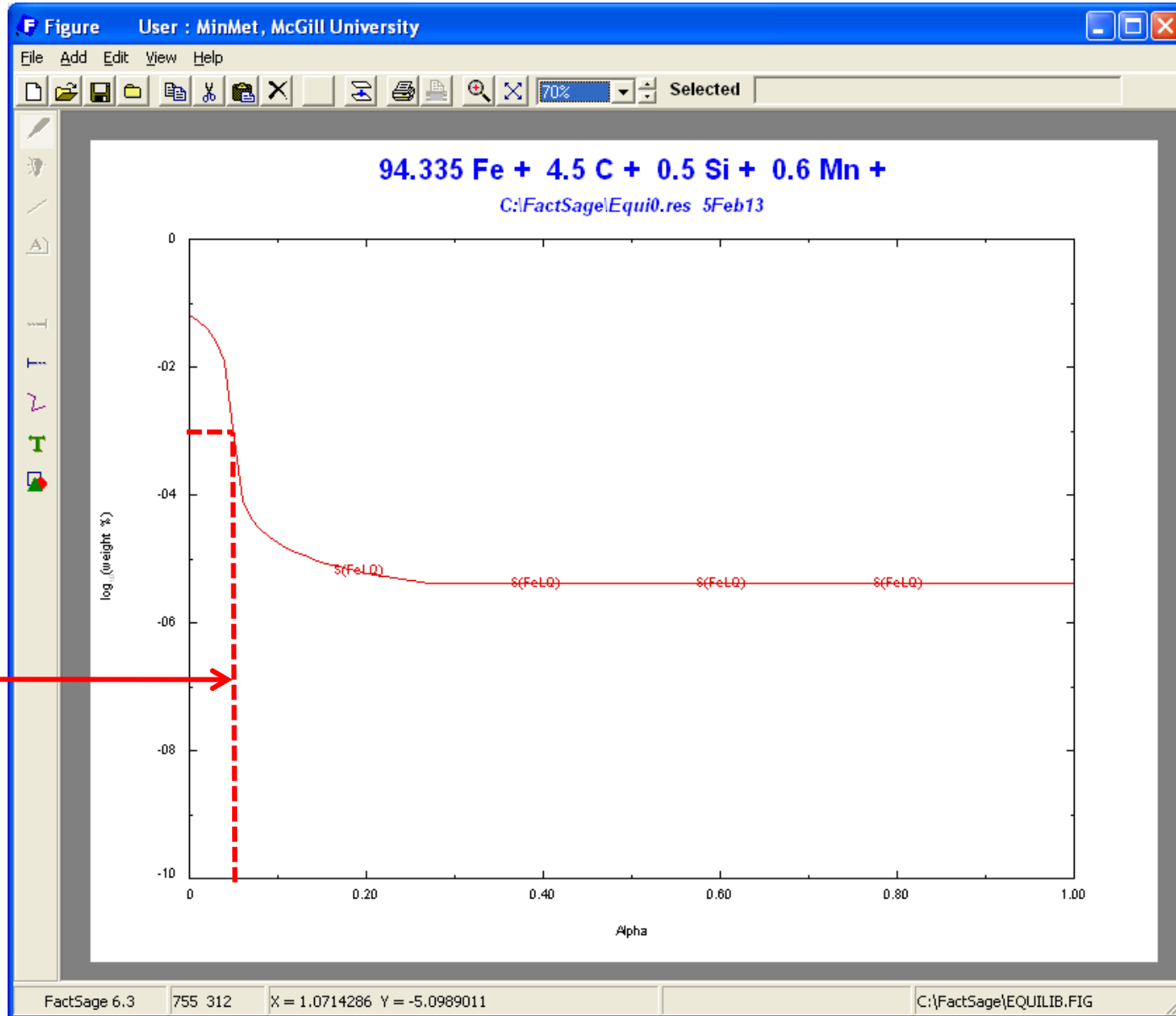
2. The "Plot" button is now activated. Click it!

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

The image shows a screenshot of the FactSage 6.3 software interface. The main window is titled "F Menu - Equilib: Hot Metal desulphurization with Mg". It displays a list of reactants and products. A context menu is open over the "FTmisc-FeLQ" entry in the "Products" list. A yellow callout box with the text "1. Right-click on the Ftmisc-FeLQ selection" has a red arrow pointing to the "FTmisc-FeLQ" entry. Another yellow callout box with the text "2. Click on 'composition target'" has a red arrow pointing to the "C - composition target ..." option in the context menu. A third yellow callout box with the text "3. This window will pop-up" has a red arrow pointing to the "Composition Target" dialog box that is open in the foreground. The dialog box has a "Variable" section with radio buttons for "species composition", "log10 (species composition)", "element composition", "log10 (element composition)", "species activity", "log10(species activity)", and "- none (removes targets) -". The "Species" section has a "Code numbers (93-98)" field with "Fe, C, Mn, ..." and a dropdown menu showing "93" and "Fe". The "Element" section has a dropdown menu showing "C". The "Values" section has a text box with the instruction "Enter a single value - or enter a range of values 'first last step'" and three input fields. The dialog box has "Cancel", "Help", and "OK" buttons.

1. Right-click on the Ftmisc-FeLQ selection

2. Click on "composition target"

3. This window will pop-up

Desulphurization of Hot Metal using Mg: Composition target

F Composition Target

Solution MI53-FeLQ

Variable

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

Species

Code numbers (93-98)
Fe, C, Mn, ...

93

Element

Elements C Mg Si S Mn Fe

Element:

Values

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

Element S:

mass fraction: (0.001%)

Cancel Help OK

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

F Menu - Equilib: Hot Metal desulphurization with Mg

File Units Parameters Help

T(C) P(atm) Energy(J) Mass(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 41
 suppress duplicates apply
* - custom selection species: 41

Solution species

| * | Base-Phase | Full Name |
|---|---------------|-------------------|
| C | FTmisc-FeLQ | Fe-liq |
| | FTmisc-MATT | Matte |
| | FTmisc-FeS_ | FeS-liq |
| | FTmisc-MAT2C | CLiq(Matte/Metal) |
| | FTmisc-PYRRRC | CPyrrhotite |
| | FTmisc-BCCS | bcc |
| | FTmisc-FCCS | fcc |
| | FTmisc-MS-c | MeS_cu |

Legend
C - composition target
- element: S

Custom Solutions
 fixed activities
 ideal solutions
 activity coefficients
Details ...

Pseudonyms

Composition target
Element S - FTmisc-FeLQ
Estimate ALPHA: 0.5
Mass(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
Calculate >>

FactSage 6.3 C:\FactSage\EquiCase2-1.DAT

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 <A> value for reducing sulphur content to 0.001% is 0.0494g.

Results - Equilib 1400 C, A=0.0494

Output Edit Show Pages

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

FactSage 6.3

```
(gram) 94.335 Fe + 4.5 C + 0.5 Si + 0.6 Mn +  
(gram) 0.065 S + <A> Mg =  
  
99.937 gram Fe-liq  
(99.937 gram, 2.0927 mol)  
(1400 C, 1 atm, a=1.0000)  
( 94.395 wt.% Fe FTmisc  
+ 4.5028 wt.% C FTmisc  
+ 0.60038 wt.% Mn FTmisc  
+ 1.0000E-03 wt.% S FTmisc  
+ 0.50032 wt.% Si FTmisc  
+ 8.9384E-04 wt.% Mg FTmisc)
```

| System component | Mole fraction | Mass fraction |
|------------------|---------------|---------------|
| Fe | 0.80721 | 0.94395 |
| Mn | 5.2188E-03 | 6.0038E-03 |
| S | 1.4893E-05 | 1.0000E-05 |
| Si | 8.5071E-03 | 5.0032E-03 |
| Mg | 1.7562E-05 | 8.9384E-06 |
| C | 0.17904 | 4.5028E-02 |

```
+ 0.11251 gram MgS_solid FactPS  
(0.11251 gram, 1.9960E-03 mol)  
(1400 C, 1 atm, S1, a=1.0000)  
  
+ 0 gram C_graphite FactPS  
(1400 C, 1 atm, S1, a=0.81669)
```

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

Desulphurization of Hot Metal using CaC_2

In the same manner, we can calculate the desulphurization ability of CaC_2



F Reactants - Equilib

File Edit Table Units Data Search Help

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

1 - 6

| Mass(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> | CaC2 | | | | 1 | |

Initial Conditions

Next >>

FactSage 6.3 Compound: 2/19 databases Solution: 1/19 databases

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

This example can be found in EquiCase2-2.dat

Desulphurization of Hot Metal using CaC_2

The same conditions are selected

F Menu - Equilib: last system

File Units Parameters Help

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

- gas ideal real 0
- aqueous 0
- pure liquids 0
- * + pure solids 44
- suppress duplicates apply
- * - custom selection species: 44

Solution species

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

Legend

+ - selected 1 Show all selected

species: 6

solutions: 1

Custom Solutions

- fixed activities
- ideal solutions
- activity coefficients

Pseudonyms

apply

include molar volumes

Total Species (max 1500) 50

Total Solutions (max 40) 1

Target

- none -

Estimate ALPHA:

Mass(g):

Final Conditions

| <A> | | T(C) | P(atm) | Product H(J) |
|-----|-----|------|--------|--------------|
| 0 | 1 | 0.01 | 1400 | 1 |

steps Table

Equilibrium

- normal normal + transitions
- transitions only
- open

FactSage 6.3 C:\FactSage\EquiCase2-1.DAT

Desulphurization of Hot Metal using CaC_2

After addition of 0.14g of CaC_2 , the amount of S in the hot metal becomes so small, that the reaction does not proceed and CaC_2 is precipitated as a solid phase.

F Results - Equilib A=0.14 (page 15/101)

Output Edit Show Pages

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

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 |
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 |

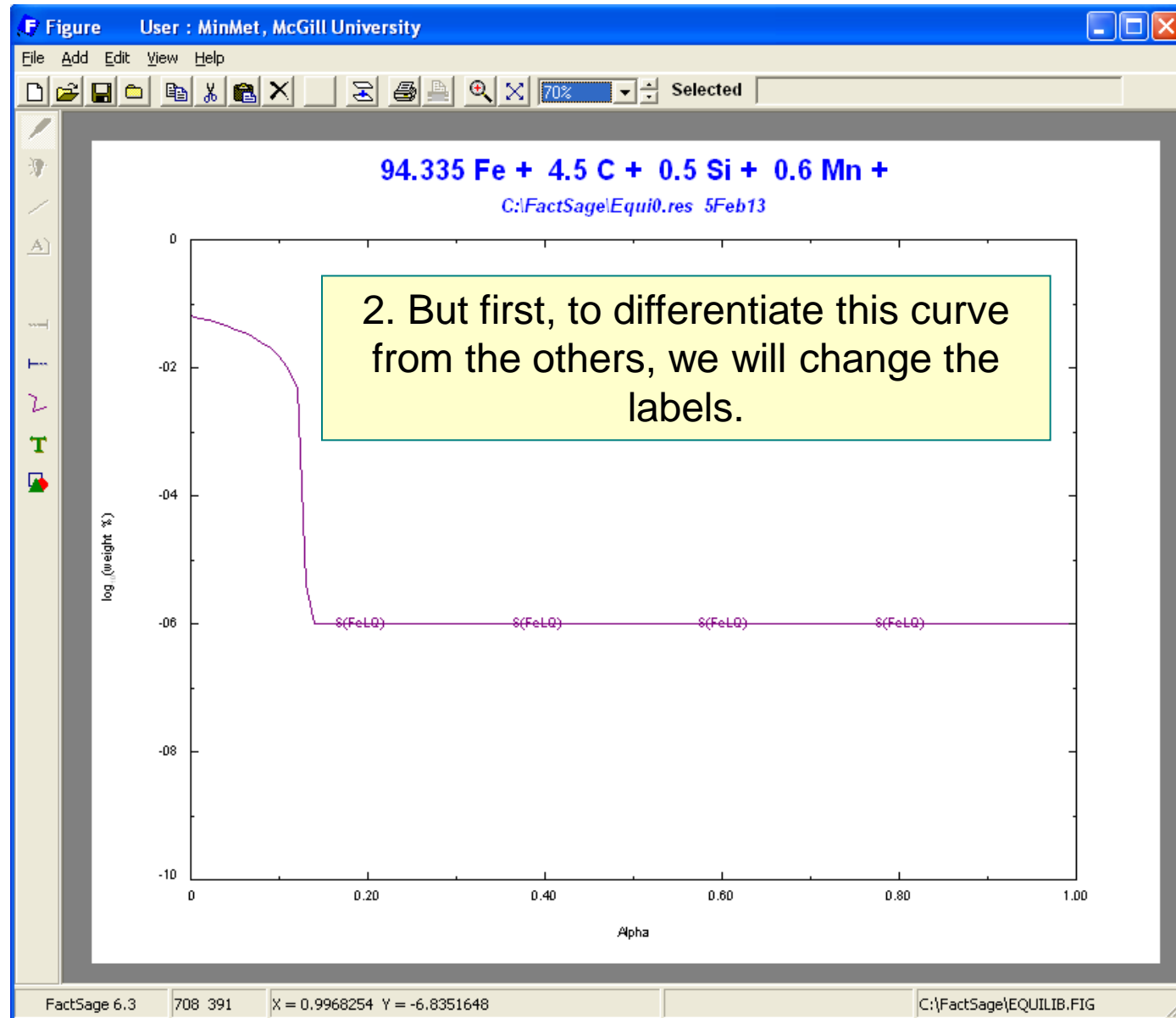
```
(gram) 94.335 Fe + 4.5 C + 0.5 Si + 0.6 Mn +  
(gram) 0.065 S + <A> CaC2 =  
  
99.984 gram Fe-liq  
(99.984 gram, 2.0967 mol)  
(1400 C, 1 atm, a=1.0000)  
( 94.350 wt.% Fe FTmisc  
+ 4.5495 wt.% C FTmisc  
+ 1.8227E-04 wt.% Ca FTmisc  
+ 0.60010 wt.% Mn FTmisc  
+ 9.8228E-07 wt.% S FTmisc  
+ 0.50008 wt.% Si FTmisc)  
  
System component Mole fraction Mass fraction  
Fe 0.80567 0.94350  
Mn 5.2089E-03 6.0010E-03  
Ca 2.1687E-06 1.8227E-06  
S 1.4608E-08 9.8228E-09  
Si 8.4909E-03 5.0008E-03  
C 0.18063 4.5495E-02  
  
+ 0.14624 gram CaS_solid FactPS  
(0.14624 gram, 2.0271E-03 mol)  
(1400 C, 1 atm, S1, a=1.0000)  
  
+ 9.7725E-03 gram CaC2_solid-b T FactPS  
(9.7725E-03 gram, 1.5246E-04 mol)  
(1400 C, 1 atm, S2, a=1.0000)
```

Desulphurization of Hot Metal using CaC_2

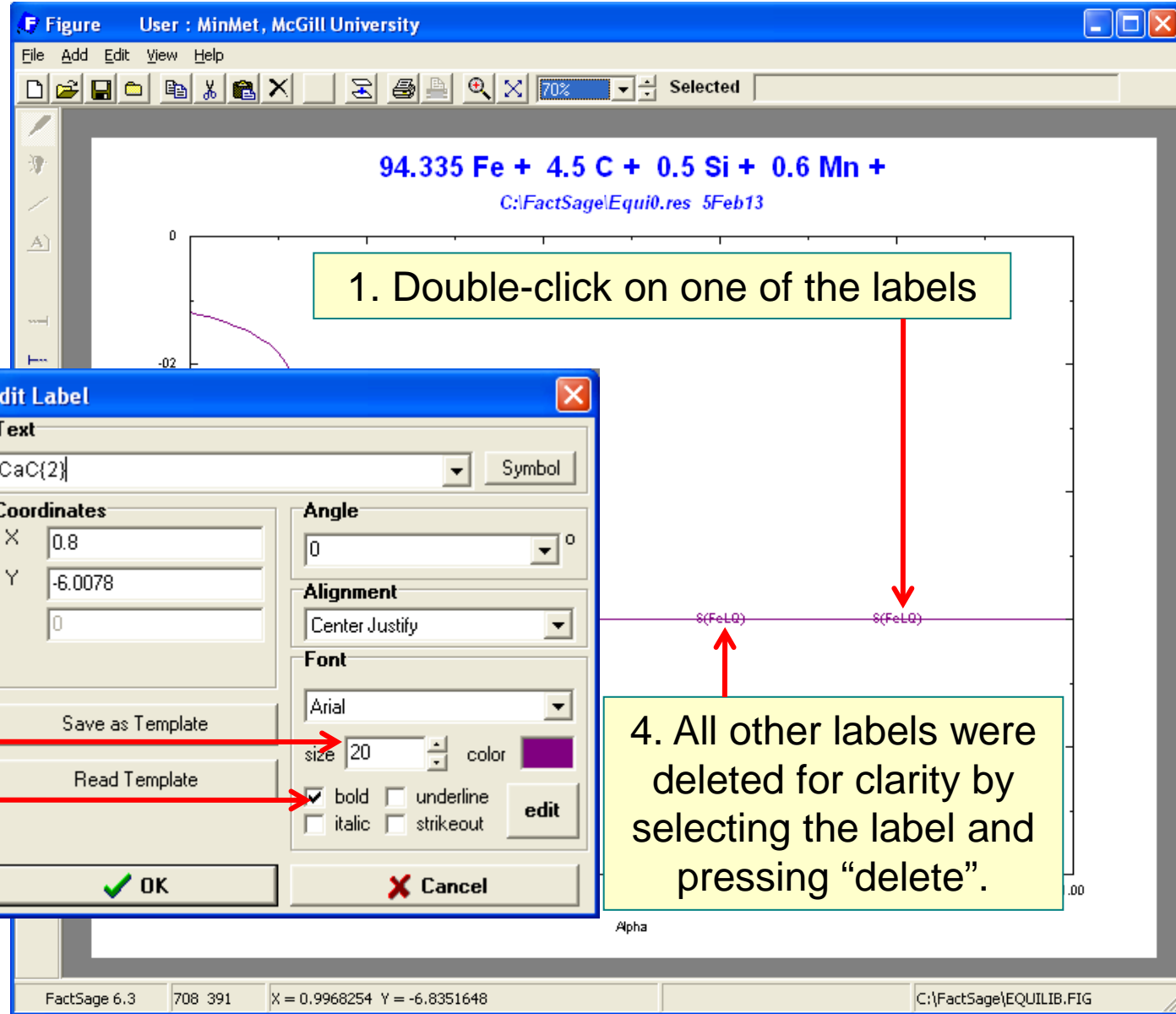
This can also be seen on the graph – after $\langle A \rangle = 0.14$, the sulphur level remains constant.

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

2. But first, to differentiate this curve from the others, we will change the labels.



Desulphurization of Hot Metal using CaC_2



1. Double-click on one of the labels

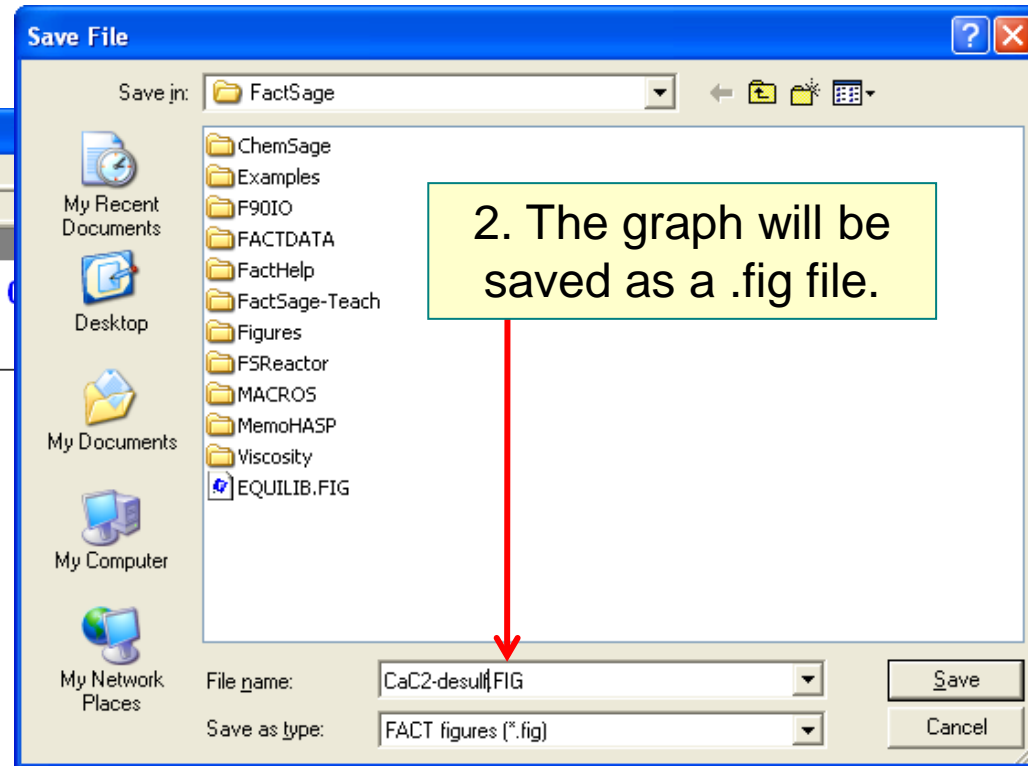
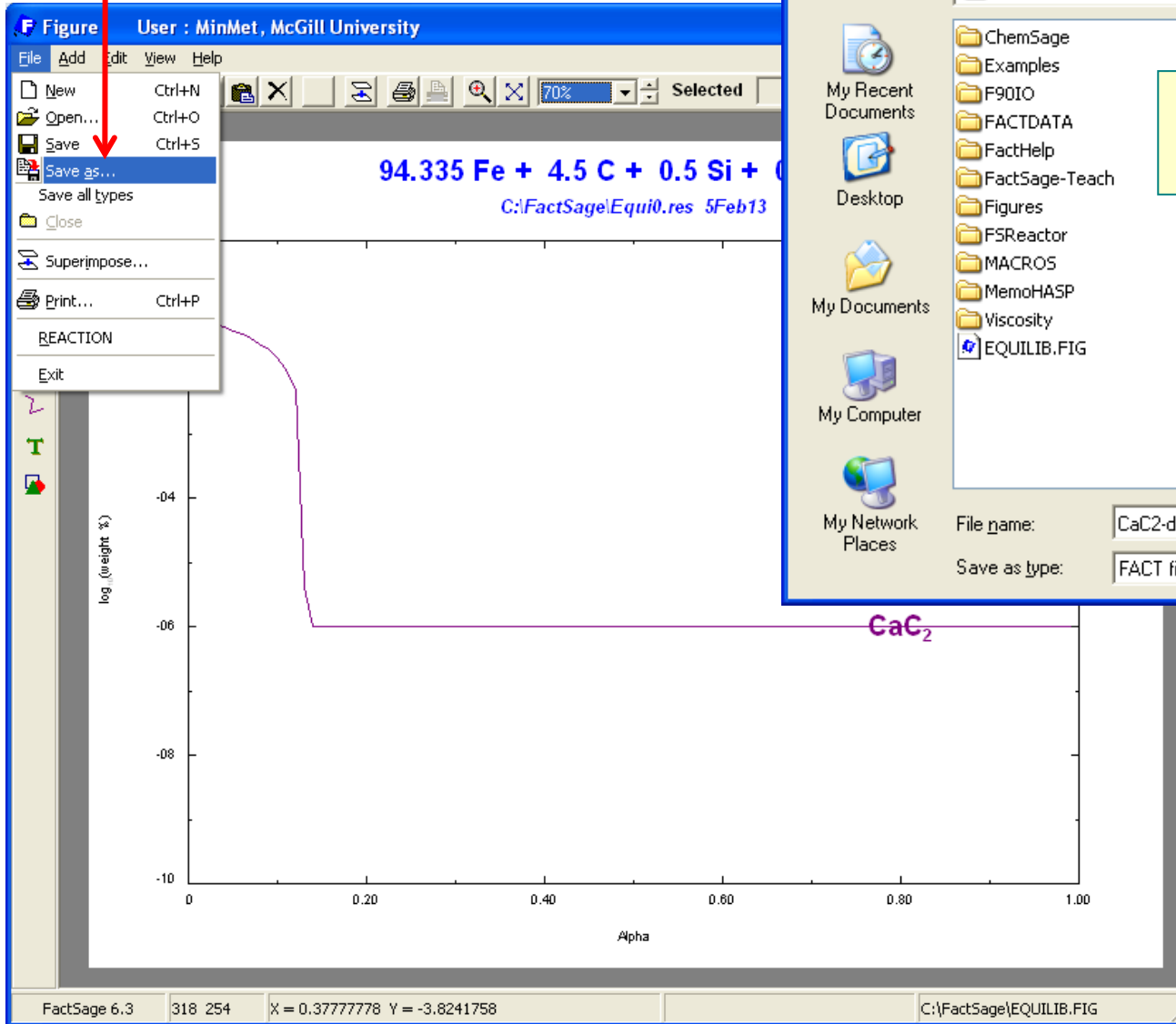
2. Edit the text
{curvy brackets
are for subscript}

3. Can increase
the text size to
see better and
make it bold

4. All other labels were
deleted for clarity by
selecting the label and
pressing "delete".

Desulphurization of Hot Metal using CaC_2

1. Press "File" → "Save as..."



2. The graph will be saved as a .fig file.

Desulphurization of Hot Metal using CaC_2 : Composition target

With CaC_2 , the amount needed to bring the sulphur level down to 0.001% is 0.1279g.

F Results - Equilib 1400 C, A=0.1279

Output Edit Show Pages

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

FactSage 6.3

```
(gram) 94.335 Fe + 4.5 C + 0.5 Si + 0.6 Mn +  
(gram) 0.065 S + <A> CaC2 =  
  
99.984 gram Fe-liq  
(99.984 gram, 2.0966 mol)  
(1400 C, 1 atm, a=1.0000)  
( 94.350 wt.% Fe FTmisc  
+ 4.5487 wt.% C FTmisc  
+ 1.7898E-07 wt.% Ca FTmisc  
+ 0.60010 wt.% Mn FTmisc  
+ 1.0000E-03 wt.% S FTmisc  
+ 0.50008 wt.% Si FTmisc)  
  
System component Mole fraction Mass fraction  
Fe 0.80568 0.94350  
Mn 5.2090E-03 6.0010E-03  
Ca 2.1296E-09 1.7898E-09  
S 1.4872E-05 1.0000E-05  
Si 8.4911E-03 5.0008E-03  
C 0.18060 4.5487E-02  
  
+ 0.14399 gram CaS_solid FactPS  
(0.14399 gram, 1.9960E-03 mol)  
(1400 C, 1 atm, S1, a=1.0000)  
  
+ 0 gram C_graphite FactPS  
(1400 C, 1 atm, S1, a=0.83715)
```

Desulphurization of Hot Metal using CaO

With CaO, CO gas is evolved during the reaction, so we must select the gas species as possible products.



This example can be found in EquiCase2-3.dat

F Menu - Equilib: last system

File Units Parameters Help

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

Reactants (6)

[gram] 94.335 Fe + 4.5 C + 0.5 Si + 0.6 Mn + 0.065 S + <A> CaO

Products

Compound species

- gas ideal real 47
- aqueous 0
- pure liquids 0
- pure solids 101
- suppress duplicates apply
- * - custom selection species: 148

Solution species

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

Legend
+ - selected 1

Show all selected

species: 10
solutions: 1 **Select**

Custom Solutions

- fixed activities
- ideal solutions
- activity coefficients

Details ...

Pseudonyms

apply **List ...**

include molar volumes

Total Species [max 1500] 158
Total Solutions [max 40] 1

Default

Final Conditions

| <A> | | T(C) | P(atm) | Product H(J) |
|-----|------|------|--------|--------------|
| 0.1 | 0.01 | 1400 | 1 | |

10 steps Table **101 calculations**

Equilibrium

- normal normal + transitions
- transitions only
- open

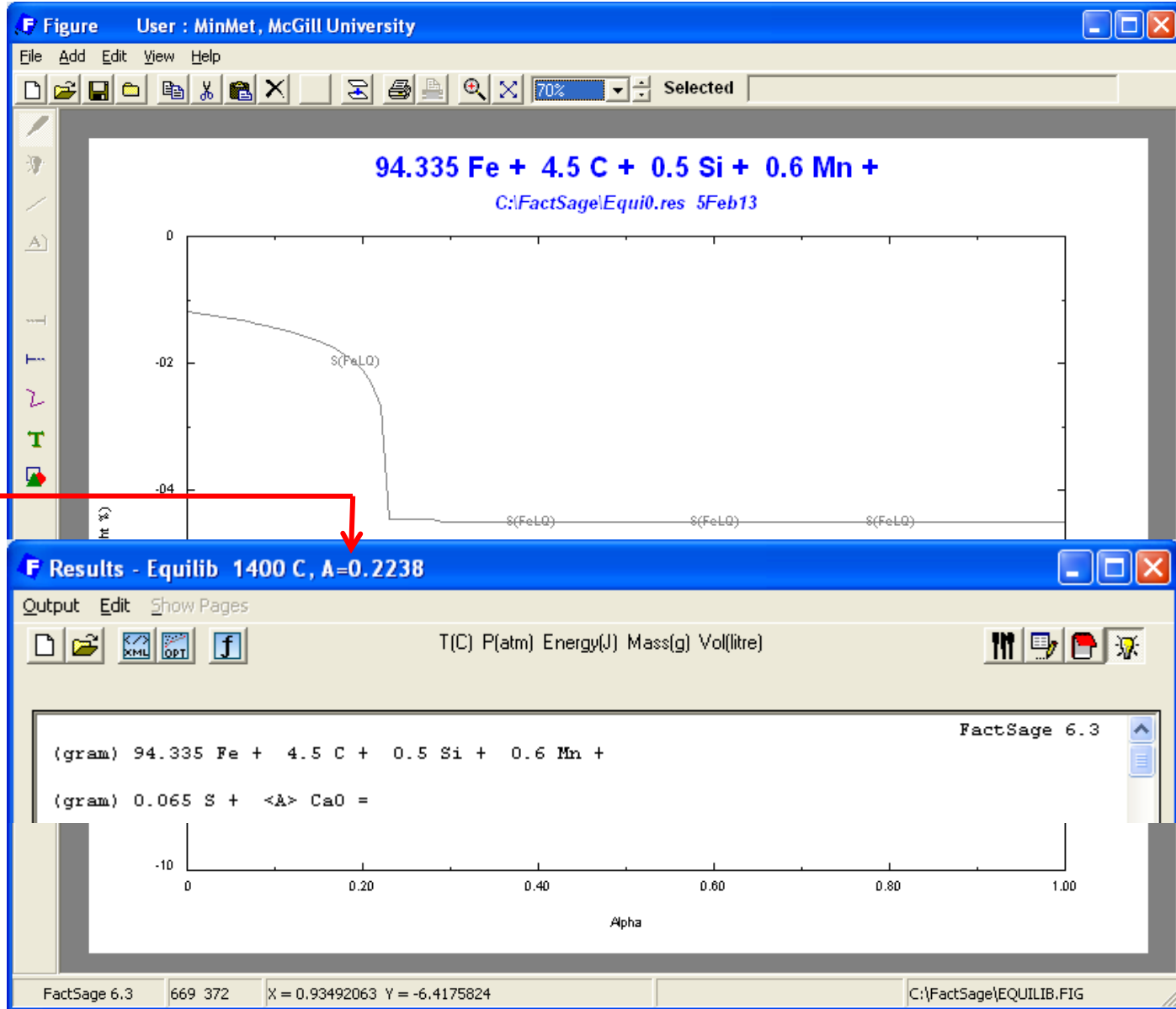
Calculate >>

FactSage 6.3 C:\FactSage\EquiCase2-2.DAT

Desulphurization of Hot Metal using CaO

The following curve is obtained with CaO

Using Composition Target, it is found that 0.2238g of CaO is needed to bring the sulphur level down to 0.001%



Desulphurization of Hot Metal using CaO+Mg

For the CaO+Mg mixture, no gas was selected and all solids were selected.

The value <A> was given for CaO and for Mg



This example can be found in EquiCase2-4.dat

Menu - Equilib: last system

File Units Parameters Help

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

Reactants (7)

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

Products

Compound species
 gas ideal real 0
 aqueous 0
 pure liquids 0
 pure solids 126
 suppress duplicates apply
* - custom selection species: 126

Solution species

| * | + | Base-Phase | Full Name |
|---|---|--------------|-------------------|
| | + | FTmisc-FeLQ | Fe-liq |
| | | FTmisc-MAT | Matte |
| | | FTmisc-FeS_ | FeS-liq |
| | | FTmisc-MAT2C | CLiq(Matte/Metal) |
| | | FTmisc-PYRRC | CPyrrhotite |
| | | FTmisc-BCCS | bcc |
| | | FTmisc-FCCS | fcc |
| | | FTmisc-MS-c | MeS_cubic |

Legend
+ - selected 1
 Show all selected
species: 12
solutions: 1 Select

Custom Solutions
 fixed activities
 ideal solutions
 activity coefficients
Details ...

Pseudonyms
apply List ...
 include molar volumes
Total Species (max 1500) 138
Total Solutions (max 40) 1
Default

Final Conditions

| <A> | | T(C) | P(atm) | Product H(J) |
|-----|-----|------|--------|--------------|
| 0 | 1 | 0.01 | 1400 | 1 |

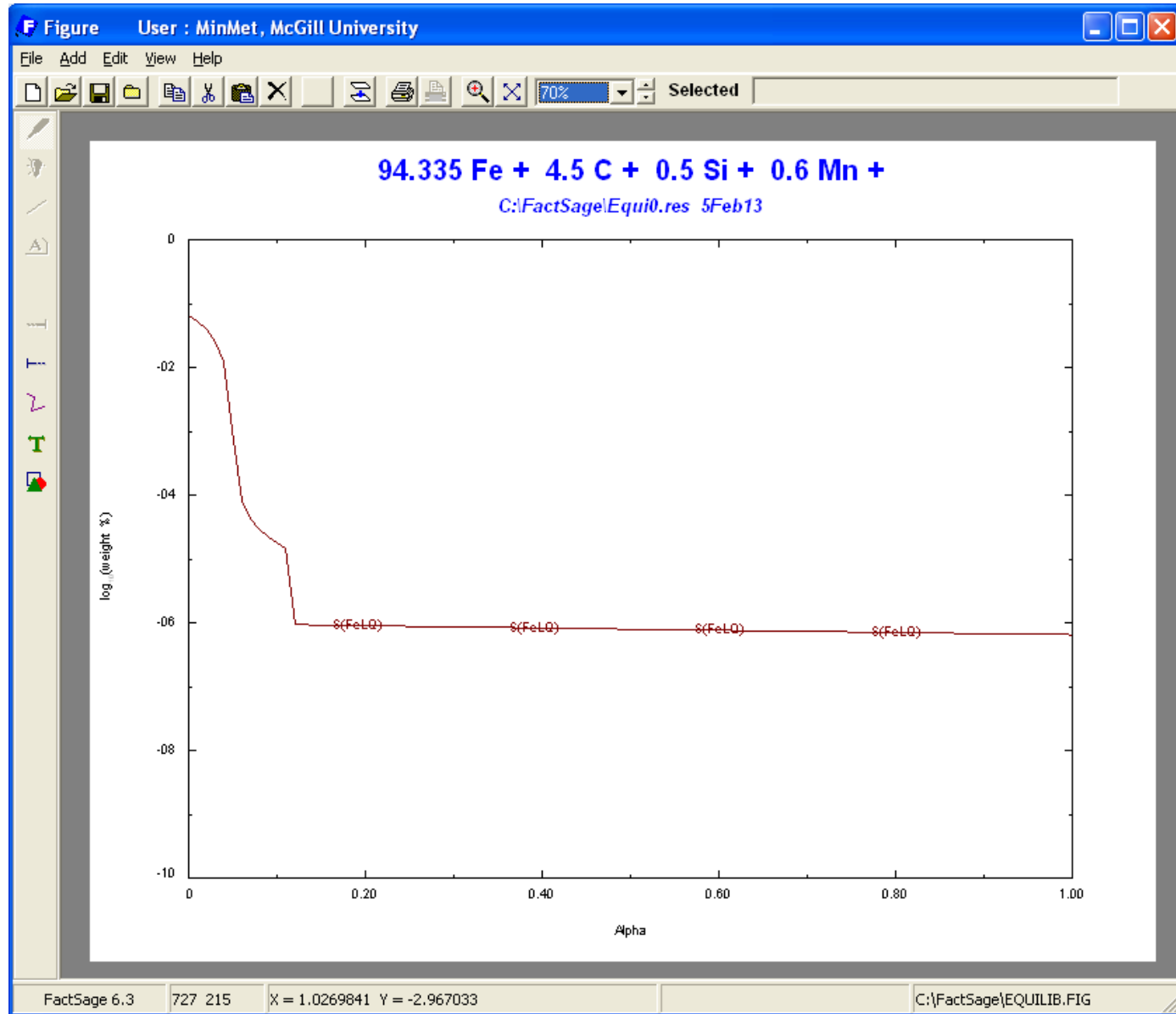
10 steps Table 101 calculations

Equilibrium
 normal normal + transitions
 transitions only
 open
Calculate >>

FactSage 6.3 C:\FactSage\EquiCase2-3.DAT

Desulphurization of Hot Metal using CaO+Mg

The drop at $\alpha=0.11$ is due to CaC_2 precipitating instead of MgS.



Desulphurization of Hot Metal using CaO+Mg: Composition target

With CaO+Mg, the amount needed to bring the sulphur level down to 0.001% is 0.0494g CaO + 0.0494g Mg.

F Results - Equilib 1400 C, A=0.0494

Output Edit Show Pages

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

FactSage 6.3

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

```
99.937 gram Fe-liq
(99.937 gram, 2.0927 mol)
(1400 C, 1 atm, a=1.0000)
( 94.395 wt.% Fe FTmisc
+ 4.5028 wt.% C FTmisc
+ 1.7427E-07 wt.% Ca FTmisc
+ 0.60038 wt.% Mn FTmisc
+ 1.8304E-07 wt.% O FTmisc
+ 1.0000E-03 wt.% S FTmisc
+ 0.50032 wt.% Si FTmisc
+ 8.9384E-04 wt.% Mg FTmisc
+ 3.9658E-05 wt.% MgO FTmisc
+ 1.4531E-07 wt.% CaO FTmisc
+ 2.6586E-08 wt.% SiO FTmisc
+ 1.0479E-08 wt.% MnO FTmisc)
```

| System component | Mole fraction | Mass fraction |
|------------------|---------------|---------------|
| Fe | 0.80720 | 0.94395 |
| Mn | 5.2188E-03 | 6.0038E-03 |
| Ca | 3.3139E-09 | 2.7812E-09 |
| S | 1.4893E-05 | 1.0000E-05 |
| Si | 8.5071E-03 | 5.0032E-03 |
| Mg | 1.8032E-05 | 9.1776E-06 |
| O | 4.7695E-07 | 1.5979E-07 |
| C | 0.17904 | 4.5028E-02 |

Desulphurization of Hot Metal using CaO+Al



This example can be found in EquiCase2-5.dat

For the CaO+Al mixture, no gas was selected and all solids were selected.

The value <A> was given for CaO and <2A> for Al

Since there is no CaO-Al₂O₃ solid solution incorporating S, we must choose the pure solids where a combination of CaO-Al₂O₃ compounds and CaS will simulate this solution.

Reactants (7)

(gram) 94.335 Fe + 4.5 C + 0.5 Si + 0.6 Mn + 0.065 S + <A> CaO + <2A> Al

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- * + pure solids 133
- suppress duplicates apply
- * - custom selection species: 133

Target: none

Estimate ALPHA: 0.5

Mass(g): 0

Solution species

| * | + | Base-Phase | Full Name |
|---|---|---------------|-------------------|
| | + | FTmisc-FeLQ | Fe-liq |
| | | FTmisc-MATT | Matte |
| | | FTmisc-FeS_ | FeS-liq |
| | | FTmisc-MAT2C | CLiq(Matte/Metal) |
| | | FTmisc-PYRRRC | CPyrrhotite |
| | | FTmisc-BCCS | bcc |
| | | FTmisc-FCCS | fcc |
| | | FTmisc-MS-c | MeS_cubic |

Legend: +- selected 1

Show all selected

species: 13

solutions: 1

Final Conditions

| <A> | | T(C) | P(atm) | Product H(J) |
|-----|------|------|--------|--------------|
| 0.1 | 0.01 | 1400 | 1 | |

10 steps Table 101 calculations

Equilibrium

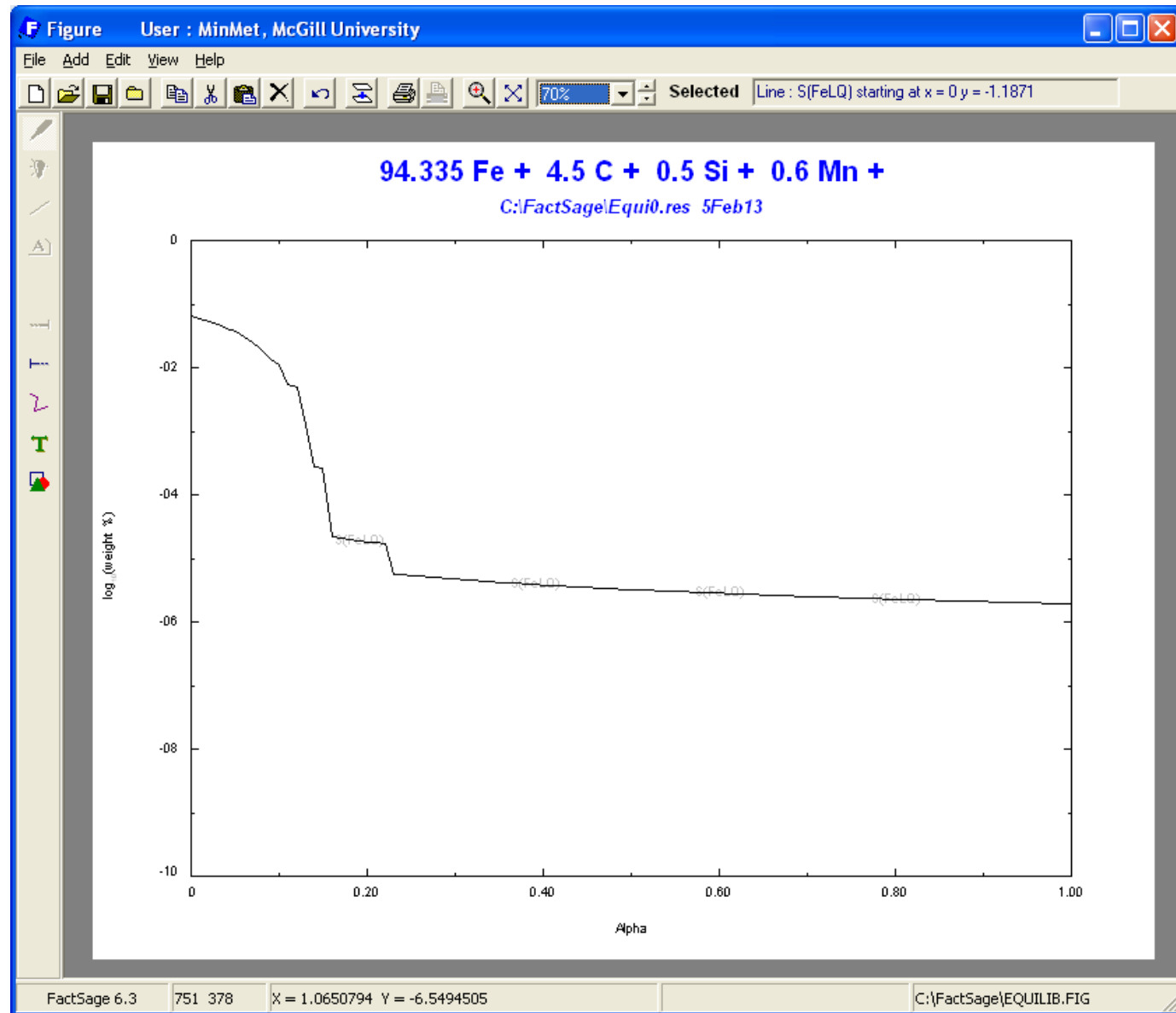
- normal normal + transitions
- transitions only
- open

Calculate >>

FactSage 6.3 C:\FactSage\EquiCase2-4.DAT

Desulphurization of Hot Metal using CaO+Al

The change of stable phase between different CaO-Al₂O₃ compounds creates the steps in this graph.



Desulphurization of Hot Metal using CaO+Al: Composition target

With CaO+Al, the amount needed to bring the sulphur level down to 0.001% is 0.1305g CaO + 0.2610g Al.

FactSage 6.3

```
(gram) 94.335 Fe + 4.5 C + 0.5 Si + 0.6 Mn +  
(gram) 0.065 S + <A> CaO + <2A> Al =  
  
100.16 gram Fe-liq  
(100.16 gram, 2.1010 mol)  
(1400 C, 1 atm, a=1.0000)  
( 94.183 wt.% Fe FTmisc  
+ 0.22448 wt.% Al FTmisc  
+ 4.4927 wt.% C FTmisc  
+ 1.7648E-07 wt.% Ca FTmisc  
+ 0.59903 wt.% Mn FTmisc  
+ 2.5096E-06 wt.% O FTmisc  
+ 1.0000E-03 wt.% S FTmisc  
+ 0.49919 wt.% Si FTmisc  
+ 1.9733E-06 wt.% CaO FTmisc  
+ 1.5704E-04 wt.% AlO FTmisc  
+ 3.7072E-07 wt.% SiO FTmisc  
+ 1.4299E-07 wt.% MnO FTmisc  
+ 4.0763E-04 wt.% Al2O FTmisc)
```

| System component | Mole fraction | Mass fraction |
|------------------|---------------|---------------|
| Fe | 0.80401 | 0.94183 |
| Mn | 5.1982E-03 | 5.9903E-03 |
| Ca | 1.8875E-08 | 1.5868E-08 |
| S | 1.4868E-05 | 1.0000E-05 |
| Si | 8.4734E-03 | 4.9919E-03 |
| Al | 3.9735E-03 | 2.2489E-03 |
| O | 4.6160E-06 | 1.5492E-06 |
| - | - | - |

Desulphurization of Hot Metal using $\text{CaO} + \text{Al}_2\text{O}_3$

The species selection for this reaction is the same as for the previous example.



This example can be found in EquiCase2-6.dat

Menu - Equilib: Hot Metal desulphurization with CaO and Al

File Units Parameters Help

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

Reactants (7)

(gram) 94.335 Fe + 4.5 C + 0.5 Si + 0.6 Mn + 0.065 S + <A> CaO + <A> Al2O3

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- * pure solids 133
- suppress duplicates apply
- * - custom selection species: 133

Target

- none -

Estimate ALPHA: 0.5

Mass(g): 0

Solution species

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

Legend

+ - selected 1

Show all selected

species: 13

solutions: 1 **Select**

Custom Solutions

- fixed activities
- ideal solutions
- activity coefficients

Details ...

Pseudonyms

apply **List ...**

include molar volumes

Total Species (max 1500) 146

Total Solutions (max 40) 1

Default

Final Conditions

| <A> | | T(C) | P(atm) | Product H(J) |
|-----|-----|------|--------|--------------|
| 0 | 1 | 0.01 | 1400 | 1 |

10 steps Table **101 calculations**

Equilibrium

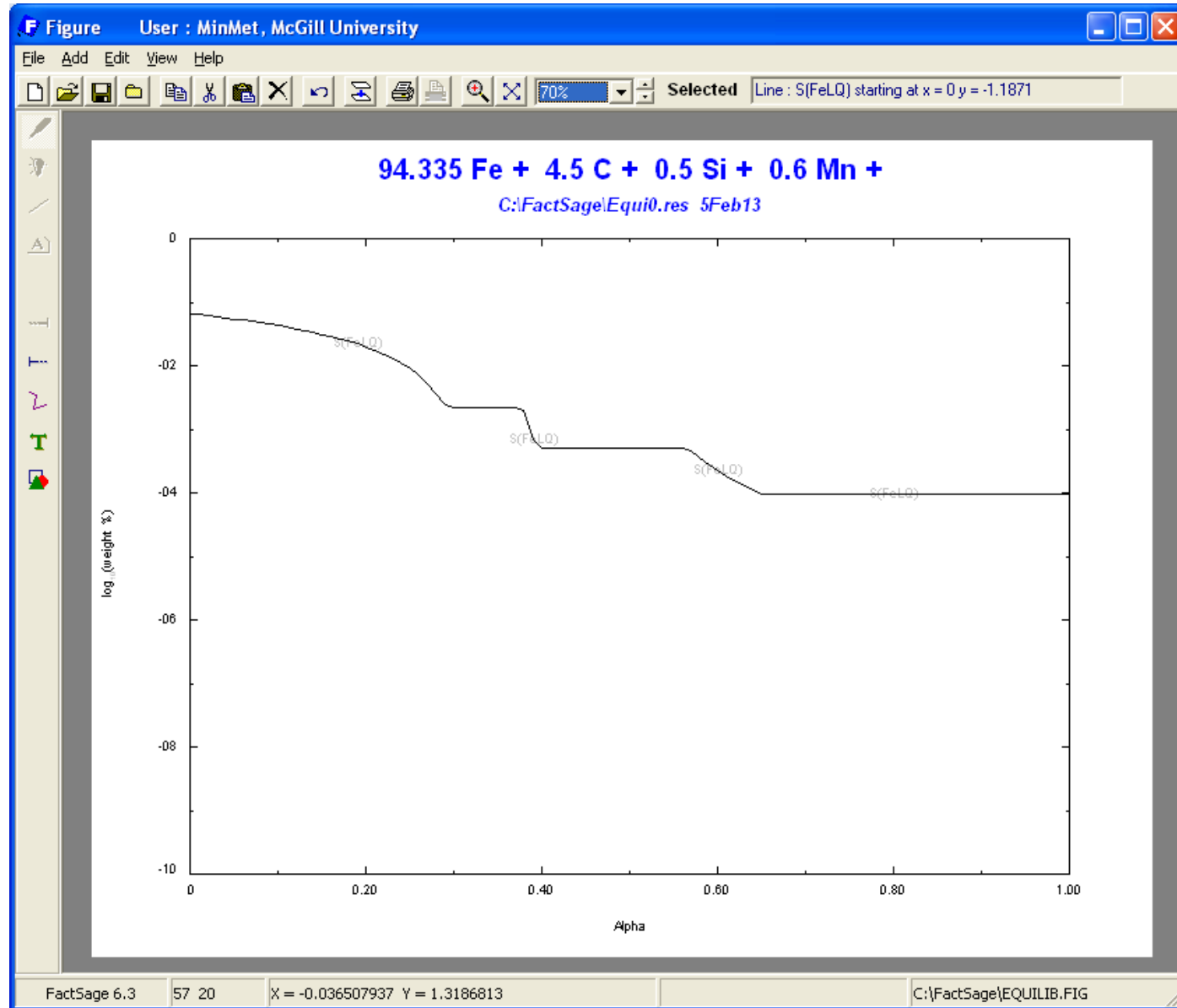
- normal normal + transitions
- transitions only
- open

Calculate >>

FactSage 6.3 C:\FactSage\EquiCase2-5.DAT

Desulphurization of Hot Metal using $\text{CaO} + \text{Al}_2\text{O}_3$

The change of stable phase between different $\text{CaO}-\text{Al}_2\text{O}_3$ compounds creates the steps in this graph.



Desulphurization of Hot Metal using CaO+Al₂O₃: Composition target

With CaO+Al₂O₃,
the amount
needed to bring
the sulphur level
down to 0.001%
is 0.3874g CaO +
0.3874g Al₂O₃.

F Results - Equilib 1400 C, A=0.3874

Output Edit Show Pages

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

FactSage 6.3

```
(gram) 94.335 Fe + 4.5 C + 0.5 Si + 0.6 Mn +  
(gram) 0.065 S + <A> CaO + <A> Al2O3 =  
  
99.911 gram Fe-liq  
(99.911 gram, 2.0918 mol)  
(1400 C, 1 atm, a=1.0000)  
( 94.419 wt.% Fe FTmisc  
+ 1.2418E-02 wt.% Al FTmisc  
+ 4.5040 wt.% C FTmisc  
+ 1.7374E-07 wt.% Ca FTmisc  
+ 0.60054 wt.% Mn FTmisc  
+ 1.2113E-05 wt.% O FTmisc  
+ 1.0000E-03 wt.% S FTmisc  
+ 0.46270 wt.% Si FTmisc  
+ 9.6523E-06 wt.% CaO FTmisc  
+ 4.1714E-05 wt.% AlO FTmisc  
+ 1.6202E-06 wt.% SiO FTmisc  
+ 6.9591E-07 wt.% MnO FTmisc  
+ 5.9588E-06 wt.% Al2O FTmisc)
```

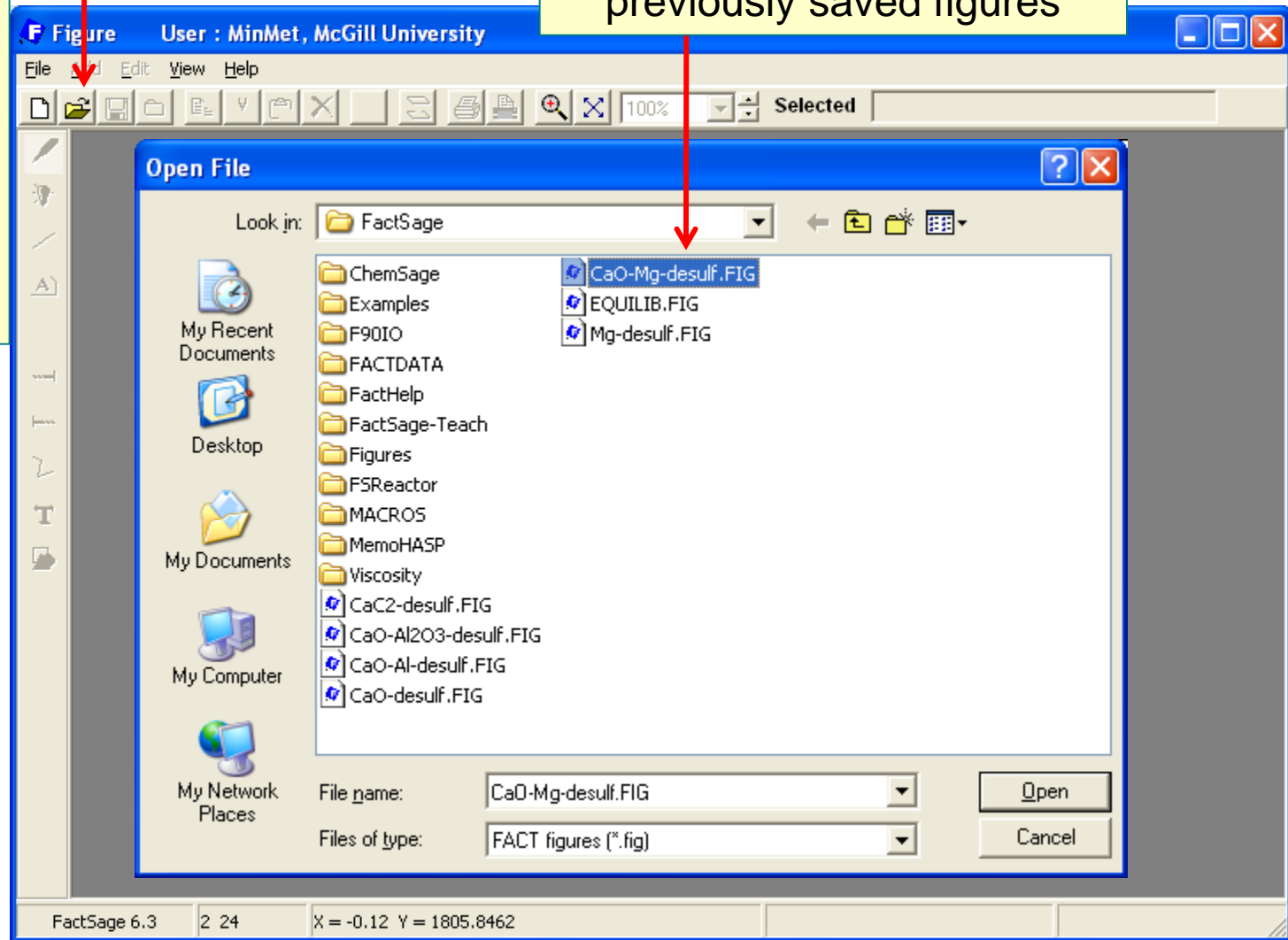
| System component | Mole fraction | Mass fraction |
|------------------|---------------|---------------|
| Fe | 0.80756 | 0.94419 |
| Mn | 5.2211E-03 | 6.0054E-03 |
| Ca | 8.4283E-08 | 7.0721E-08 |
| S | 1.4896E-05 | 1.0000E-05 |
| Si | 7.8689E-03 | 4.6270E-03 |
| Al | 2.2037E-04 | 1.2448E-04 |
| O | 9.7030E-07 | 3.2502E-07 |
| - | - | - |

Desulphurization of Hot Metal

1. To compare the different desulphurization methods, it is convenient to plot all the obtained curves on one graph.

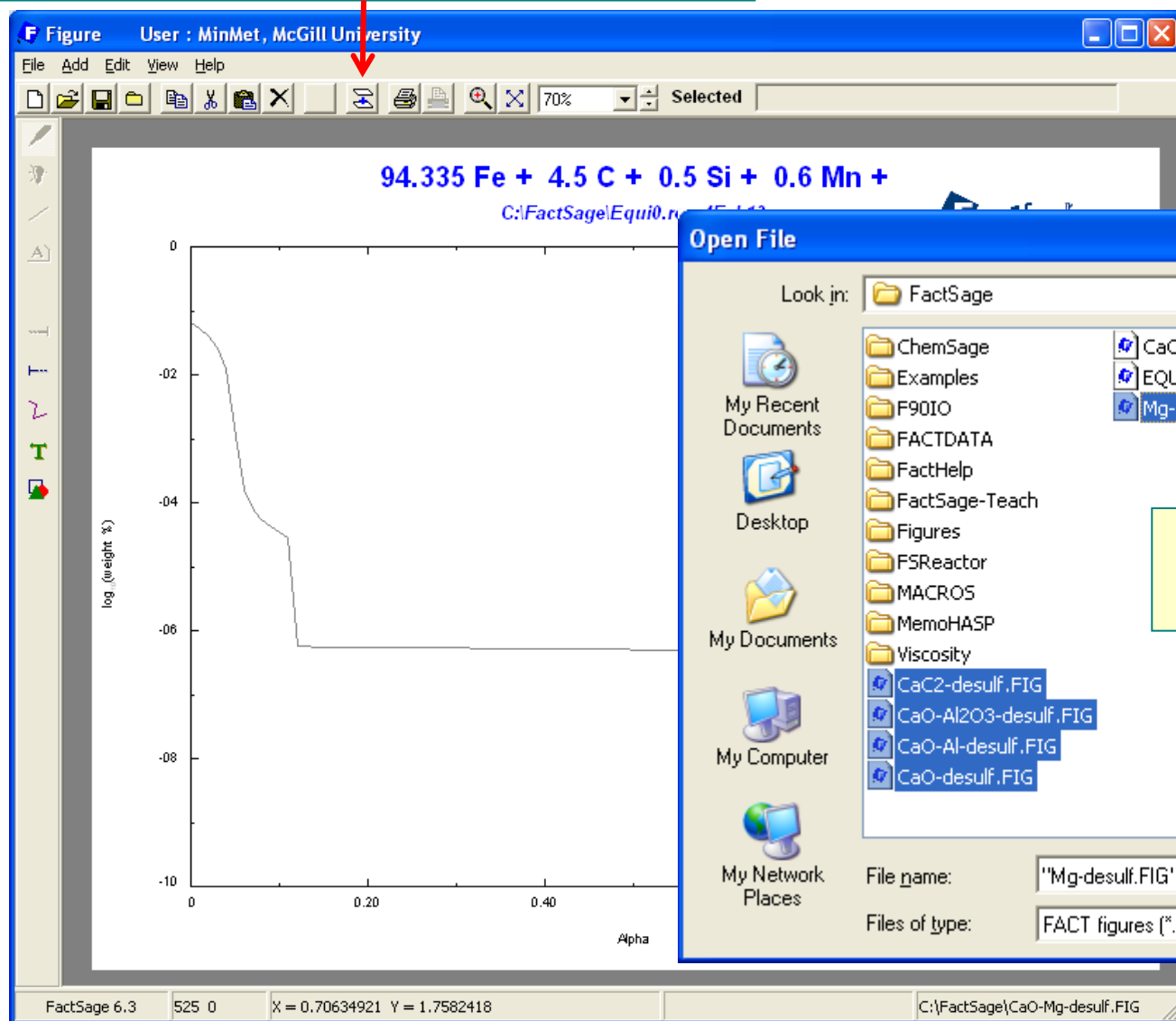
2. Press "Open"

3. Select one of the previously saved figures



Desulphurization of Hot Metal

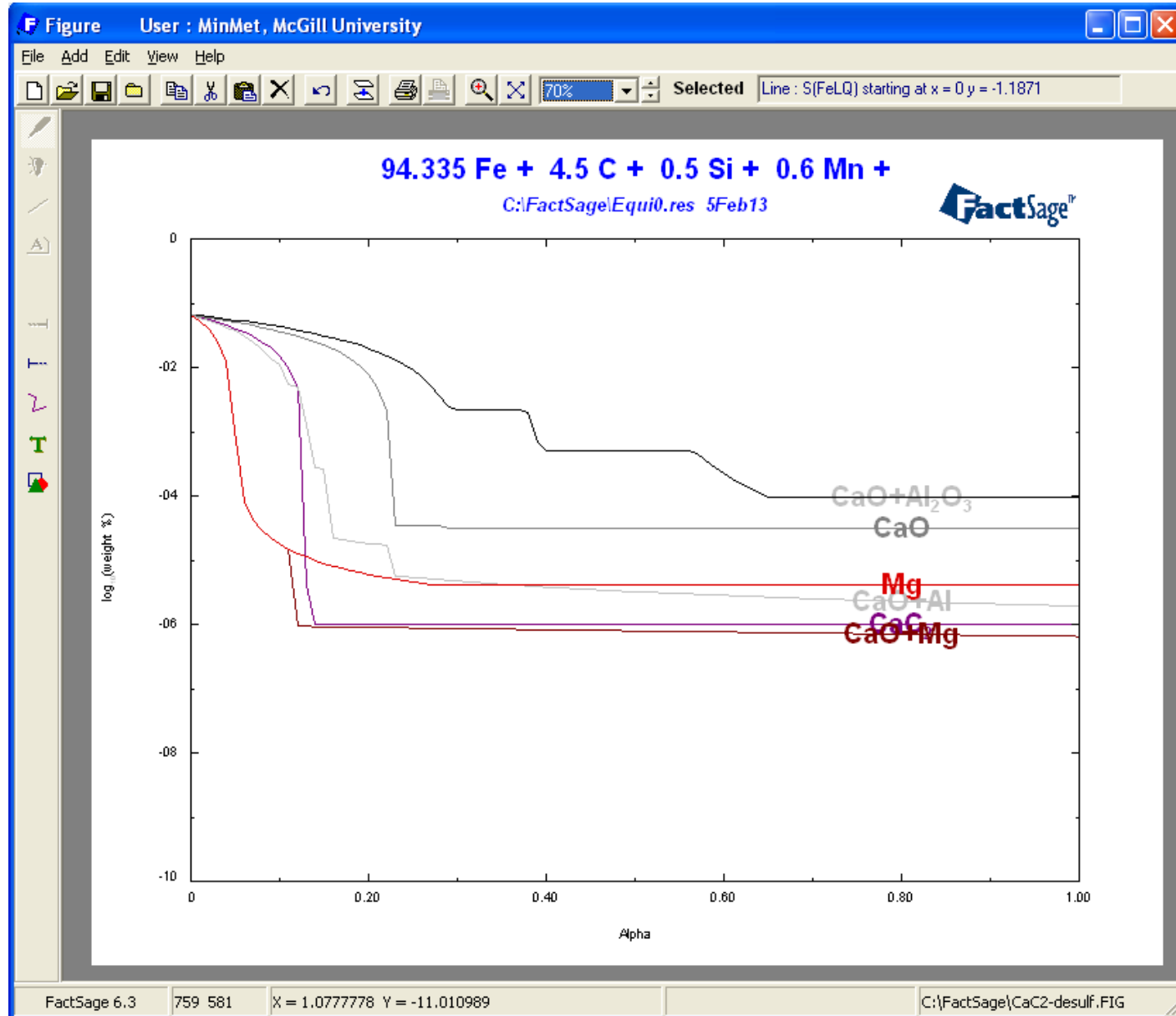
1. Press “superimposed figure”



2. Select all the other saved figures.

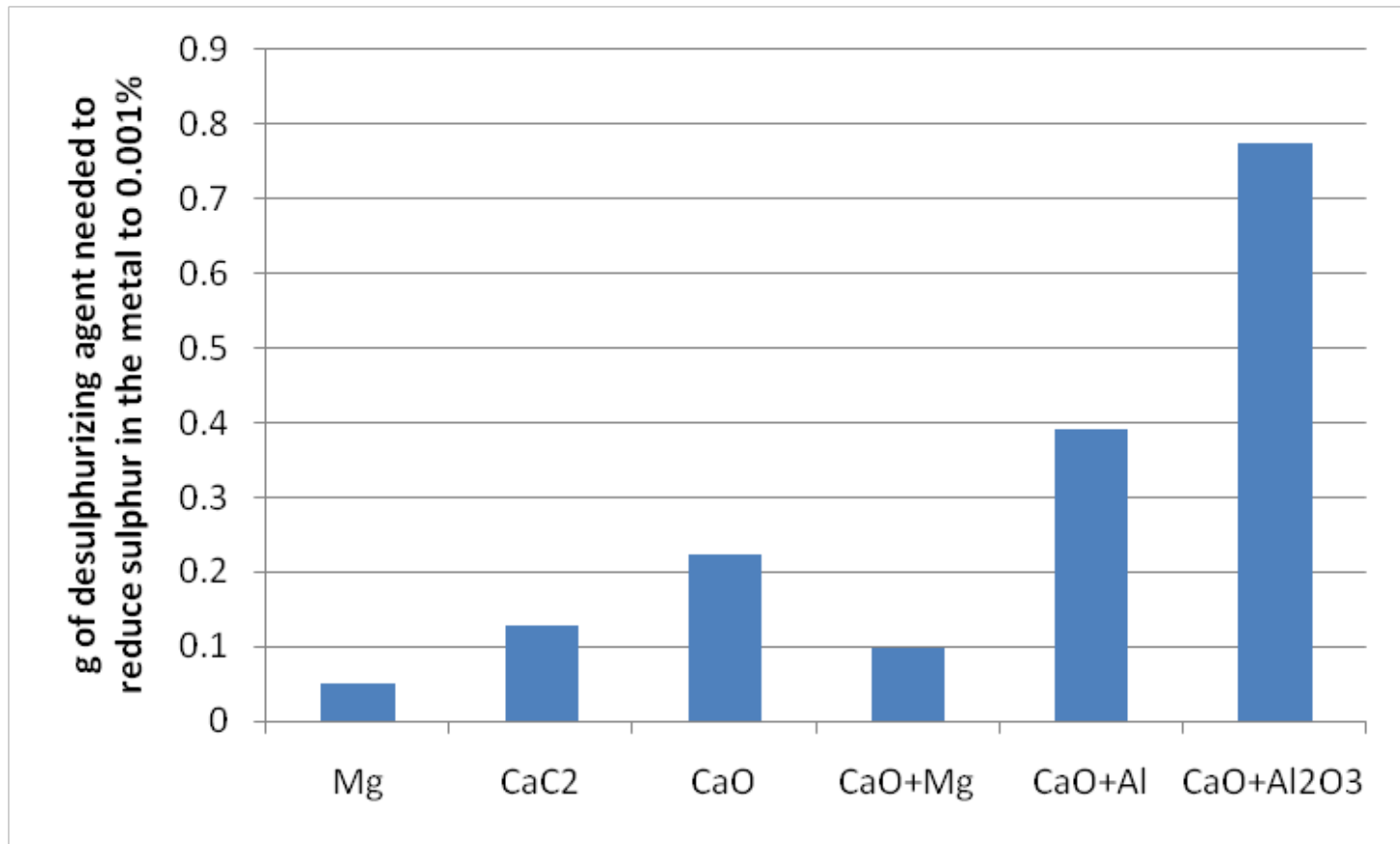
Desulphurization of Hot Metal

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

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% Al_2O_3 , 10% MgO and 10% SiO_2 . The ratio of slag to metal is 1/10

Desulphurization of Steel using Mg

1. Enter the metal and slag composition

This example can be found in EquiCase2-7.dat

2. In "Data Search" select FTmisc and FToxid

Reactants - Equilib

| Mass(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 - 3/19 compound databases, 2/19 solution databases

| Fact | FactSage | SGTE |
|--------------------------------------------|---------------------------------|---------------------------------|
| <input checked="" type="checkbox"/> FactPS | <input type="checkbox"/> FScopp | <input type="checkbox"/> BINS |
| <input checked="" type="checkbox"/> FToxid | <input type="checkbox"/> FSlead | <input type="checkbox"/> SGPS |
| <input type="checkbox"/> FTsalt | <input type="checkbox"/> FSlite | <input type="checkbox"/> SGTE |
| <input checked="" type="checkbox"/> FTmisc | <input type="checkbox"/> FSstel | <input type="checkbox"/> SGnobl |
| <input type="checkbox"/> FTball | <input type="checkbox"/> FSnobl | <input type="checkbox"/> SGsold |
| <input type="checkbox"/> FTOfCN | <input type="checkbox"/> FSupsi | <input type="checkbox"/> SGnucl |
| <input type="checkbox"/> FTfritz | | |
| <input type="checkbox"/> FTthelp | | |
| <input type="checkbox"/> FTpulp | <input type="checkbox"/> ELEM | Other |
| <input type="checkbox"/> FTlite | <input type="checkbox"/> FTdemo | <input type="checkbox"/> TDnucl |

Miscellaneous

EXAM SGTE# SGTE*

compounds only
solutions only
no database

Clear All
Select All
Add/Remove Data
RefreshDatabases

Options

Include

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

Limits

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

Cancel Summary ... OK

Desulphurization of Steel using Mg

2. Select liquid steel and SlagA as the solutions

Reactants (9)
(gram) 99.84 Fe + 0.05 C + 0.1 Mn + 0.01 S + 4 CaO + 4 Al2O3 + SiO2 + MgO + <A> Mg

Products

Compound species:
 gas ideal real 0
 aqueous 0
 pure liquids 0
 pure solids 165
 suppress duplicates apply
* - custom selection species: 165

Solution species

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

Custom Solutions:
 fixed activities
 ideal solutions
 activity coefficients
Details ...

Pseudonyms:
apply List ...

include molar volumes
Total Species (max 1500) 212
Total Solutions (max 40) 3
Default

Final Conditions

| <A> | | T(C) | P(atm) | Product H(J) |
|-----|------|------|--------|--------------|
| 0.1 | 0.01 | 1600 | 1 | |

10 steps Table 101 calculations

Equilibrium
 normal normal + transitions
 transitions only
 open
Calculate >>

FactSage 6.3

1. Enter the <A> and Temperature

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

4. Press "Calculate"

Desulphurization of Steel using Mg

Results show a slag phase and a metal phase

Solid periclase (MgO) appears as <A> is increased

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

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

Output Edit Show Pages

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

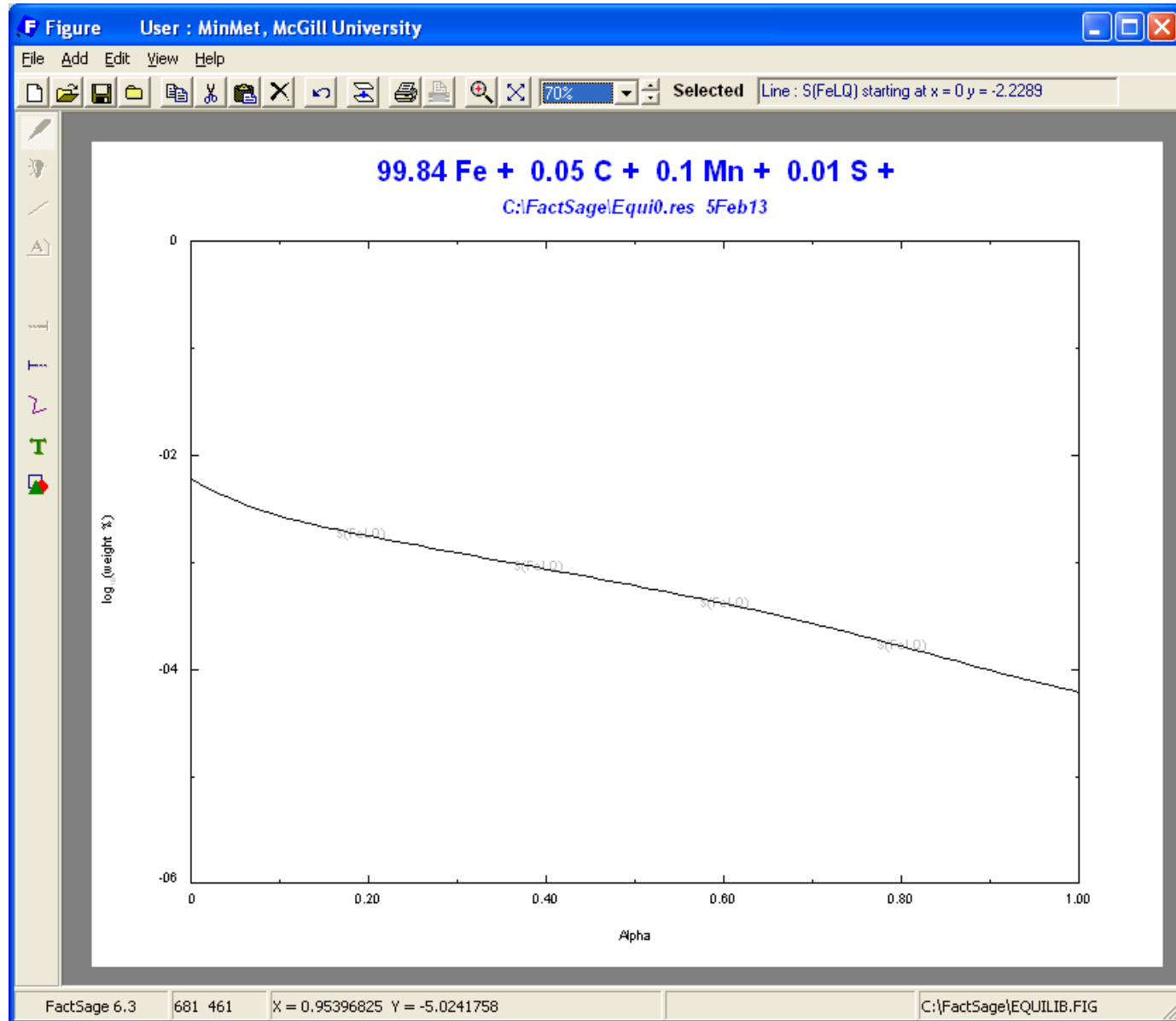
A=0.13 | A=0.14 | A=0.15 | A=0.16 | A=0.17 | A=0.18 | A=0.19 | A=0.2 | A=0.21 | A=0.22 | A=0.23 | A=0.24 |
A=0 | A=0.01 | A=0.02 | A=0.03 | A=0.04 | A=0.05 | A=0.06 | A=0.07 | A=0.08 | A=0.09 | A=0.1 | A=0.11 | A=0.12 |

FactSage 6.3

```
(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 FTmisc  
+ 6.9289E-04 wt.% Al FTmisc  
+ 5.0012E-02 wt.% C FTmisc  
+ 2.0349E-08 wt.% Ca FTmisc  
+ 8.9970E-02 wt.% Mn FTmisc  
+ 1.3134E-03 wt.% O FTmisc  
+ 5.9036E-03 wt.% S FTmisc  
+ 6.6985E-03 wt.% Si FTmisc  
+ 1.1551E-05 wt.% Mg FTmisc  
+ 1.0662E-03 wt.% MgO FTmisc  
+ 4.2218E-04 wt.% CaO FTmisc  
+ 5.4542E-05 wt.% AlO FTmisc  
+ 4.9024E-07 wt.% SiO FTmisc  
+ 2.0219E-05 wt.% MnO FTmisc  
+ 1.2528E-07 wt.% Al2O FTmisc  
  
System component Mole fraction Mass fraction  
Fe 0.99643 0.99844  
Mn 9.1287E-04 8.9985E-04
```

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” → “Save
or Print As ...”

2. Select “Open Text
Spreadsheet”

3. Press “Spreadsheet
Setup”

The screenshot shows the FactSage 6.3 software interface. The main window is titled "F Results - Equilib A=0 (page 1/101)". The "Output" menu is open, showing options like "Save or Print", "Plot", "Equilib Results file", etc. The "Save or Print" option is selected, and a sub-menu is visible with "Save or Print As ..." highlighted. A red arrow points from the text box "1. Press 'Output' → 'Save or Print' → 'Save or Print As ...'" to the "Save or Print" menu item. Another red arrow points from the text box "2. Select 'Open Text Spreadsheet'" to the "Open Text Spreadsheet" option in the "Type of Output" section of the "Output" dialog box. A third red arrow points from the text box "3. Press 'Spreadsheet Setup'" to the "Spreadsheet setup ..." button in the same dialog box. The "Output" dialog box has "Page Range" set to "All 101 pages" and "Type of Output" set to "Open Text Spreadsheet". The "OK" button is visible at the bottom right of the dialog box. The background window shows chemical composition data for a system component (Fe) with mole fraction 0.99643 and mass fraction 0.99843.

Desulphurization of Steel using Mg

1. Select "Alpha" as the property column

FactSage 6.3

(gram) 99.84 Fe + 0.05 C + 0.1 Mn + 0.01 S +
(gram) 4 CaO + 4 Al2O3 + SiO2 + MgO +
(gram) 99.84 Fe + 0.05 C + 0.1 Mn + 0.01 S +
(gram) 4 CaO + 4 Al2O3 + SiO2 + MgO +
+ 1.2528E-07 wt.% Al2O3

Property columns: 1

| | |
|-----------|-------|
| Column: | - 1 - |
| Variable: | Alpha |

Columns per species: 1

order species order props.

| | |
|-----------|-------|
| Column: | - 1 - |
| Variable: | Wt% |

Species

Columns: 3

Select ...

Selected: 2

Cancel

Default

OK

File fraction Mass f

| | |
|------------|------|
| 0.99643 | 0.99 |
| 9.1287E-04 | 8.99 |

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

F Spreadsheet - Equilib Page 1/101 : T(C) = 1600, P(atm) = 1

File Edit Show

Selected: 2/200 Spreadsheet Species 1 Pages: 1 - 101 [page]

Page 1/101 : T(C) = 1600, P(atm) = 1

| + Code | Species | Data | Phase | T | V | Activity | Minimum | Maximum |
|--------|--------------|--------|---------------|---|---|------------|------------------|-----------------|
| 399 | FeS(SLAGA) | FToxid | FToxid-SLAGA | | | 6.4260E-04 | 7.0718E-06 [101] | 6.4260E-04 [1] |
| 400 | Fe2S3(SLAGA) | FToxid | FToxid-SLAGA | | | 1.1685E-36 | 1.5775E-42 [101] | 1.1685E-36 [1] |
| 401 | MgS(SLAGA) | FToxid | FToxid-SLAGA | | | 4.4588E-04 | 3.8331E-04 [101] | 8.2982E-04 [18] |
| 402 | MnS(SLAGA) | FToxid | FToxid-SLAGA | | | 2.9142E-04 | 3.4643E-06 [101] | 2.9142E-04 [1] |
| 403 | Mn2S3(SLAGA) | FToxid | FToxid-SLAGA | | | 2.2626E-43 | 3.5642E-49 [101] | 2.2626E-43 [1] |
| | | | | | | 0.1138 | 0.1138 | 0.1138 |
| 785 | Solution | | FTmisc-FeLQ | | | 1.000 | 1.000 | 1.000 |
| 793 | Solution | | FToxid-SLAGA# | | | 1.000 | 1.000 | 1.000 |
| 833 | All Elements | | FTmisc-FeLQ | | | | | |
| + 841 | All Elements | | FToxid-SLAGA# | | | | | |

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

Select All Clear OK

2. Press "OK"

Desulphurization of Steel using Mg

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

Output Edit Show Pages

T(C) P(atm) Energy(J) Mass(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 6.3

(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
Selected: 2

Buttons: Cancel, Default, **OK**

+ 4.1738E-05 wt.% MnS FSstel
+ 1.5244E-08 wt.% Ca FSstel
+ 4.1689E-04 wt.% CaO FSstel
+ 3.2943E-11 wt.% CaS FSstel
+ 1.2018E-09 wt.% MgS FSstel)

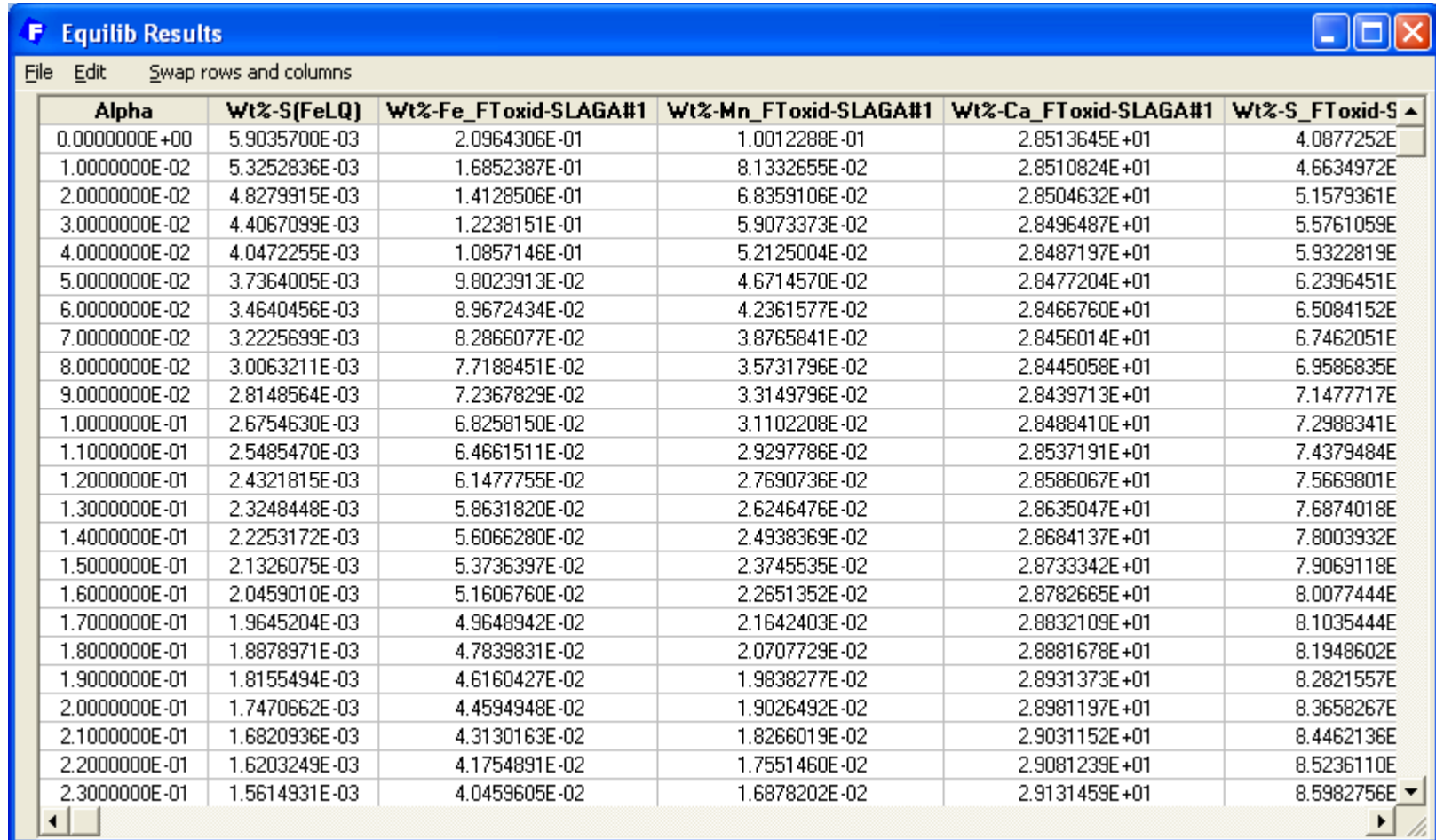
| System component | Mole fraction | Mass fraction |
|------------------|---------------|---------------|
| Fe | 0.99643 | 0.99843 |

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.



The screenshot shows a window titled "Equilib Results" with a menu bar containing "File", "Edit", and "Swap rows and columns". The window displays a table with 6 columns and 21 rows of data. The columns are labeled as follows:

- Alpha
- Wt%-S(FeLQ)
- Wt%-Fe_FToxid-SLAGA#1
- Wt%-Mn_FToxid-SLAGA#1
- Wt%-Ca_FToxid-SLAGA#1
- Wt%-S_FToxid-S

The data in the table is as follows:

| Alpha | Wt%-S(FeLQ) | Wt%-Fe_FToxid-SLAGA#1 | Wt%-Mn_FToxid-SLAGA#1 | Wt%-Ca_FToxid-SLAGA#1 | Wt%-S_FToxid-S |
|--------------|---------------|-----------------------|-----------------------|-----------------------|----------------|
| 0.000000E+00 | 5.9035700E-03 | 2.0964306E-01 | 1.0012288E-01 | 2.8513645E+01 | 4.0877252E |
| 1.000000E-02 | 5.3252836E-03 | 1.6852387E-01 | 8.1332655E-02 | 2.8510824E+01 | 4.6634972E |
| 2.000000E-02 | 4.8279915E-03 | 1.4128506E-01 | 6.8359106E-02 | 2.8504632E+01 | 5.1579361E |
| 3.000000E-02 | 4.4067099E-03 | 1.2238151E-01 | 5.9073373E-02 | 2.8496487E+01 | 5.5761059E |
| 4.000000E-02 | 4.0472255E-03 | 1.0857146E-01 | 5.2125004E-02 | 2.8487197E+01 | 5.9322819E |
| 5.000000E-02 | 3.7364005E-03 | 9.8023913E-02 | 4.6714570E-02 | 2.8477204E+01 | 6.2396451E |
| 6.000000E-02 | 3.4640456E-03 | 8.9672434E-02 | 4.2361577E-02 | 2.8466760E+01 | 6.5084152E |
| 7.000000E-02 | 3.2225699E-03 | 8.2866077E-02 | 3.8765841E-02 | 2.8456014E+01 | 6.7462051E |
| 8.000000E-02 | 3.0063211E-03 | 7.7188451E-02 | 3.5731796E-02 | 2.8445058E+01 | 6.9586835E |
| 9.000000E-02 | 2.8148564E-03 | 7.2367829E-02 | 3.3149796E-02 | 2.8439713E+01 | 7.1477717E |
| 1.000000E-01 | 2.6754630E-03 | 6.8258150E-02 | 3.1102208E-02 | 2.8488410E+01 | 7.2988341E |
| 1.100000E-01 | 2.5485470E-03 | 6.4661511E-02 | 2.9297786E-02 | 2.8537191E+01 | 7.4379484E |
| 1.200000E-01 | 2.4321815E-03 | 6.1477755E-02 | 2.7690736E-02 | 2.8586067E+01 | 7.5669801E |
| 1.300000E-01 | 2.3248448E-03 | 5.8631820E-02 | 2.6246476E-02 | 2.8635047E+01 | 7.6874018E |
| 1.400000E-01 | 2.2253172E-03 | 5.6066280E-02 | 2.4938369E-02 | 2.8684137E+01 | 7.8003932E |
| 1.500000E-01 | 2.1326075E-03 | 5.3736397E-02 | 2.3745535E-02 | 2.8733342E+01 | 7.9069118E |
| 1.600000E-01 | 2.0459010E-03 | 5.1606760E-02 | 2.2651352E-02 | 2.8782665E+01 | 8.0077444E |
| 1.700000E-01 | 1.9645204E-03 | 4.9648942E-02 | 2.1642403E-02 | 2.8832109E+01 | 8.1035444E |
| 1.800000E-01 | 1.8878971E-03 | 4.7839831E-02 | 2.0707729E-02 | 2.8881678E+01 | 8.1948602E |
| 1.900000E-01 | 1.8155494E-03 | 4.6160427E-02 | 1.9838277E-02 | 2.8931373E+01 | 8.2821557E |
| 2.000000E-01 | 1.7470662E-03 | 4.4594948E-02 | 1.9026492E-02 | 2.8981197E+01 | 8.3658267E |
| 2.100000E-01 | 1.6820936E-03 | 4.3130163E-02 | 1.8266019E-02 | 2.9031152E+01 | 8.4462136E |
| 2.200000E-01 | 1.6203249E-03 | 4.1754891E-02 | 1.7551460E-02 | 2.9081239E+01 | 8.5236110E |
| 2.300000E-01 | 1.5614931E-03 | 4.0459605E-02 | 1.6878202E-02 | 2.9131459E+01 | 8.5982756E |

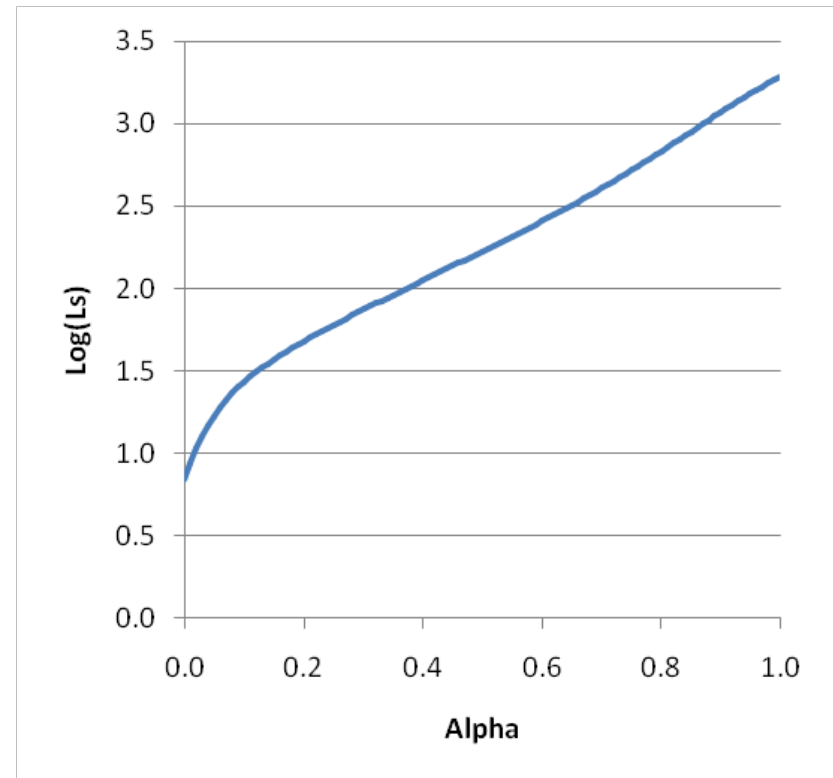
Desulphurization of Steel using Mg

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 .

| | A | B | C | D | E |
|---|----------|-------------|----------------------|-------------|---|
| 1 | Alpha | Wt%-S(FeLQ) | Wt%-S_FToxid-SLAGA#1 | log(Ls) | |
| 2 | 0.00E+00 | 5.90E-03 | 4.09E-02 | 0.840367 | |
| 3 | 1.00E-02 | 5.33E-03 | 4.66E-02 | 0.942369 | |
| 4 | 2.00E-02 | 4.83E-03 | 5.16E-02 | 1.028709 | |
| 5 | 3.00E-02 | 4.41E-03 | 5.58E-02 | =LOG(C5/B5) | |
| 6 | 4.00E-02 | 4.05E-03 | 5.93E-02 | 1.166064 | |
| 7 | 5.00E-02 | 3.74E-03 | 6.24E-02 | 1.222706 | |

3. Plotting Alpha against log(Ls)



Desulphurization of Steel using Mg: Composition target

As before, it is possible to calculate the composition target for liquid steel at 0.001% S

Here, we see that 0.3558g Mg is needed to attain the desired sulphur composition.

F Results - Equilib 1600 C, A=0.3558

Output Edit Show Pages

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

FactSage 6.3

```
(gram) 99.84 Fe + 0.05 C + 0.1 Mn + 0.01 S +
(gram) 4 CaO + 4 Al2O3 + SiO2 + MgO +
(gram) <A> Mg =

100.19 gram Fe-liq
(100.19 gram, 1.8011 mol)
(1600 C, 1 atm, a=1.0000)
( 99.643 wt.% Fe FTmisc
+ 1.1852E-02 wt.% Al FTmisc
+ 4.9903E-02 wt.% C FTmisc
+ 2.4844E-07 wt.% Ca FTmisc
+ 9.8773E-02 wt.% Mn FTmisc
+ 1.6314E-04 wt.% O FTmisc
+ 1.0000E-03 wt.% S FTmisc
+ 0.19301 wt.% Si FTmisc
+ 1.1836E-04 wt.% Mg FTmisc
+ 1.3037E-03 wt.% MgO FTmisc
+ 6.1035E-04 wt.% CaO FTmisc
+ 1.1886E-04 wt.% AlO FTmisc
+ 1.8364E-06 wt.% SiO FTmisc
+ 2.7238E-06 wt.% MnO FTmisc
+ 4.7829E-06 wt.% Al2O FTmisc)
```

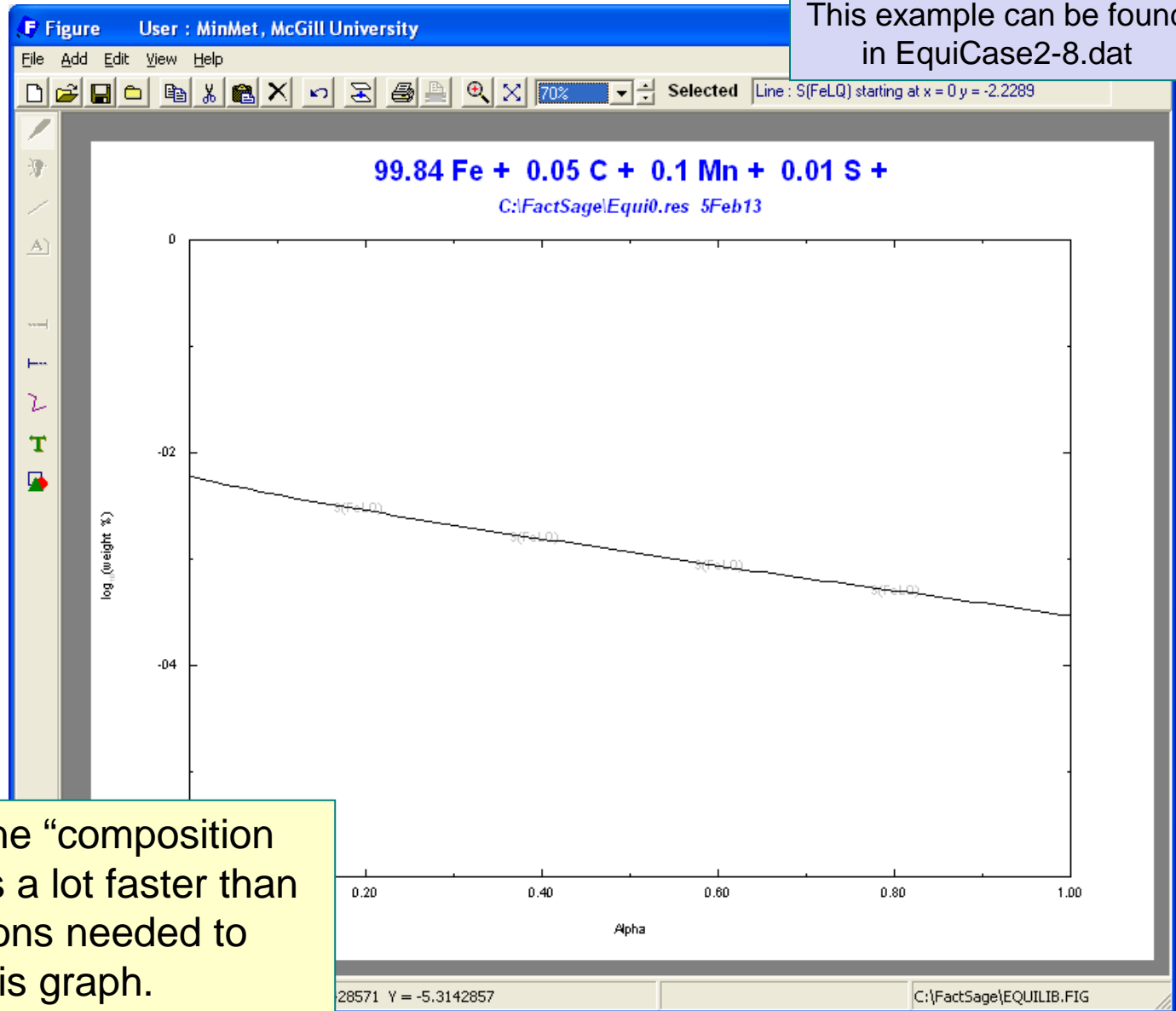
| System component | Mole fraction | Mass fraction |
|------------------|---------------|---------------|
| Fe | 0.99254 | 0.99643 |
| Mn | 1.0001E-03 | 9.8775E-04 |
| Ca | 6.0580E-06 | 4.3646E-06 |
| .. | | |

Desulphurization of Steel using CaC_2

Performing the same operations using CaC_2 , the following graph is obtained.

Using “composition target” it was found that 0.5446g of CaC_2 is needed to obtain the desired sulphur composition.

Performing only one “composition target” calculation is a lot faster than the 101 calculations needed to construct this graph.

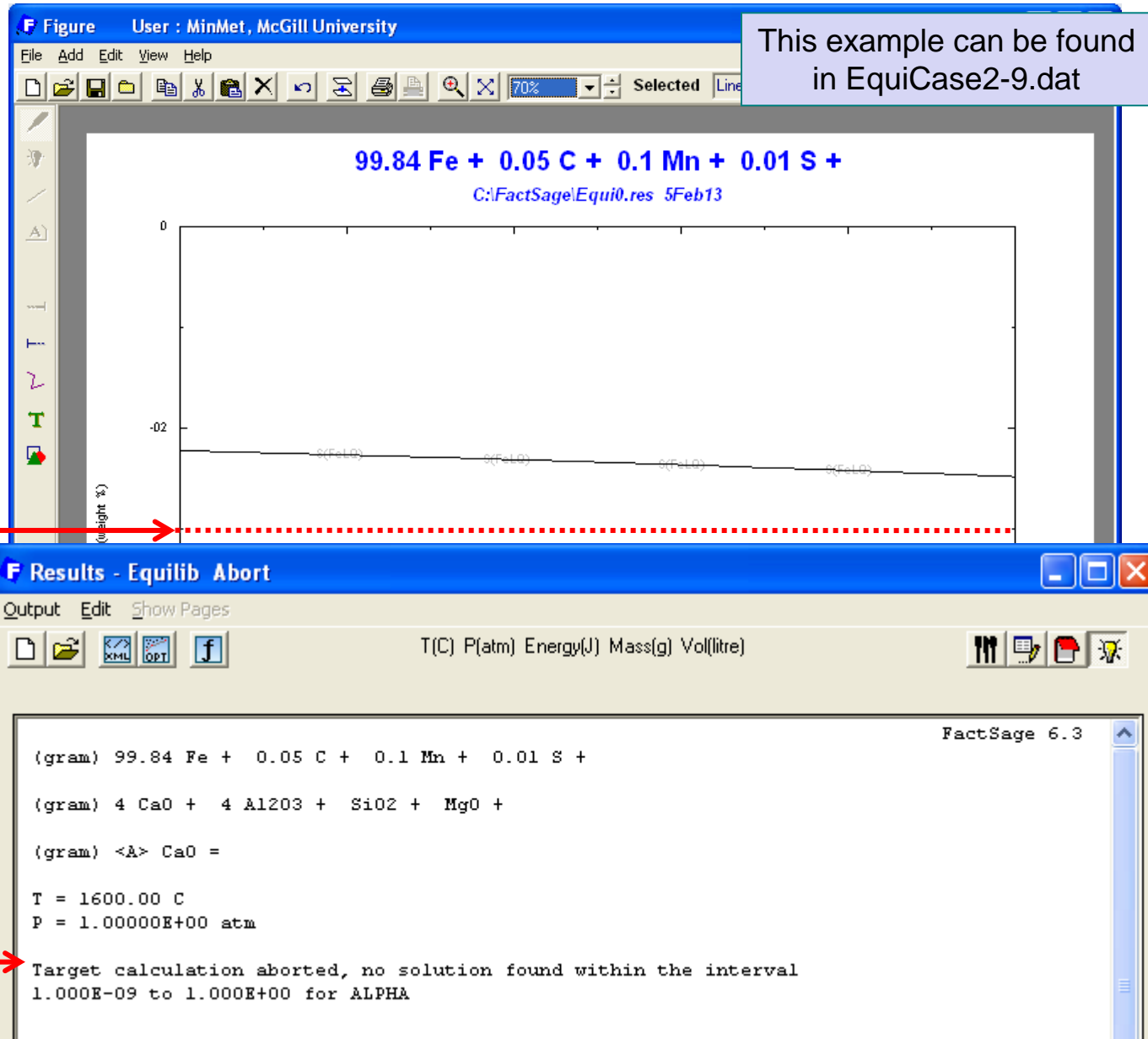


Desulphurization of Steel using CaO

1. Performing the same operations using CaO, the following graph is obtained.

2. It can be seen from this graph, that there is no value of Alpha for which $\log(\text{wt}\%S) = -3$

3. "Composition target" scans Alpha values from 0 to 1 only. So no solution is found for the composition target calculation.



Desulphurization of Steel using CaO

1. Because we need to go outside the 0 to 1 range, the amount of CaO was selected to be <10A>

2. It was then found that 2.368g of CaO is necessary to obtain 0.001% S

F Results - Equilib 1600 C, A=0.2368

Output Edit Show Pages

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

FactSage 6.3

```
(gram) 99.84 Fe + 0.05 C + 0.1 Mn + 0.01 S +  
(gram) 4 CaO + 4 Al2O3 + SiO2 + MgO +  
(gram) <10A> CaO =
```

99.969 gram Fe-liq
(99.969 gram, 1.7935 mol)
{1600 C, 1 atm, a=1.0000}

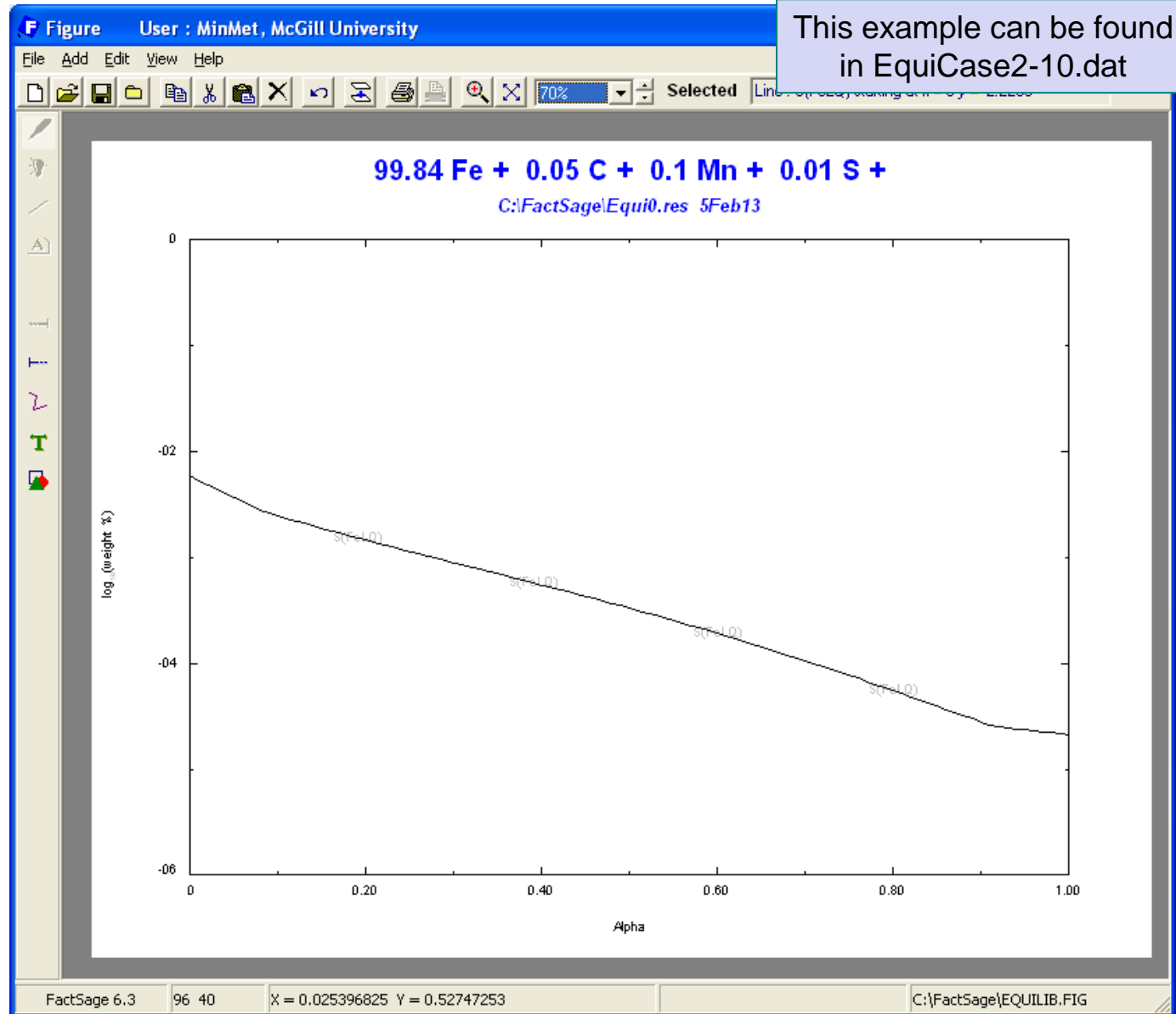
| | | |
|--------------|-----------|---------|
| { 99.845 | wt.% Fe | FTmisc |
| + 8.0433E-04 | wt.% Al | FTmisc |
| + 5.0016E-02 | wt.% C | FTmisc |
| + 1.1939E-07 | wt.% Ca | FTmisc |
| + 9.5877E-02 | wt.% Mn | FTmisc |
| + 6.5627E-04 | wt.% O | FTmisc |
| + 1.0000E-03 | wt.% S | FTmisc |
| + 3.5858E-03 | wt.% Si | FTmisc |
| + 2.8145E-05 | wt.% Mg | FTmisc |
| + 1.3009E-03 | wt.% MgO | FTmisc |
| + 1.2405E-03 | wt.% CaO | FTmisc |
| + 3.1660E-05 | wt.% AlO | FTmisc |
| + 1.3111E-07 | wt.% SiO | FTmisc |
| + 1.0791E-05 | wt.% MnO | FTmisc |
| + 8.4362E-08 | wt.% Al2O | FTmisc) |

| System component | Mole fraction | Mass fraction |
|------------------|---------------|---------------|
| Fe | 0.99652 | 0.99845 |
| Mn | 9.7279E-04 | 9.5885E-04 |
| Ca | 1.2331E-05 | 8.8668E-06 |
| .. | | |

Desulphurization of Steel using CaO+Mg

Performing the same operations using CaO+Mg, the following graph is obtained.

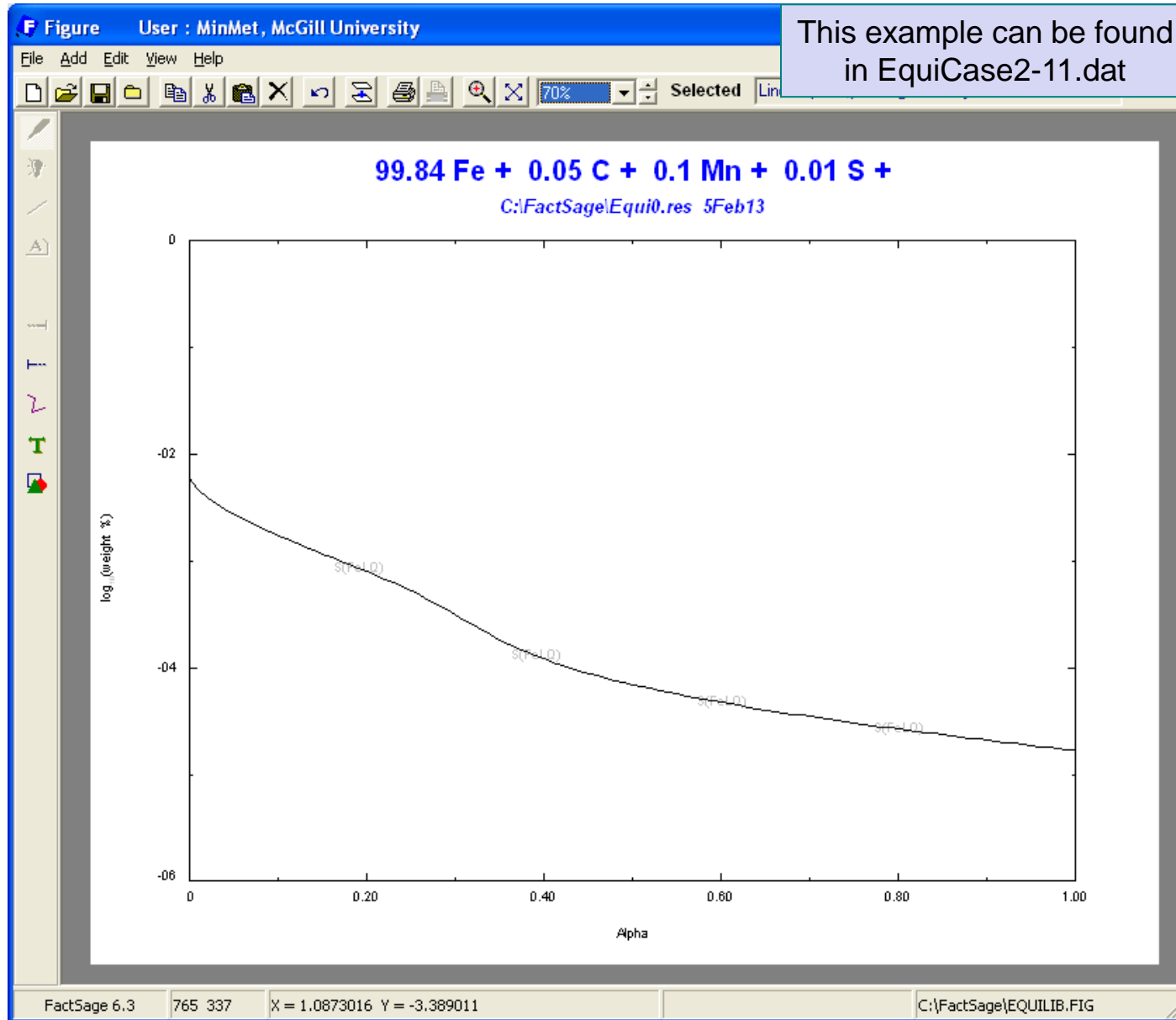
Using “composition target” it was found that 0.2746g of CaO and 0.2746g Mg is needed to obtain the desired sulphur composition.



Desulphurization of Steel using CaO+Al

Performing the same operations using CaO+Al, the following graph is obtained.

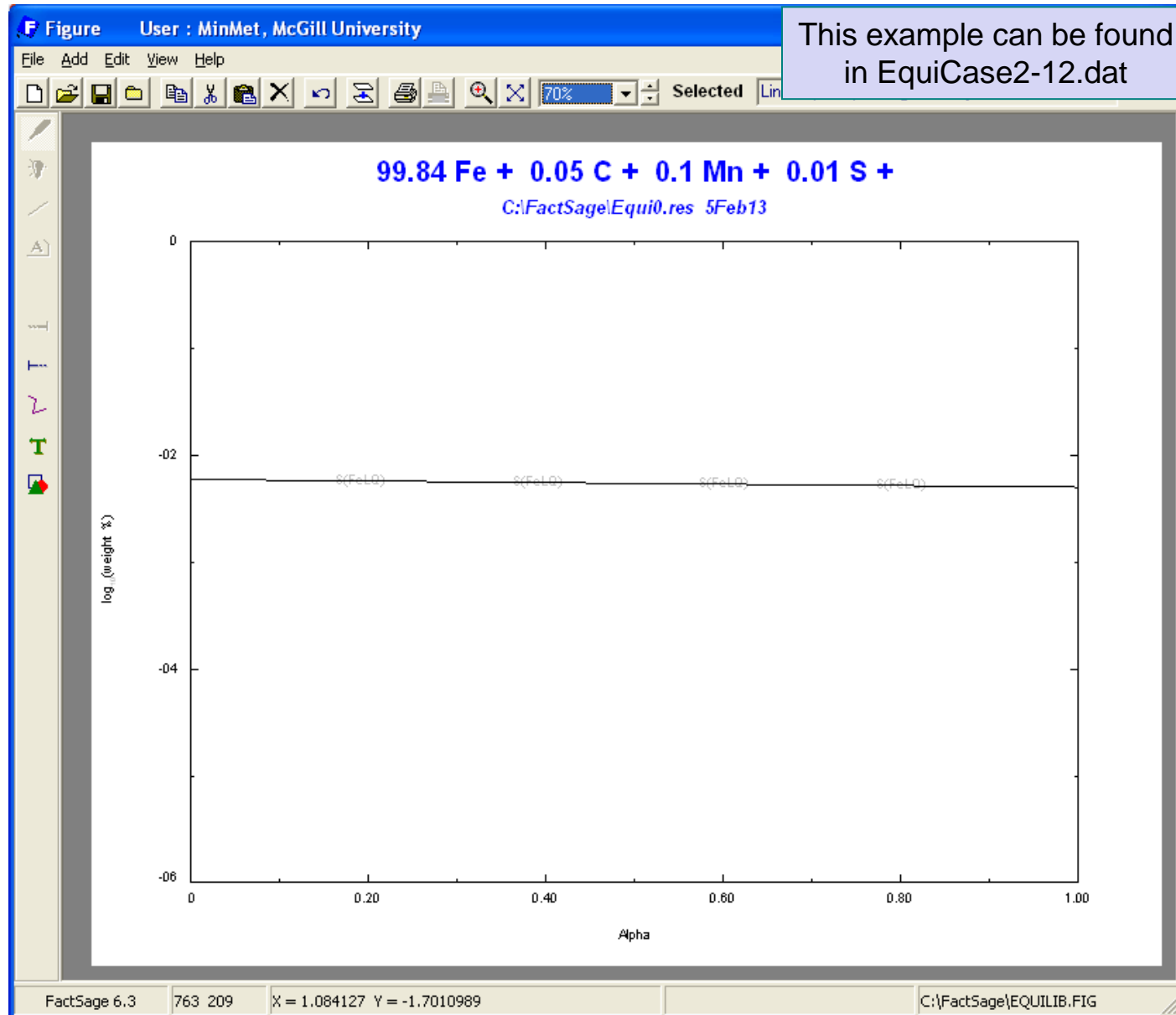
Using “composition target” it was found that 0.1699g of CaO and 0.3398g Al is needed to obtain the desired sulphur composition.



Desulphurization of Steel using $\text{CaO} + \text{Al}_2\text{O}_3$

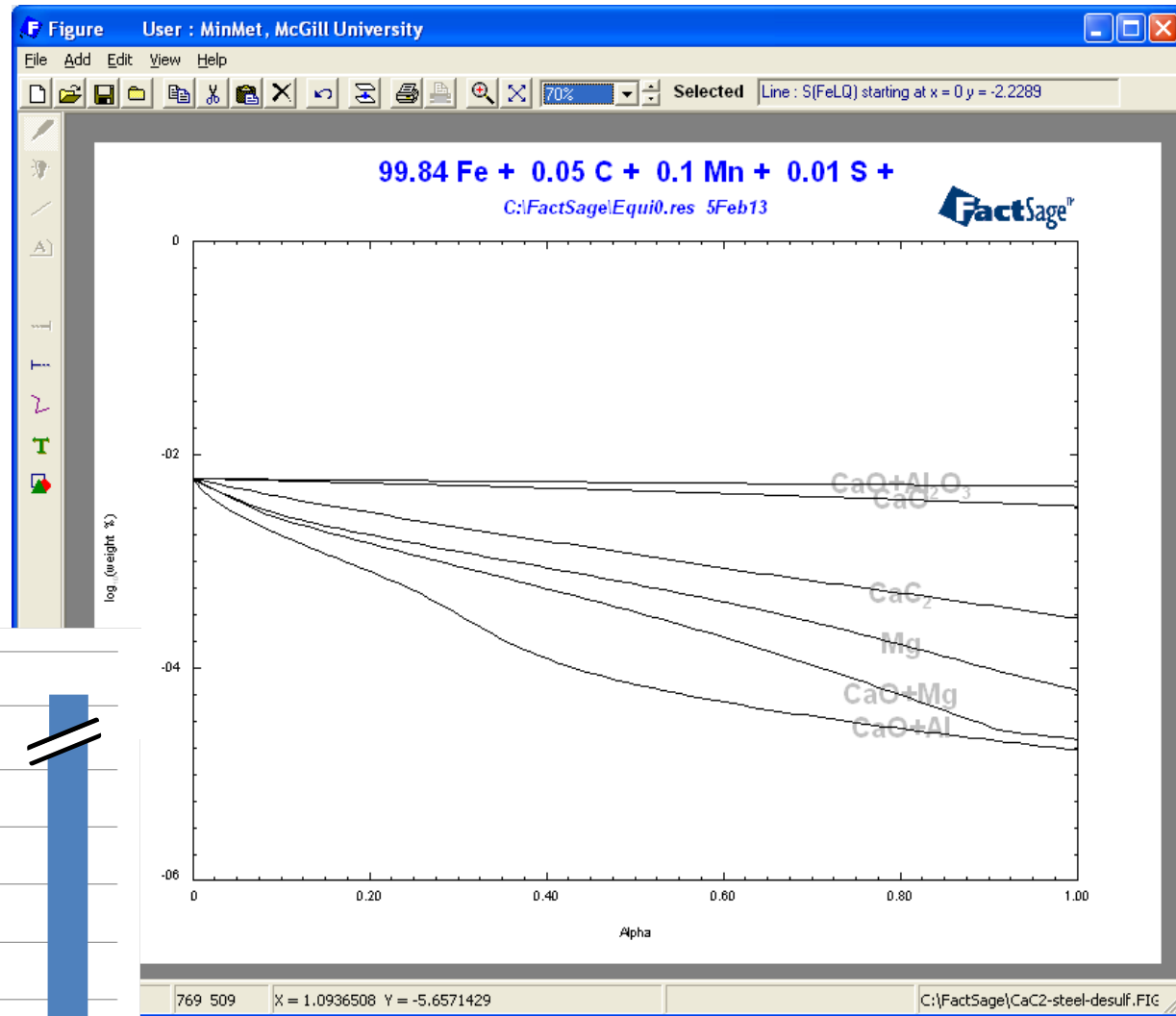
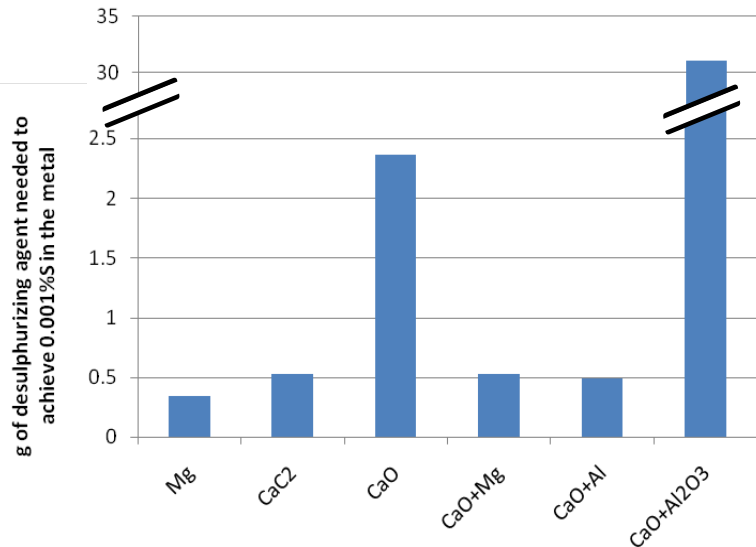
Performing the same operations using $\text{CaO} + \text{Al}_2\text{O}_3$, the following graph is obtained.

Using “composition target” it was found that 15.49g of CaO and 15.49g Al_2O_3 is needed to obtain the desired sulphur composition.



Desulphurization of Steel

Comparing the different desulphurization agents.



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 displays two windows from the FactSage 6.3 software. The background window is titled "F Reactants - Equilib" and shows a table of reactants. The foreground window is titled "F Data Search" and shows the process of selecting databases for the calculation.

| Mass(g) | Species |
|---------|---------|
| 44 | CaO |
| 9 | MgO |
| 13 | SiO2 |
| 1.8 | Al2O3 |
| 18 | Fe |
| 4.5 | MnO |
| 0.07 | S |
| 2 | P2O5 |
| 1 | TiO2 |

The "Data Search" dialog box shows the following database selection options:

- FactPS
- Ftoxid
- FTsalt
- FTmisc
- FTball
- FT0xCN
- FTfrtz
- FTelg
- FTpulp
- FTlite
- FScopp
- FSlead
- FSlite
- FSstel
- FSnobl
- FSupsi
- ELEM
- FTdemo
- BINS
- SGPS
- SGTE
- SGnobl
- SGSold
- SGnucl
- TDnucl

The "Miscellaneous" section includes:

- EXAM
- SGTE#
- SGTE*

The "Options" section includes:

- Include: gaseous ions (plasmas), aqueous species, limited data compounds (25C)
- Limits: Organic species CxHy..., X(max) = 2, Minimum solution components: 1, 2 cpts

2. Select FactPS and Ftoxid databases

Calculating Slag Sulphide Capacity

1. Select gas and SlagA as possible products

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 ideal real 57
 aqueous 0
 pure liquids 0
 pure solids 0
 suppress duplicates
species: 57

Target
- none -
Estimate T(K):
Mass(g):

Solution species

| * | Base-Phase | Full Name |
|---|--------------|--------------------------------|
| 1 | FToxid-SLAGA | ASlag-liq all oxides + S |
| | FToxid-SLAGB | BSlag-liq with SO ₄ |
| | FToxid-SLAGC | CSlag-liq with PO ₄ |
| | FToxid-SLAG? | ?Slag-liq |
| | FToxid-SPINA | ASpinel |
| | FToxid-SPINB | BSpinel |
| | FToxid-SPIN? | ?Spinel |
| | FToxid-MeO_A | AMonoxide |

Legend
I - immiscible 1
 Show all selected
species: 40
solutions: 2

Custom Solutions
 fixed activities
 ideal solutions
 activity coefficients

Pseudonyms
apply
 include molar volumes
Total Species (max 1500) 97
Total Solutions (max 40) 2

Final Conditions

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

10 steps Table

Equilibrium
 normal normal + transitions
 transitions only
 open

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

3. Press "Calculate"

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.

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

Output Edit Show Pages

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

1580 C | 1600 C | 1620 C |

FactSage 6.3

(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
(11.932 gram, 0.25836 mol, 39.287 litre, 3.0372E-04 gram/cm3)
(1580 C, 1 atm, a=1.0000)

| | | |
|--------------|------|--------|
| 0.41820 | Fe | FactPS |
| + 0.31005 | Mg | FactPS |
| + 0.21581 | Mn | FactPS |
| + 5.4274E-02 | P2 | FactPS |
| + 1.4880E-03 | Ca | FactPS |
| + 1.2400E-04 | P4 | FactPS |
| + 2.9676E-05 | P | FactPS |
| + 1.7530E-05 | Mg2 | FactPS |
| + 1.0246E-05 | SiO | FactPS |
| + 3.9334E-07 | PO | FactPS |
| + 5.5574E-08 | FeO | FactPS |
| + 7.8883E-09 | Si | FactPS |
| + 2.0124E-09 | Ca2 | FactPS |
| + 1.8430E-09 | MgO | FactPS |
| + 1.8372E-09 | FeS | FactPS |
| + 1.7628E-09 | SiS | FactPS |
| + 1.0575E-09 | PS | FactPS |
| + 7.1669E-10 | MgS | FactPS |
| + 1.8919E-10 | CaO | FactPS |
| + 1.1979E-10 | Al2O | FactPS |

Calculating Slag Sulphide Capacity

The first way is to use Excel

1. Save the results in a spreadsheet

The screenshot shows the FactSage 6.3 interface. The main window title is "F Results - Equilib 1580 C (page 1/3)". The "Output" menu is open, showing options like "Save or Print", "Plot", "Equilib Results file", "Stream File", "Format", "Fact-XML", "Fact-Optimal", "Fact-Function-Builder", and "Refresh ...". The "Save or Print As ..." option is selected, and a sub-menu is open with "Repeat Save" and "Spreadsheet setup ...". The "Spreadsheet setup ..." dialog box is also open, showing "Page Range" (All 3 pages selected) and "Type of Output" (Open Text Spreadsheet selected). The "Spreadsheet setup ..." button is highlighted with a red arrow pointing to it from a yellow box containing the text "2. Press 'Spreadsheet setup'".

2. Press "Spreadsheet setup"

Calculating Slag Sulphide Capacity

1. Set T(C) as the system property

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% | a |

Species

Columns: 5

Select ...

Species: 2

Cancel

Default

OK

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

Calculating Slag Sulphide Capacity

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

Spreadsheet - Equilib Page 1/3 : T(C) = 1580, P(atm) = 1

File Edit Show

Selected: 4/81 Spreadsheet Species

Page 1/3 : T(C) = 1580 [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 | | | 1.7208E-13 | 1.7208E-13 [1] | 5.8032E-13 [3] |
| + | 2 | O ₂ (g) | FactPS | gas | | | 7.6267E-19 | 7.6267E-19 [1] | 4.3095E-18 [3] |
| | 3 | O ₃ (g) | FactPS | gas | | | 1.7227E-35 | 1.7227E-35 [1] | 2.8251E-34 [3] |
| | 26 | S(g) | FactPS | gas | | | 1.3536E-12 | 1.3536E-12 [1] | 3.8752E-12 [3] |
| + | 27 | S ₂ (g) | FactPS | gas | | | 1.4389E-18 | 1.4389E-18 [1] | 6.4939E-18 [3] |
| | 28 | S ₃ (g) | FactPS | gas | | | 8.5282E-30 | 8.5282E-30 [1] | 7.6427E-29 [3] |
| | 921 | Gas | | GAS | | | 1.000 | 1.000 | 1.000 |
| | 925 | Solution | | FToxid-SLAGA# | | | 1.000 | 1.000 | 1.000 |
| | 968 | All Elements | | GAS | | | | | |
| + | 972 | All Elements | | 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

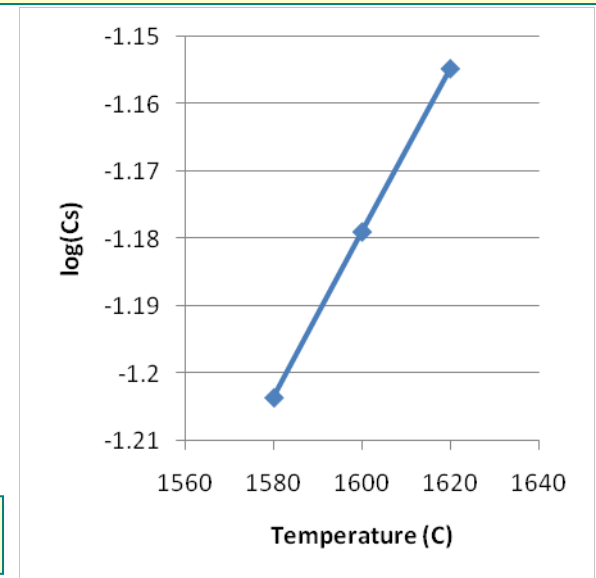
1. All the needed results (and even more) appear in the spreadsheet.

| T(C) | Wt%-O2(g) | Wt%-S2(g) | a-O2(g) | a-S2(g) | Wt%-Fe_FToxid-SLAGA#1 | Wt%-Mn_FToxid-SLAGA#1 |
|---------------|---------------|---------------|---------------|---------------|-----------------------|-----------------------|
| 1.5800000E+03 | 5.2840192E-17 | 1.9979179E-16 | 7.6266917E-19 | 1.4388711E-18 | 1.4693761E+01 | 5.1810549E-01 |
| 1.6000000E+03 | 1.2689259E-16 | 4.2841627E-16 | 1.8306754E-18 | 3.0839938E-18 | 1.4683709E+01 | 5.3768839E-01 |
| 1.6200000E+03 | 2.9884777E-16 | 9.0252038E-16 | 4.3095187E-18 | 6.4939392E-18 | 1.4673537E+01 | 5.5742466E-01 |

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

| | A | B | C | D | E | F | G |
|---|----------|----------|----------|----------------------|----------------------|---|---|
| 1 | T(C) | a-O2(g) | a-S2(g) | Wt%-S_FToxid-SLAGA#1 | | | |
| 2 | 1.58E+03 | 7.63E-19 | 1.44E-18 | 8.60E-02 | | | |
| 3 | 1.60E+03 | 1.83E-18 | 3.08E-18 | 8.60E-02 | | | |
| 4 | 1.62E+03 | 4.31E-18 | 6.49E-18 | 8.59E-02 | | | |
| | | | | | log(Cs) | | |
| | | | | | -1.20357 | | |
| | | | | | -1.17899 | | |
| | | | | | =LOG(D4*SQRT(B4/C4)) | | |

4. Plot log(Cs) versus temperature



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

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

The screenshot shows the FactSage 6.3 interface with the 'Fact-Function-Builder' menu open. The menu options are:

- Save or Print
- Plot
- Equilib Results file
- Stream File
- Format
- Fact-XML
- Fact-Optimal
- Fact-Function-Builder**
 - Select function group(s)
 - Always calculate function groups(s) - (nothing selected)
 - Refresh Results ...
 - Edit function group
 - Edit/create functions ...**
 - Summary of function groups ...
 - Fact-Function-Builder Slide Show ...
- Refresh ...

The background window displays the following chemical formula and data:

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

MgO + 13 SiO2 + 1.8 Al2O3 +
5 MnO + 0.07 S + 2 P2O5 +

| Value | Component | Value |
|--------------|-----------|--------|
| + 0.418 | | FactPS |
| + 0.310 | | FactPS |
| + 0.215 | | FactPS |
| + 5.427 | | FactPS |
| + 1.488 | | FactPS |
| + 1.240 | | FactPS |
| + 2.9676E-05 | P | FactPS |
| + 1.7530E-05 | Mg2 | FactPS |
| + 1.0246E-05 | Si0 | FactPS |
| + 3.9334E-07 | P0 | FactPS |
| + 8.3962E-08 | Al | FactPS |
| + 5.5574E-08 | Fe0 | FactPS |
| + 7.8883E-09 | Si | FactPS |
| + 2.0124E-09 | Ca2 | FactPS |
| + 1.8430E-09 | Mg0 | FactPS |
| + 1.8372E-09 | FeS | FactPS |
| + 1.7628E-09 | SiS | FactPS |
| + 1.0575E-09 | PS | FactPS |
| + 7.1669E-10 | MgS | FactPS |
| + 1.8919E-10 | Ca0 | FactPS |
| | | |

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' is empty. The 'Functions' section is empty. The 'Variable selection' dropdown is set to 'Amount/Composition'. The 'Selection' table is displayed below, with 'S (total)' selected. A context menu is open over 'S (total)' with the option 'Add to variables list' highlighted. The unit selection at the bottom is set to 'Wt. %'.

| Species | Phase | Data | Amount/Co... | MIN | MAX | Pseudonym |
|------------|------------|--------|--------------|-----------|-----------|-----------|
| Mn2S3 | Slag-liq#1 | FToxid | 6.716E-08 | 6.716E-08 | 1.035E-07 | |
| Fe (total) | Slag-liq#1 | | 1.469E+01 | 6.716E-08 | 1.469E+01 | |
| Mn (total) | Slag-liq#1 | | 5.181E-01 | 6.716E-08 | 1.469E+01 | |
| Ti (total) | Slag-liq#1 | | 7.360E-01 | 6.716E-08 | 1.469E+01 | |
| Ca (total) | Slag-liq#1 | | 3.860E+01 | 6.716E-08 | 3.860E+01 | |
| S (total) | Slag-liq#1 | | 8.596E-02 | 6.716E-08 | 3.860E+01 | |
| P (total) | Slag-liq#1 | | 0.000E+00 | 0.000E+00 | 3.860E+01 | |
| Si (total) | Slag-liq#1 | | 7.462E+00 | 0.000E+00 | 3.860E+01 | |
| Al (total) | Slag-liq#1 | | 1.170E+00 | 0.000E+00 | 3.860E+01 | |
| Mg (total) | Slag-liq#1 | | 4.273E+00 | 0.000E+00 | 3.860E+01 | |
| O (total) | Slag-liq#1 | | 3.247E+01 | 0.000E+00 | 3.860E+01 | |
| Al2O3 | Slag-liq#2 | FToxid | 0.000E+00 | 0.000E+00 | 0.000E+00 | |

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

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 window. The 'Variables List' contains the variable 'A : Amount/Composition (S (total)/Slag-liq#1)) wt.%'. A right-click context menu is open over this variable, with 'Rename' selected. A 'Name' dialog box is open, showing the new variable name 'wtS' entered in the text field. The 'Functions' section is empty. The 'Variable selection' section shows a table of species and phases. The 'Selection' section is set to 'Species/phases:'. The 'Species' column lists various elements and compounds, and the 'Phase' column lists 'Gas'. The 'Data' column lists 'FactPS'. The 'Amount/Co...' column lists values in scientific notation. The 'MIN' and 'MAX' columns list values in scientific notation. The 'Pseudonym' column lists values in scientific notation. The 'mol' radio button is selected in the bottom right corner.

| Species | Phase | Data | Amount/Co... | MIN | MAX | Pseudonym |
|---------|-------|--------|--------------|-----------|-----------|-----------|
| O | Gas | FactPS | 5.961E-12 | 5.961E-12 | 2.012E-11 | |
| O2 | Gas | FactPS | 5.284E-17 | 5.284E-17 | 2.988E-16 | |
| O3 | Gas | FactPS | 1.790E-33 | 1.790E-33 | 2.939E-32 | |
| Mg | Gas | FactPS | 1.632E+01 | 1.632E+01 | 1.640E+01 | |
| Mg2 | Gas | FactPS | 1.845E-03 | 1.763E-03 | 1.845E-03 | |
| MgO | Gas | FactPS | 1.608E-07 | 1.608E-07 | 3.474E-07 | |
| Al | Gas | FactPS | 4.905E-06 | 4.905E-06 | 6.877E-06 | |
| Al2 | Gas | FactPS | 5.346E-13 | 5.346E-13 | 8.413E-13 | |
| AlO | Gas | FactPS | 3.732E-10 | 3.732E-10 | 8.673E-10 | |
| AlO2 | Gas | FactPS | 1.884E-18 | 1.884E-18 | 9.094E-18 | |
| Al2O | Gas | FactPS | 1.815E-08 | 1.815E-08 | 2.816E-08 | |
| Al2O2 | Gas | FactPS | 1.931E-13 | 1.931E-13 | 5.057E-13 | |

Calculating Slag Sulphide Capacity

Function Builder

File Help

Variables List: clear Preview results Copy to clipboard

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

D
E
G
I
J

Functions

?1 = + Preview results

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

Variable selection

Activity ▾ + variable

Selection

Species/phases:

| | Species | Phase | Data | Activity | MIN | MAX | Pseudonym |
|--|---------|-------|--------|-----------|-----------|-----------|-----------|
| | O | Gas | FactPS | 1.721E-13 | 1.721E-13 | 5.803E-13 | |
| | O2 | Gas | FactPS | 7.627E-19 | 7.627E-19 | 4.310E-18 | |
| | O3 | Gas | FactPS | 1.723E-35 | 1.723E-35 | 2.825E-34 | |
| | Mg | Gas | FactPS | 3.101E-01 | 3.101E-01 | 3.113E-01 | |
| | Mg2 | Gas | FactPS | 1.753E-05 | 1.673E-05 | 1.753E-05 | |
| | MgO | Gas | FactPS | 1.843E-09 | 1.843E-09 | 3.978E-09 | |
| | Al | Gas | FactPS | 8.396E-08 | 8.396E-08 | 1.176E-07 | |
| | Al2 | Gas | FactPS | 4.575E-15 | 4.575E-15 | 7.194E-15 | |
| | AlO | Gas | FactPS | 4.010E-12 | 4.010E-12 | 9.311E-12 | |
| | AlO2 | Gas | FactPS | 1.475E-20 | 1.475E-20 | 7.115E-20 | |
| | Al2O | Gas | FactPS | 1.198E-10 | 1.198E-10 | 1.857E-10 | |
| | Al2O2 | Gas | FactPS | 1.037E-15 | 1.037E-15 | 2.715E-15 | |

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(Cs)

2. Press "preview results"

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

Variables List

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

Functions

?1 = $\log(\text{wtS} * \text{SQRT}(\text{aO2}/\text{aS2}))$

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

Preview results

| Page | ?1 = log(wtS*SQRT(aO2/aS2)) |
|------|-----------------------------|
| 1 | -1.203570 |
| 2 | -1.178994 |
| 3 | -1.154799 |

Variable selection

Amount/Composition

Selection

Species/phases:

| Species | Phase | Data | Amount/Co... | MIN | MAX | Pseudonym |
|---------|-------|--------|--------------|-----------|-----------|-----------|
| O | Gas | FactPS | 5.961E-12 | 5.961E-12 | 2.012E-11 | |
| O2 | Gas | FactPS | 5.284E-17 | 5.284E-17 | 2.988E-16 | |
| O3 | Gas | FactPS | 1.790E-33 | 1.790E-33 | 2.939E-32 | |
| Mg | Gas | FactPS | 1.632E+01 | 1.632E+01 | 1.640E+01 | |
| Mg2 | Gas | FactPS | 1.845E-03 | 1.763E-03 | 1.845E-03 | |
| MgO | Gas | FactPS | 1.608E-07 | 1.608E-07 | 3.474E-07 | |
| Al | Gas | FactPS | 4.905E-06 | 4.905E-06 | 6.877E-06 | |
| Al2 | Gas | FactPS | 5.346E-13 | 5.346E-13 | 8.413E-13 | |
| AlO | Gas | FactPS | 3.732E-10 | 3.732E-10 | 8.673E-10 | |
| AlO2 | Gas | FactPS | 1.884E-18 | 1.884E-18 | 9.094E-18 | |
| Al2O | Gas | FactPS | 1.815E-08 | 1.815E-08 | 2.816E-08 | |
| Al2O2 | Gas | FactPS | 1.931E-13 | 1.931E-13 | 5.057E-13 | |

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

Close

Calculating Slag Sulphide Capacity

1. Save the function as "Sulphide_Capacity"

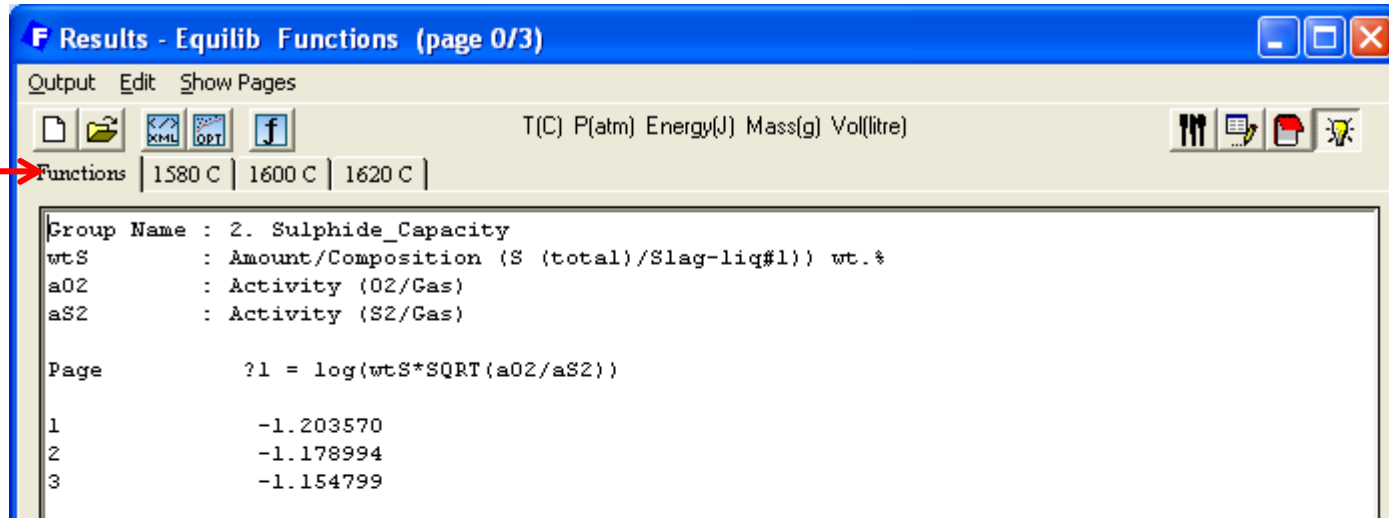
The screenshot shows the 'Function Builder' window for a function named '[Sulphide_Capacity]'. A 'Name' dialog box is open, prompting the user to enter a name for the system, with 'Sulphide_Capacity' entered in the text field. The background window shows the function definition $(total)/Slag-liq\#1))$ wt.%, a preview of results for three pages, and a table of species/amounts.

| Species | Phase | Data | Amount/Co... | MIN | MAX | Pseudonym |
|---------|-------|--------|--------------|-----------|-----------|-----------|
| O | Gas | FactPS | 5.961E-12 | 5.961E-12 | 2.012E-11 | |
| O2 | Gas | FactPS | 5.284E-17 | 5.284E-17 | 2.988E-16 | |
| O3 | Gas | FactPS | 1.790E-33 | 1.790E-33 | 2.939E-32 | |
| Mg | Gas | FactPS | 1.632E+01 | 1.632E+01 | 1.640E+01 | |
| Mg2 | Gas | FactPS | 1.845E-03 | 1.763E-03 | 1.845E-03 | |
| MgO | Gas | FactPS | 1.608E-07 | 1.608E-07 | 3.474E-07 | |
| Al | Gas | FactPS | 4.905E-06 | 4.905E-06 | 6.877E-06 | |
| Al2 | Gas | FactPS | 5.346E-13 | 5.346E-13 | 8.413E-13 | |
| AlO | Gas | FactPS | 3.732E-10 | 3.732E-10 | 8.673E-10 | |
| AlO2 | Gas | FactPS | 1.884E-18 | 1.884E-18 | 9.094E-18 | |
| Al2O | Gas | FactPS | 1.815E-08 | 1.815E-08 | 2.816E-08 | |
| Al2O2 | Gas | FactPS | 1.931E-13 | 1.931E-13 | 5.057E-13 | |

2. Close the window

Calculating Slag Sulphide Capacity

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



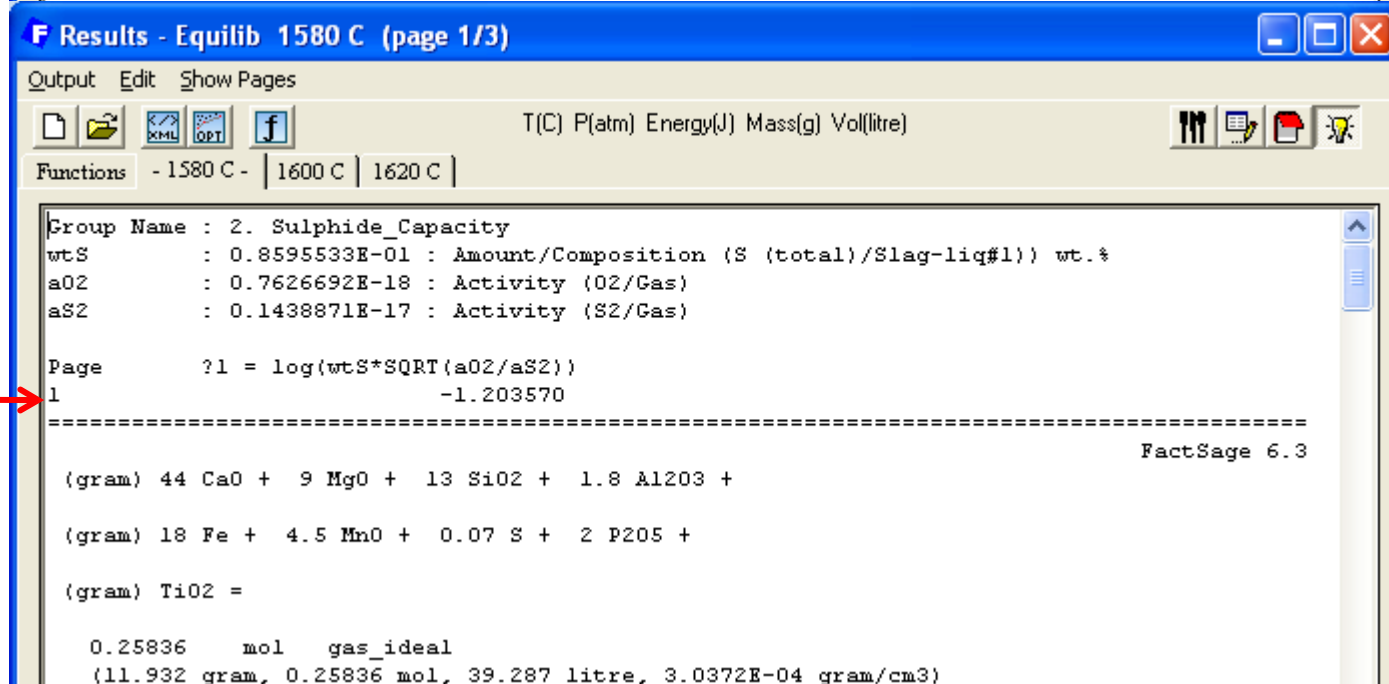
```
Results - Equilib Functions (page 0/3)
Output Edit Show Pages
T(C) P(atm) Energy(J) Mass(g) Vol(litre)
Functions | 1580 C | 1600 C | 1620 C |

Group Name : 2. Sulphide_Capacity
wtS       : Amount/Composition (S (total)/Slag-liq#1)) wt.%
aO2       : Activity (O2/Gas)
aS2       : Activity (S2/Gas)

Page      ?1 = log(wtS*SQRT(aO2/aS2))

1         -1.203570
2         -1.178994
3         -1.154799
```

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



```
Results - Equilib 1580 C (page 1/3)
Output Edit Show Pages
T(C) P(atm) Energy(J) Mass(g) Vol(litre)
Functions | -1580 C - | 1600 C | 1620 C |

Group Name : 2. Sulphide_Capacity
wtS       : 0.8595533E-01 : Amount/Composition (S (total)/Slag-liq#1)) wt.%
aO2       : 0.7626692E-18 : Activity (O2/Gas)
aS2       : 0.1438871E-17 : Activity (S2/Gas)

Page      ?1 = log(wtS*SQRT(aO2/aS2))
1         -1.203570
-----
FactSage 6.3

(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
(11.932 gram, 0.25836 mol, 39.287 litre, 3.0372E-04 gram/cm3)
```

Calculating Slag Sulphide Capacity

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

2. Then select "Graph" → "Setup"

3. Import the "Sulphide_Capacity" function

The screenshot displays the FactSage software interface with three overlapping windows. The top window, titled "Results - Equilib Functions (page 0/3)", shows a toolbar with an "XML" button highlighted by a red arrow. Below it, the "XML Viewer - [C:\FACTSAGE\Xml_out.xml]" window has its "Graph" menu open, with the "Setup..." option selected by a red arrow. The bottom window, "Graph - Setup", shows the "Import" menu open, with "1 - Sulphide Capacity" selected by a red arrow. The Y-axis is labeled "Activity" and the X-axis is labeled "Page #".

| Species | Phase | Data | Activity | MIN | MAX | Pseudonym |
|---------|-------|------|----------|-----|-----|-----------|
| | | | | | | |

Calculating Slag Sulphide Capacity

1. Select "Functions" as the Y-Axis

2. Select "Temperature" as the X-axis

Graph - Setup

Variables

- wtS : Amount/Composition
- aO2 : Activity (O2 Gas)
- aS2 : Activity (S2 Gas)
- E
- G
- I
- L

Figure Settings

- Font size : 10
- # labels per line : 0
- line colors... Title
- Full Screen

Y-Axis

Functions Y + variable

?1 = $\log(\text{wtS} * \sqrt{\text{aO2} / \text{aS2}})$

MIN MAX STEP Label every

-2.8 -2.73 Default 0.01 0.006999

X-Axis

Temperature X + variable

? =

MIN MAX STEP Label every

1580 1620 Default 1 4

Species/phases:

| Species | Phase | Data | Amount/Co... | MIN | MAX | Pseudonym |
|---------|-------|------|--------------|-----|-----|-----------|
|---------|-------|------|--------------|-----|-----|-----------|

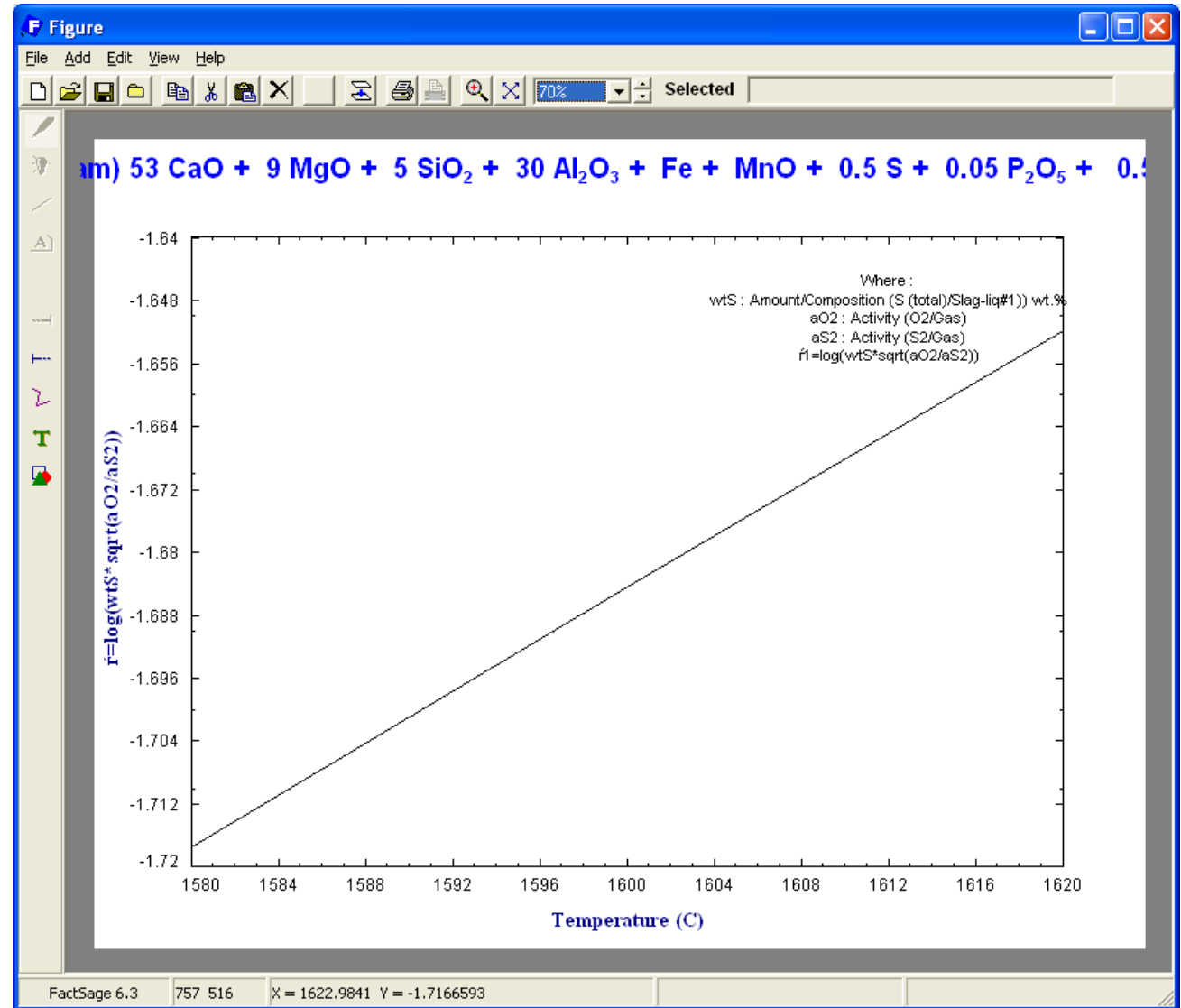
4. Press "Draw"

3. Adjust the min and max values, the step, etc.

4. Press "Draw"

Calculating Slag Sulphide Capacity

The figure is then obtained



Calculating Slag Sulphide Capacity

Repeating the same procedure for the other slag compositions, it is possible to compare the sulphide capacity of the different slags.

