Case 2: Desulphurization

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

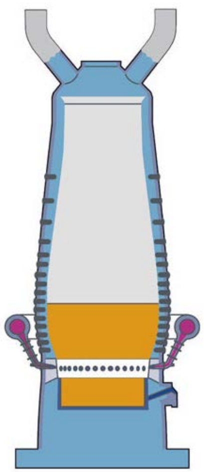
Desulphurization of Hot Metal

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.

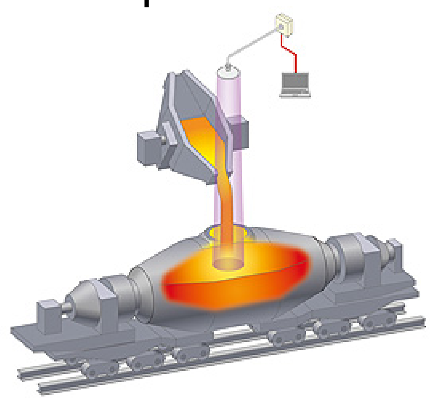
To reduce the amount of sulphur in the hot metal between the blast furnace and the oxygen converter, desulphurization is usually performed at a De-S station

Blast Furnace (BF)

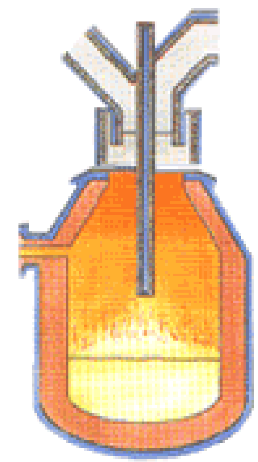


0.04-0.07% S

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:

$$Mg(s) + \underline{S} \rightarrow MgS(s)$$

$$CaC_2 + \underline{S} \rightarrow CaS(s) + 2\underline{C}$$

$$CaO + \underline{S} + \underline{C} \rightarrow CaS(s) + CO(g)$$

$$Mg + CaO + \underline{S} \rightarrow CaS(s) + MgO(s)$$

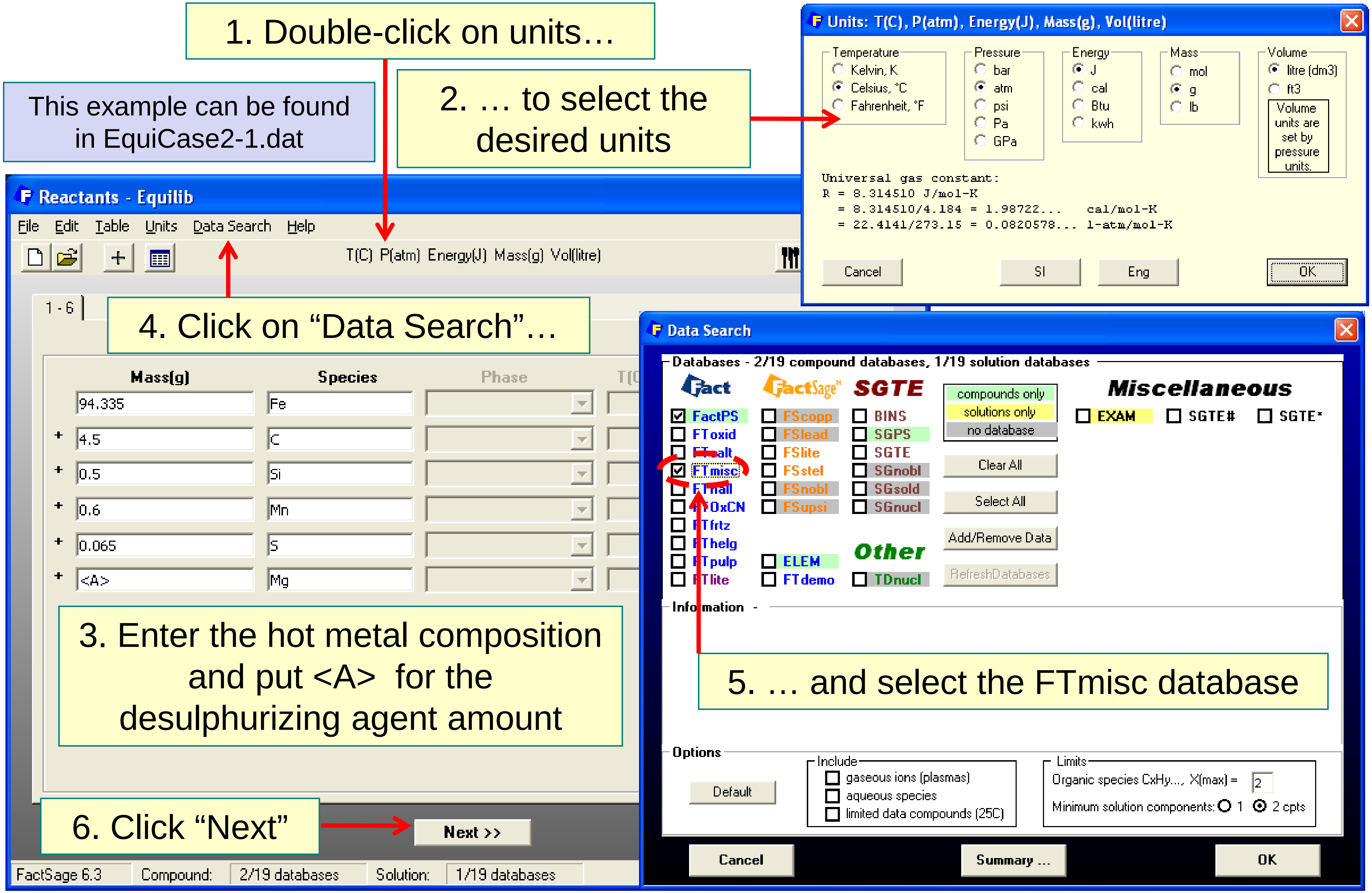
$$CaO + 2\underline{Al} + \underline{S} + 3\underline{O} \rightarrow (CaO \cdot Al_2O_3)\ (S)$$

$$(CaO \cdot Al_2O_3)(s) + \underline{S} \rightarrow (CaO \cdot Al_2O_3)\ (S)$$

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

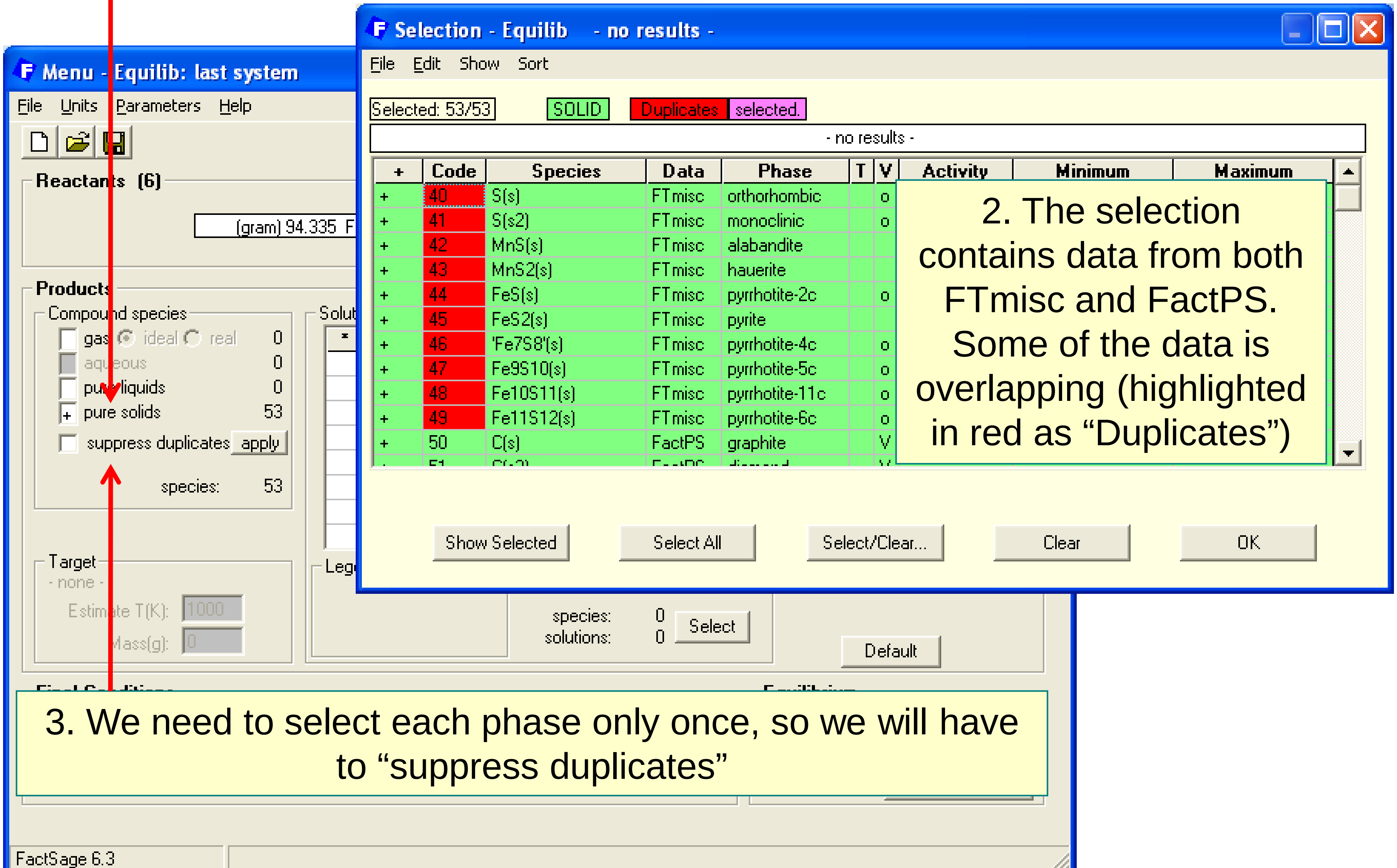
It will then be shown how the exact amount of desulphurizing agent can be selected to achieve the desired sulphur content.

Desulphurization of Hot Metal using Mg



Desulphurization of Hot Metal using Mg

1. Right-click on “pure solids”

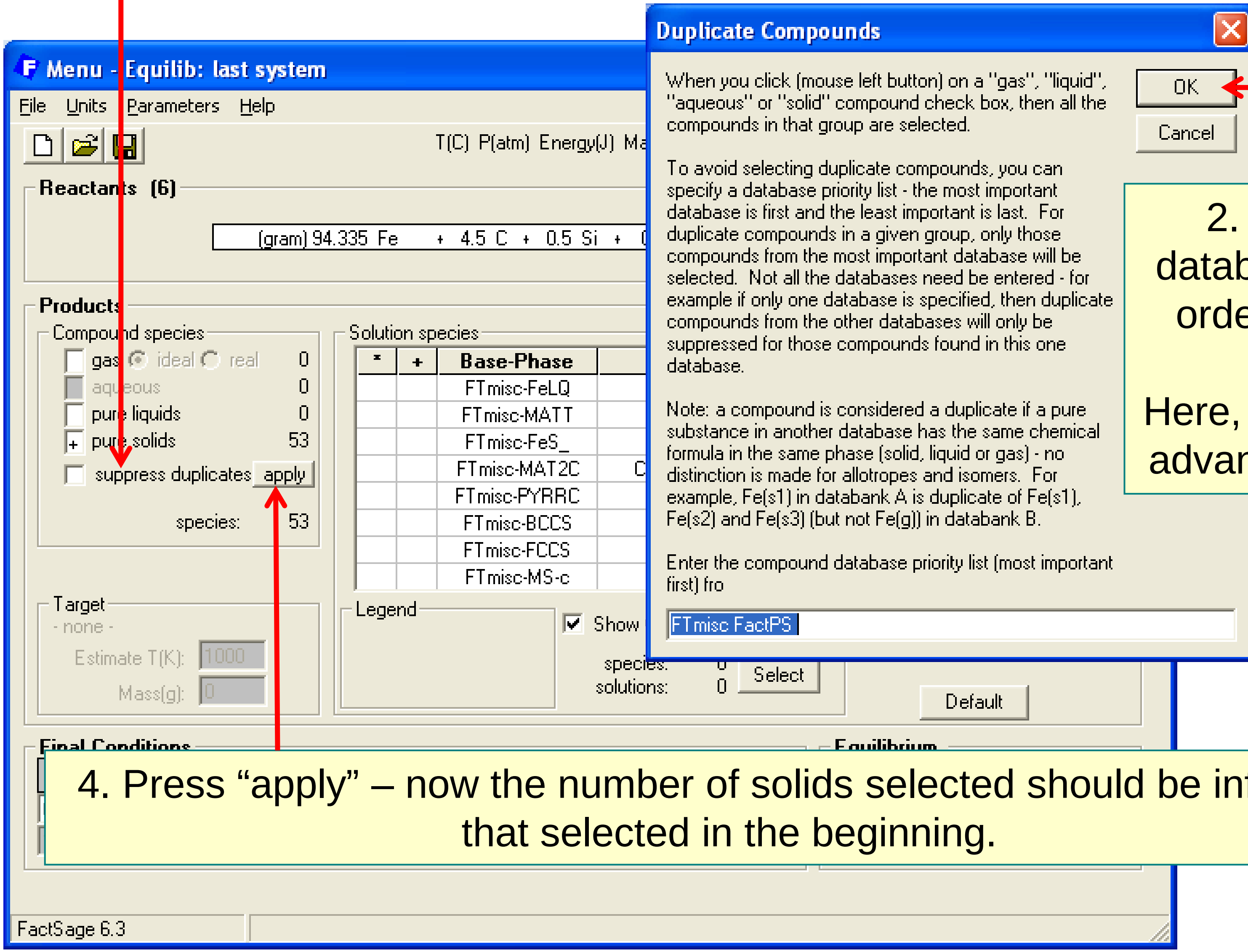


2. The selection contains data from both FTmisc and FactPS. Some of the data is overlapping (highlighted in red as “Duplicates”)

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”



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

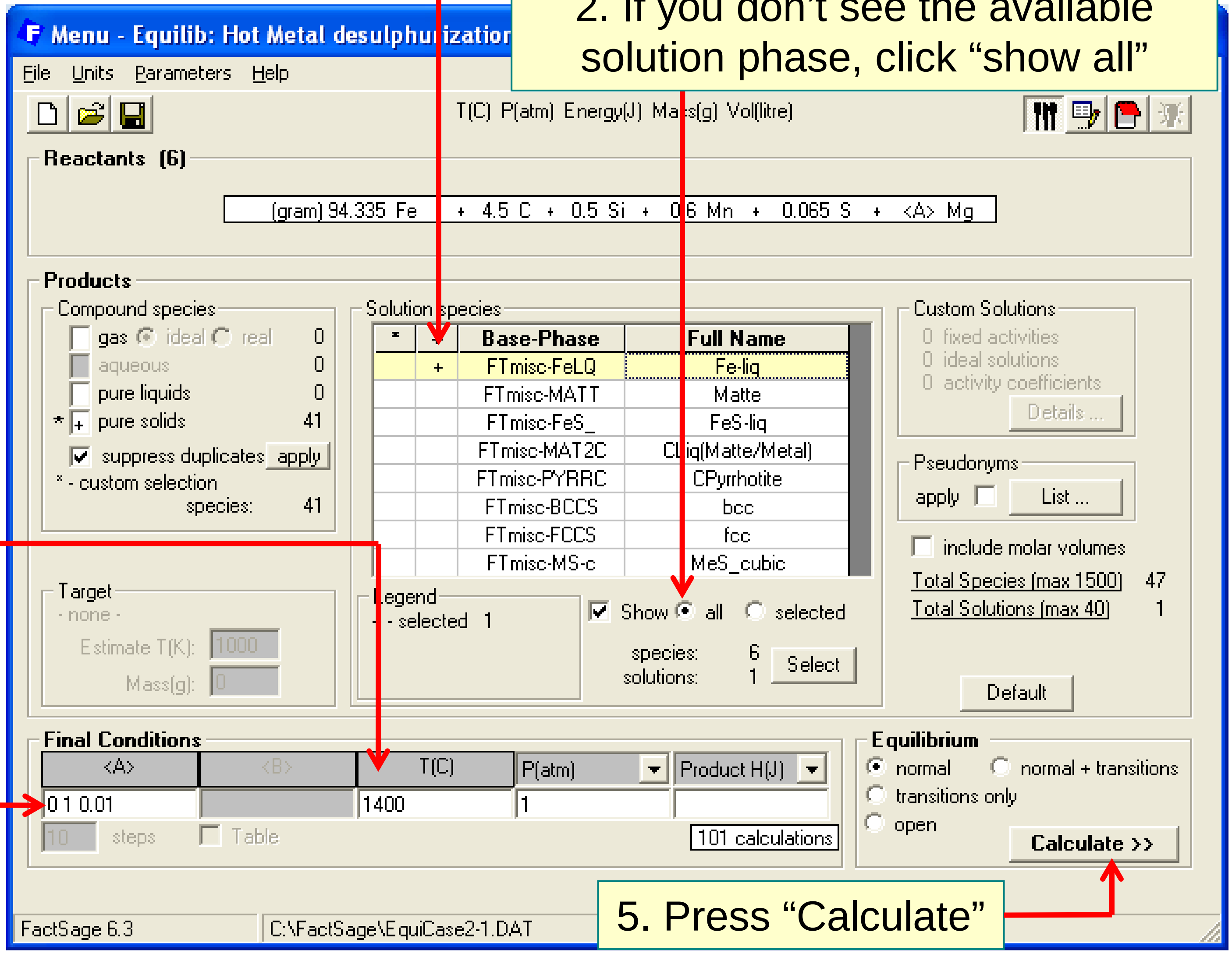
1. Left-click to select the liquid steel solution phase

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"



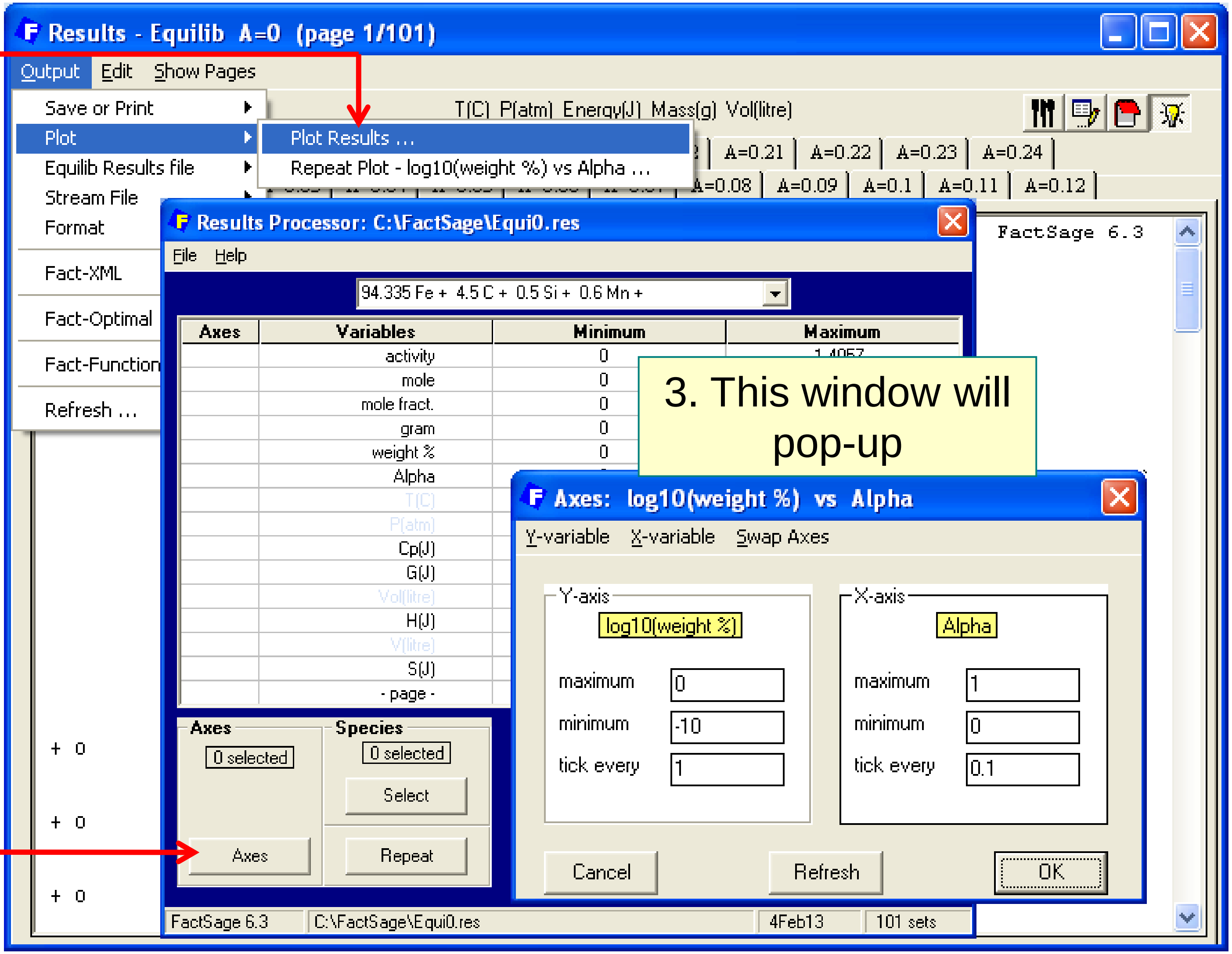
Desulphurization of Hot Metal using Mg

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…"

2. Press "Axes"

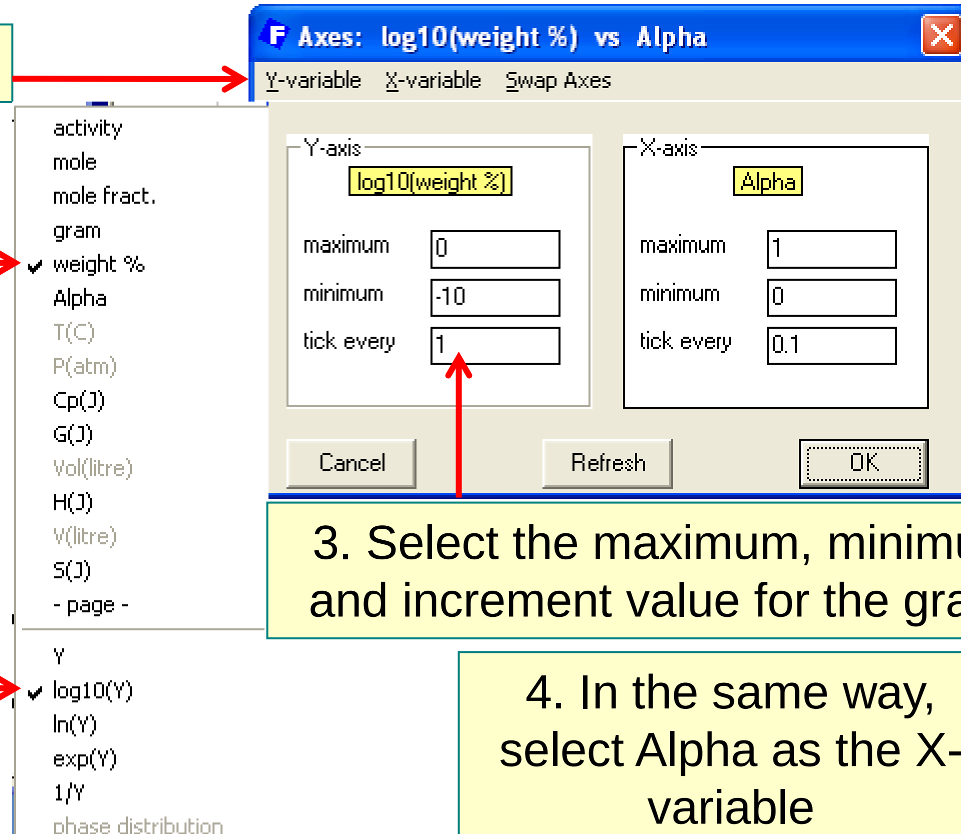
3. This window will pop-up



Desulphurization of Hot Metal using Mg

1. Press “Y-variable”

2. Select “weight %” in “log10(Y)” scale

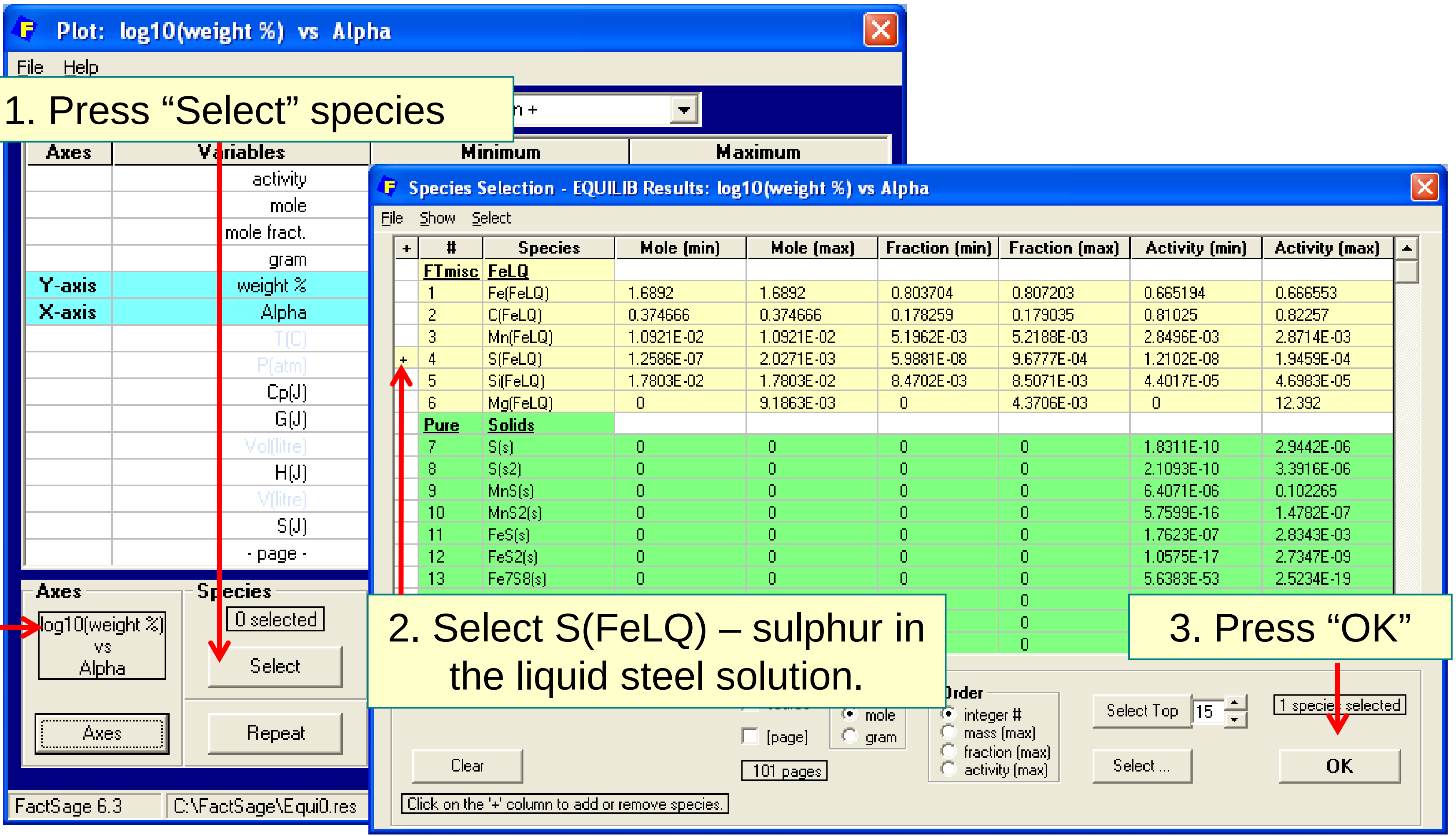


3. Select the maximum, minimum and increment value for the graph

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

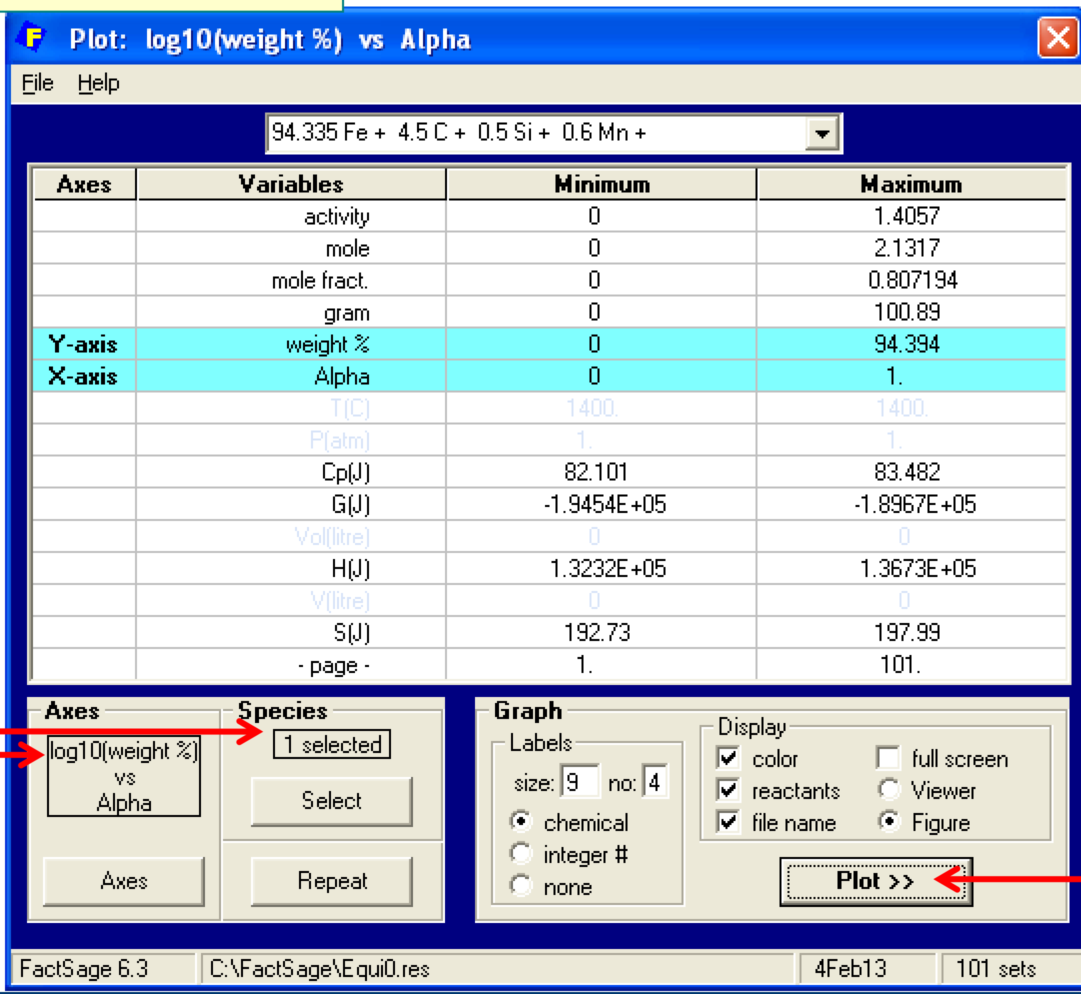
Desulphurization of Hot Metal using Mg

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



Desulphurization of Hot Metal using Mg

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



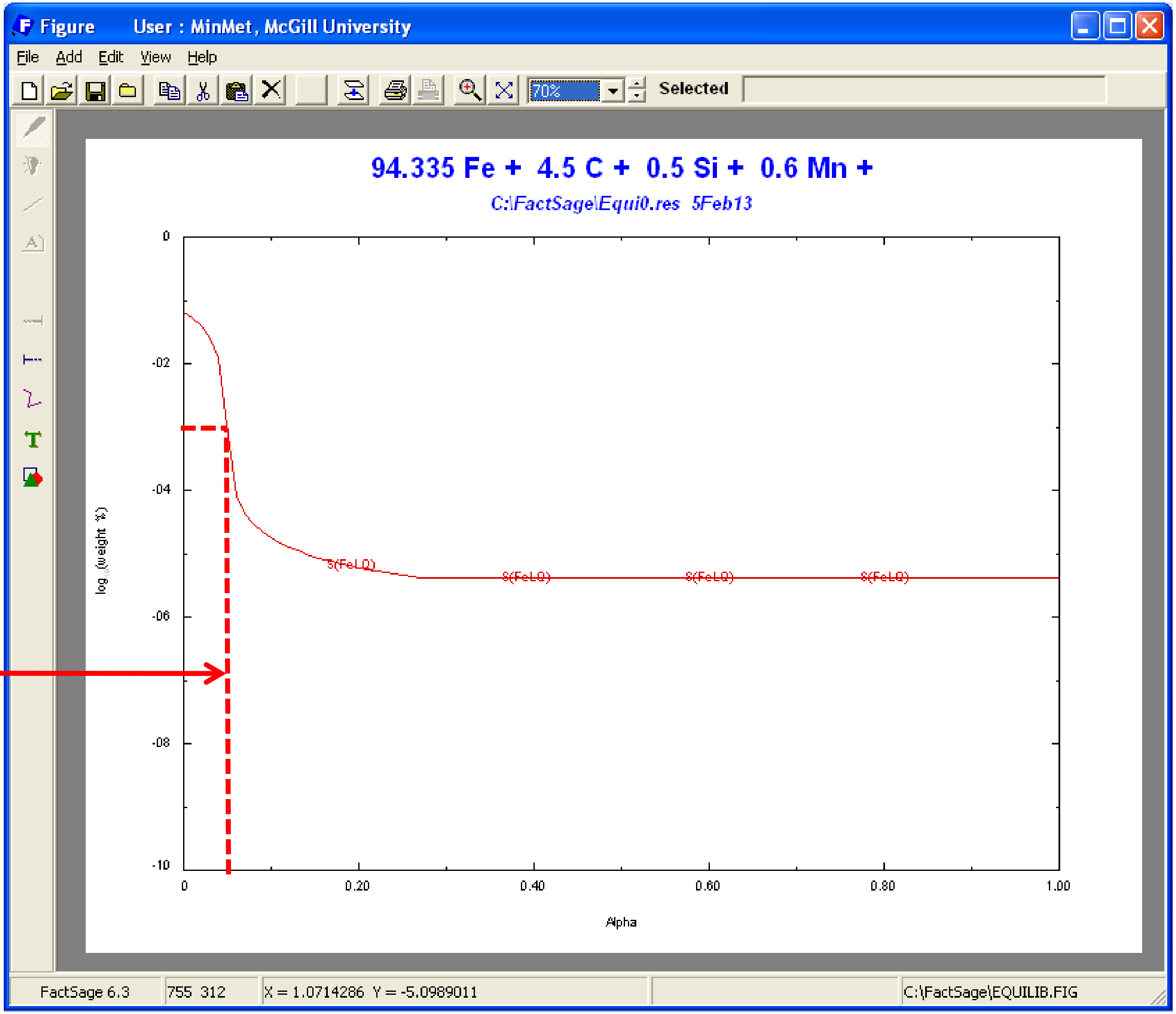
2. The “Plot” button is now activated. Click it!

Desulphurization of Hot Metal using Mg

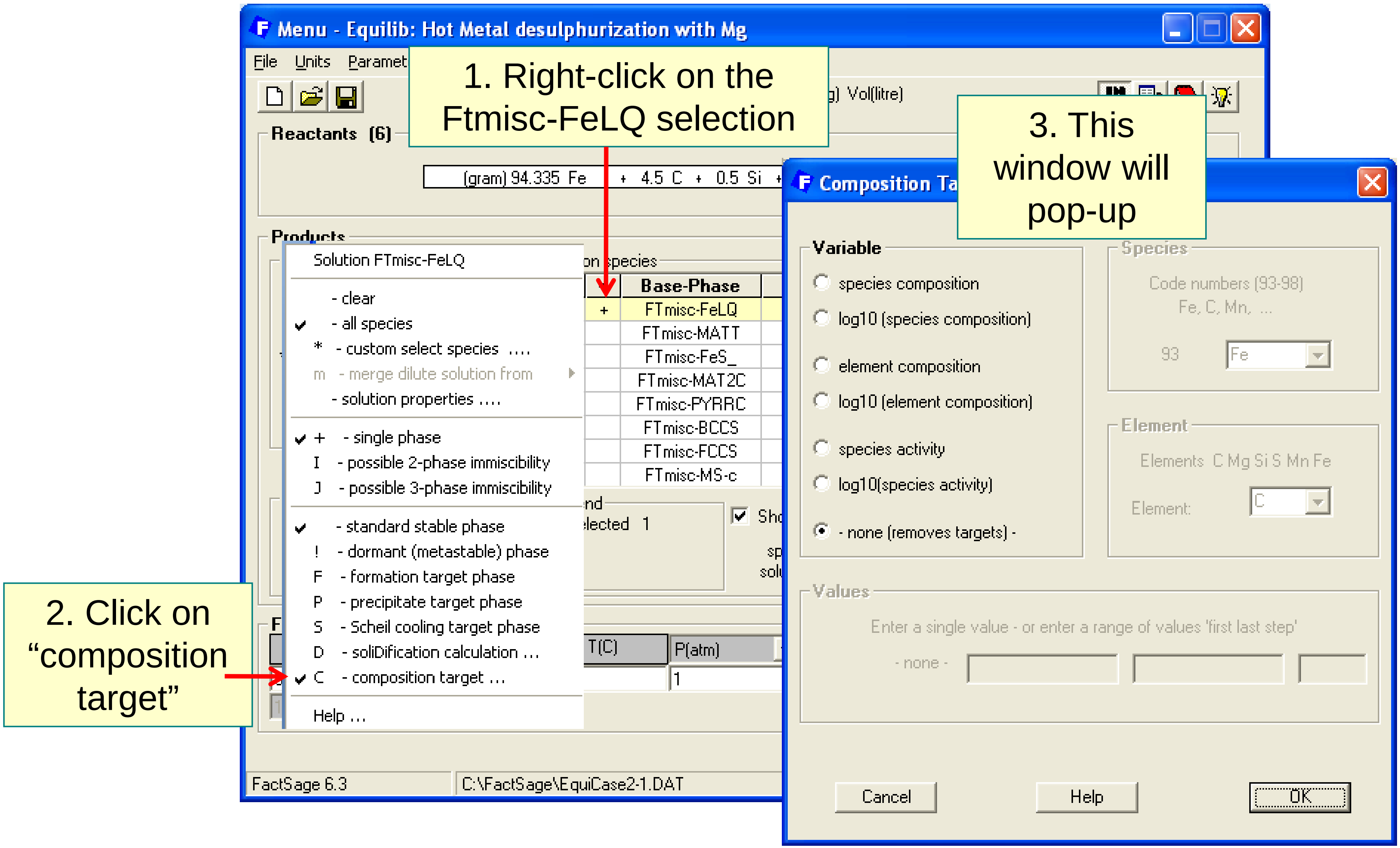
1. It can be seen that after the addition of 0.1g Mg, the desulphurization is not so effective.

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

3. However, there is a better way.



Desulphurization of Hot Metal using Mg: Composition target



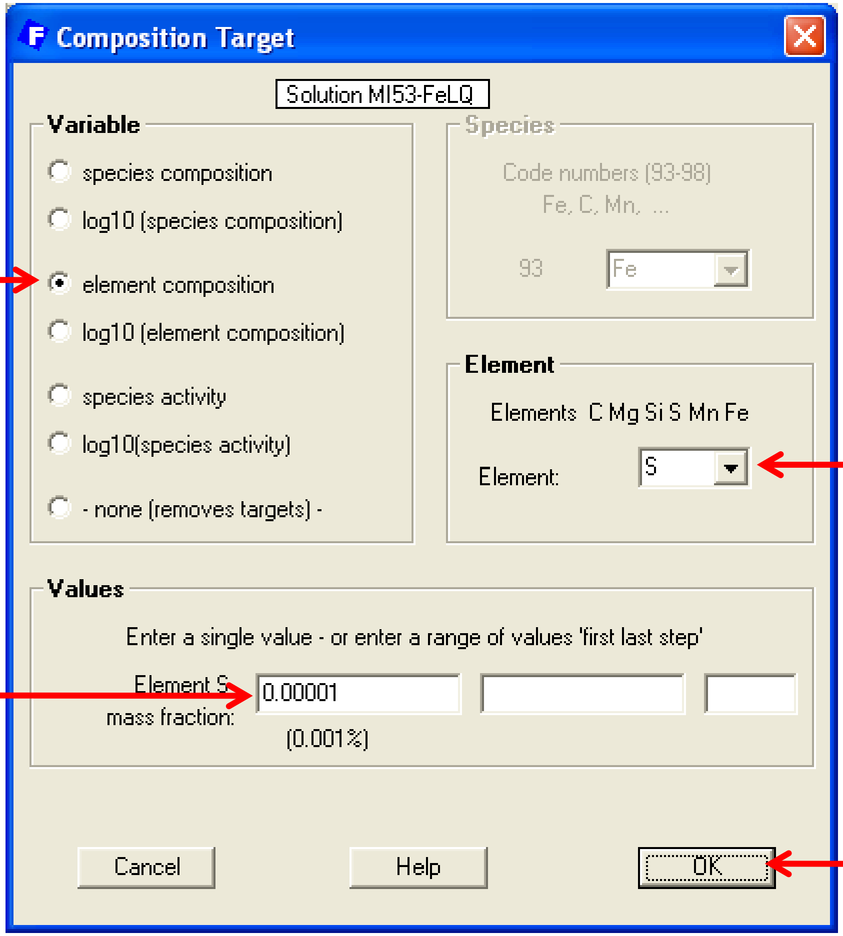
Desulphurization of Hot Metal using Mg: Composition target

1. Select "element composition"

2. Choose element S

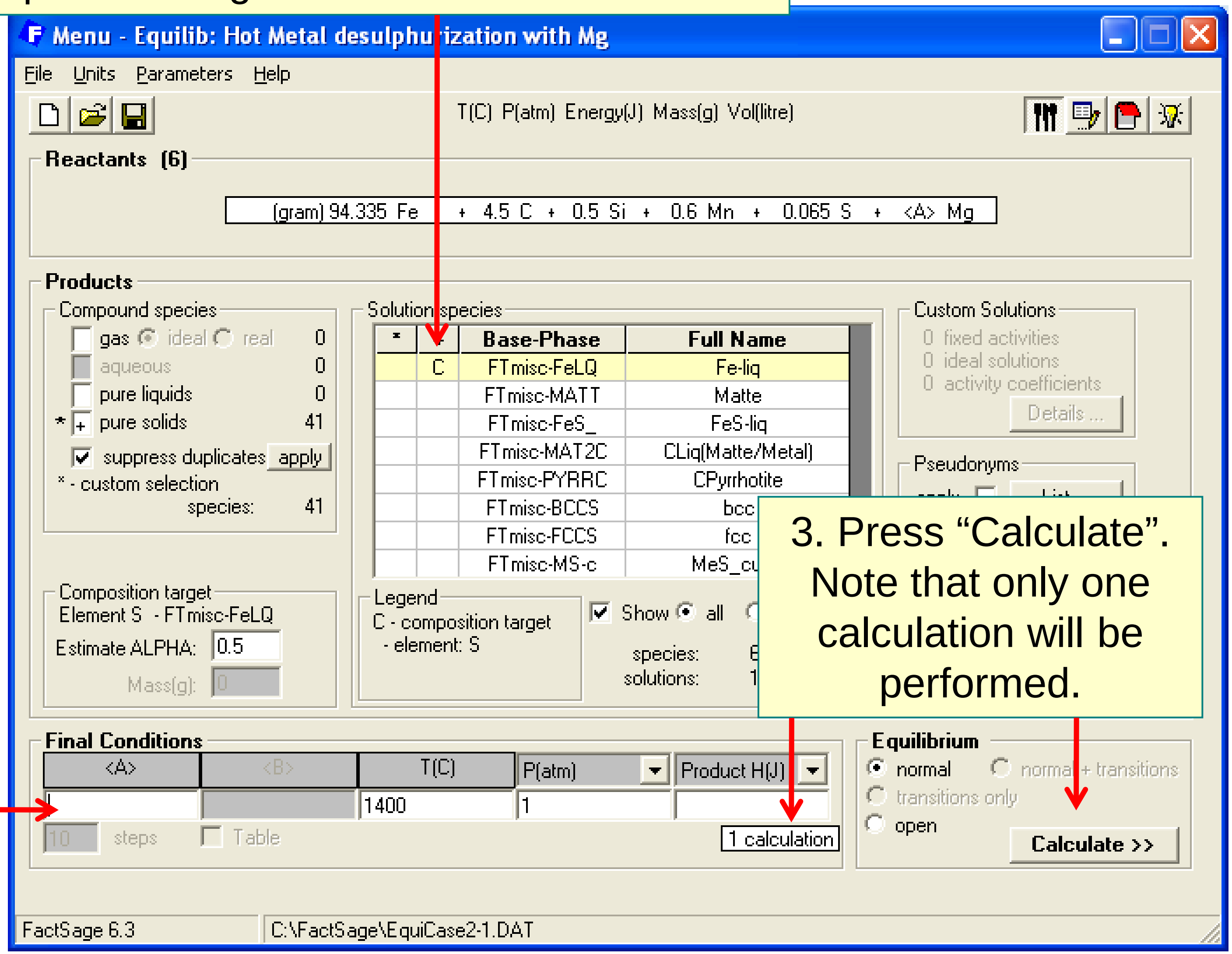
3. Enter the desired value (here – 0.001%)

4. Press "OK"



Desulphurization of Hot Metal using Mg: Composition target

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

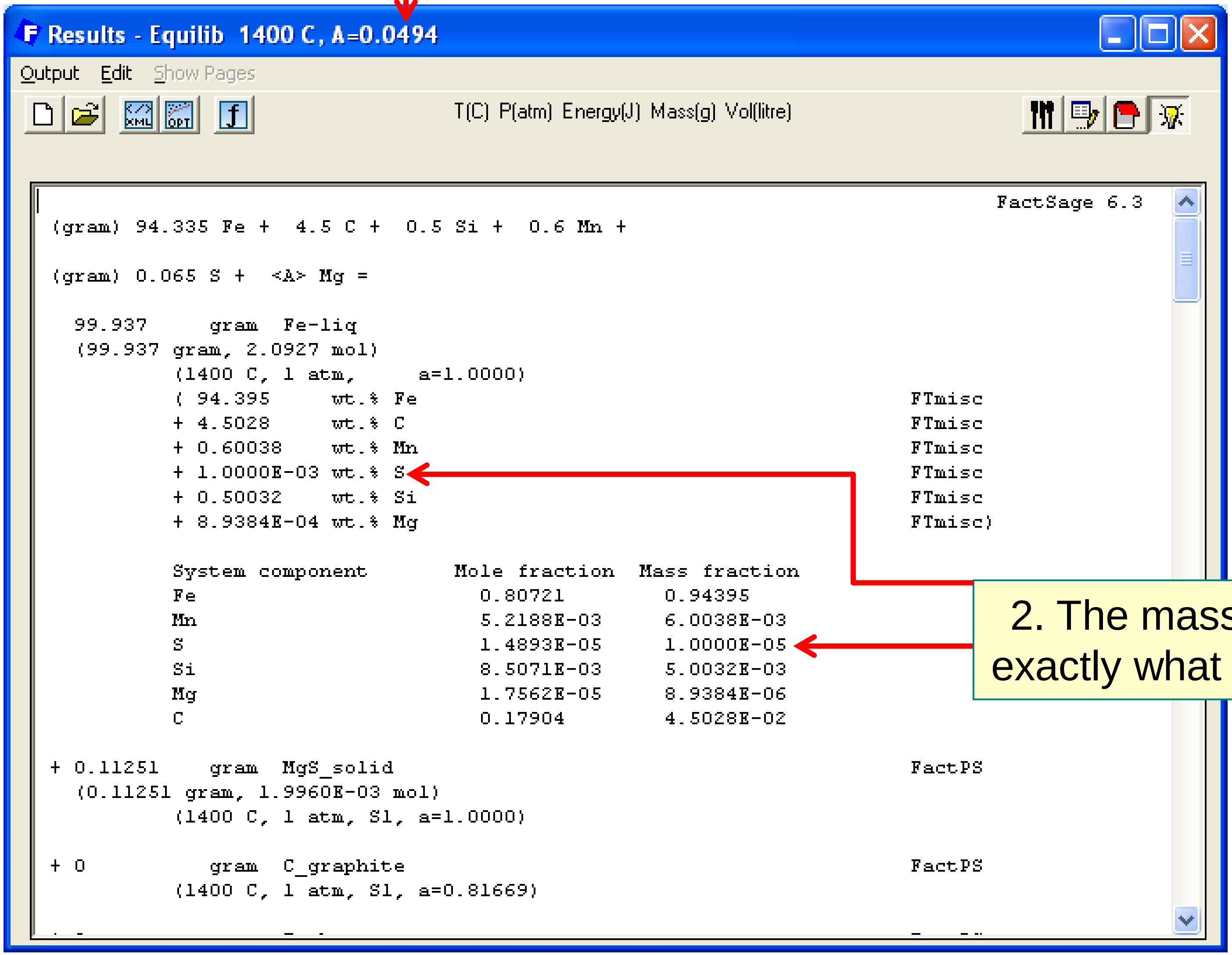


2. We must leave the <A> field blank, because <A> is what we want to calculate.

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.



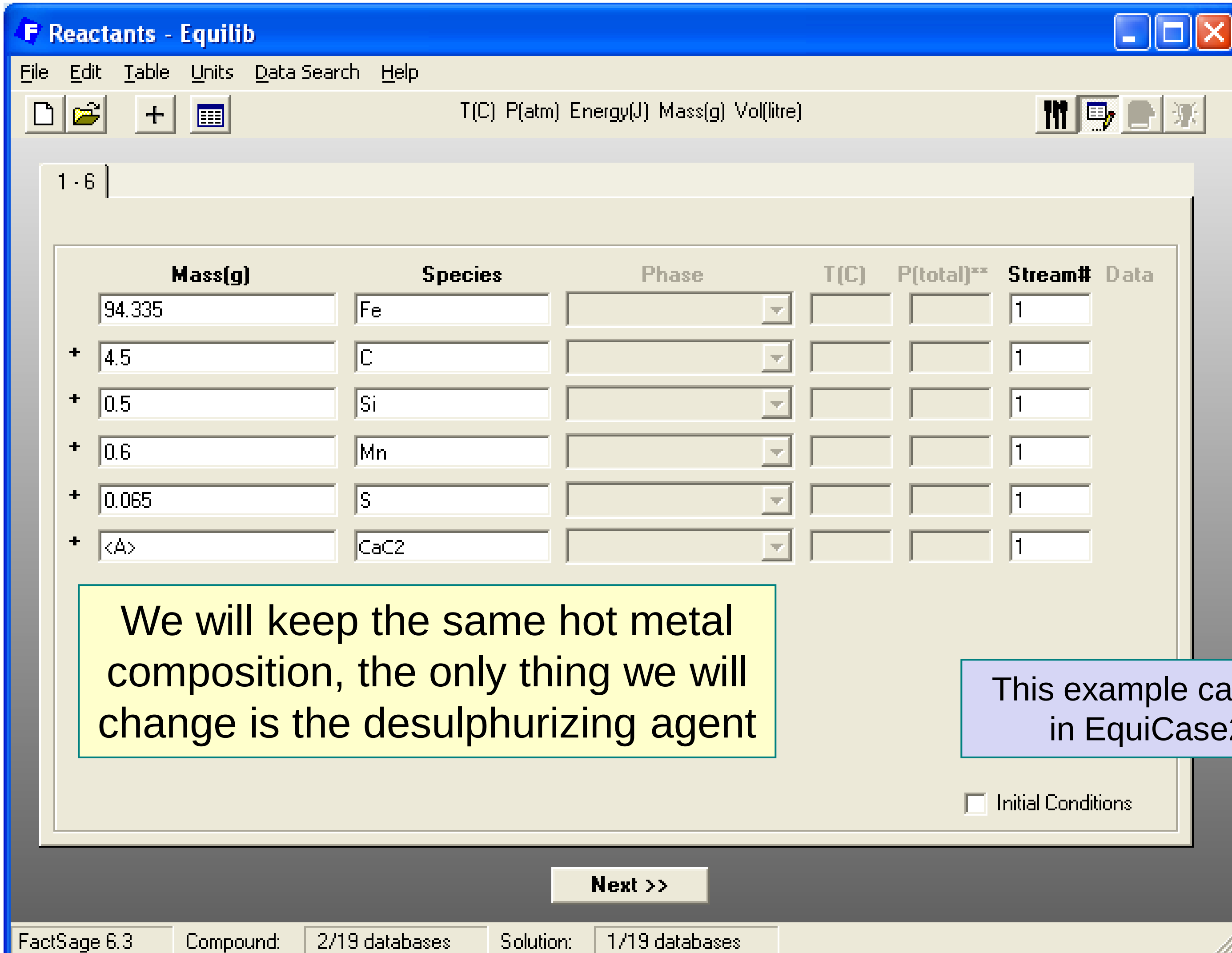
```
Results - Equilib  1400 C, A=0.0494
Output  Edit  Show Pages
T(C)  P(atm)  Energy(J)  Mass(g)  Vol(litre)

                                                                   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

$$CaC_2 + \underline{S} \rightarrow CaS(s) + 2\underline{C}$$

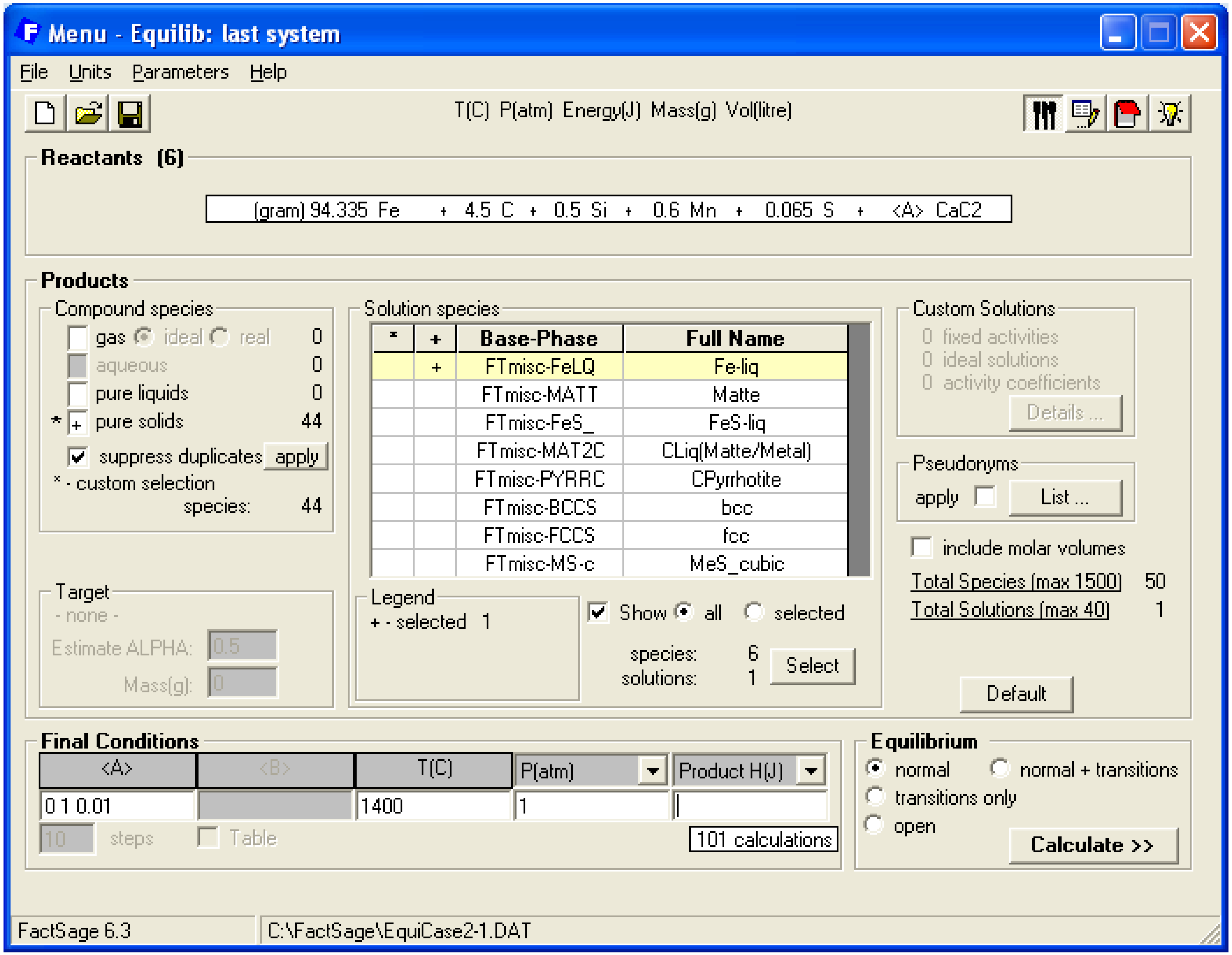


We will keep the same hot metal composition, the only thing we will change is the desulphurizing agent

This example can be found in EquiCase2-2.dat

Desulphurization of Hot Metal using CaC_2

The same conditions are selected



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.

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

Output Edit Show Pages

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

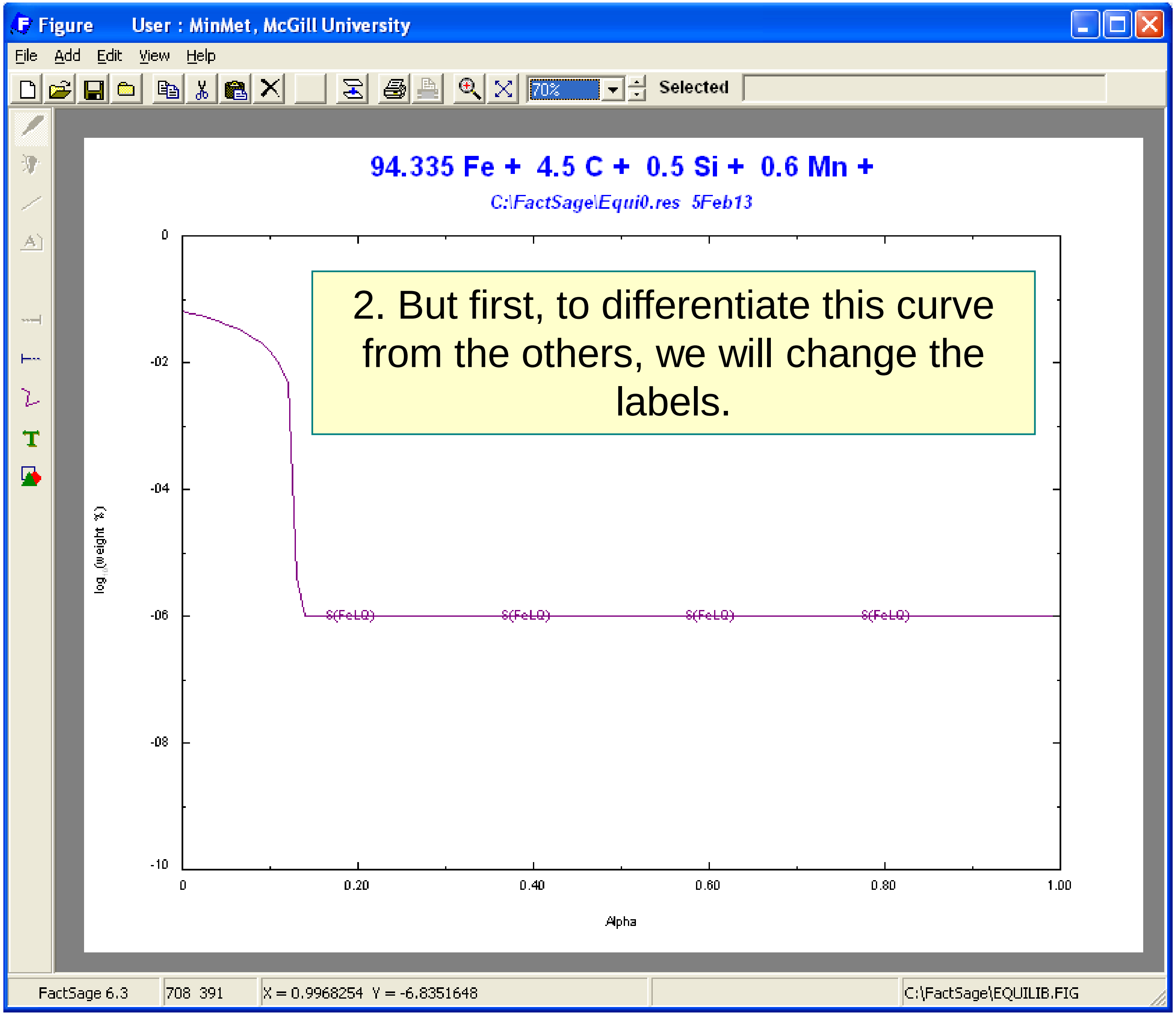
A=0 | A=0.01 | A=0.02 | A=0.03 | A=0.04 | A=0.05 | A=0.06 | A=0.07 | A=0.08 | A=0.09 | A=0.1 | A=0.11 | A=0.12 | A=0.13 | - A=0.14 - | A=0.15 | A=0.16 | A=0.17 | A=0.18 | A=0.19 | A=0.2 | A=0.21 | A=0.22 | A=0.23 | A=0.24

```
(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)
```

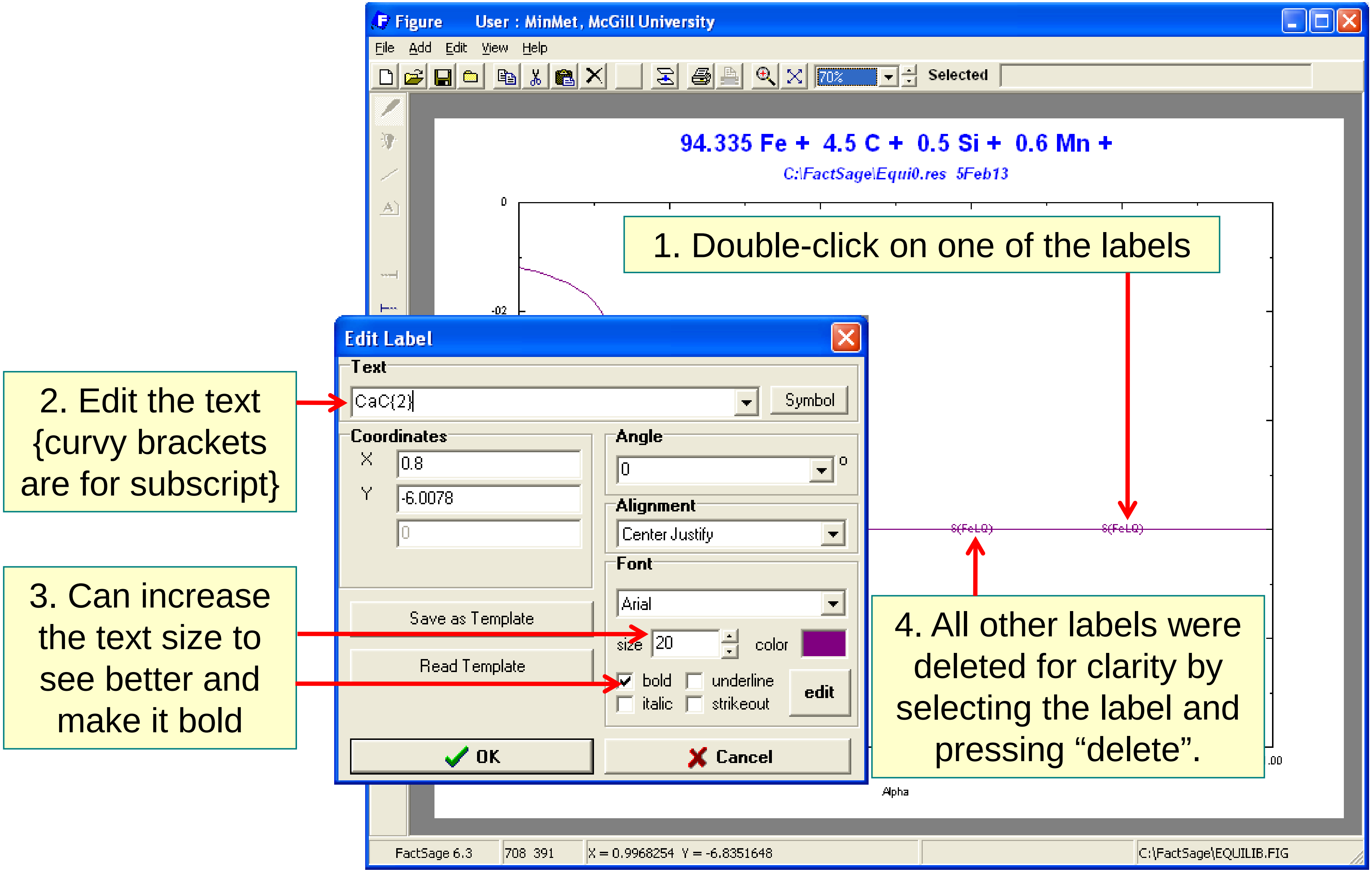
Desulphurization of Hot Metal using CaC_2

This can also be seen on the graph – after <A>=0.14, the sulphur level remains constant.

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



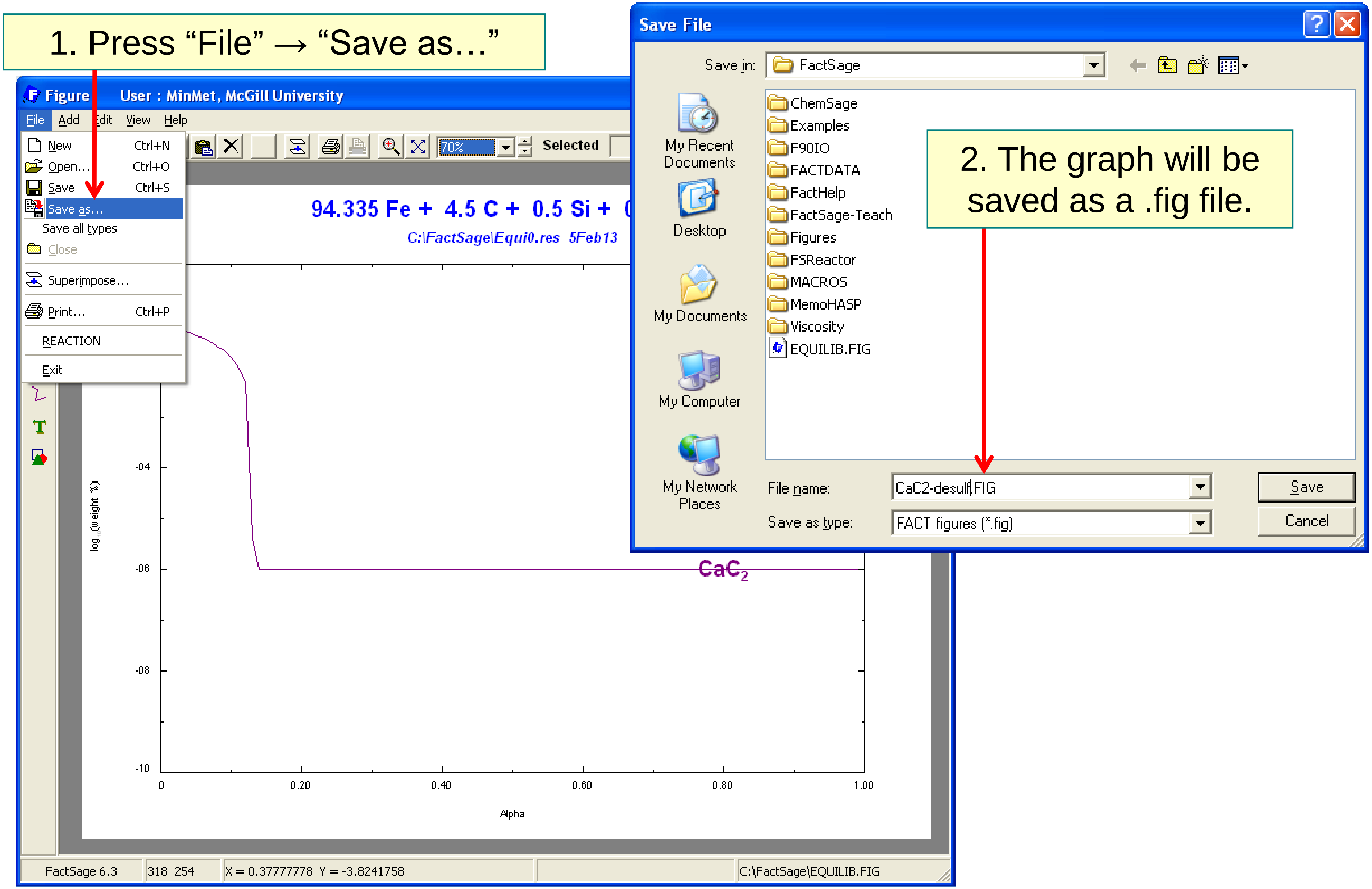
Desulphurization of Hot Metal using CaC_2



Desulphurization of Hot Metal using CaC_2

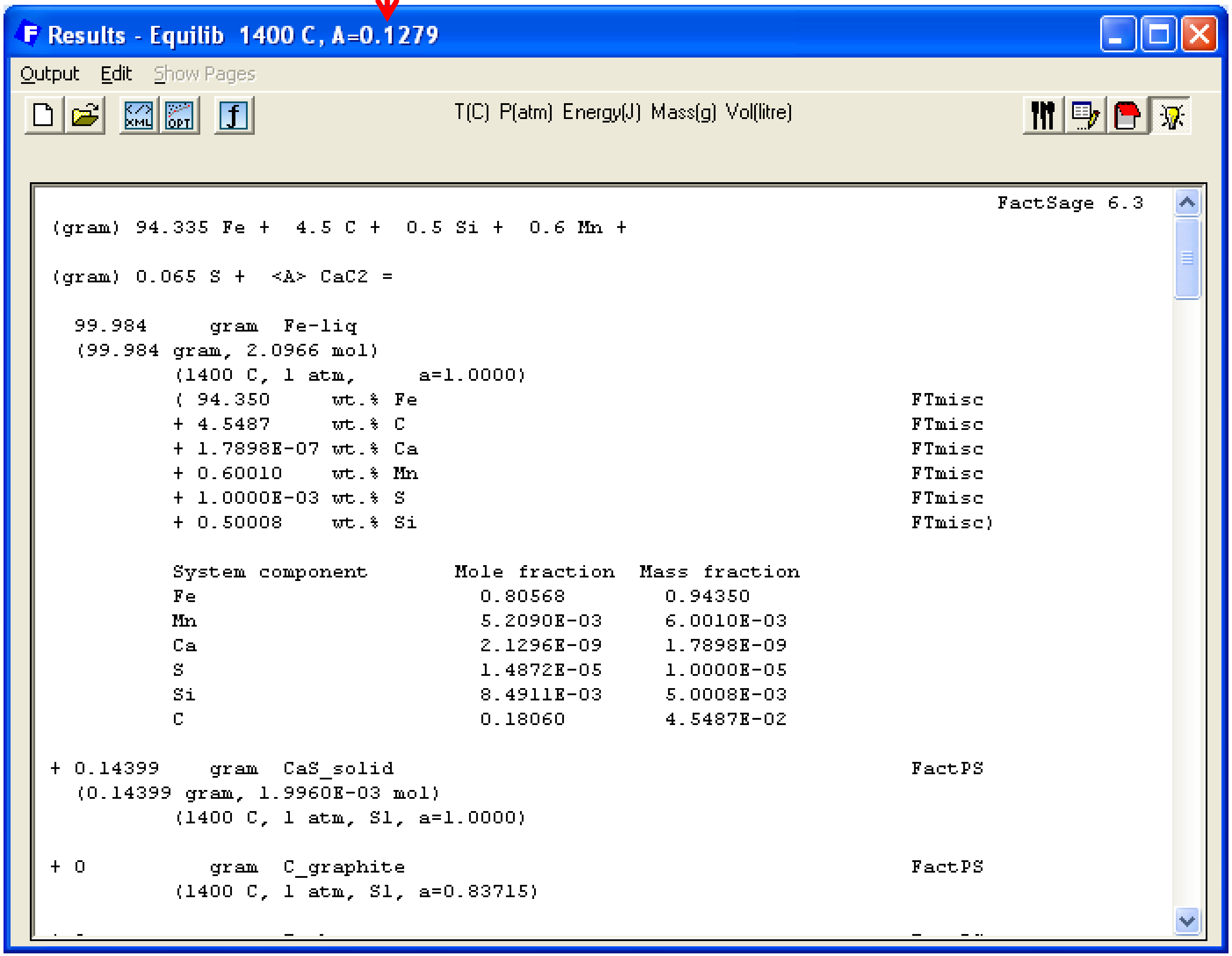
1. Press “File” → “Save as…”

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.

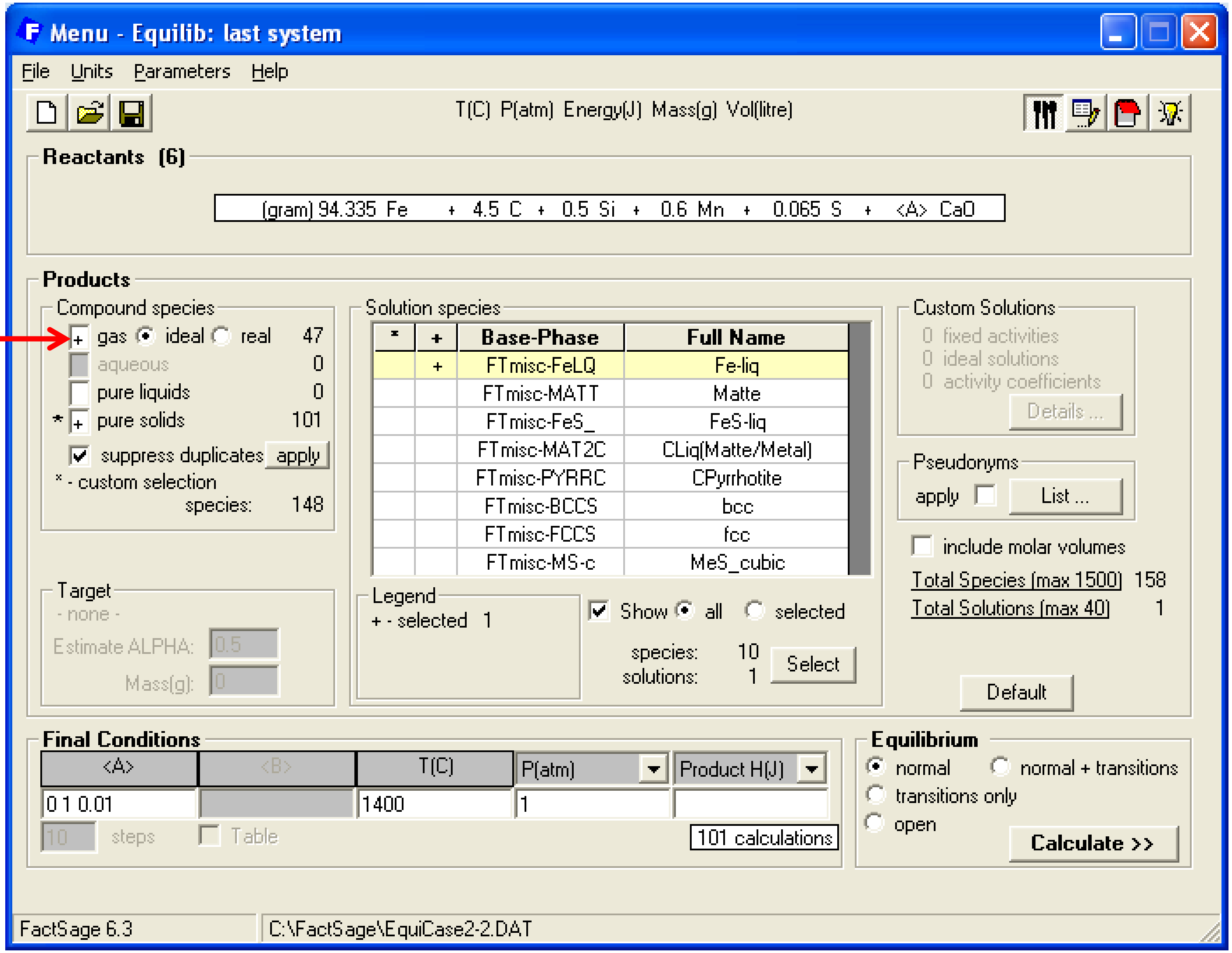


Desulphurization of Hot Metal using CaO

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

$$CaO + \underline{S} + \underline{C} \rightarrow CaS(s) + CO(g)$$

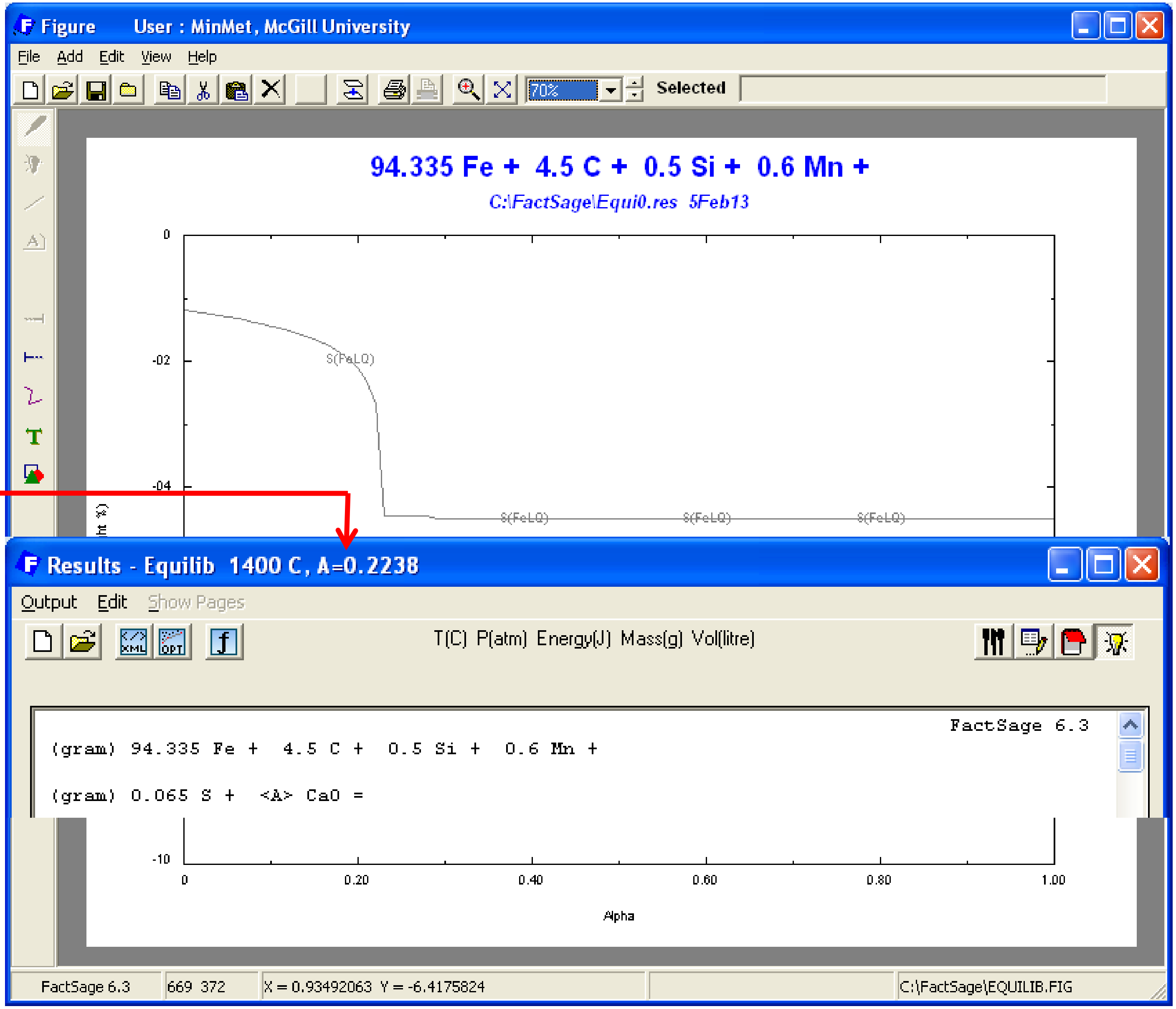
This example can be found in EquiCase2-3.dat



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%



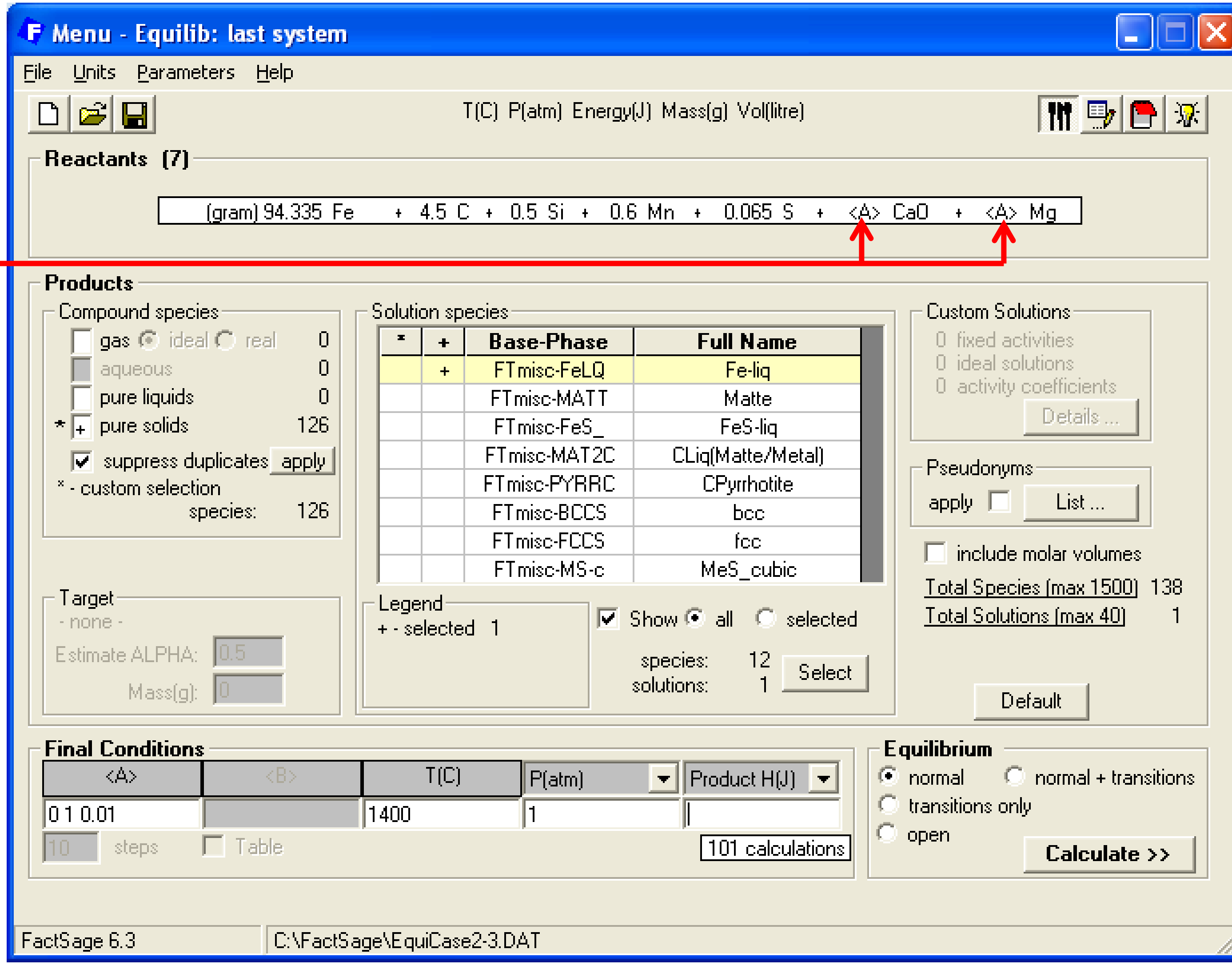
Desulphurization of Hot Metal using CaO+Mg

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

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

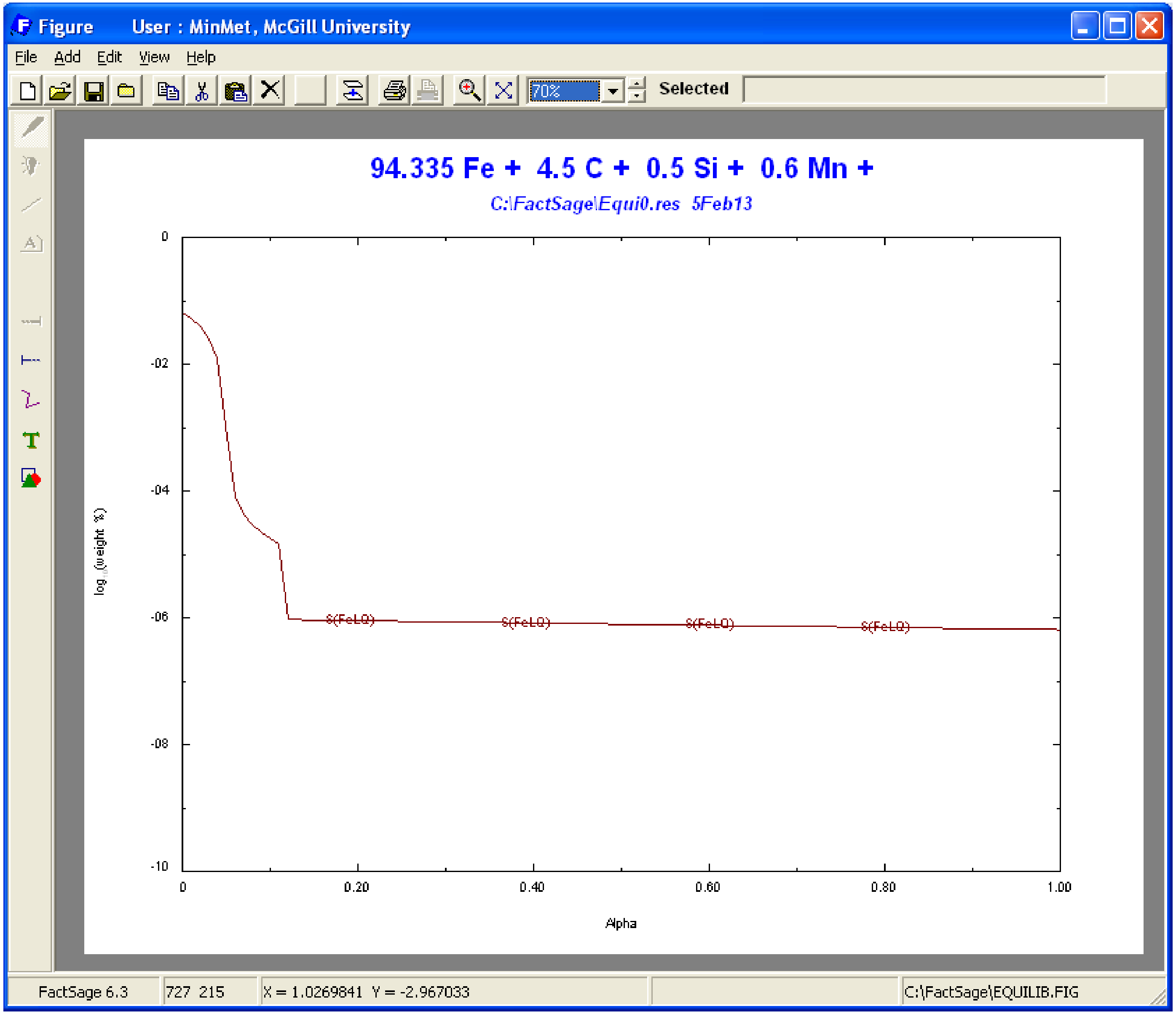
$$Mg + CaO + \underline{S} \rightarrow CaS(s) + MgO(s)$$

This example can be found in EquiCase2-4.dat



Desulphurization of Hot Metal using CaO+Mg

The drop at <A>=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.

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

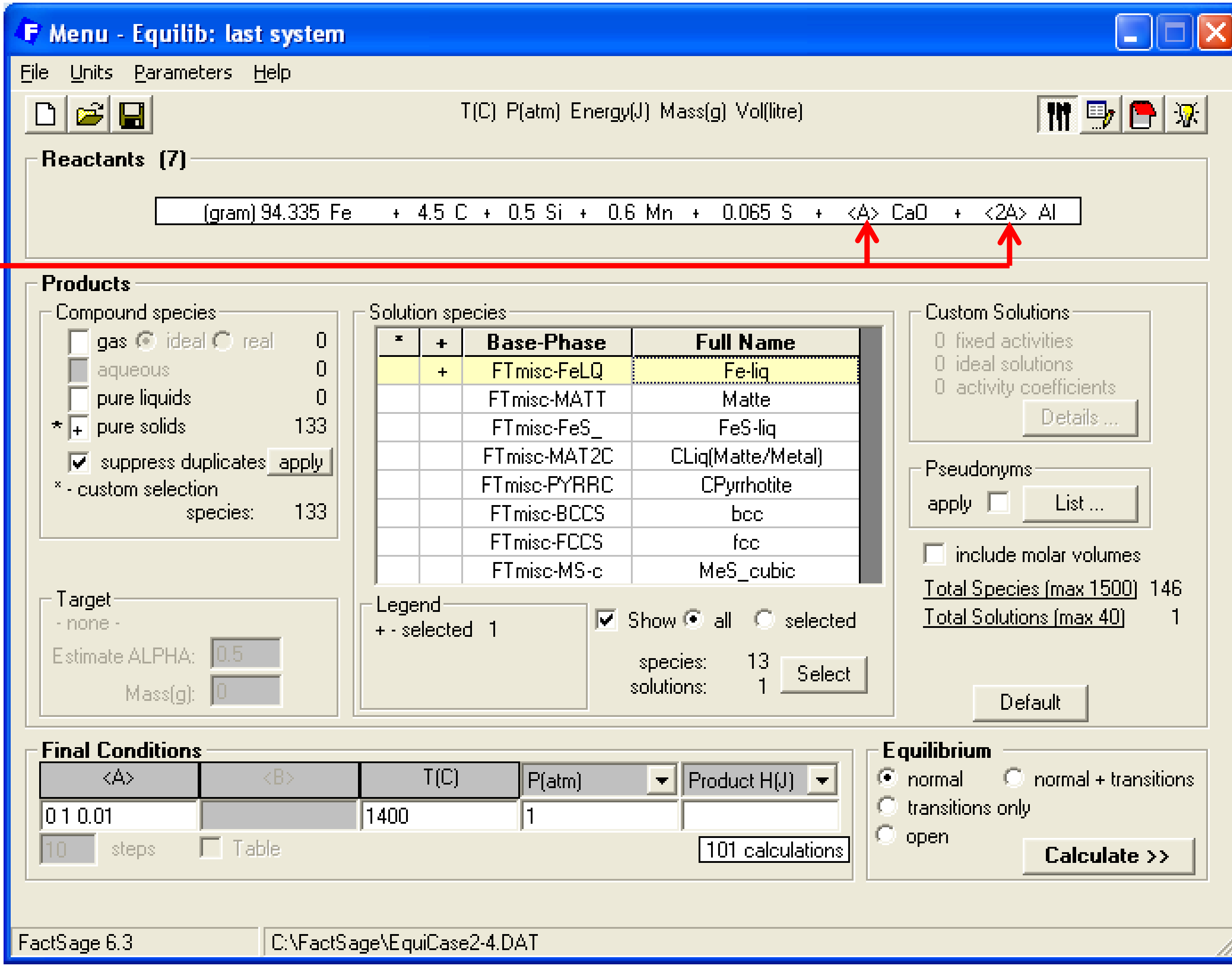
$$CaO + 2\underline{Al} + \underline{S} + 3\underline{O} \rightarrow (CaO \cdot Al_2O_3)\ (S)$$

This example can be found in EquiCase2-5.dat

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

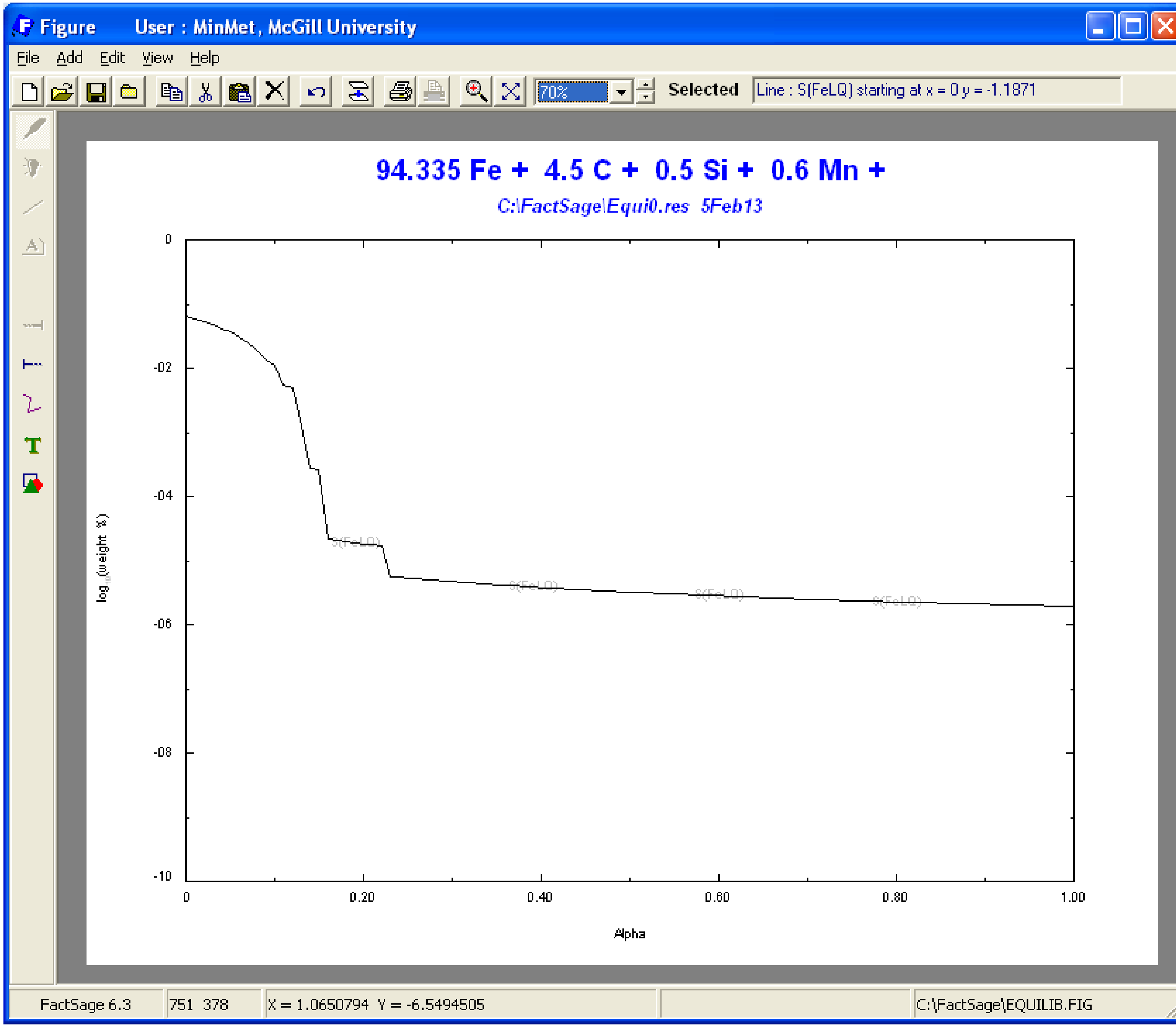
The value <A> was given for CaO and <2A> for Al

Since there is no $CaO-Al_2O_3$ solid solution incorporating S, we must choose the pure solids where a combination of $CaO-Al_2O_3$ compounds and CaS will simulate this solution.



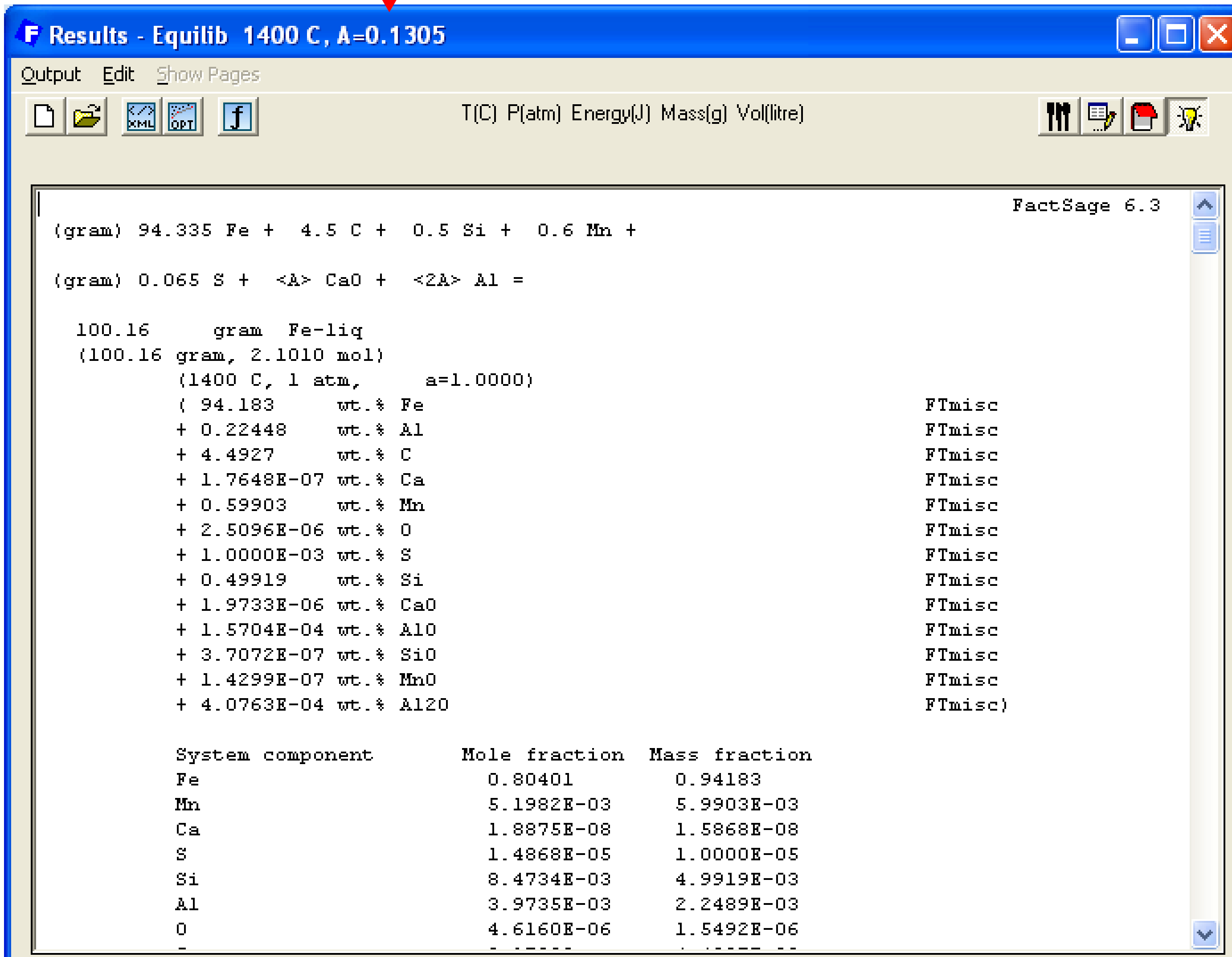
Desulphurization of Hot Metal using CaO+Al

The change of stable phase between different $CaO\text{-}Al_2O_3$ 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.

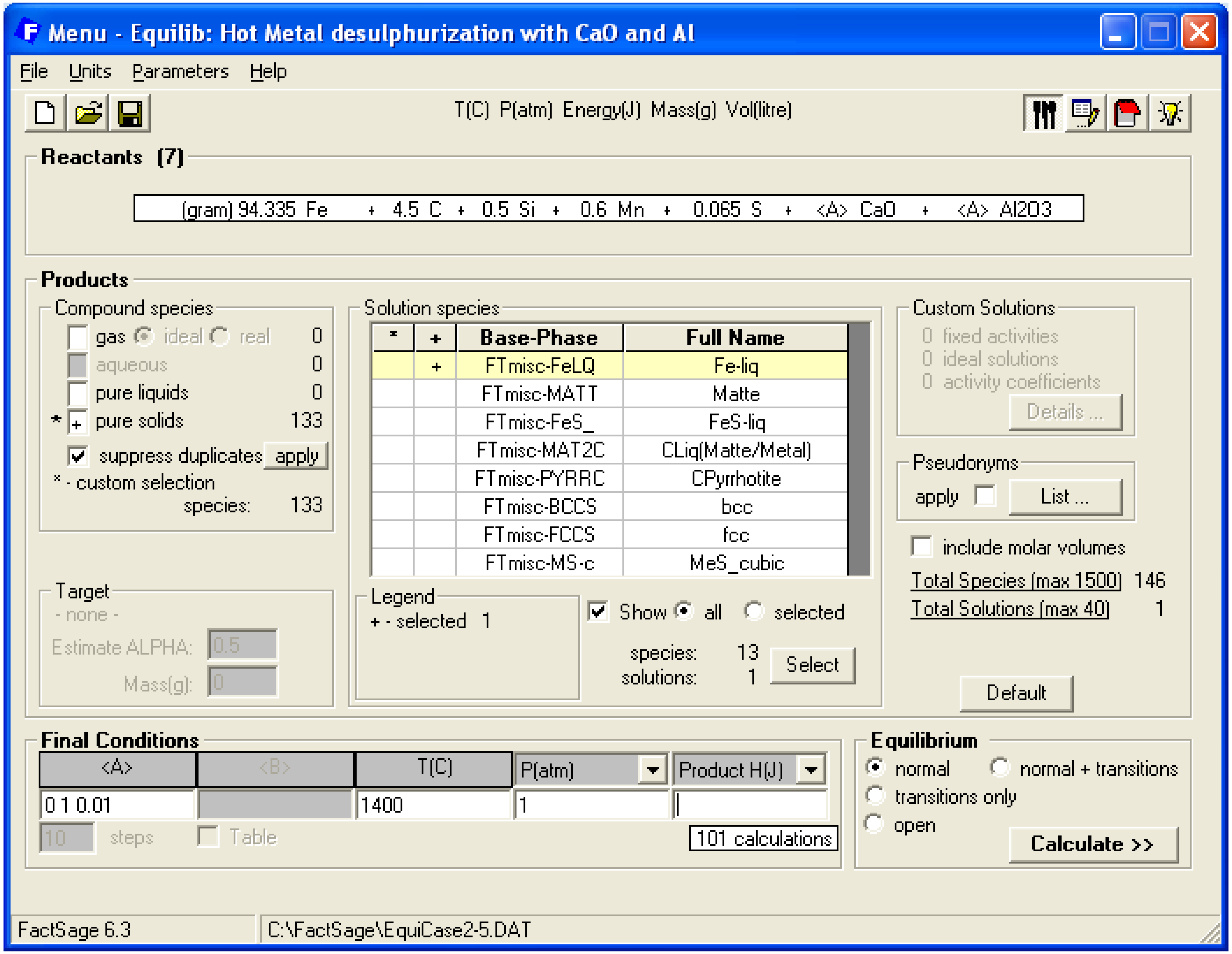


Desulphurization of Hot Metal using $CaO+Al_2O_3$

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

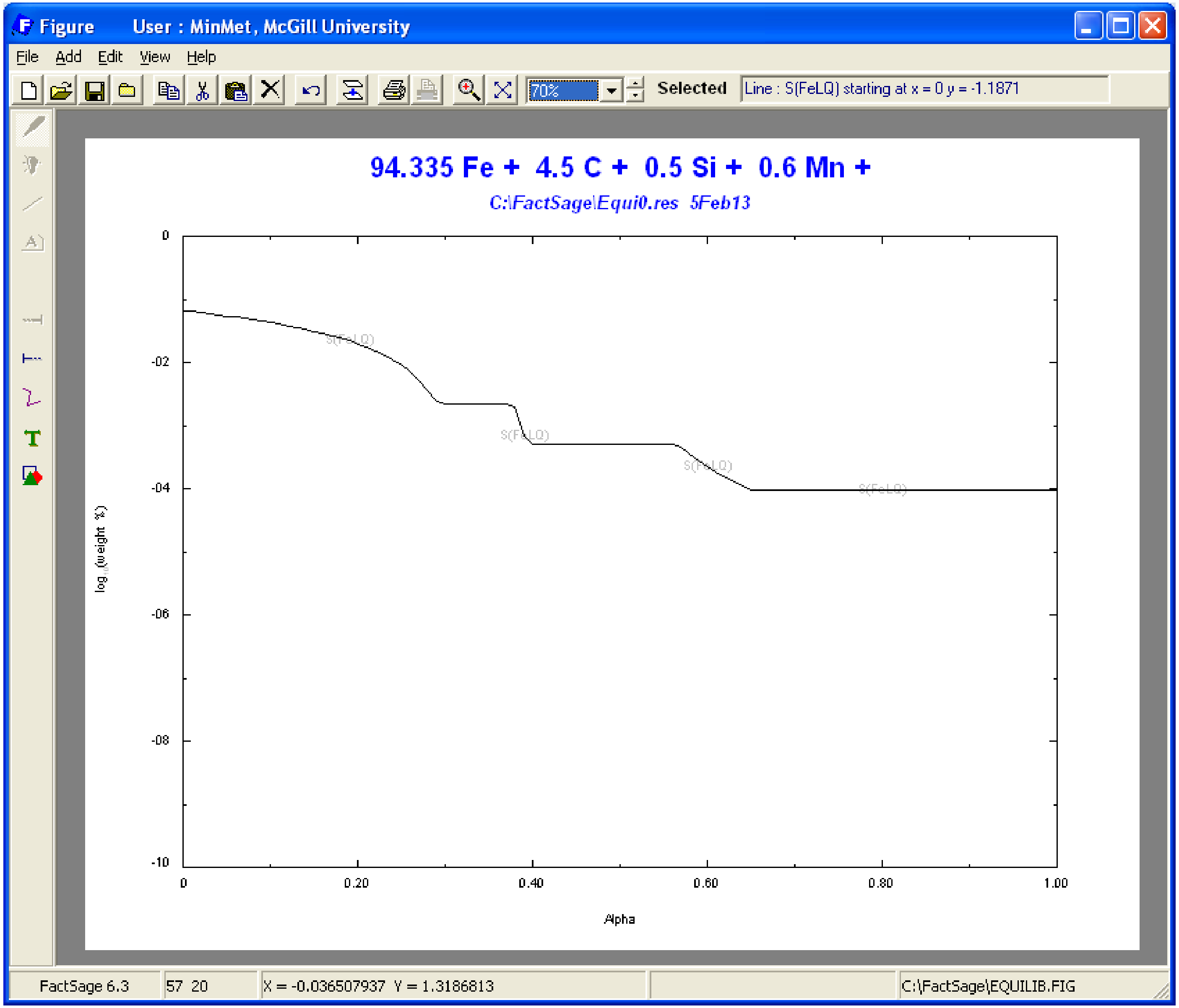
$$(CaO \cdot Al_2O_3)(s) + \underline{S} \rightarrow (CaO \cdot Al_2O_3)\ (S)$$

This example can be found in EquiCase2-6.dat



Desulphurization of Hot Metal using $CaO+Al_2O_3$

The change of stable phase between different $CaO-Al_2O_3$ compounds creates the steps in this graph.



Desulphurization of Hot Metal using $CaO+Al_2O_3$: Composition target

With $CaO+Al_2O_3$, the amount needed to bring the sulphur level down to 0.001% is 0.3874g CaO + 0.3874g Al_2O_3.

Results - Equilib 1400 C, A=0.3874

Output Edit Show Pages

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

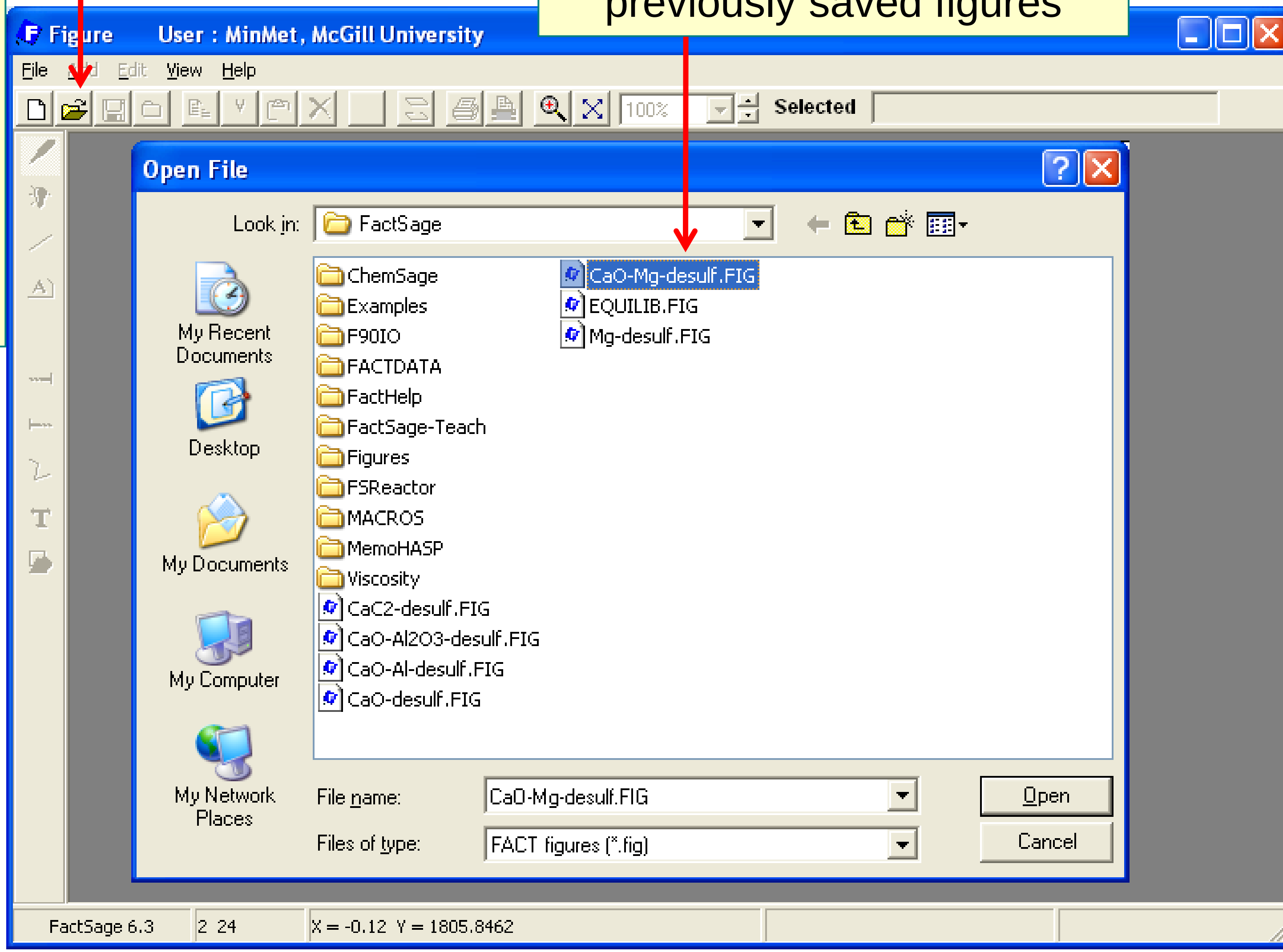
```
                                                               FactSage 6.3
(gram) 94.335 Fe +  4.5 C +  0.5 Si +  0.6 Mn +

(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.

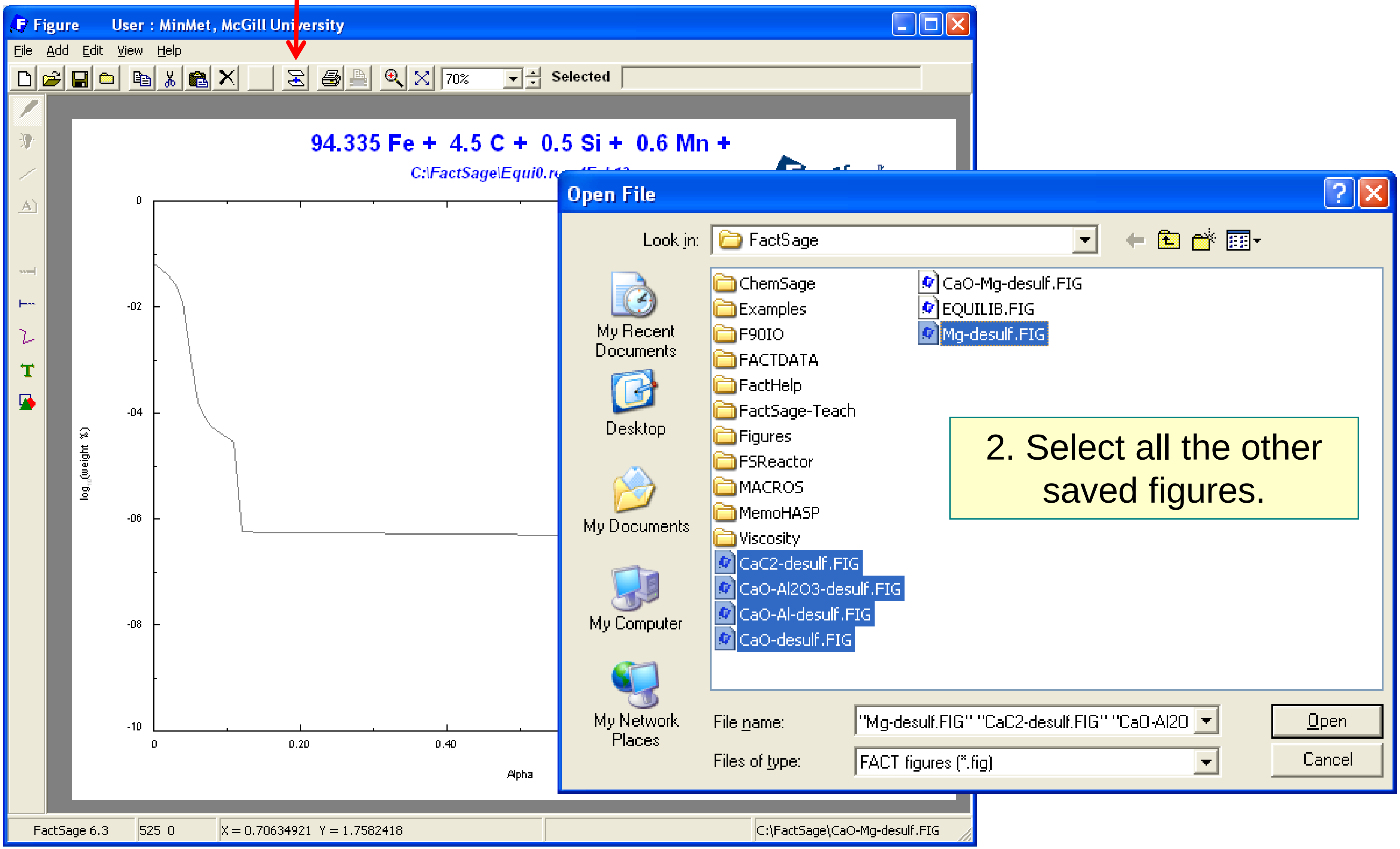
2. Press “Open”

3. Select one of the previously saved figures



Desulphurization of Hot Metal

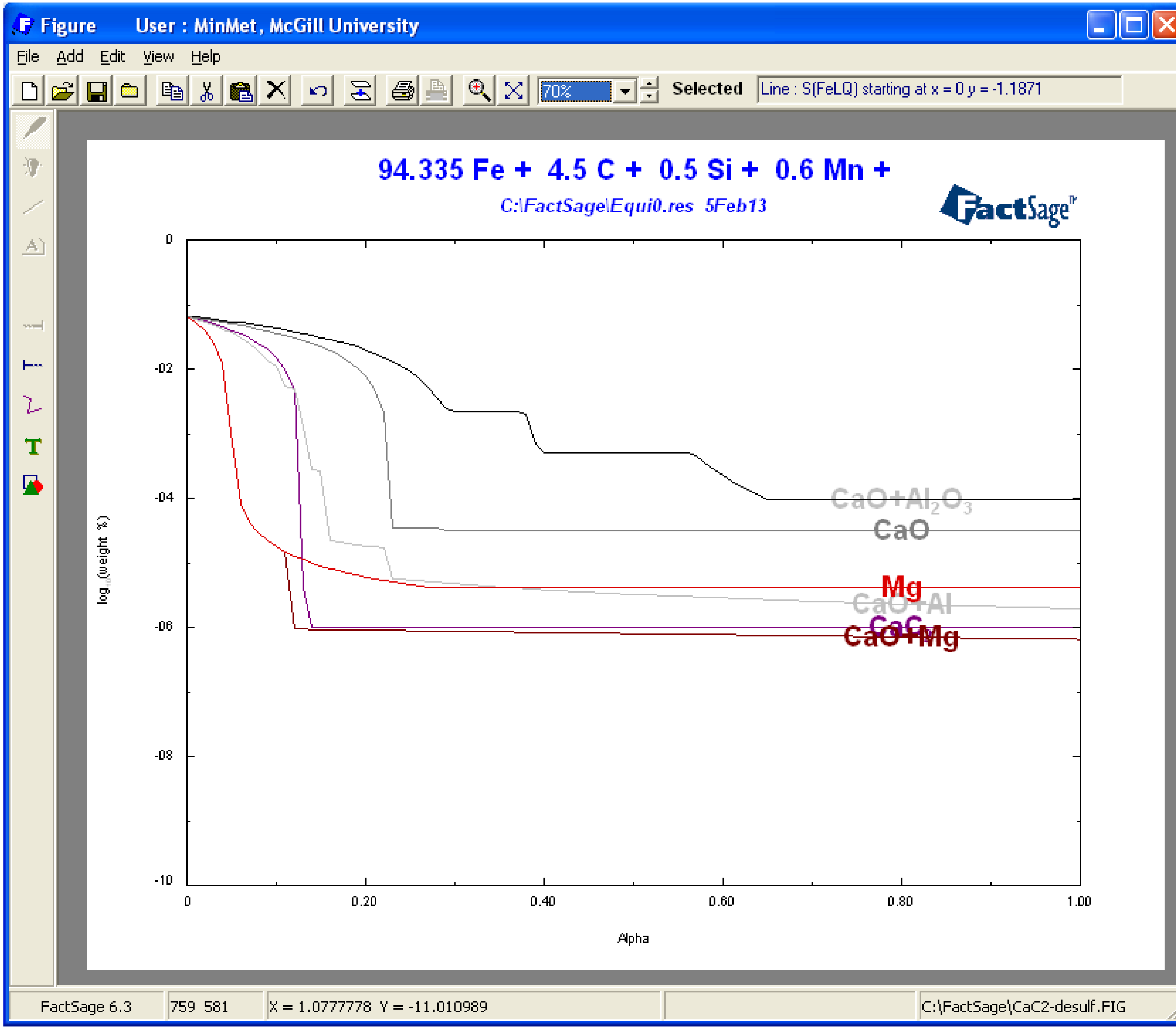
1. Press “superimposed figure”



2. Select all the other saved figures.

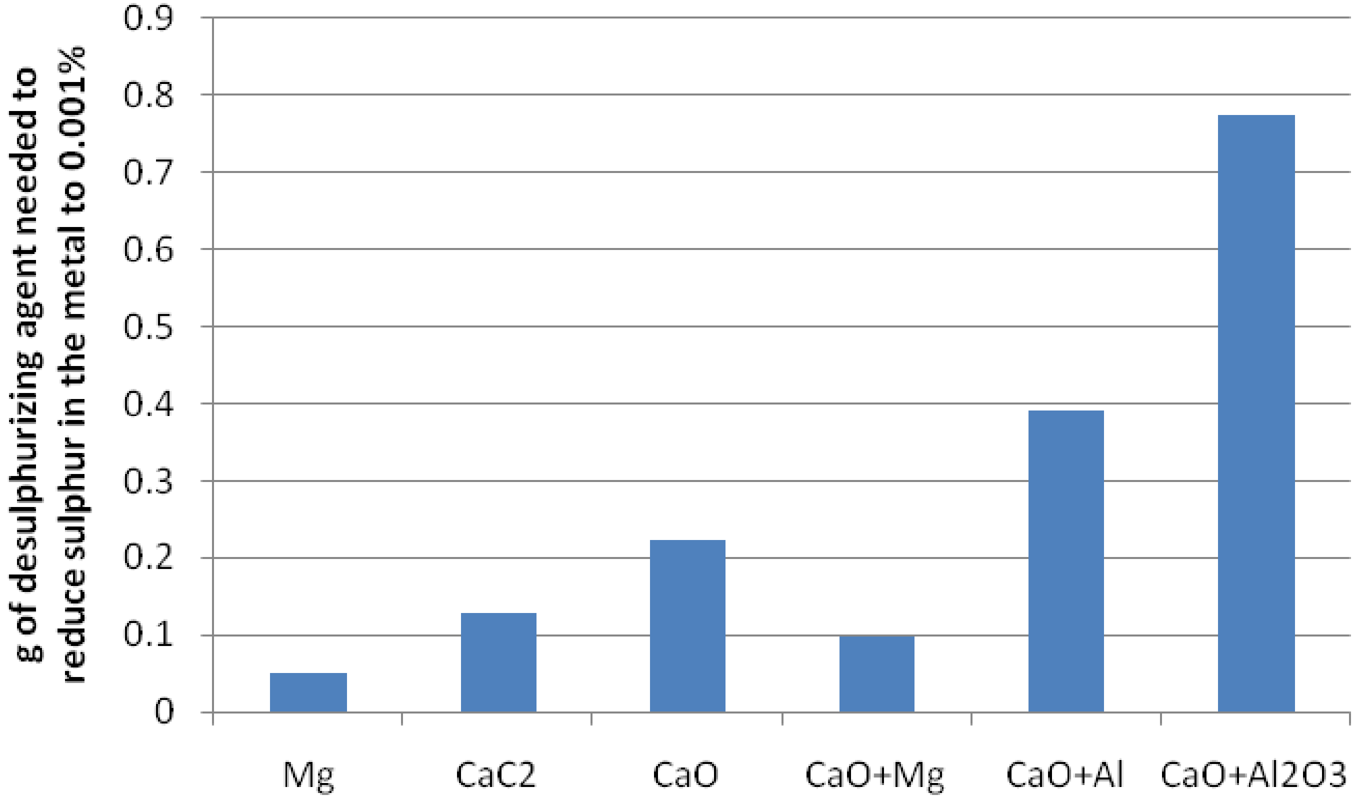
Desulphurization of Hot Metal

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

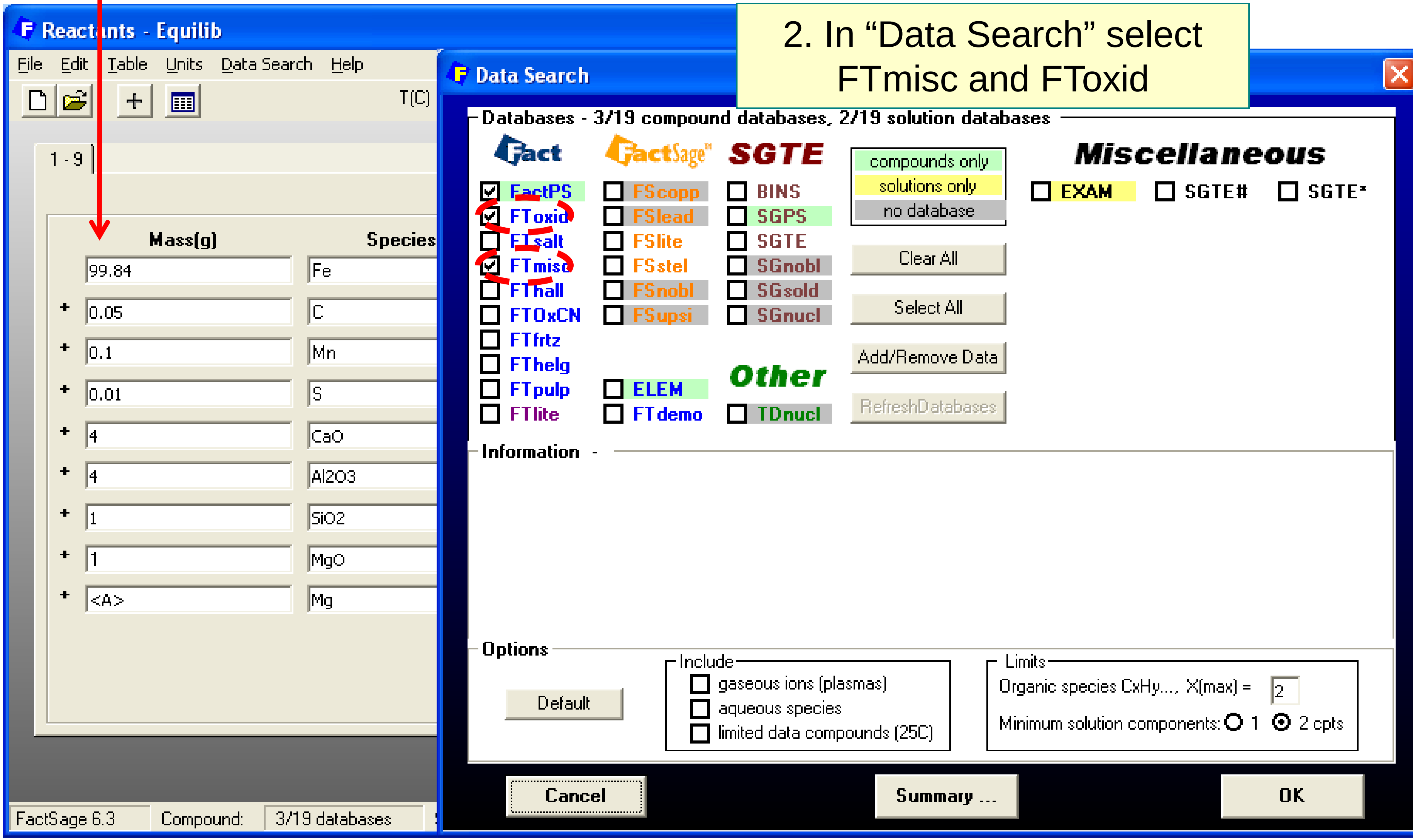
We will also assume that a slag is present in the ladle. It consists of 40% CaO, 40% Al_2O_3, 10% MgO and 10% SiO_2. The ratio of slag to metal is 1/10

Desulphurization of Steel using Mg

1. Enter the metal and slag composition

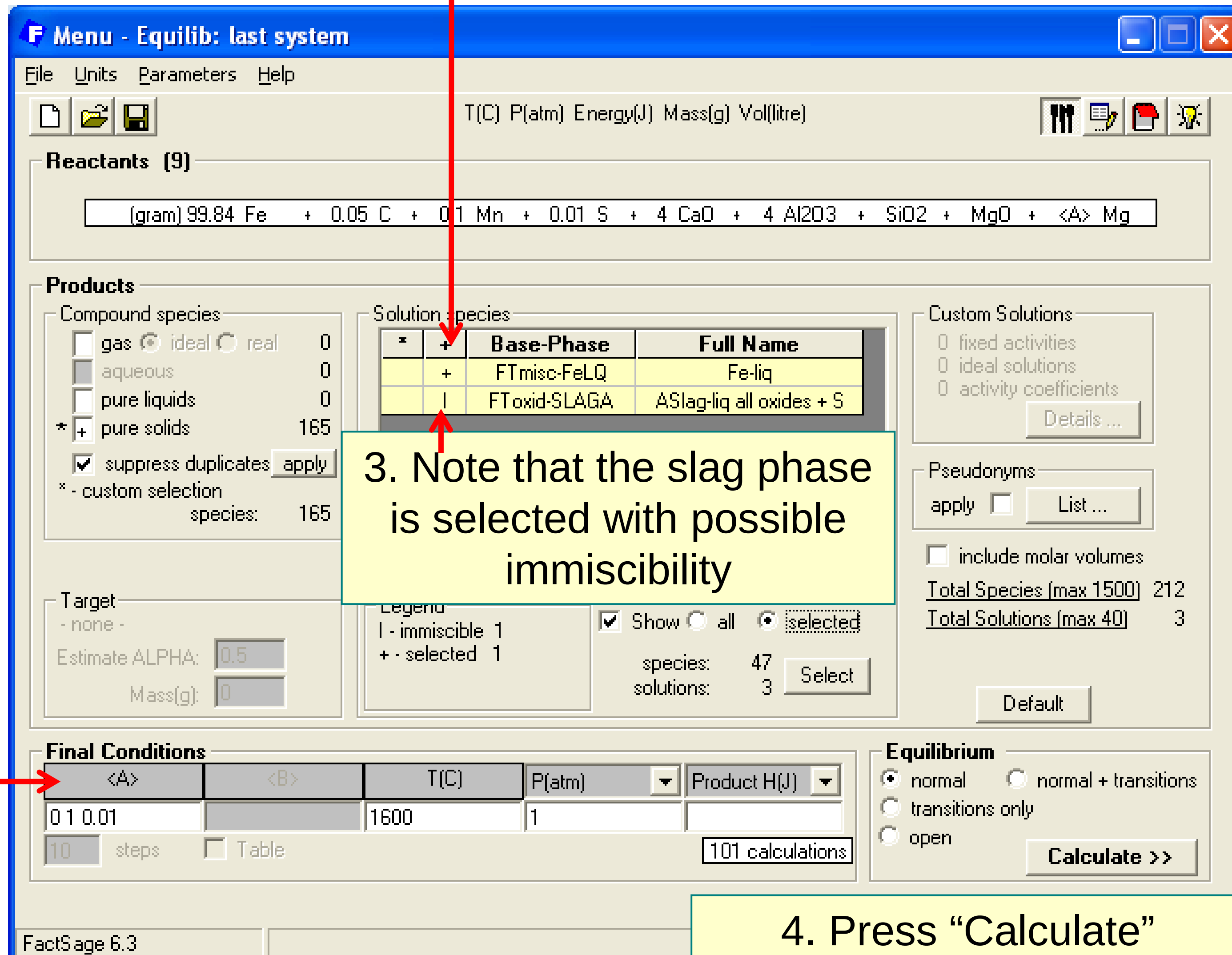
This example can be found in EquiCase2-7.dat

2. In “Data Search” select FTmisc and FToxid



Desulphurization of Steel using Mg

2. Select liquid steel and SlagA as the solutions



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

1. Enter the <A> and Temperature

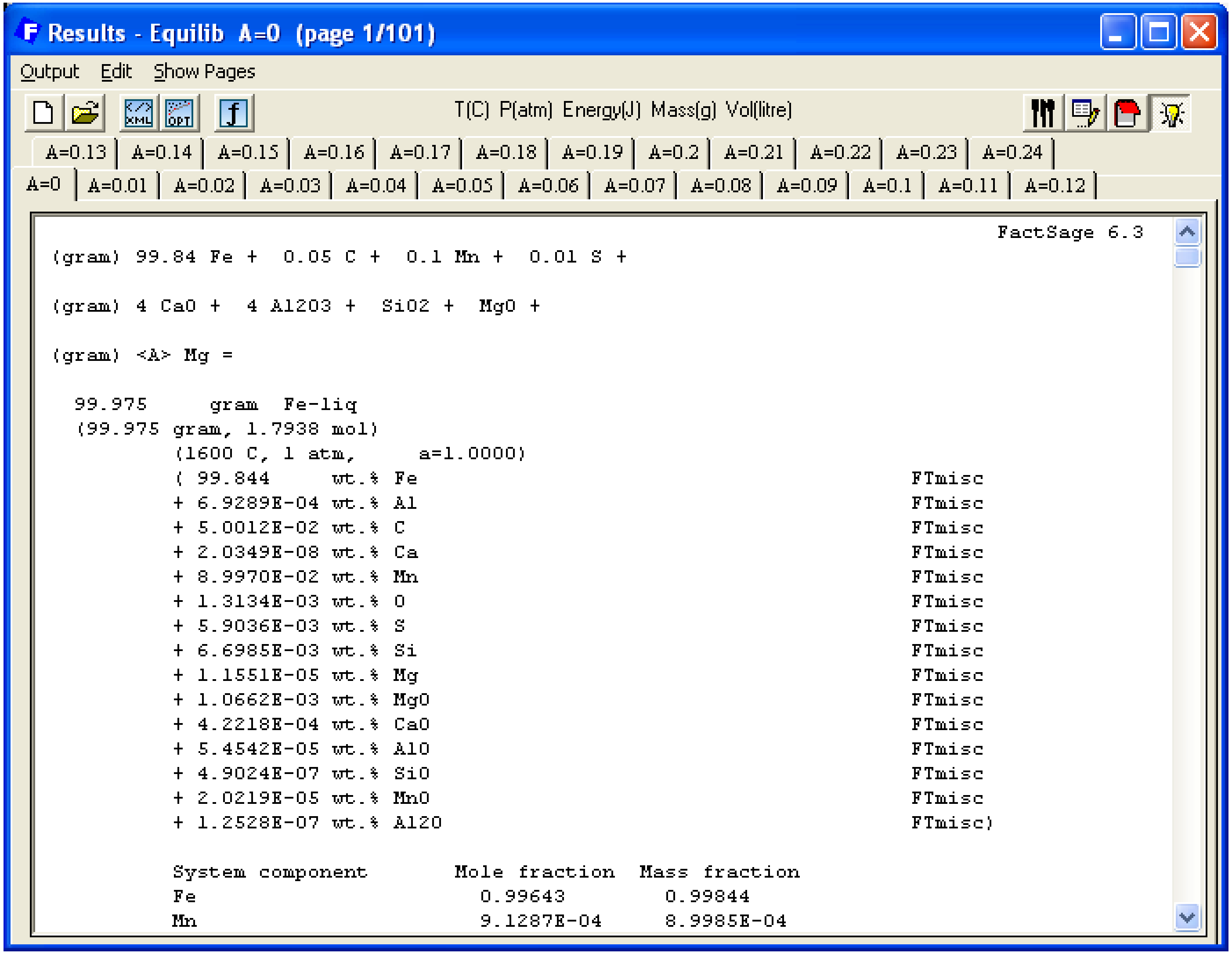
4. Press “Calculate”

Desulphurization of Steel using Mg

Results show a slag phase and a metal phase

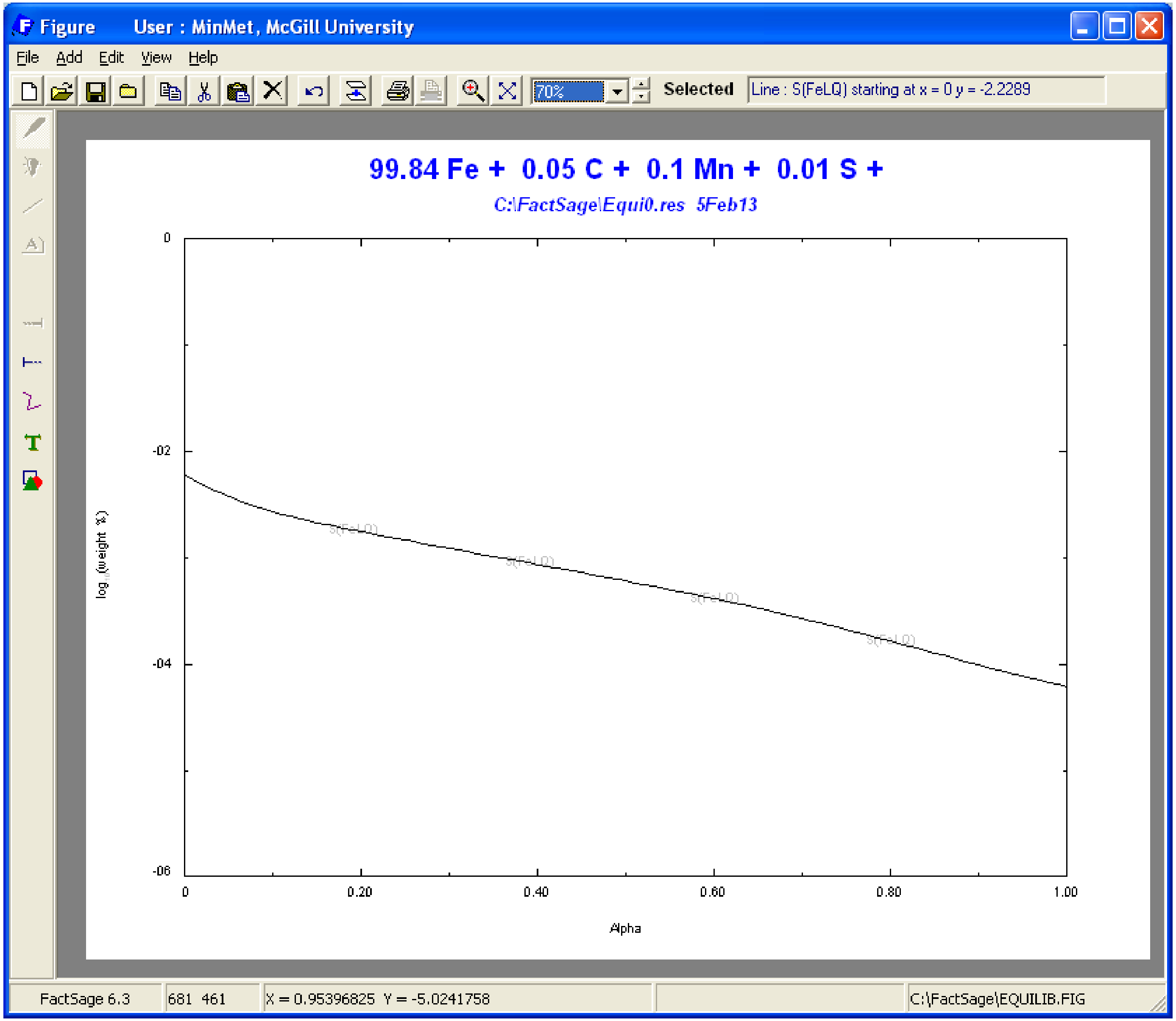
Solid periclase (MgO) appears as <A> is increased

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



Desulphurization of Steel using Mg

A constant decrease in metal sulphur content is observed



Desulphurization of Steel using Mg

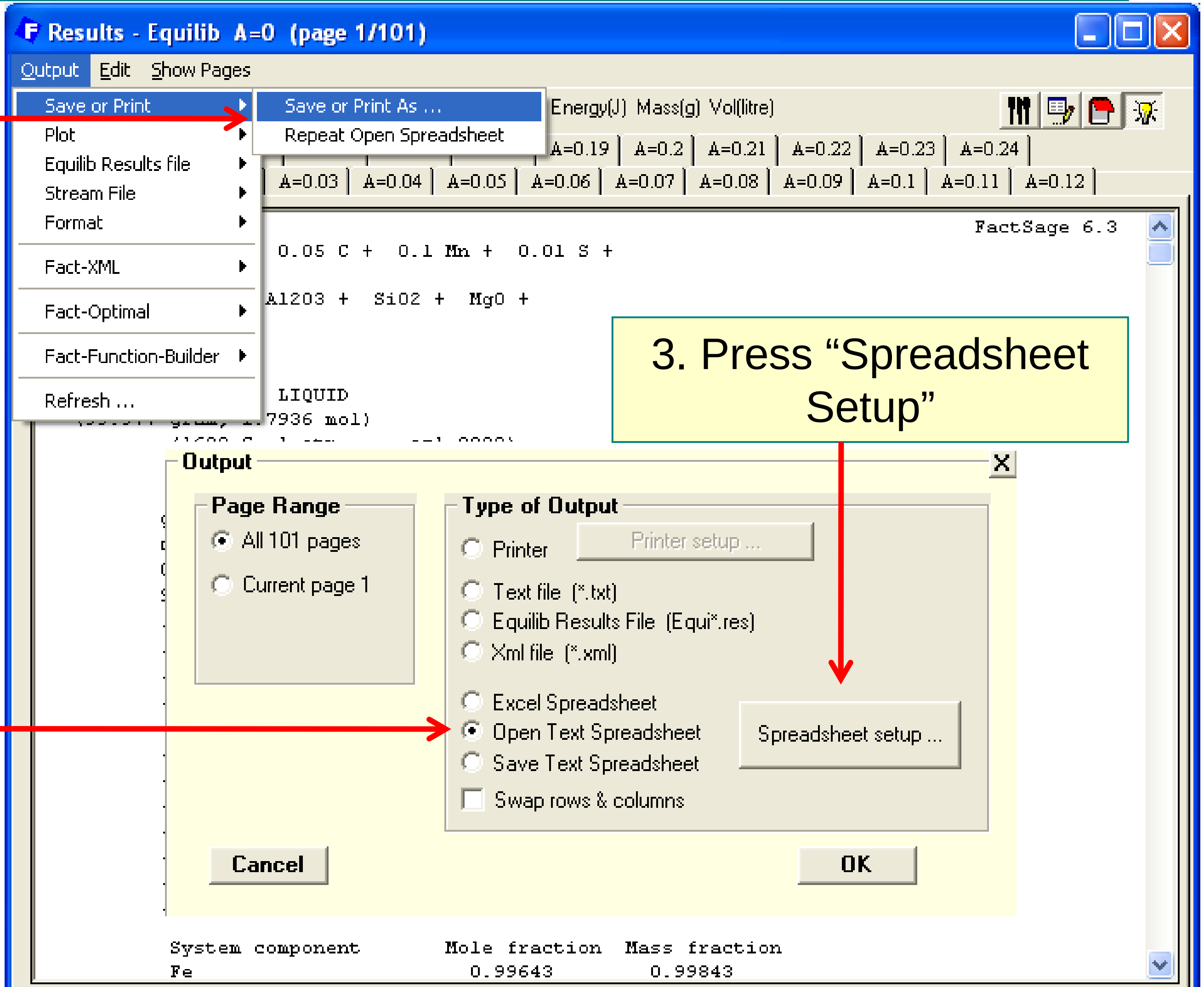
Another useful way to visualize these results, is the sulphur partition coefficient:

$Ls=(S_{in\ slag})/[S_{in\ metal}]$

1. Press “Output” → “Save or Print” → “Save or Print As …”

2. Select “Open Text Spreadsheet”

3. Press “Spreadsheet Setup”

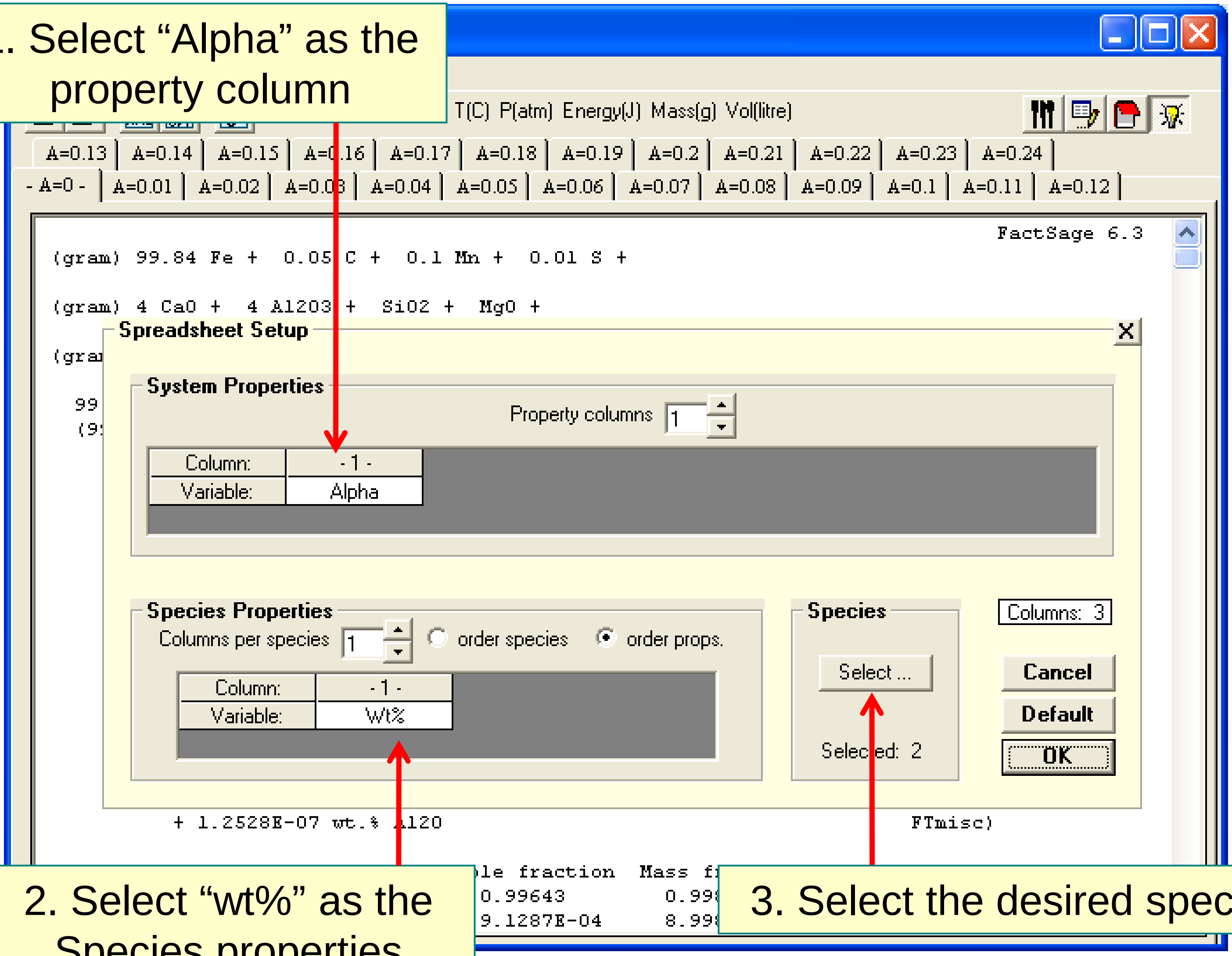


Desulphurization of Steel using Mg

1. Select "Alpha" as the property column

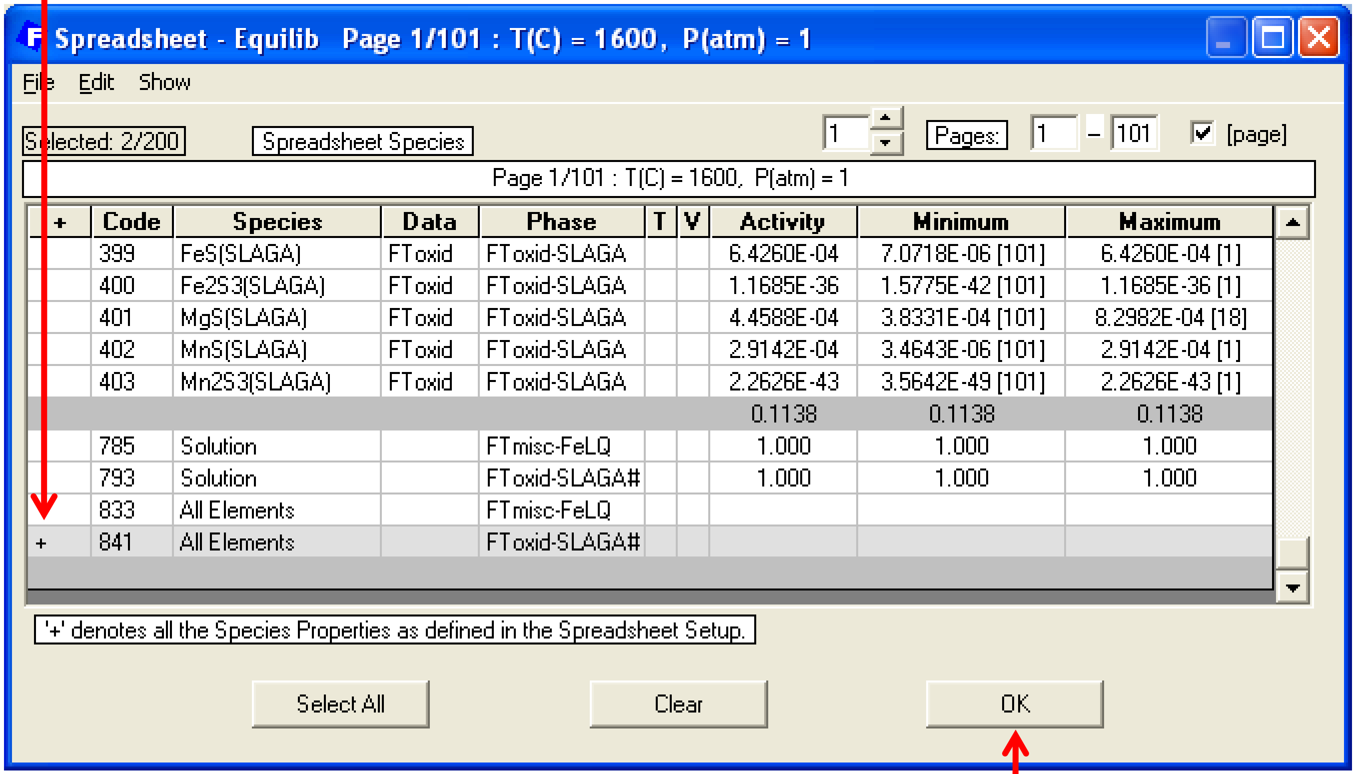
2. Select "wt%" as the Species properties

3. Select the desired species



Desulphurization of Steel using Mg

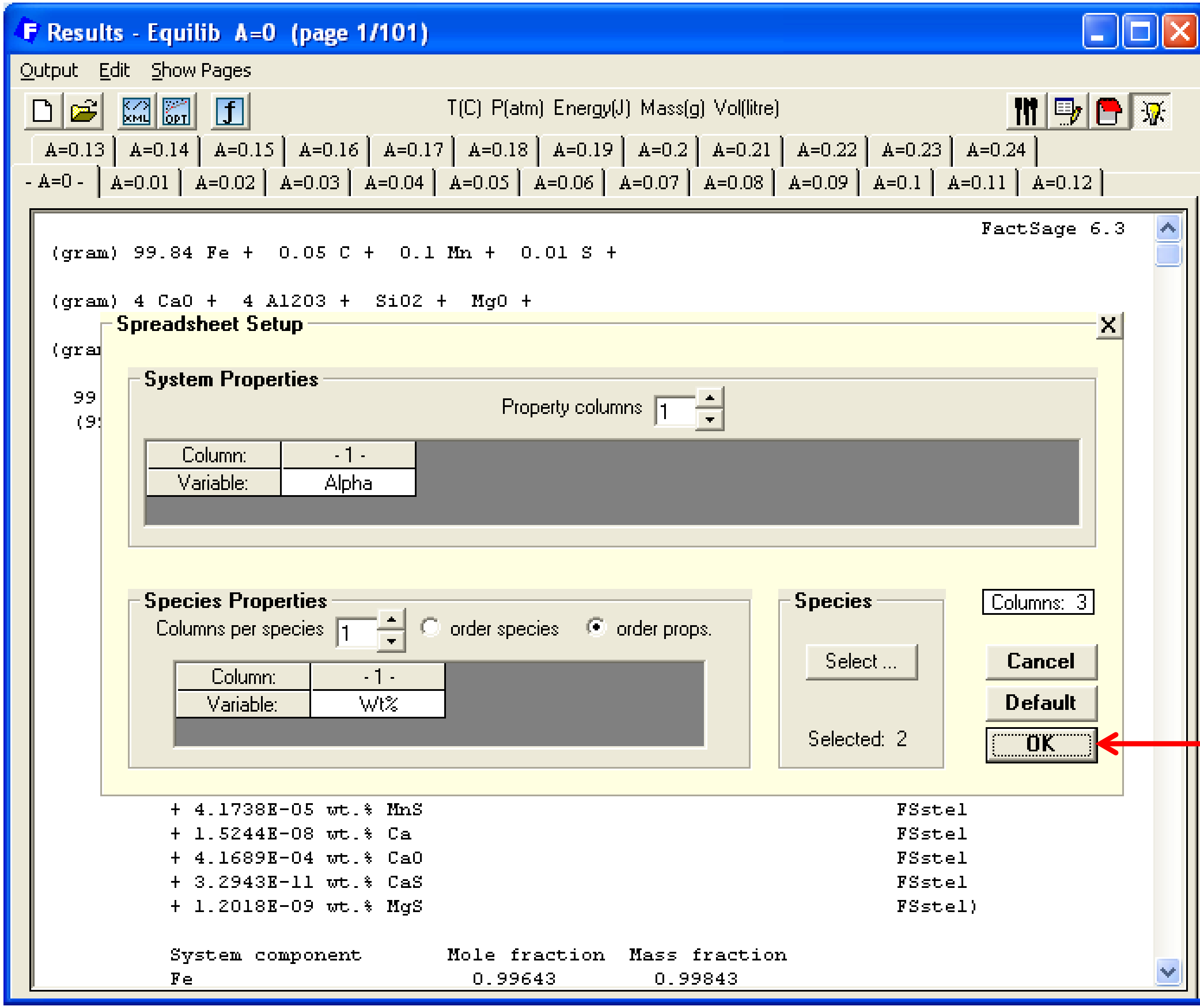
1. Select sulphur from liquid steel and all elements from the slag



+	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#					

2. Press “OK”

Desulphurization of Steel using Mg



1. Press "OK" on this window and the next one

Desulphurization of Steel using Mg

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

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

Equilib Results

File Edit Swap rows and columns

Alpha	Wt%-S(FeLQ)	Wt%-Fe_FToxid-SLAGA#1	Wt%-Mn_FToxid-SLAGA#1	Wt%-Ca_FToxid-SLAGA#1	Wt%-S_FToxid-S
0.0000000E+00	5.9035700E-03	2.0964306E-01	1.0012288E-01	2.8513645E+01	4.0877252E
1.0000000E-02	5.3252836E-03	1.6852387E-01	8.1332655E-02	2.8510824E+01	4.6634972E
2.0000000E-02	4.8279915E-03	1.4128506E-01	6.8359106E-02	2.8504632E+01	5.1579361E
3.0000000E-02	4.4067099E-03	1.2238151E-01	5.9073373E-02	2.8496487E+01	5.5761059E
4.0000000E-02	4.0472255E-03	1.0857146E-01	5.2125004E-02	2.8487197E+01	5.9322819E
5.0000000E-02	3.7364005E-03	9.8023913E-02	4.6714570E-02	2.8477204E+01	6.2396451E
6.0000000E-02	3.4640456E-03	8.9672434E-02	4.2361577E-02	2.8466760E+01	6.5084152E
7.0000000E-02	3.2225699E-03	8.2866077E-02	3.8765841E-02	2.8456014E+01	6.7462051E
8.0000000E-02	3.0063211E-03	7.7188451E-02	3.5731796E-02	2.8445058E+01	6.9586835E
9.0000000E-02	2.8148564E-03	7.2367829E-02	3.3149796E-02	2.8439713E+01	7.1477717E
1.0000000E-01	2.6754630E-03	6.8258150E-02	3.1102208E-02	2.8488410E+01	7.2988341E
1.1000000E-01	2.5485470E-03	6.4661511E-02	2.9297786E-02	2.8537191E+01	7.4379484E
1.2000000E-01	2.4321815E-03	6.1477755E-02	2.7690736E-02	2.8586067E+01	7.5669801E
1.3000000E-01	2.3248448E-03	5.8631820E-02	2.6246476E-02	2.8635047E+01	7.6874018E
1.4000000E-01	2.2253172E-03	5.6066280E-02	2.4938369E-02	2.8684137E+01	7.8003932E
1.5000000E-01	2.1326075E-03	5.3736397E-02	2.3745535E-02	2.8733342E+01	7.9069118E
1.6000000E-01	2.0459010E-03	5.1606760E-02	2.2651352E-02	2.8782665E+01	8.0077444E
1.7000000E-01	1.9645204E-03	4.9648942E-02	2.1642403E-02	2.8832109E+01	8.1035444E
1.8000000E-01	1.8878971E-03	4.7839831E-02	2.0707729E-02	2.8881678E+01	8.1948602E
1.9000000E-01	1.8155494E-03	4.6160427E-02	1.9838277E-02	2.8931373E+01	8.2821557E
2.0000000E-01	1.7470662E-03	4.4594948E-02	1.9026492E-02	2.8981197E+01	8.3658267E
2.1000000E-01	1.6820936E-03	4.3130163E-02	1.8266019E-02	2.9031152E+01	8.4462136E
2.2000000E-01	1.6203249E-03	4.1754891E-02	1.7551460E-02	2.9081239E+01	8.5236110E
2.3000000E-01	1.5614931E-03	4.0459605E-02	1.6878202E-02	2.9131459E+01	8.5982756E

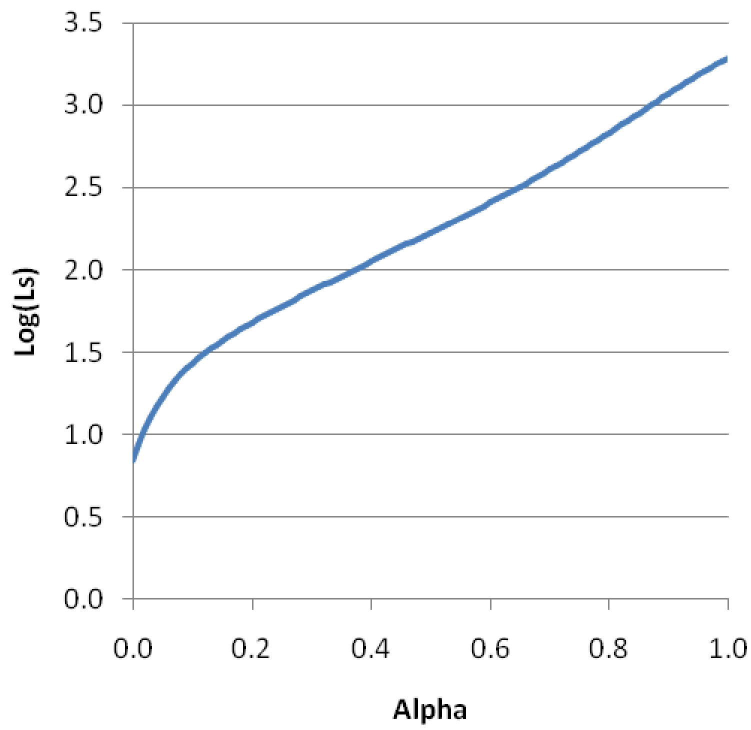
Desulphurization of Steel using Mg

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 Ls.

	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-(	=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.

Results - Equilib 1600 C, A=0.3558

Output Edit Show Pages

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

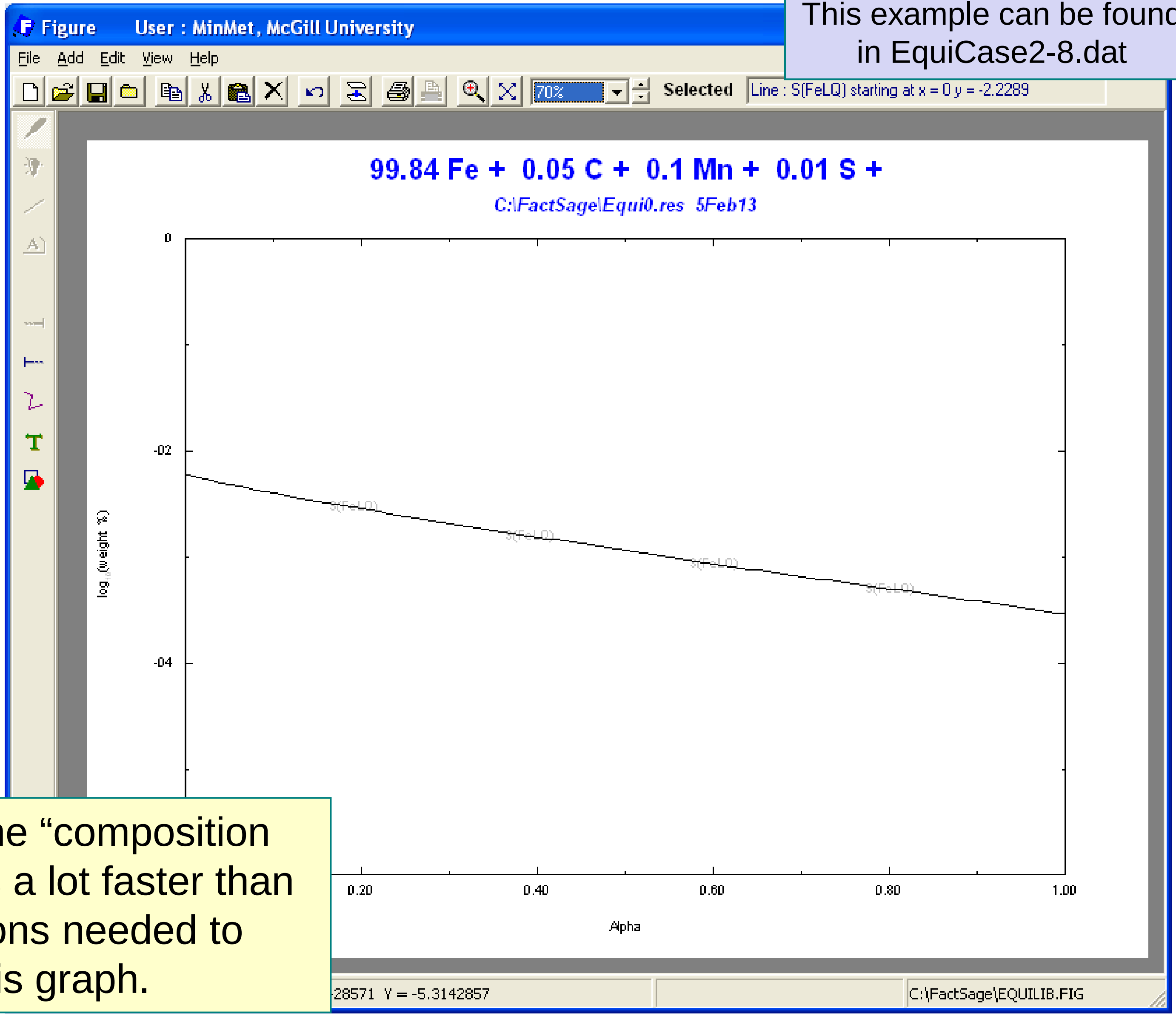
```
                                                                  FactSage 6.3
(gram) 99.84 Fe +  0.05 C +  0.1 Mn +  0.01 S +

(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.

This example can be found in EquiCase2-8.dat



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

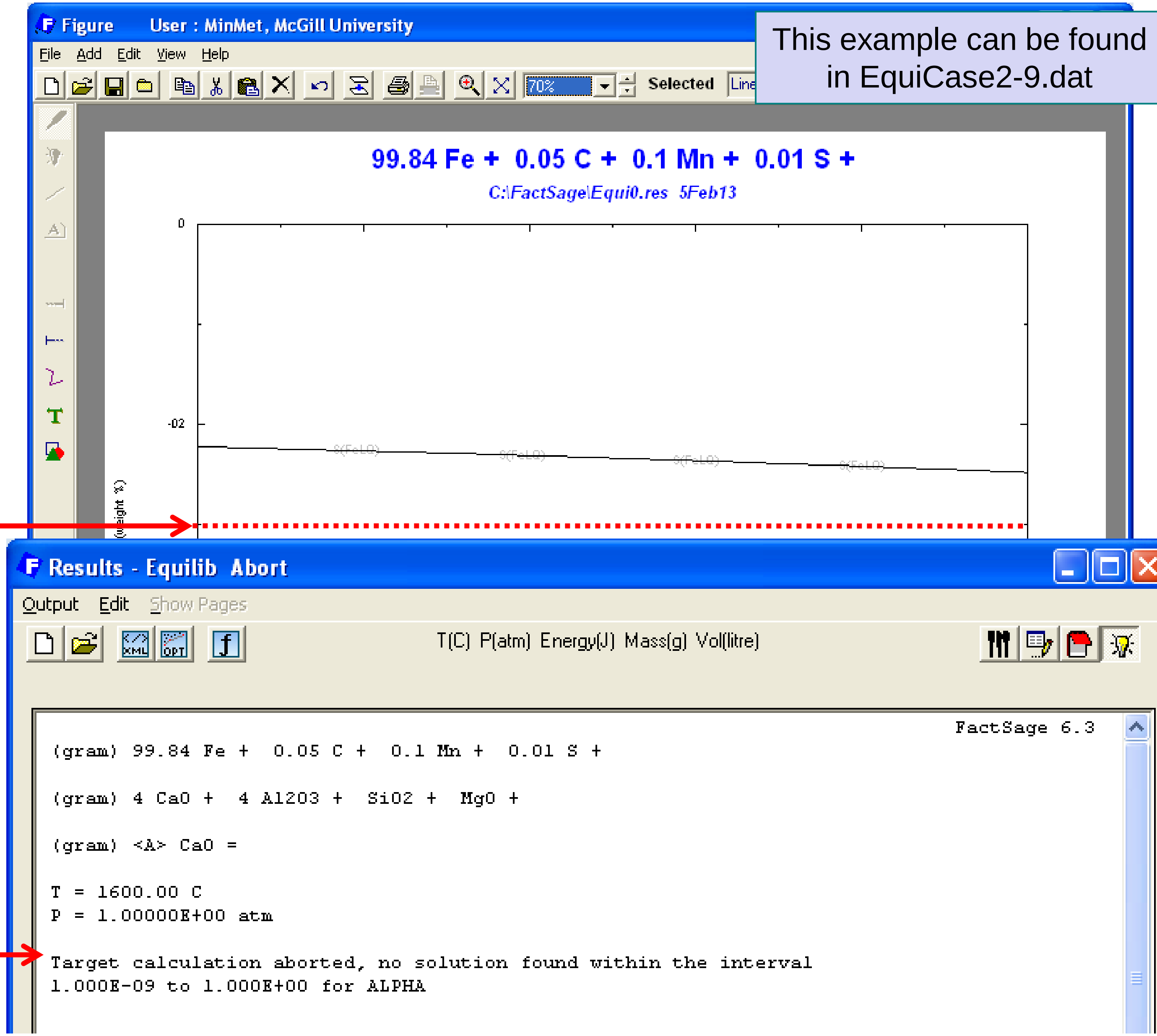
Desulphurization of Steel using CaO

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(wt%S)=-3

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

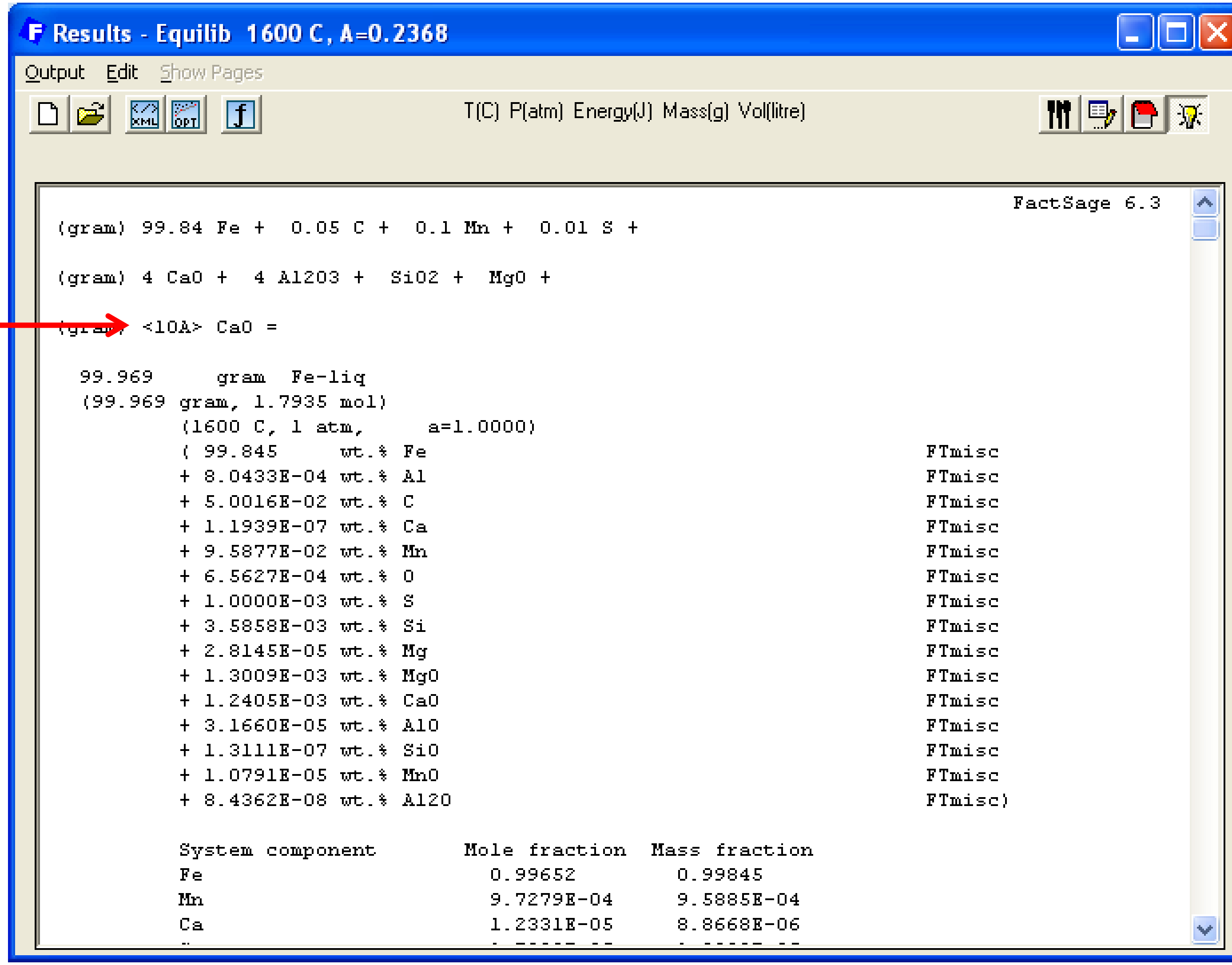
This example can be found in EquiCase2-9.dat



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

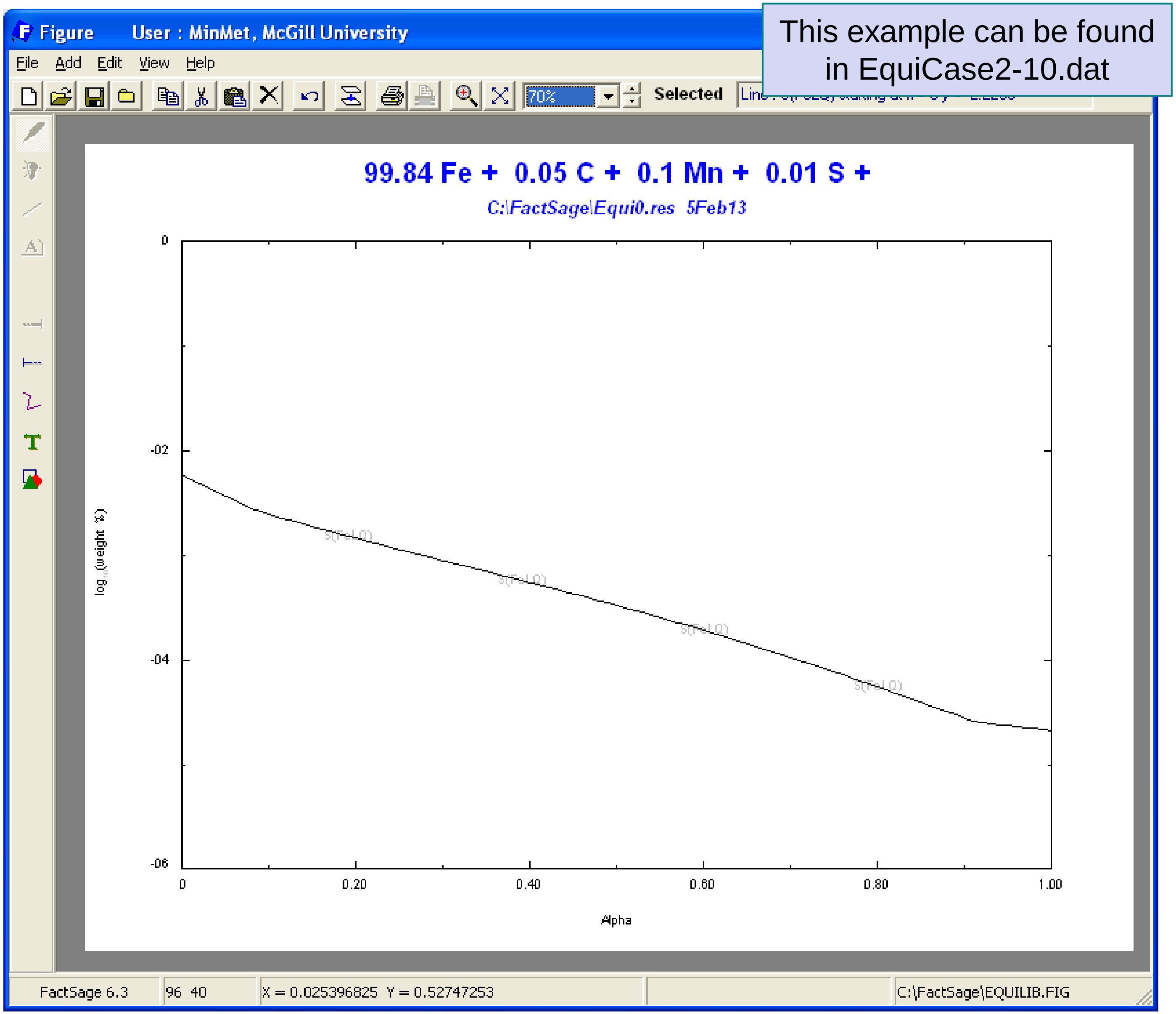


Desulphurization of Steel using CaO+Mg

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.

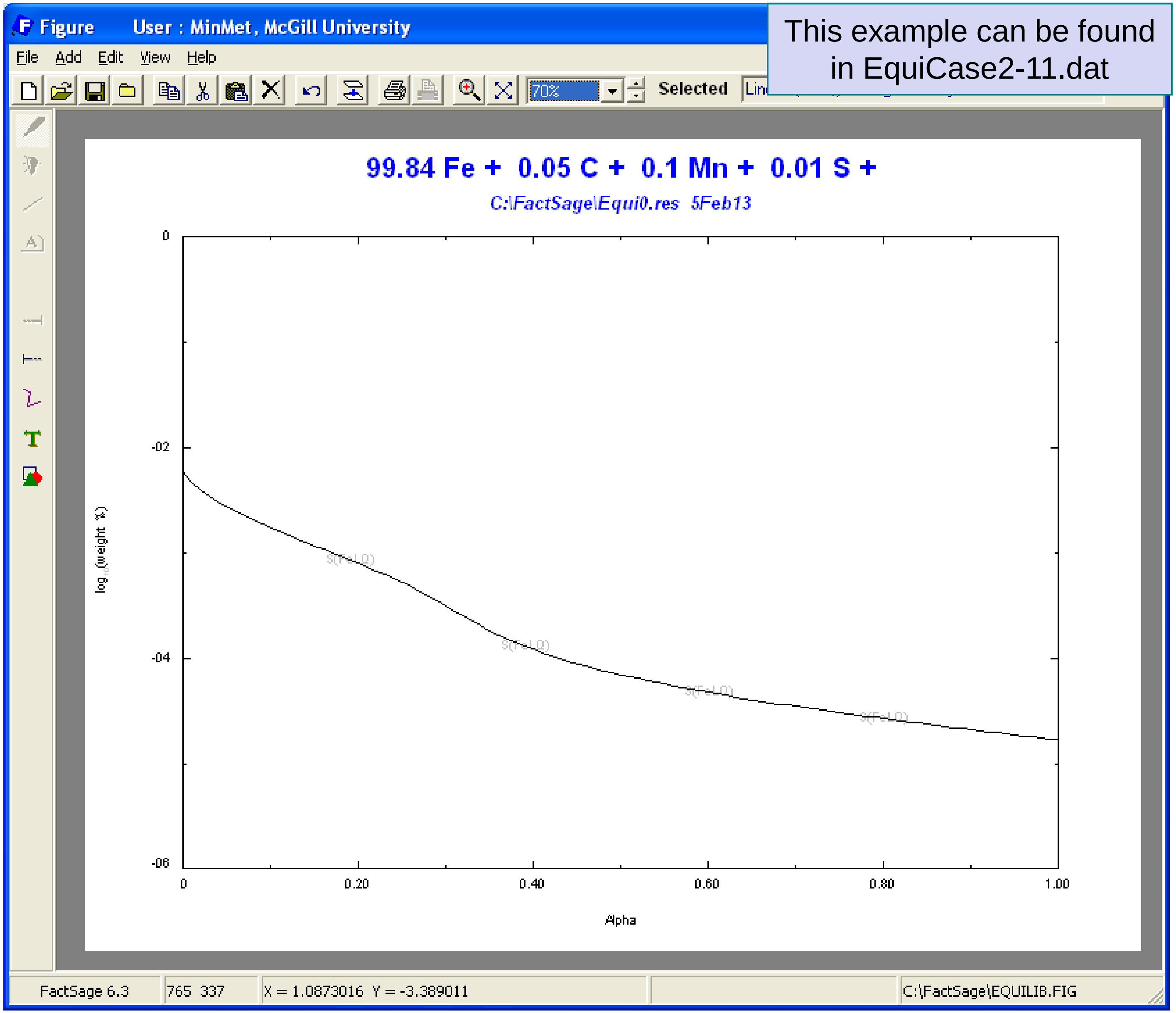
This example can be found in EquiCase2-10.dat



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.

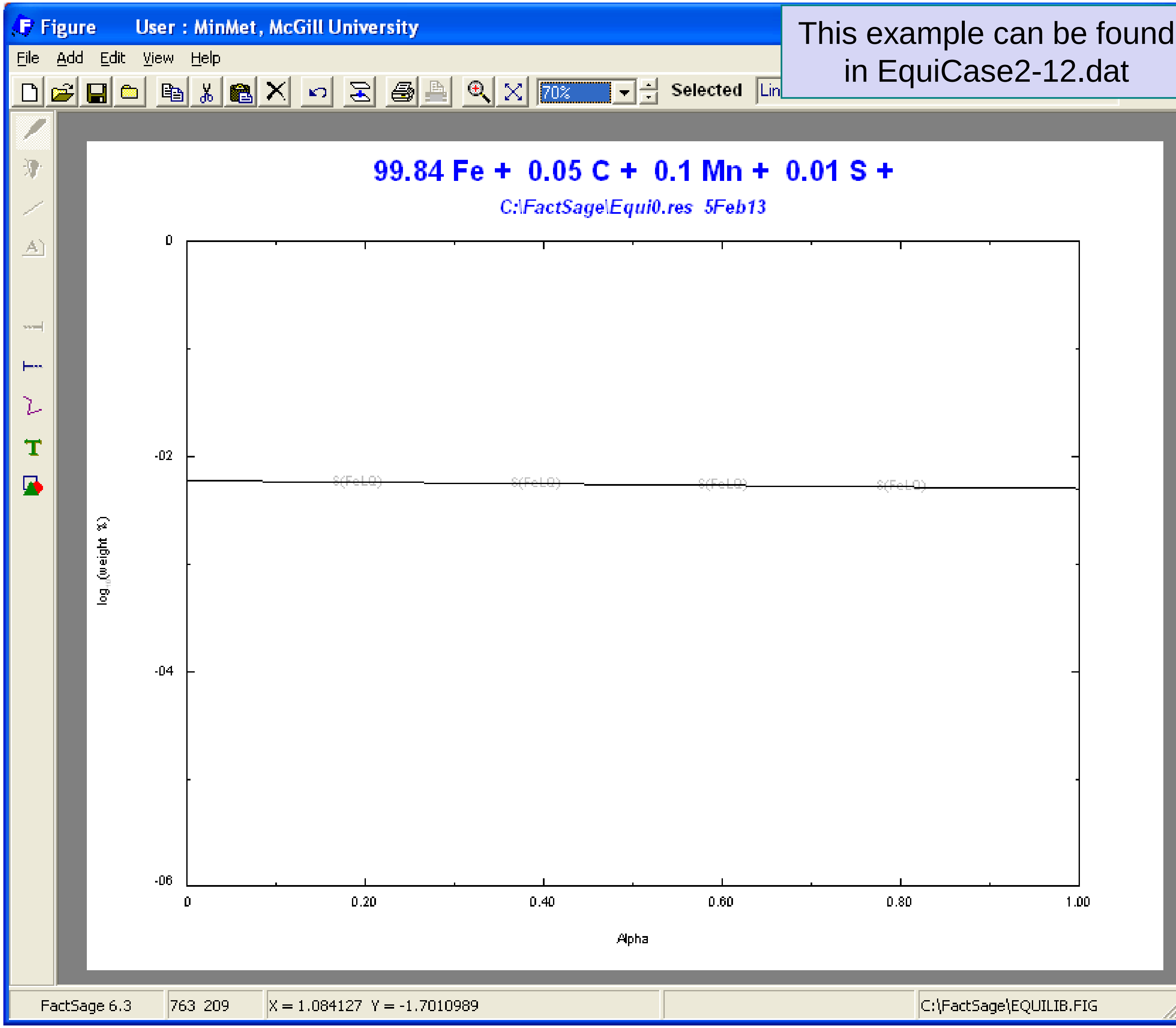


This example can be found in EquiCase2-11.dat

Desulphurization of Steel using $CaO+Al_2O_3$

Performing the same operations using $CaO+Al_2O_3$, the following graph is obtained.

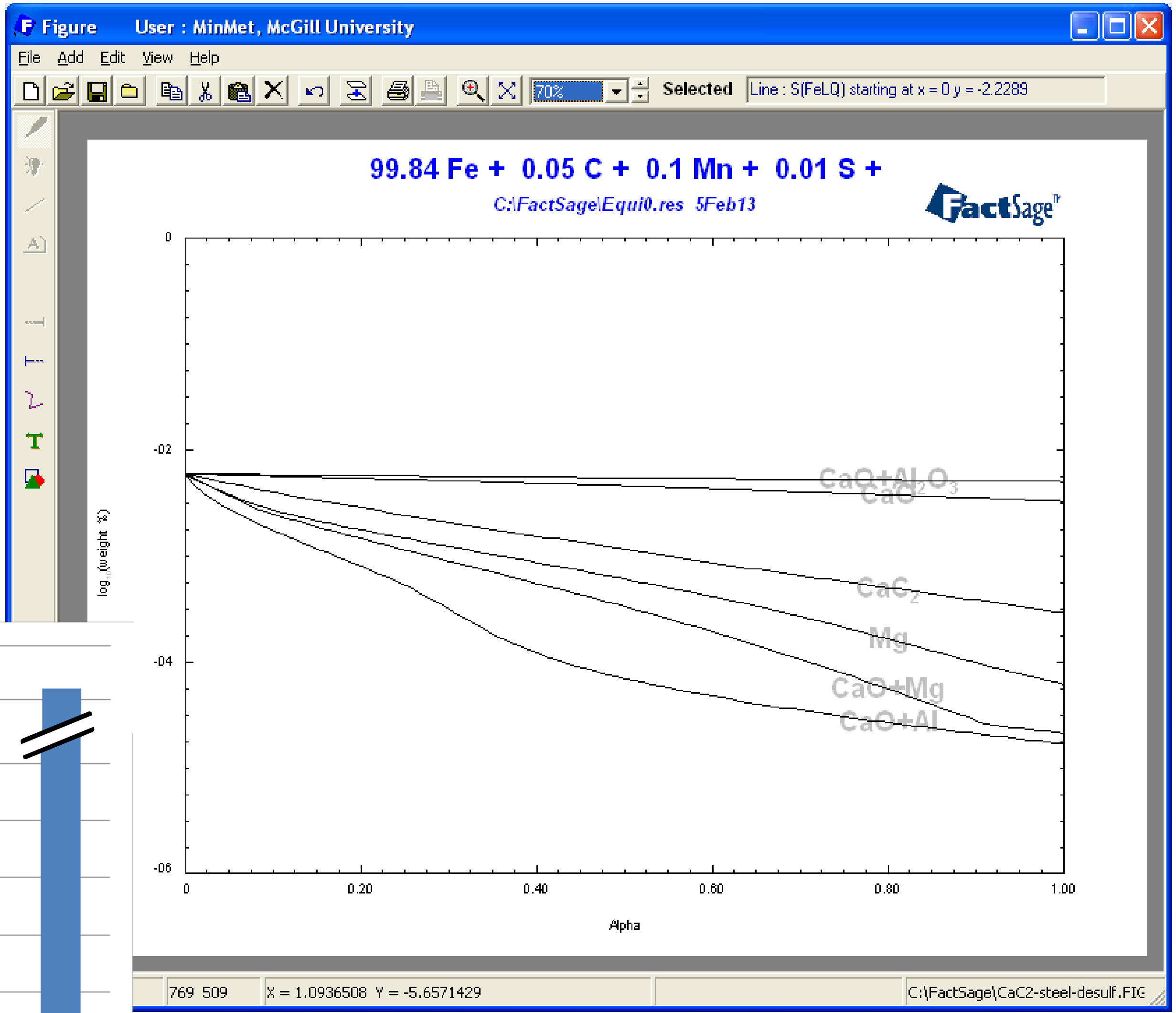
Using “composition target” it was found that 15.49g of CaO and 15.49g Al_2O_3 is needed to obtain the desired sulphur composition.

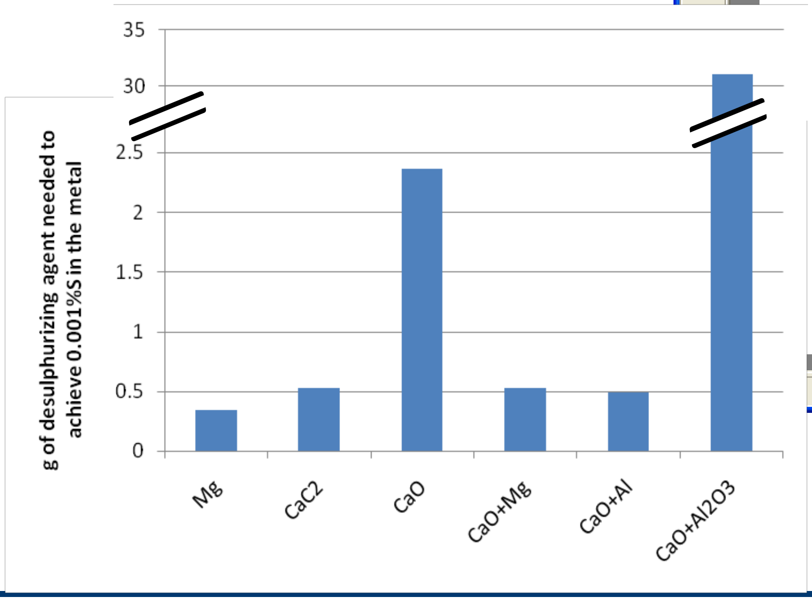


This example can be found in EquiCase2-12.dat

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:

$$C_S=(S_{in\ slag})*(P_{O2}/P_{S2})^{1/2}$$

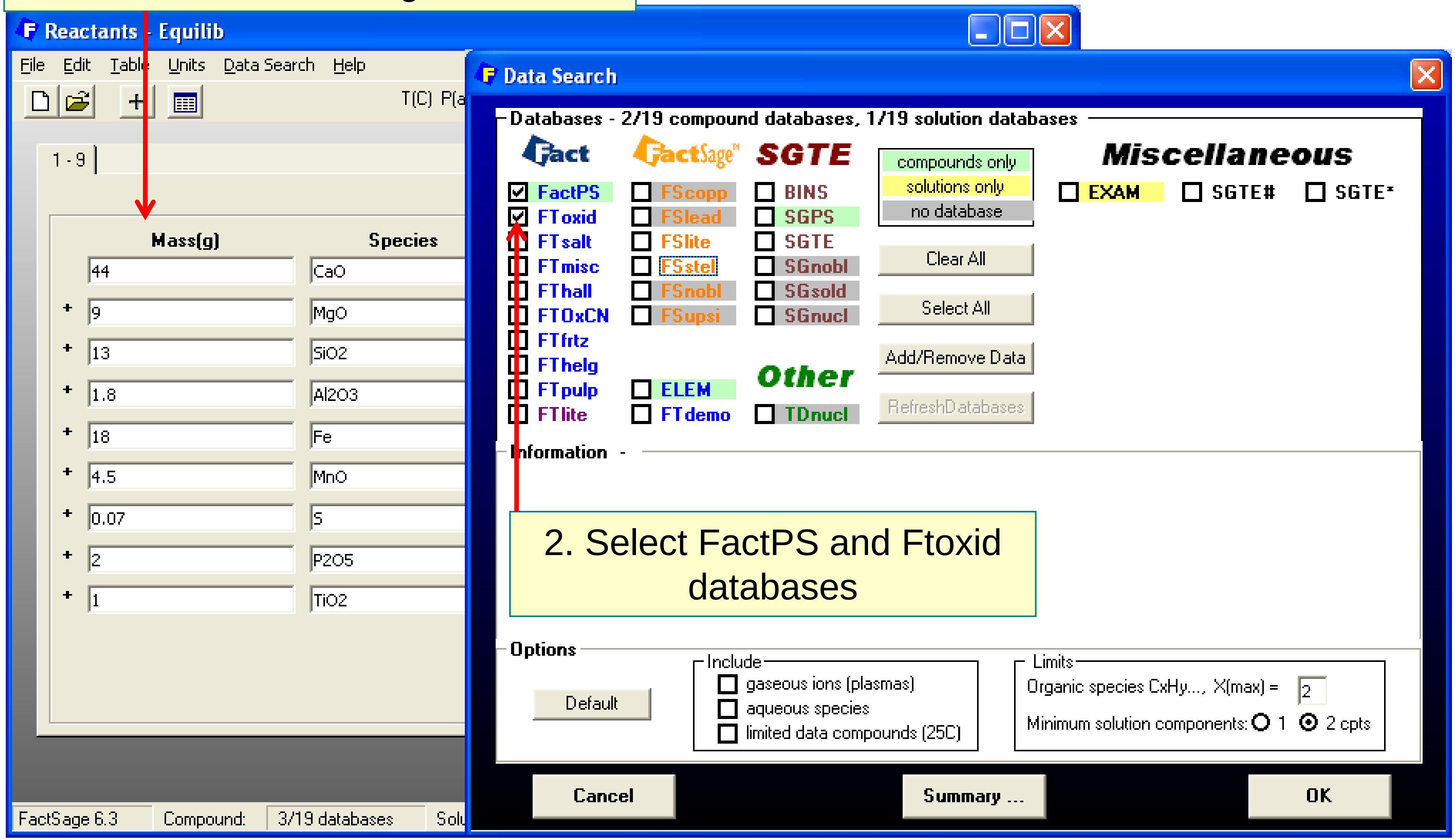
In the following slides, the sulphide capacity of four different slags will be calculated

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
SiO2	13.0	14.0	5.0	20.0
Al2O3	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
P2O5	2.00	3.50	0.05	0.05
TiO2	1.0	<0.5	<0.5	<0.5
Slag Basicity (CaO / SiO2)	3.4	3.9	10.6	2.8
Slag Basicity (CaO +MgO) / (SiO2+Al2O3)	3.6	3.7	1.8	2.0

Calculating Slag Sulphide Capacity

1. Enter the amount and species for the first slag

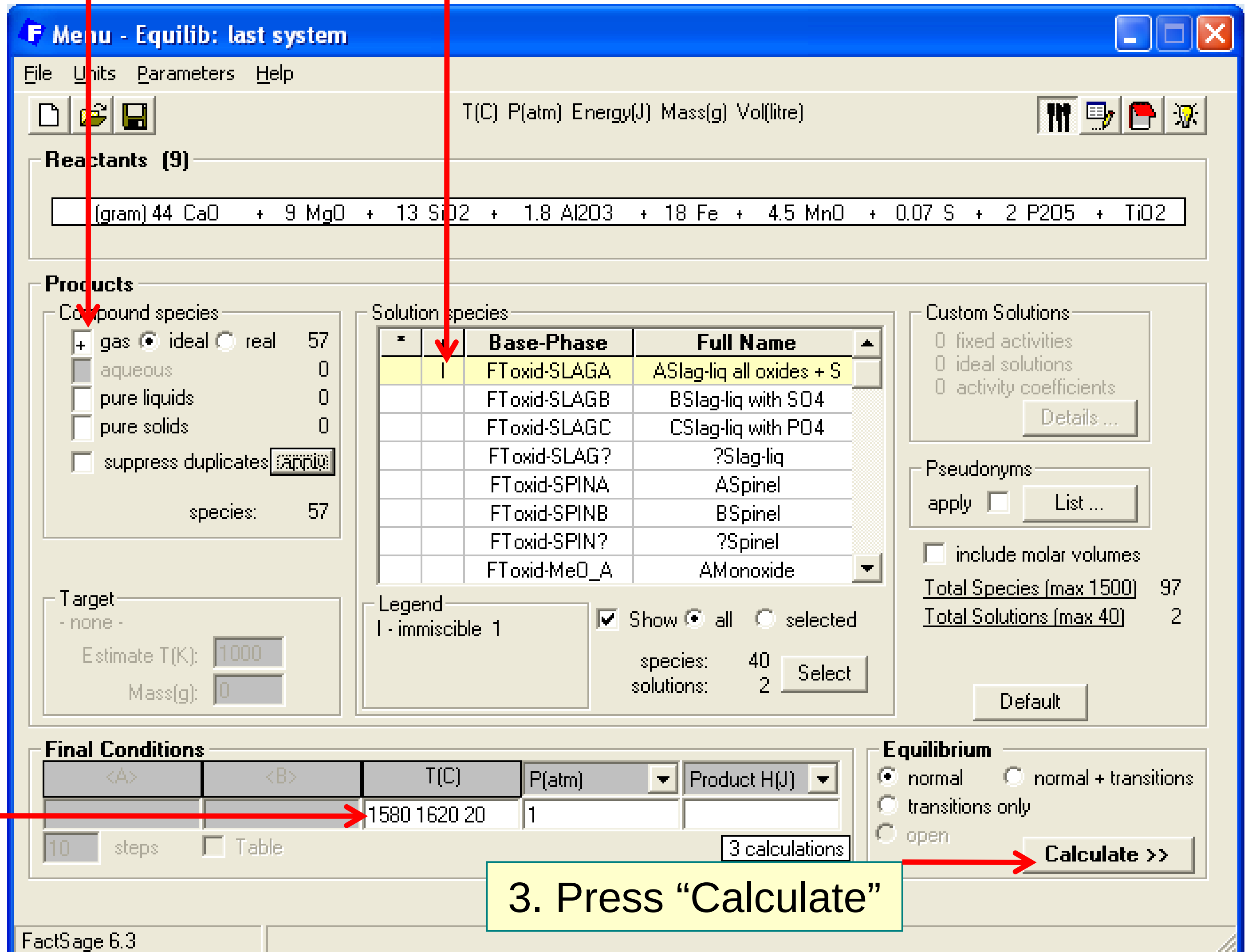
This example can be found in EquiCase2-13.dat



2. Select FactPS and Ftoxid databases

Calculating Slag Sulphide Capacity

1. Select gas and SlagA as possible products



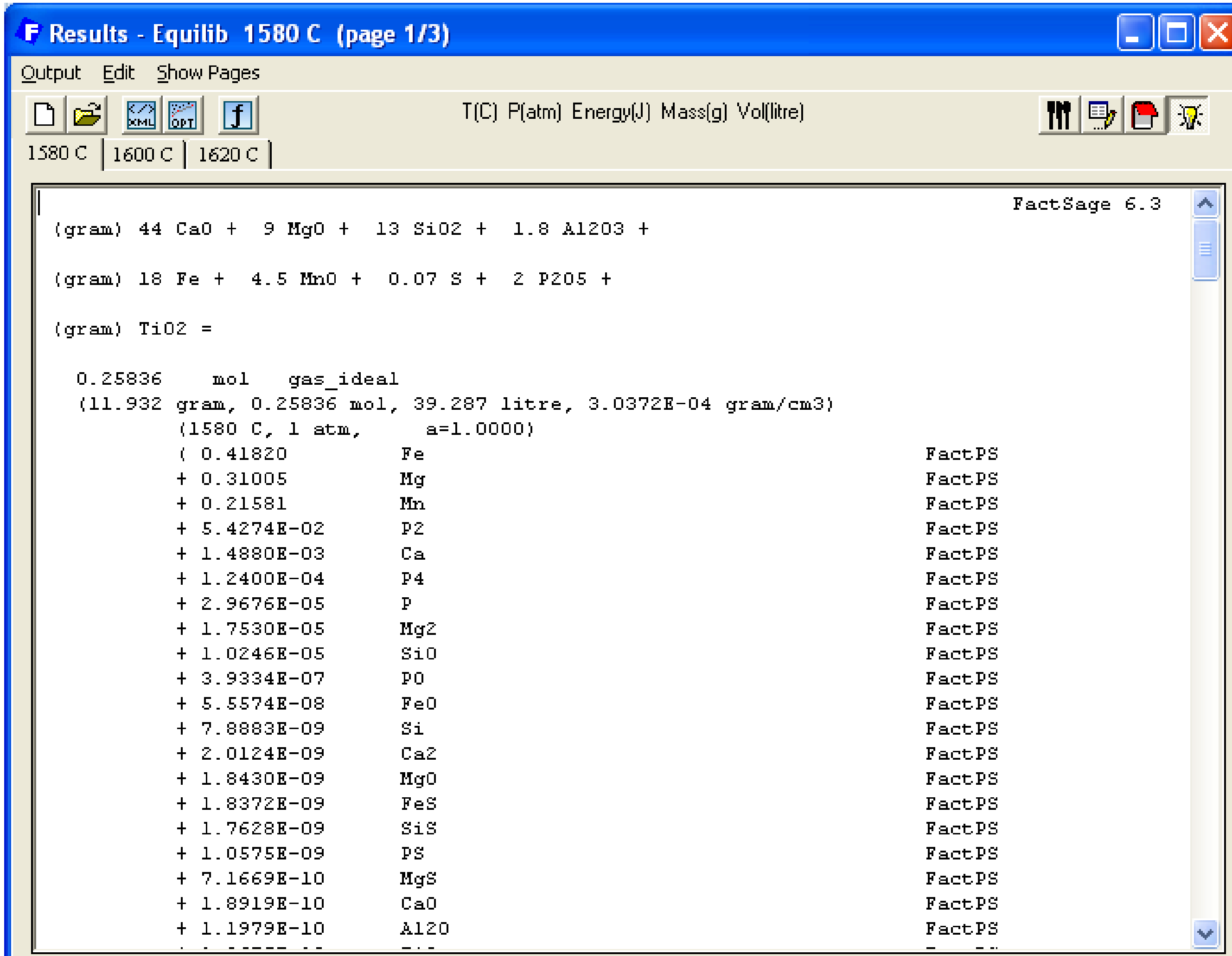
2. We will calculate the sulphide capacity at three temperatures: 1580, 1600 and 1620°C

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.

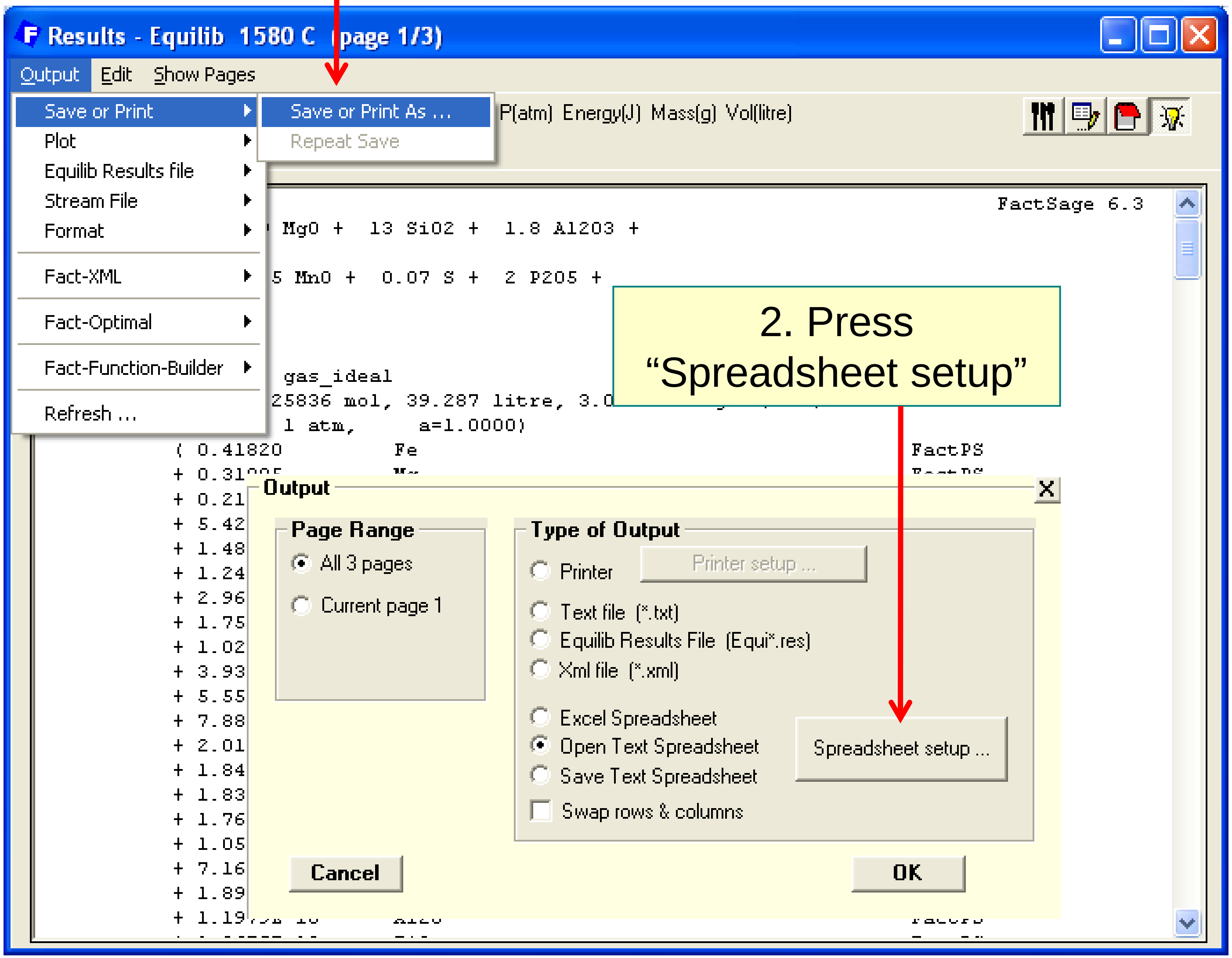


Calculating Slag Sulphide Capacity

The first way is to use Excel

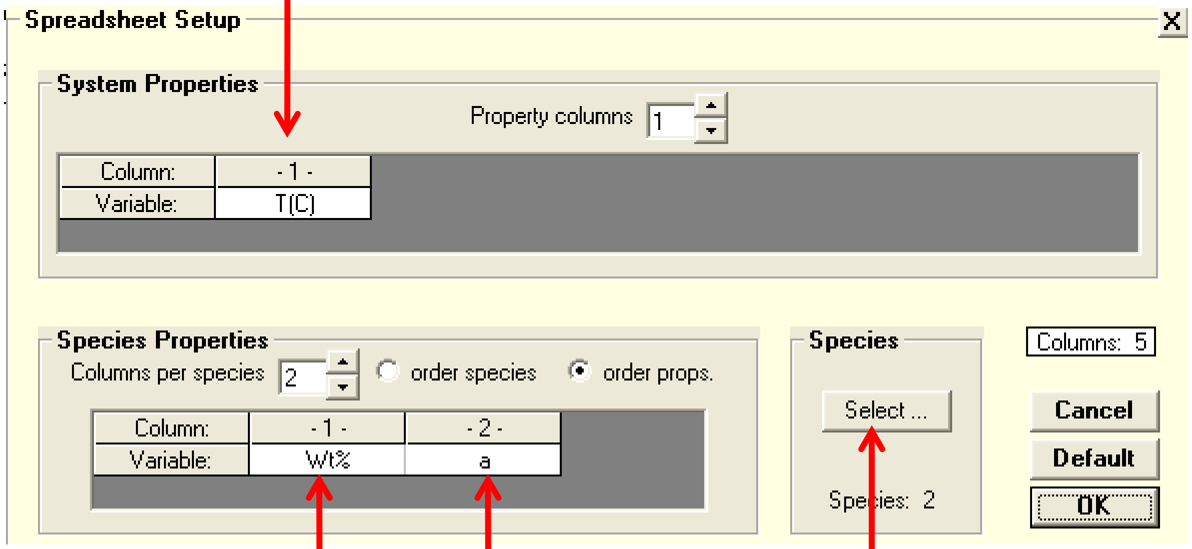
1. Save the results in a spreadsheet

2. Press "Spreadsheet setup"



Calculating Slag Sulphide Capacity

1. Set T(C) as the system property

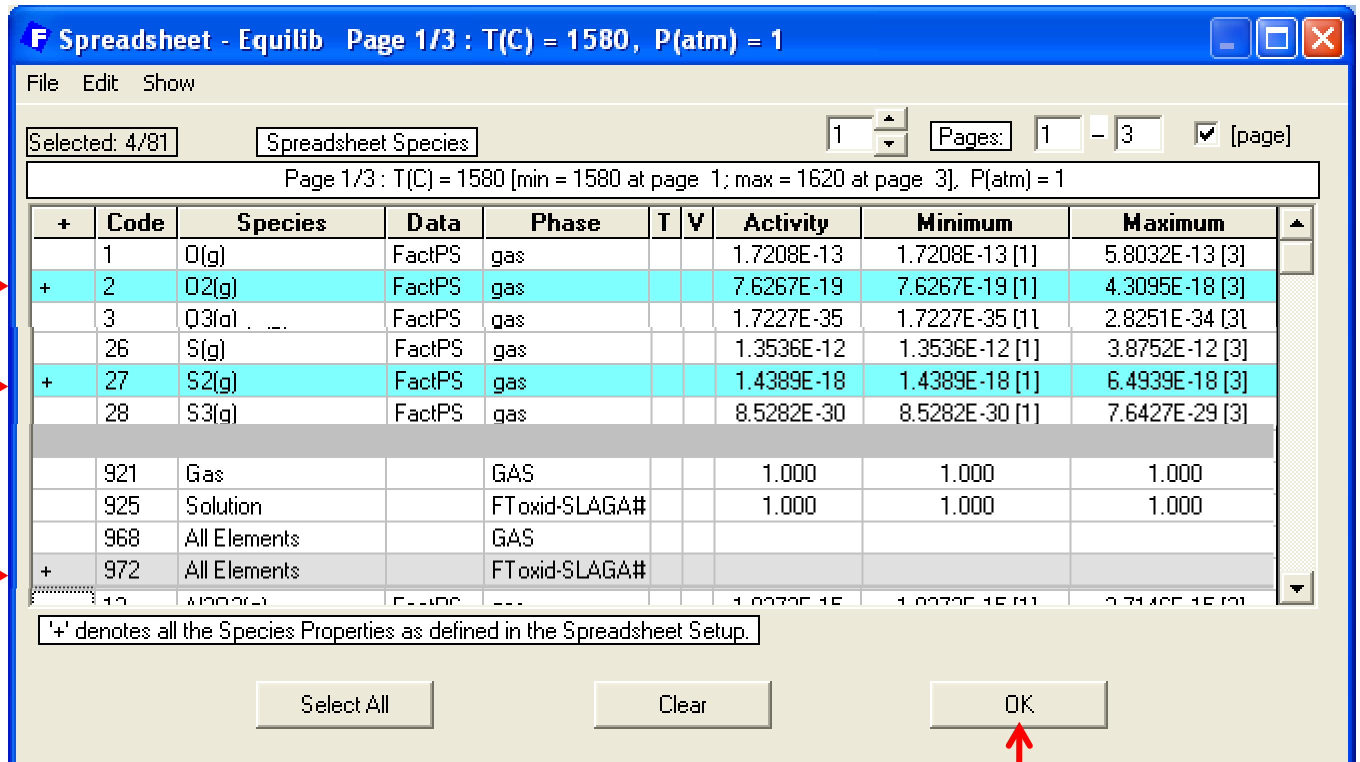


2. We need wt%S and the activity of O_2 and S_2 in the gas, so select "wt%" and "a" as the species properties.

3. Select the species

Calculating Slag Sulphide Capacity

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



2. Press “OK” on all three screens

Calculating Slag Sulphide Capacity

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

Equilib Results

File Edit Swap rows and columns

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

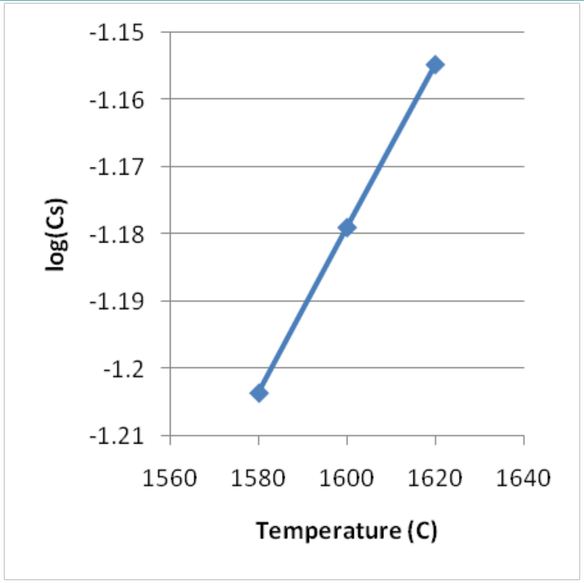
2. Copy the results in Excel and delete the unnecessary columns

	A	B	C	D
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

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

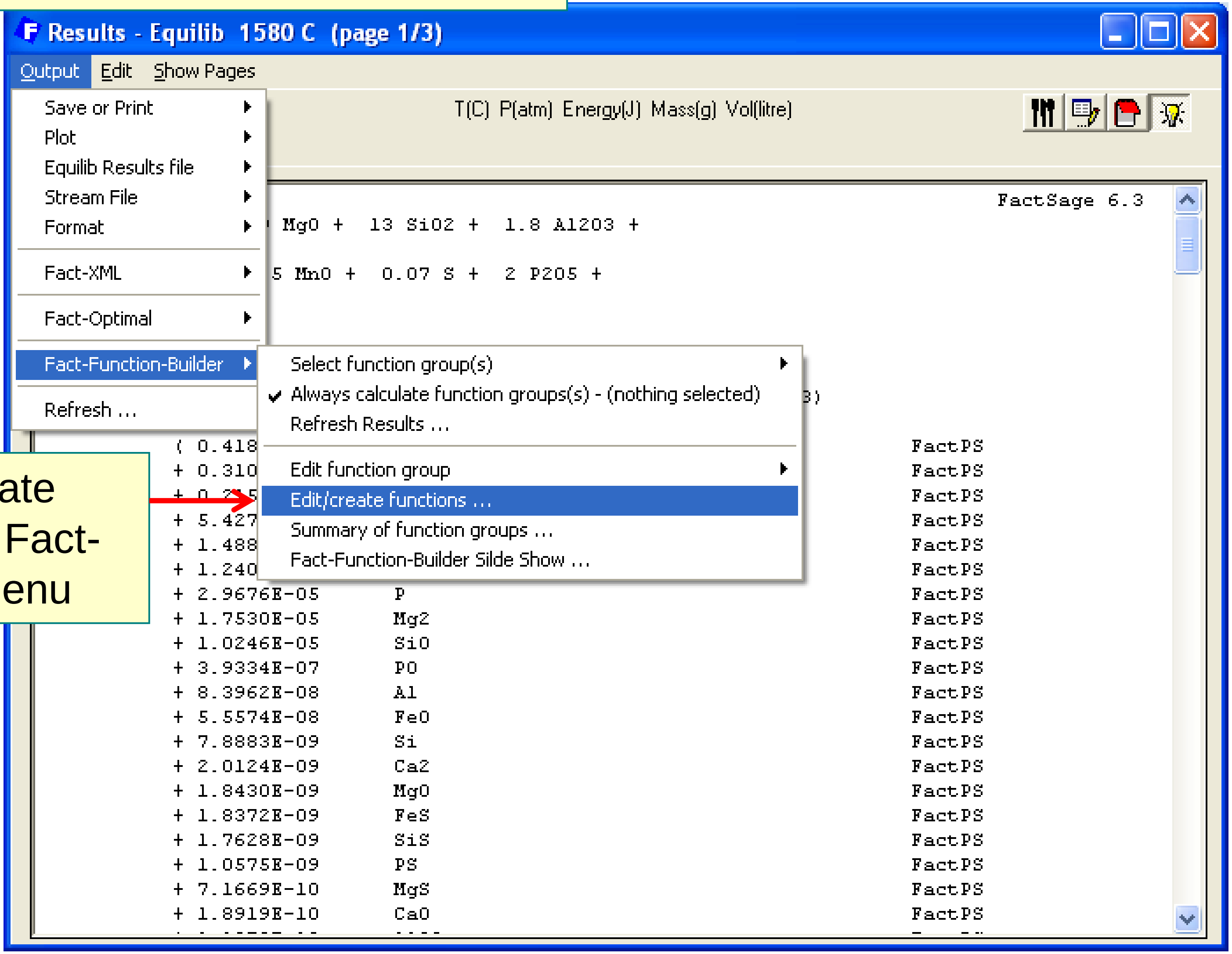
3. Calculate the sulphide capacity in a separate column.

4. Plot log(Cs) versus temperature



Calculating Slag Sulphide Capacity

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



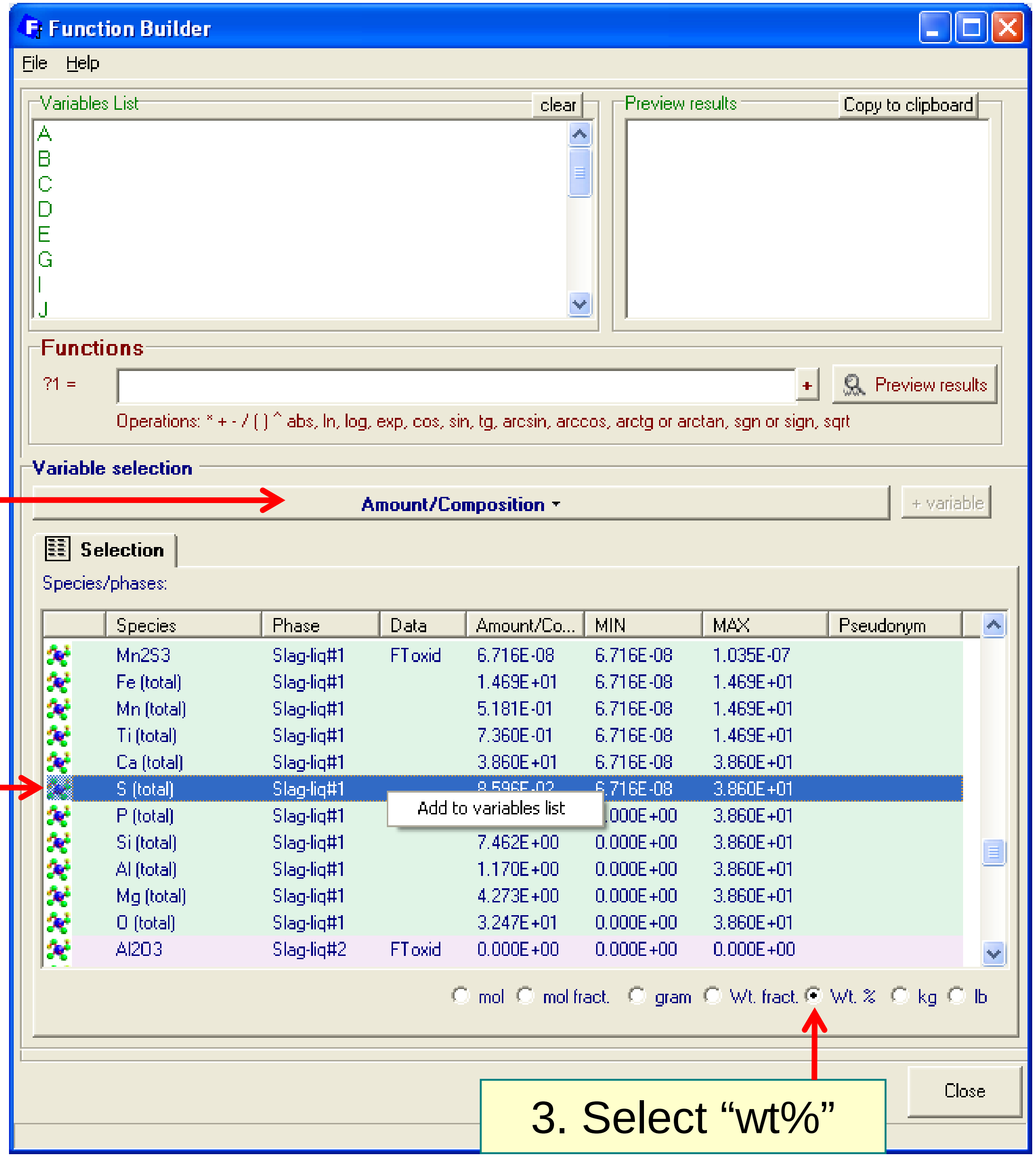
1. Press "Edit/Create functions" under the Fact-Function-Builder Menu

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



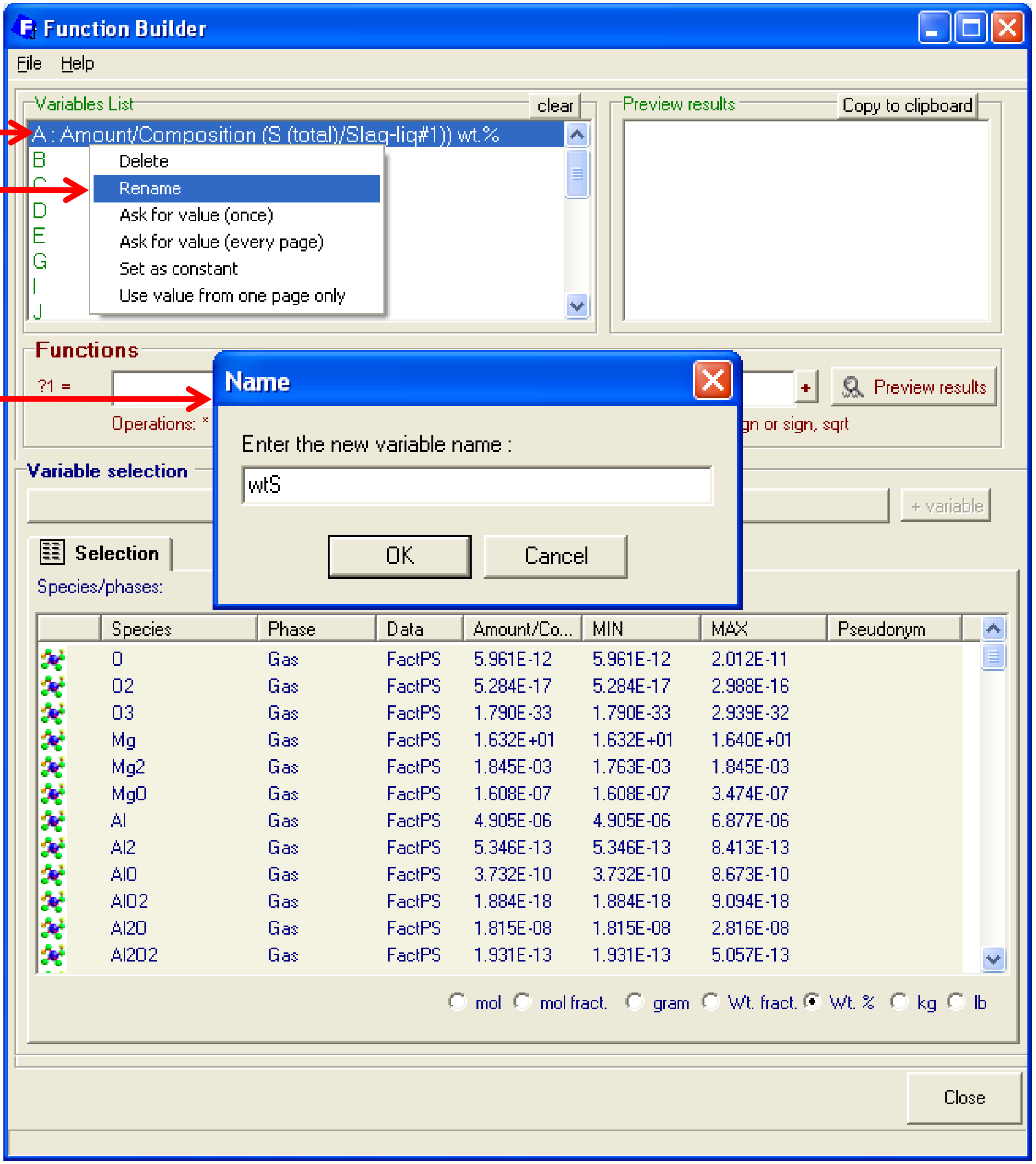
3. Select “wt%”

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 O_2 and S_2 in the gas as the two other variables.

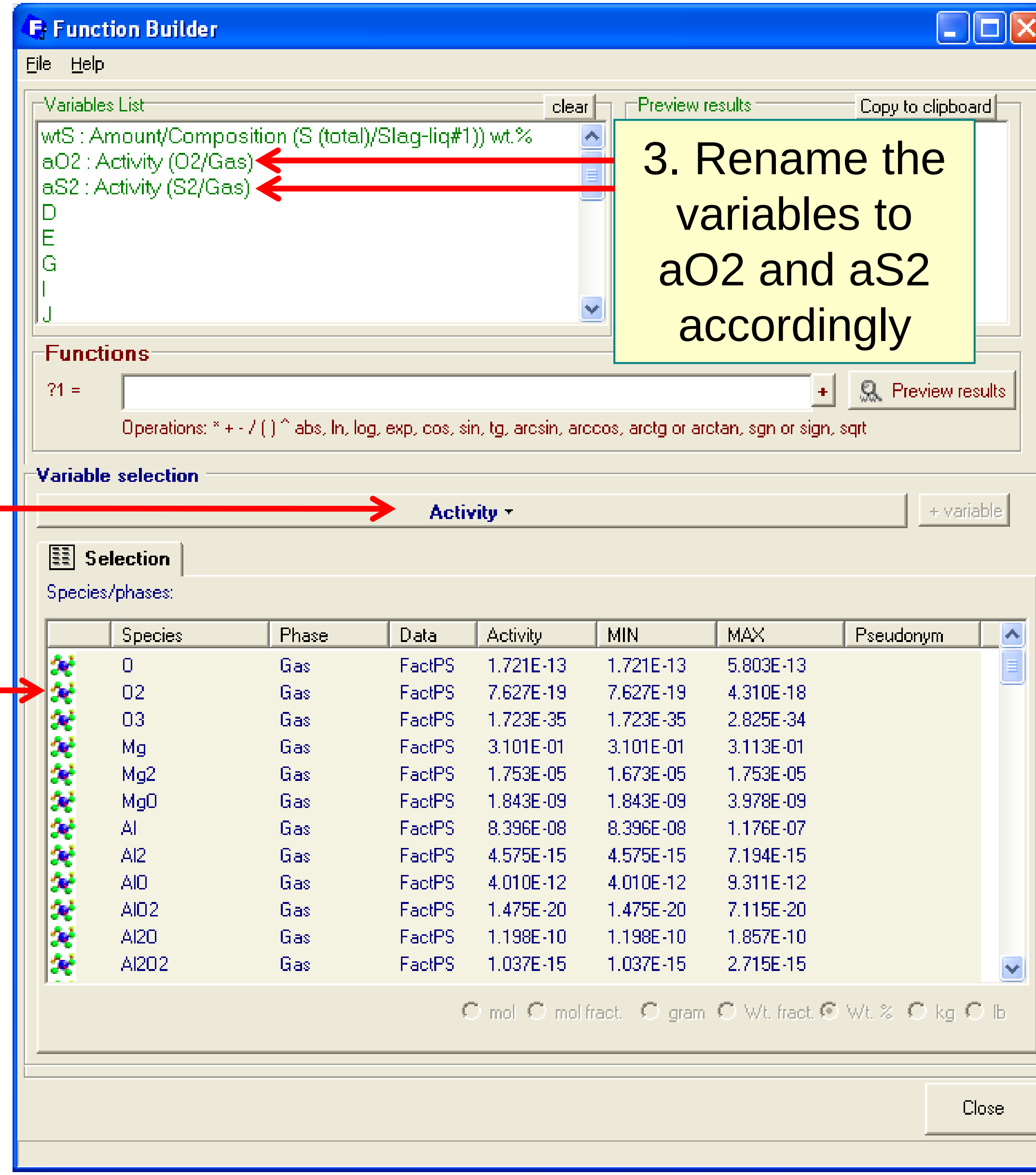


Calculating Slag Sulphide Capacity

1. Select “Activity” under “Variable Selection”

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

3. Rename the variables to aO2 and aS2 accordingly

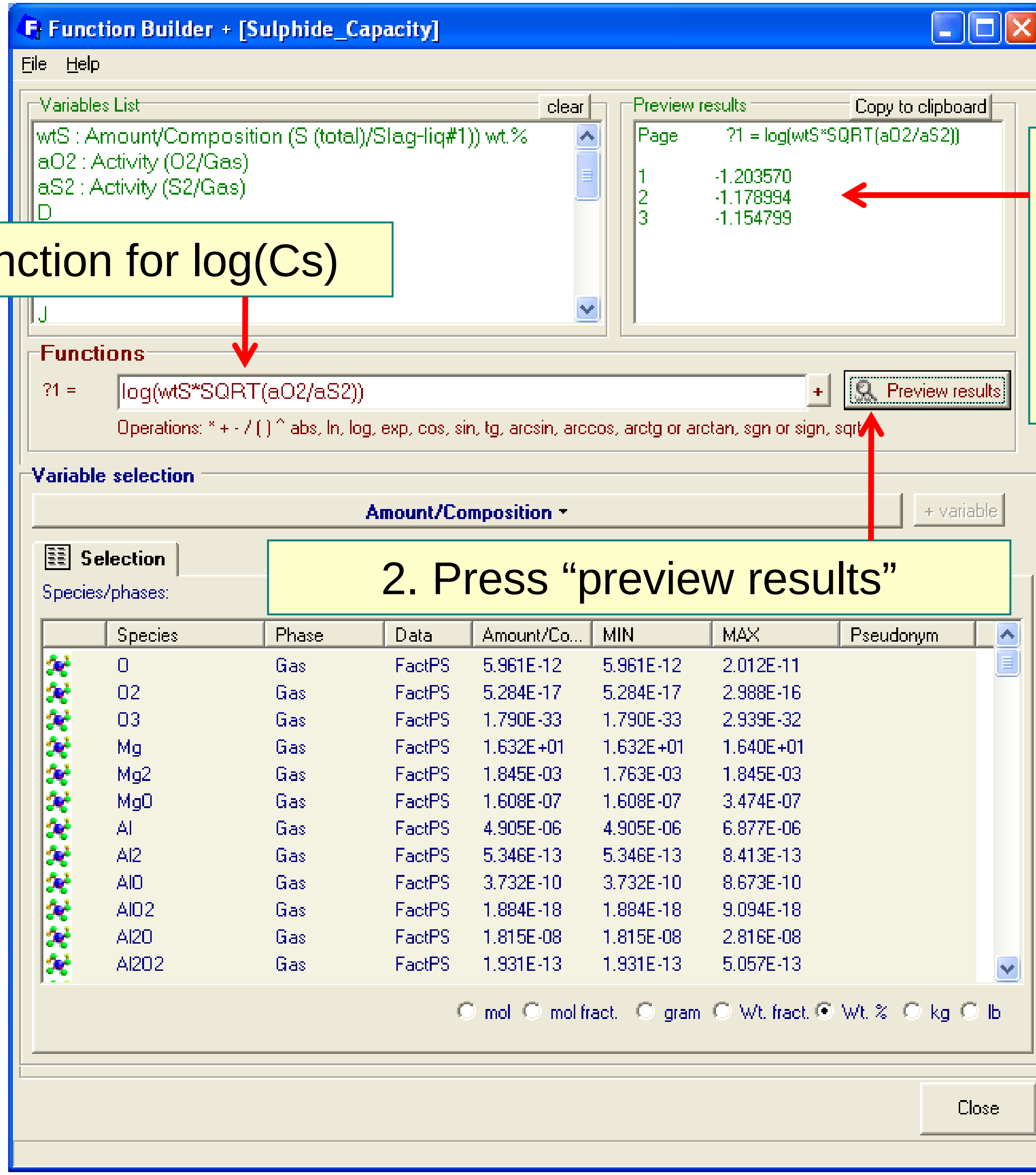


Calculating Slag Sulphide Capacity

1. Enter the function for log(Cs)

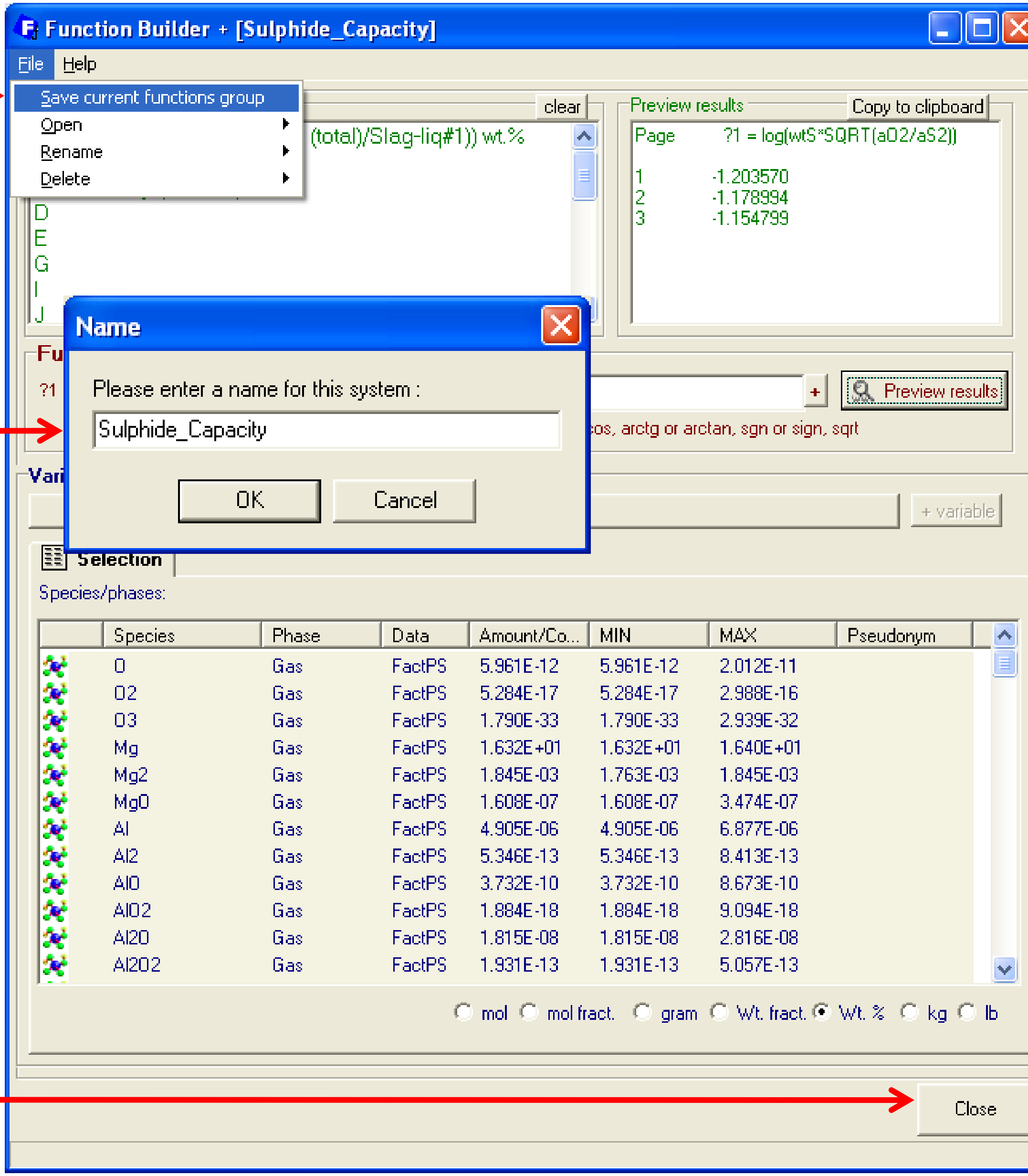
2. Press "preview results"

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



Calculating Slag Sulphide Capacity

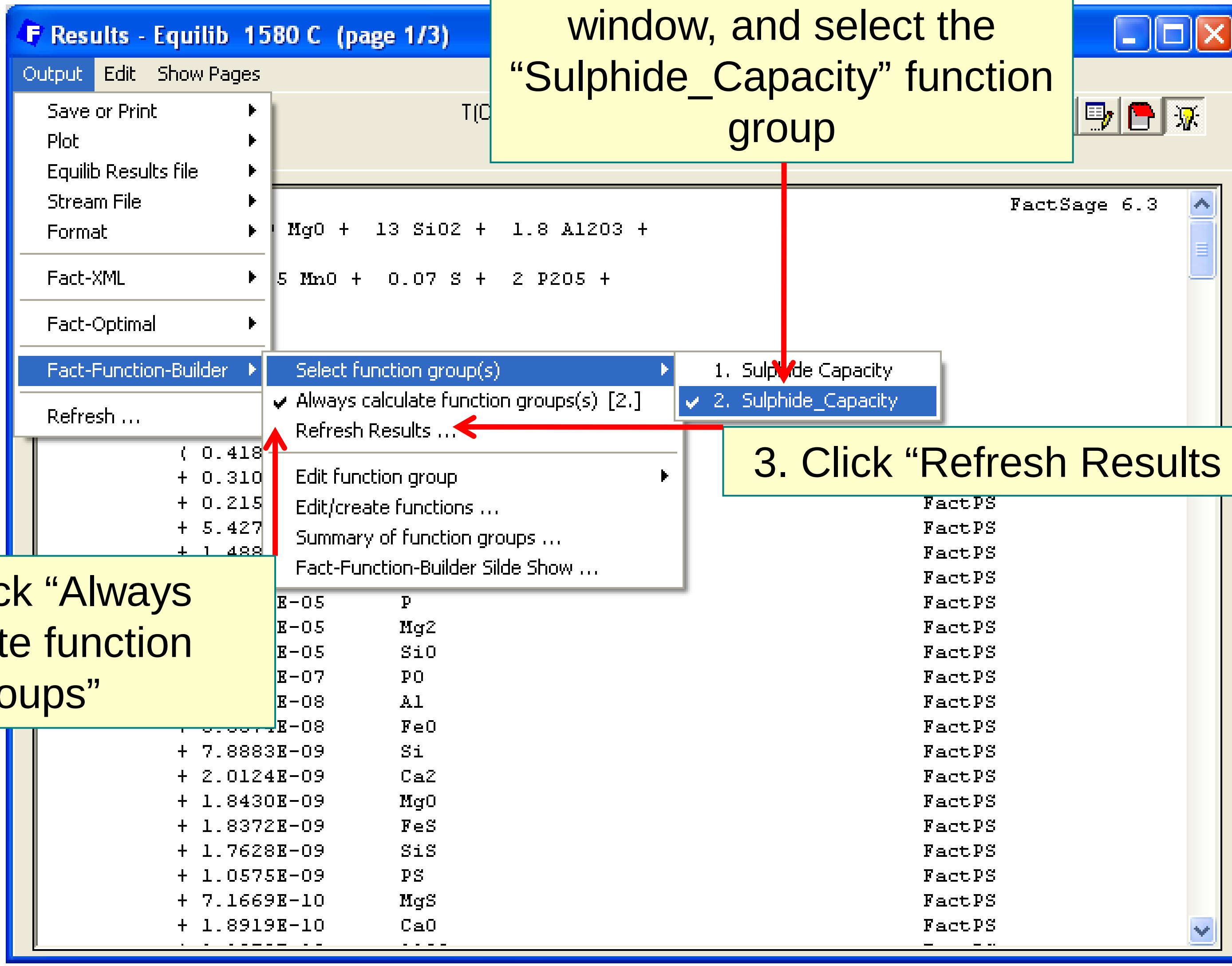
1. Save the function as "Sulphide_Capacity"



2. Close the window

Calculating Slag Sulphide Capacity

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

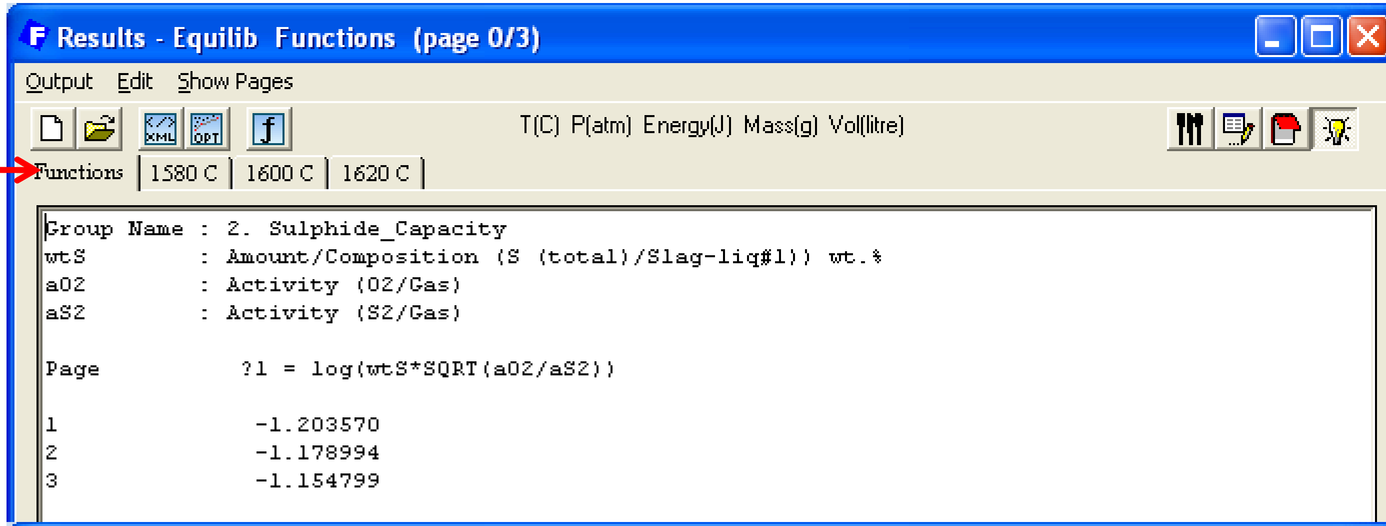


2. Check "Always calculate function groups"

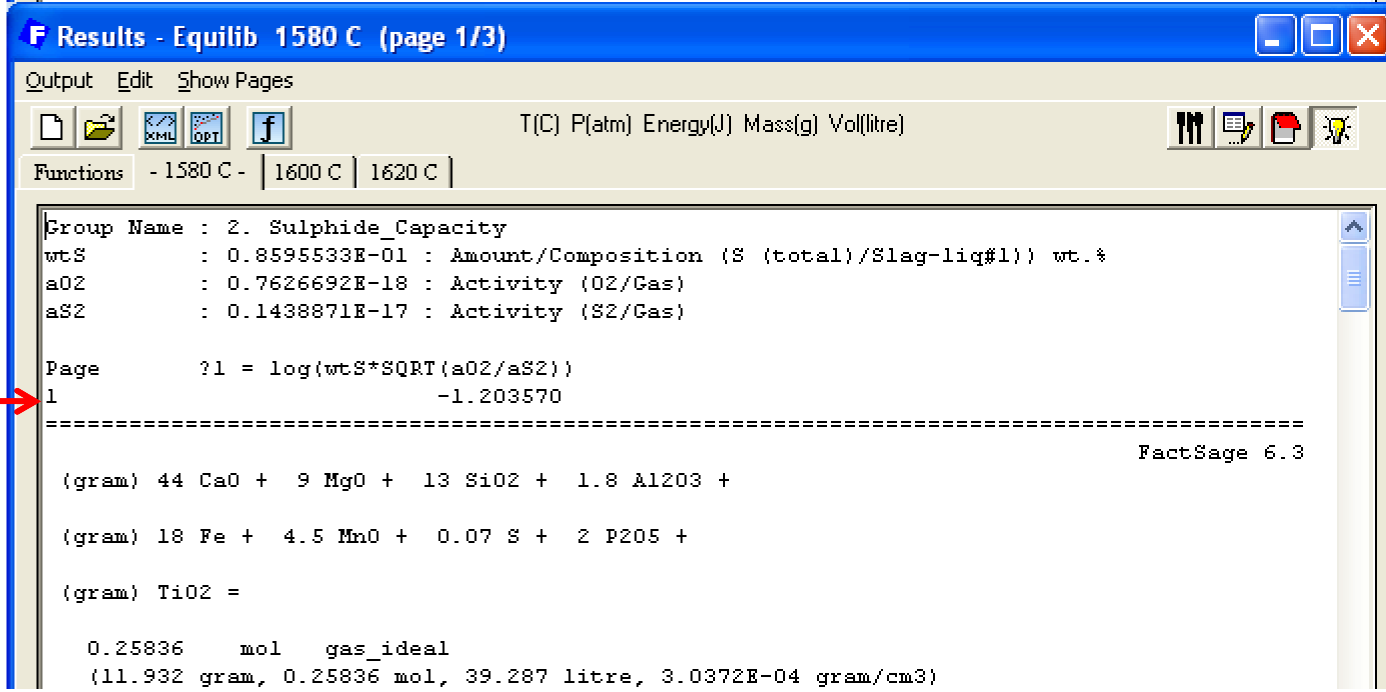
3. Click "Refresh Results …"

Calculating Slag Sulphide Capacity

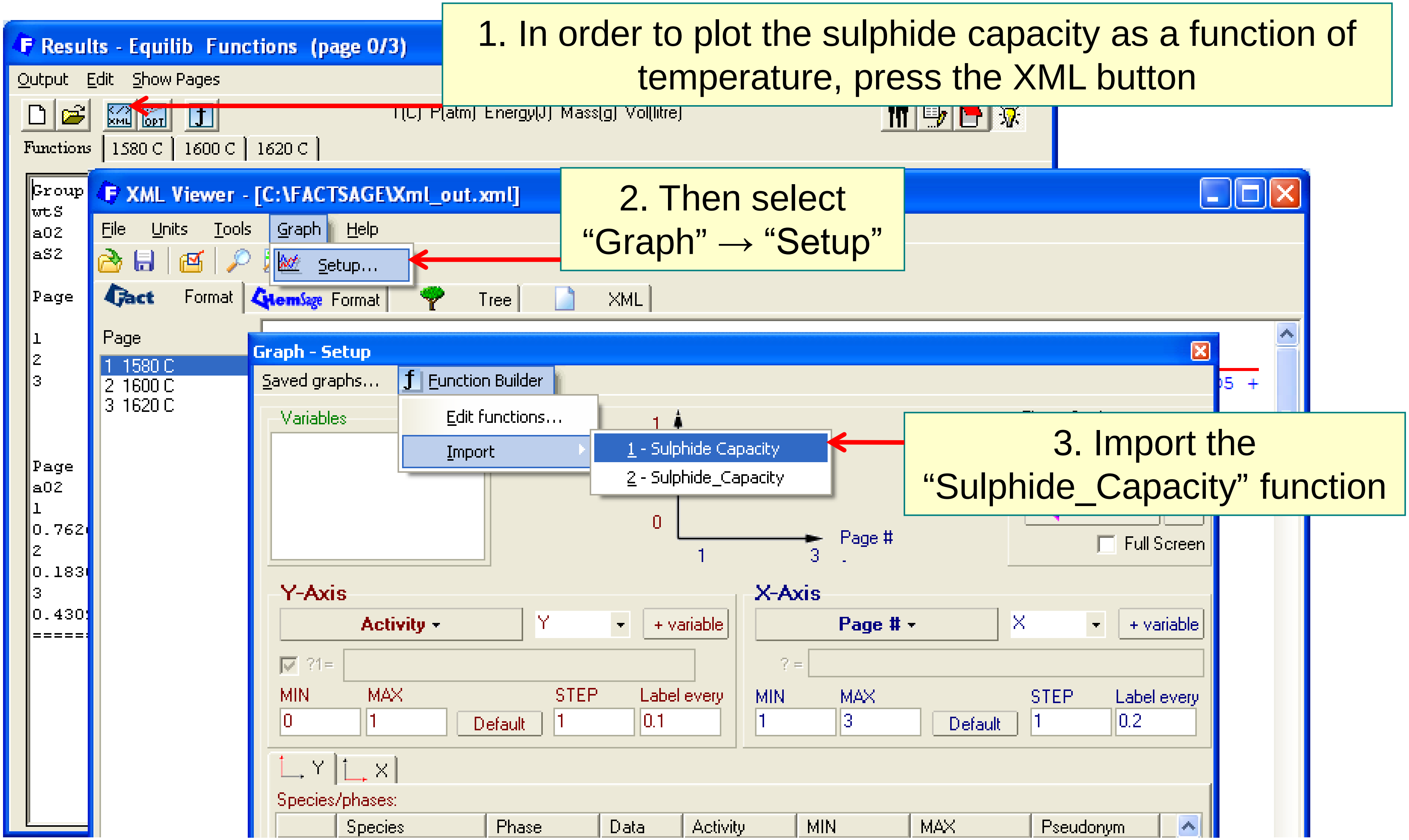
1. A separate "Functions" tab will appear with the results of the calculations



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



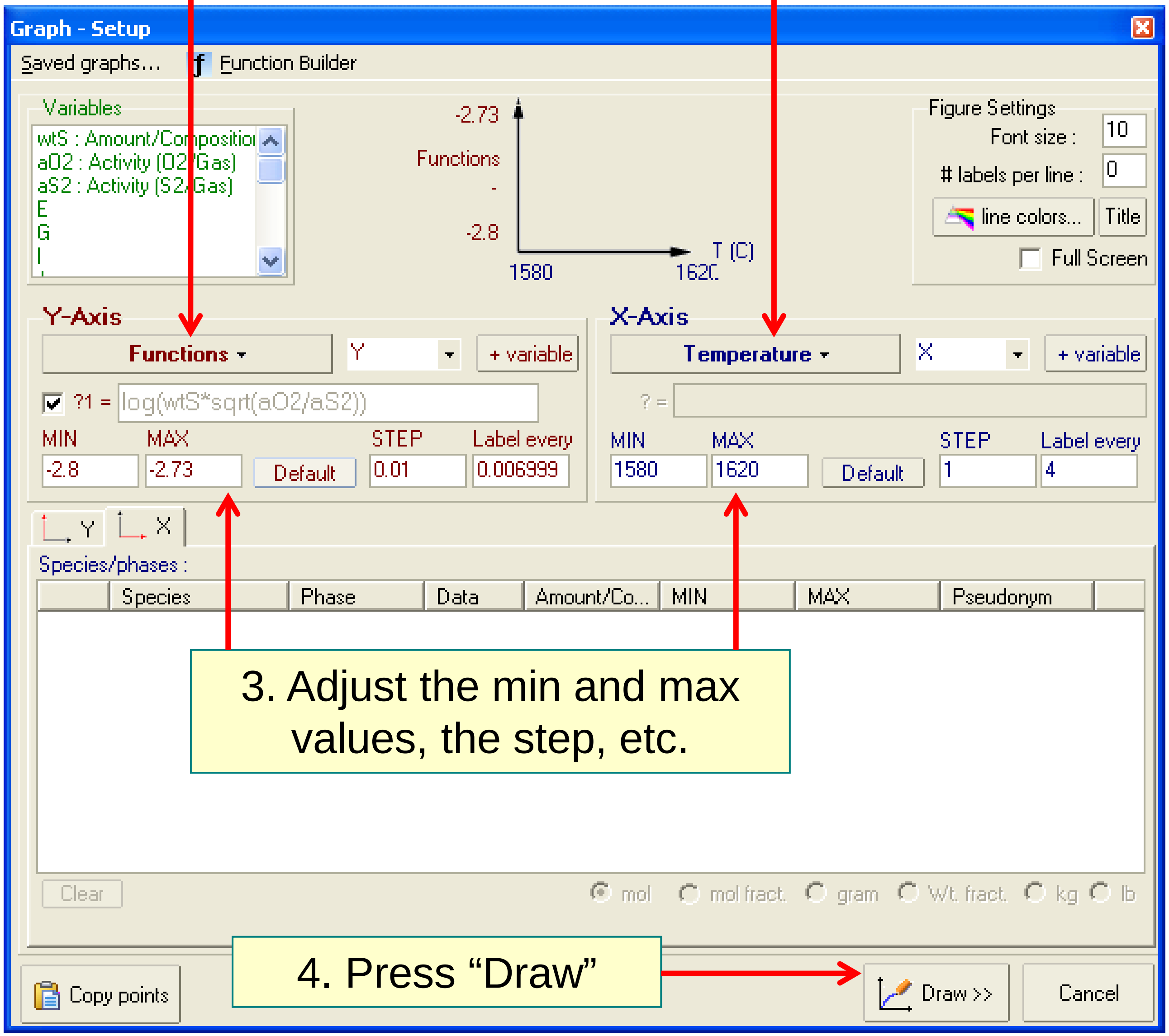
Calculating Slag Sulphide Capacity



Calculating Slag Sulphide Capacity

1. Select "Functions" as the Y-Axis

2. Select "Temperature" as the X-axis

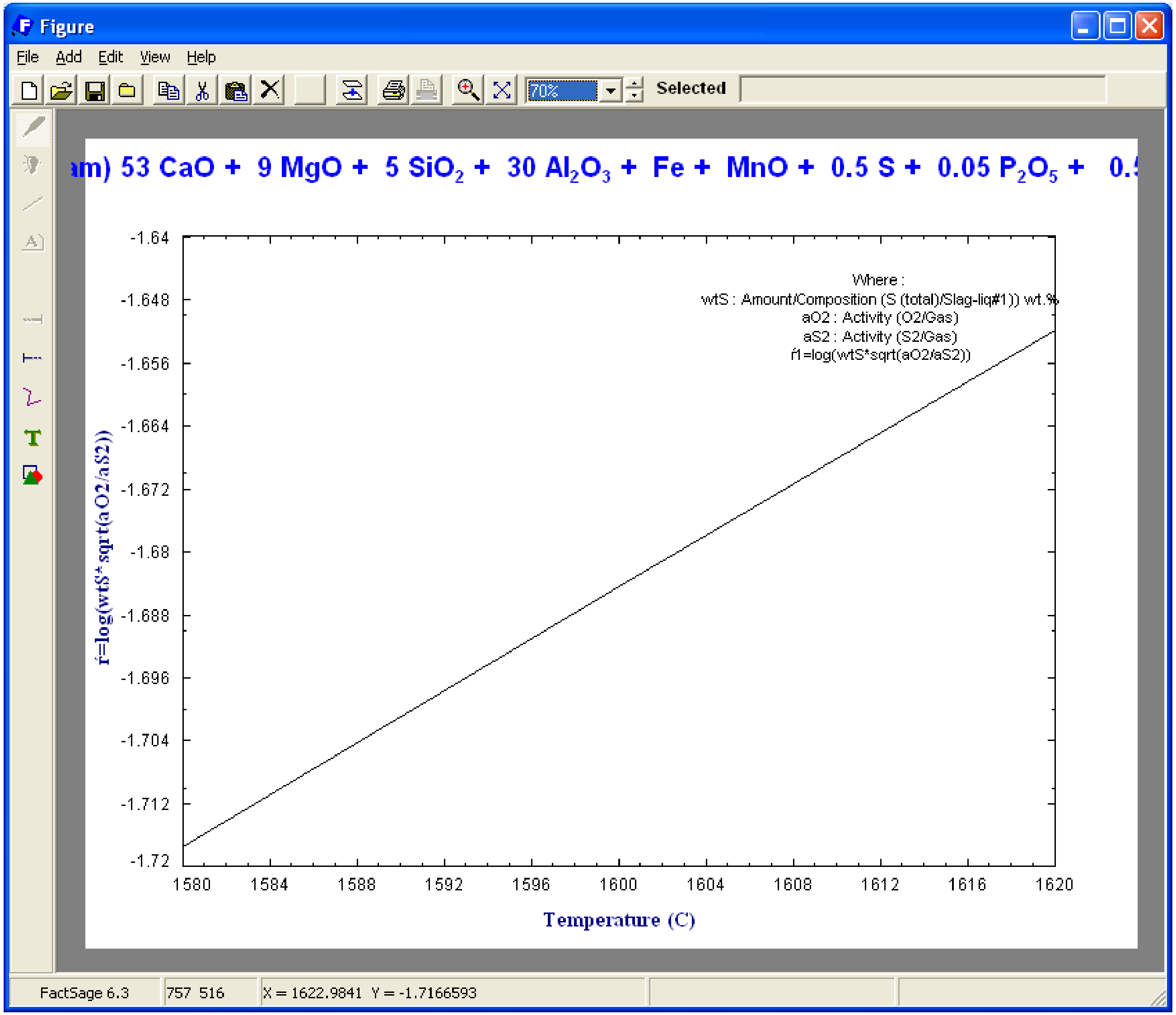


3. Adjust the min and max values, the step, etc.

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.