Fact-Function-Builder

Manipulating the ***Equilib*** results

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Introduction - **Fact-Function-Builder**

Fact-Function-Builder is an add-in to the ***Equilib*** program that employs the function builder algorithm of ***Fact-XML*** and enables you to calculate and display user-defined functions after each ***Equilib*** calculation.

The functions can contain expressions using values employed or calculated by ***Equilib***. These include temperature, pressure, volume and thermochemical variables such as compound, solution and species activities, amounts, fractions, partial or integral properties, etc. The functions can include the common mathematic operators * + - / () ^ abs, ln, log, exp, cos, sin, etc. as well as other functions – see ***Example 1: Sievert's Law***.

After an ***Equilib*** calculation you can also import the calculated functions into ***Fact-XML*** and manipulate the values in other ways such as create graphs – see ***Example 2: Plotting slag sulfide capacity***.

Example 1 - **Sievert's Law**

We will use a simple example to demonstrate the basic principles of the **Fact-Function-Builder**. Let us examine the dissolution of N_2(gas) in Fe(liquid) at elevated temperatures:

$$\tfrac{1}{2}\, N_2(g) \quad = \quad \underline{N}(\%\text{ in Fe-liq})$$

The Wt.% solubility of nitrogen in the steel may be represented by **Sievert's Law**:

$$\%N \quad = \quad S.p(N_2)^{1/2}$$

where **S**, Sievert's parameter, is constant at a given temperature and moderate pressure $p(N_2)$. We will use the **Fact-Function-Builder** to calculate **S**.

Setting up the example involves 3 steps:

Step 1: Calculating the equilibrium using **Equilib**.

Step 2: Defining the functions using the **Fact-Function-Builder**.

Step 3: Displaying the calculated functions in the **Results Window**.

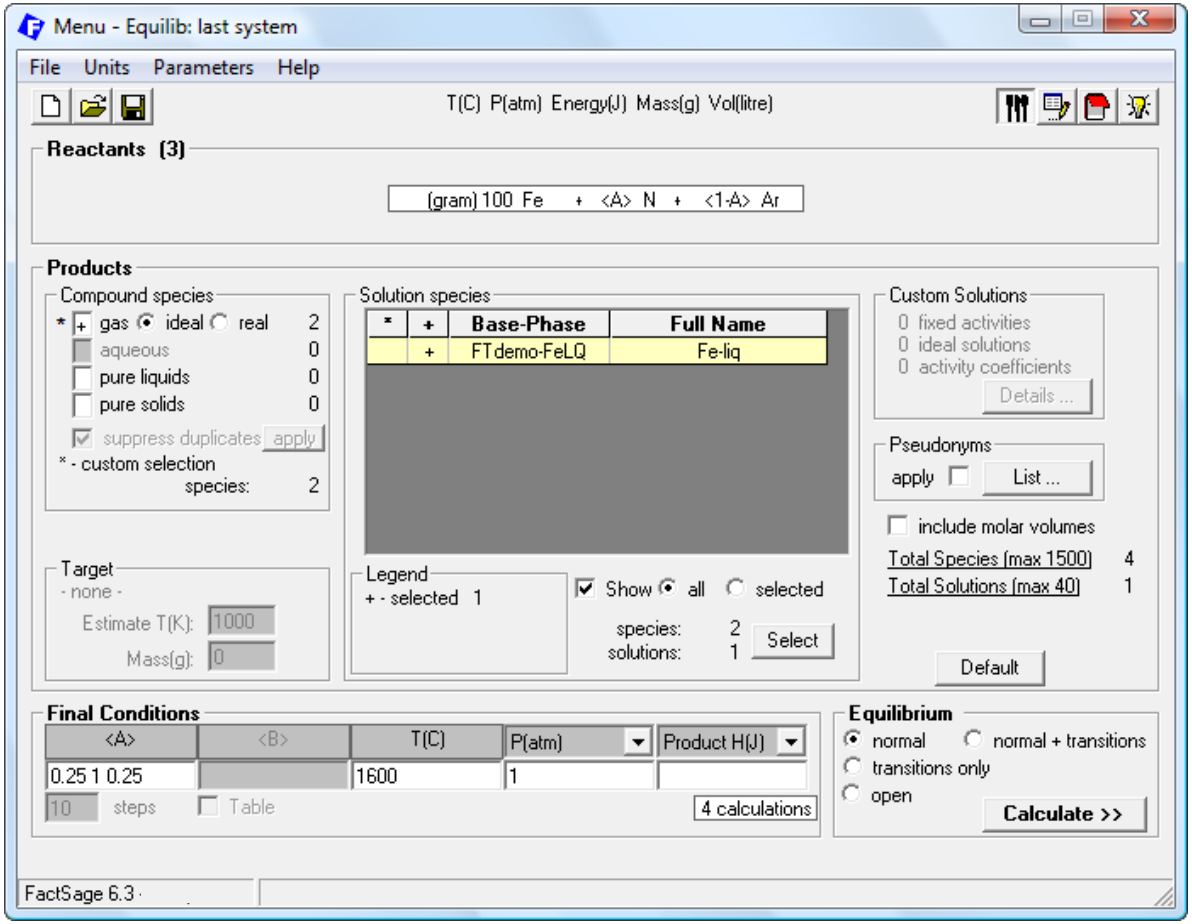
Step 1: *Equilib* input

The reaction is based on **(gram) 100 Fe + <A> N + <1-A> Ar** at 1600°C and 1 atm.

Argon stablizes the gas phase so that $p(N_2)$ is calculated

For simplicity only 2 species are selected in the gas phase : **N_2(g), Ar(g)**

The liquid steel phase is **FeLQ** taken from the **FTdemo** database. This is fine for demonstration purposes but for precise calculations you should use the **FSstel** database.



4 pages of results will be calculated with <A> = 0.25, 0.5, 0.75 and 1

Step 1: *Equilib* output

The **Results Window** contains 4 pages generated at 1600°C and 1 atm with <A> = 0.25, 0.5, 0.75 and 1.

Here the results at page 4 (<A> = 1) show the solubility is 0.046847 wt.% N and $p(N_2)$ = 1 atm.

S = %N / $p(N_2)^{1/2}$

= 0.046847

Results - Equilib A=1 (page 4/4)

Output Edit Show Pages

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

A=0.25 | A=0.5 | A=0.75 | - A=1 -

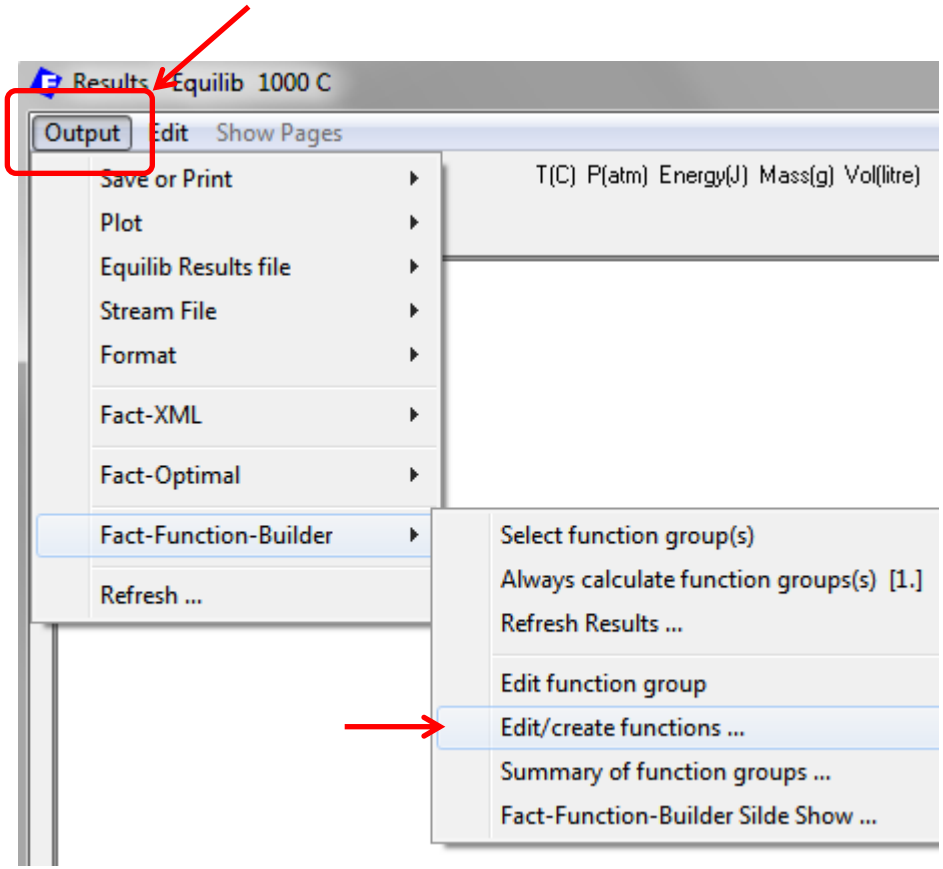
```
(gram) 100 Fe +  <A> N +  <1-A> Ar =

  3.4024E-02 mol   gas_ideal
  (0.95313 gram, 3.4024E-02 mol, 5.2297 litre, 1.8225E-04 gram/cm3)
          (1600 C, 1 atm,     a=1.0000)
          ( 1.0000          N2)

+ 100.05     gram  Fe-liq
  (100.05 gram, 1.7940 mol)
          (1600 C, 1 atm,     a=1.0000)
          ( 99.953     wt.% Fe
          + 4.6847E-02 wt.% N)

          System component       Mole fraction  Mass fraction
          Fe                       0.99813        0.99953
          N                        1.8652E-03     4.6847E-04

where "A" on the reactant side is 1
```

The **Fact-Function-Builder** will now be employed to automatically calculate the function ***f*1 = S.** In addition a second function will be calculated: ***f*2 = *f*1 – *f*1(page 1)** where ***f*2** is the difference between ***f*1** at the page of interest and ***f*1** at **page 1**.

Step 2: Open the **Fact-Function-Builder**

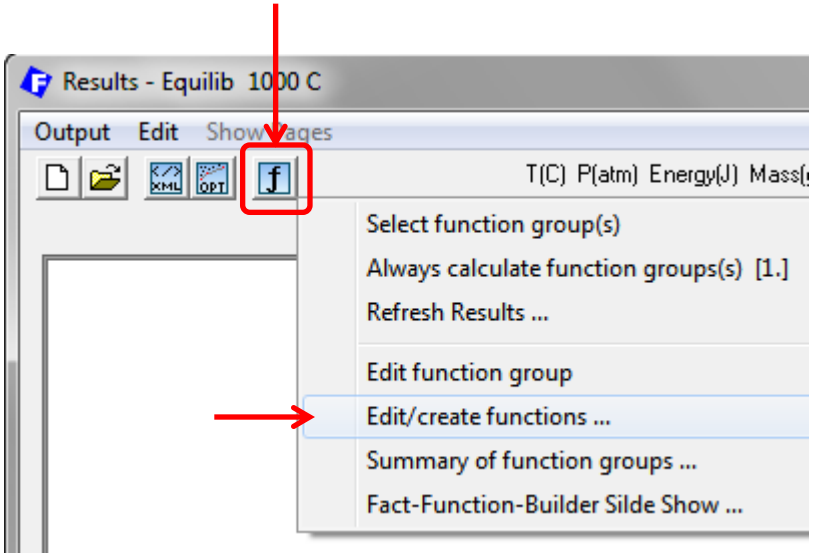
You access the **Fact-Function-Builder** by clicking on *'Edit/create functions …'*

via the *Output menu*



<u>or</u>

via the **Function** button

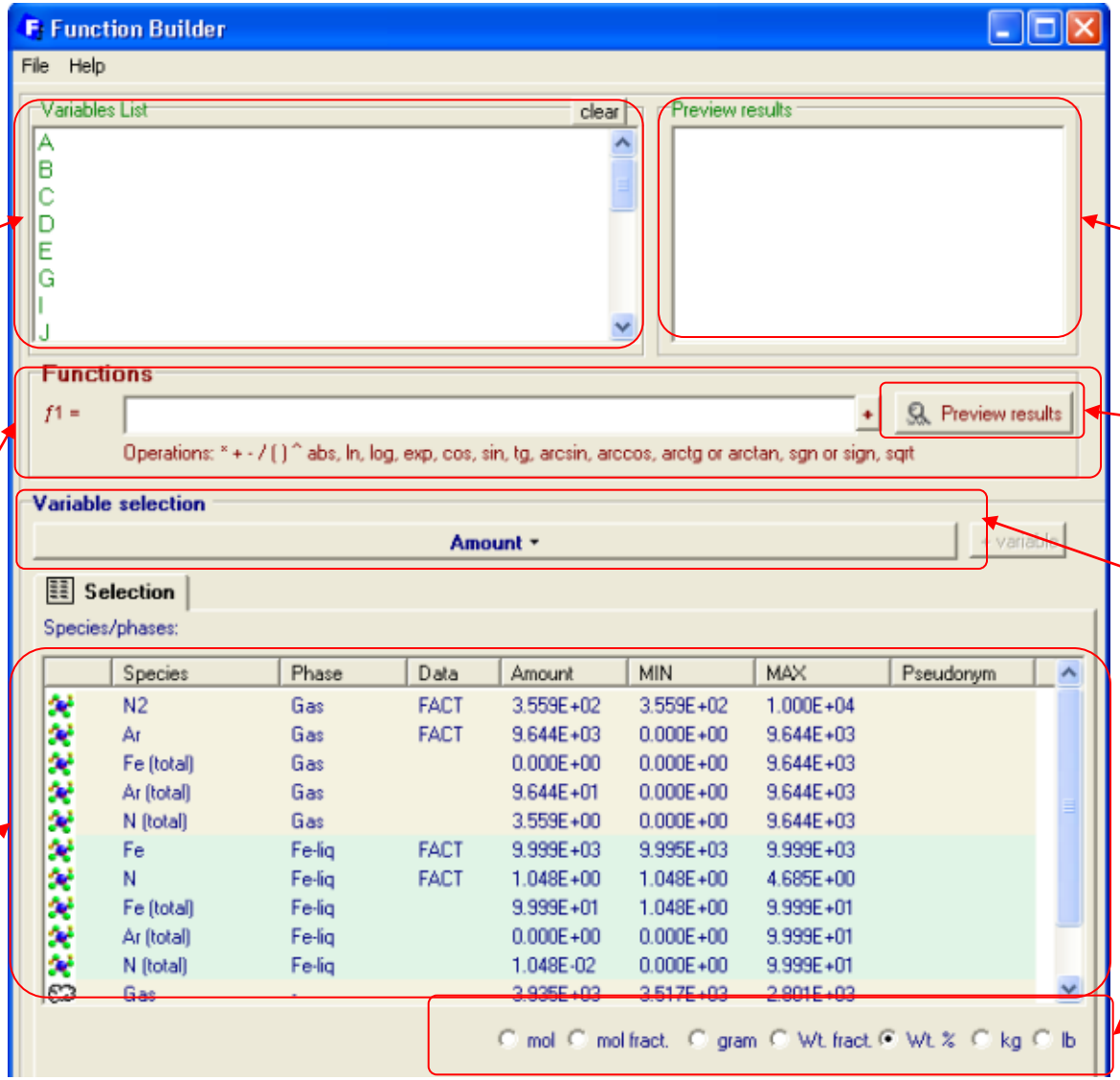


Step 2: **Function Builder** Dialog Box

Variables list display

Functions frame

Variables selection panel – the view differs with the variable selected



Preview results display

Preview results button

Variable selection button

Composition units

Step 2: Define the variable **WtPctN**

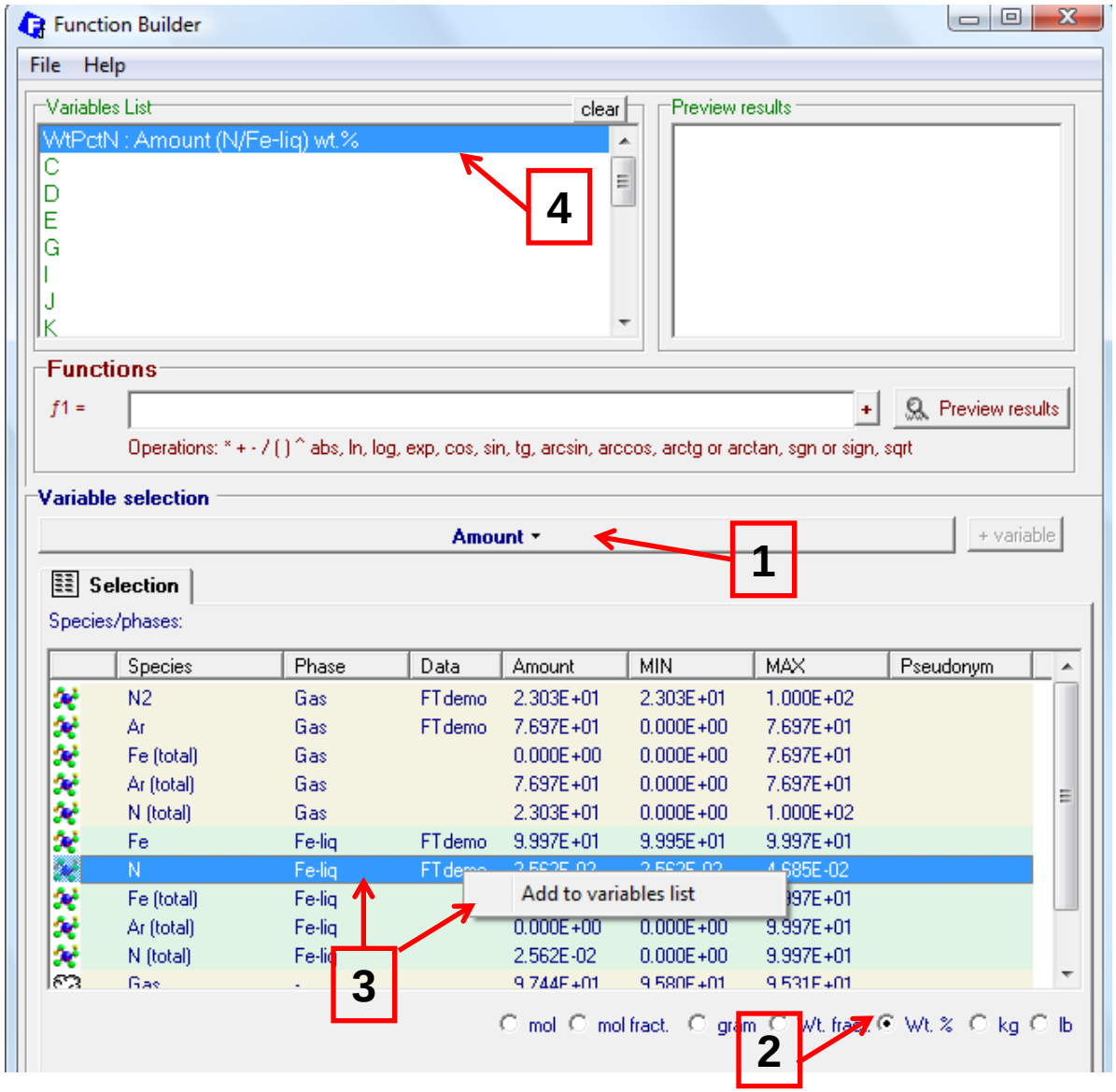
Defining the variable **WtPctN**, the Wt.% of N in Fe-liq:

1. Click the **Variable selection** button and select **Amount/Composition** .

2. Select the units of **Composition** – **Wt.%** .

3. In the **Variables** panel *mouse-right-click* on **N / Fe-liq** and click on *'Add to variables list'* .

4. In the **Variables list** display *mouse-right-click* on **N/Fe-liq** and rename the variable as **WtPctN**. The name must be *alphanumeric* – that is, it starts with a letter and contains only letters and numbers.



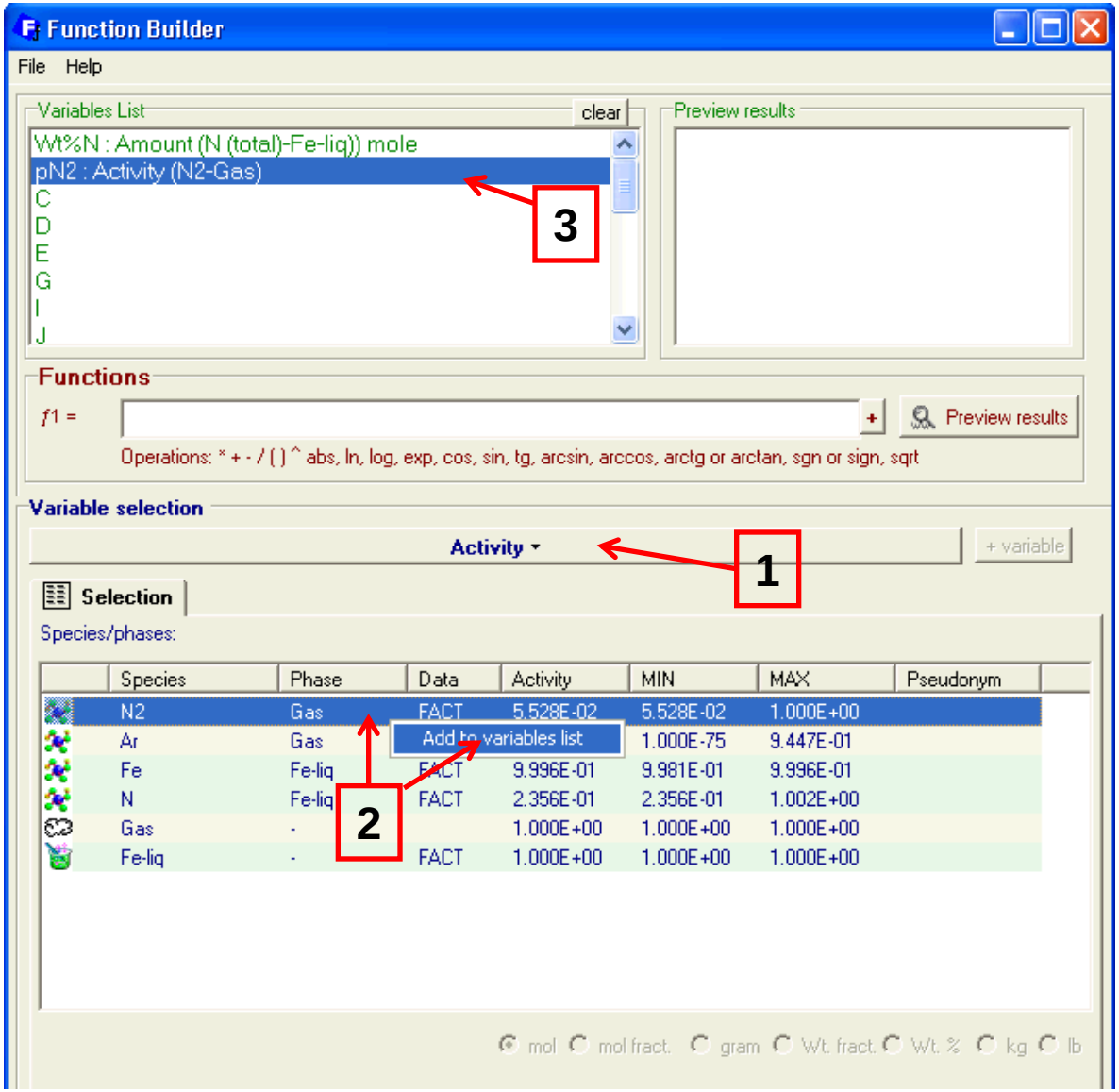
Step 2: Define the variable **pN2**

Defining the variable **pN2**, the pressure of N_2(g):

1. Click the **Variable selection** button and select **Activity**.

2. In the **Variables** panel *mouse-right-click* on **N2 / Gas** and click on *'Add to variables list'* .

3. In the **Variables list** display *mouse-right-click* on **Activity (N2-Gas)** rename the variable as **pN2** (*alphanumeric* variable).



Step 2: Define the functions – *f*1, *f*2

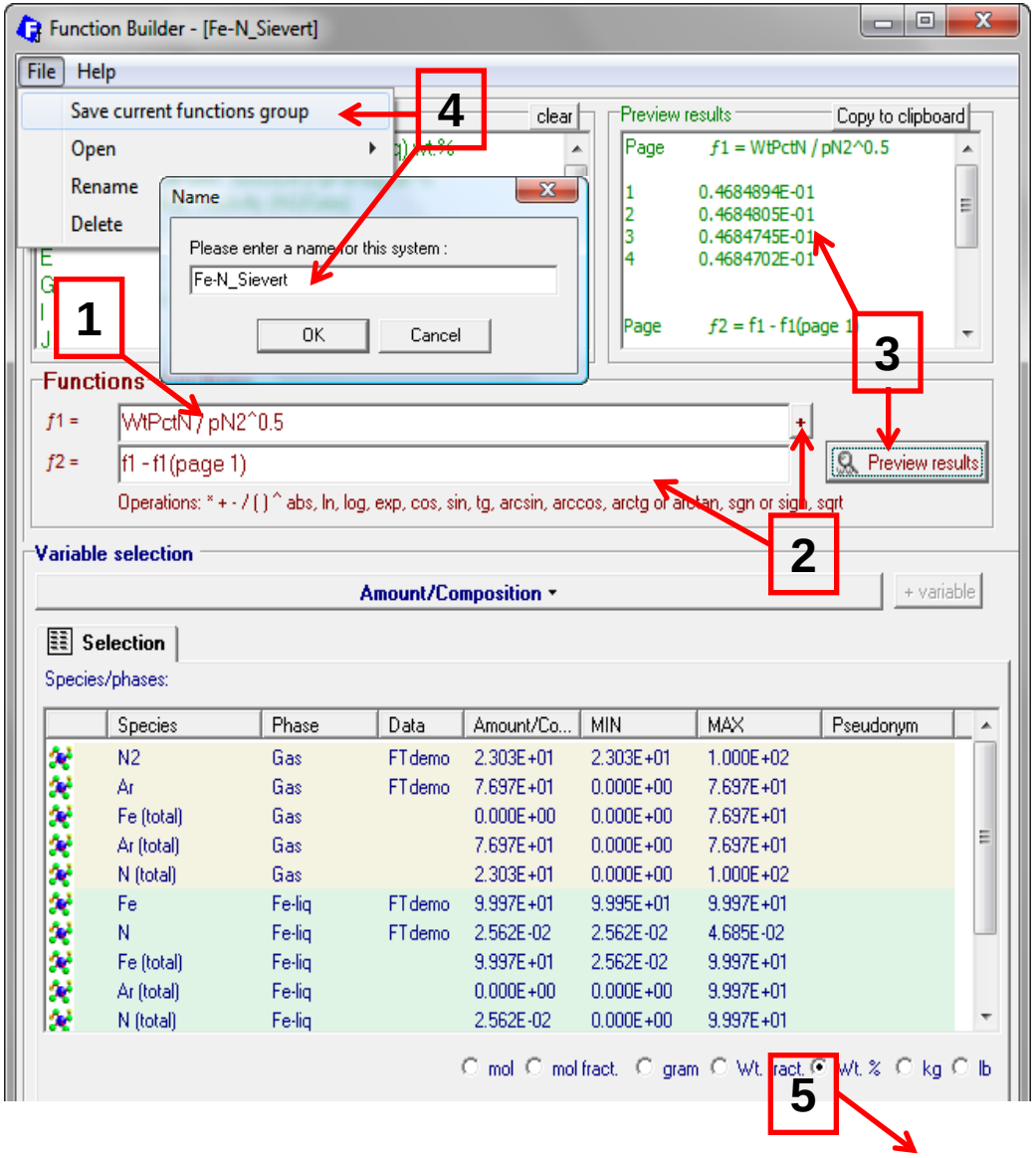
1. Define function: ***f*1 = %N / p(N_2)$^{1/2}$**
- in the **Functions *f*1** input box enter **WtPctN / pN2^0.5**.

2. Define function: ***f*2 = *f*1- *f*1(page 1)**
- click on **Functions '+'** button and in the ***f*2** input box enter ***f*1 – *f*1(page 1)** .

3. Verify the functions - click on **Functions Preview results** for calculated values shown in the **Preview results** display.

4. Save the functions group - click on menu ' File > Save current functions group …' and enter the name **Fe-N_Sievert**.

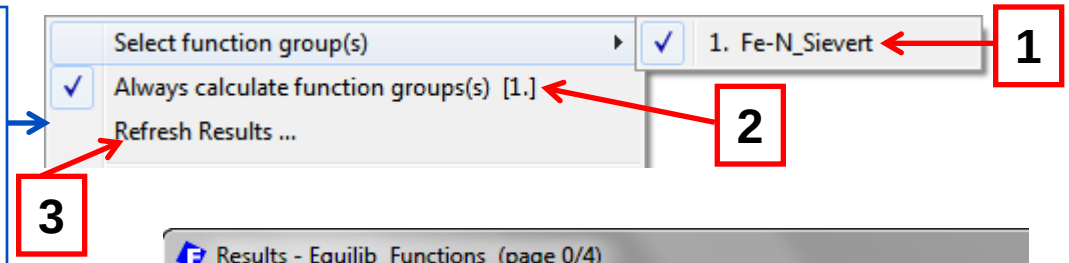
5. 'Close' – (not shown here) to return to the *Results Window*.



Step 3: Display *f*1, *f*2 for all pages

Open the **Fact-Function-Builder** Toolbox menu :

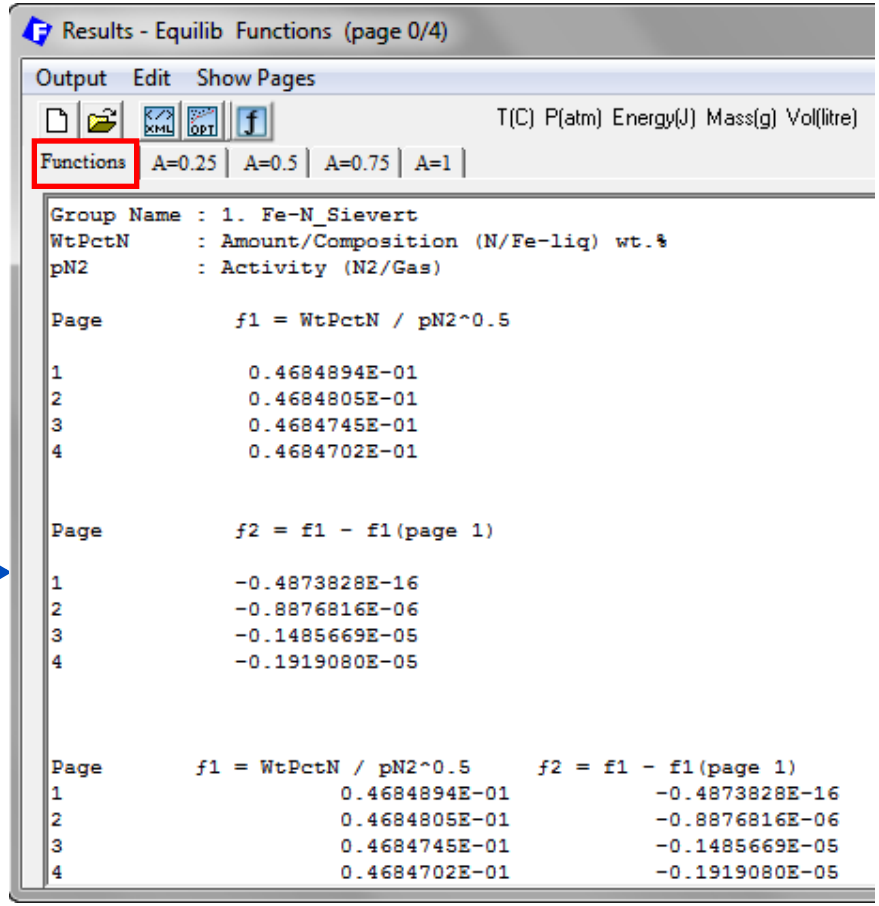
1. Click on '*Select function group(s) >* '
   Check √ **Fe-N_Sievert**
2. Check √ '*Always calculate function ...*'
3. Click on '*Refresh Results ....*'



After the results are refreshed the **"Functions" page** displays ***f*1** and ***f*2** for all the pages.

It is seen that ***f*1** is fairly constant and ***f*2** is close to zero for all pages – **Sievert's law** applies well in this example.

(Note the round off error – ***f*2** at Page 1 should be zero and not -0.487…E-16.)



Step 3: Display *f*1, *f*2 for each page

This slide displays the results in ***FACT Format***

The calculated functions are displayed at the top of each page.

Here page 2 shows :

<A> = 0.5

$P(N_2)$ = 0.56992 atm

N = 0.035367 Wt.%

***f*1 = 0.046848**

***f*2 = -0.887.. x 10^{-6}**

Results - Equilib A=0.5 (page 2/4)

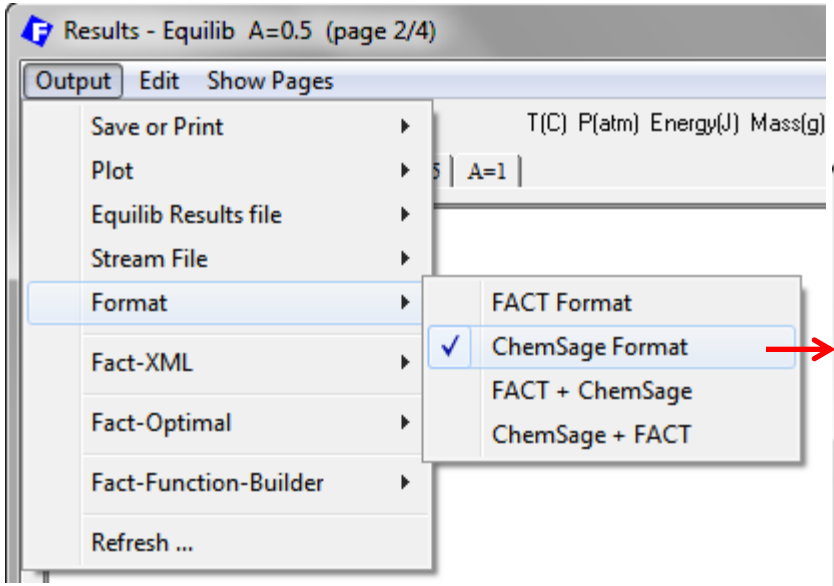
Output Edit Show Pages

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

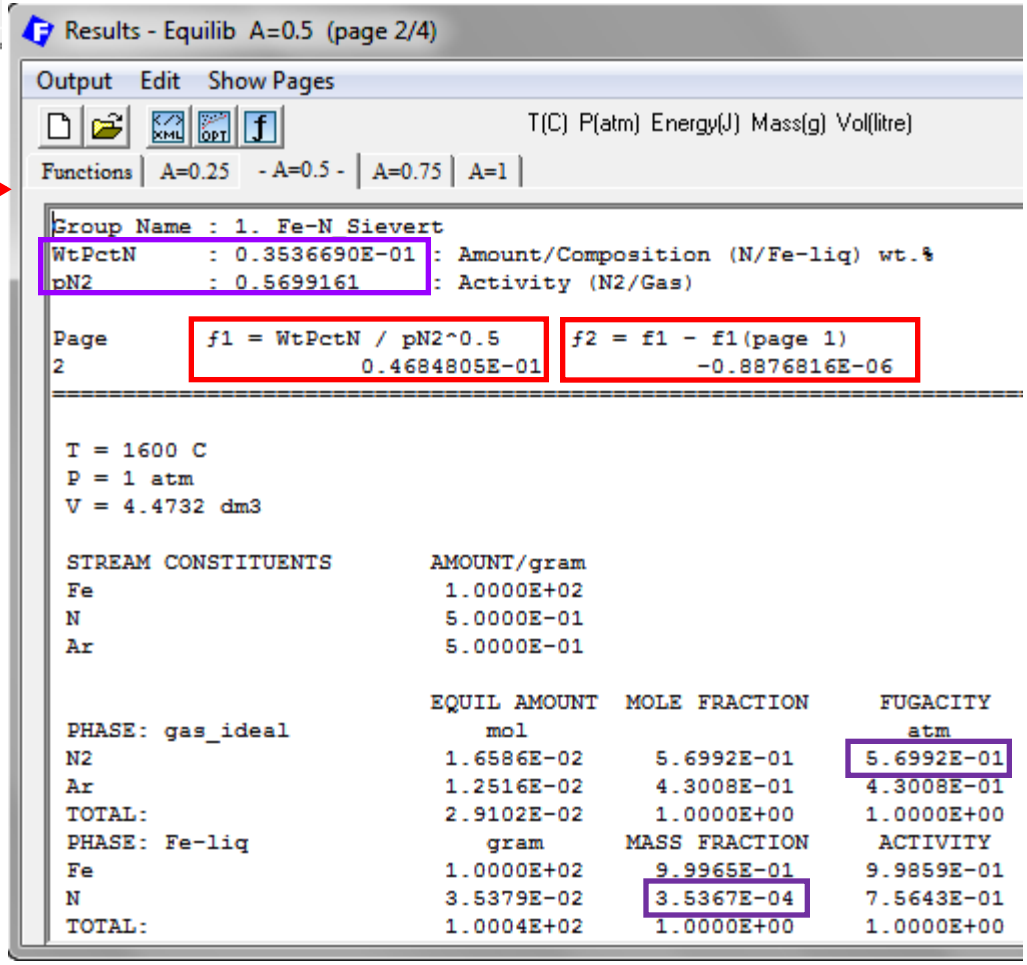
Functions | A=0.25 | - A=0.5 - | A=0.75 | A=1

```
Group Name : 1. Fe-N Sievert
WtPctN      : 0.3536690E-01 : Amount/Composition (N/Fe-liq) wt.%
pN2         : 0.5699161     : Activity (N2/Gas)

Page        f1 = WtPctN / pN2^0.5     f2 = f1 - f1(page 1)
2                     0.4684805E-01            -0.8876816E-06
==================================================================

 (gram) 100 Fe +  <A> N +  <1-A> Ar =

   2.9102E-02 mol   gas_ideal
   (0.96462 gram, 2.9102E-02 mol, 4.4732 litre, 2.1565E-04 gram/cm3)
            (1600 C, 1 atm,     a=1.0000)
            ( 0.56992          N2
            + 0.43008          Ar)

 + 100.04     gram  Fe-liq
   (100.04 gram, 1.7932 mol)
            (1600 C, 1 atm,     a=1.0000)
            ( 99.965     wt.% Fe
            + 3.5367E-02 wt.% N)

            System component       Mole fraction  Mass fraction
            Fe                       0.99859        0.99965
            N                        1.4086E-03     3.5367E-04

 where "A" on the reactant side is 0.50000
```

Step 3: Display *f*1, *f*2 for each page



This slide displays the same results in ***ChemSage Format***.



<u>Note</u>: the special function ***f*i(page n)** - e.g. ***f*1(page 1)** - that enables you to refer to the value of a function calculated on another page.

***f*i(page n)** is ***f*i** on page n
***f*i(page+1)** is ***f*i** on the next page
***f*i(page-1)** is ***f*i** on the previous page

Example 2 – **Plotting slag sulfide capacity**

This example shows how calculated functions can be plotted by **Fact-XML**. The sulfide capacity of a slag may defined as:

$$Cs = (wt\ S)\ \ x\ (Po_2/Ps_2)^{1/2}$$

where **wt S** is the Wt.% solubility of sulfur in the slag, and Po_2 and Ps_2 are the equilibrium partial pressures of $O_2(g)$ and $S_2(g)$.

In this example **wt S** is calculated across the SiO_2 – MnO binary system at 1650°C with the partial pressures fixed at $Po_2 = 10^{-10}$ and $Ps_2 = 10^{-6}$ bar. The sulfide capacity of a slag **Cs** is calculated using the **Fact-Function-Builder.** The results are then imported and plotted by **Fact-XML**. The example involves 4 steps:

Step 1: Calculating the equilibrium using **Equilib**

Step 2: Defining the sulfide capacity using the **Fact-Function-Builder**

Step 3: Displaying the sulfide capacity in the **Results Window**

Step 4: Plotting the sulfide capacity in **Fact-XML**.

Step 1: *Equilib* input

The reaction is based on **<1-A> SiO2 + <A> MnO + 0 S** at 1650°C and 1 bar.

Sulfur is present but the amount is not defined – it will be calculated.

There are 2 species selected in the gas phase :

S_2(g), O_2(g)

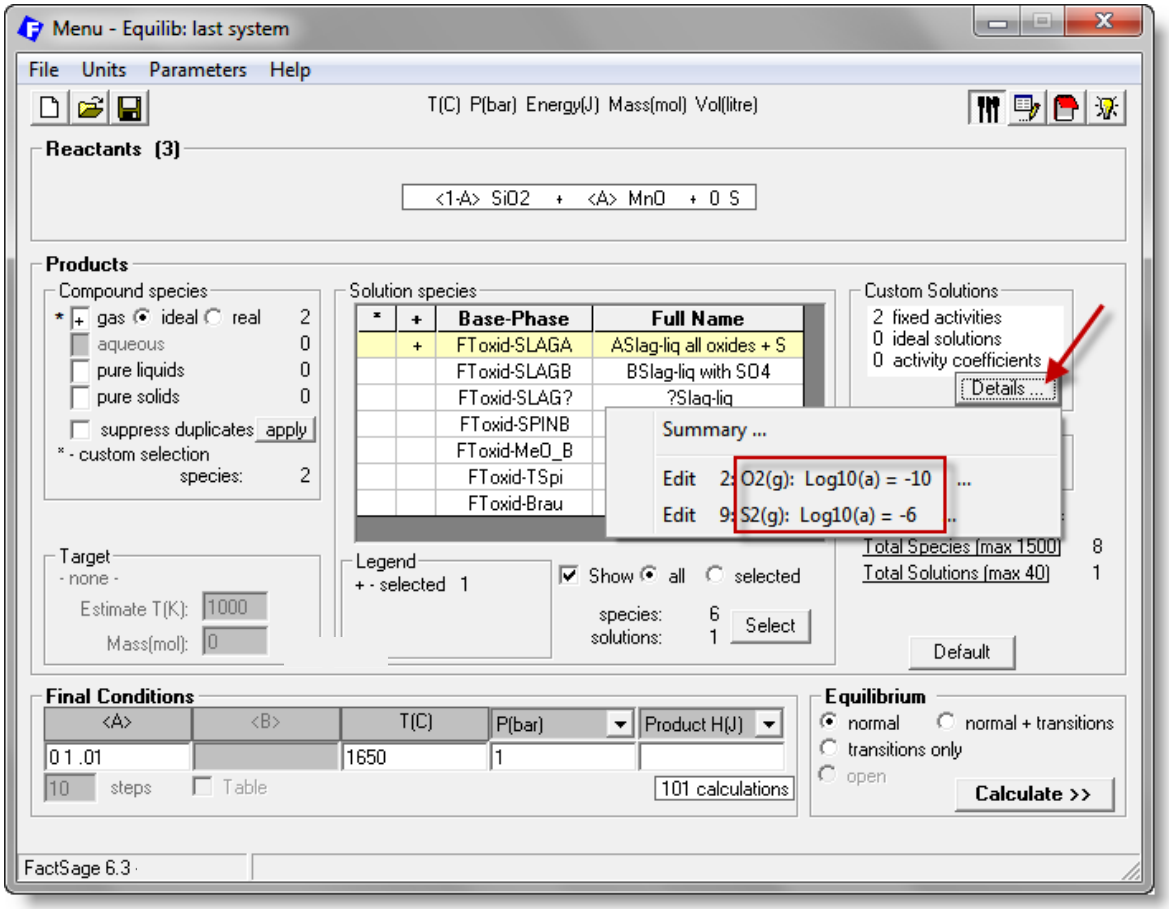
and their equilibrium partial pressures are fixed:

log(Po_2) = -10

log(Ps_2) = -6

- how this is done is shown in the slide <u>on the next page</u>.

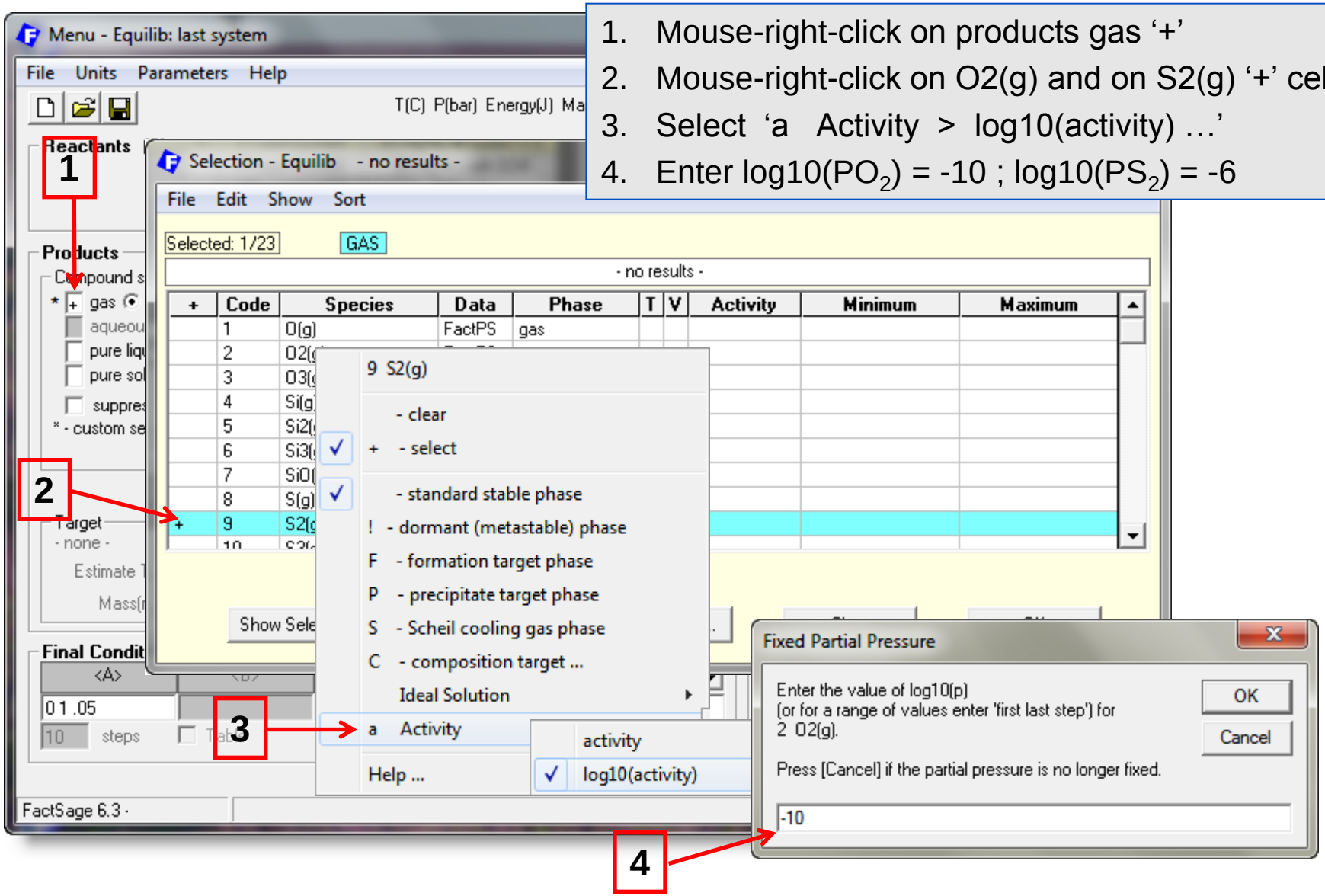
The liquid oxide slag phase is **SLAGA** taken from the **FToxid** database.



101 pages of results will be calculated with <A> = 0, 0.01, 0.02. …1.

Step 1: Defining ***Equilib*** $P(O_2)$ and $P(S_2)$

1. Mouse-right-click on products gas '+'
2. Mouse-right-click on O2(g) and on S2(g) '+' cells
3. Select 'a Activity > log10(activity) …'
4. Enter $\log10(PO_2) = -10$; $\log10(PS_2) = -6$



Step 1: ***Equilib*** output

The ***Results Window*** contains 101 pages with <A> = 0, 0.01, 0.02,… 1.

This is the ***Equilib*** output at page 51 where

<A> = 0.5

The equilibrium partial pressures (bar) are :

$P(S_2) = 10^{-6}$

$P(O_2) = 10^{-10}$

The calculated weight fraction of S dissolved in the slag is 3.0094 x 10^{-3}

Wt% S = 0.30094

Results - Equilib A=0.5 (page 51/101)

Output Edit Show Pages

T(C) P(bar) Energy(J) Mass(mol) Vol(litre)

A=0.62 | A=0.63 | A=0.64 | A=0.65 | A=0.66 | A=0.67 | A=0.68 | A=0.69 | A=0.7 | A=0.71 | A=0.72 | A=0.73

A=0.49 | - A=0.5 - | A=0.51 | A=0.52 | A=0.53 | A=0.54 | A=0.55 | A=0.56 | A=0.57 | A=0.58 | A=0.59 | A=0.6 | A=0.61

```
                                                                    FactSage 6.3
 SiO2 +  <A> MnO +  0 S =

27E-03 O2

89E-03 S2

       mol   gas_ideal
    (1650 C, 1 bar,      a=1.0001E-06)
    ( 1.0000E-06       S2                                          FactPS
    + 1.0000E-10       O2                                          FactPS)

997    mol   ASlag-liq
610 gram, 0.99997 mol)
    (1650 C, 1 bar,      a=1.0000)
    ( 0.49796          SiO2                                        FToxid
    + 0.49790          MnO                                         FToxid
    + 3.2248E-05       Mn2O3                                       FToxid
    + 2.0526E-03       SiS2                                        FToxid
    + 2.0524E-03       MnS                                         FToxid
    + 1.3293E-07       Mn2S3                                       FToxid)

    Site fraction of sublattice constituents:
    Si                        0.50000
    Mn2+                      0.49994
    Mn3+                      6.4759E-05
    ------------------------------------
    O                         0.99589
    S                         4.1051E-03

    System component       Mole fraction  Mass fraction
    Mn                        0.20000        0.41867
    S                         2.4631E-03     3.0094E-03
    Si                        0.20000        0.21403
    O                         0.59754        0.36429
```

Step 2: Defining the **slag sulfide capacity**

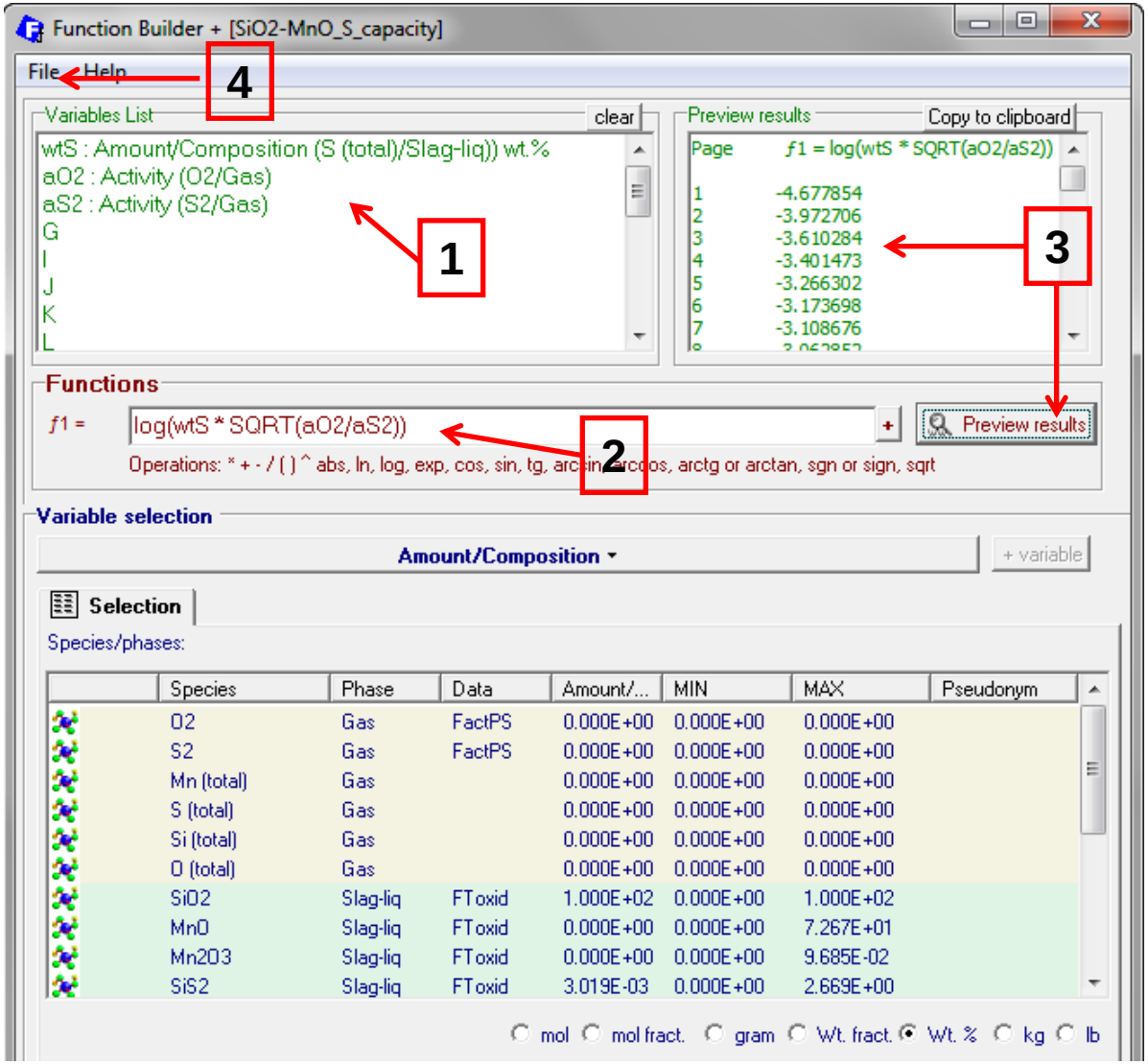
See ***Example 1 (slide 4.3)*** for details on how to make the following entries:

1. Create the **Variable List** containing the 3 variables: **wtS aO2 aS2**

2. In the **Functions input box** enter the expression: ***f*1 = log(wtS * SQRT(aO2/aS2))**

3. Click on **Functions Preview results** to check the calculated values

4. Save the functions group (click on *'File > Save …'*) as **SiO2-MnO_S_capacity**



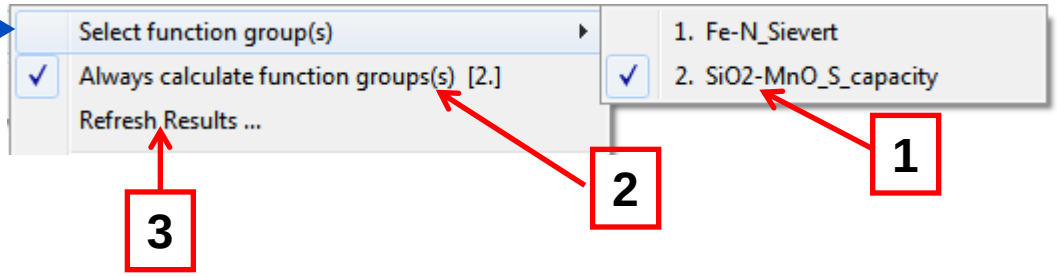
Step 3: Display **sulfide capacity** for all pages

Open the **Fact-Function-Builder** Toolbox menu :

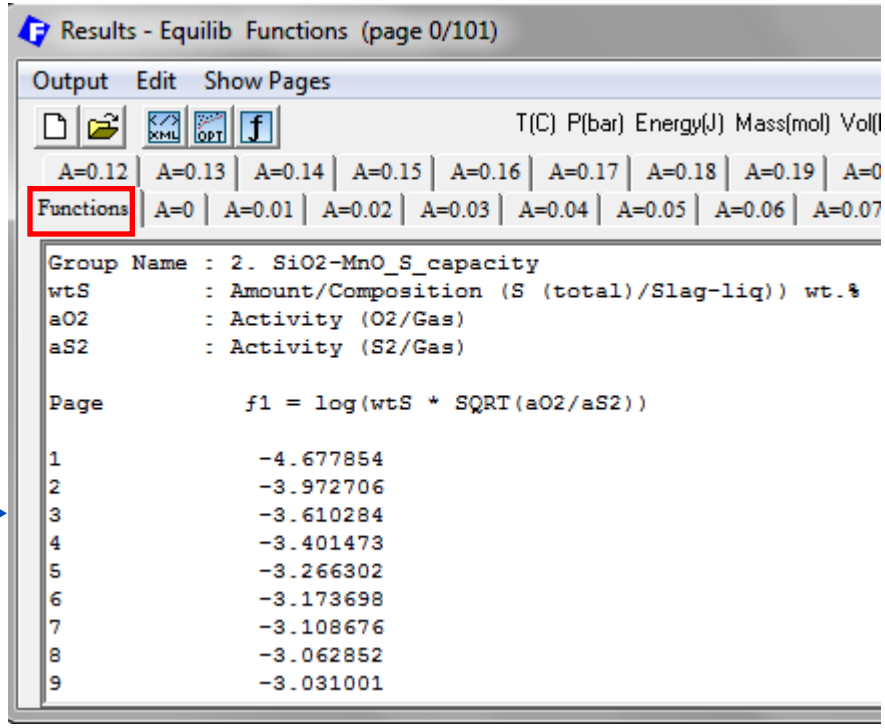
1. Click '*Select function group(s)* > '
   Check √ **SiO2-MnO_S_capacity**

2. Check √ '*Always calculate function* '

3. Click on '*Refresh Results ….*'



After the results are refreshed the **"Functions" page** displays ***f*1 - slag sulfide capacity -** for all the pages..



Step 3: Display **sulfide capacity** for each page

The calculated **slag sulfide capacity** is displayed at the top of each page.

Here page 51 shows :

<A> = 0.5

S = 0.30094 Wt.%

$P(O_2) = 10^{-6}$ bar

$P(S_2) = 10^{-6}$ bar

***f*1 (i.e. log(Cs))**

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

= -2.521514

Results - Equilib A=0.5 (page 51/101)

Output Edit Show Pages

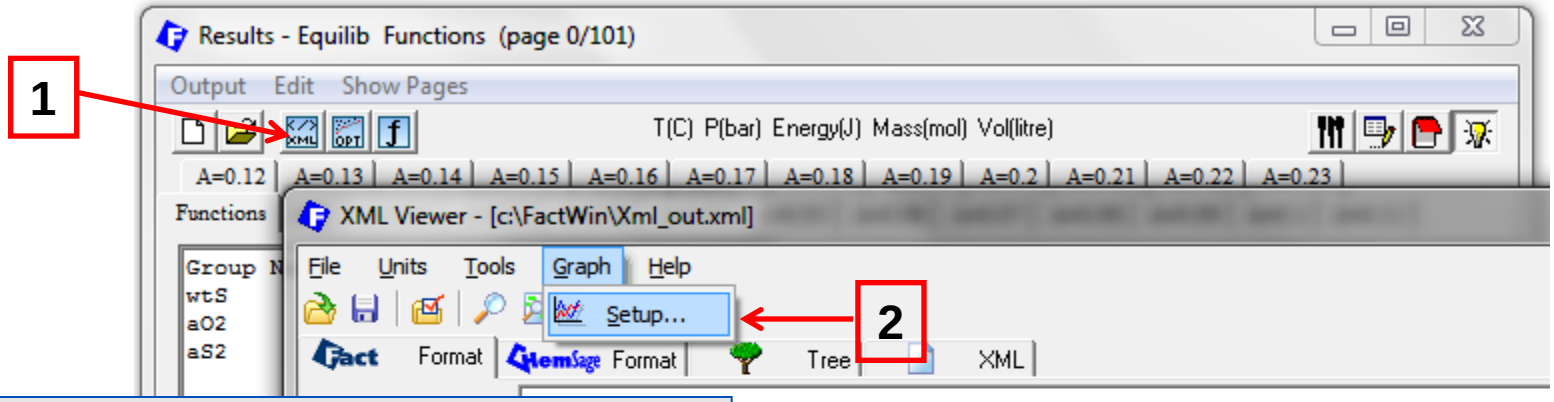
T(C) P(bar) Energy(J) Mass(mol) Vol(litre)

A=0.62 | A=0.63 | A=0.64 | A=0.65 | A=0.66 | A=0.67 | A=0.68 | A=0.69 | A=0.7 | A=0.71 | A=0.72

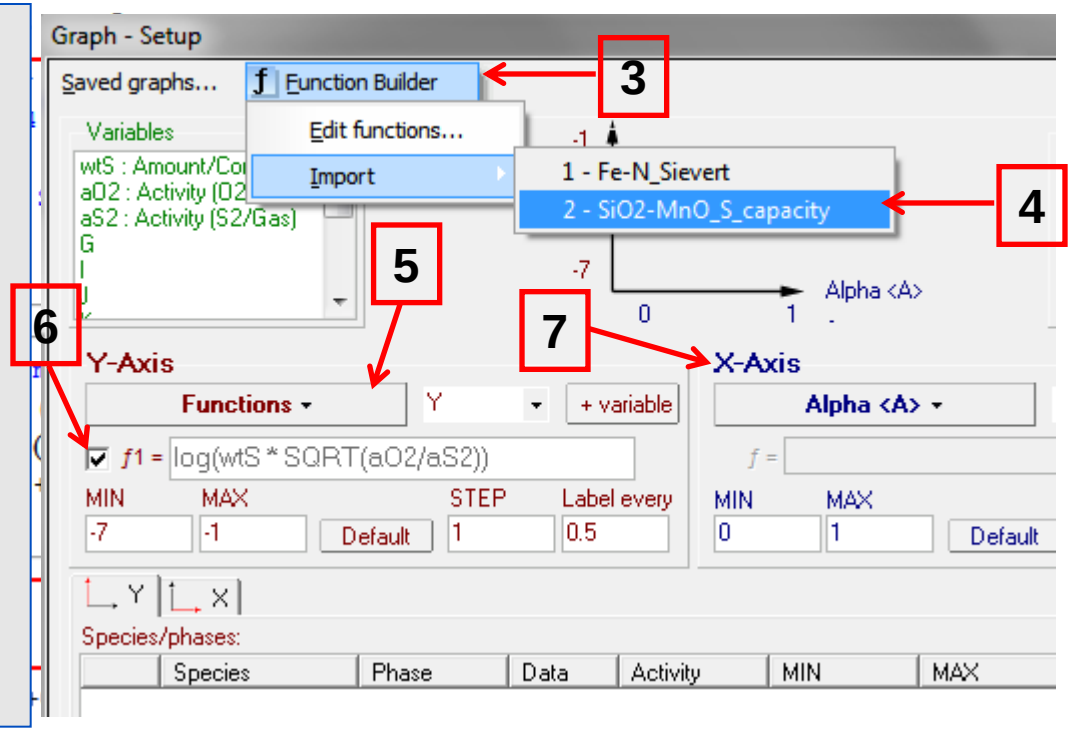
A=0.49 | - A=0.5 - | A=0.51 | A=0.52 | A=0.53 | A=0.54 | A=0.55 | A=0.56 | A=0.57 | A=0.58 | A=0.59

```
Group Name  : 2. SiO2-MnO S capacity
wtS         : 0.3009442        Amount/Composition (S (total)/Slag-liq)) wt.%
aO2         : 0.1000000E-09    Activity (O2/Gas)
aS2         : 0.1000000E-05    Activity (S2/Gas)

Page        f1 = log(wtS * SQRT(aO2/aS2))
51                                -2.521514
==================================================================================

  <1-A> SiO2 +  <A> MnO +  0 S =

 - 3.0627E-03 O2

 + 3.0789E-03 S2

   0          mol   gas_ideal
            (1650 C, 1 bar,     a=1.0001E-06)
            ( 1.0000E-06      S2
            + 1.0000E-10      O2      )

 + 0.99997    mol   ASlag-liq
   (65.610 gram, 0.99997 mol)
            (1650 C, 1 bar,     a=1.0000)
            ( 0.49796         SiO2
            + 0.49790         MnO
            + 3.2248E-05      Mn2O3
            + 2.0526E-03      SiS2
            + 2.0524E-03      MnS
            + 1.3293E-07      Mn2S3   )
```

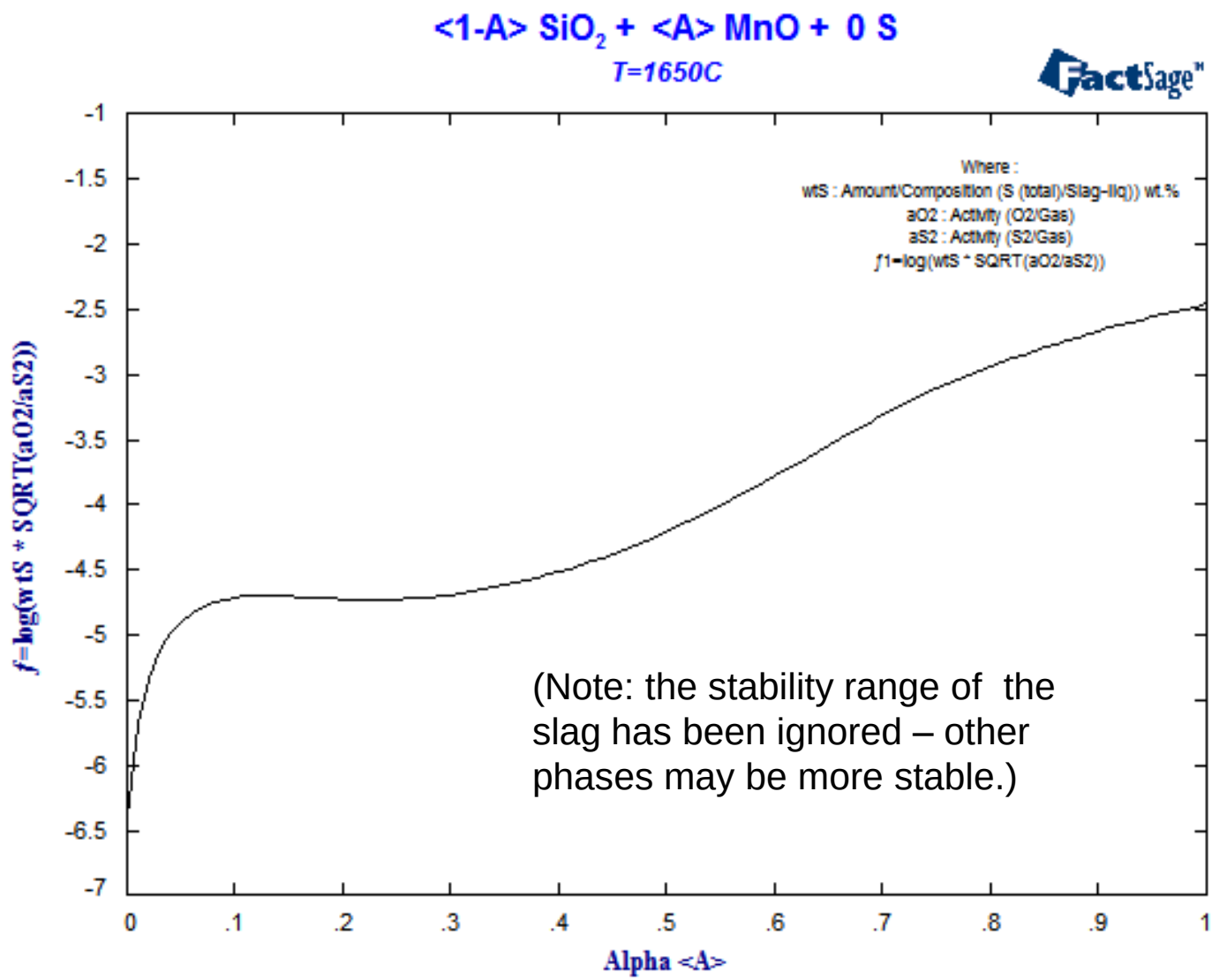
Step 4: Importing **functions** into **Fact-XML**



1. To activate **Fact-XML** click on the **XML** menu button.
2. Click on **Graph > Setup ….**
3. Click on **Function Builder**.
4. **Import** function group: **SiO2-MnO_S_capacity**
5. Select **Functions** from the Y-Axis menu.
6. Check √ the functions you wish to plot: set **MIN**, **MAX**, **STEP**, etc
7. Select X-Axis **Alpha <A>**, etc.
8. Click on **Draw** (not shown here).

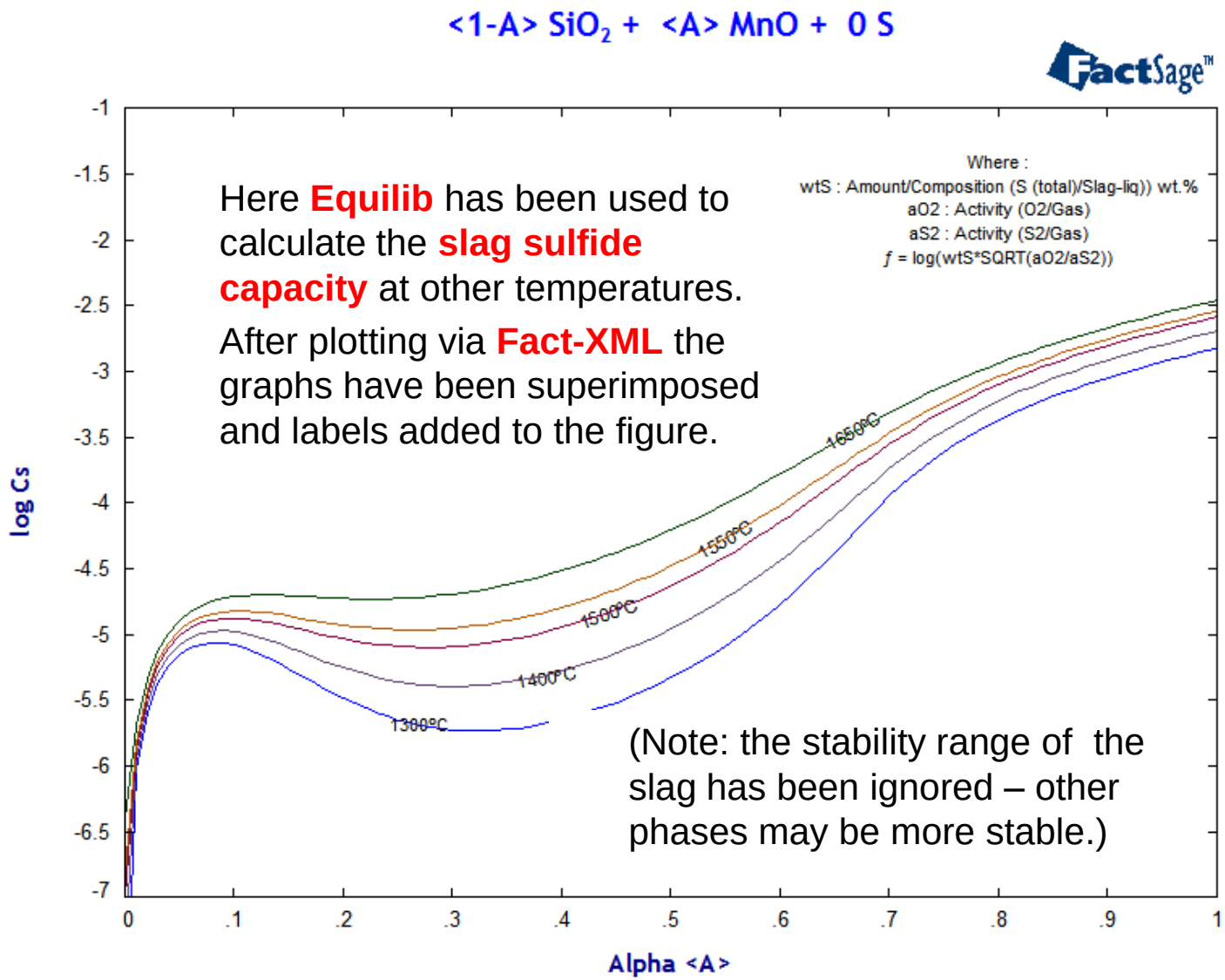


Step 4: Plot of **slag sulfide capacity** at 1650°C



(Note: the stability range of the slag has been ignored – other phases may be more stable.)

Step 4: **Slag sulfide capacity** at 1300 -1650°C

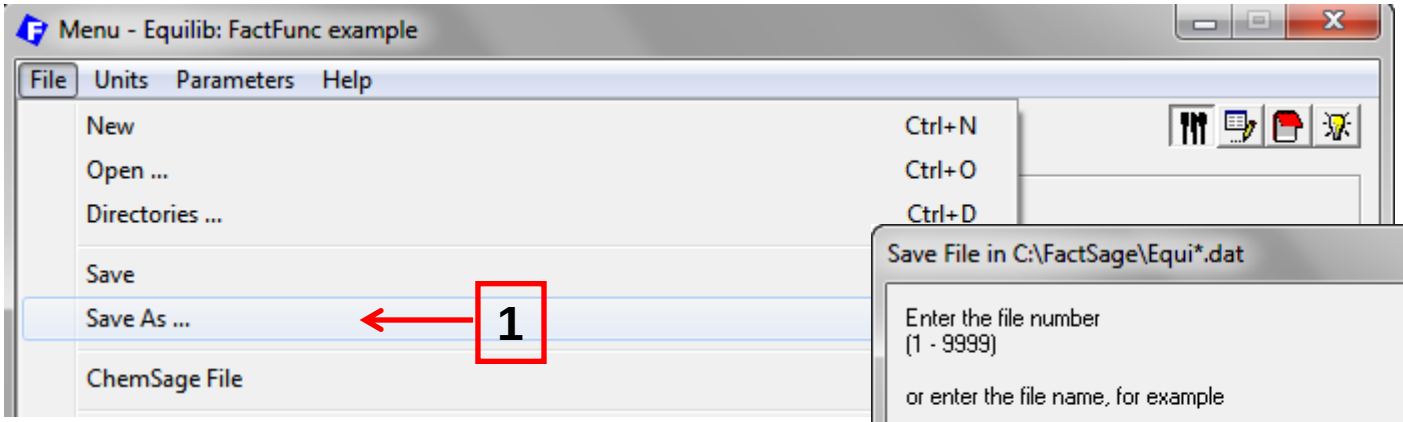


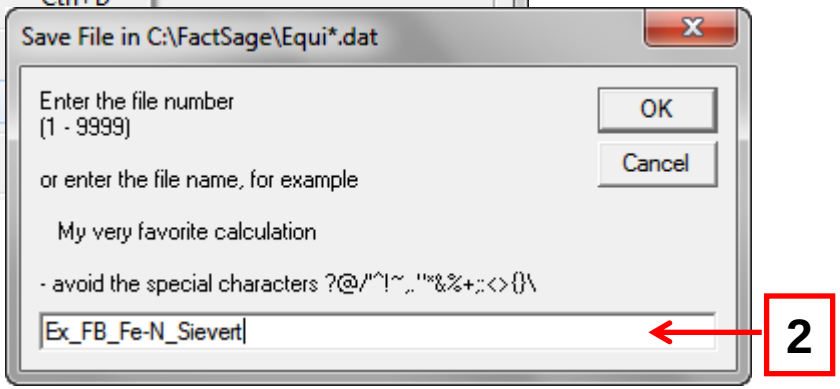
Here **Equilib** has been used to calculate the **slag sulfide capacity** at other temperatures.

After plotting via **Fact-XML** the graphs have been superimposed and labels added to the figure.

(Note: the stability range of the slag has been ignored – other phases may be more stable.)

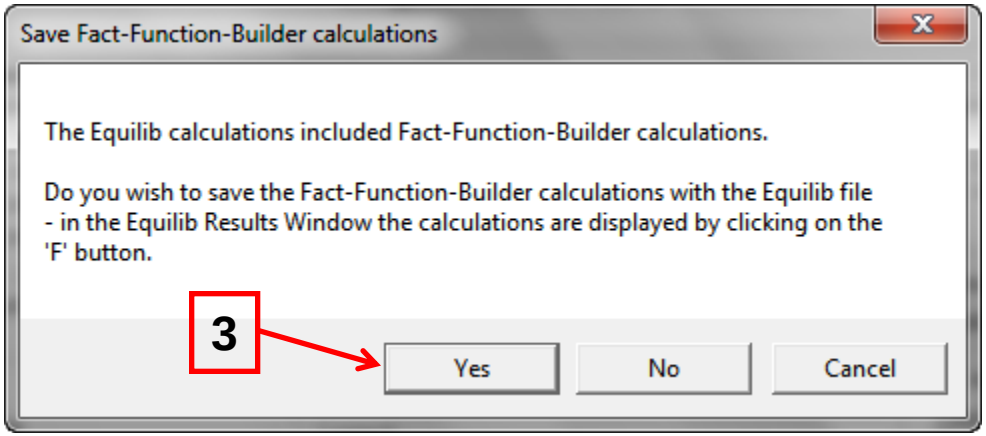
Saving **Equilib** and **Function-Builder** Files





To save the **Equilib** and the **Fact-Function-Builder** calculations :

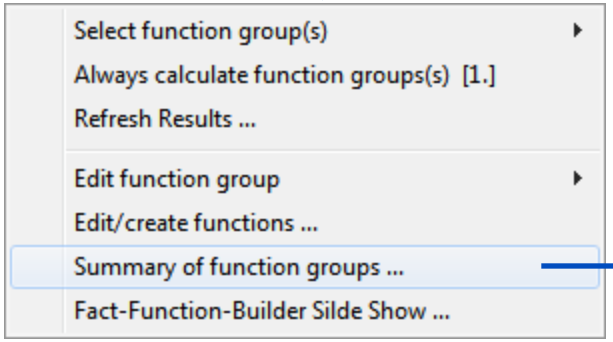
1. In the *Menu Window* click on *'File > Save As ….'*
2. Enter the name of the **Equilib** file.
3. Save the **Fact-Function-Builder** file – click on 'Yes'

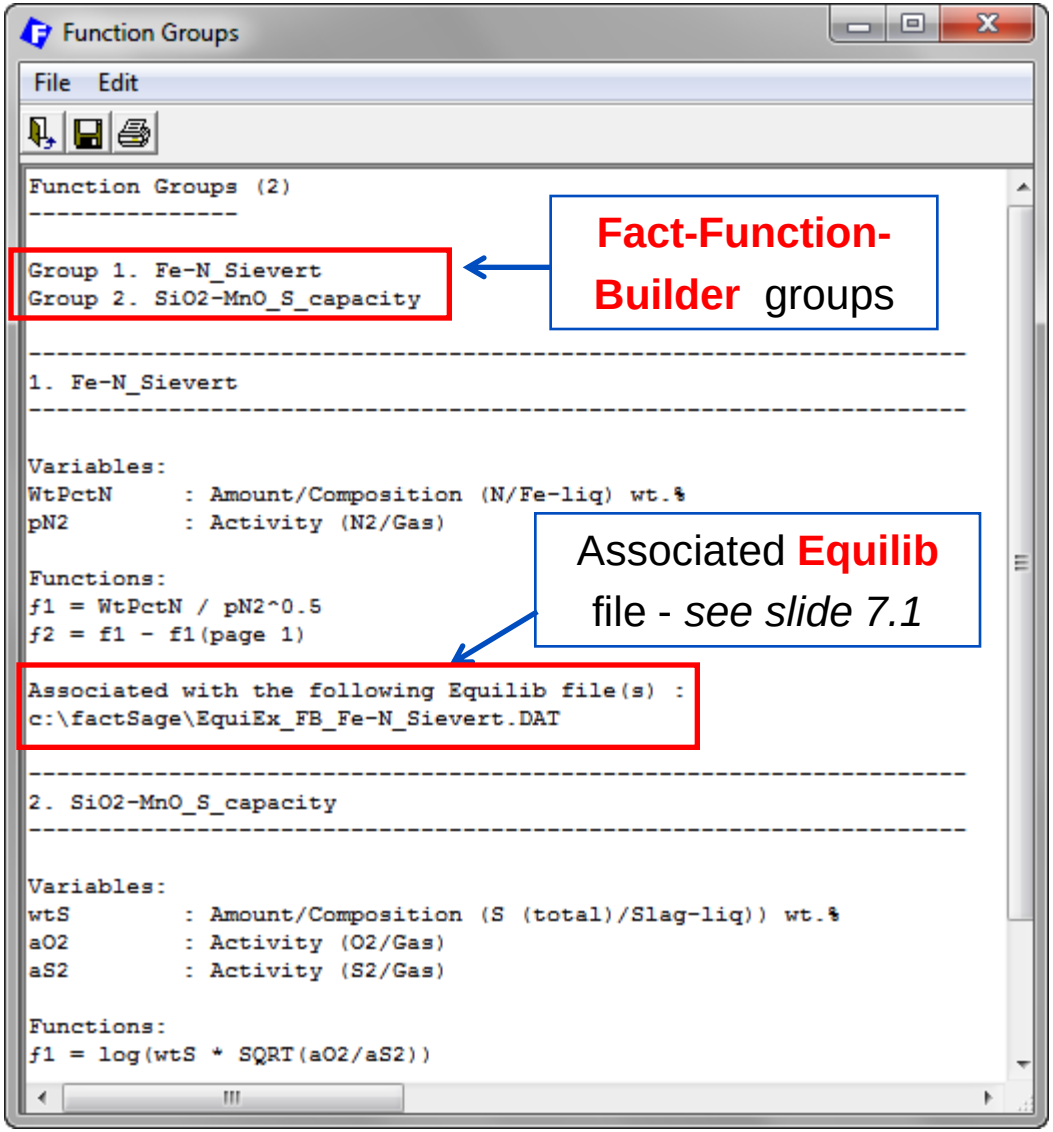


Summary of stored **Function-Builder** groups

Open the **Fact-Function-Builder** Toolbox menu :

Click on
'Summary of function groups …'





Fact-Function-Builder groups

Associated **Equilib** file - *see slide 7.1*