Fact-Function-Builder & FactOptimal in FactSage 6.3

Dr. Stephan Petersen, GTT-Technologies, Herzogenrath, Germany
GTT-Technologies Gunnar Eriksson Symposium and 14th Annual Workshop
July 11-13, 2012, Herzogenrath, Germany

Fact-Function-Builder

Manipulating the
Equilib results

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**

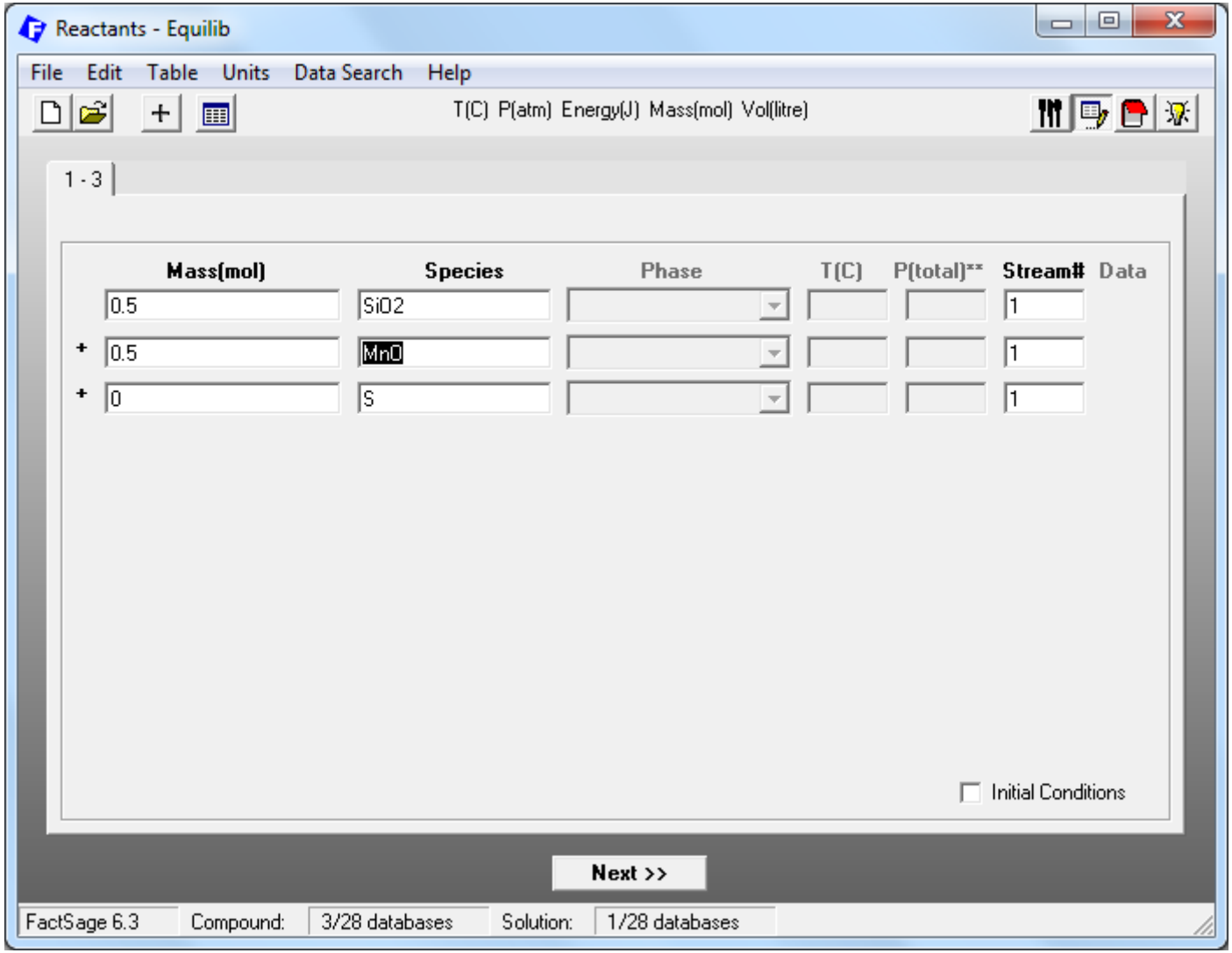
Step 2: Defining the sulfide capacity using the **Fact-Function-Builder**

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

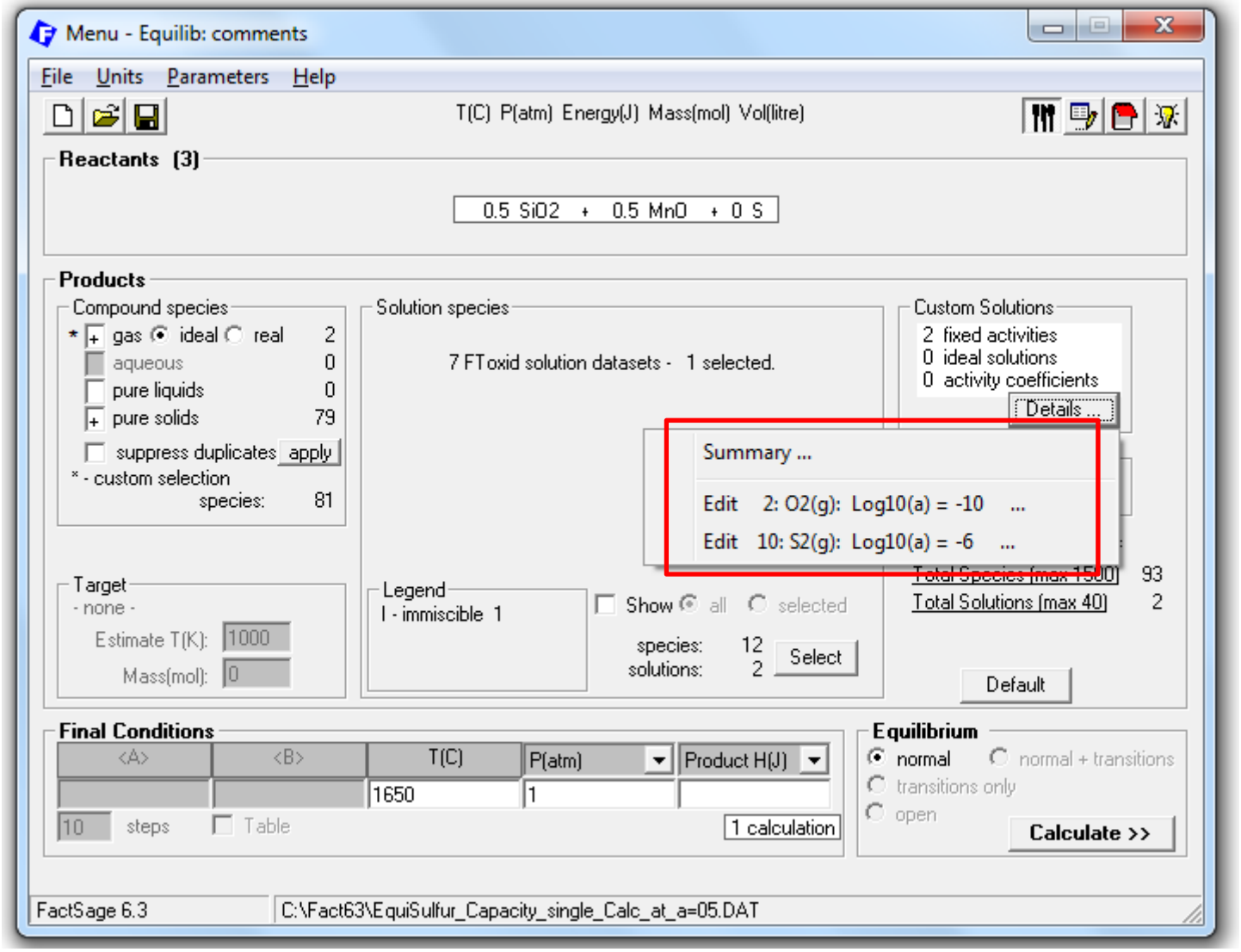
Step 4: Plotting the sulfide capacity in **Fact-XML**.

Example 2 – **Plotting slag sulfide capacity**

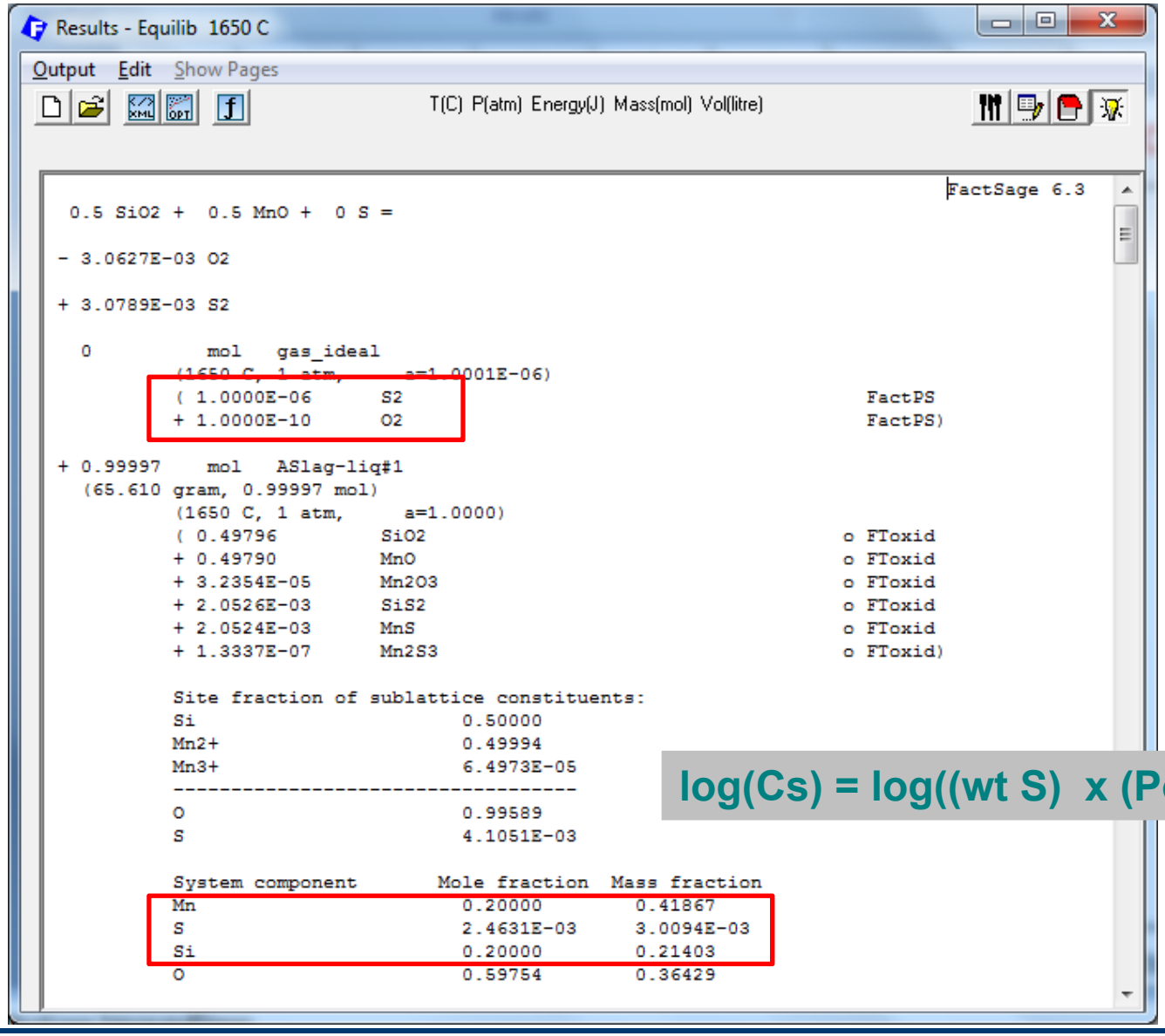
A simple Equilib point calculation and manual calculation of the sulfide capacity



Example 2 – **Plotting slag sulfide capacity**



Example 2 – Plotting slag sulfide capacity



$\log(Cs) = \log((\text{wt S}) \times (Po_2/Ps_2)^{1/2}) = -2.521514$

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 :

$S_2(g)$, $O_2(g)$

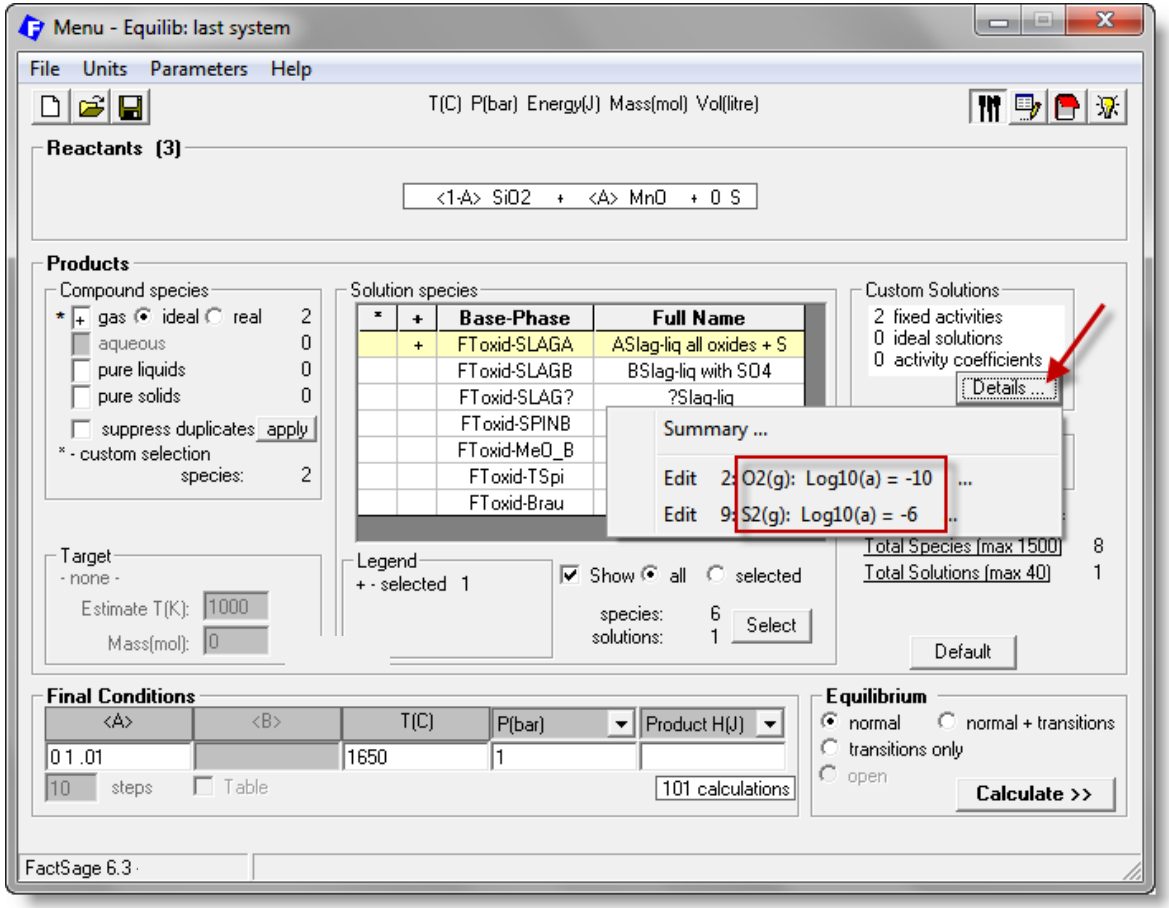
and their equilibrium partial pressures are fixed:

$\log(Po_2) = -10$

$\log(Ps_2) = -6$

- how this is done is shown in the slide on the next page.

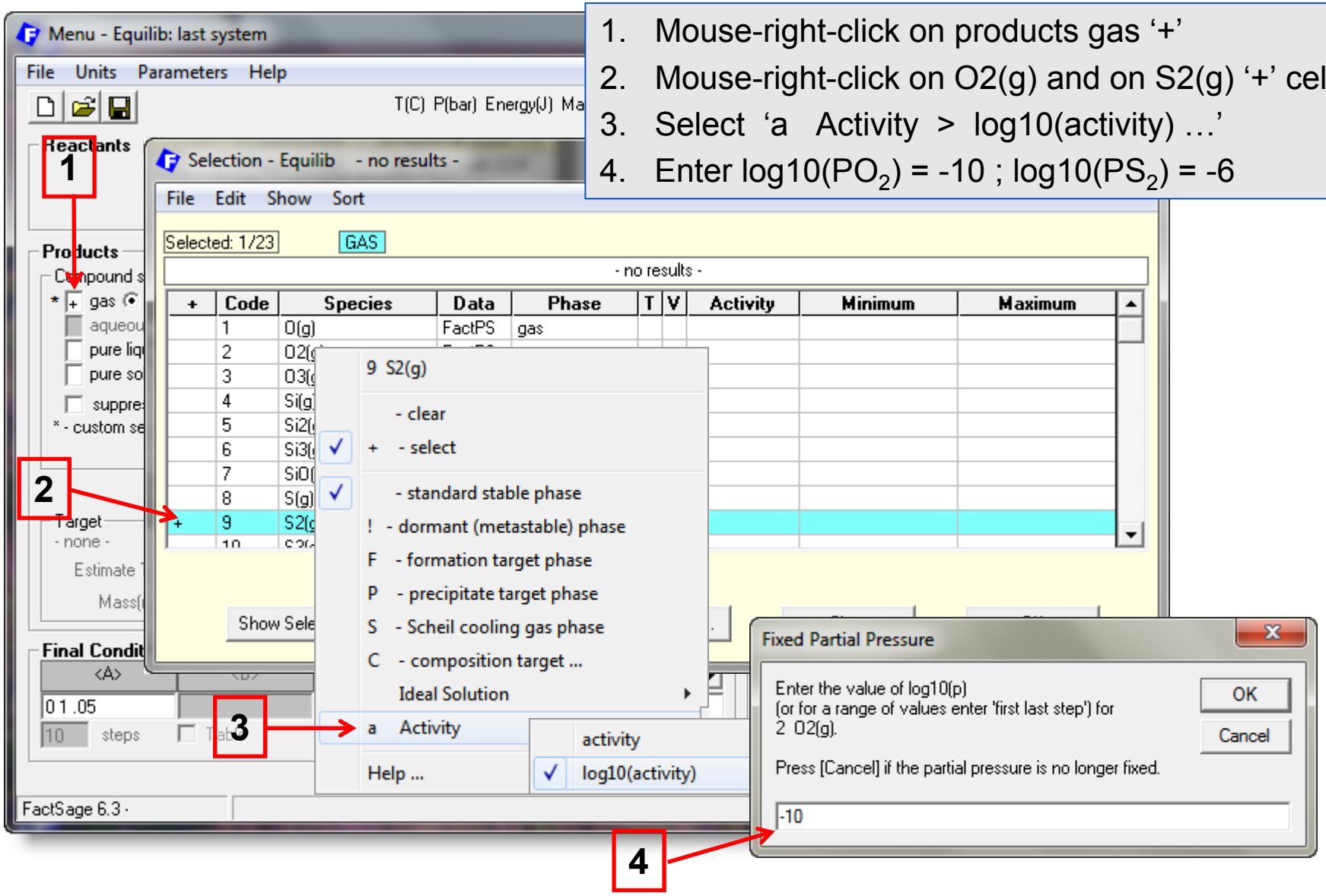
The liquid oxide slag phase is **SLAGA** taken from the **FToxid** database.



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

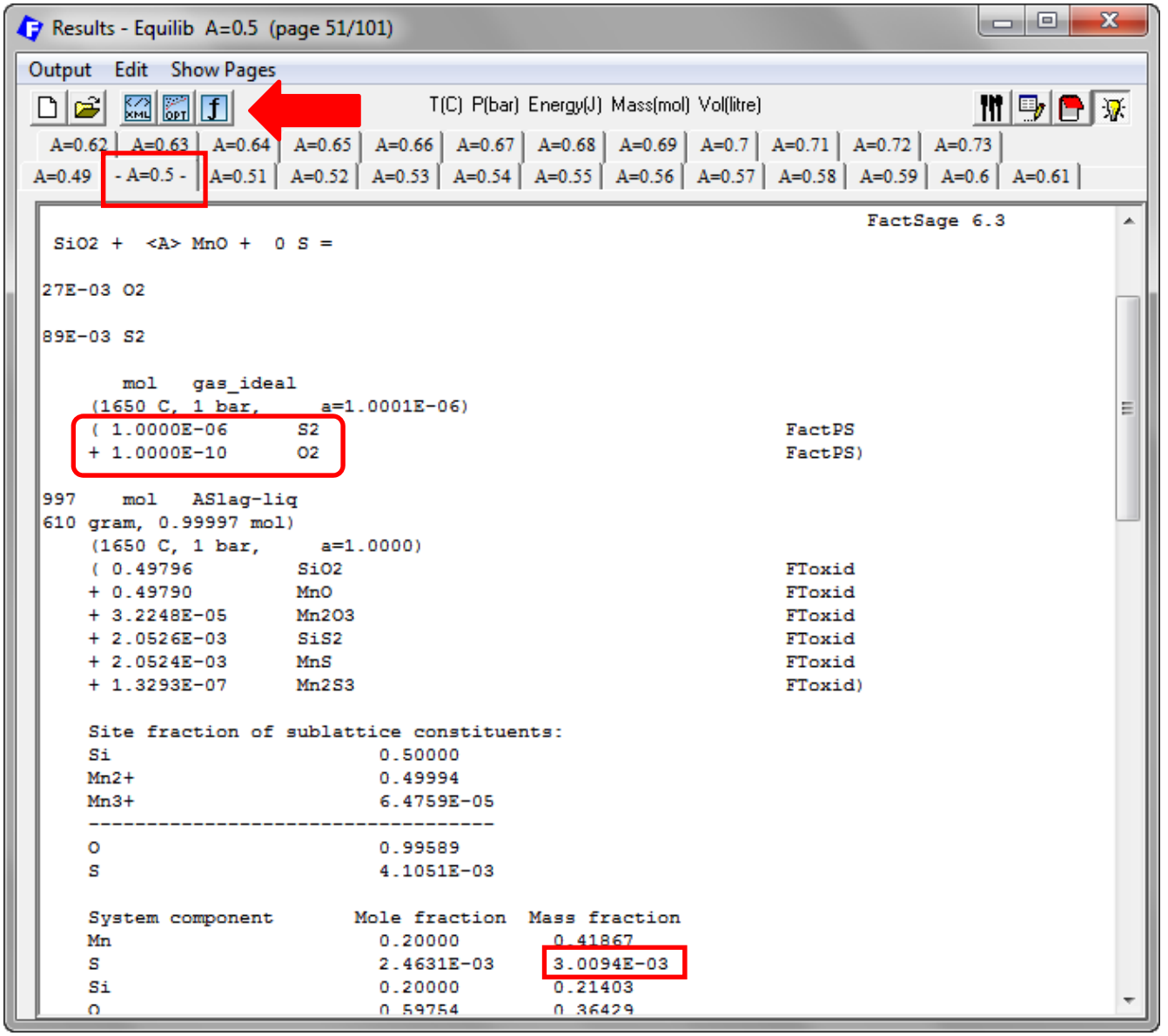
The equilibrium partial pressures (bar) are :

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

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

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

Wt% S = 0.30094



Step 2: Defining the slag sulfide capacity

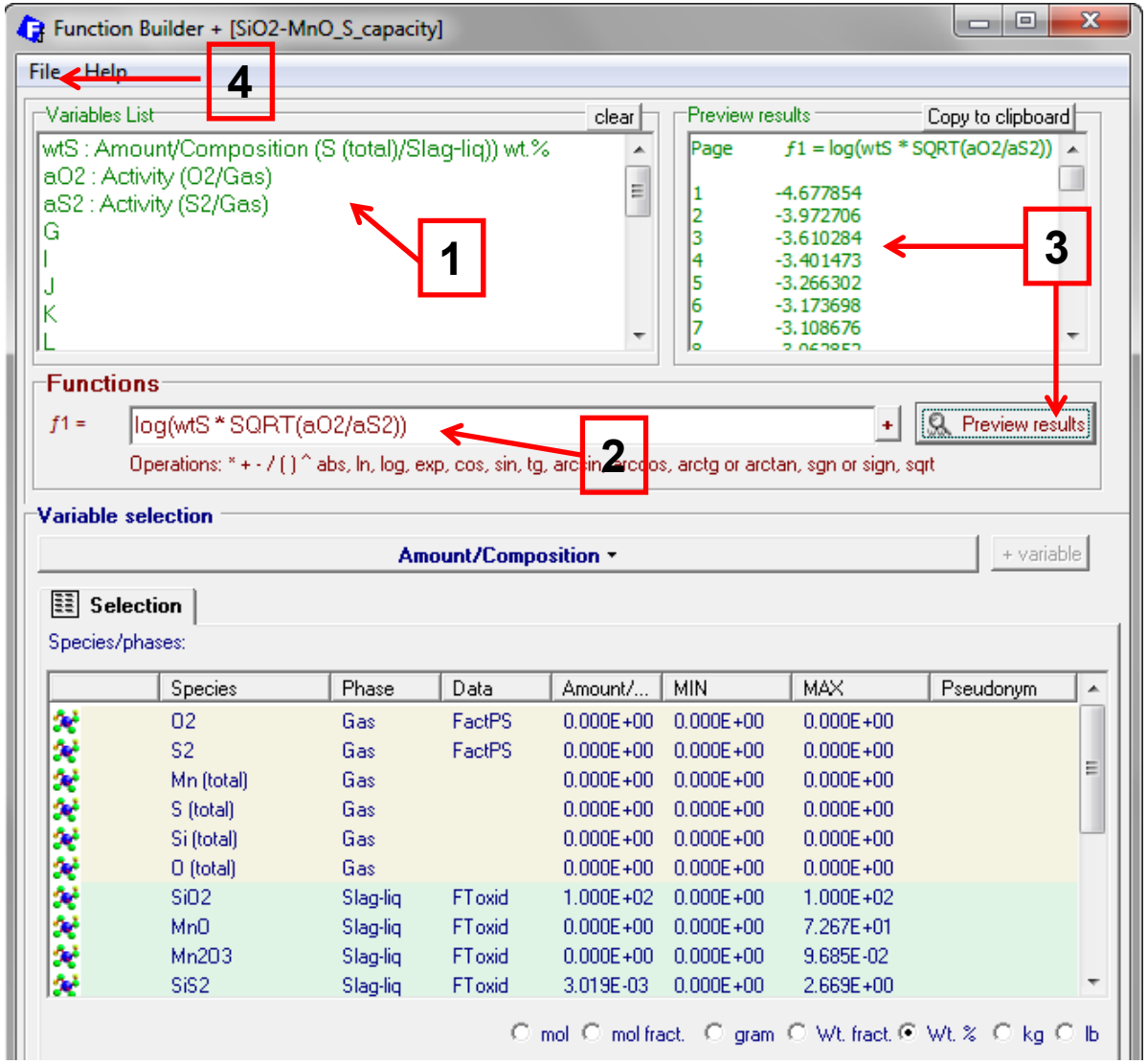
See ***Example 1 (slide 4.3)*** for details on how to make the following entries:

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

2. In the **Functions input box** enter the expression: ***ƒ1 = log(wtS * SQRT(aO2/aS2))***

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

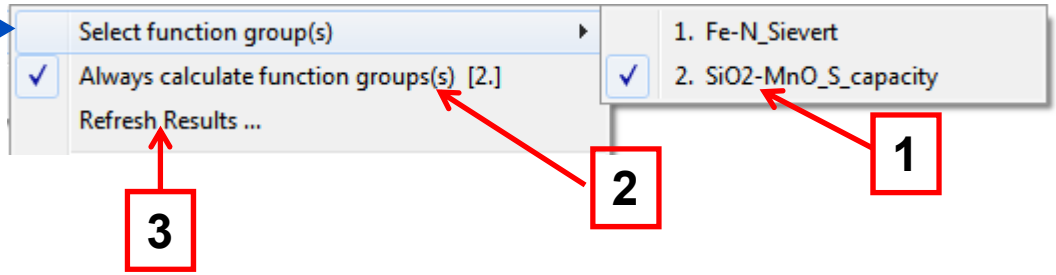
4. Save the functions group (click on *'File > Save …'*) as **SiO2-MnO_S_capacity**



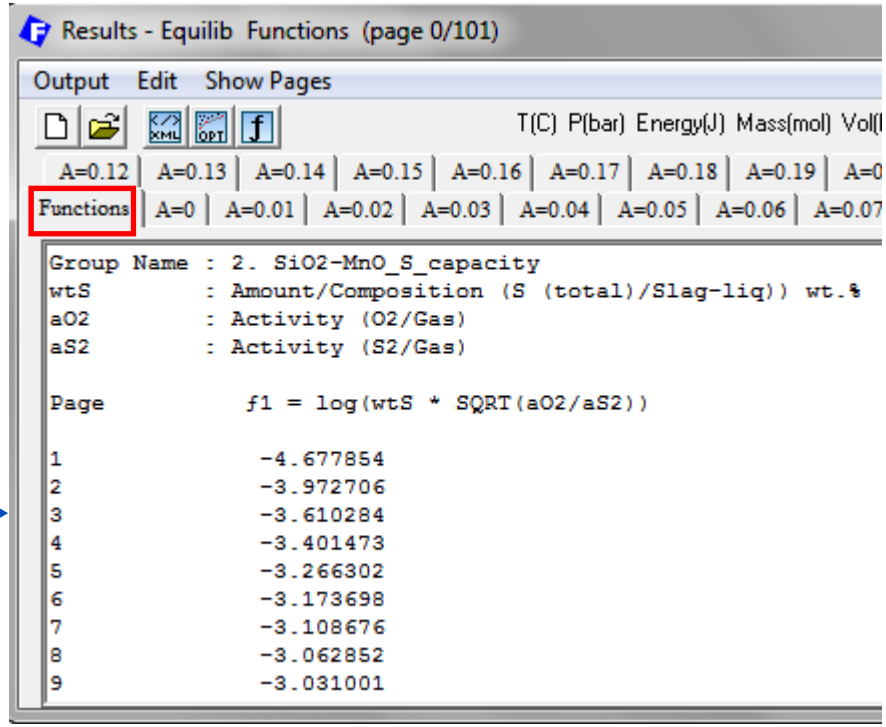
Step 3: Display **sulfide capacity** for all pages

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 ***ƒ1*** **- slag sulfide capacity -** for all the pages..



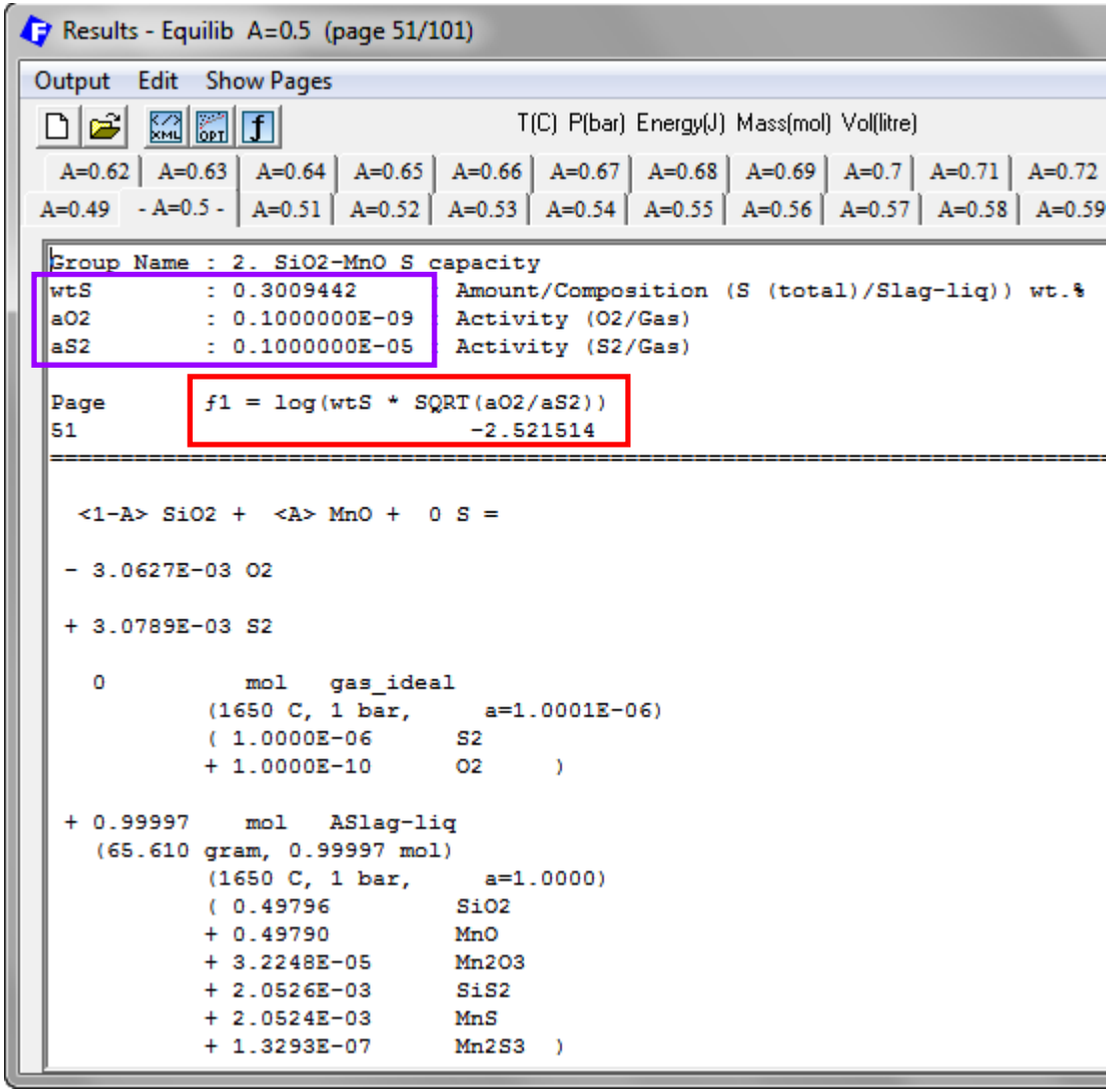
Step 3: Display **sulfide capacity** for each page

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

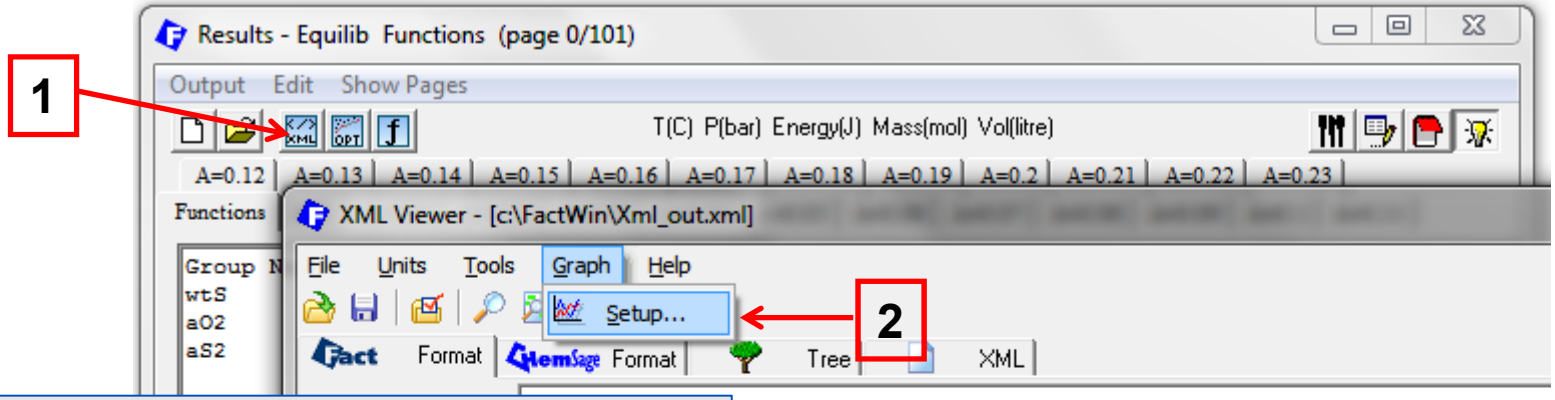
Here page 51 shows :

<A> = 0.5
S = 0.30094 Wt.%
$P(O_2) = 10^{-6}$ bar
$P(S_2) = 10^{-6}$ bar

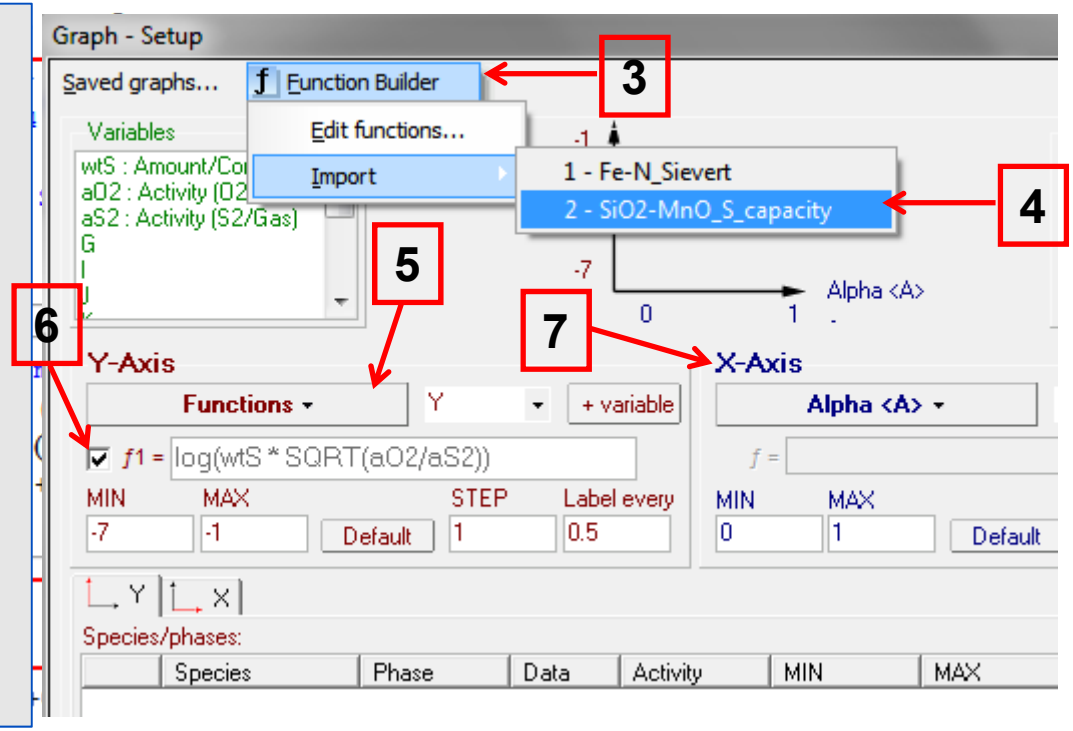
***f*1 (i.e. log(Cs))**
= log(wtS * SQRT(aO2/aS2))
= -2.521514



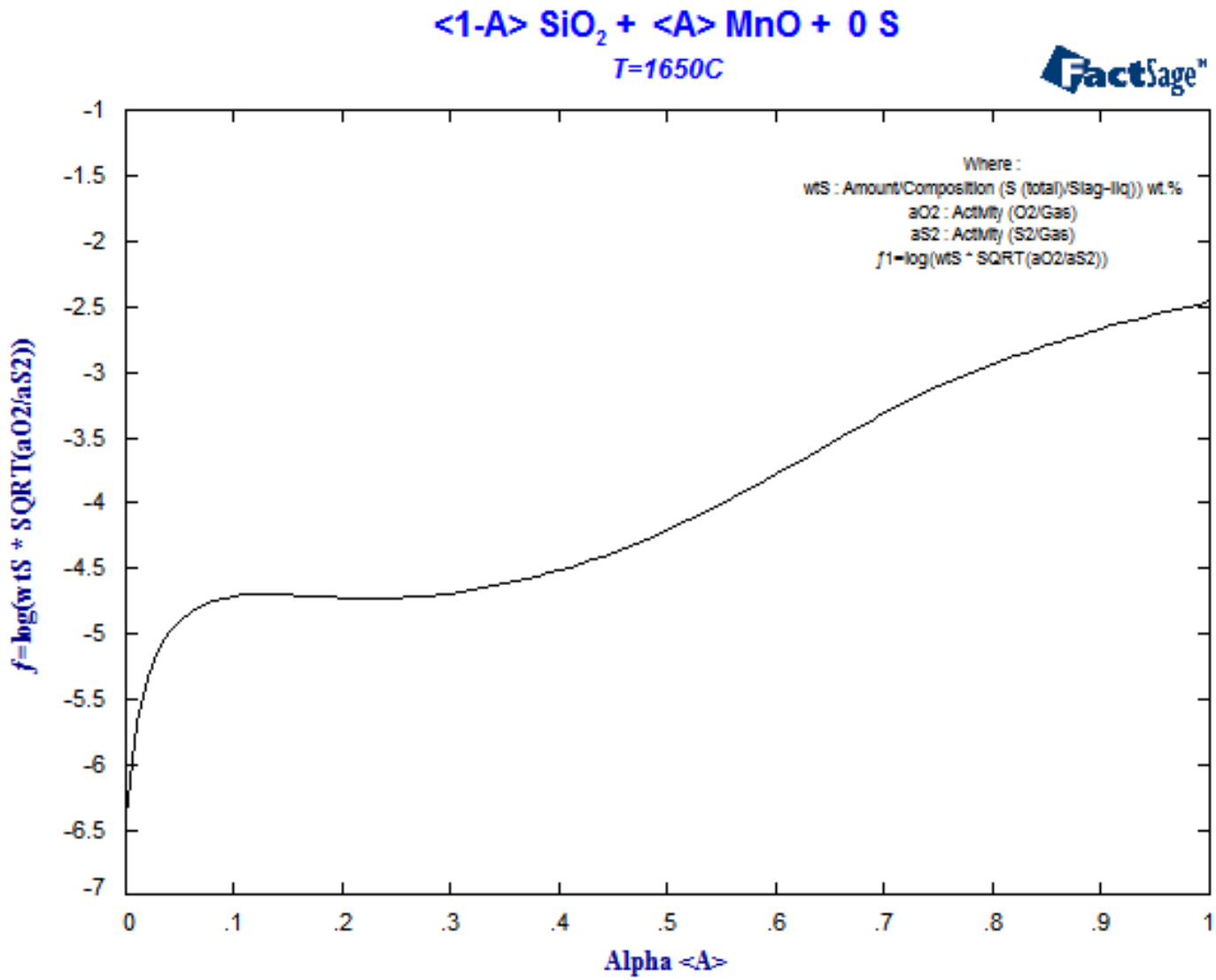
Step 4: Importing **functions** into **Fact-XML**



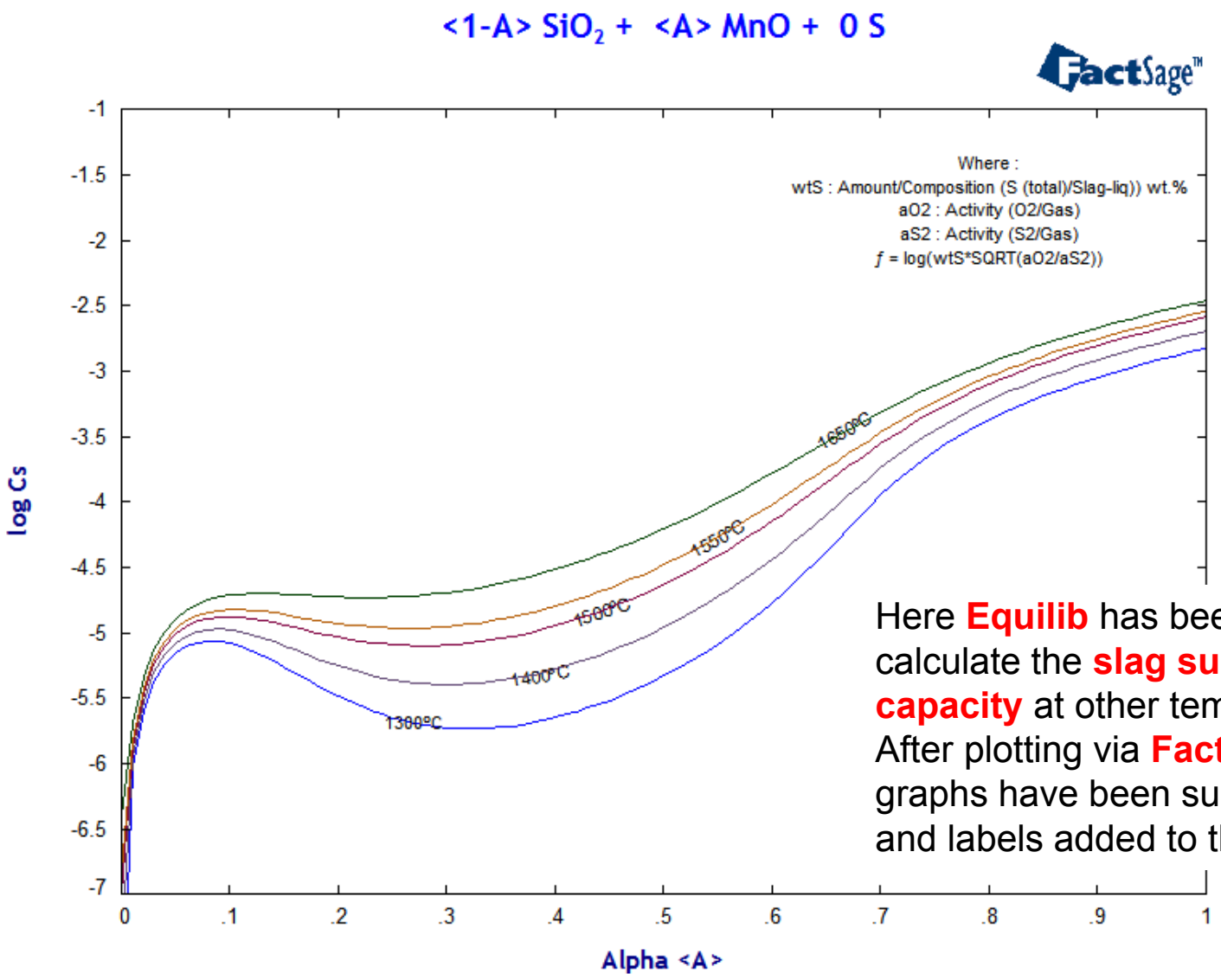
1. To activate **Fact-XML** click on the **XML** menu button.
2. Click on **Graph > Setup ….**
3. Click on **Function Builder**.
4. **Import** function group: **SiO2-MnO_S_capacity**
5. Select **Functions** from the Y-Axis menu.
6. Check √ the functions you wish to plot: set **MIN**, **MAX**, **STEP**, 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



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.

FactOptimal

***FactOptimal** is programmed to identify the optimal conditions for alloy and process design using thermodynamic and property databases, FactSage software and the Mesh Adaptive Direct Search Algorithm.*

A.Gheribi, E. Bélisle, C.W. Bale and A.D. Pelton CRCT, École Polytechnique de Montréal

S. Le Digabel and C. Audet, GERAD, École Polytechnique de Montréal

The *FactOptimal* Module

***FactOptimal** is programmed to identify the optimal conditions for alloy and process design using thermodynamic and property databases, FactSage software and the Mesh Adaptive Direct Search Algorithm.*

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Table of contents

Introduction - 1

- The **Equilib** module can be used to screen potential systems, searching for compositions having a desired set of properties and phase constitution, under a given set of constraints

- For instance, one could search for alloys within a given composition range, with a liquidus temperature below x°C, with a desired freezing range, with a maximum or minimum amount of precipates after annealing at y°C, with a density or shrinkage ratio within a given range, etc. One could also search for optimal annealing or rolling temperatures, for example.

- However, to perform such searches “by hand” for a multicomponent alloy by simply performing thousands of calculations over a grid of compositions is extremely time-consuming.

- **FactOptimal** extends the capability of **Equilib** by coupling it with a **Mesh Adaptive Direct Search** method algorithm (MADS) developed at GERAD by S. Le Digabel and C. Audet, Ecole Polytechnique de Montreal

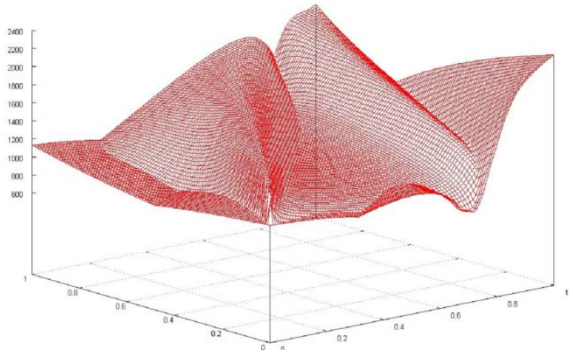
The *FactOptimal* Module

What's New In FactOptimal 6.3 ?

- Target calculations : in addition to minimizing/maximizing one can now target a specific value.
- Additional new property for optimization : activity of a phase/species.
- Additional new variables : temperature and pressure.
- Additional new property constraint : activity of a phase/species.
- The sum of composition variables can now be greater than 1.
- Thus, variables can now be of type integer or real.
- When using two input files, the "linked" button is now activated in order to use the temperature from the first file in the second file.
- When using two input files, properties constraints can now apply to each of the input files.
- Latest optimizations are saved with **Equilib** files and can be recalled by using the "Recent" button
- Convenient MIN/MAX buttons to set all minimum/maximum values of composition variables
- For a Scheil cooling system, the mass of specific species/phase(s) can now be optimized
- Better optimization for composition constraints having equality rules
- Table display of result for the special points option
- Use of cache file to restart any optimization from the latest calculation

Introduction - 2

- **The purpose of FactOptimal is to minimize and/or maximize a set of functions: {$f_1(x_1,x_2..T, P)$; $f_2(x_1,x_2....T, P)$}**



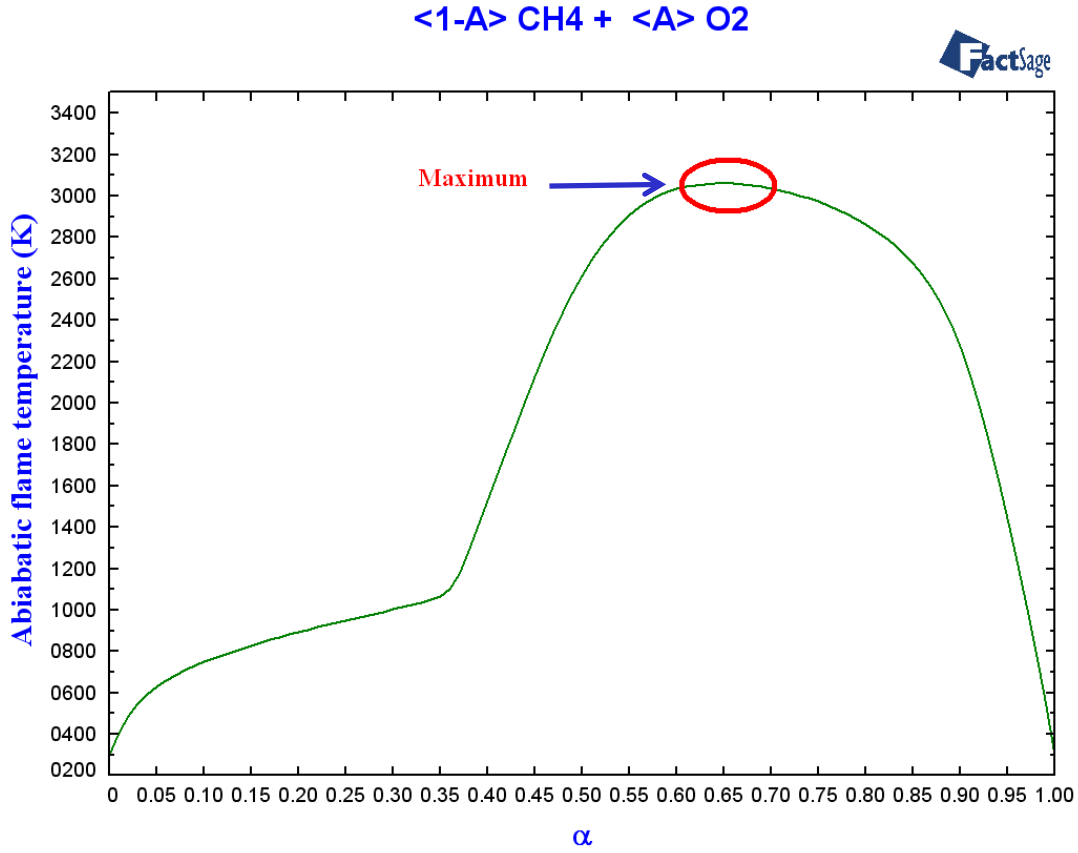
- The functions are calculated by **Equilib**
- The functions may be non-smooth (e.g. liquidus)
- The estimation of derivatives is problematic
- Evaluations of *f* can be time consuming
- The function calculation may fail unexpectedly at some points
- The constraints may be non-linear, non-smooth or Boolean

Example 1: Maximize an adiabatic flame temperature - 1

The objective is <u>to maximize the adiabatic flame temperature</u> of : **(1-A) CH_4 + (A) O_2**

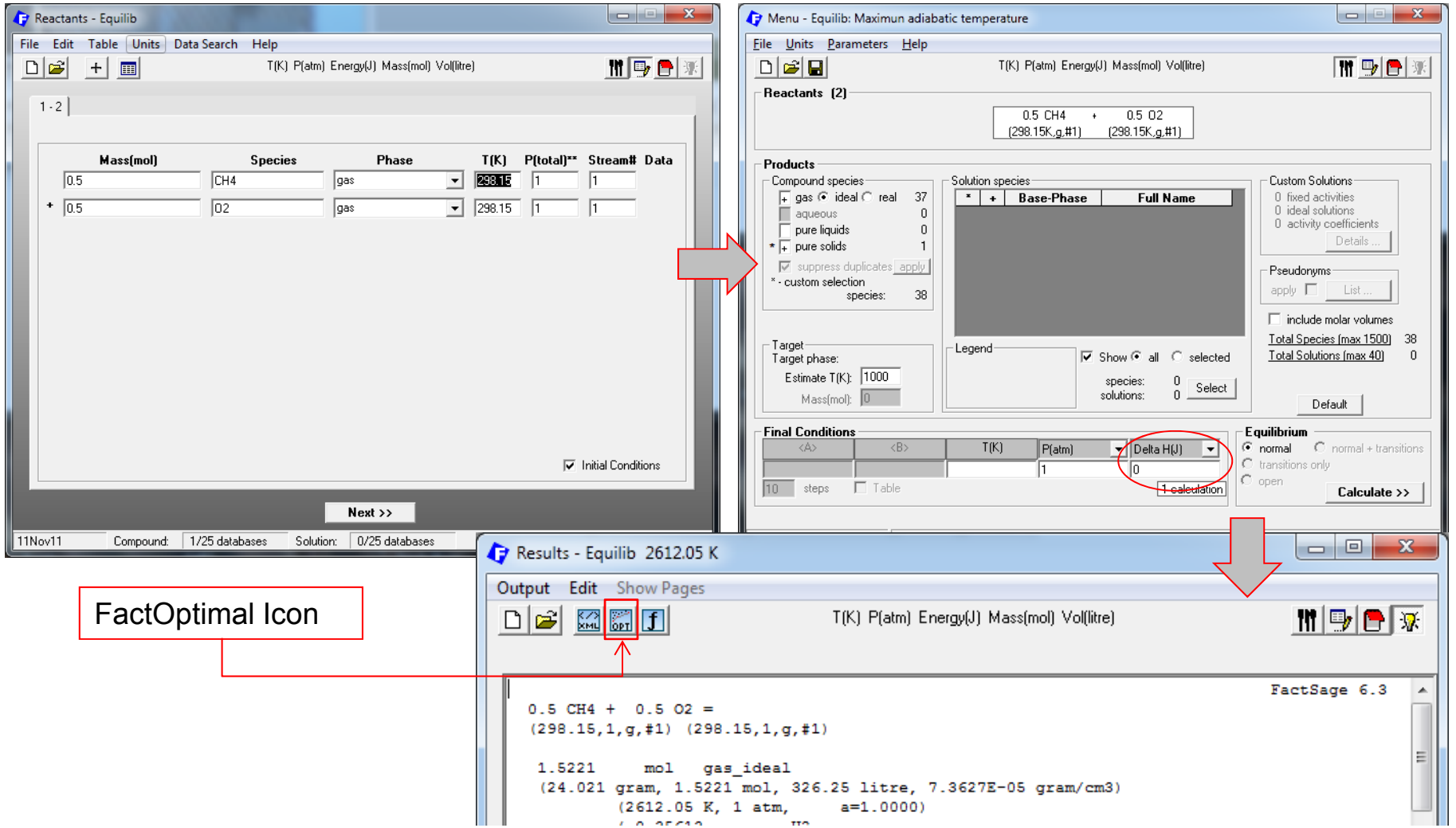
By varying A from 0 to 1 in steps of 0.01, you can calculate the adiabatic flame temperature as a function of A using the **Equilib** module (see **Equilib** regular slide show, section 10).

Plotting the results you find that: $T_{ad,max}$ ~3075 K when A ~0.65



Example 1: Maximize an adiabatic flame temperature - 2

To calculate the maximum temperature with **FactOptimal**, the first step is to perform a single equilibrium calculation at any arbitrary composition and then open **FactOptimal**.



FactOptimal Icon

Example 1: Maximize an adiabatic flame temperature - 3

When you “click” on the **FactOptimal** icon the first window of the module appears. If you are using the stored example files, click on “Recent...” to load the FactOptimal file. There are 5 tabs.

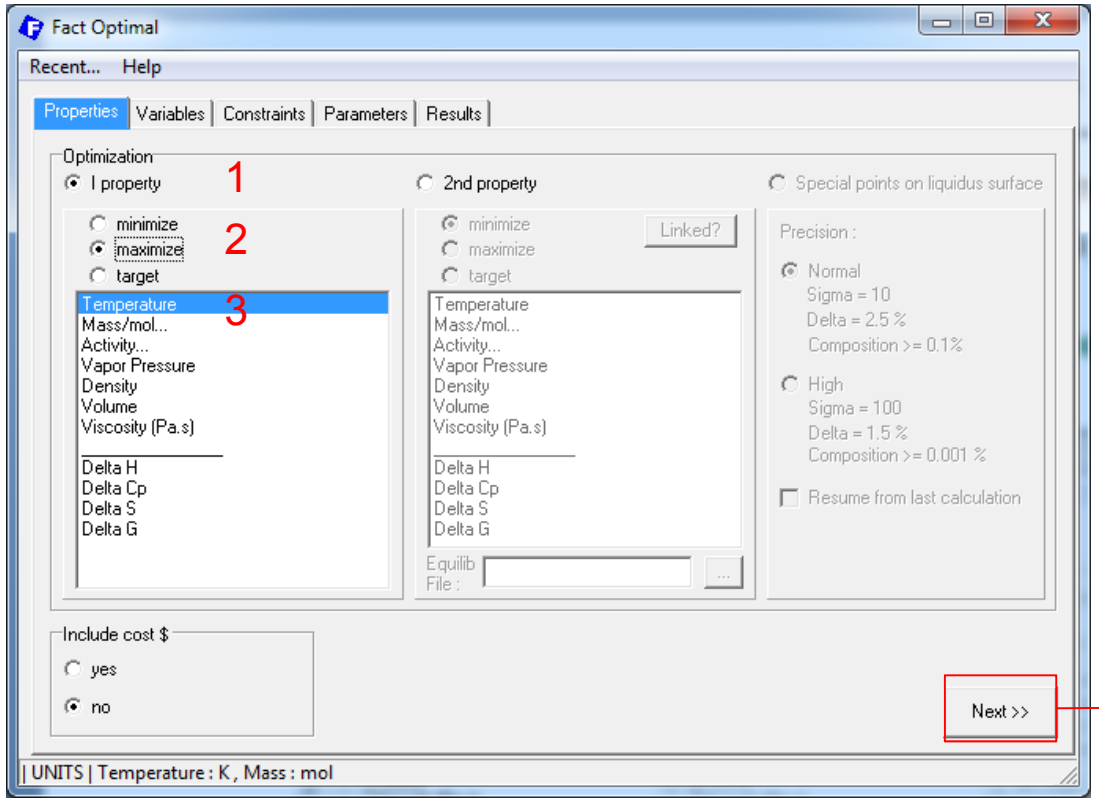
The first tab is “Properties” where we define the quantities to minimize and/or maximize.

In this example, we specify that :

1 - we consider **one property**

2 - we want to **maximize this property**

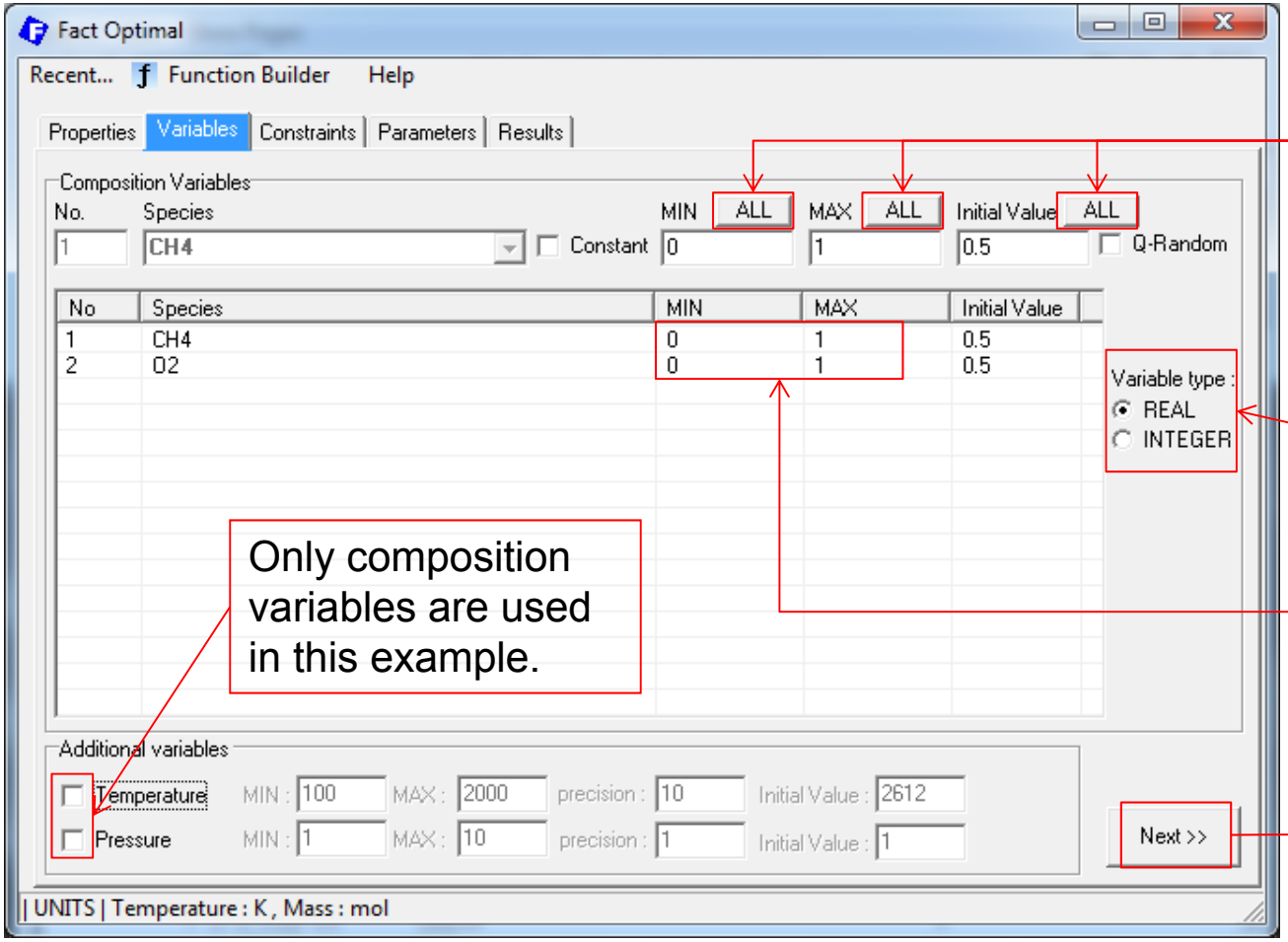
3 - the property is **temperature**



Click on Next to go to the Variables tab

Example 1: Maximize an adiabatic flame temperature - 4

In the “Variables” tab we define the permissible range of composition and the initial values for the first estimate. Alternatively, select “Q-Random” and let the program choose the initial values. (see page 3.9)



Use “ALL” buttons to set the same value for all variables.

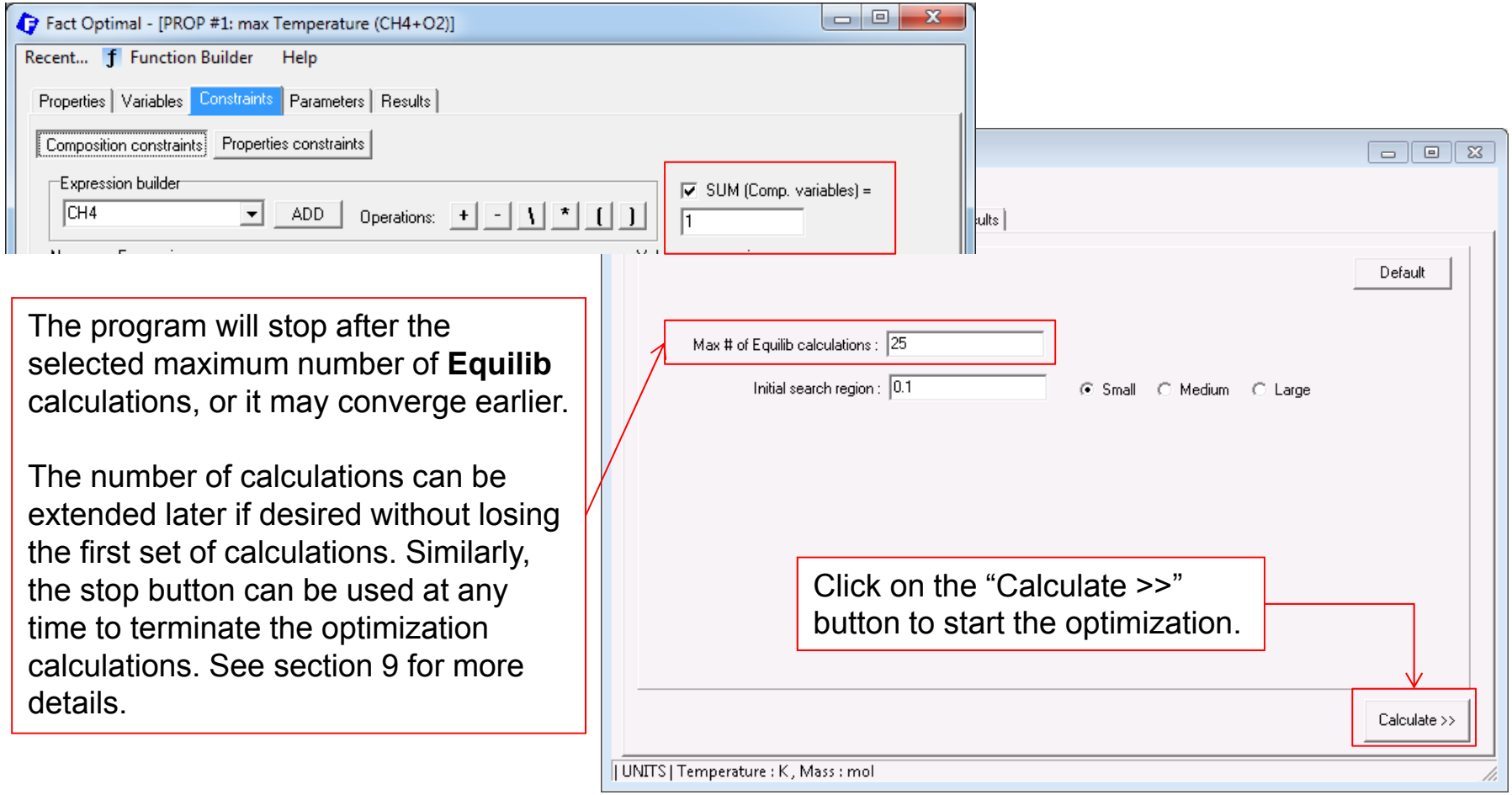
REAL type is chosen with values varying from 0 to 1. For INTEGER type, see example in section 3.7.

Only composition variables are used in this example.

Click on Next to go to the Constraints tab.

Example 1: Maximize an adiabatic flame temperature - 5

In the “Constraints” tab the sum of composition variables is set by default to 1. In the “Parameters” tab we define the maximum number of **Equilib** calculations and the search region. If the initial point is a good estimate of the expected answer, choose Small (0.1), otherwise choose Large (1) or Medium (0.5).



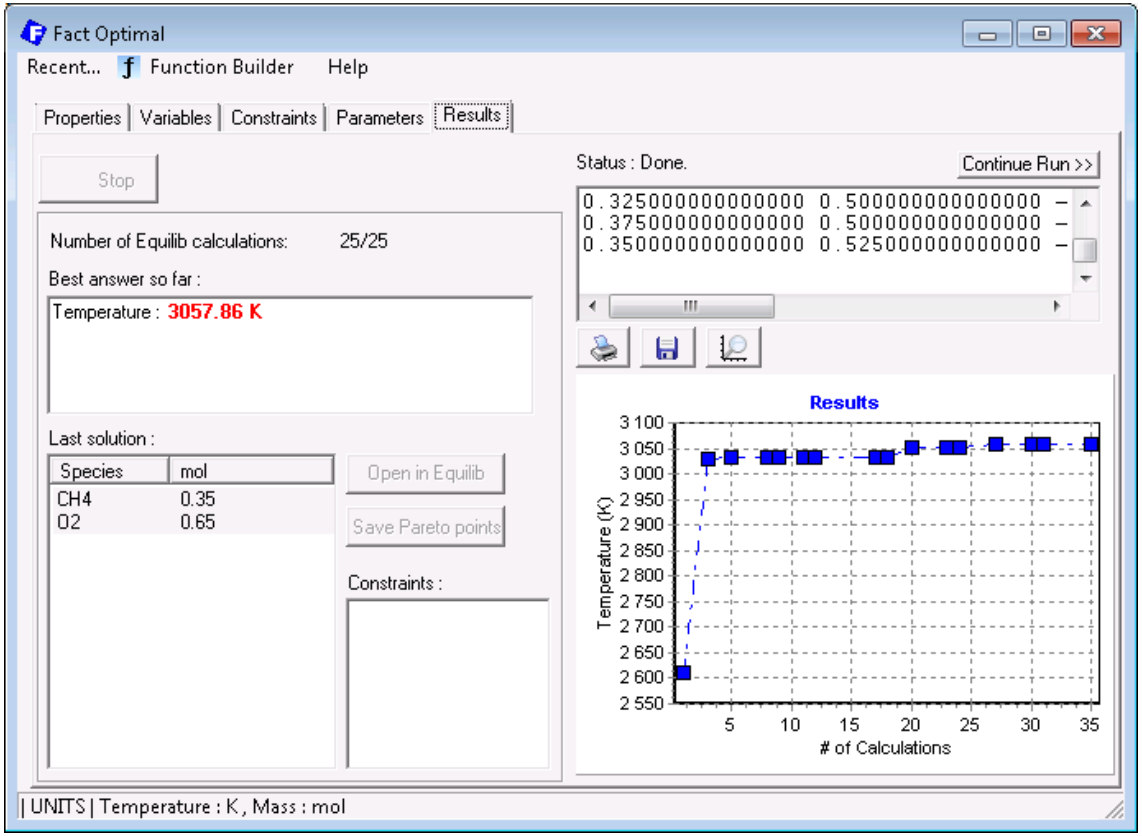
The program will stop after the selected maximum number of **Equilib** calculations, or it may converge earlier.

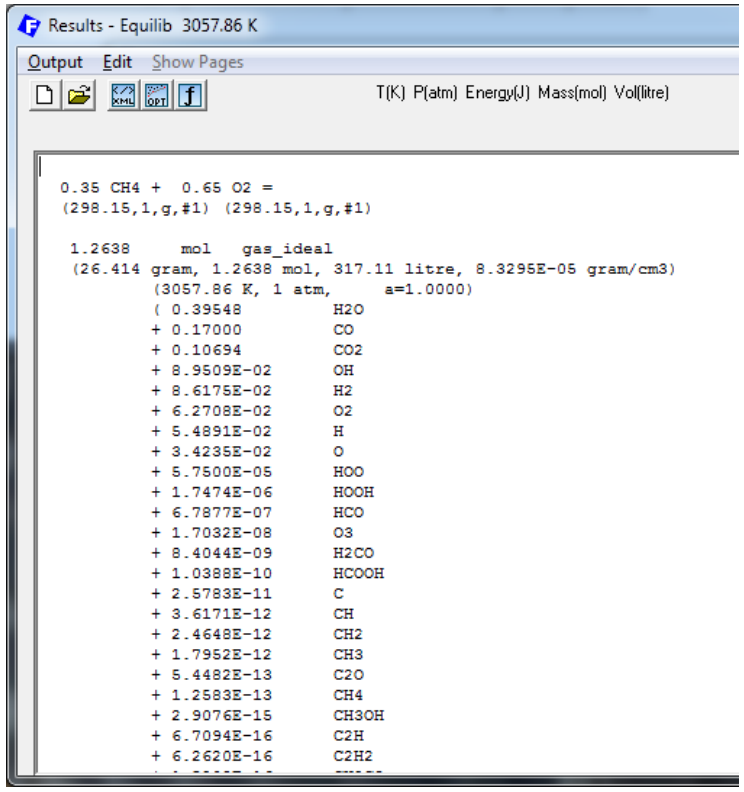
The number of calculations can be extended later if desired without losing the first set of calculations. Similarly, the stop button can be used at any time to terminate the optimization calculations. See section 9 for more details.

Click on the “Calculate >>” button to start the optimization.

Example 1: Maximize an adiabatic flame temperature - 6

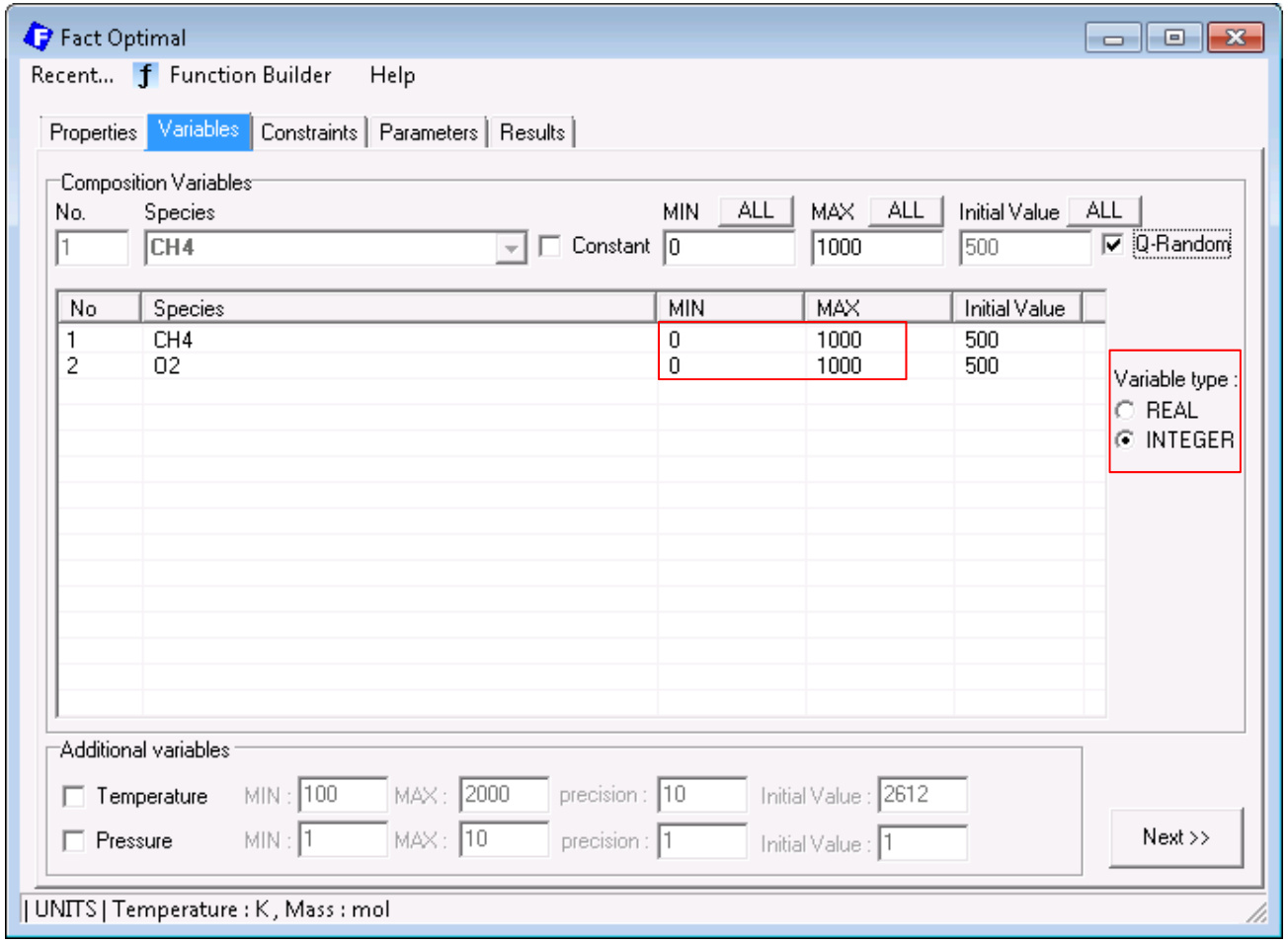
We obtain the results after 25 **Equilib** Calculations. The *Equilib Results Window* with the equilibrium calculation corresponds to the calculated maximum adiabatic flame temperature.



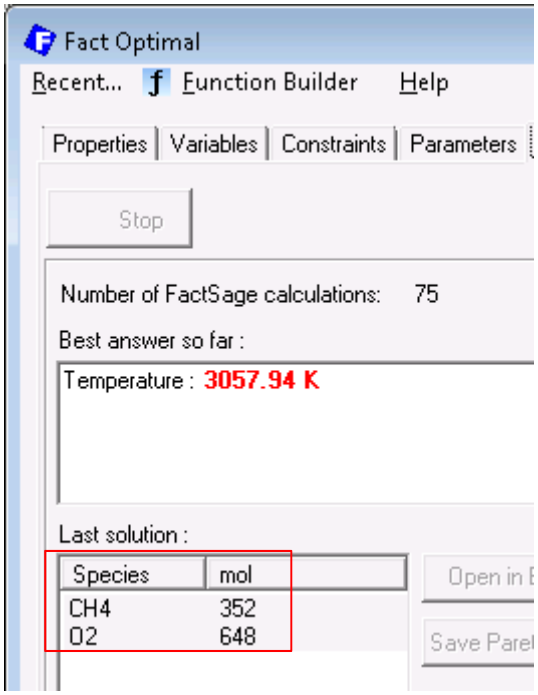


Example 1: Maximize an adiabatic flame temperature - 7

To decrease the number of significant digits and thereby decrease the computation time, you can choose to work with INTEGER type variables.

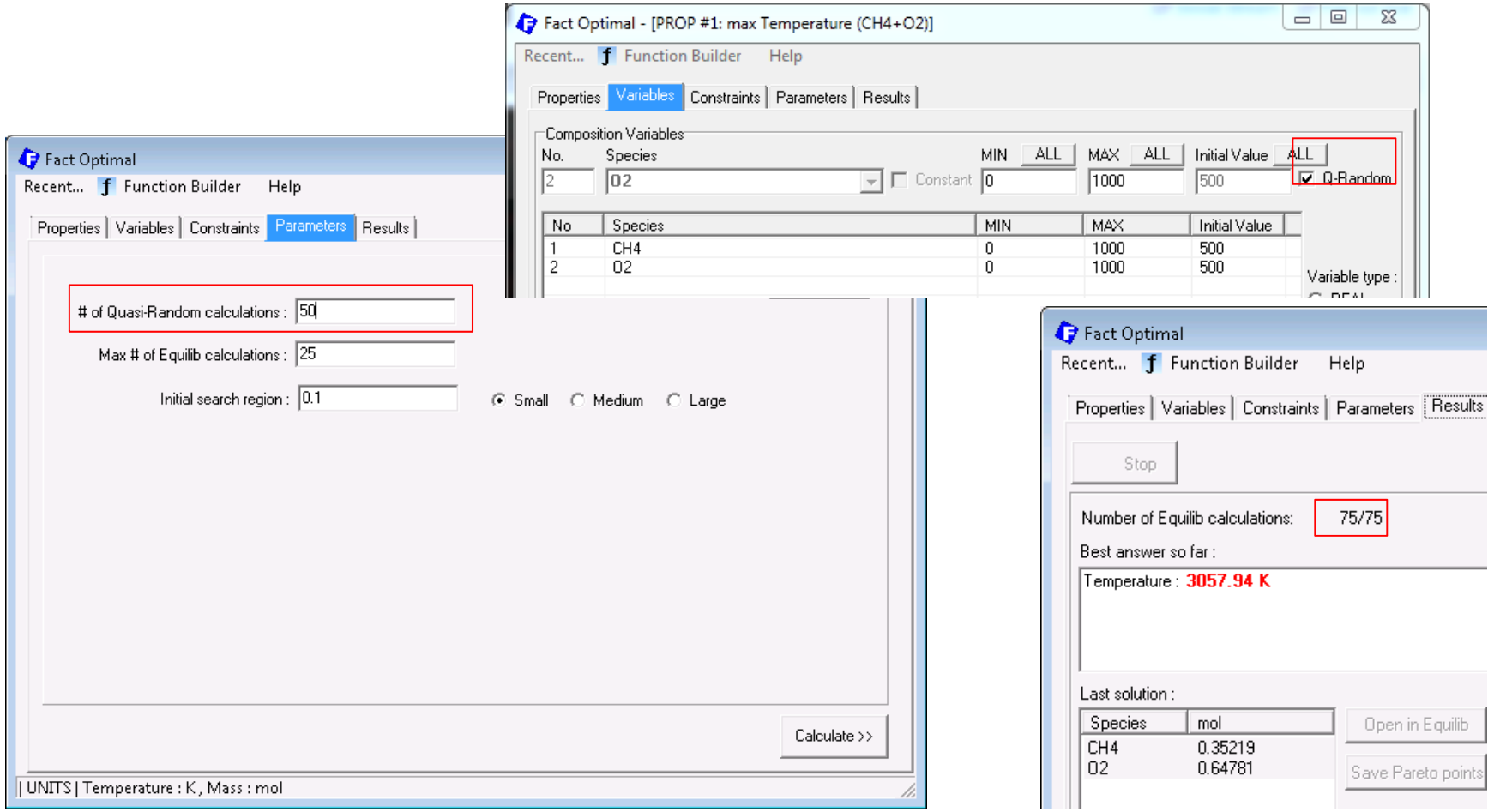


Using the same example, INTEGER type is chosen with values varying from 0 to 1000. By selecting this option as opposed to real values varying from 0 to 1, we are limiting the number of significant digits to 3.



Example 1: Maximize an adiabatic flame temperature - 8

When choosing the Quasi-Random option, we have to define the number of such calculations. In the present example 50 quasi-random calculations will be performed in order to get the best initial point, then 25 subsequent **Equilib** calculations will be performed to determine the *Pareto Front* (see slide 7.1) for a total of 75 calculations.

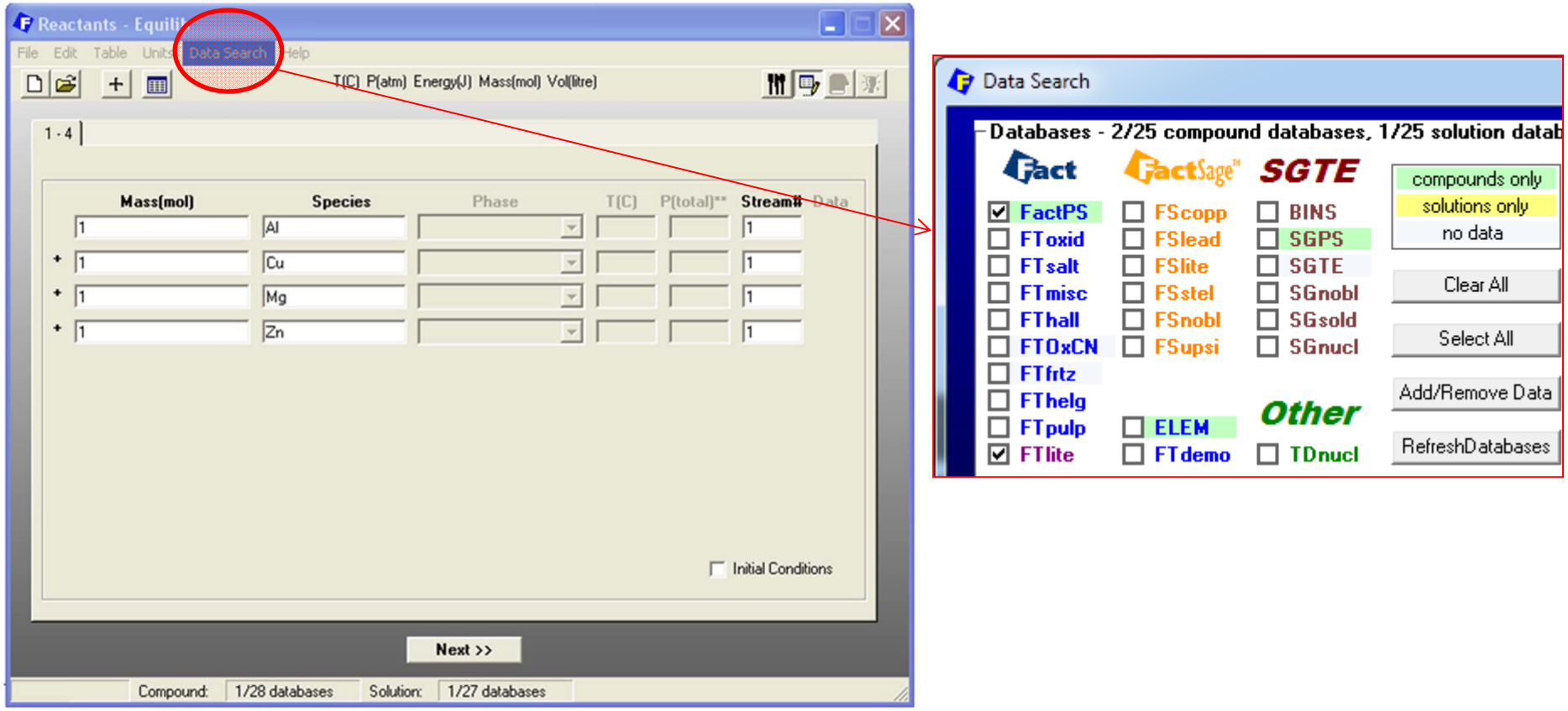


Example 2 : Minimize the liquidus temperature under constraints - 1

System: Al-Cu-Mg-Zn. Constraints:

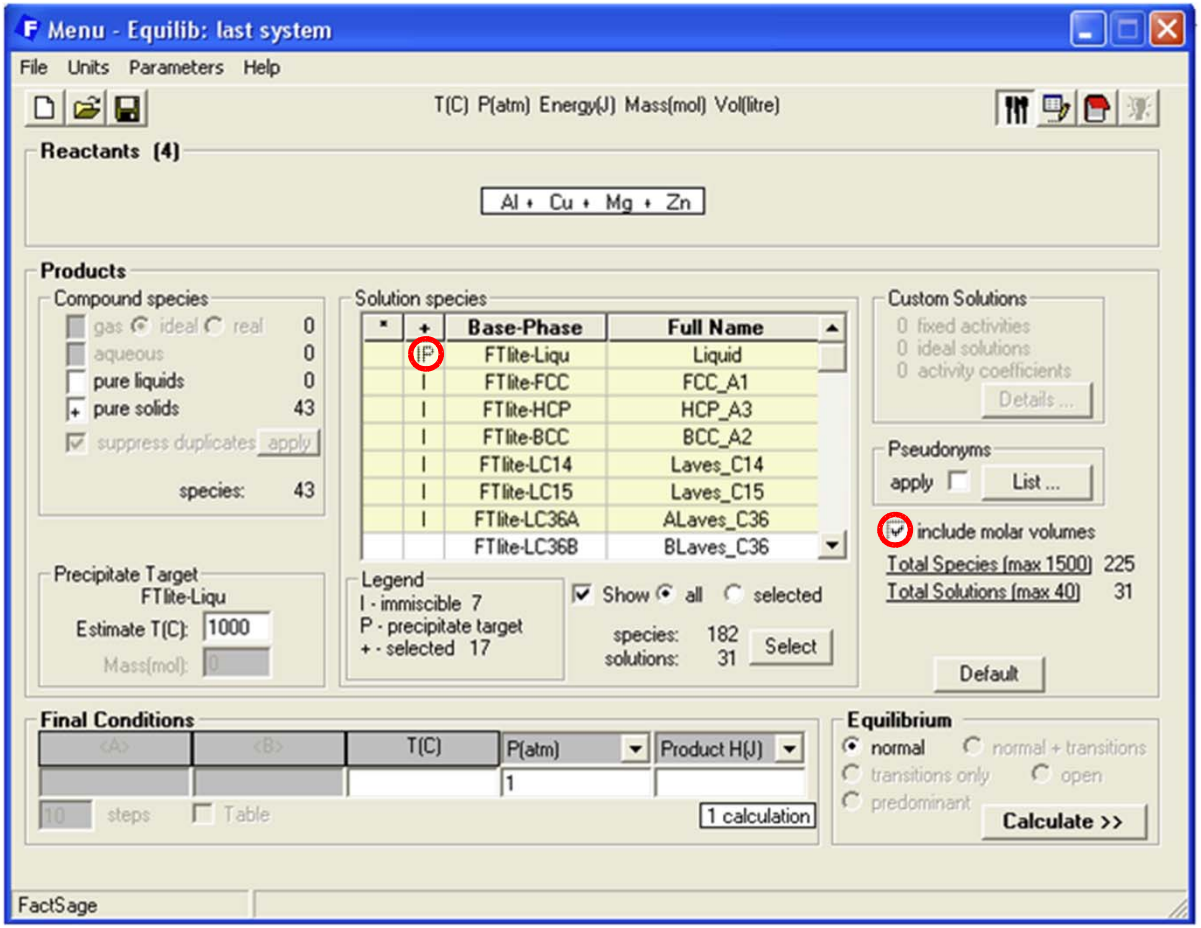
- **Sum of mole fractions (X_{Al} + X_{Cu}) < 0.2**
- **Density < 2.2 g/ml**
- **Cost < 2900 $/ton**

Step 1: Using **Equilib** define the system and select the appropriate databases: **FTlite**.



Example 2 : Minimize the liquidus temperature under constraints - 2

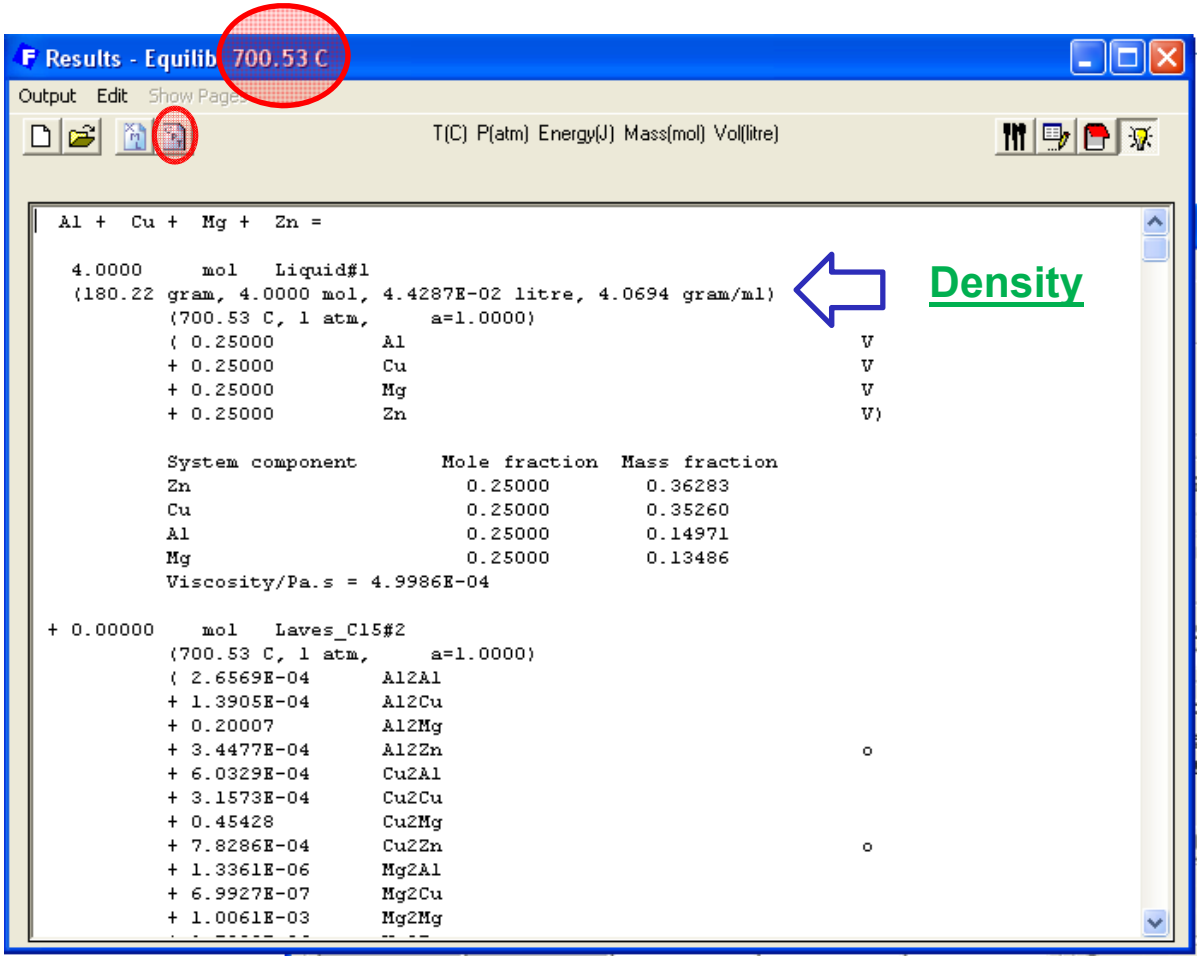
Step 2: Perform a single equilibrium calculation at an arbitrary composition and specify a precipitate (P) calculation on the liquid (i.e. liquidus temperature calculation) and “include molar volumes” (for the calculation of the density):



Example 2 : Minimize the liquidus temperature under constraints - 3

Equilib Results Window

Calculated liquidus temperature : 700.53°C

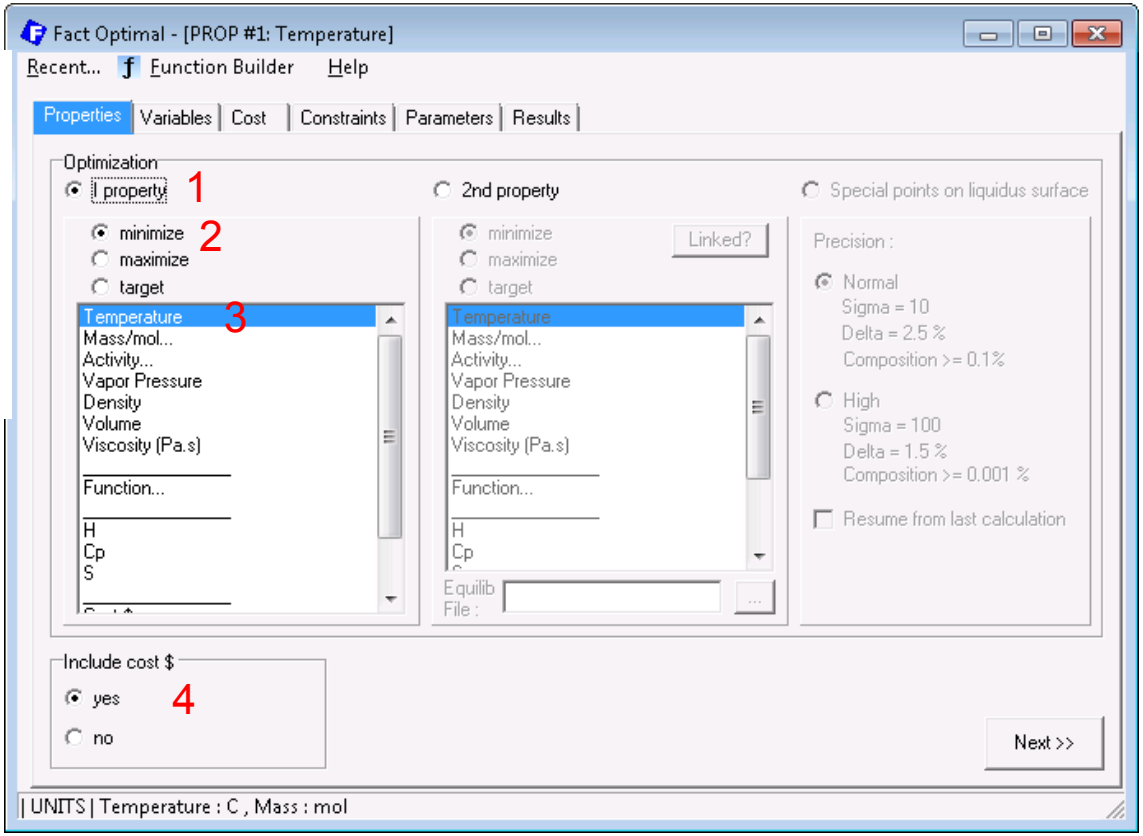


Example 2 : Minimize the liquidus temperature under constraints - 4

Step 3: Click on the **FactOptimal** icon and set up the calculation.

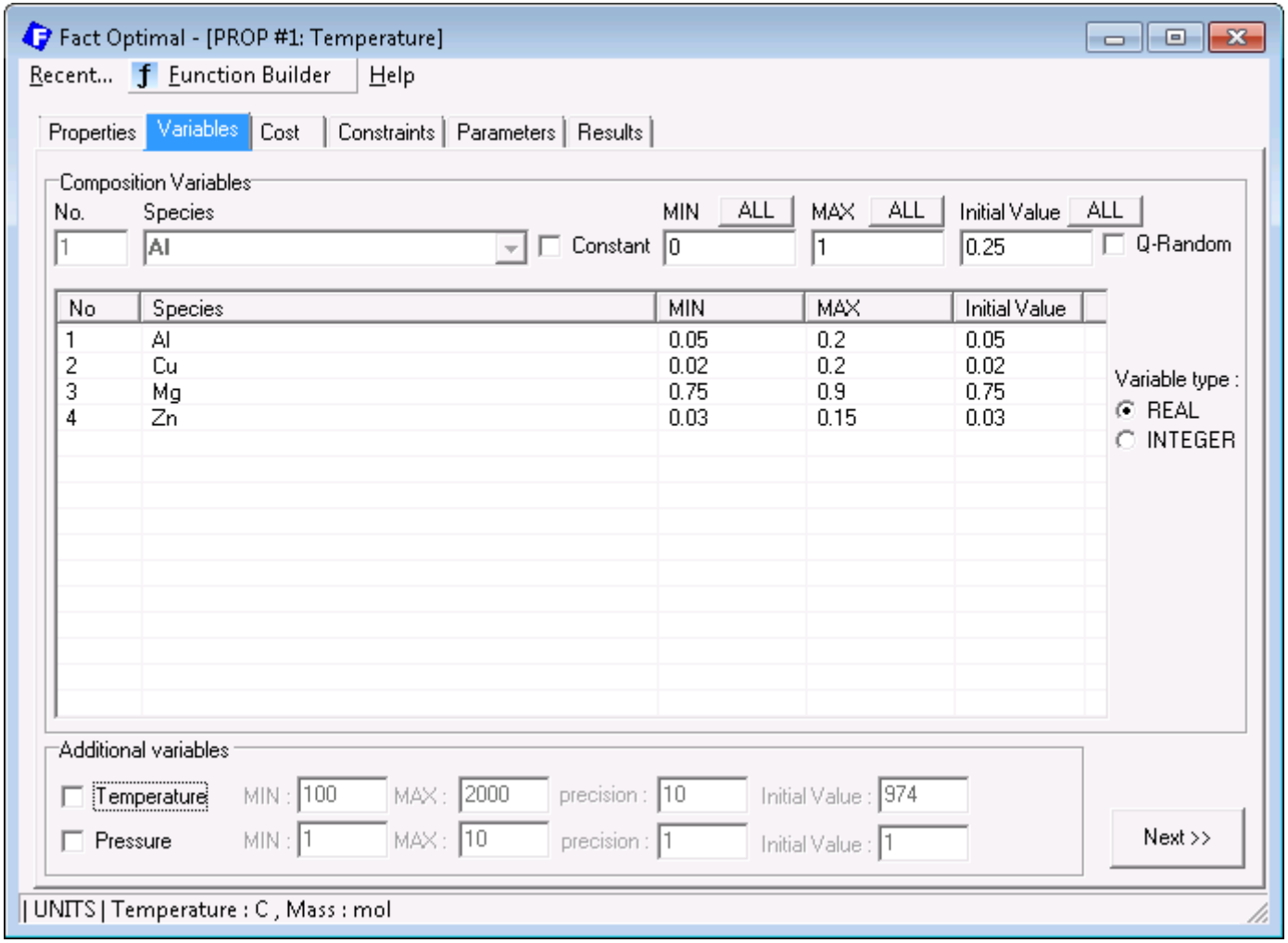
If you are using the stored example files, click on “Recent...” to load the Fact Optimal file. In this example, we specify that:

1. we consider **one property**
2. we want to **minimize this property**
3. the property is **temperature**
4. the **Cost** is to be included in the optimization



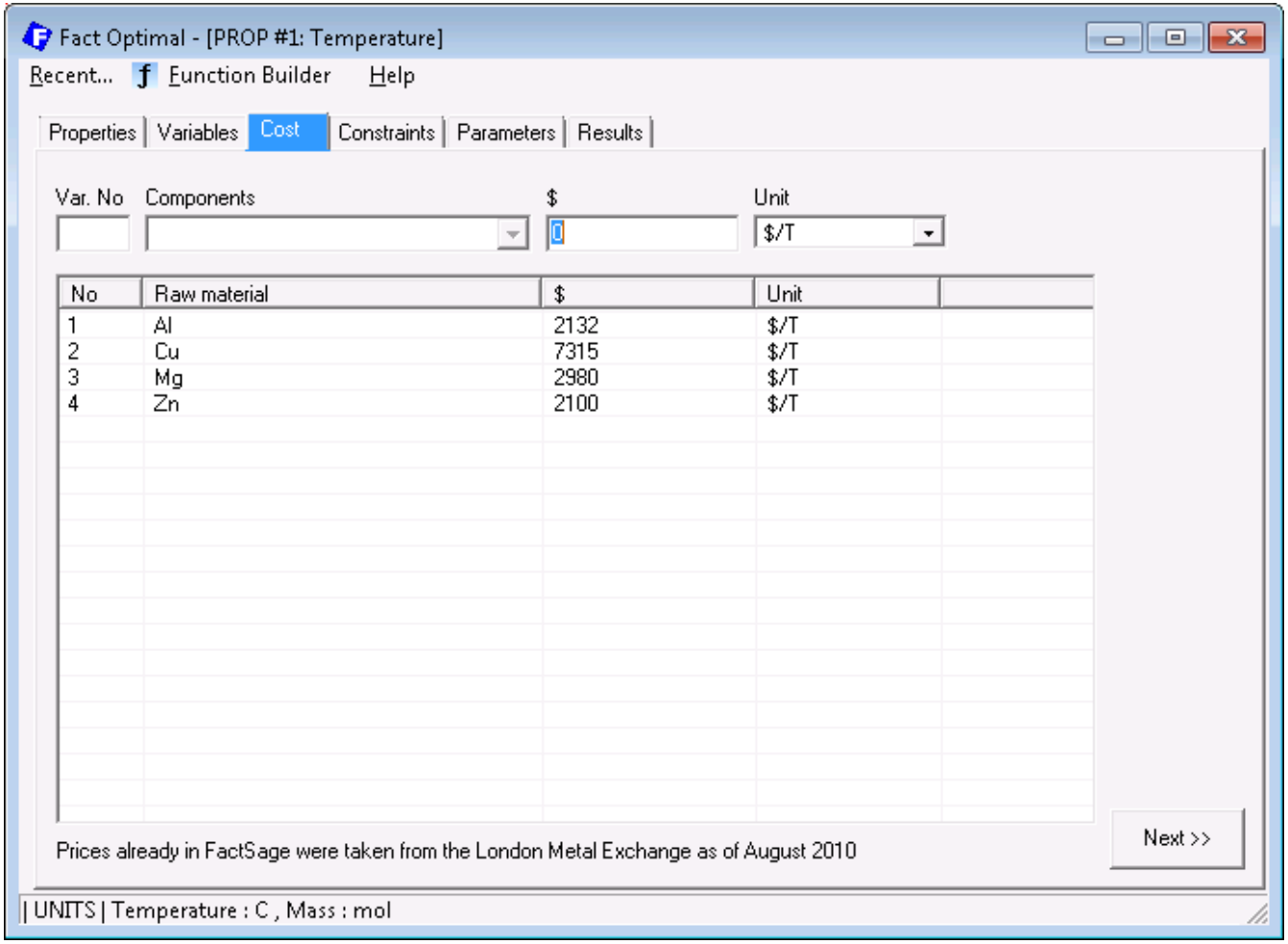
Example 2 : Minimize the liquidus temperature under constraints - 5

Step 4: Define the permissible composition range and a set of initial estimates



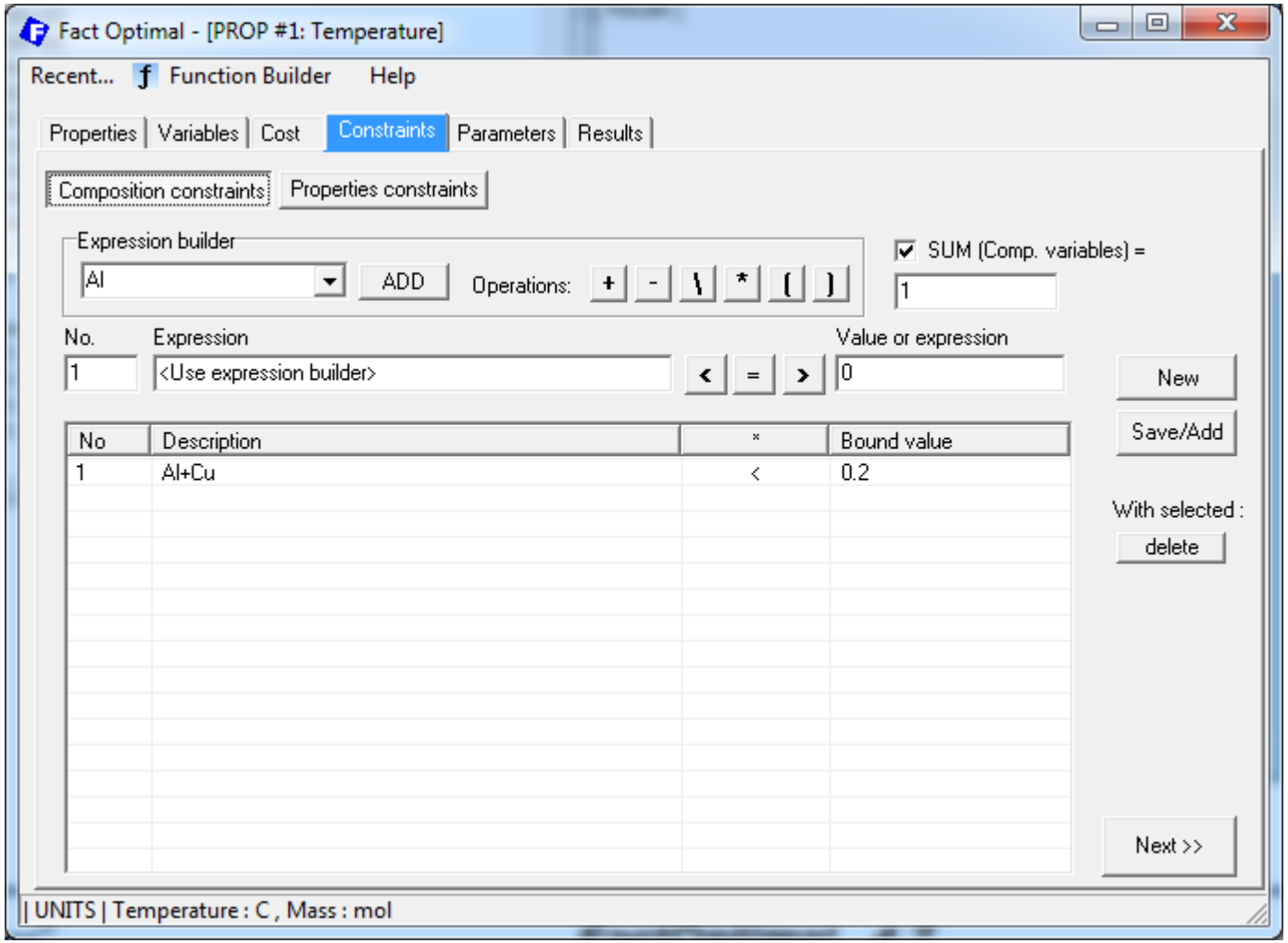
Example 2 : Minimize the liquidus temperature under constraints - 6

The materials costs can either be defined (if they are not available) or updated using the tab “cost”.



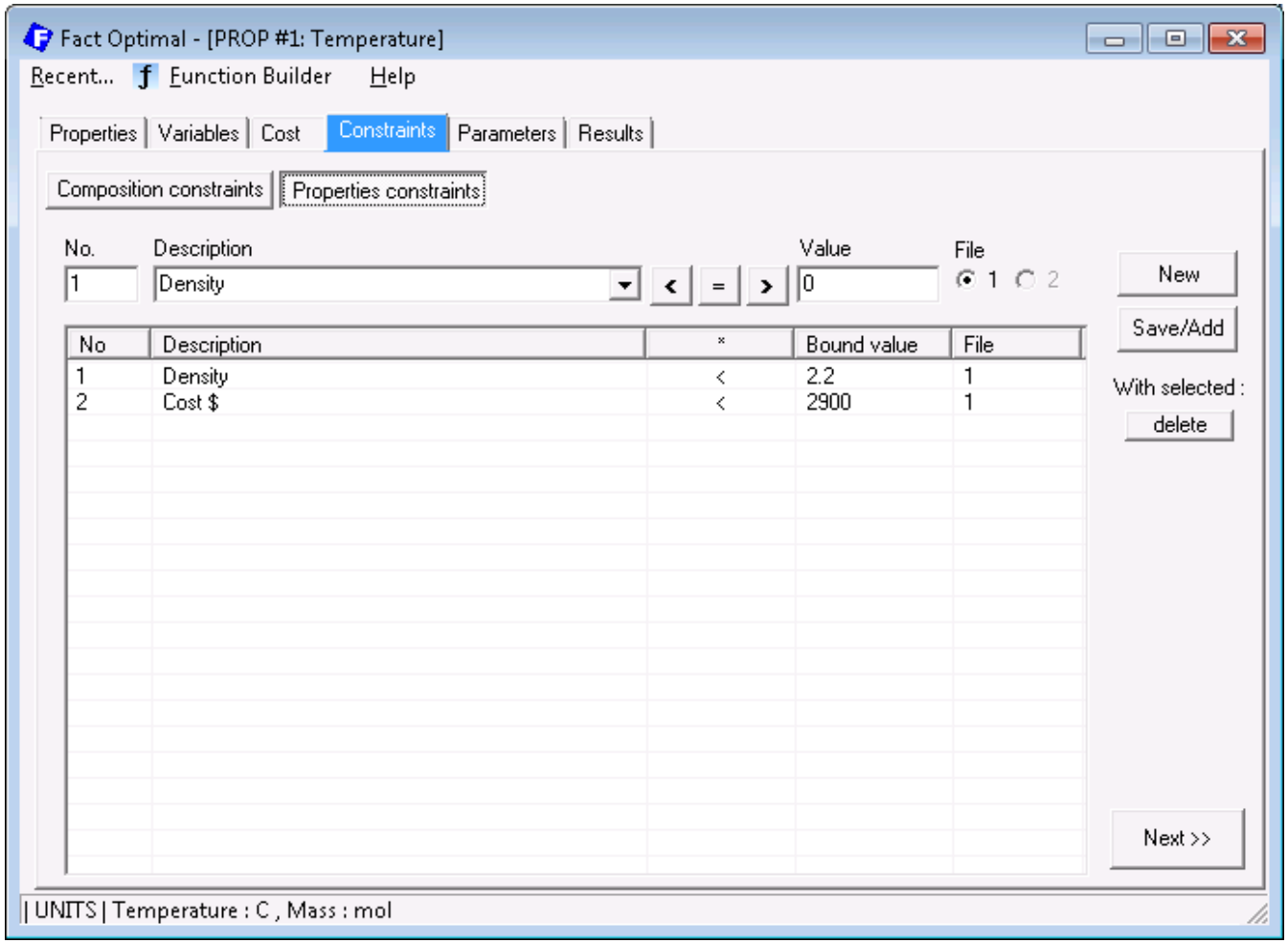
Example 2 : Minimize the liquidus temperature under constraints - 7

Step 5: Define the constraints on composition: **X(Al) + X(Cu) < 0.2**



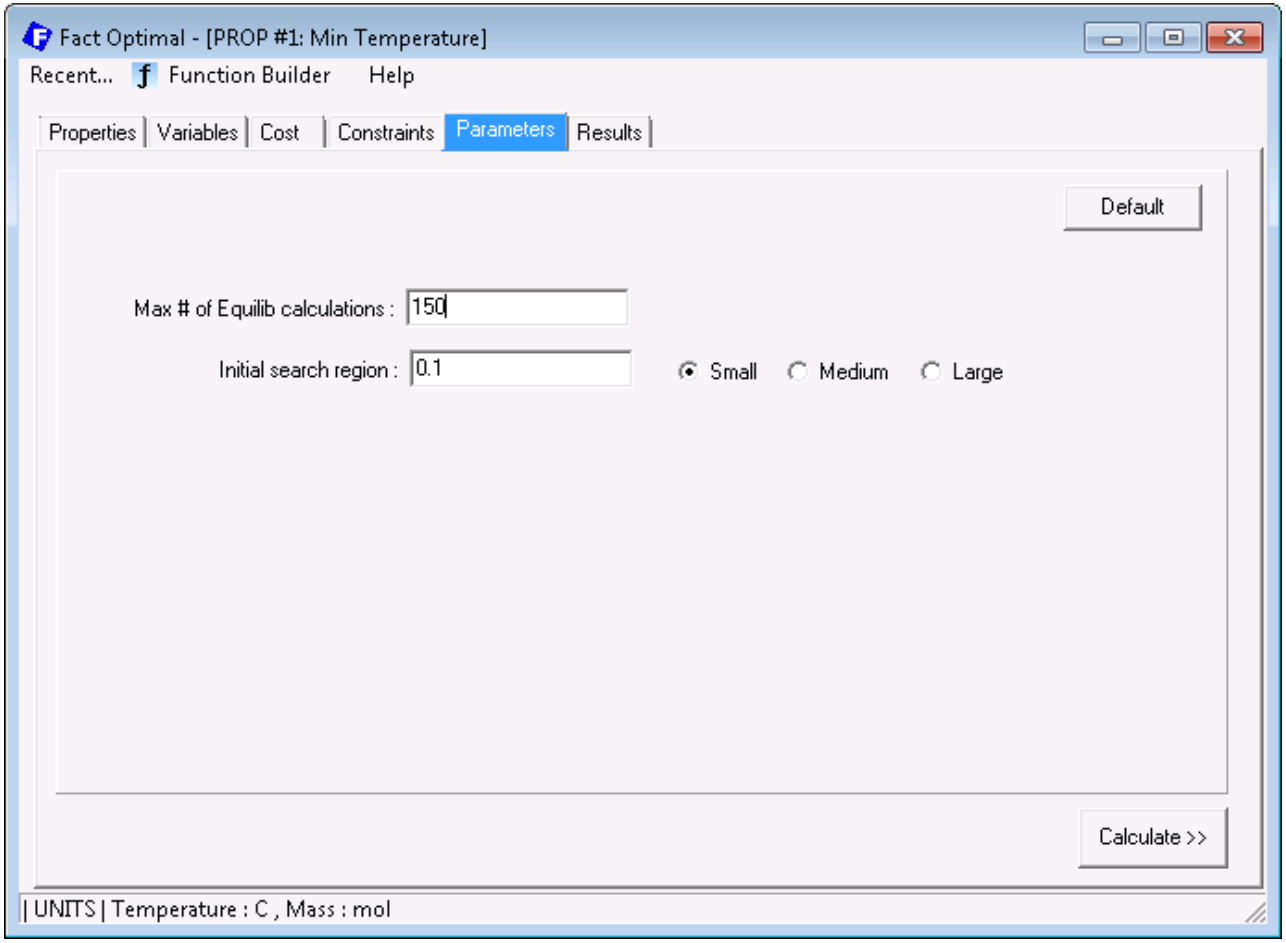
Example 2 : Minimize the liquidus temperature under constraints - 8

Step 6: Define the constraints on properties : **ρ < 2.2 g/ml cost < 2900 $/Ton**



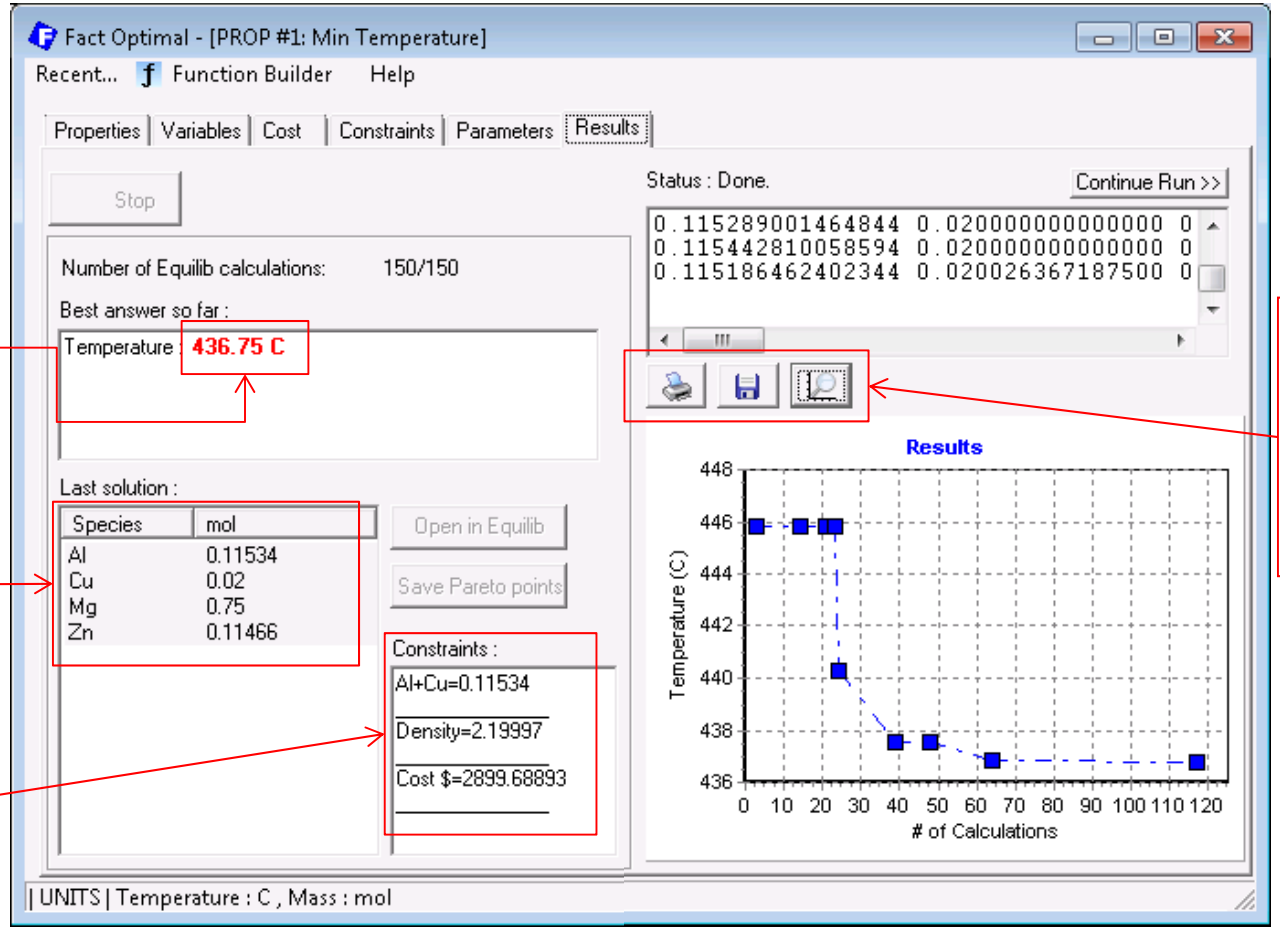
Example 2 : Minimize the liquidus temperature under constraints - 9

Enter the maximum number of **Equilib** calculations
and the initial search region (see slide 3.5).



Example 2 : Minimize the liquidus temperature under constraints - 10

FactOptimal Results Window



Minimum

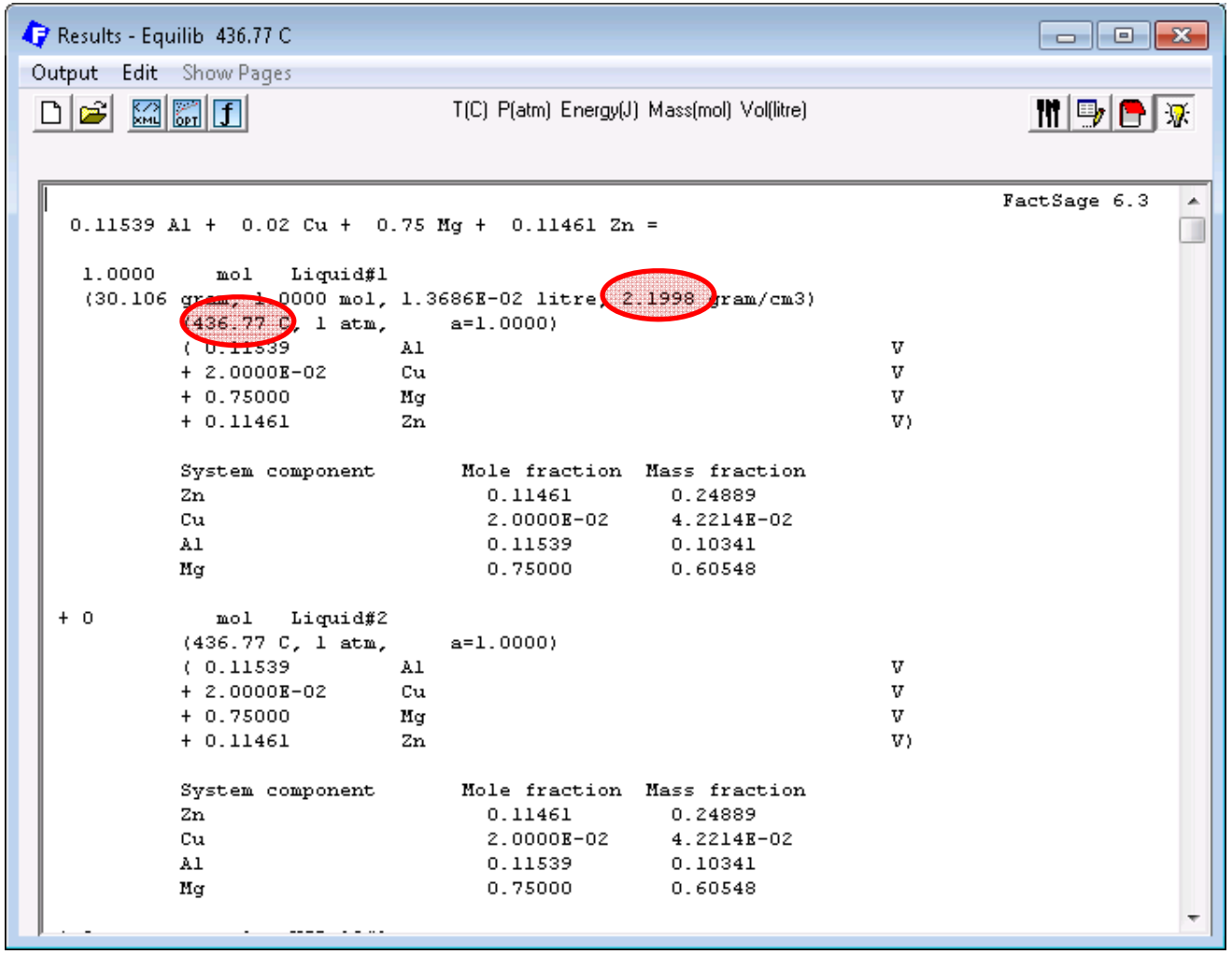
Composition at the minimum

Values of the chosen constraints

Save and print the graph or change the axis scale

Example 2 : Minimize the liquidus temperature under constraints - 11

Equilib Results Window



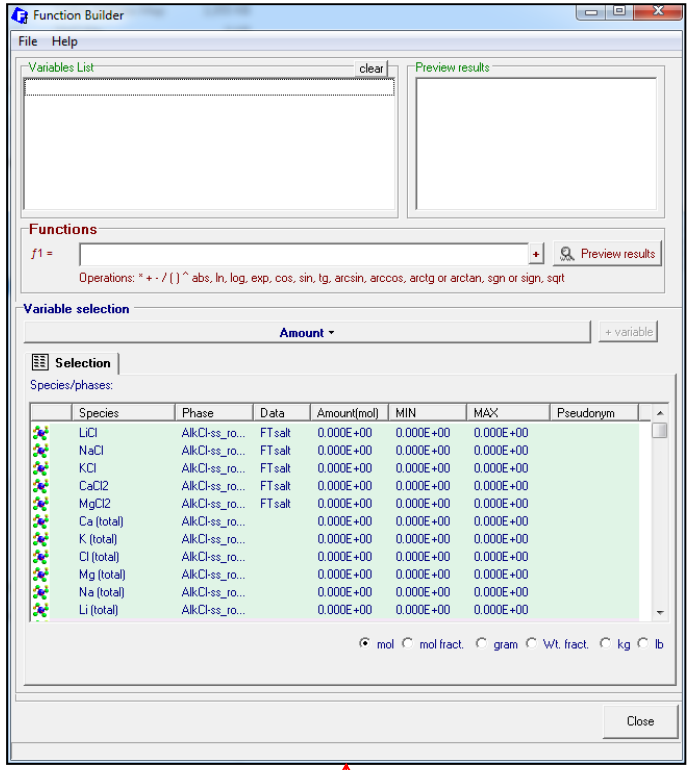
Optimization using the Function Builder - 1

In addition to optimizing properties that can be calculated by **Equilib**, **FactOptimal** also allows optimization of user-defined properties, in the form of functions of properties calculated by **Equilib**.

For example, Redkin [1] has proposed that the electrical conductivity σ of molten chloride solutions can be expressed as :

ln(σ) = 4.9*exp[-(2747-33724/V)/T]*exp(53.7/V)

where V is the volume of the solution in litres. This formula can be saved in the ***Function Builder*** and then chosen as a property to be optimized.



[1] A. Redkin, Relationship between Electrical Conductivity and Thermodynamic Properties of Binary Molten Salt Mixtures http://www.electrochem.org/dl/ma/201/pdfs/1420.pdf

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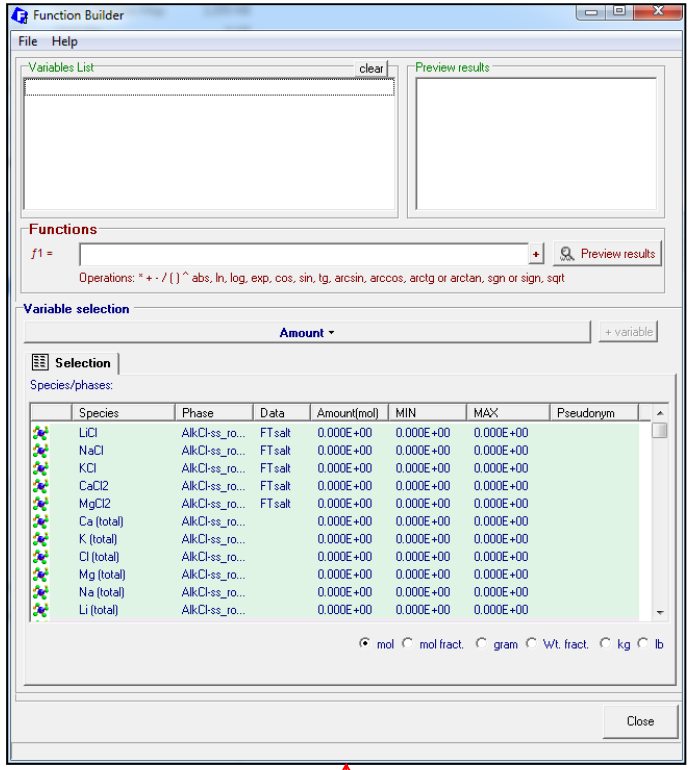
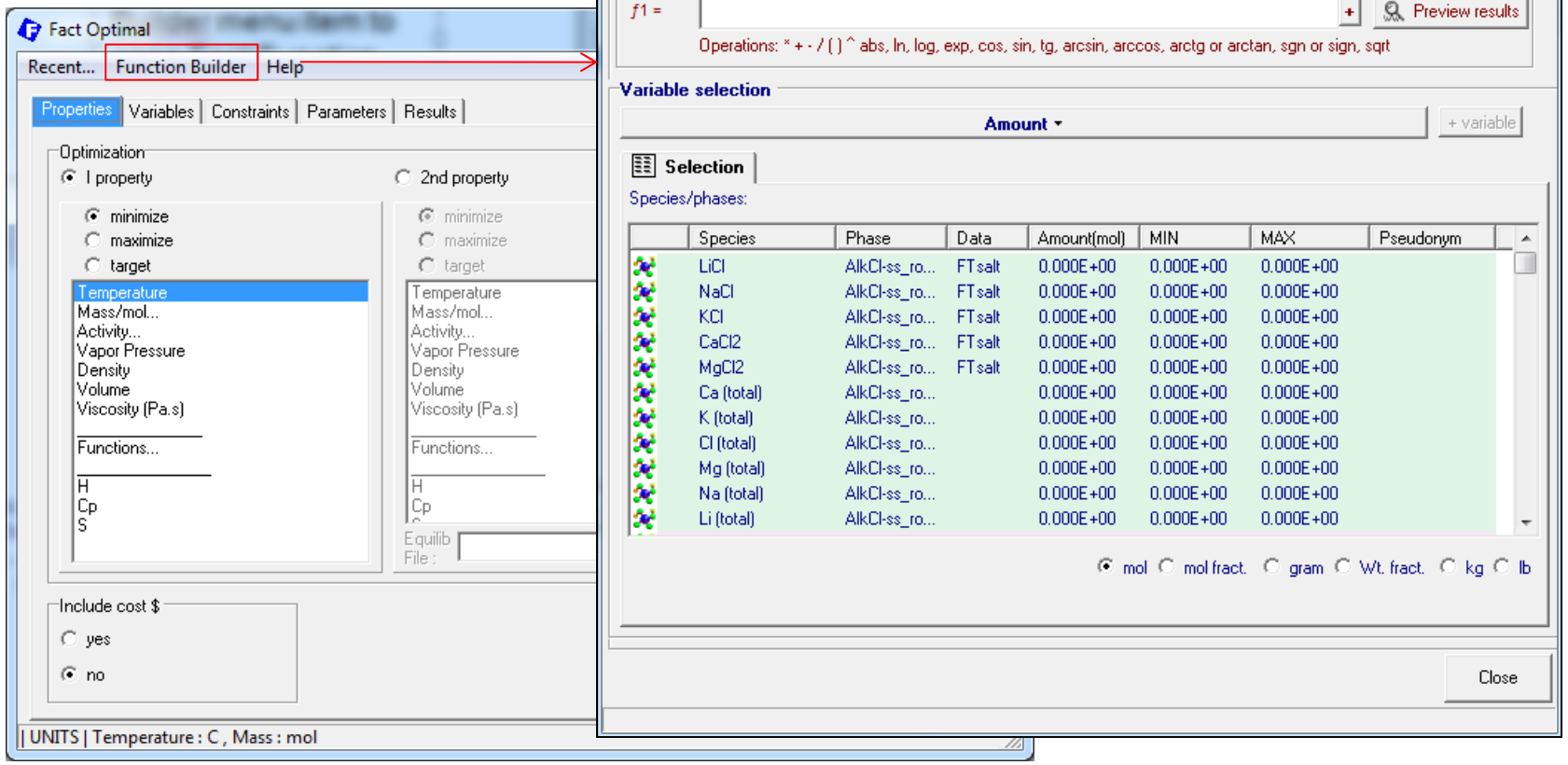


[1] A. Redkin, Relationship between Electrical Conductivity and Thermodynamic Properties of Binary Molten Salt Mixtures http://www.electrochem.org/dl/ma/201/pdfs/1420.pdf

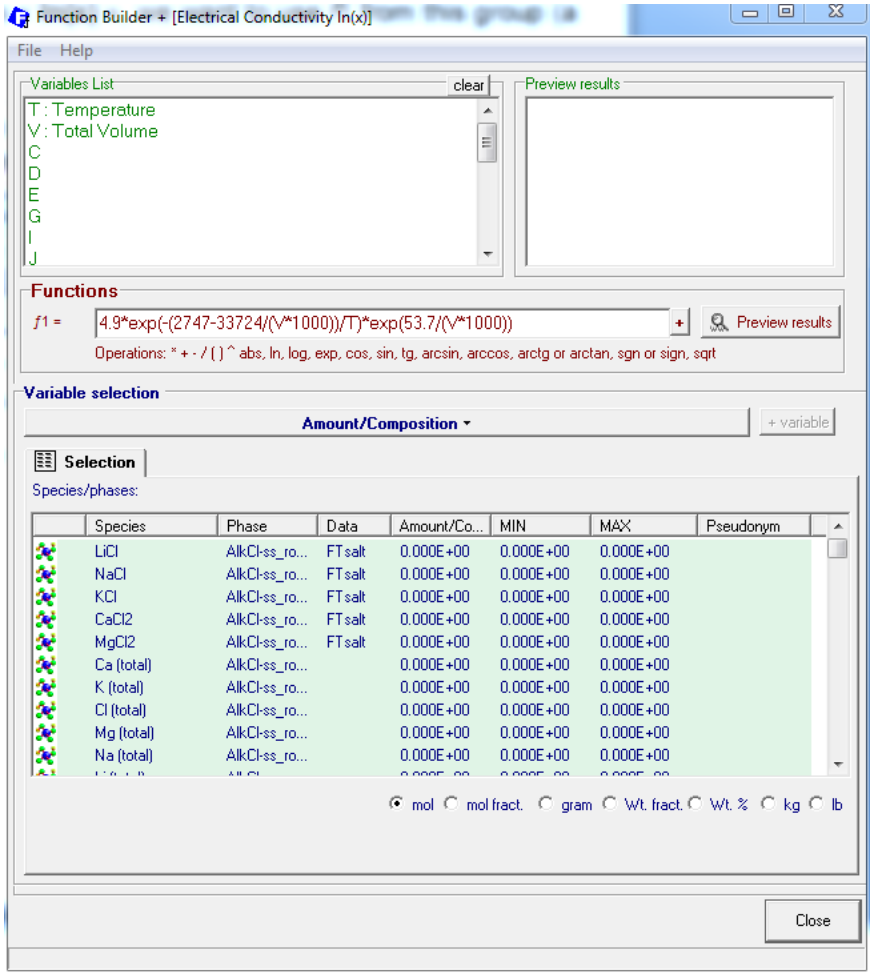
Optimization using the Function Builder - 2

Click on the *Function Builder* icon to open the *FactSage Function Builder*. Edit or build a new group of functions, then save it. For help click on the *Function Builder* icon and then on *'Help > PDF SlideShow'*

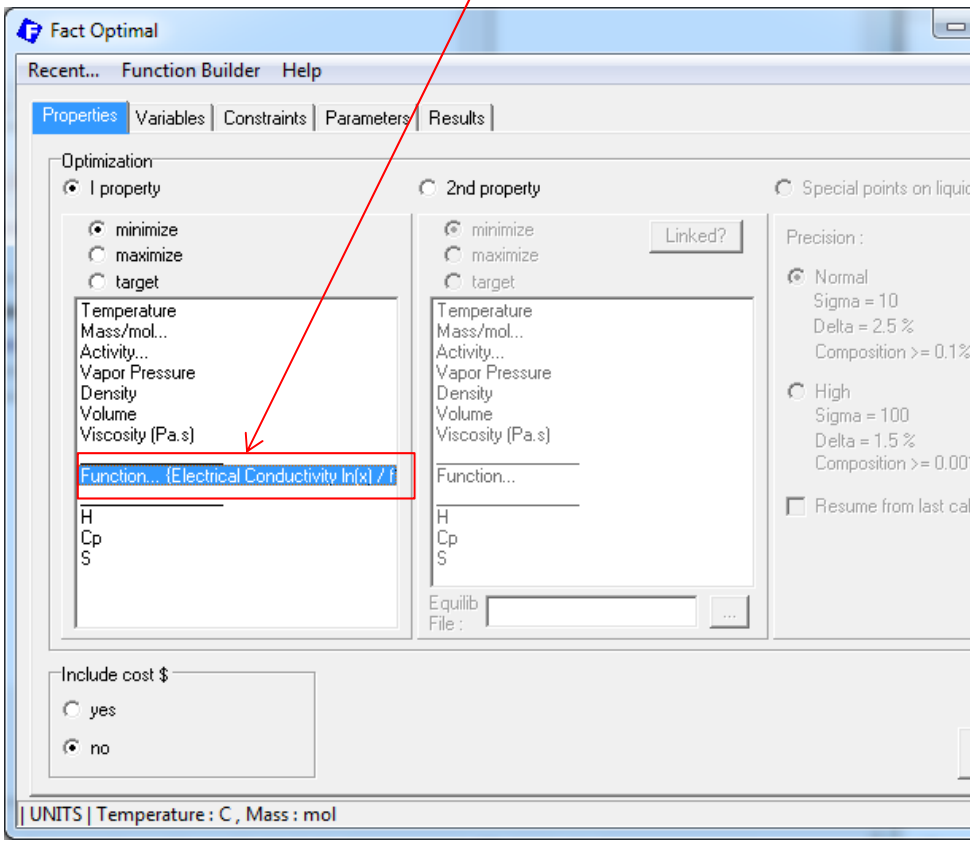


Optimization using the Function Builder - 3

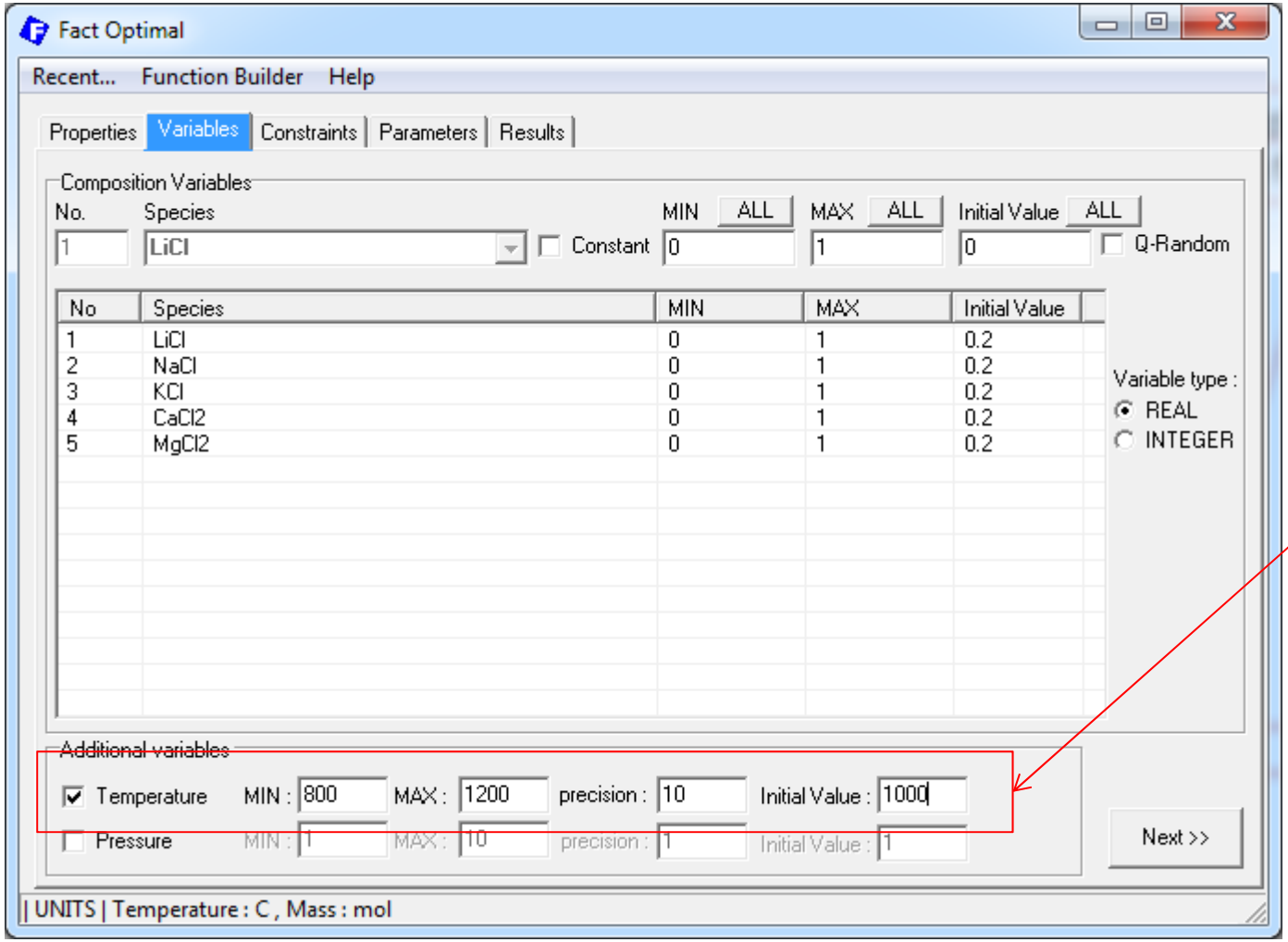
Here we enter the formula for electrical conductivity in the *Function Builder*. A group of functions is created in Function Builder, saved as « **Electrical Conductivity ln(x)** ». We want to use the fuction *f*1 from this group (a group can contain up to 10 functions *f*1, *f*2, *f*3, etc.)



To minimize the Electrical Conductivity, select the saved function as the first property.



Optimization using the Function Builder - 4



In this example, the temperature is set as an additional variable. FactOptimal will now determine the composition and temperature which minimize the electrical conductivity.

Additional options can then be selected and the Electrical Conductivity can be optimized.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