

# 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 be defined as:

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

where **wt S** is the Wt.% solubility of sulfur in the slag, and **Po<sub>2</sub>** and **Ps<sub>2</sub>** are the equilibrium partial pressures of O<sub>2</sub>(g) and S<sub>2</sub>(g).

In this example **wt S** is calculated across the SiO<sub>2</sub> – MnO binary system at 1650°C with the partial pressures fixed at **Po<sub>2</sub>** = 10<sup>-10</sup> and **Ps<sub>2</sub>** = 10<sup>-6</sup> 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

Reactants - Equilib

File Edit Table Units Data Search Help

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

1 - 3

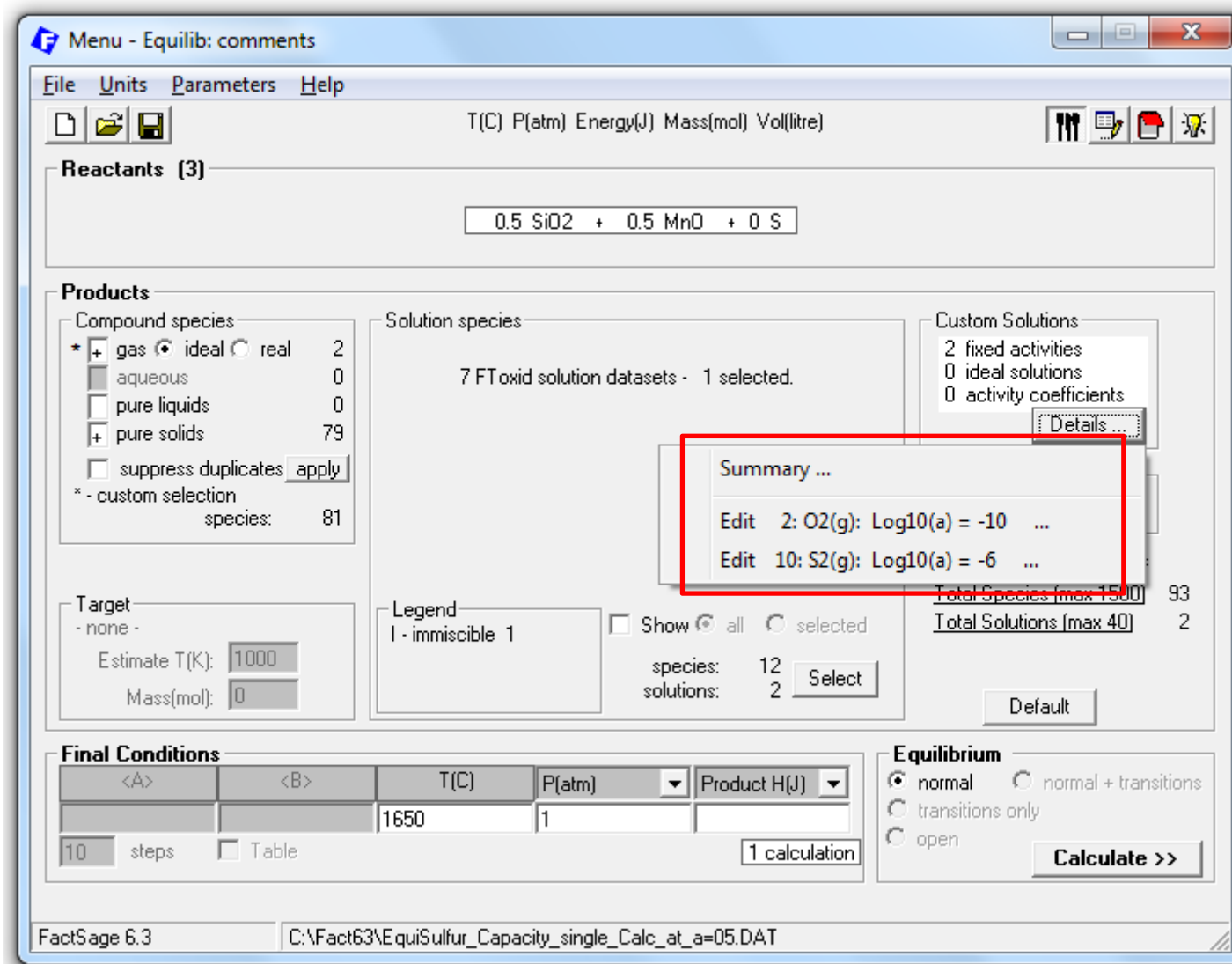
Mass(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
0.5	SiO2				1	
+ 0.5	MnO				1	
+ 0	S				1	

☐ Initial Conditions

Next >>

FactSage 6.3 Compound: 3/28 databases Solution: 1/28 databases

## Example 2 – Plotting slag sulfide capacity



## Example 2 – Plotting slag sulfide capacity

Results - Equilib 1650 C

Output Edit Show Pages

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

FactSage 6.3

0.5 SiO2 + 0.5 MnO + 0 S =

- 3.0627E-03 O2

+ 3.0789E-03 S2

0 mol gas\_ideal  
(1650 C, 1 atm, a=1.0001E-06)

( 1.0000E-06 S2  
+ 1.0000E-10 O2

FactPS  
FactPS)

+ 0.99997 mol ASlag-liq#1  
(65.610 gram, 0.99997 mol)  
(1650 C, 1 atm, a=1.0000)

( 0.49796 SiO2  
+ 0.49790 MnO  
+ 3.2354E-05 Mn2O3  
+ 2.0526E-03 SiS2  
+ 2.0524E-03 MnS  
+ 1.3337E-07 Mn2S3

o FToxid  
o FToxid  
o FToxid  
o FToxid  
o FToxid  
o FToxid)

Site fraction of sublattice constituents:

Si 0.50000  
Mn2+ 0.49994  
Mn3+ 6.4973E-05

-----

O 0.99589  
S 4.1051E-03

System component Mole fraction Mass fraction

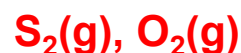
Mn 0.20000 0.41867  
S 2.4631E-03 3.0094E-03  
Si 0.20000 0.21403  
O 0.59754 0.36429

$$\log(C_s) = \log((\text{wt S}) \times (P_{\text{O}_2}/P_{\text{S}_2})^{1/2}) = -2.521514$$

# Step 1: *Equilib* input

The reaction is based on  $\text{<1-A> SiO}_2 + \text{<A> MnO} + 0 \text{ S}$  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 :



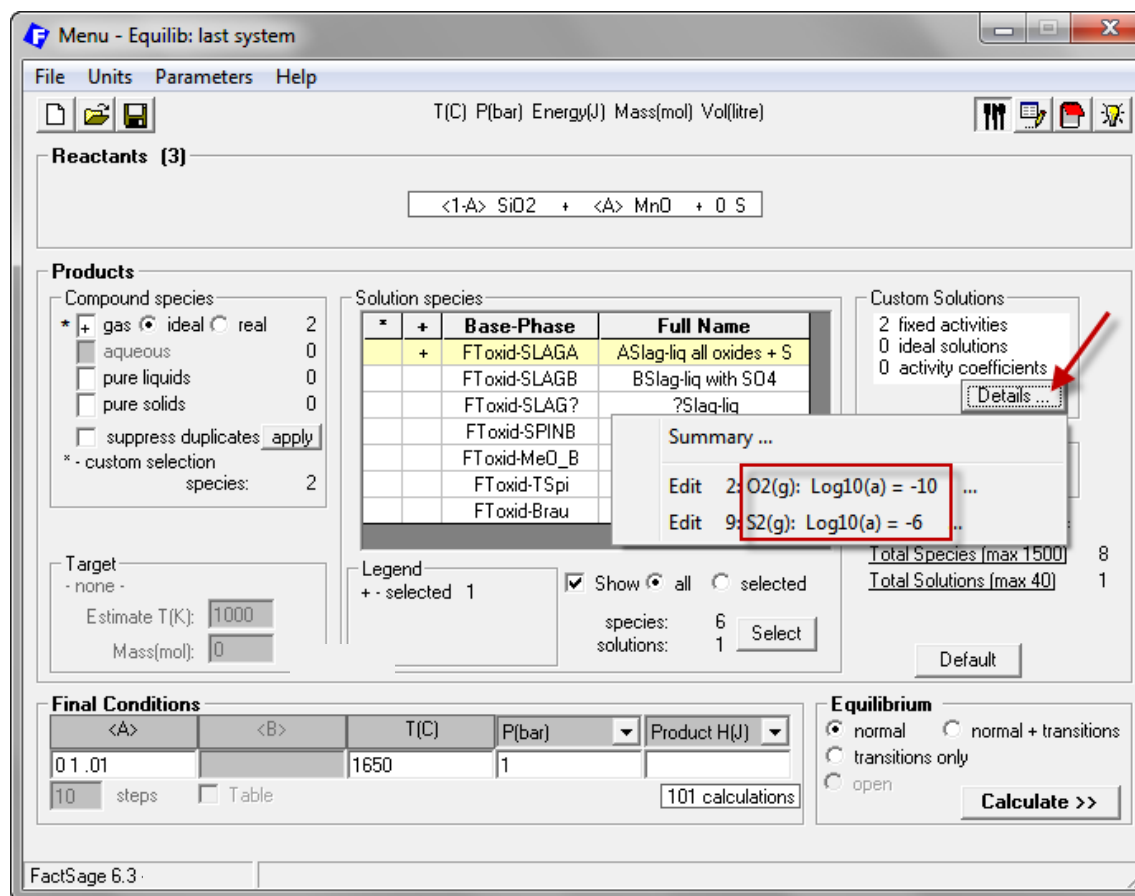
and their equilibrium partial pressures are fixed:

$$\log(P_{\text{O}_2}) = -10$$

$$\log(P_{\text{S}_2}) = -6$$

- 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  $\text{<A>} = 0, 0.01, 0.02, \dots, 1$ .

# Step 1: Defining *Equilib* P(O<sub>2</sub>) and P(S<sub>2</sub>)

The screenshot shows the FactSage 6.3 interface with the 'Equilib' tab selected. The 'Reactants' list on the left contains '1' (highlighted with a red box and arrow labeled '1'). The 'Products' list contains '2' (highlighted with a red box and arrow labeled '2'). A context menu is open over the '2' in the products list, showing options like 'clear', 'select', 'standard stable phase', etc. The 'Activity' option is selected (highlighted with a red box and arrow labeled '3'). A 'Fixed Partial Pressure' dialog box is open, showing the input field for log10(p) with the value '-10' entered (highlighted with a red box and arrow labeled '4').

1. Mouse-right-click on products gas '+'

2. Mouse-right-click on O<sub>2</sub>(g) and on S<sub>2</sub>(g) '+' cells

3. Select 'a Activity > log10(activity) ...'

4. Enter log10(P<sub>O<sub>2</sub></sub>) = -10 ; log10(P<sub>S<sub>2</sub></sub>) = -6

+	Code	Species	Data	Phase	T	V	Activity	Minimum	Maximum
1	O(g)	FactPS	gas						
2	O <sub>2</sub> (g)								
3	O <sub>3</sub> (g)								
4	Si(g)								
5	Si <sub>2</sub> (g)								
6	Si <sub>3</sub> (g)								
7	SiO(g)								
8	S(g)								
9	S <sub>2</sub> (g)								
10	S <sub>2</sub> (g)								

Fixed Partial Pressure

Enter the value of log10(p)  
(or for a range of values enter 'first last step') for  
2 O<sub>2</sub>(g).

Press [Cancel] if the partial pressure is no longer fixed.

-10



# Step 1: *Equilib* output

The *Results Window* contains 101 pages with  $\langle A \rangle = 0, 0.01, 0.02, \dots 1$ .

This is the *Equilib* output at page 51 where

$$\langle A \rangle = 0.5$$

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  $3.0094 \times 10^{-3}$

$$\text{Wt\% S} = 0.30094$$

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  
+ 1.0000E-10 O2 FactPS  
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: **f1 = 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**

The screenshot shows the 'Function Builder + [SiO2-MnO\_S\_capacity]' window. It includes a 'Variables List' on the left, a 'Functions' input box in the center, a 'Preview results' table on the right, and a 'Variable selection' table at the bottom. Red arrows and boxes highlight key steps: 1 points to the variable list, 2 points to the function input box, 3 points to the 'Preview results' button, and 4 points to the 'File' menu.

**Variables List**

- wtS : Amount/Composition (S (total)/Slag-liq)) wt. %
- aO2 : Activity (O2/Gas)
- aS2 : Activity (S2/Gas)
- G
- I
- J
- K
- L

**Functions**

f1 =  $\log(\text{wtS} * \text{SQRT}(\text{aO2}/\text{aS2}))$

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

**Preview results**

Page	f1 = log(wtS * SQRT(aO2/aS2))
1	-4.677854
2	-3.972706
3	-3.610284
4	-3.401473
5	-3.266302
6	-3.173698
7	-3.108676
8	-3.067857

**Variable selection**

Amount/Composition

**Selection**

Species/phases:

	Species	Phase	Data	Amount/...	MIN	MAX	Pseudonym
	O2	Gas	FactPS	0.000E+00	0.000E+00	0.000E+00	
	S2	Gas	FactPS	0.000E+00	0.000E+00	0.000E+00	
	Mn (total)	Gas		0.000E+00	0.000E+00	0.000E+00	
	S (total)	Gas		0.000E+00	0.000E+00	0.000E+00	
	Si (total)	Gas		0.000E+00	0.000E+00	0.000E+00	
	O (total)	Gas		0.000E+00	0.000E+00	0.000E+00	
	SiO2	Slag-liq	FToxid	1.000E+02	0.000E+00	1.000E+02	
	MnO	Slag-liq	FToxid	0.000E+00	0.000E+00	7.267E+01	
	Mn2O3	Slag-liq	FToxid	0.000E+00	0.000E+00	9.685E-02	
	SiS2	Slag-liq	FToxid	3.019E-03	0.000E+00	2.669E+00	

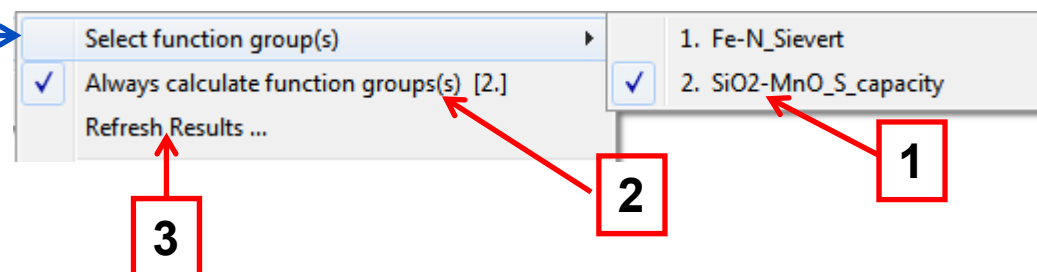
☐ mol ☐ mol fract. ☐ gram ☐ Wt. fract. ☒ Wt. % ☐ kg ☐ lb

# 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 **f1 - slag  
sulfide capacity** - for all the pages..

Results - Equilib Functions (page 0/101)

Output Edit Show Pages

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

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=0.20
Functions	A=0	A=0.01	A=0.02	A=0.03	A=0.04	A=0.05	A=0.06	A=0.07

Group Name : 2. SiO2-MnO\_S\_capacity

wtS : Amount/Composition (S (total)/Slag-liq)) wt. %

aO2 : Activity (O2/Gas)

aS2 : Activity (S2/Gas)

Page f1 = log(wtS \* SQRT(aO2/aS2))

1	-4.677854
2	-3.972706
3	-3.610284
4	-3.401473
5	-3.266302
6	-3.173698
7	-3.108676
8	-3.062852
9	-3.031001

# 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 :

$$<A> = 0.5$$

$$\underline{S} = 0.30094 \text{ Wt.}\%$$

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

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

$$f1 \text{ (i.e. } \log(Cs))$$

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

$$= -2.521514$$

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 51

$f1 = \log(wtS * \text{SQRT}(aO2/aS2))$   
-2.521514

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

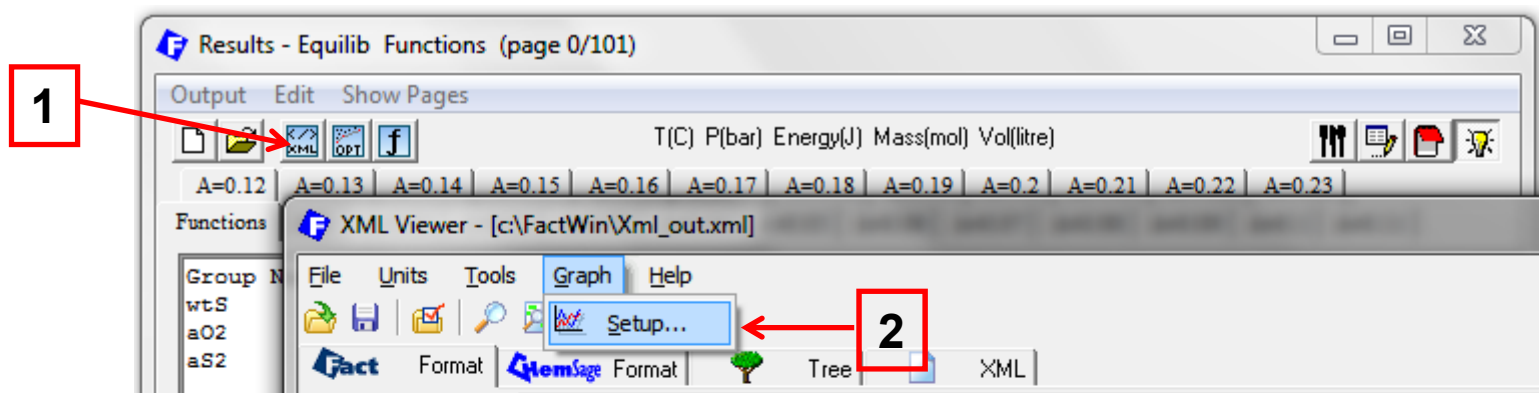
- 3.0627E-03 O2

+ 3.0789E-03 S2

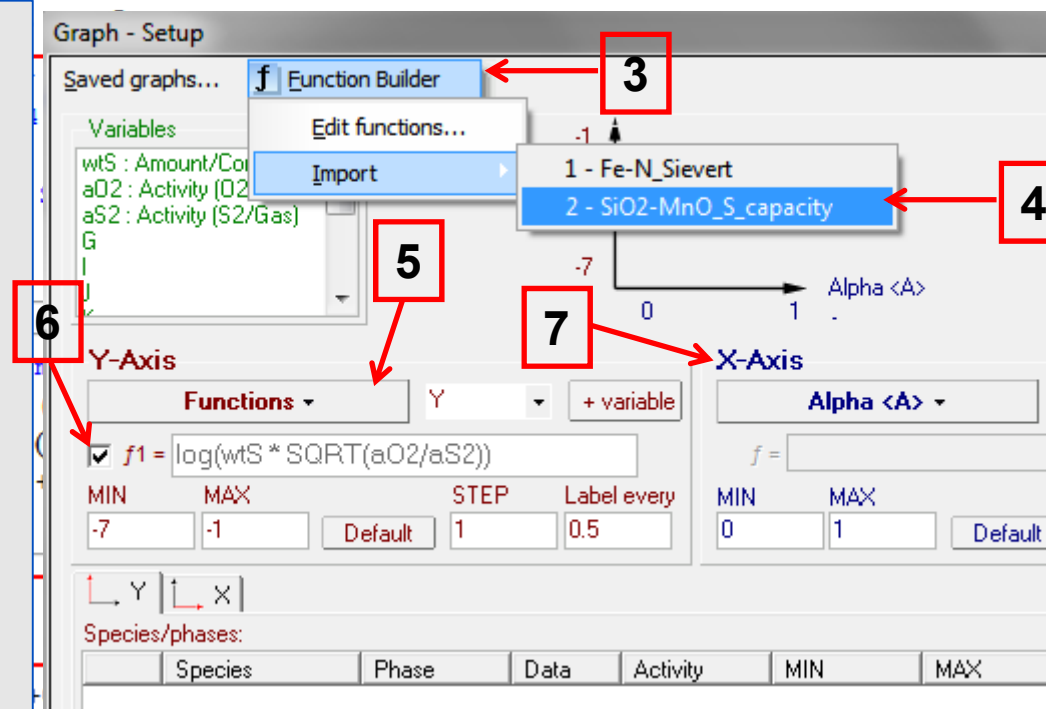
0 mol gas\_ideal  
(1650 C, 1 bar, a=1.0001E-06)  
( 1.0000E-06 S2  
+ 1.0000E-10 O2 )

+ 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 )

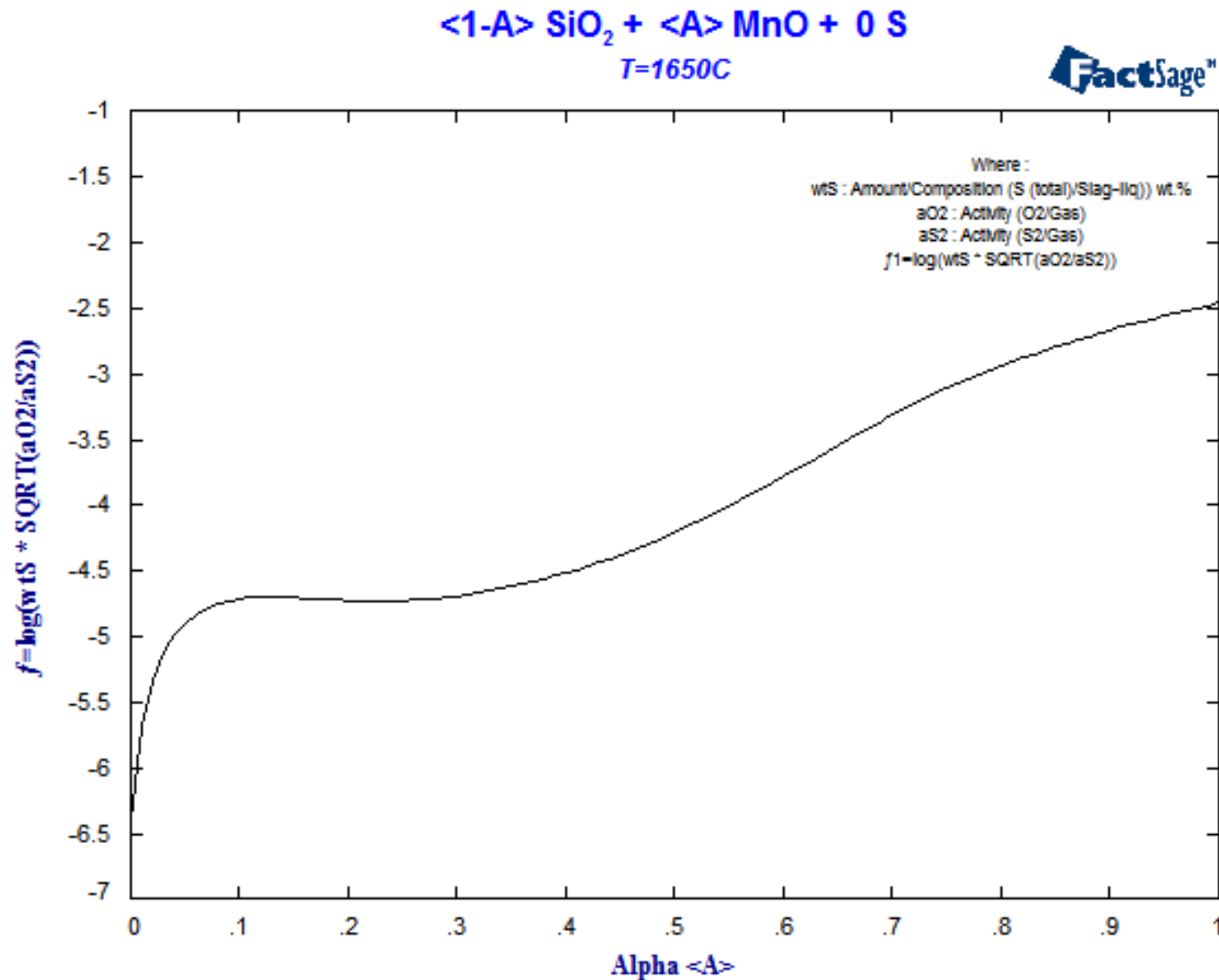
# Step 4: Importing **functions** into **Fact-XML**



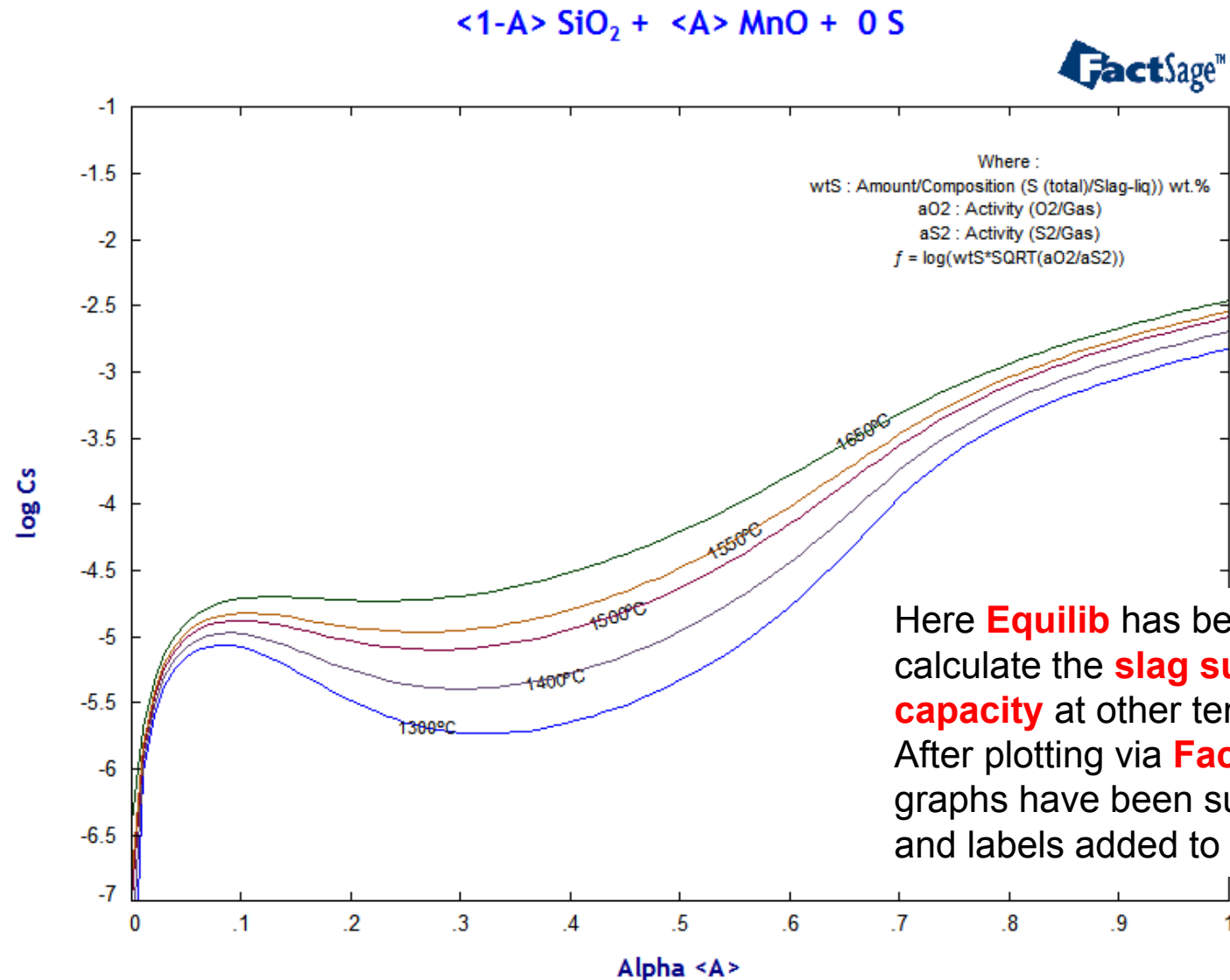
1. To activate **Fact-XML** click on the **XML** menu button.
2. Click on **Graph > Setup ....**
3. Click on **Function Builder**.
4. **Import** function group:  
**SiO2-MnO\_S\_capacity**
5. Select **Functions** from the Y-Axis menu.
6. Check ☒ the functions you wish to plot: set **MIN**, **MAX**, **STEP**,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



## 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.*

A.Gheribi, E. Bélisle, C.W. Bale and A.D. Pelton CRCT, Ecole Polytechnique de Montréal  
S. Le Digabel and C. Audet, GERAD, Ecole Polytechnique de Montréal

## Table of contents

<u>Section</u>	<u>1</u>	<u>Introduction</u>
<u>Section</u>	<u>2</u>	<u>How does FactOptimal Work</u>
<u>Section</u>	<u>3</u>	<u>Example 1 : Maximize an adiabatic flame temperature</u>
<u>Section</u>	<u>4</u>	<u>Example 2 : Calculation of minimum liquidus temperature under constraints</u>
<u>Section</u>	<u>5</u>	<u>Example 3 : How to use equality constraints</u> <b>NEW</b>
<u>Section</u>	<u>6</u>	<u>Example 4 : FactOptimal coupled with solidification software</u>
<u>Section</u>	<u>7</u>	<u>Introduction to the Pareto concept</u>
<u>Section</u>	<u>8</u>	<u>Example 5 : Optimize 2 properties with two files (linked)</u> <b>NEW</b> <u>P<sub>gas</sub> vs density (T2 = T1+20)</u>
<u>Section</u>	<u>9</u>	<u>Example 6 : Application using the cache option (Next Run)</u> <b>NEW</b>
<u>Section</u>	<u>10</u>	<u>Example 7 : Target optimization</u> <b>NEW</b>
<u>Section</u>	<u>11</u>	<u>Optimization using the Function Builder</u> <b>NEW</b>
<u>Section</u>	<u>12</u>	<u>Example 8 : Calculation of special points on the liquidus surface</u>
<u>Section</u>	<u>13</u>	<u>Special points – reciprocal systems</u> <b>NEW</b>

# 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  $x^{\circ}\text{C}$ , with a desired freezing range, with a maximum or minimum amount of precipitates after annealing at  $y^{\circ}\text{C}$ , 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

---

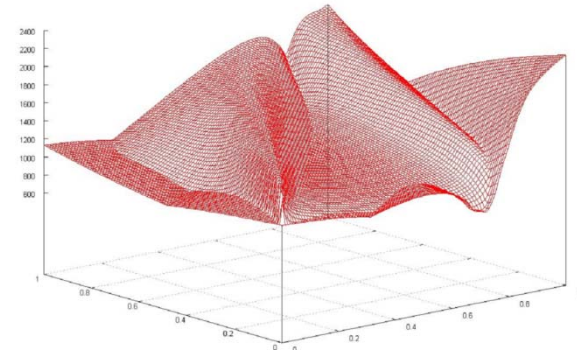
## *What's New In FactOptimal 6.3 ?*

- 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:  $\{f_1(x_1, x_2 \dots T, P); f_2(x_1, x_2 \dots T, P)\}$
- 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

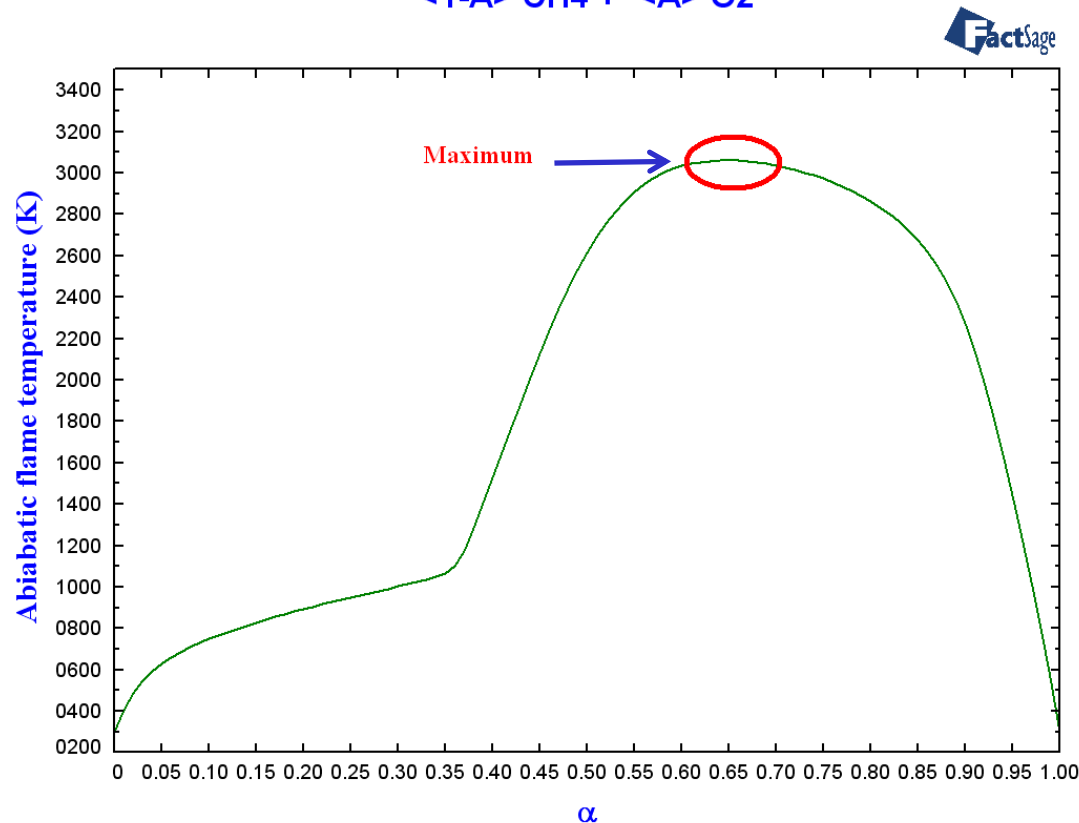


# Example 1: Maximize an adiabatic flame temperature - 1

The objective is to maximize the adiabatic flame temperature of :  $(1-A) \text{CH}_4 + (A) \text{O}_2$

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:  $T_{\text{ad,max}} \sim 3075 \text{ K}$  when  $A \sim 0.65$   
 $<1-A> \text{CH}_4 + <A> \text{O}_2$



# 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**.

The screenshot displays the FactSage 6.3 software interface, showing the process of maximizing adiabatic flame temperature.

**Reactants - Equilib** window shows the input composition:

Mass(mol)	Species	Phase	T(K)	P(total)**	Stream#	Data
0.5	CH4	gas	298.15	1	1	
+ 0.5	O2	gas	298.15	1	1	

**Menu - Equilib: Maximun adiabatic temperature** window shows the calculation settings:

- Reactants (2): 0.5 CH4 (298.15K,g,#1) + 0.5 O2 (298.15K,g,#1)
- Products: Compound species (gas, ideal, real, aqueous, pure liquids, pure solids) and Solution species (Base-Phase, Full Name).
- Target: Target phase: Estimate T(K): 1000, Mass(mol): 0.
- Final Conditions: T(K), P(atm), Delta H(J), 10 steps, Table.
- Equilibrium: normal + transitions, transitions only, open.

**Results - Equilib 2612.05 K** window shows the output:

```
0.5 CH4 + 0.5 O2 =  
(298.15,1,g,#1) (298.15,1,g,#1)  
  
1.5221 mol gas_ideal  
(24.021 gram, 1.5221 mol, 326.25 litre, 7.3627E-05 gram/cm3)  
(2612.05 K, 1 atm, a=1.0000)
```

A red box highlights the **FactOptimal** icon in the Results window, which is used to open the FactOptimal interface for further optimization.

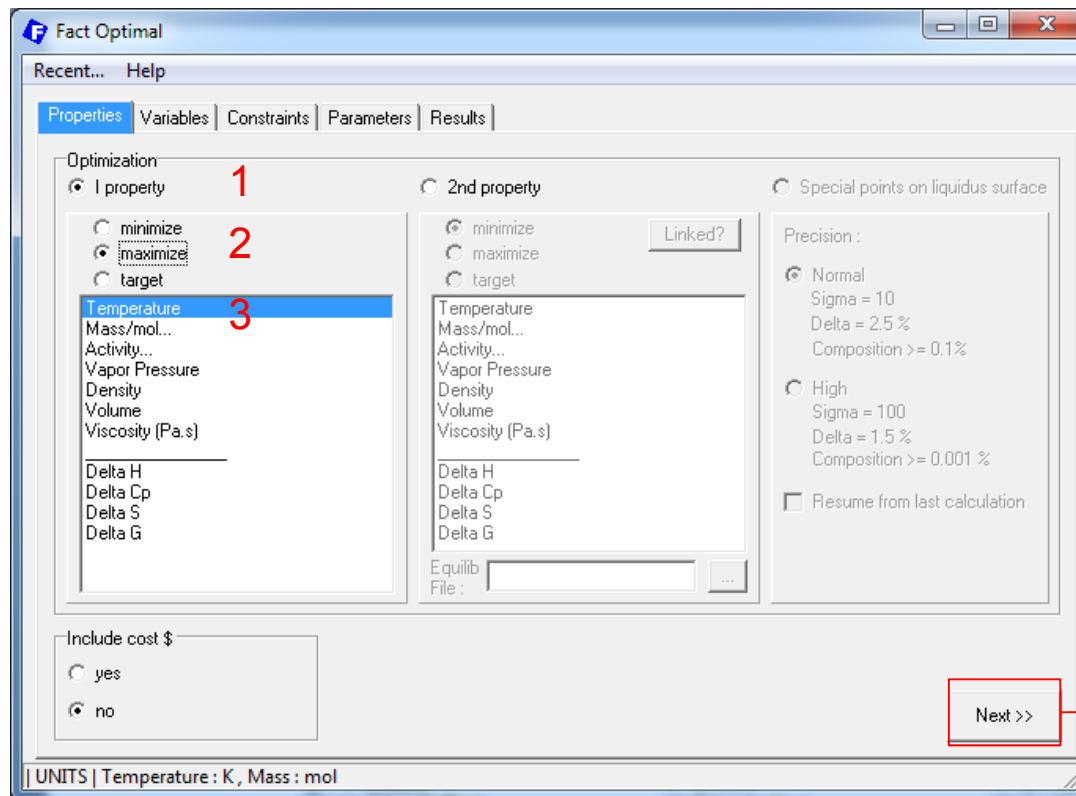
# Example 1: Maximize an adiabatic flame temperature - 3

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)

Fact Optimal

Recent... f Function Builder Help

Properties Variables Constraints Parameters Results

Composition Variables

No. Species MIN MAX Initial Value

1 CH4 0 1 0.5

2 O2 0 1 0.5

Variable type:  
☒ REAL  
☐ INTEGER

Additional variables

☒ Temperature MIN: 100 MAX: 2000 precision: 10 Initial Value: 2612

☒ Pressure MIN: 1 MAX: 10 precision: 1 Initial Value: 1

Next >>

UNITS | Temperature : K, Mass : mol

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 screenshot displays the Fact Optimal window for the property 'max Temperature (CH4+O2)'. The 'Constraints' tab is active, showing 'Composition constraints' with a checked box for 'SUM (Comp. variables) = 1'. The 'Parameters' tab is also visible, showing 'Max # of Equilib calculations : 25' and 'Initial search region : 0.1' with radio buttons for 'Small', 'Medium', and 'Large'. A 'Calculate >>' button is located at the bottom right. Red boxes and arrows highlight these key settings and the calculation button.

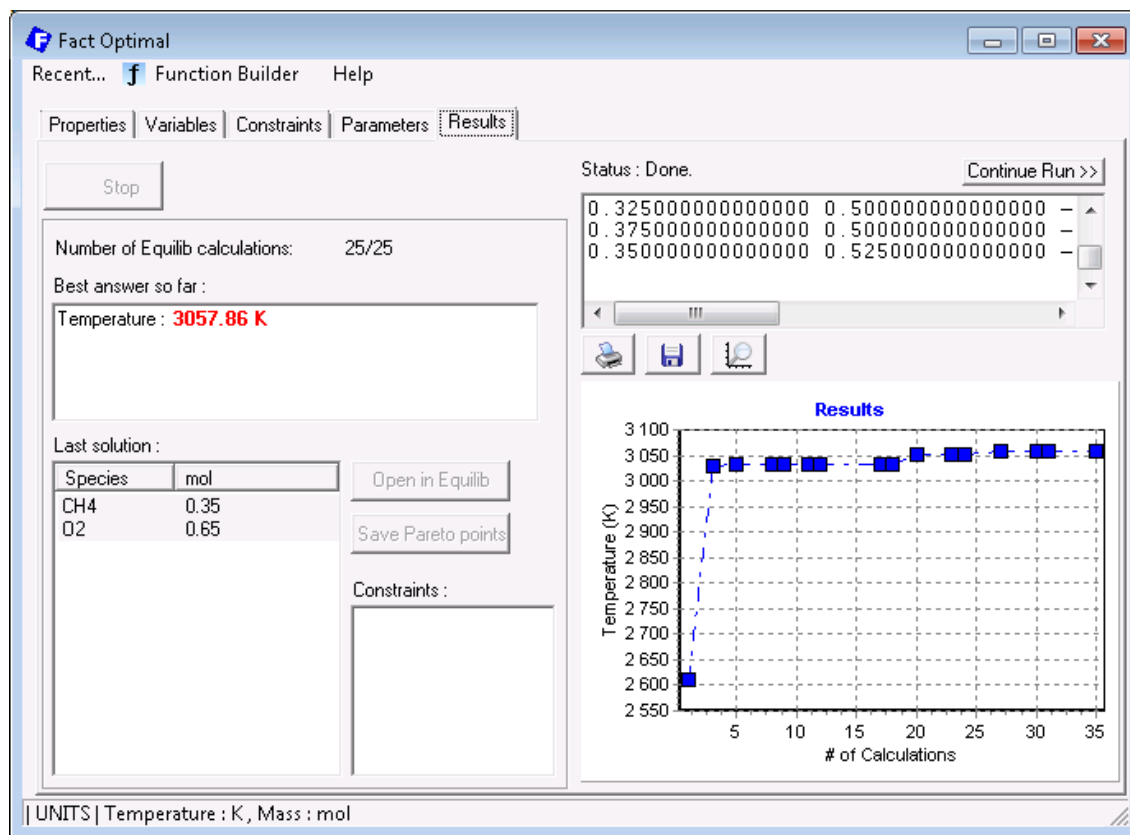
The program will stop after the selected maximum number of **Equilib** calculations, or it may converge earlier.

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.



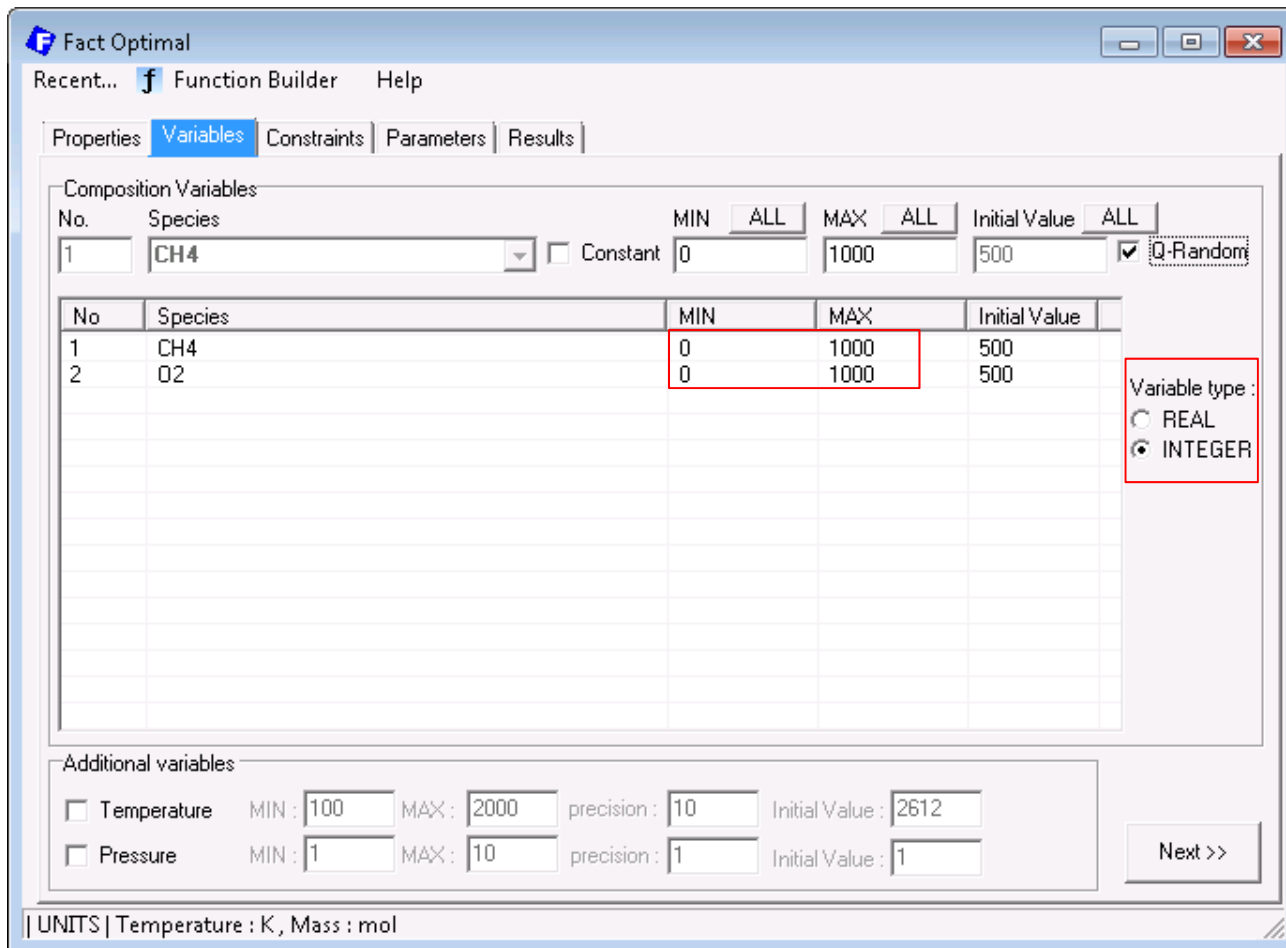
The screenshot shows the 'Results - Equilib 3057.86 K' window. The 'Output' tab is active, displaying the chemical composition of the equilibrium mixture. The input reaction is 0.35 CH4 + 0.65 O2 = (298.15, 1, g, #1) (298.15, 1, g, #1). The output shows the equilibrium composition at 3057.86 K and 1 atm, with a standard state of a=1.0000. The composition is listed as follows:

mol	gas_ideal
1.2638	(26.414 gram, 1.2638 mol, 317.11 litre, 8.3295E-05 gram/cm3)
(0.39548	H2O
+ 0.17000	CO
+ 0.10694	CO2
+ 8.9509E-02	OH
+ 8.6175E-02	H2
+ 6.2708E-02	O2
+ 5.4891E-02	H
+ 3.4235E-02	O
+ 5.7500E-05	HOO
+ 1.7474E-06	HOOH
+ 6.7877E-07	HCO
+ 1.7032E-08	O3
+ 8.4044E-09	H2CO
+ 1.0388E-10	HCOOH
+ 2.5783E-11	C
+ 3.6171E-12	CH
+ 2.4648E-12	CH2
+ 1.7952E-12	CH3
+ 5.4482E-13	C2O
+ 1.2583E-13	CH4
+ 2.9076E-15	CH3OH
+ 6.7094E-16	C2H
+ 6.2620E-16	C2H2

# 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.

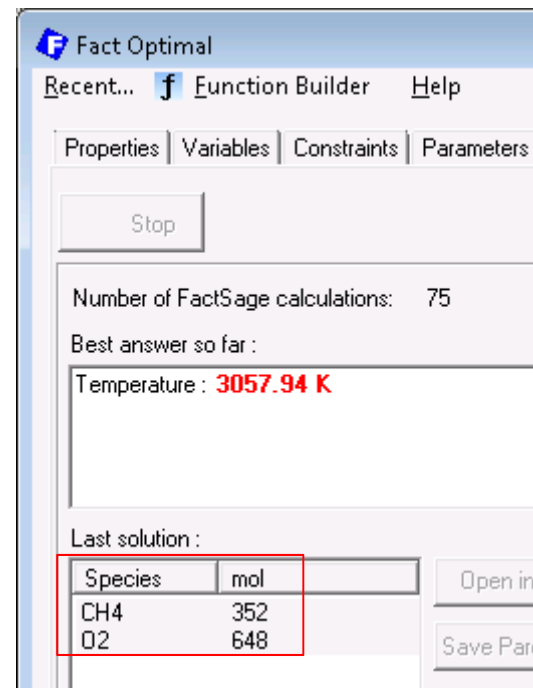


The screenshot shows the 'Variables' tab in the Fact Optimal window. It displays a table of composition variables with columns for No., Species, MIN, MAX, and Initial Value. The first two rows are CH4 and O2, both with MIN values of 0 and MAX values of 1000. A red box highlights these MIN and MAX values. Below the table, there is a 'Variable type' section with radio buttons for 'REAL' and 'INTEGER', where 'INTEGER' is selected. At the bottom, there are fields for 'Additional variables' such as Temperature and Pressure, with their respective MIN, MAX, precision, and Initial Value settings.

No.	Species	MIN	MAX	Initial Value
1	CH4	0	1000	500
2	O2	0	1000	500

Variable type :  
☐ REAL  
☒ INTEGER

Additional variables:  
☐ Temperature MIN: 100 MAX: 2000 precision: 10 Initial Value: 2612  
☐ Pressure MIN: 1 MAX: 10 precision: 1 Initial Value: 1



The screenshot shows the 'Results' tab in the Fact Optimal window. It displays the 'Best answer so far' and the 'Last solution'. The 'Best answer so far' shows a Temperature of 3057.94 K. The 'Last solution' table shows the species and their mole fractions: CH4 at 352 and O2 at 648. A red box highlights the 'Last solution' table.

Number of FactSage calculations: 75  
Best answer so far :  
Temperature : 3057.94 K

Last solution :

Species	mol
CH4	352
O2	648

# 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.

The image displays three screenshots of the FactSage Fact Optimal software interface, illustrating the setup and results of an optimization process.

**Top Screenshot (Function Builder):** Shows the 'Variables' tab. The 'Composition Variables' table lists two species: CH<sub>4</sub> and O<sub>2</sub>. The 'Initial Value' column is set to 500 for both. The 'MIN' and 'MAX' columns are set to 0 and 1000, respectively. The 'Initial Value' column is set to 500. The 'Variable type' is set to 'ALL'. The 'Quasi-Random' checkbox is checked.

**Bottom Left Screenshot (Parameters):** Shows the 'Parameters' tab. The '# of Quasi-Random calculations' is set to 50. The 'Max # of Equilib calculations' is set to 25. The 'Initial search region' is set to 0.1. The 'Calculate >>' button is visible.

**Bottom Right Screenshot (Results):** Shows the 'Results' tab. The 'Number of Equilib calculations' is 75/75. The 'Best answer so far' is 'Temperature : 3057.94 K'. The 'Last solution' table shows the composition of the final solution:

Species	mol
CH <sub>4</sub>	0.35219
O <sub>2</sub>	0.64781

Buttons for 'Open in Equilib' and 'Save Pareto points' are also visible.

## 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**.

The screenshot shows the FactSage Equilib software interface. The main window is titled "Reactants - Equilib" and contains a table for defining the system. The "Data Search" dialog box is open, showing a list of databases to select from. A red circle highlights the "Data Search" button in the main window, and a red arrow points from it to the "Data Search" dialog box.

**Reactants - Equilib**

Mass(mol)	Species	Phase	T(C)	P(atm)	Energy(J)	Mass(mol)	Vol(litre)
1	Al						
+ 1	Cu						
+ 1	Mg						
+ 1	Zn						

**Data Search**

Databases - 2/25 compound databases, 1/25 solution databases

Fact	FactSage™	SGTE
<input checked="" type="checkbox"/> FactPS	<input type="checkbox"/> FScopp	<input type="checkbox"/> BINS
<input type="checkbox"/> FToxid	<input type="checkbox"/> FSlead	<input checked="" type="checkbox"/> SGPS
<input type="checkbox"/> FTsalt	<input type="checkbox"/> FSlite	<input type="checkbox"/> SGTE
<input type="checkbox"/> FTmisc	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGnobl
<input type="checkbox"/> FThall	<input type="checkbox"/> FSnobl	<input type="checkbox"/> SGsold
<input type="checkbox"/> FT0xCN	<input type="checkbox"/> FSupsi	<input type="checkbox"/> SGnucl
<input type="checkbox"/> FTfrtz		
<input type="checkbox"/> FThelg	<input type="checkbox"/> ELEM	<b>Other</b>
<input type="checkbox"/> FTpulp	<input type="checkbox"/> FTdemo	<input type="checkbox"/> TDnucl
<input checked="" type="checkbox"/> FTlite		

compounds only  
solutions only  
no data

Clear All  
Select All  
Add/Remove Data  
RefreshDatabases

Next >>

Compound: 1/28 databases Solution: 1/27 databases

## 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):

**F Menu - Equilib: last system**

File Units Parameters Help

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

**Reactants (4)**

Al + Cu + Mg + Zn

**Products**

Compound species

- ☐ gas ☒ ideal ☐ real 0
- ☐ aqueous 0
- ☐ pure liquids 0
- ☒ pure solids 43
- ☒ suppress duplicates **apply**

species: 43

Precipitate Target

FTlite-Liqu

Estimate T(C): 1000

Mass(mol): 0

**Solution species**

*	+	Base-Phase	Full Name
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	FTlite-Liqu	Liquid
<input type="checkbox"/>	<input type="checkbox"/>	FTlite-FCC	FCC_A1
<input type="checkbox"/>	<input type="checkbox"/>	FTlite-HCP	HCP_A3
<input type="checkbox"/>	<input type="checkbox"/>	FTlite-BCC	BCC_A2
<input type="checkbox"/>	<input type="checkbox"/>	FTlite-LC14	Laves_C14
<input type="checkbox"/>	<input type="checkbox"/>	FTlite-LC15	Laves_C15
<input type="checkbox"/>	<input type="checkbox"/>	FTlite-LC36A	ALaves_C36
<input type="checkbox"/>	<input type="checkbox"/>	FTlite-LC36B	BLaves_C36

Legend

- I - immiscible 7
- P - precipitate target
- + - selected 17

☒ Show ☒ all ☐ selected

species: 182

solutions: 31 **Select**

**Custom Solutions**

- ☐ fixed activities
- ☐ ideal solutions
- ☐ activity coefficients

**Pseudonyms**

**include molar volumes** ☒

Total Species (max 1500) 225

Total Solutions (max 40) 31

**Final Conditions**

<A>  <B>  T(C)  P(atm)  Product H(J)

10 steps ☐ Table **1 calculation**

**Equilibrium**

- ☒ normal ☐ normal + transitions
- ☐ transitions only ☐ open
- ☐ predominant

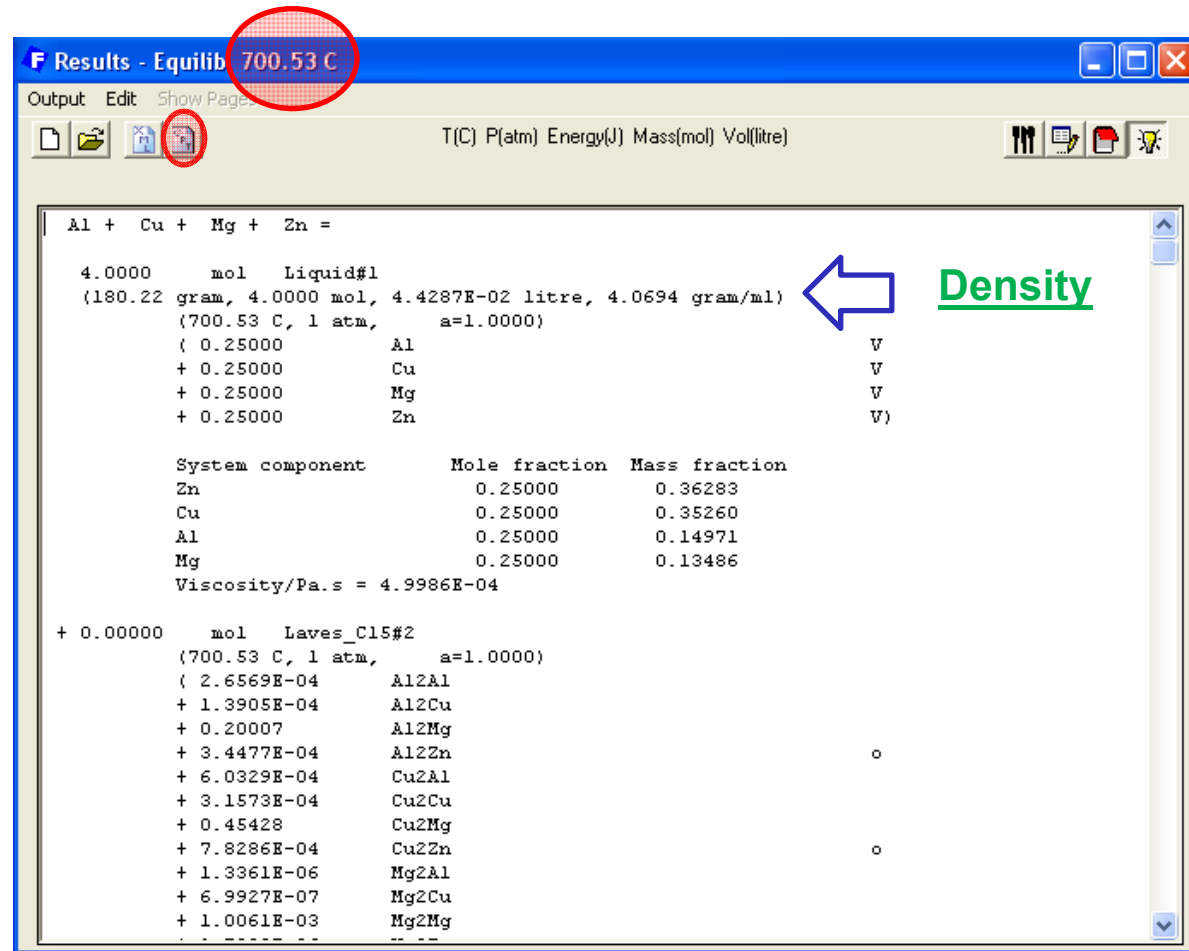
**Calculate >>**

FactSage

## Example 2 : Minimize the liquidus temperature under constraints - 3

### Equilib Results Window

Calculated liquidus temperature : 700.53°C

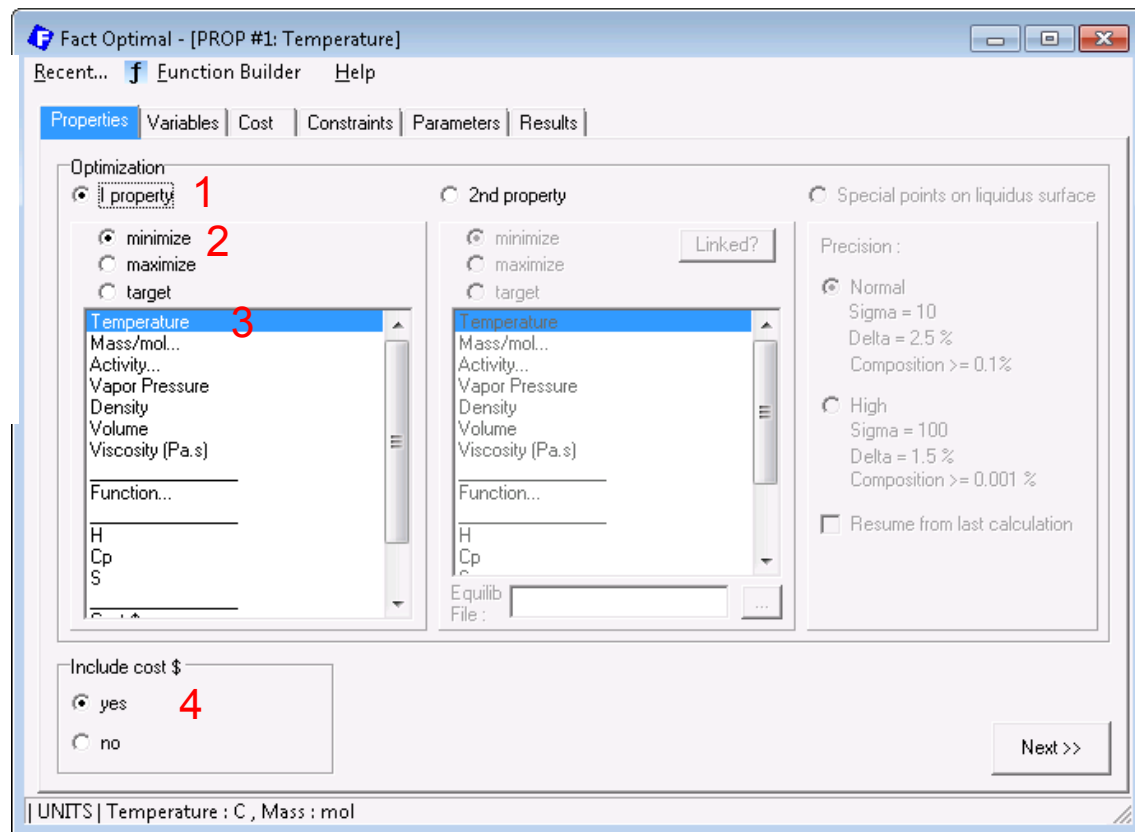


## Example 2 : Minimize the liquidus temperature under constraints - 4

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

Fact Optimal - [PROP #1: Temperature]

Recent... **f** Function Builder Help

Properties **Variables** Cost Constraints Parameters Results

Composition Variables

No.	Species	MIN	ALL	MAX	ALL	Initial Value	ALL
1	Al	0		1		0.25	

☐ Constant ☐ Q-Random

No	Species	MIN	MAX	Initial Value
1	Al	0.05	0.2	0.05
2	Cu	0.02	0.2	0.02
3	Mg	0.75	0.9	0.75
4	Zn	0.03	0.15	0.03

Variable type :  
☒ REAL  
☐ INTEGER

Additional variables

☐ Temperature MIN : 100 MAX : 2000 precision : 10 Initial Value : 974

☐ Pressure MIN : 1 MAX : 10 precision : 1 Initial Value : 1

Next >>

| UNITS | Temperature : C , Mass : mol

### 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”.

[illegible]



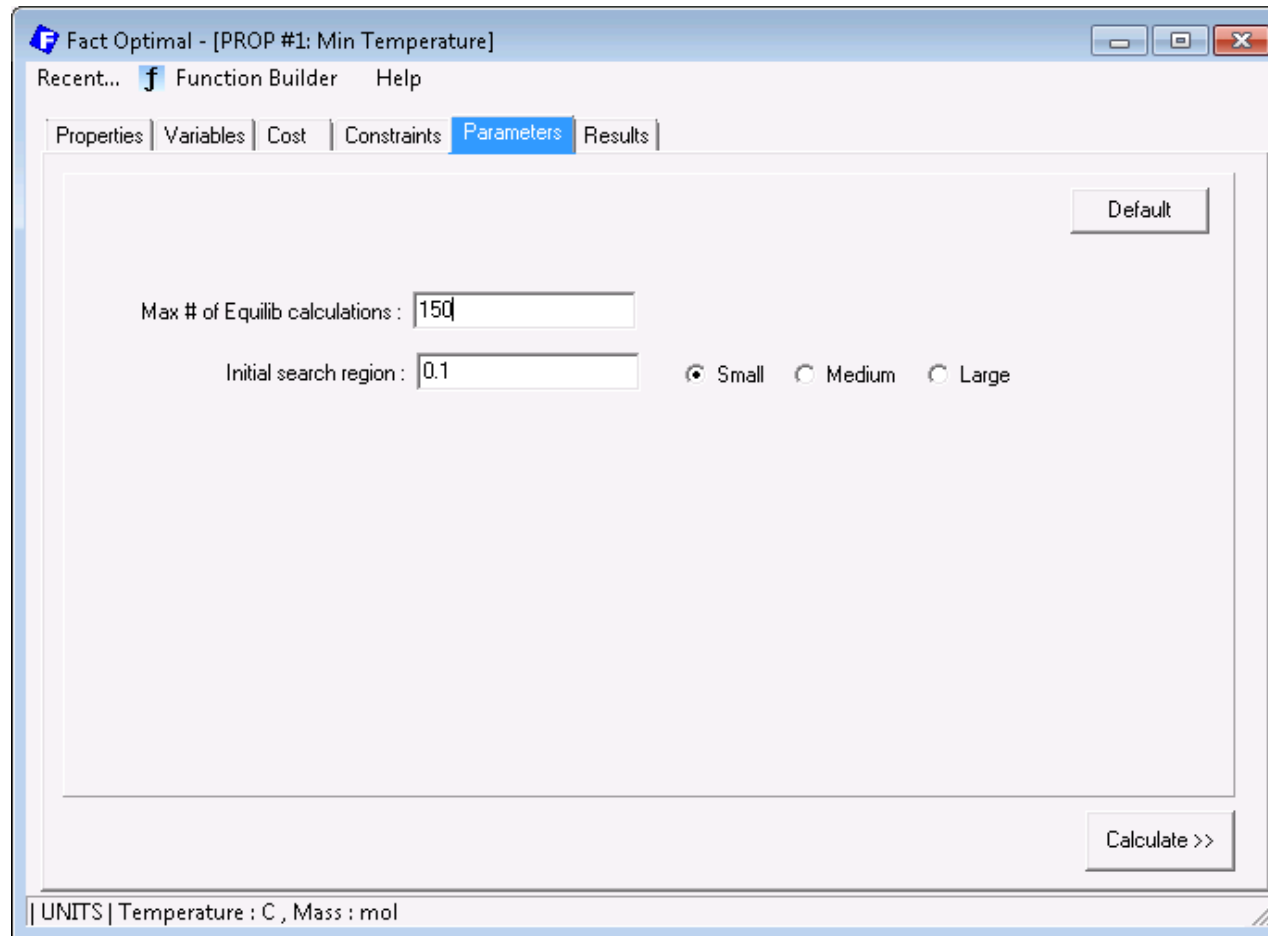
Step 6: Define the constraints on properties :  $\rho < 2.2 \text{ g/ml}$      $\text{cost} < 2900 \text{ \$/Ton}$



## 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).



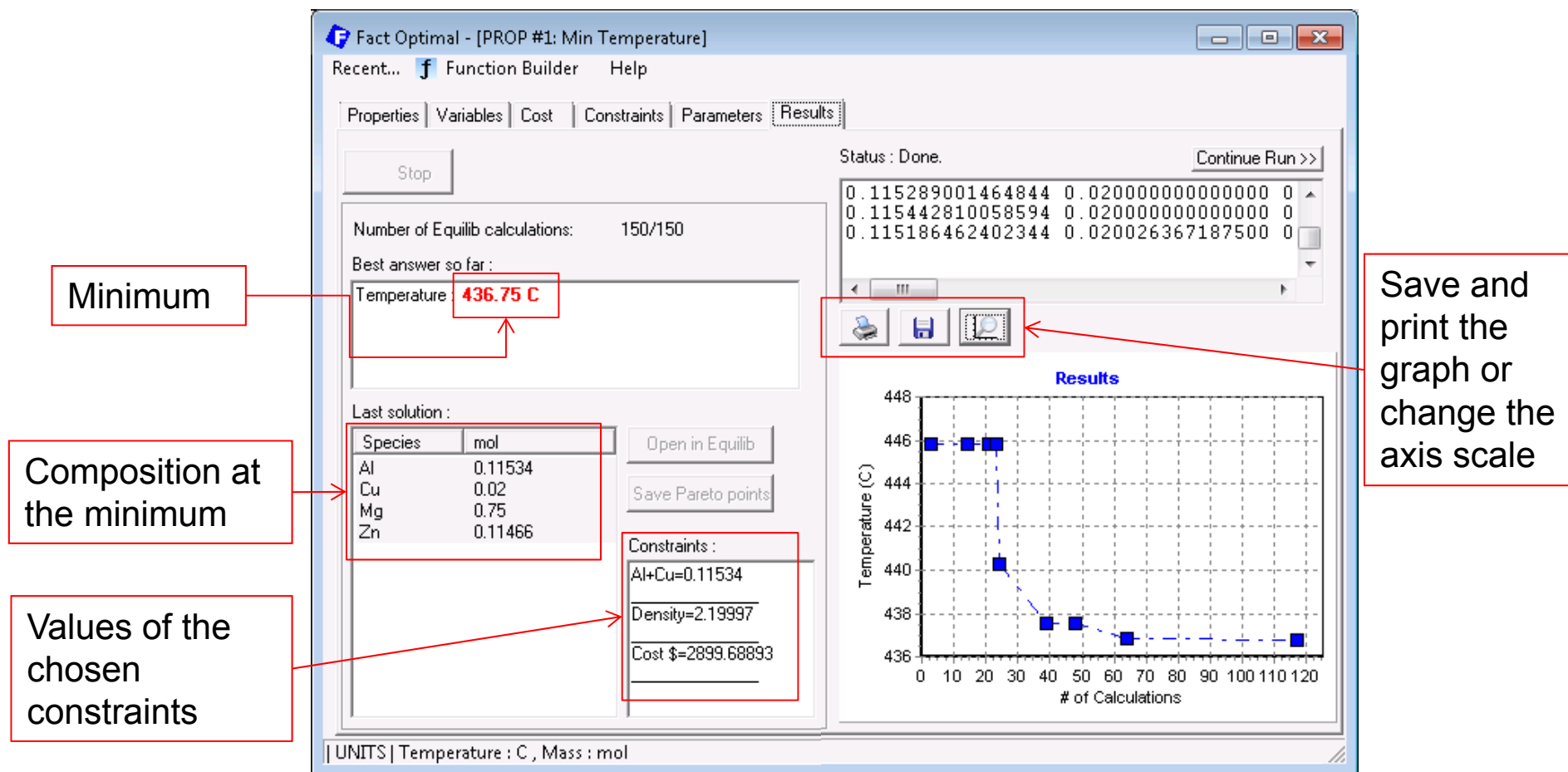
The screenshot shows the 'Fact Optimal - [PROP #1: Min Temperature]' window. The 'Parameters' tab is selected, displaying the following settings:

- Max # of Equilib calculations : 150
- Initial search region : 0.1
- Search region options: ☒ Small, ☐ Medium, ☐ Large

Buttons for 'Default' and 'Calculate >>' are visible. The status bar at the bottom indicates 'UNITS | Temperature : C , Mass : mol'.

## Example 2 : Minimize the liquidus temperature under constraints - 10

### FactOptimal Results Window



## Example 2 : Minimize the liquidus temperature under constraints - 11

### Equilib Results Window

Results - Equilib 436.77 C

Output Edit Show Pages

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

FactSage 6.3

0.11539 Al + 0.02 Cu + 0.75 Mg + 0.11461 Zn =

1.0000 mol Liquid#1  
(30.106 gram, 1.0000 mol, 1.3686E-02 litre, 2.1998 gram/cm3)  
(436.77 C, 1 atm, a=1.0000)

( 0.11539 Al V  
+ 2.0000E-02 Cu V  
+ 0.75000 Mg V  
+ 0.11461 Zn V)

System component	Mole fraction	Mass fraction
Zn	0.11461	0.24889
Cu	2.0000E-02	4.2214E-02
Al	0.11539	0.10341
Mg	0.75000	0.60548

+ 0 mol Liquid#2  
(436.77 C, 1 atm, a=1.0000)

( 0.11539 Al V  
+ 2.0000E-02 Cu V  
+ 0.75000 Mg V  
+ 0.11461 Zn V)

System component	Mole fraction	Mass fraction
Zn	0.11461	0.24889
Cu	2.0000E-02	4.2214E-02
Al	0.11539	0.10341
Mg	0.75000	0.60548

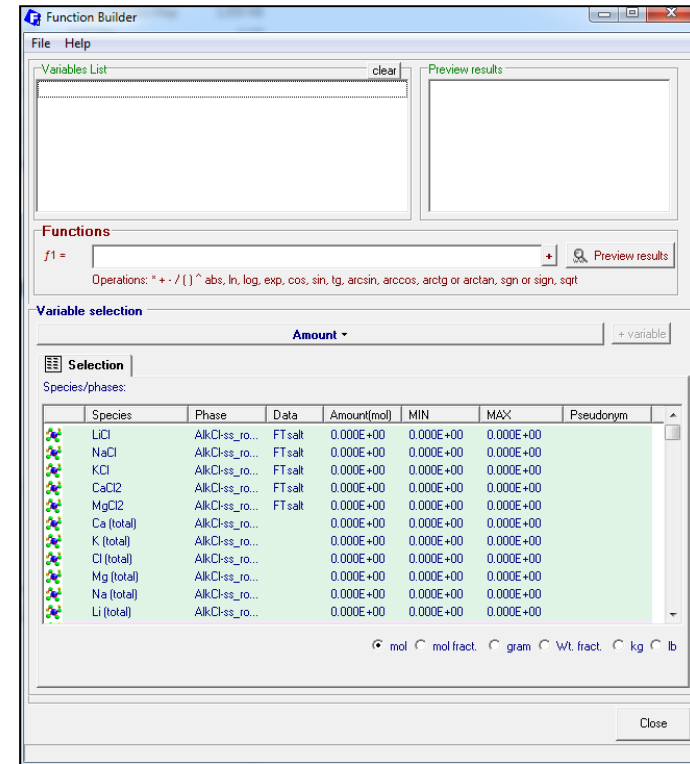
# Optimization using the Function Builder - 1

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 <sup>[1]</sup> has proposed that the electrical conductivity  $\sigma$  of molten chloride solutions can be expressed as :

$$\ln(\sigma) = 4.9 \cdot \exp[-(2747 - 33724/V)/T] \cdot \exp(53.7/V)$$

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>



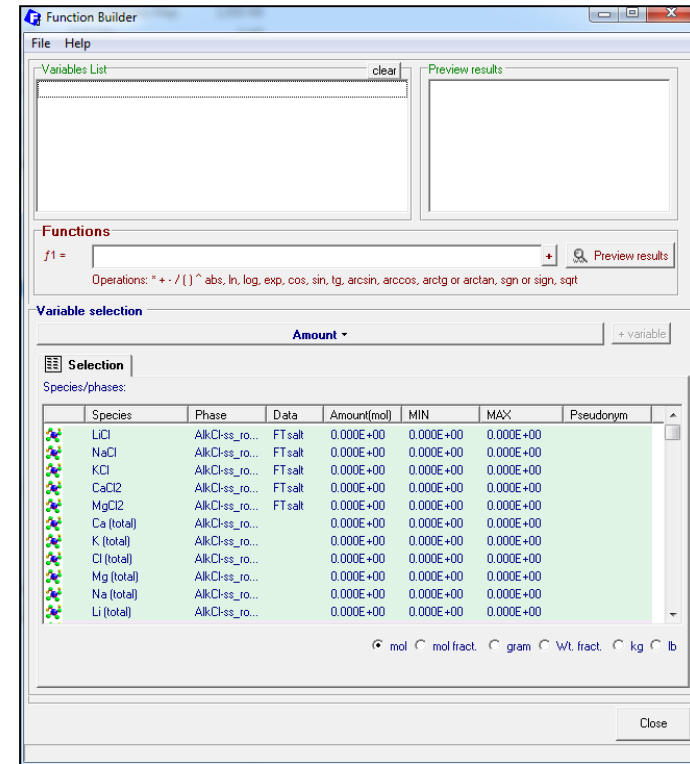
# Optimization using the Function Builder - 1

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 <sup>[1]</sup> has proposed that the electrical conductivity  $\sigma$  of molten chloride solutions can be expressed as :

$$\ln(\sigma) = 4.9 \cdot \exp[-(2747 - 33724/V)/T] \cdot \exp(53.7/V)$$

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>

# 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'

The image shows two windows from the FactSage software. The 'Fact Optimal' window on the left has the 'Function Builder' tab selected, indicated by a red arrow. The 'Function Builder' window on the right is open, showing a 'Variables List' and a 'Functions' section with a formula editor. Below the functions section is a 'Variable selection' area with a table of species/phases.

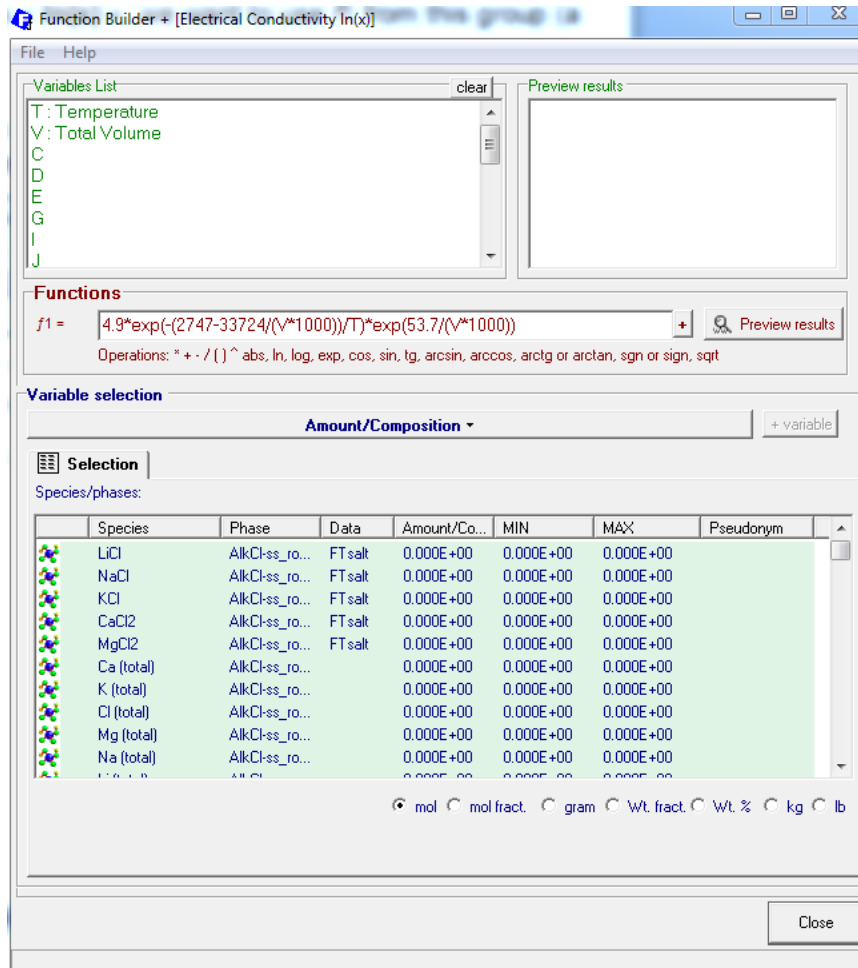
**Variable selection table:**

	Species	Phase	Data	Amount(mol)	MIN	MAX	Pseudonym
	LiCl	AlkCl-ss_ro...	FTsalt	0.000E+00	0.000E+00	0.000E+00	
	NaCl	AlkCl-ss_ro...	FTsalt	0.000E+00	0.000E+00	0.000E+00	
	KCl	AlkCl-ss_ro...	FTsalt	0.000E+00	0.000E+00	0.000E+00	
	CaCl2	AlkCl-ss_ro...	FTsalt	0.000E+00	0.000E+00	0.000E+00	
	MgCl2	AlkCl-ss_ro...	FTsalt	0.000E+00	0.000E+00	0.000E+00	
	Ca (total)	AlkCl-ss_ro...		0.000E+00	0.000E+00	0.000E+00	
	K (total)	AlkCl-ss_ro...		0.000E+00	0.000E+00	0.000E+00	
	Cl (total)	AlkCl-ss_ro...		0.000E+00	0.000E+00	0.000E+00	
	Mg (total)	AlkCl-ss_ro...		0.000E+00	0.000E+00	0.000E+00	
	Na (total)	AlkCl-ss_ro...		0.000E+00	0.000E+00	0.000E+00	
	Li (total)	AlkCl-ss_ro...		0.000E+00	0.000E+00	0.000E+00	

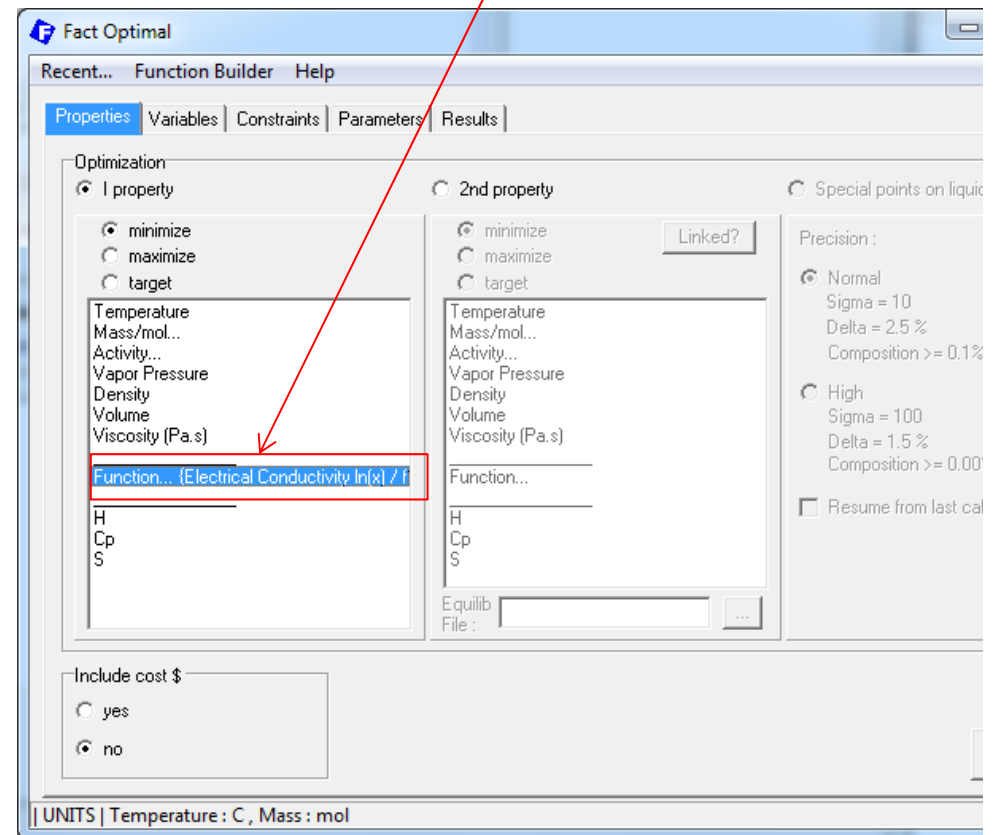
Units: Temperature : C, Mass : mol

# 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 function  $f1$  from this group (a group can contain up to 10 functions  $f1$ ,  $f2$ ,  $f3$ , etc.)



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



## Optimization using the Function Builder - 4

The screenshot shows the 'Fact Optimal' software interface with the 'Function Builder' tab selected. The 'Variables' sub-tab is active, displaying a table of composition variables and a section for additional variables.

**Composition Variables**

No.	Species	MIN	MAX	Initial Value
1	LiCl	0	1	0.2
2	NaCl	0	1	0.2
3	KCl	0	1	0.2
4	CaCl <sub>2</sub>	0	1	0.2
5	MgCl <sub>2</sub>	0	1	0.2

**Additional variables**

Variable	MIN	MAX	precision	Initial Value
<input checked="" type="checkbox"/> Temperature	800	1200	10	1000
<input type="checkbox"/> Pressure	1	10	1	1

Variable type:   
☒ REAL   
☐ INTEGER

Next >>

UNITS | Temperature : C , Mass : mol

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.

