# 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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# 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$^{o}$C, with a desired freezing range, with a maximum or minimum amount of precipates after annealing at y$^{o}$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

## *What's New In FactOptimal 7.0 ?*

- FactOptimal was first introduced in FactSage 6.1. The module computes optimal conditions for material and process design by coupling FactSage with the Mesh Adaptive Direct Search (MADS) algorithm for nonlinear optimization developed by the GERAD research group at the Ecole Polytechnique de Montréal.

- In FactSage 7.0 the stability of the module has been improved and fewer unwanted error messages are now issued. All the examples have been thoroughly checked and revised where necessary. The Slide Show has been updated with the revised examples.

## *What's New In FactOptimal 6.4 ?*

- Double Target calculations: one can now **target two properties** simultaneously.
- Continue run after a target calculation: it is now possible to click on "continue run" to calculate another composition corresponding to the desired target.
- Additional properties for optimization or constraints : physical properties (density, thermal expansion, viscosity, thermal conductivity, electrical conductivity…) are now available.
- For cooling calculations, the annealing temperature can now be chosen as an optimizable variable.
- Logarithmic values: one can optimize the logarithm of a property e.g log(activity) or log(P). In certain cases this may present a numerical advantage, increasing speed and precision.
- When using two input files, the "linked" button previously allowed using the temperature from the first file as a variable for the second file. In FactOptimal 6.4, **amount of reactants** and **pressure** can also be used.
- A function saved with Function Builder can now be used as a property constraint.
- When characteristic points on a liquidus surface are calculated, the results are now shown in a table as well as on a graph, displaying detailed compositions, temperature and the solid phases in equilibrium with the liquid.

## *What's New In FactOptimal 6.4 ? (cont.)*

- There is now an option to calculate the minimum or maximum on a liquidus surface closest to the initial composition.
- When calculating characteristic points on a liquidus surface, there is a new option either to calculate the lowest minimum first or to calculate all minima with no priority.
- There is a new parameter to limit the maximum time for the optimization.
- When working with variables of type "real", a new parameter is available: the decimal precision.
- Results displayed in a table (target type calculations or characteristic points on a liquidus. surface) can now be saved as an Excel file.
- When using two input files, property constraints can now be applied on either file.
- When no feasible solution is found, FactOptimal now displays the closest solution (example on page 4.20).

## *What was 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

# General recommendations

- In general, we recommend that you perform every optimization twice, using different starting points.

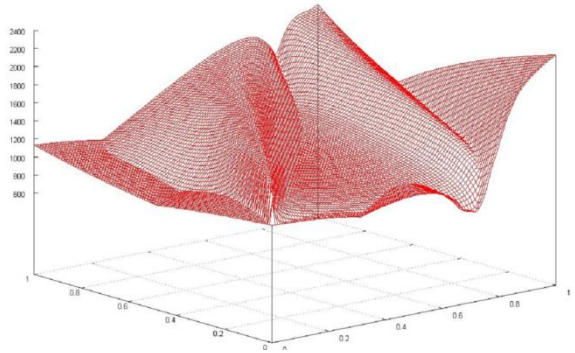
- If you are not sure of the best starting point, a good practice is to use the Q-Random option. See p. 3.8 and p. 19.5 for detailed examples.

- Do not hesitate to use the « Continue Run >> » option to make sure there is no better answer when you have completed the maximum number of calculations entered in the parameters (see example 6).

- If you need more information or if you have specific questions about FactOptimal, please contact Aimen Gheribi (aimen.gheribi@polymtl.ca) or Eve Bélisle (eve.belisle@polymtl.ca).

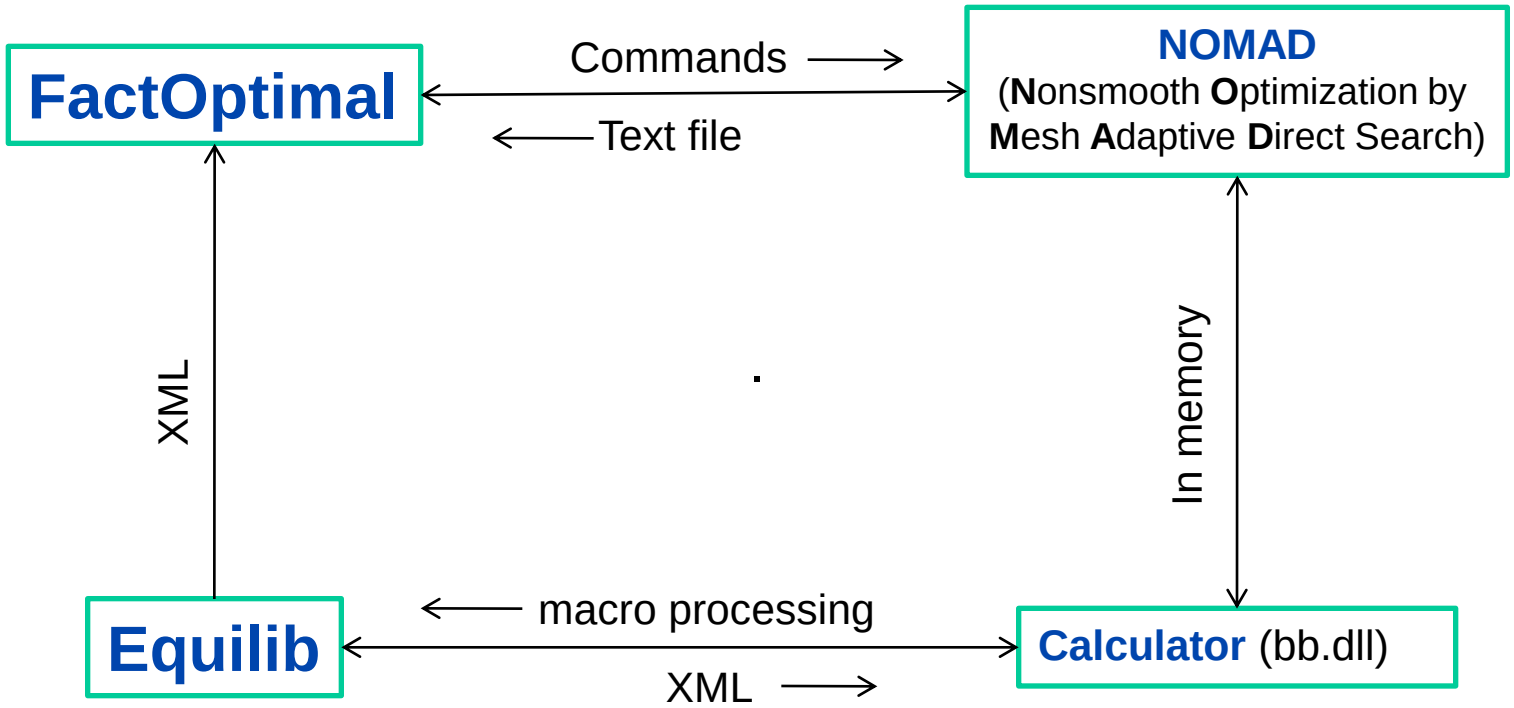
# Introduction - 2

- **The purpose of FactOptimal is to minimize <u>and/or</u> 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 <u>non-smooth</u> (e.g. liquidus )
- The estimation of <u>derivatives is problematic</u>
- Evaluations of *f* can be <u>time consuming</u>
- The function calculation may <u>fail unexpectedly</u> at some points
- The constraints may be <u>non-linear</u>, <u>non-smooth</u> or <u>Boolean</u>

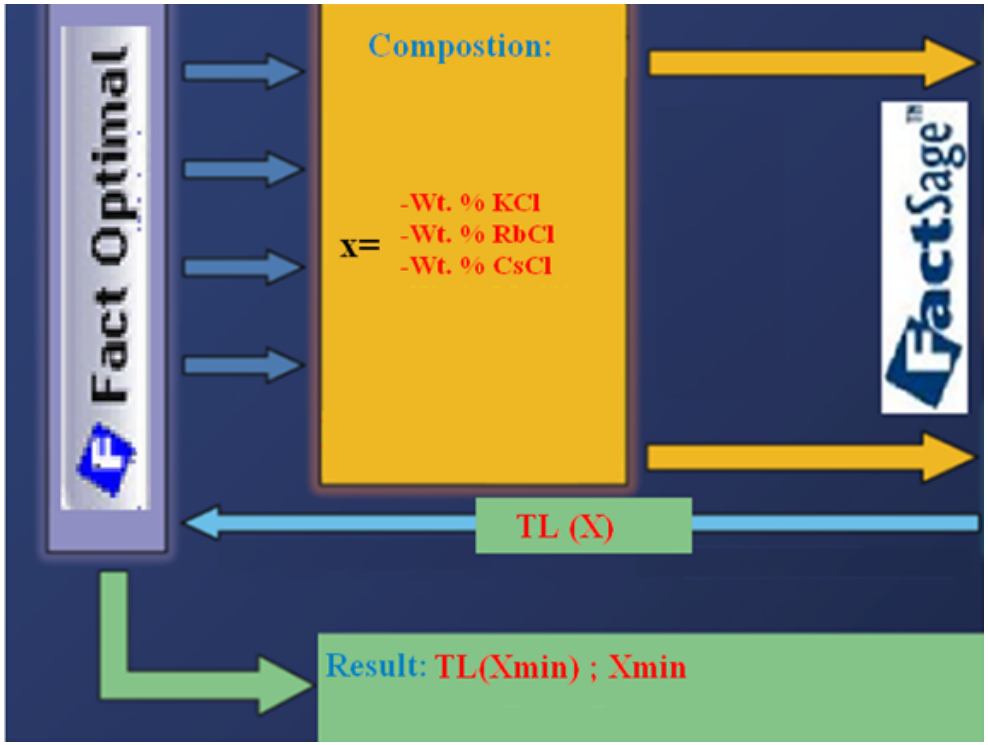
# How does **FactOptimal** work ? – 1



# How does **FactOptimal** work ? – 2

The principal of the optimization is a loop where **FactOptimal** sends compositions to **Equilib**, then **Equilib** returns the values of the properties to be optimized to **FactOptimal**. This is repeated until the properties minimum or maximum of is reached.

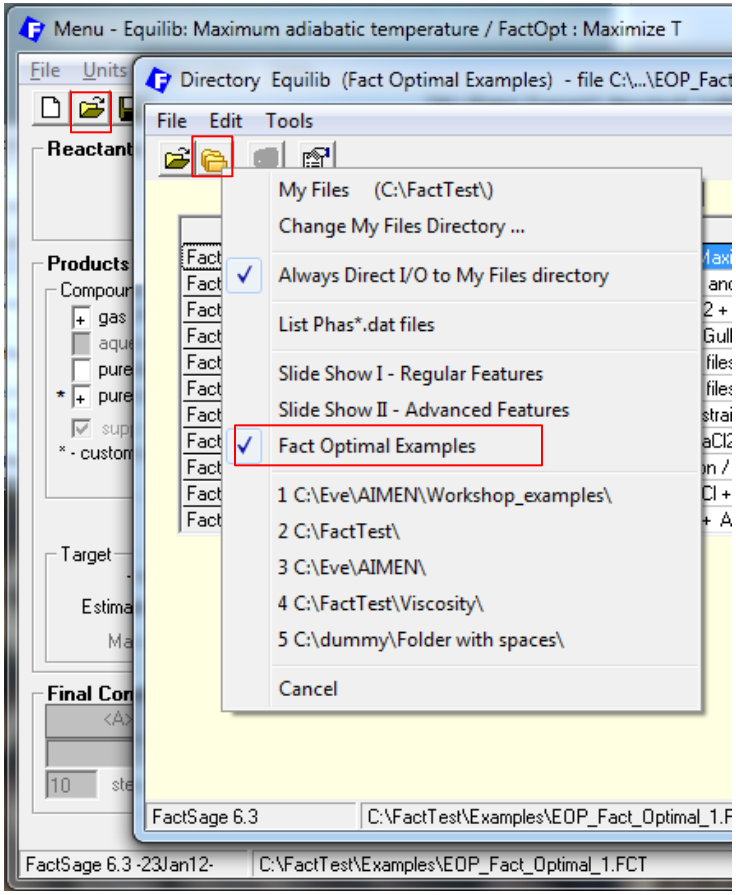
For example, the minimization of the liquidus temperature of the KCl-RbCl-CsCl salt system can be represented by :

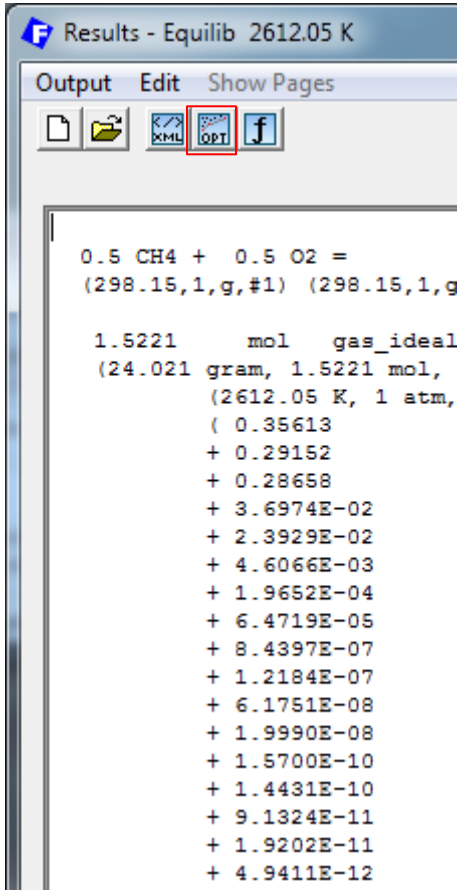


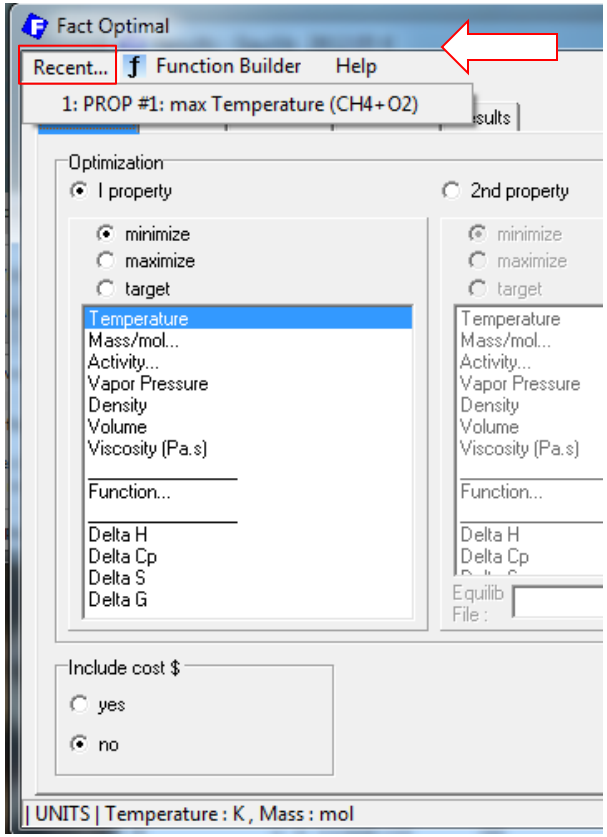
# Using the stored examples

The following examples are stored on your computer. In **Equilib** click on *'File > Open > Directory > Fact Optimal Examples' > Fact Optimal 1 (Maximum adiabatic ...')*. In the *Menu Window* click on *'Calculate '* and then in the *Results Window* click the **FactOptimal** icon.

In the *Fact Optimal Window* click on *'Recent ...'* to load the stored example.



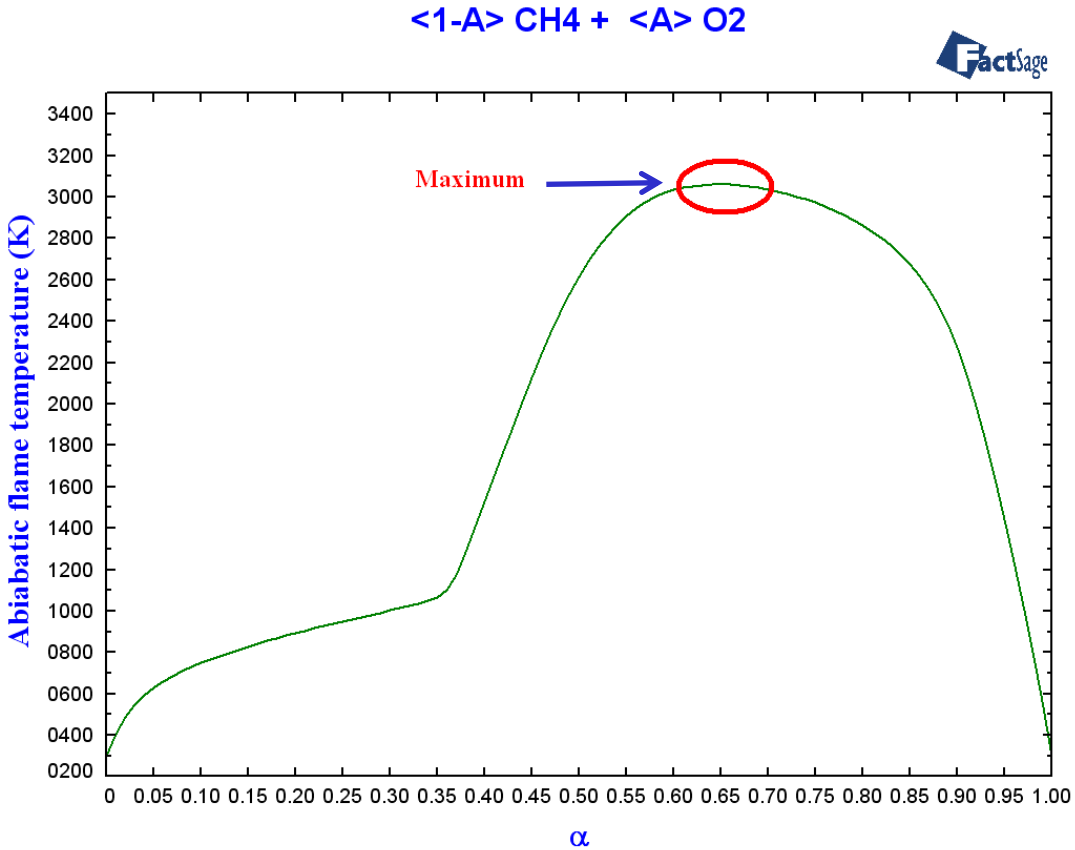
# *Examples of FactOptimal*

# 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) $O_2$**

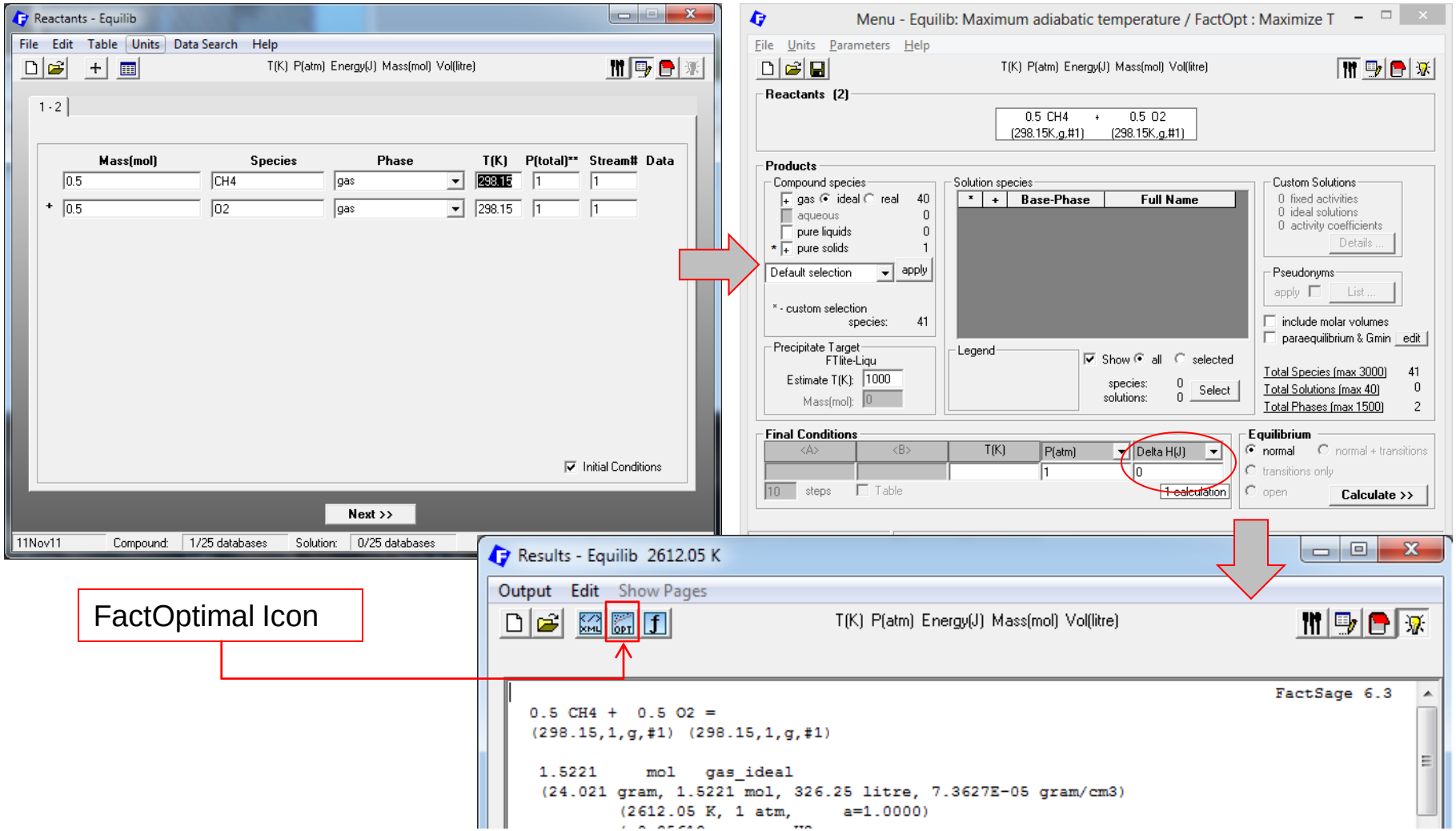
By varying A from 0 to 1 in steps of 0.01, you can calculate the adiabatic flame temperature as a function of A using the **Equilib** module (see **Equilib** regular slide show, section 10).

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**.



# 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.

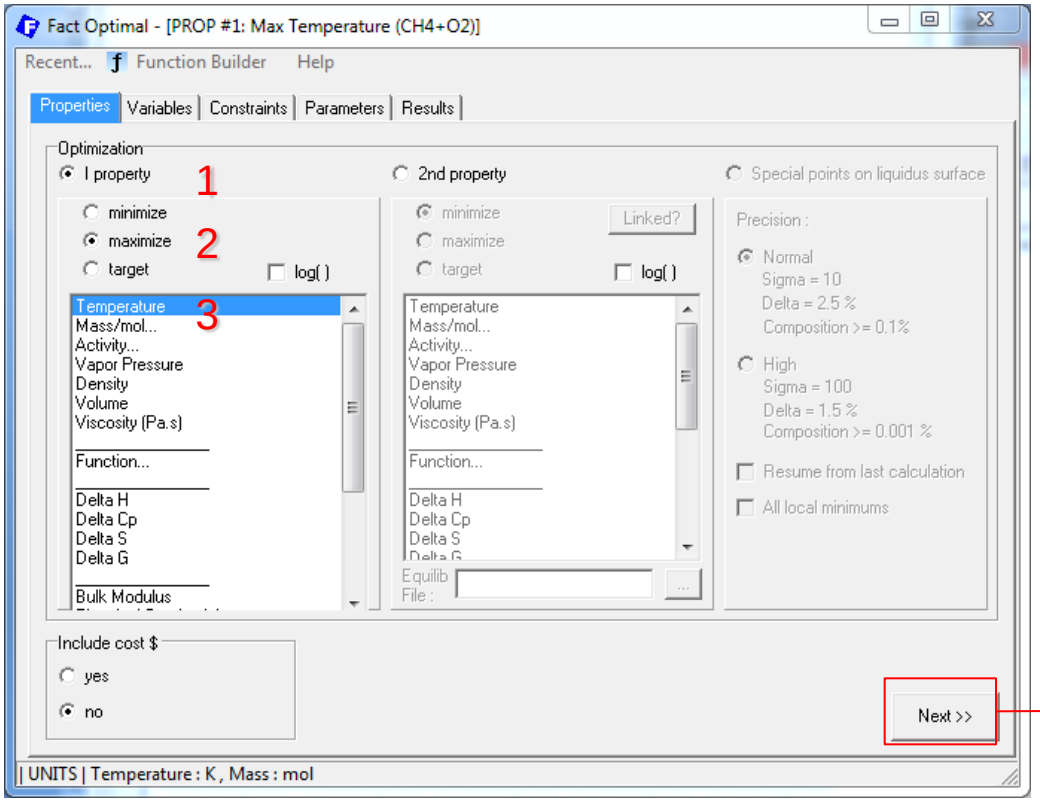
The first tab is "Properties" where we define the quantities to minimize and/or maximize.

In this example, we specify that :

1 - we consider **one property**

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

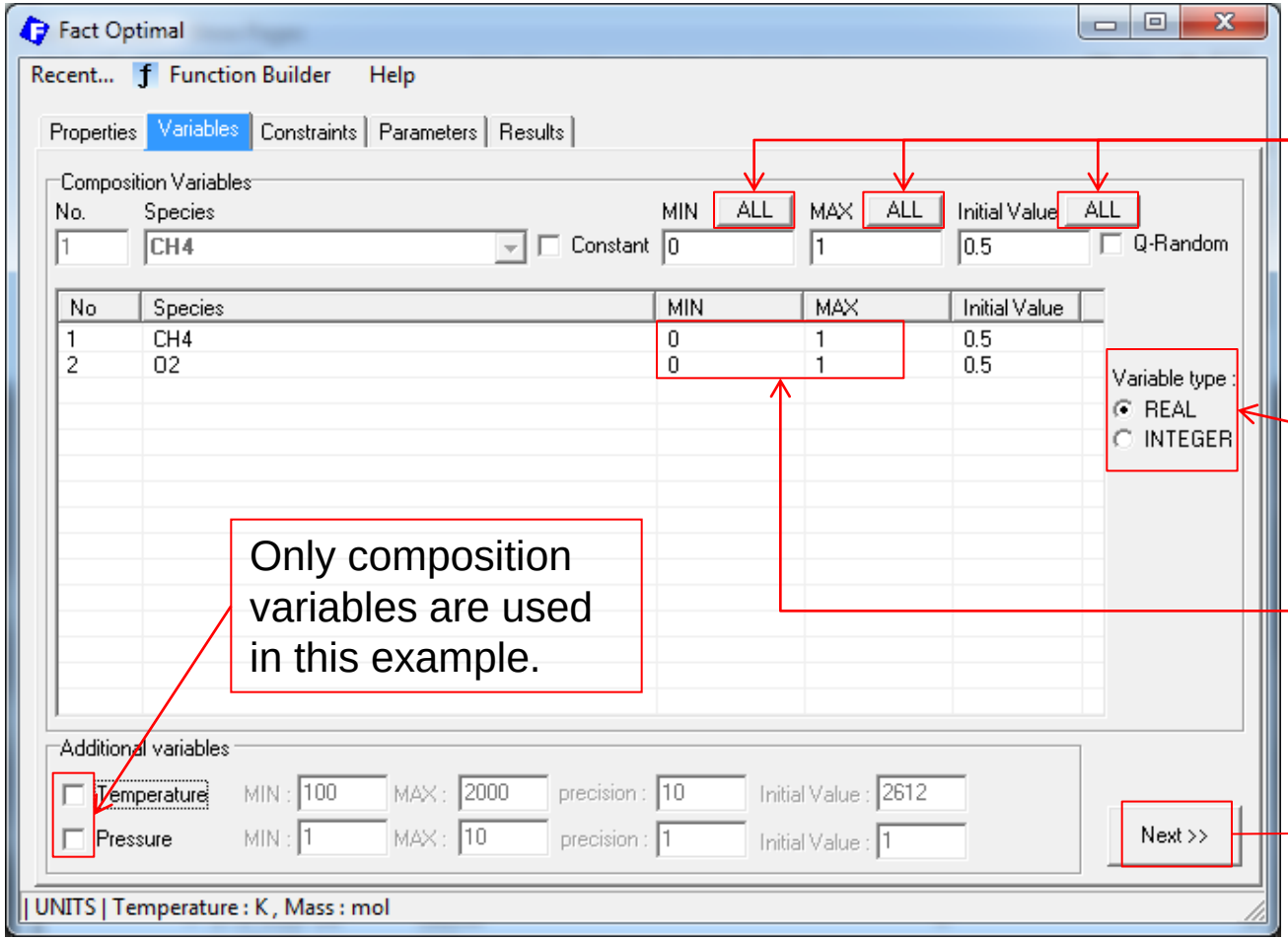
3 - the property is **temperature**




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 3.8)




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

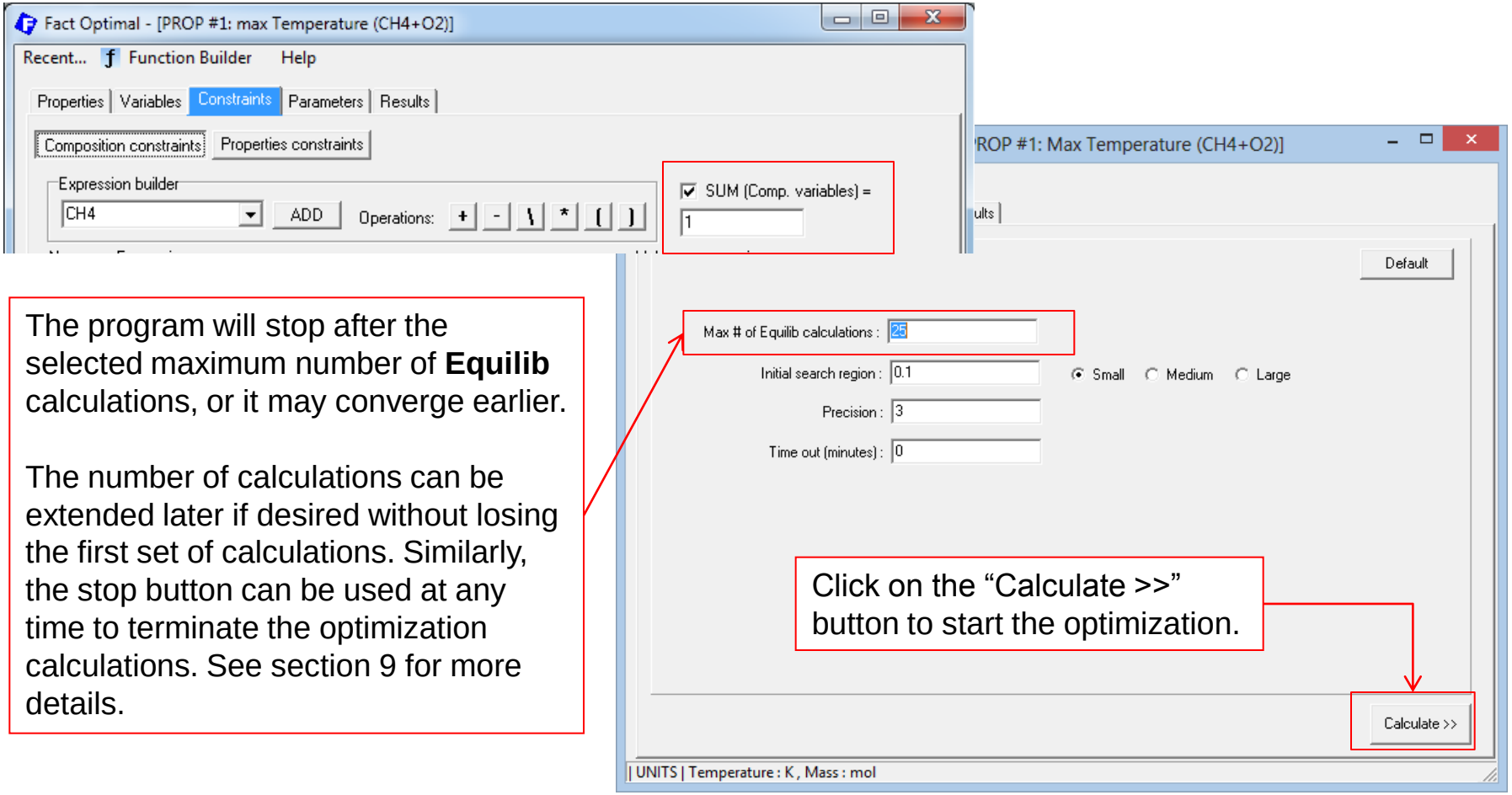
REAL type is chosen with values varying from 0 to 1. For INTEGER type, see example in section 3.7.

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).



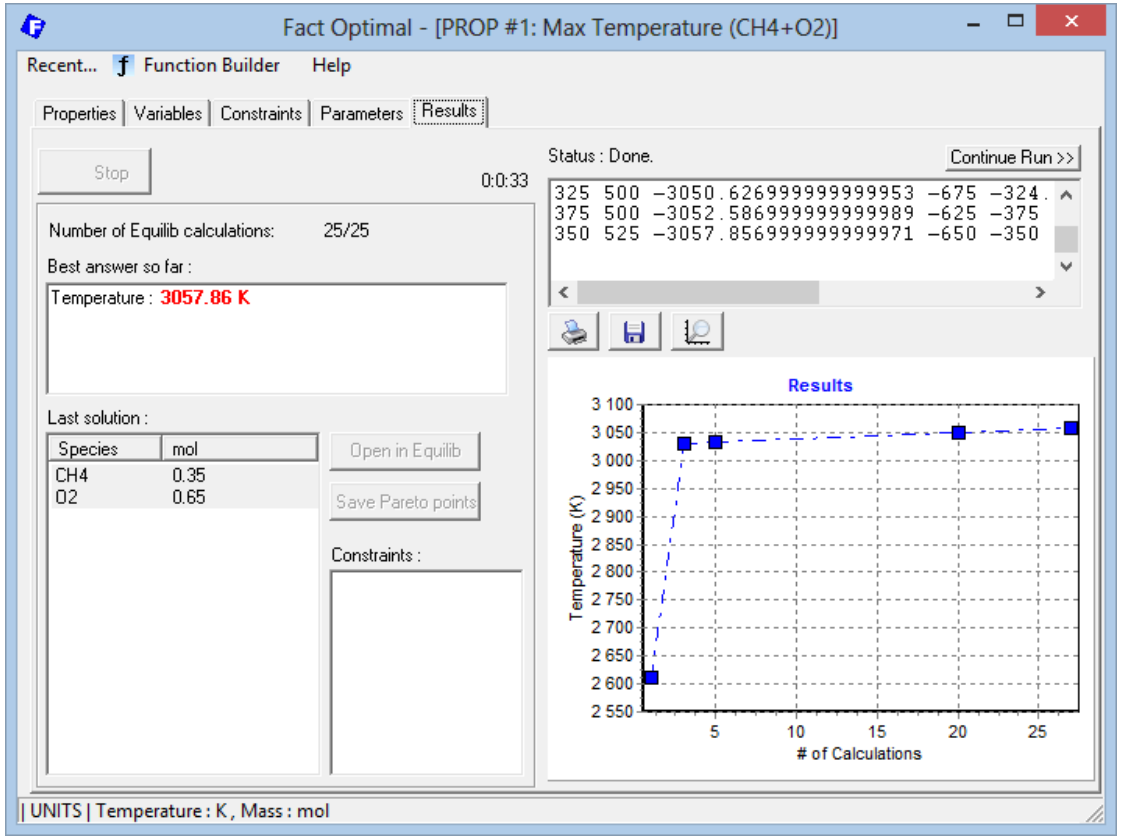

The program will stop after the selected maximum number of **Equilib** calculations, or it may converge earlier.

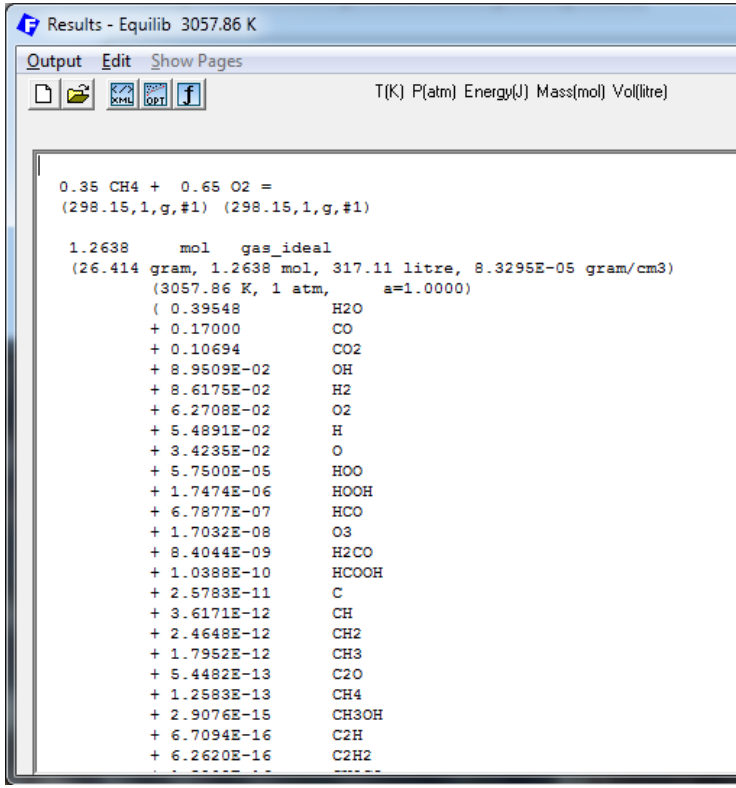
The number of calculations can be extended later if desired without losing the first set of calculations. Similarly, the stop button can be used at any time to terminate the optimization calculations. See section 9 for more details.

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.

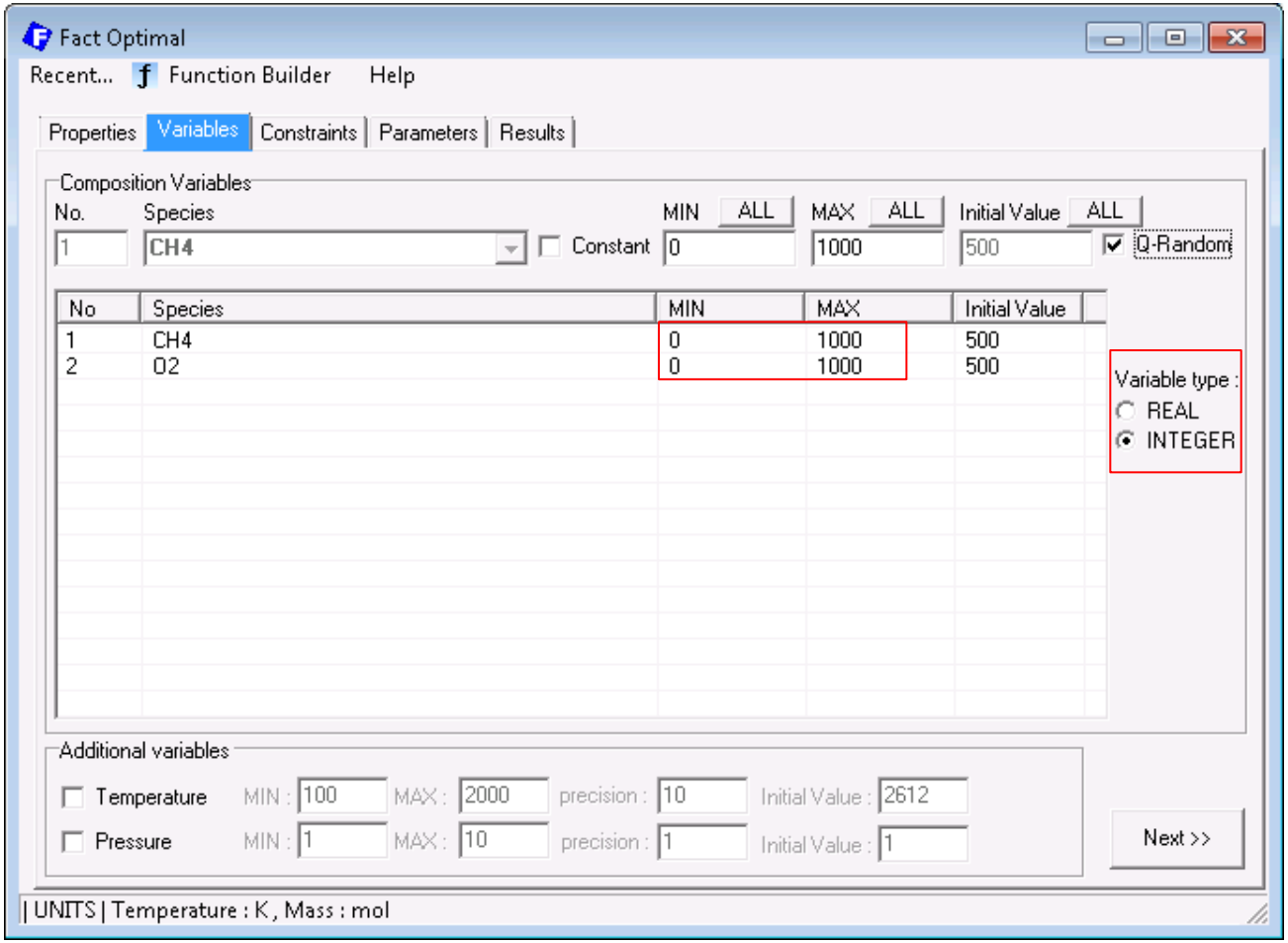


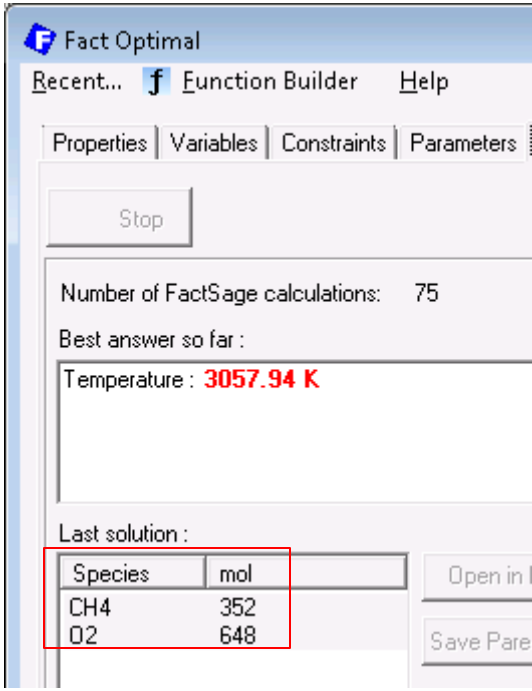



# Example 1: Maximize an adiabatic flame temperature - 7

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

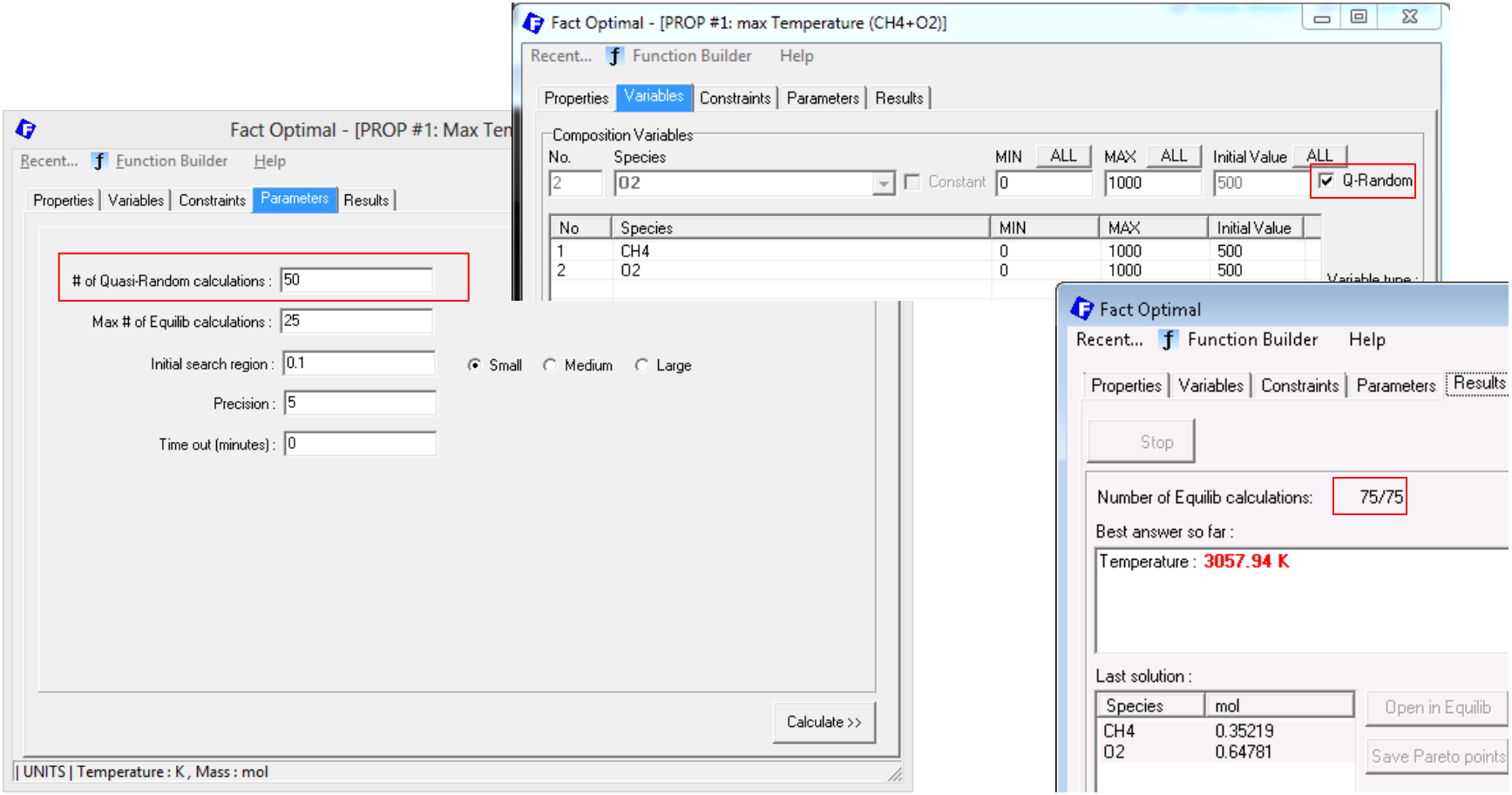
Using the same example, INTEGER type is chosen with values varying from 0 to 1000. By selecting this option as opposed to real values varying from 0 to 1, we are limiting the number of significant digits to 3.



# Example 1: Maximize an adiabatic flame temperature - 8

We also clicked the Q-Random (Quasi-Random) option, in order to let FactOptimal determine the best initial point. This is a good practice if you are not sure of what the best starting point should be. When choosing this 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 best solution for a total of 75 calculations.



## *Example 2: Minimize the liquidus temperature under constraints*

In this section we will calculate the minimum liquidus temperature of a multicomponent solution phase under various constraints of composition, cost, density, etc.

There are 2 examples –

- minimize the liquidus temperature of an Al-Cu-Mg-Zn molten alloy using data from FTlite
- minimize the liquidus temperature of a LiCl-NaCl-KCl-LiF-NaF-KF molten salt using data from FTsalt

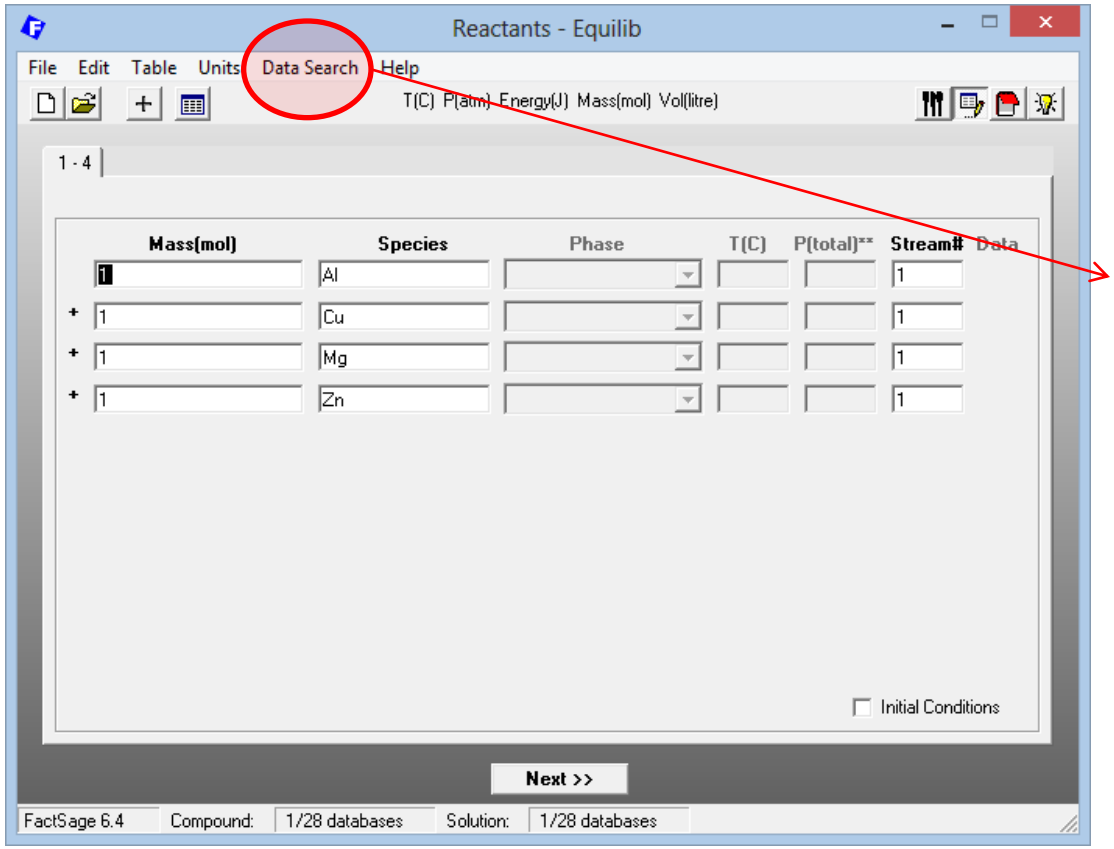
# Example 2a : Minimize the alloy liquidus temperature under constraints - 1

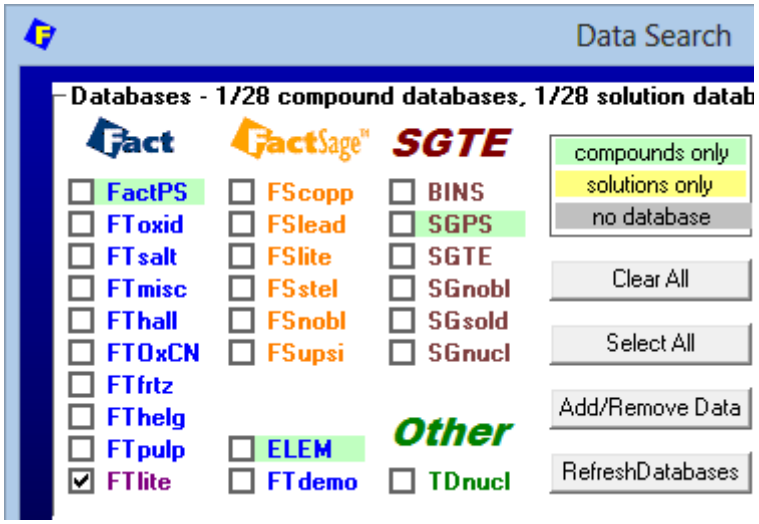
**System:** **Al-Cu-Mg-Zn.**

**Constraints:**

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

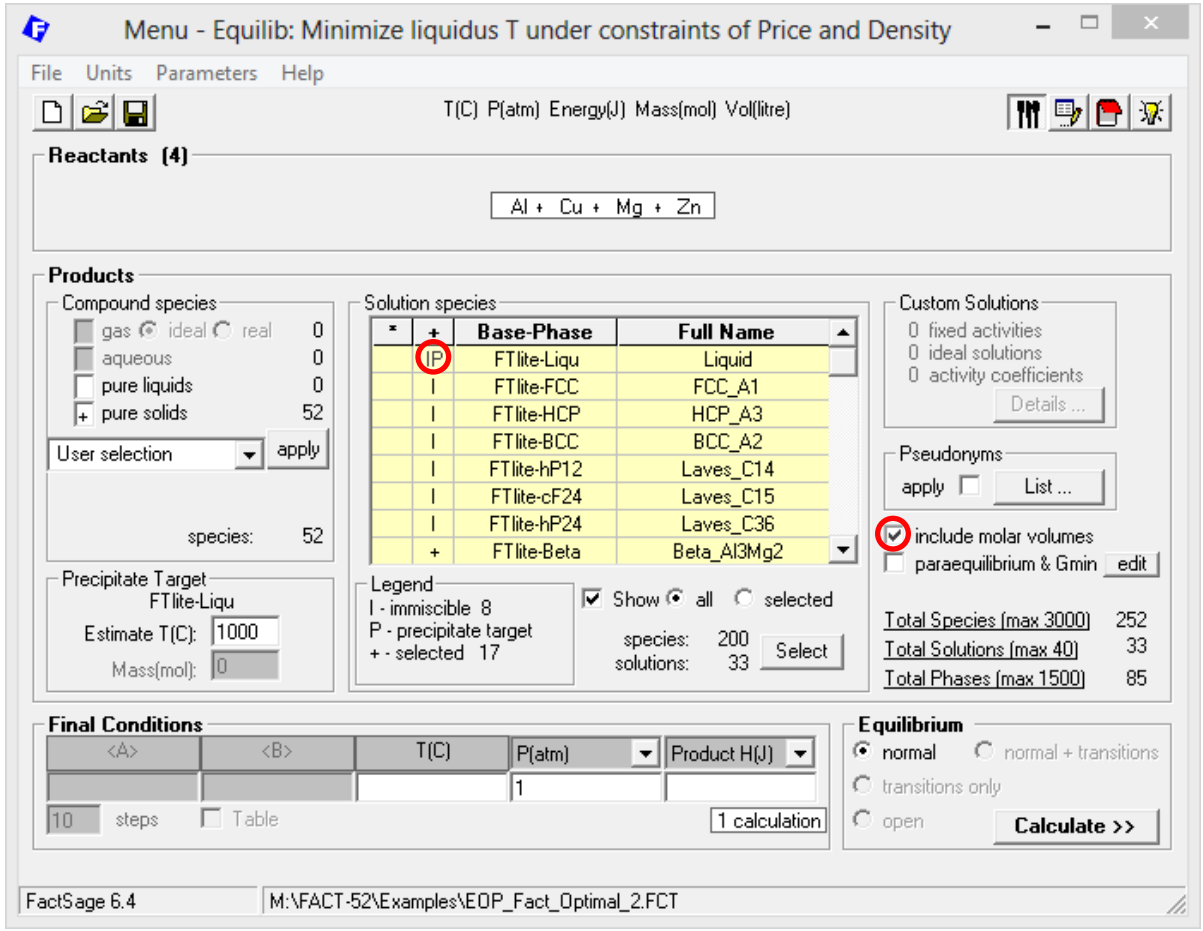
Step 1: Using **Equilib** define the system and select the appropriate database: **FTlite**.



# Example 2a : Minimize the alloy liquidus temperature under constraints - 2

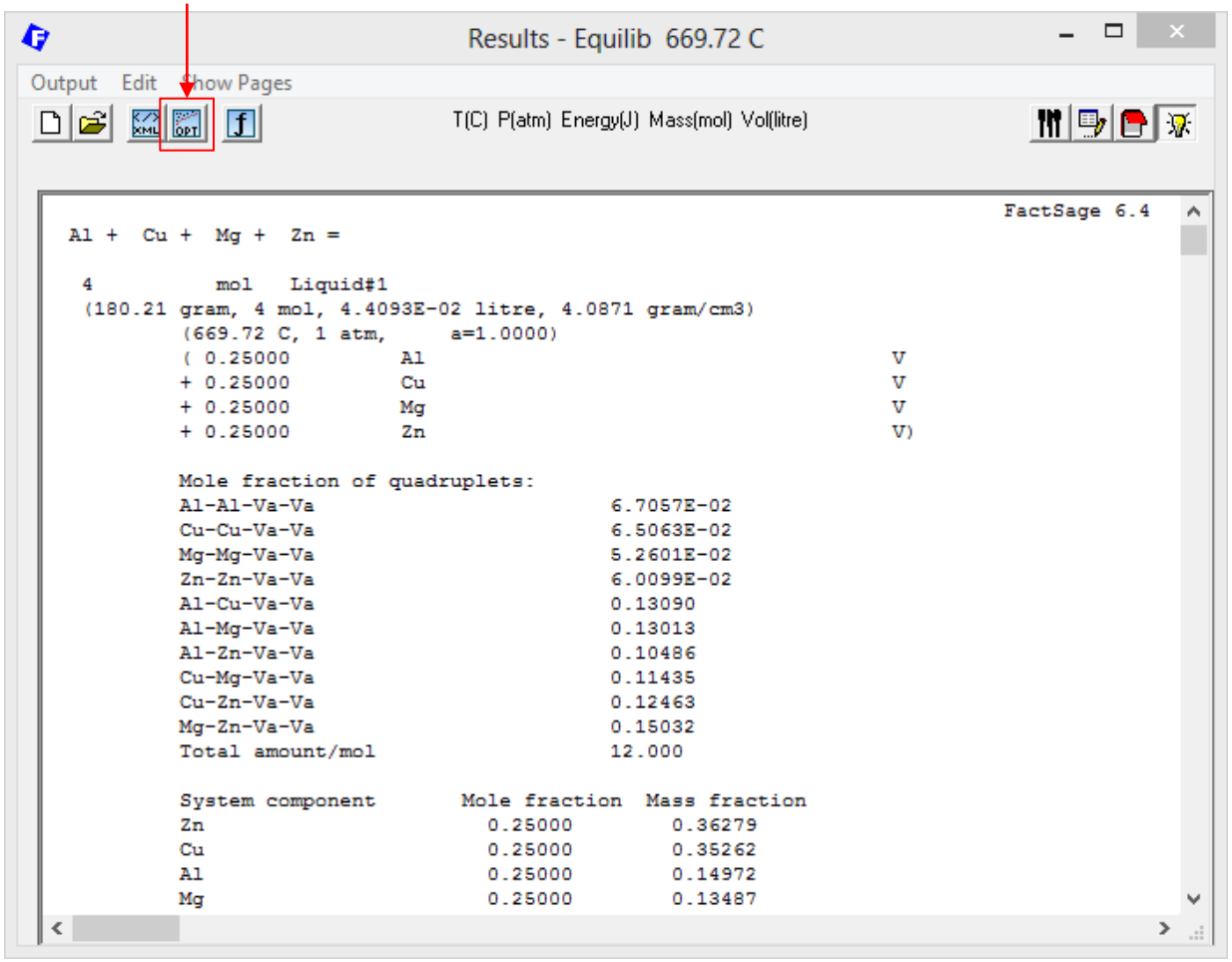
<u>Step 2</u>**:** Perform a single equilibrium calculation at an arbitrary composition and specify a precipitate (P) calculation on the liquid (i.e. liquidus temperature calculation) and “include molar volumes” (for the calculation of the density):



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

*Equilib Results Window*

**Click on the FactOptimal icon**

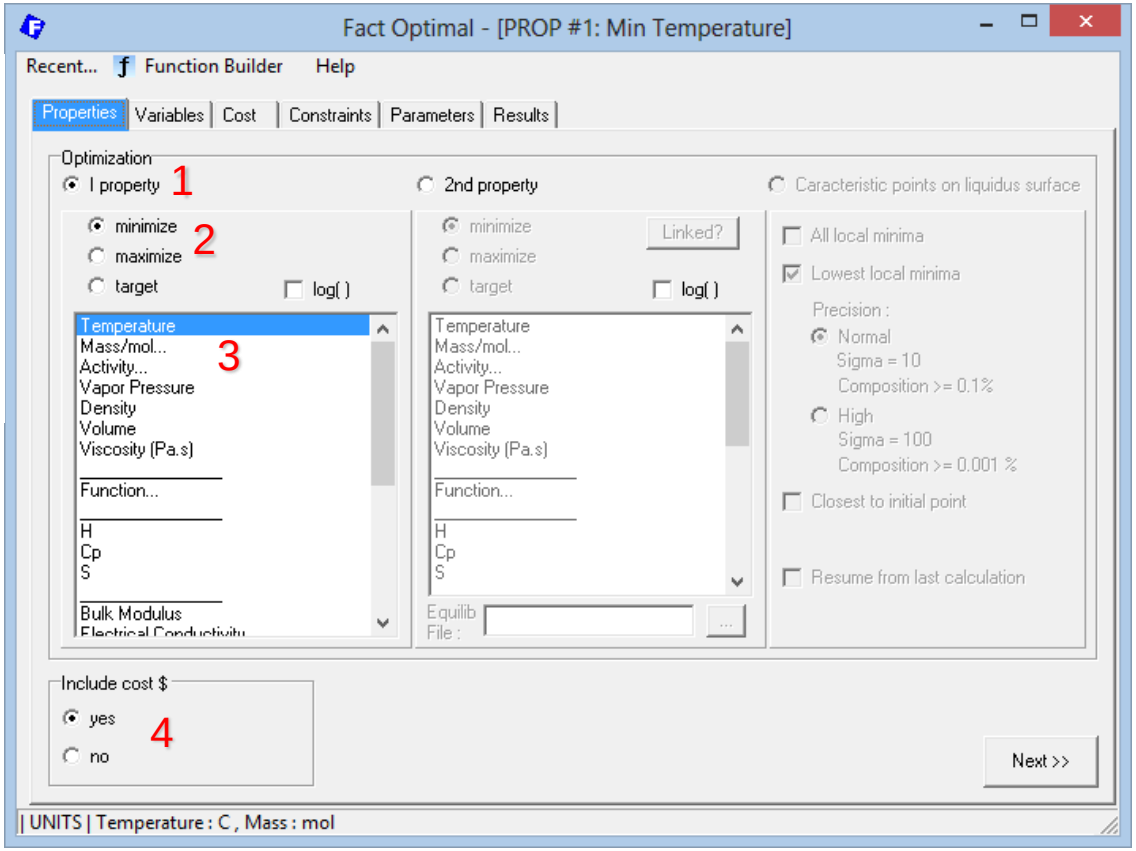


# Example 2a : Minimize the alloy liquidus temperature under constraints - 4

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

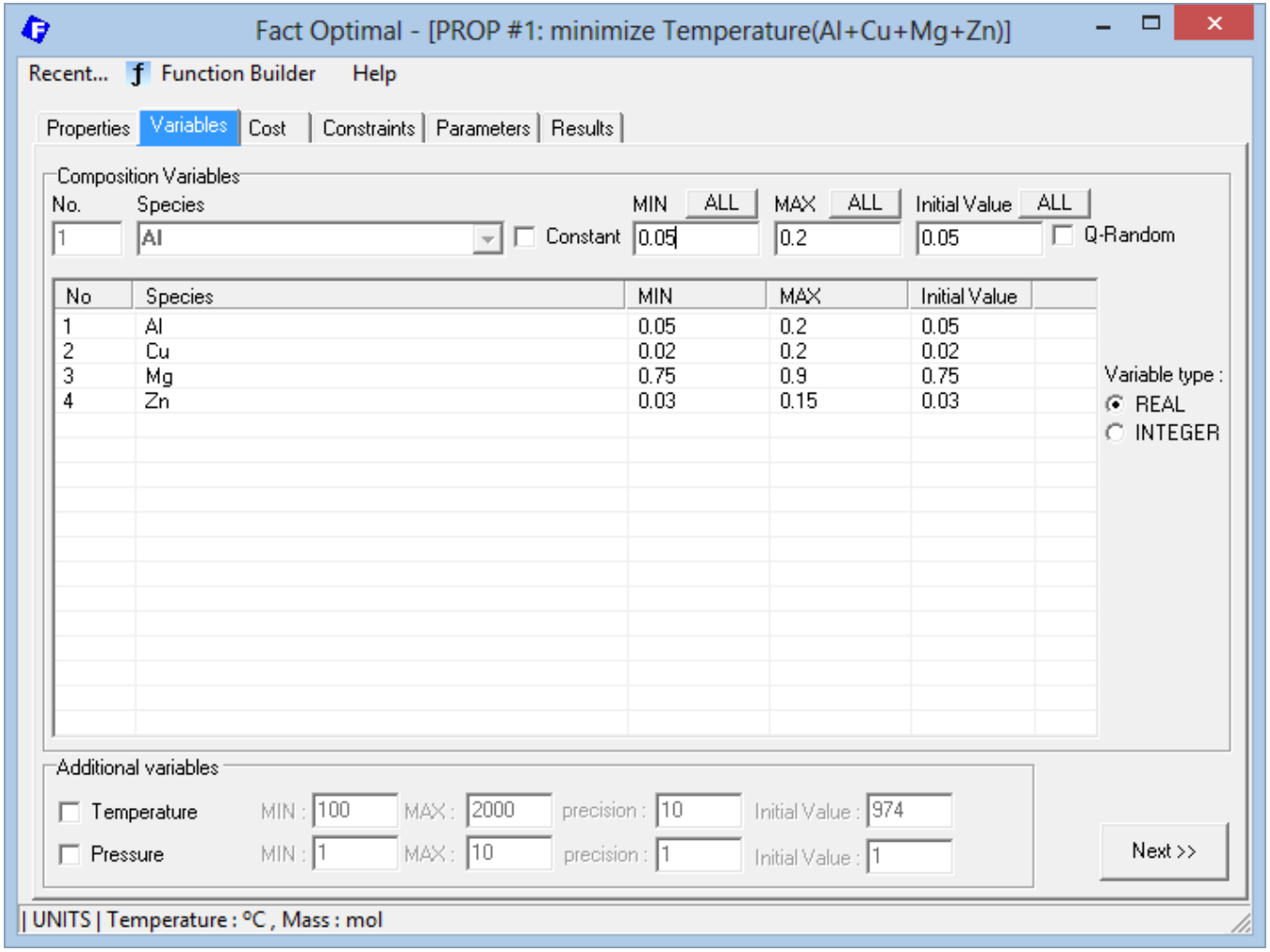
If you are using the stored example files, click on “Recent...” to load the Fact Optimal file. In this example, we specify that:

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 2a : Minimize the alloy liquidus temperature under constraints - 5

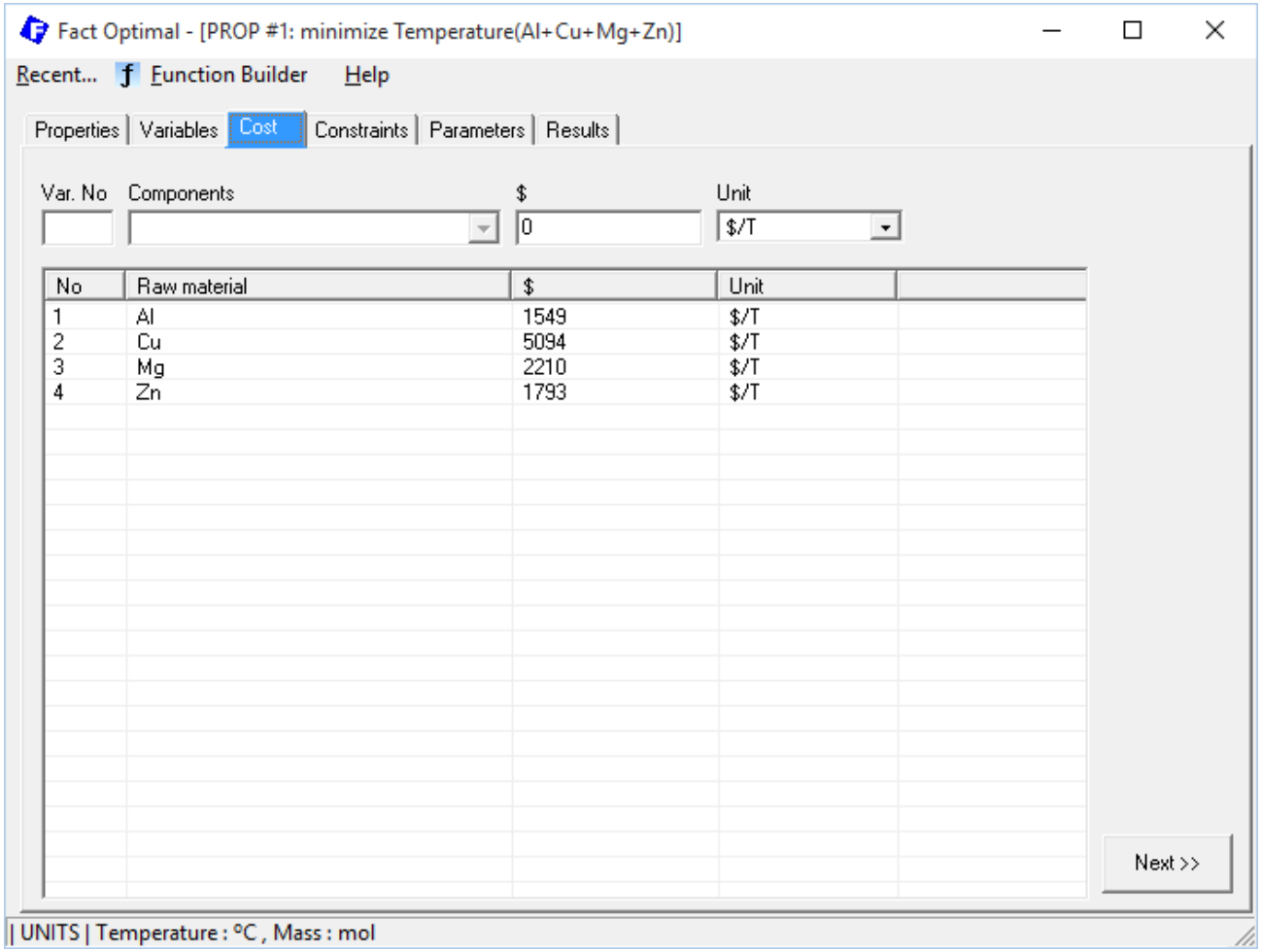
Step 4: In the "Variables" tab we define the permissible composition range (and initial estimates)




0.05 ≤ Wt.% Al ≤ 0.2 (0.05)
0.05 ≤ Wt.% Cu ≤ 0.2 (0.02)
0.75 ≤ Wt.% Mg ≤ 0.9 (0.75)
0.00 ≤ Wt.% Zn ≤ 0.15 (0.03)

# Example 2a : Minimize the alloy liquidus temperature under constraints - 6

Step 5: In the "cost" tab we define the unit price of each component.

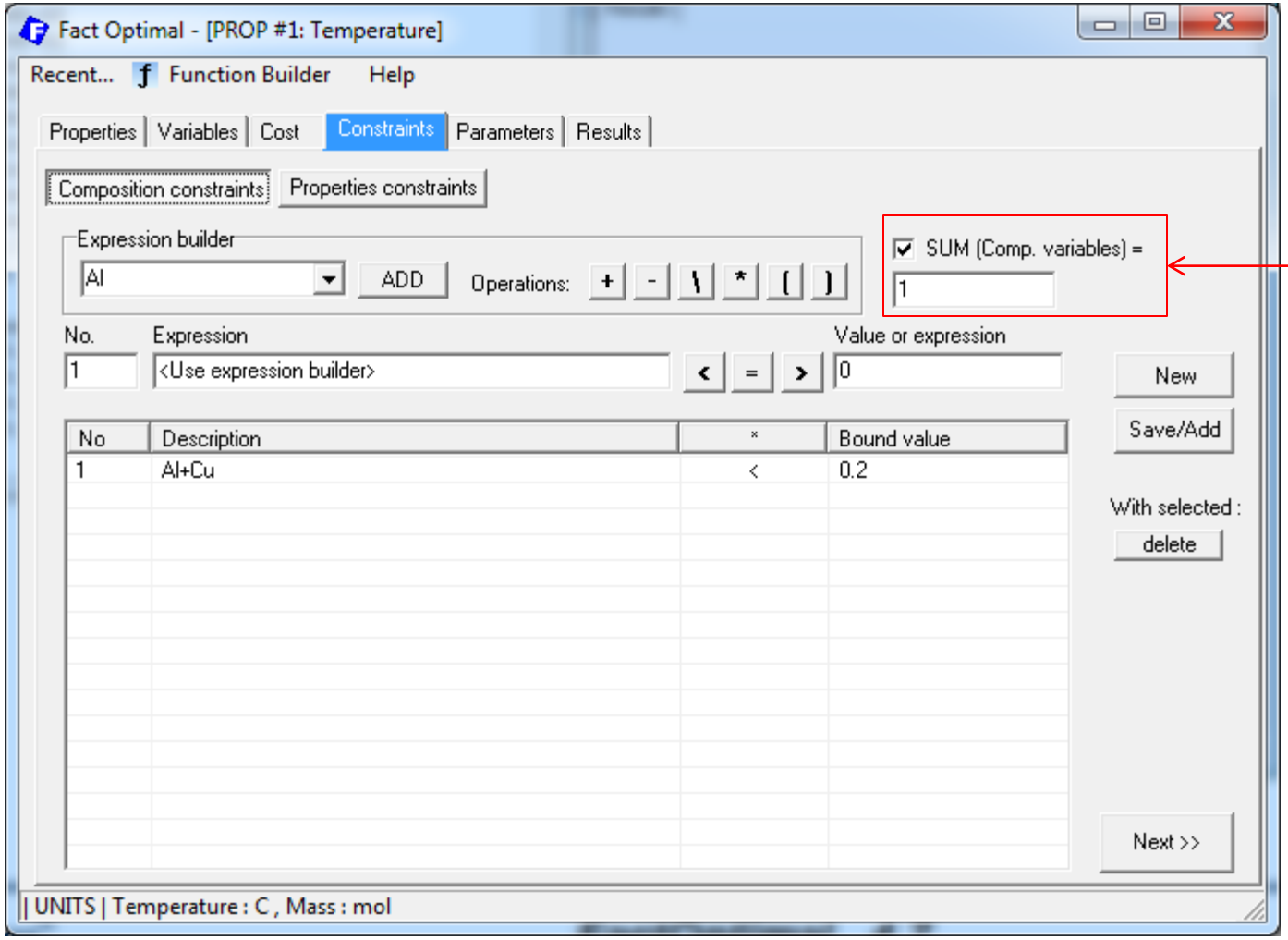



The cost per unit can be in $/ton, $/kg or $/g

$2132 per ton Al
$7315 per ton Cu
$2980 per ton Mg
$2100 per ton Zn

# Example 2a : Minimize the alloy liquidus temperature under constraints - 7

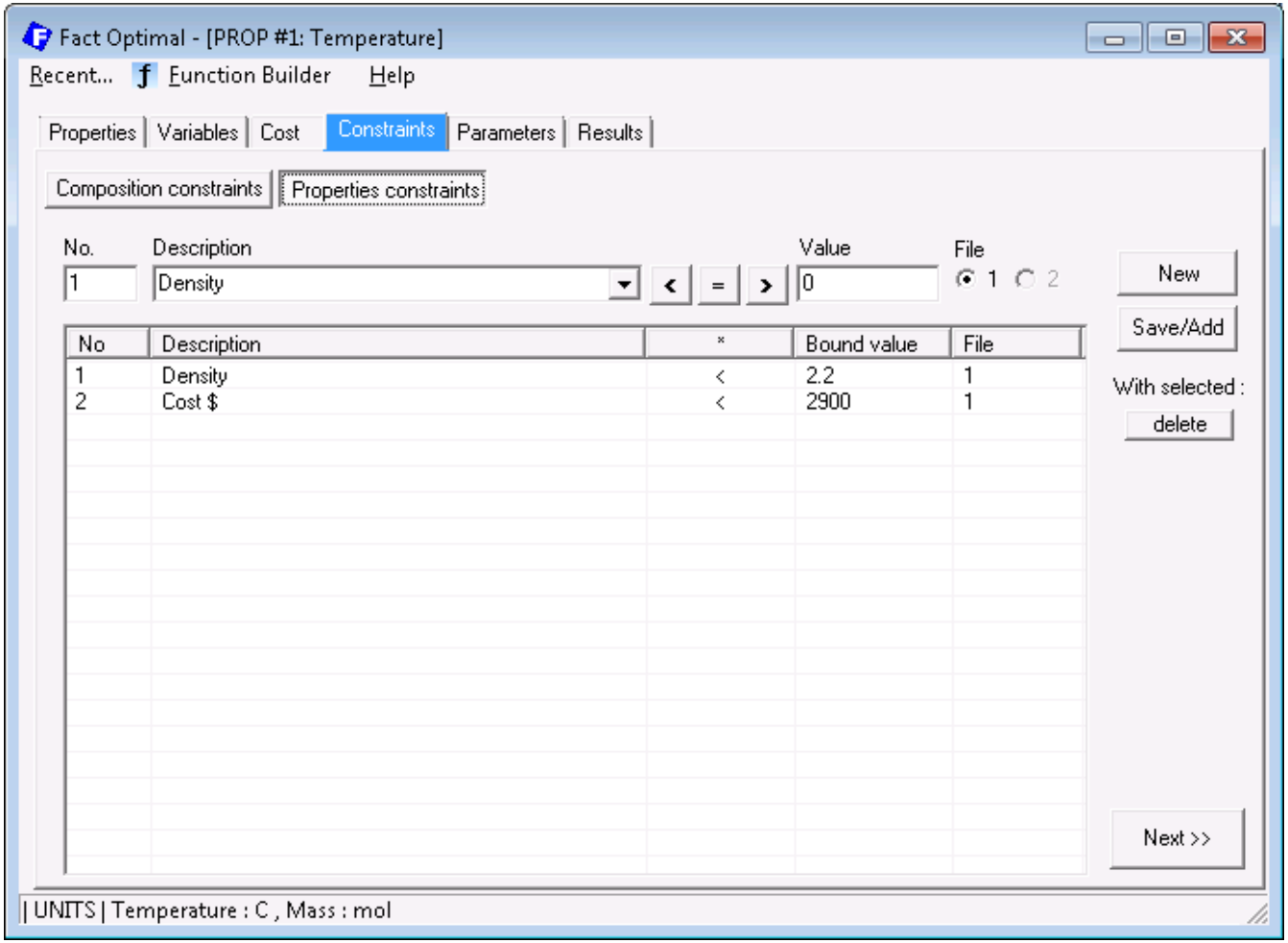
Step 6: Define the constraints on composition: **X(Al) + X(Cu) < 0.2**




SUM (Comp. Variables) = 1 therefore compositions are mole fractions

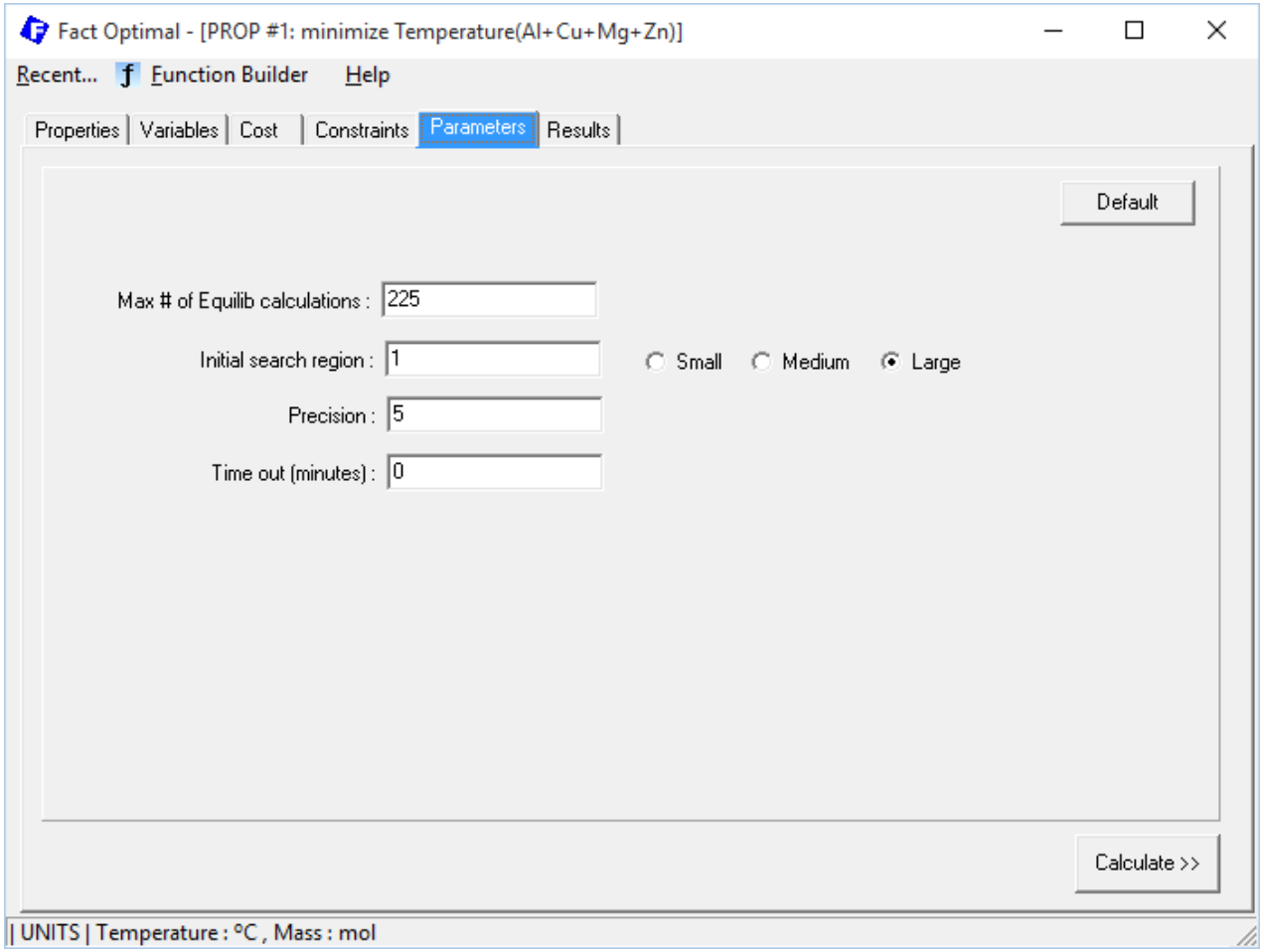
# Example 2a : Minimize the alloy liquidus temperature under constraints - 8

Step 7: Define the constraints on properties : **ρ < 2.2 g/ml  cost < 2900 $/Ton**



# Example 2a : Minimize the alloy liquidus temperature under constraints - 9

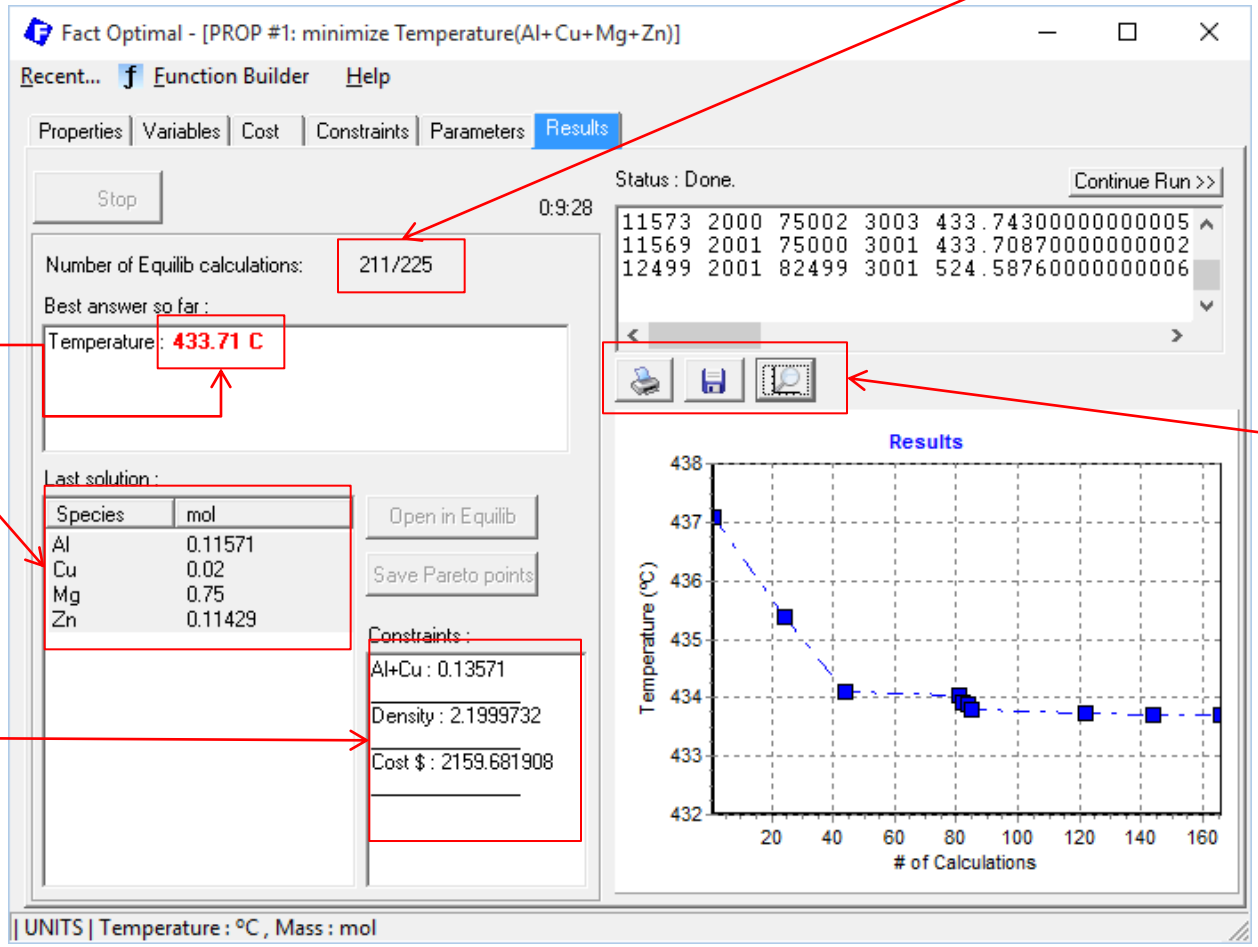
Step 8: Enter the maximum number of **Equilib** calculations and the initial search region (see slide 3.5). The max number of calculations is 150 because previous calculations have shown this number is necessary to obtain convergence.



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

FactOptimal Results Window

Here FactOptimal converged before executing all the calculations




Minimum

Composition at the minimum

Values of the defined constraints:
**X(Al) + X(Cu) < 0.2**
**ρ < 2.2 g/ml**
**cost < 2900 $/Ton**

Save and print the graph or change the axis scale

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

## Equilib Results Window

Results - Equilib 433.96 C

Output Edit Show Pages

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

```
                                                                    FactSage 6.4
0.11579 Al +  0.02 Cu +  0.75 Mg +  0.11421 Zn =

 1          mol   Liquid#1
 (30.091 gram, 1 mol, 1.3678E-02 litre, 2.1999 gram/cm3)
         (433.96 C, 1 atm,      a=1.0000)
         ( 0.11579          Al                                      V
         + 2.0000E-02       Cu                                      V
         + 0.75000          Mg                                      V
         + 0.11421          Zn                                      V)

         Mole fraction of quadruplets:
         Al-Al-Va-Va                        1.2356E-02
         Cu-Cu-Va-Va                        4.6548E-04
         Mg-Mg-Va-Va                        0.54341
         Zn-Zn-Va-Va                        7.9907E-03
         Al-Cu-Va-Va                        4.6790E-03
         Al-Mg-Va-Va                        0.18809
         Al-Zn-Va-Va                        1.4101E-02
         Cu-Mg-Va-Va                        3.0574E-02
         Cu-Zn-Va-Va                        3.8159E-03
         Mg-Zn-Va-Va                        0.19452
         Total amount/mol                   3.0000

         System component       Mole fraction  Mass fraction
         Zn                       0.11421        0.24815
         Cu                       2.0000E-02     4.2236E-02
         Al                       0.11579        0.10383
         Mg                       0.75000        0.60579
```

# Example 2b: Minimize the salt liquidus temperature under constraints - 1

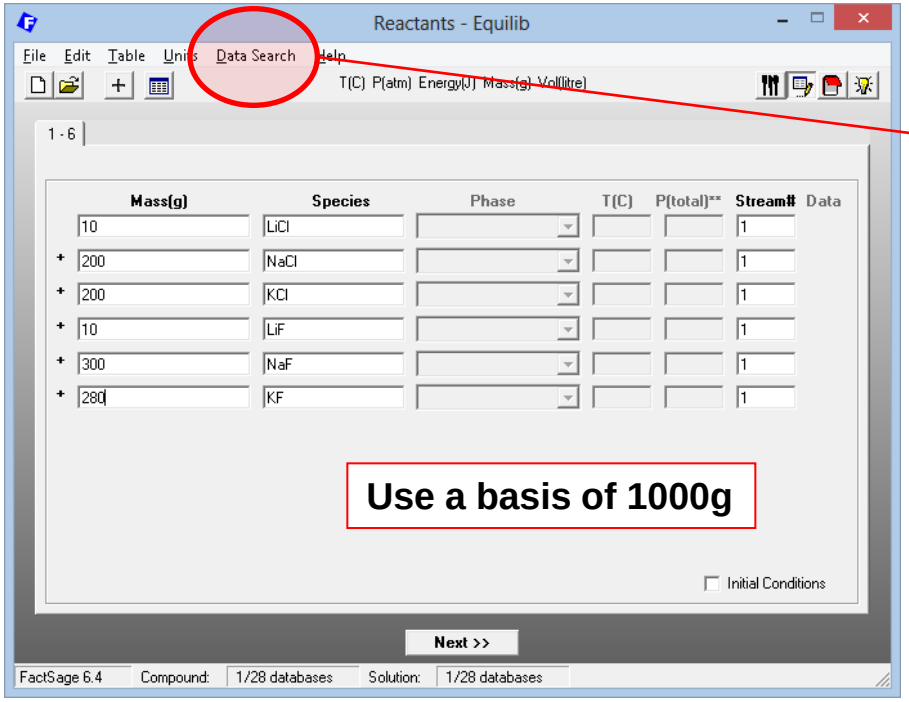
This is a typical problem to solve for the design of a molten salt medium for thermal storage

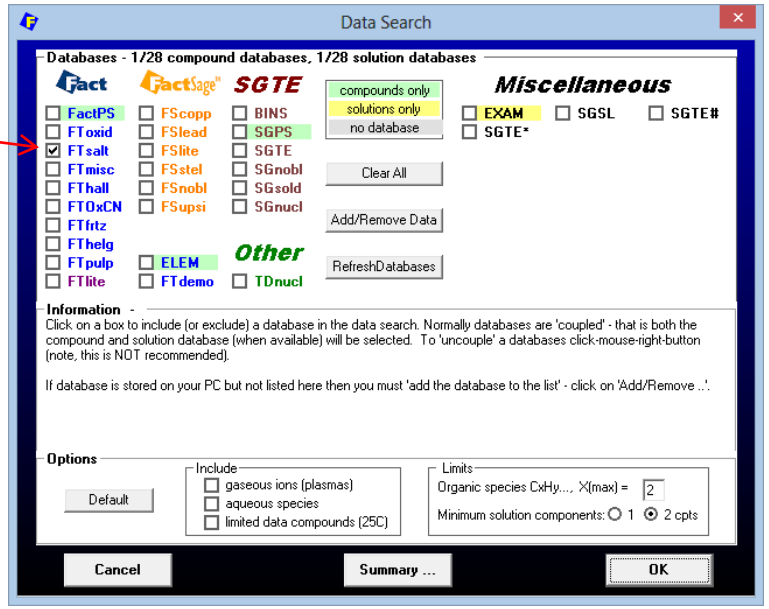
**System:** **LiCl-NaCl-KCl-LiF-NaF-KF**

**Constraints:**

- **wt.%(LiCl) + wt.%(LiF) ≤ 10**
- **wt.%(NaCl) + wt.%(KCl) ≥ 3*(wt.%(NaF) + wt.%(KF))**
- **Density ≥ 1750 kg/m$^3$**
- **Cp ≥ 1250 J/kg**
- **Cost ≤ 3.5 $/kg**

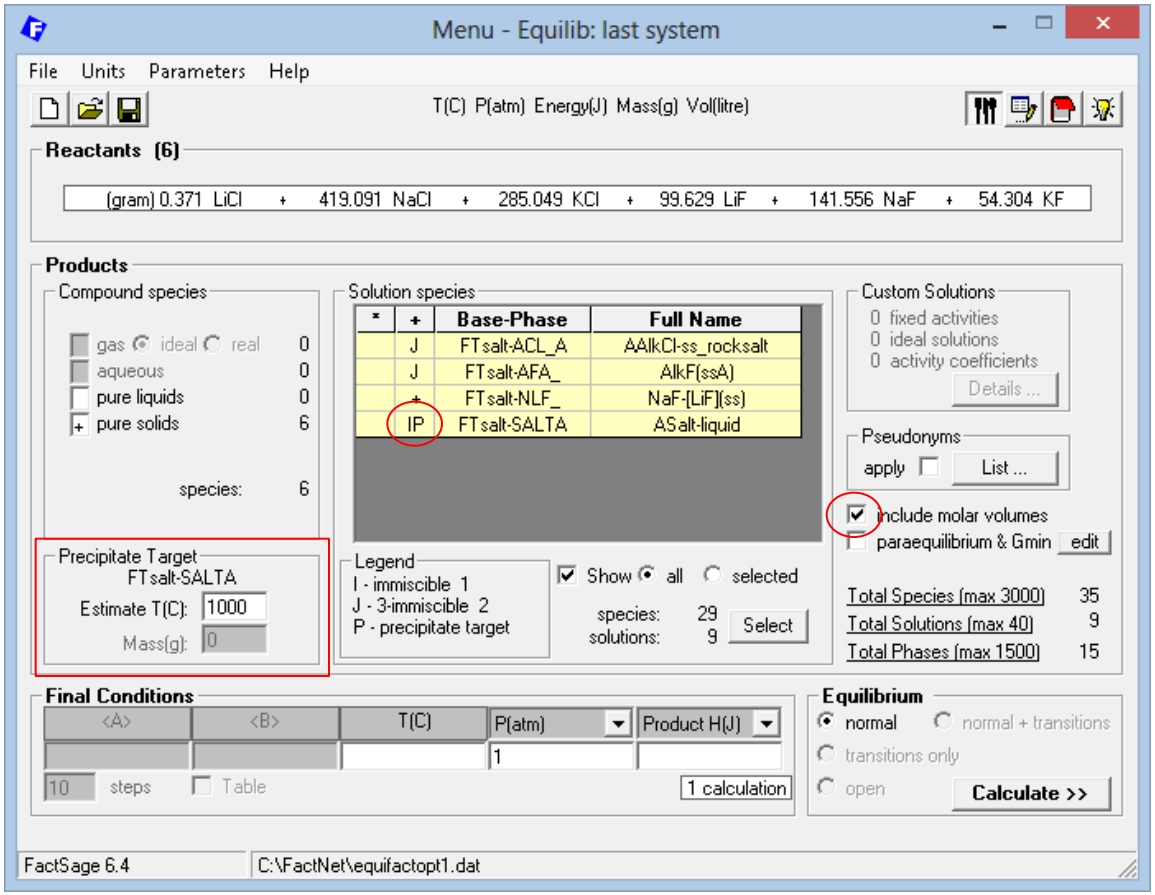
Step 1: Using **Equilib,** define the system and select the appropriate database: **FTsalt**.



# Example 2b: Minimize the salt liquidus temperature under constraints - 2

<u>Step 2</u>**:** 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):

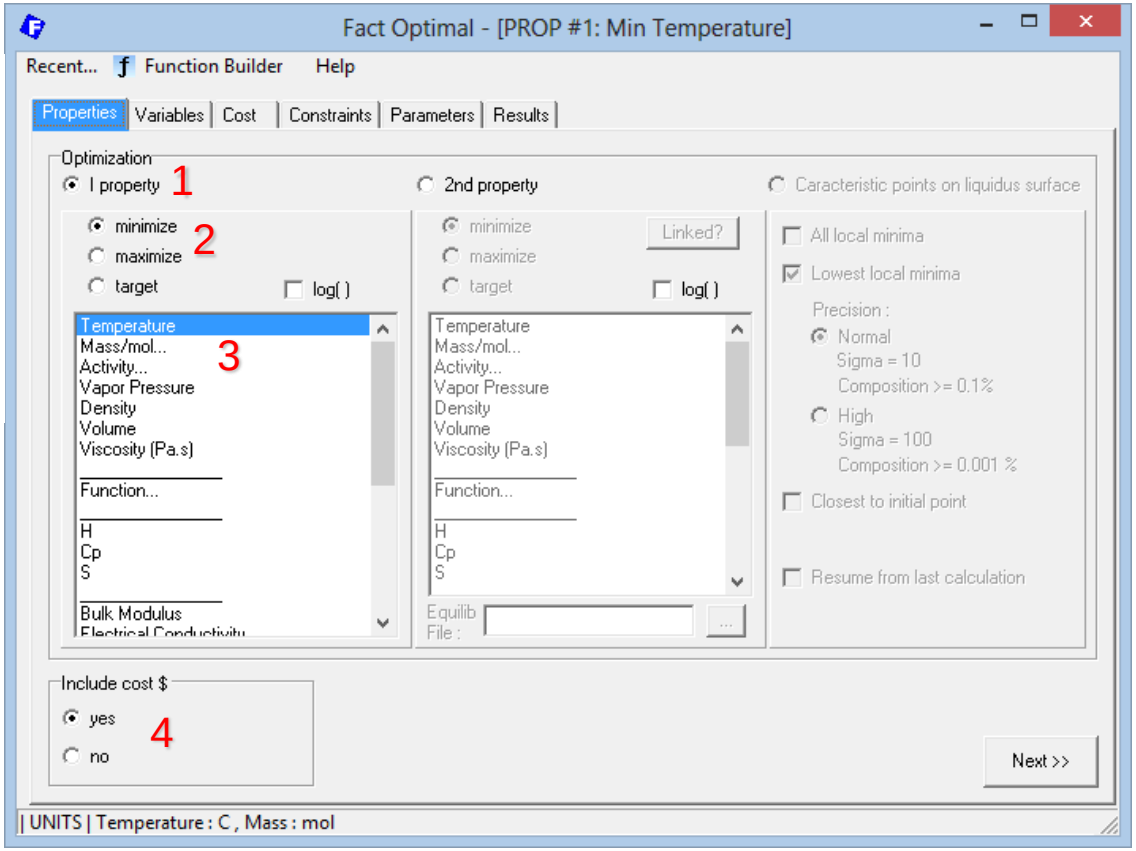


# Example 2b: Minimize the salt liquidus temperature under constraints - 4

Step 3: After doing one calculation, click on the **FactOptimal** icon and set up the optimization.

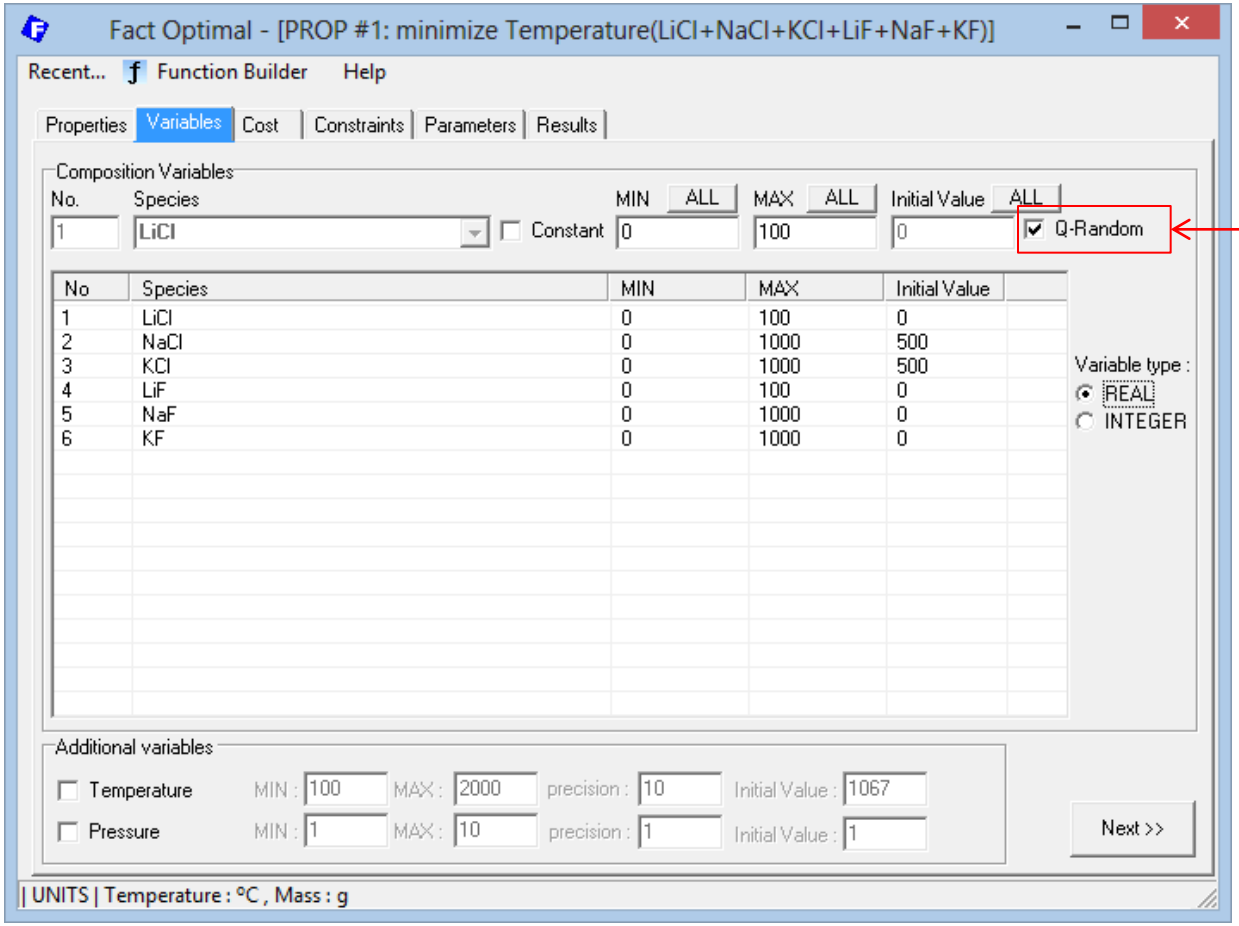
If you are using the stored example files, click on “Recent...” to load the Fact Optimal file. In this example, we specify that:

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 2b: Minimize the salt liquidus temperature under constraints - 5

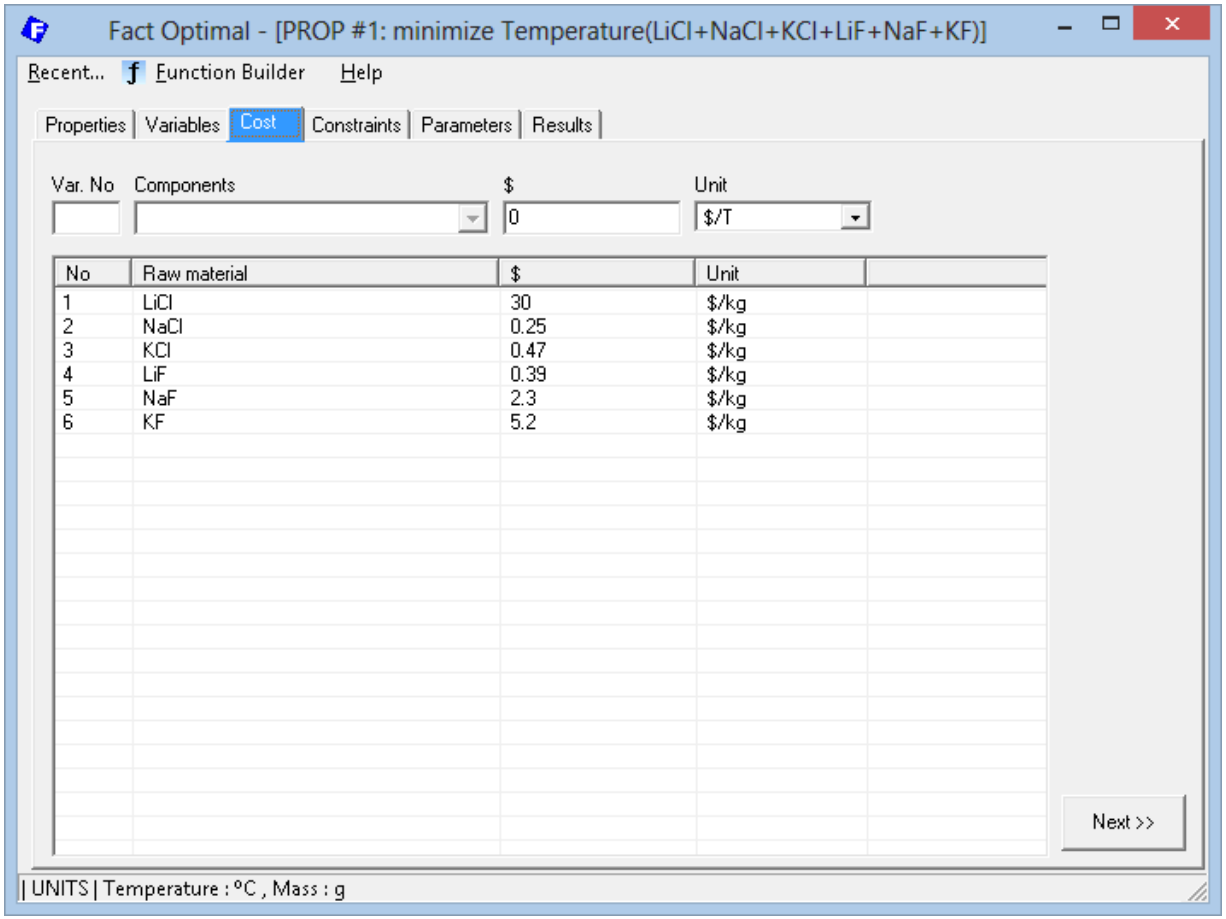
Step 4: Define the permissible composition range and a set of initial estimates.




Here we are not sure of the best starting point so we used the Q-Random option.

# Example 2b: Minimize the salt liquidus temperature under constraints - 6

Step 5: In the "cost" tab we define the unit price of each component.

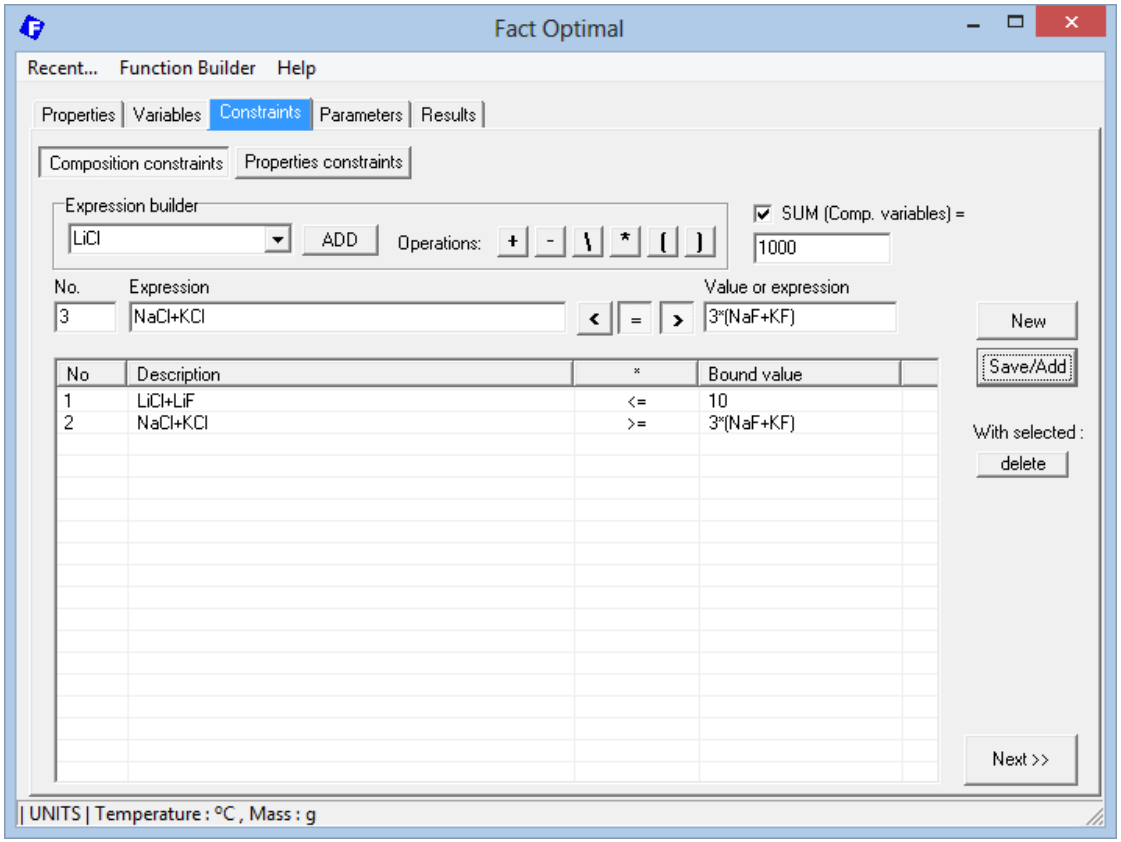



| No | Raw material | $ | Unit |
|---|---|---|---|
| 1 | LiCl | 30 | $/kg |
| 2 | NaCl | 0.25 | $/kg |
| 3 | KCl | 0.47 | $/kg |
| 4 | LiF | 0.39 | $/kg |
| 5 | NaF | 2.3 | $/kg |
| 6 | KF | 5.2 | $/kg |

# Example 2b: Minimize the salt liquidus temperature under constraints - 7

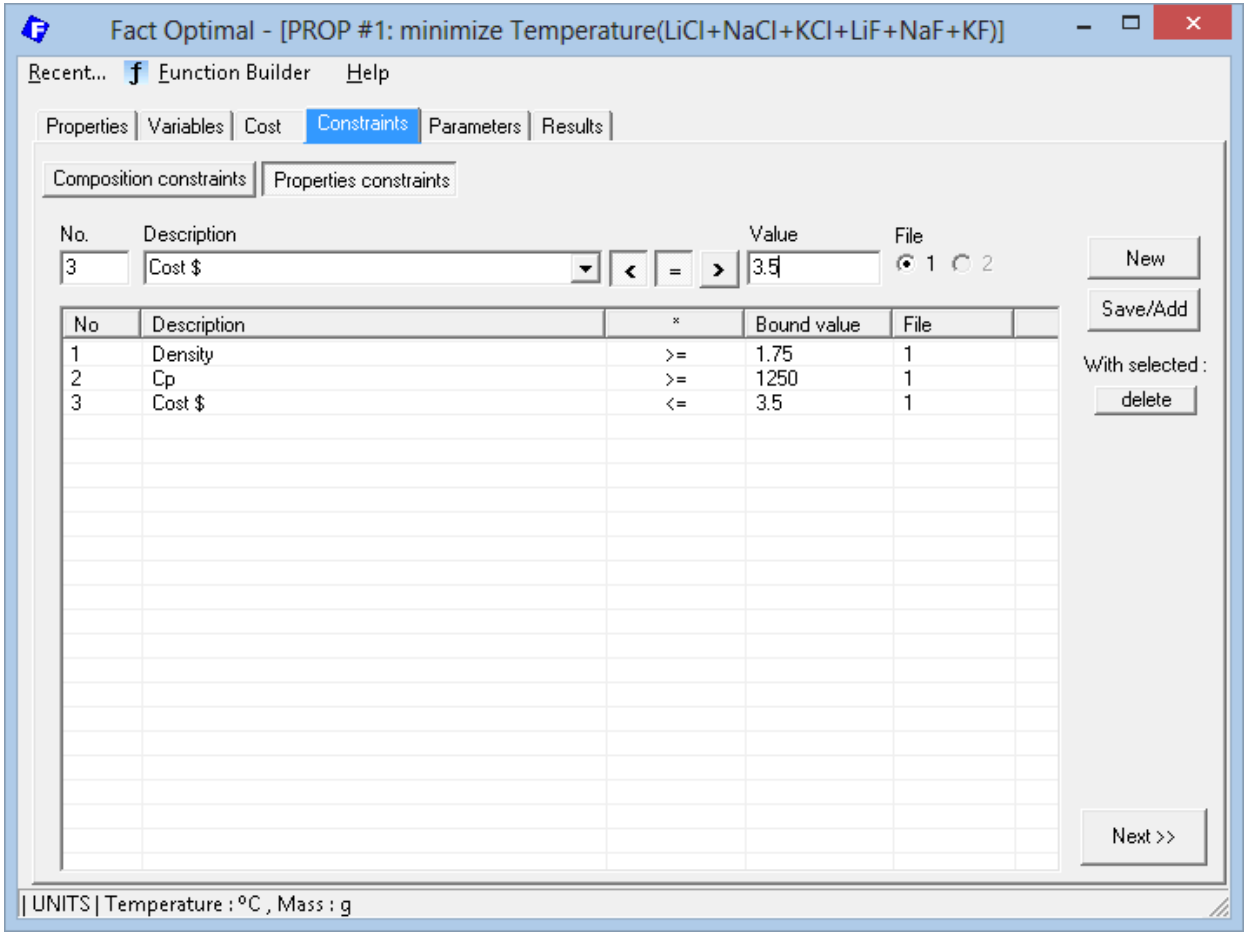
Step 5: Define the constraints on composition.

- Sum (Comp. Variables) = 1000 g
- wt.%(LiCl) + wt.%(LiF) ≤ 10
- wt.%(NaCl) + wt.%(KCl) ≥ 3*(wt.%(NaF) + wt.%(KF))



# Example 2b: Minimize the salt liquidus temperature under constraints - 8

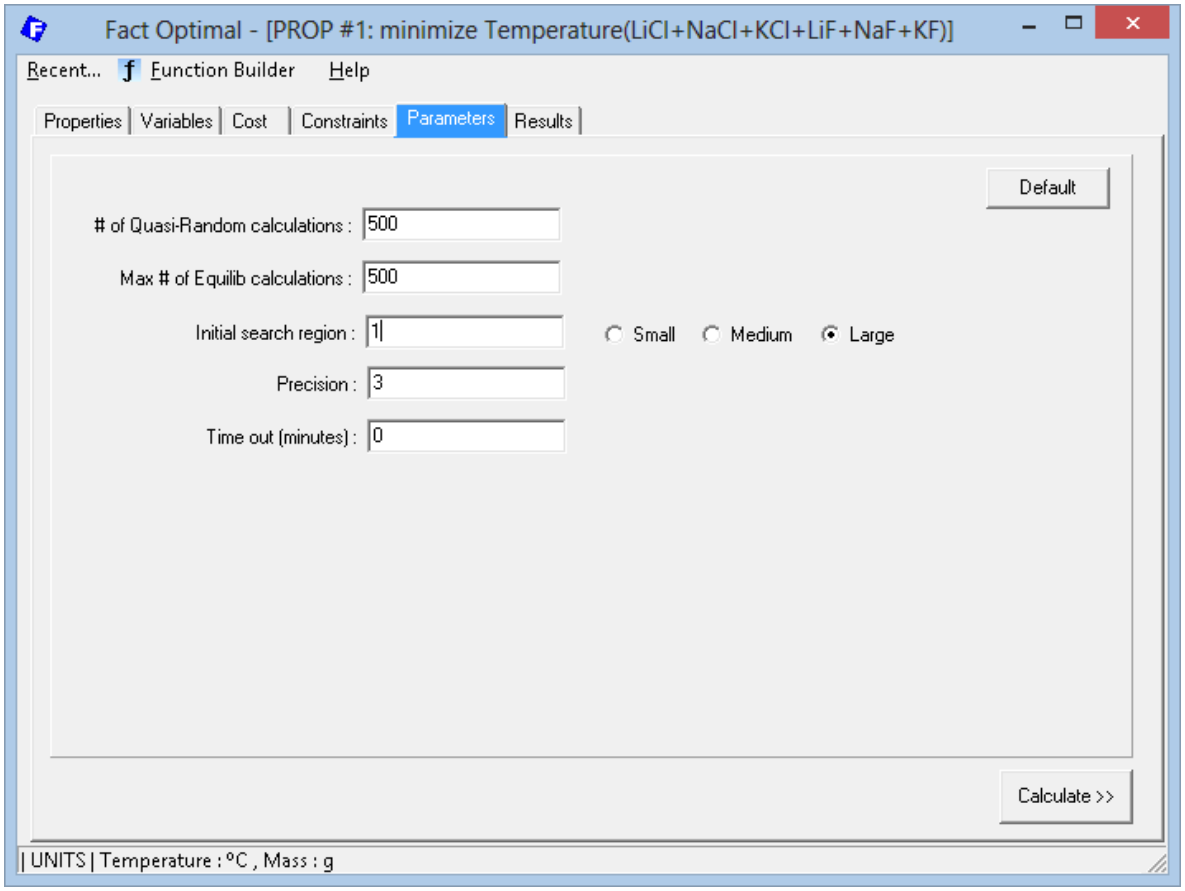
Step 6: Define the constraints on properties.




- Density ≥ 1750 kg/m$^3$
- Cp ≥ 1250 J/kg
- Cost ≤ 3.5 $/kg

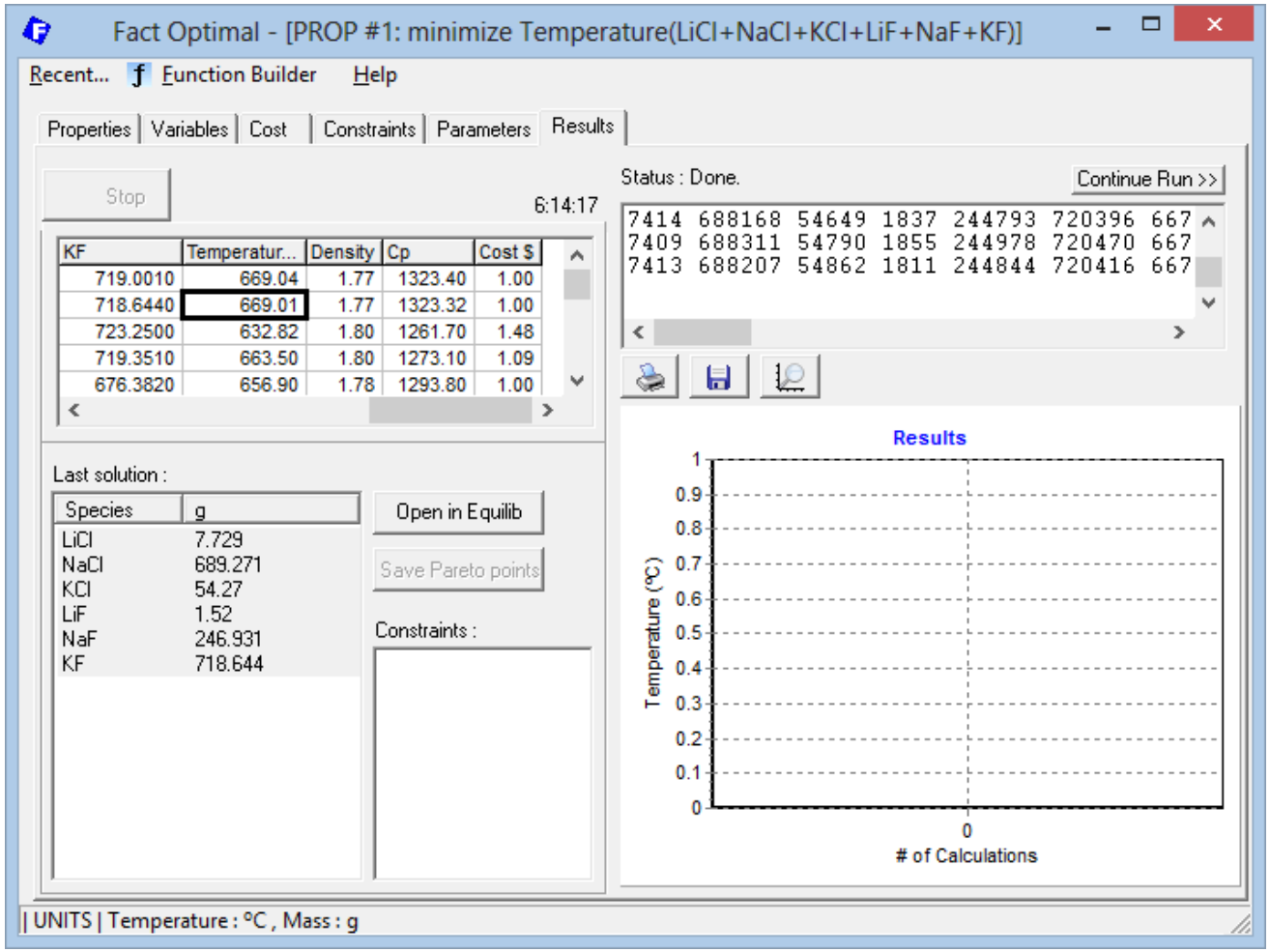
# Example 2b: Minimize the salt liquidus temperature under constraints - 9

<u>Step 7:</u> Enter the maximum number of **Equilib** calculations and the initial search region (see slide 3.5). Here we tried 500 calculations with 500 Quasoi-Random calcuations for a total of 1000 calculations. We used a large search region.



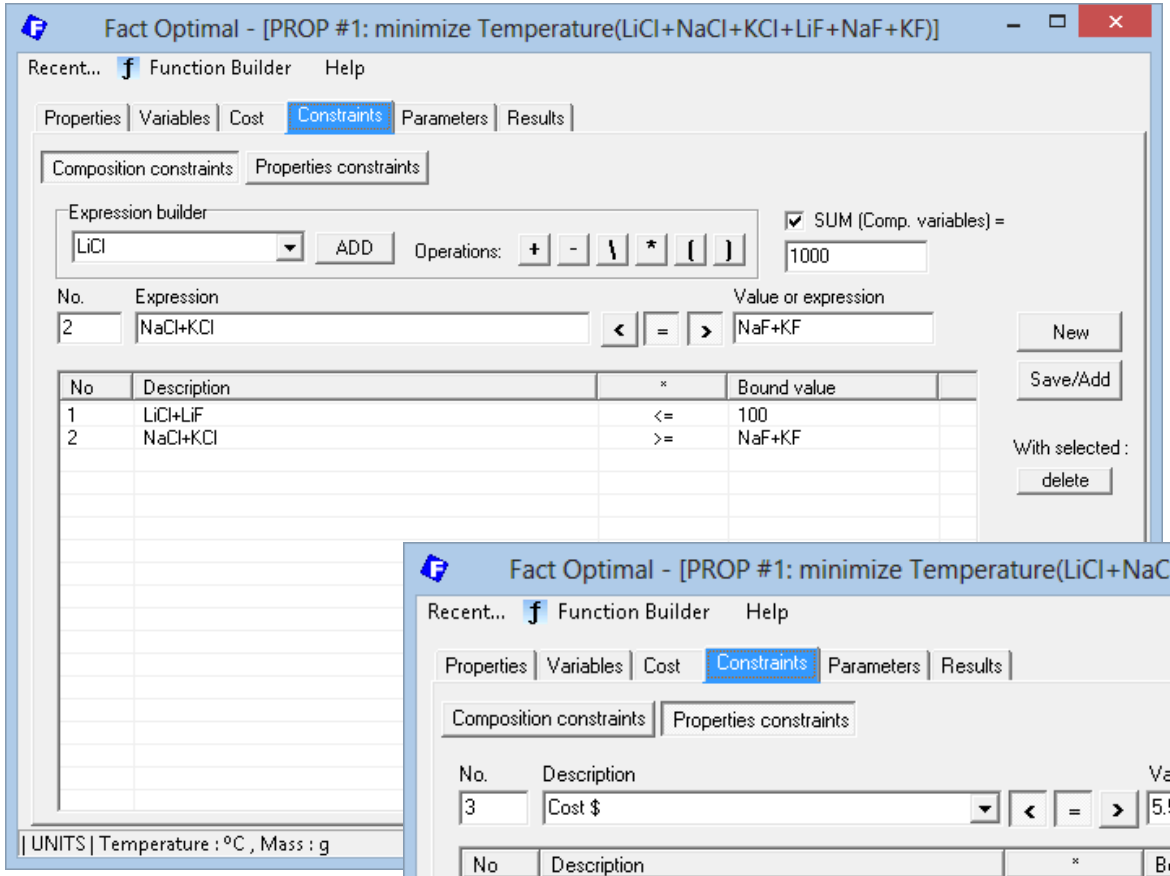
# Example 2b: Minimize the salt liquidus temperature under constraints - 10

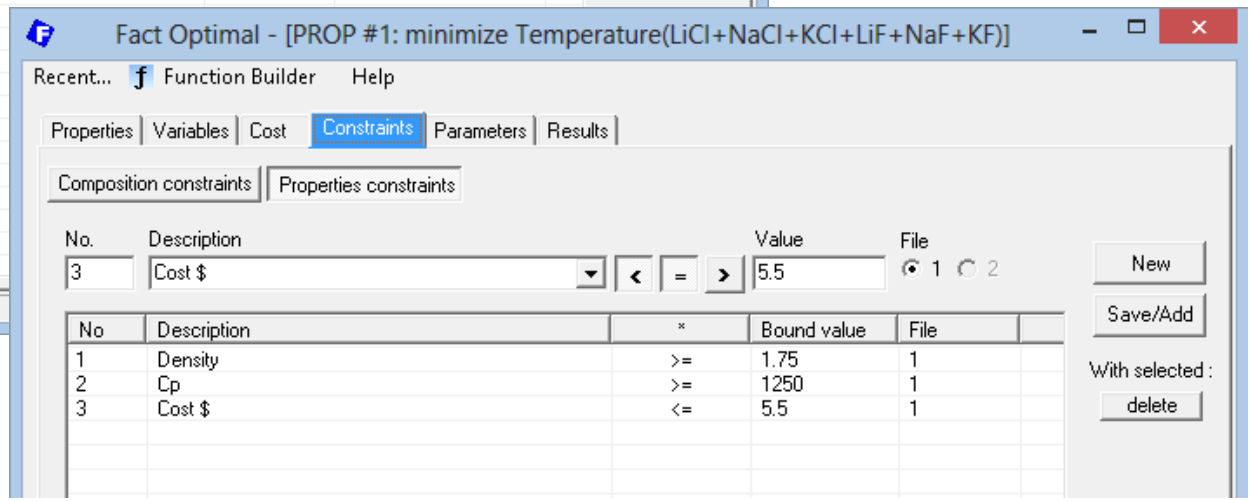
<u>FactOptimal Results Window:</u> Unfortunately, after 1000 calculations, FactOptimal did not find any answer respecting the constraints. Here the closest results are shown in a table.



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

Here we change constraints on composition and cost.




The new constraints are :

wt.%(LiCl) + wt.%(LiF) ≤ 100

wt.%(NaCl) + wt.%(KCl) ≥ (NaF + KF)

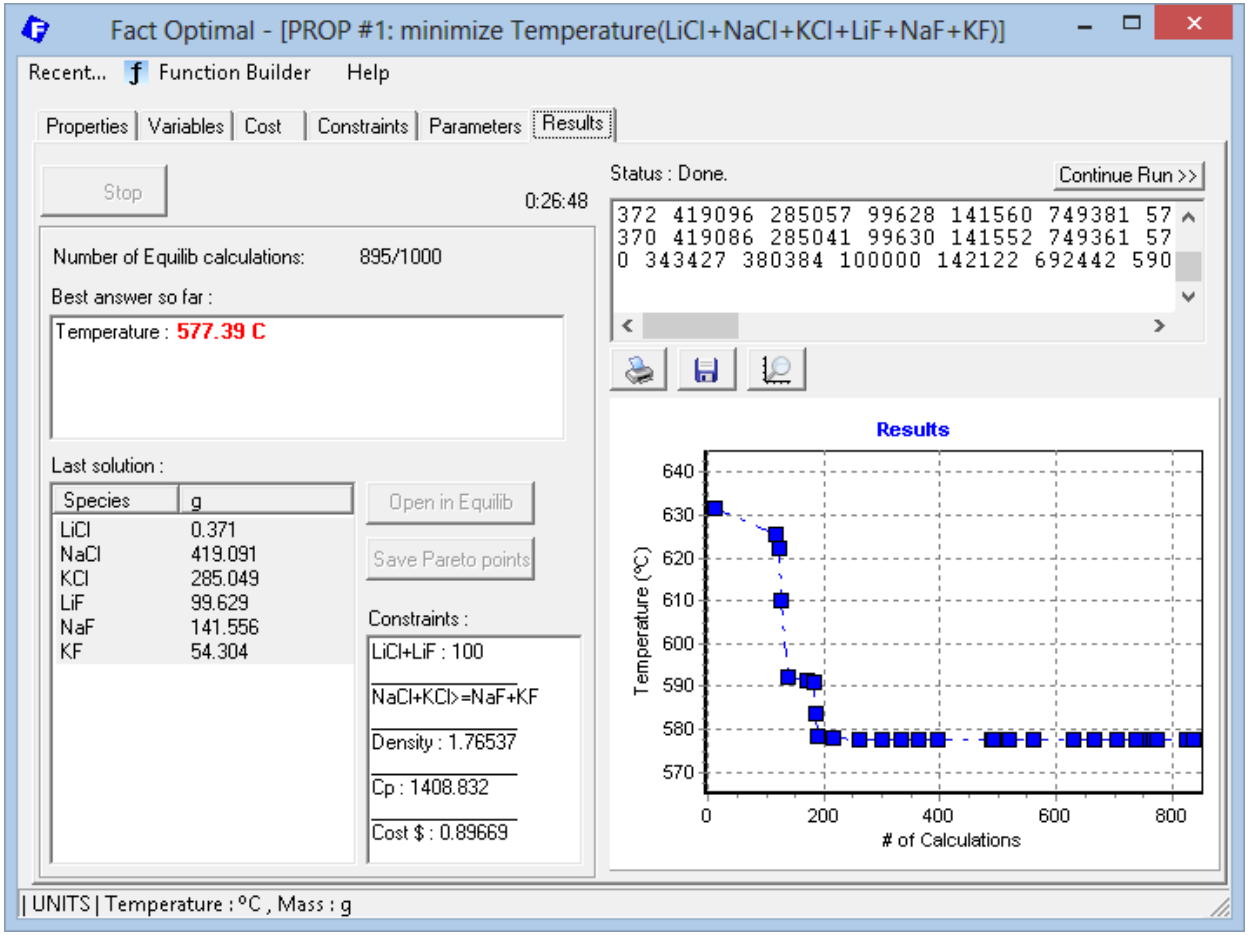
Density ≥ 1750 kg/m$^3$

Cp ≥ 1250 J/kg

Cost ≤ 5.5 $/kg

# Example 2b: Minimize the salt liquidus temperature under constraints - 12

<u>FactOptimal Results Window:</u> with the new set of constraints, FactOptimal finds the lowest liquidus temperature to be 577.39ºC.



# Example 2b: Minimize the salt liquidus temperature under constraints - 13

## Equilib Results Window

Results - Equilib 577.39 C

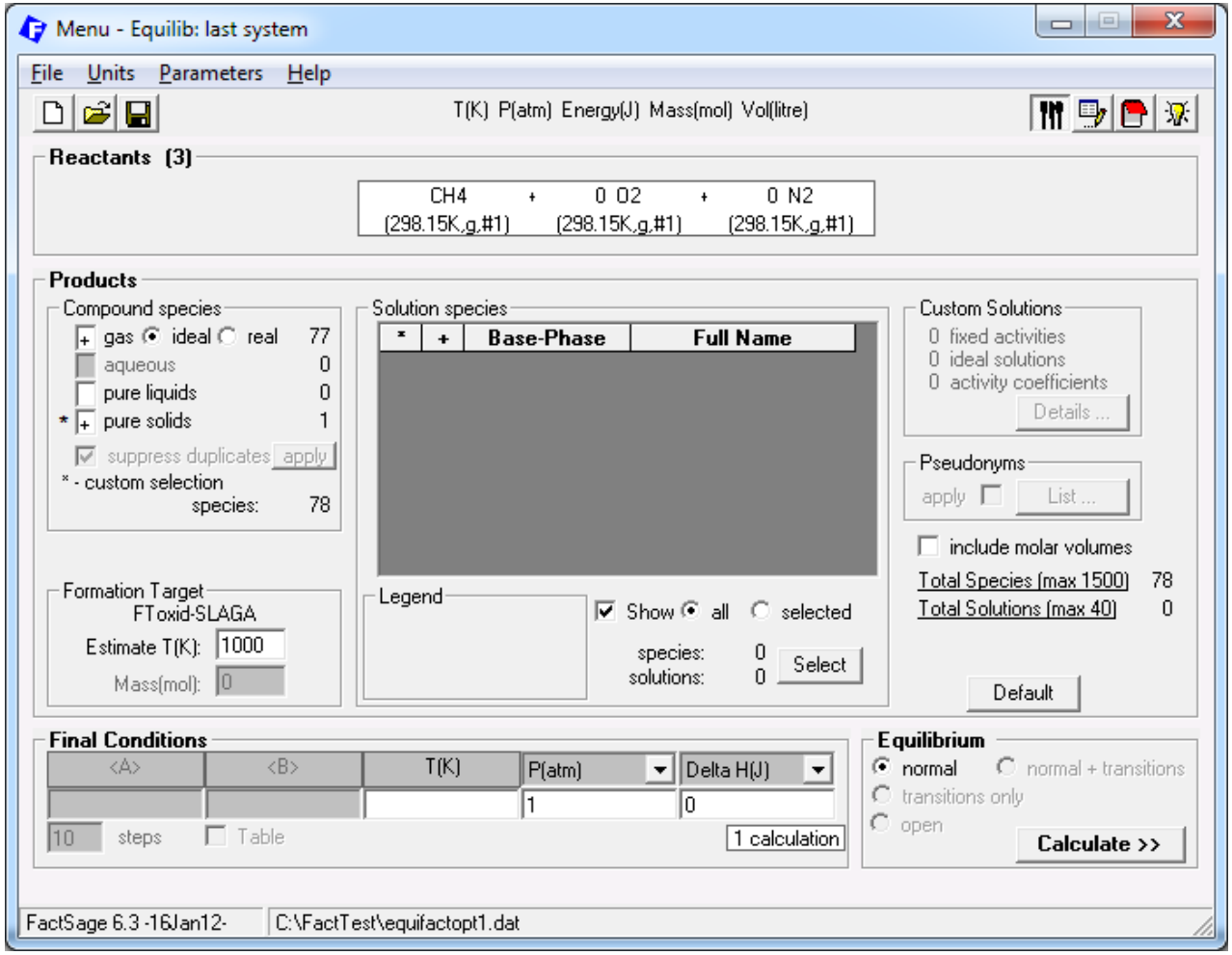
Output Edit Show Pages

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

```
                                                                    FactSage 6.4
(gram) 0.371 LiCl +  419.091 NaCl +  285.049 KCl +  99.629 LiF +

(gram) 141.556 NaF +  54.304 KF =

  1000.0      gram  ASalt-liquid#1
  (1000.0 gram, 19.150 mol, 0.56641 litre, 1.7655 gram/cm3)
          (577.39 C, 1 atm,     a=1.0000)
          ( 4.2481      wt.% LiF                                    V
          + 9.3771      wt.% LiCl                                   V
          + 18.831      wt.% NaF                                    V
          + 35.401      wt.% NaCl                                   V
          + 11.760      wt.% KF                                     V
          + 20.382      wt.% KCl                                    V)

          Site fraction of sublattice constituents:
          Li                        0.20102
          Na                        0.55051
          K                         0.24847
          ----------------------------------
          F                         0.42542
          Cl                        0.57458

          Mole fraction of quadruplets:
          Li-Li-F-F                          3.5710E-02
          Li-Li-Cl-Cl                        1.3132E-03
          Na-Na-F-F                          4.7307E-02
          Na-Na-Cl-Cl                        0.11081
          K-K-F-F                            1.5704E-03
```

# Example 3 : How to use equality constraints - 1

Using the example from section 3, we will calculate the maximum adiabatic flame temperature when O2 is replaced by air where moles O2 = moles N2/4.



# Example 3 : How to use equality constraints - 2

We want the following constraints to be respected (molar basis):

$$CH_4 + O_2 + N_2 = 1$$
$$O_2 = N_2/4$$

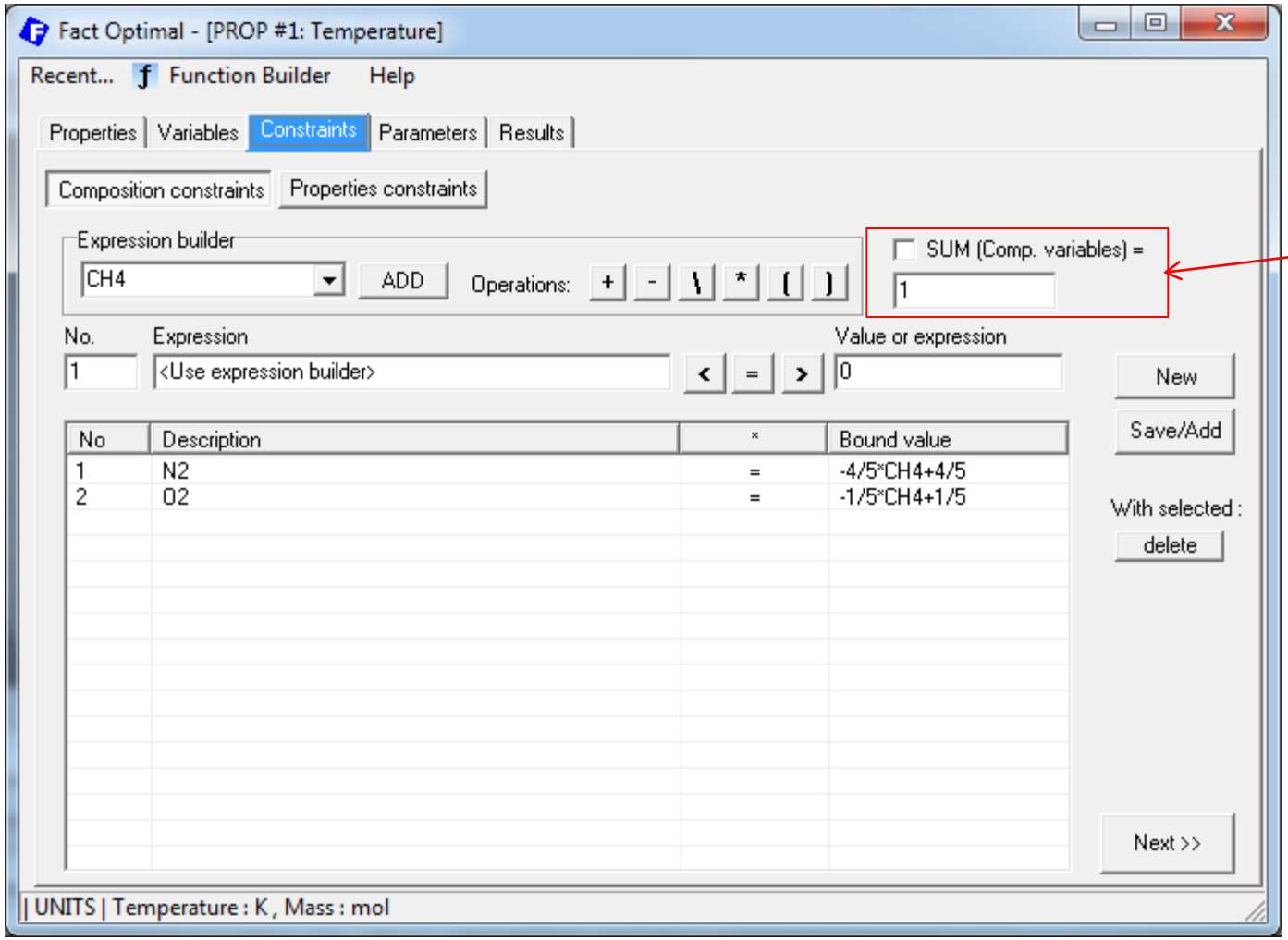
To enter these constraints in **FactOptimal**, they must be converted to allow only one degree of freedom :

$$O_2 = -1/5*CH_4 + 1/5$$
$$N_2 = -4/5*CH_4 + 4/5$$

That is, if there are m composition variables ($C_1$, $C_2$, ... $C_m$) and n equations relating these variables, then the first (m-n) variables must be expressed as functions of the remaining variables as

$$C_i = f(C_{m-n+1},...C_m); \quad i \leq (m-n)$$

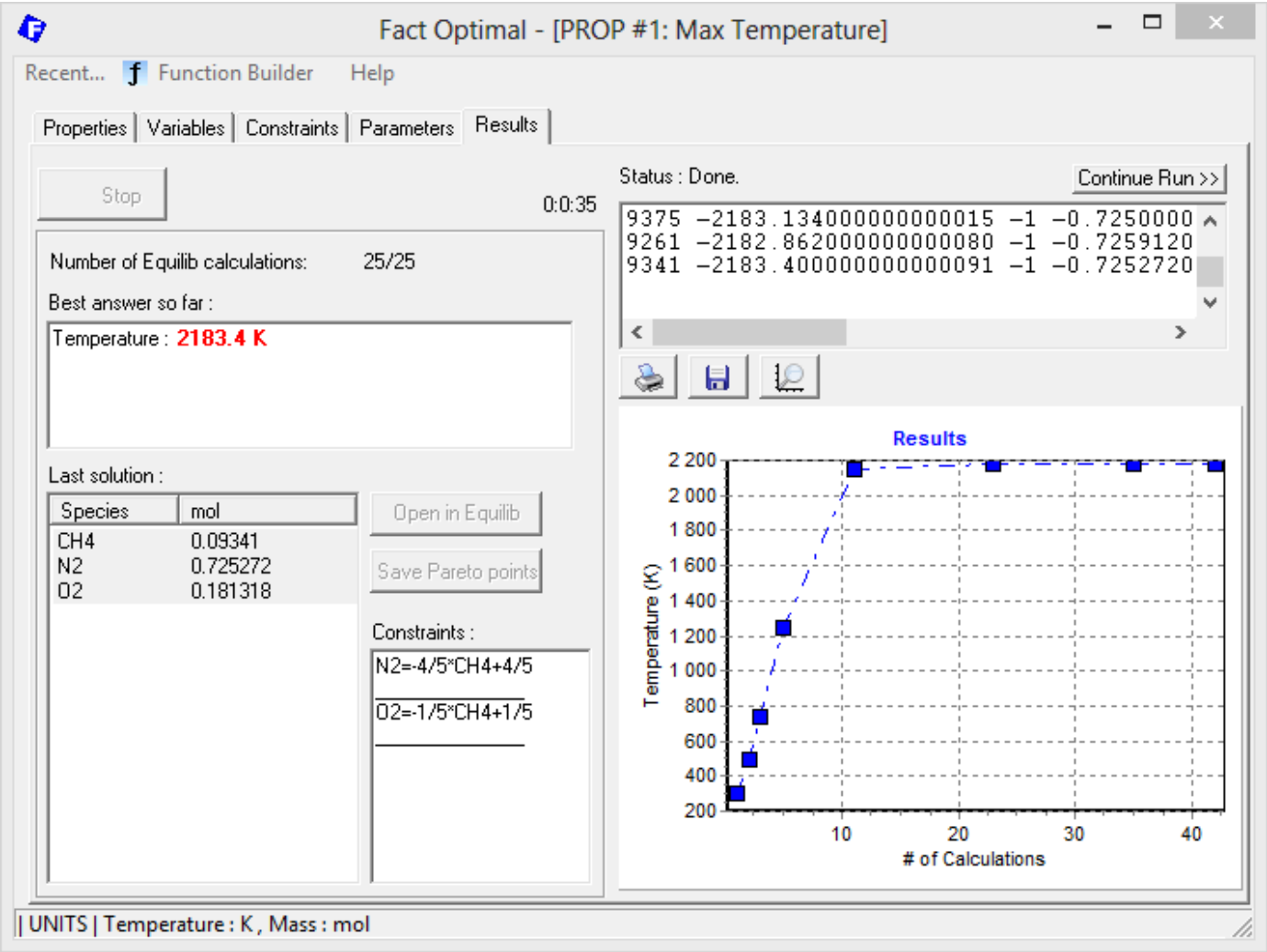
# Example 3 : How to use equality constraints - 3




The SUM (Comp. variables) option must always be unchecked when equality constraints are being used.

# Example 3 : How to use equality constraints - 4

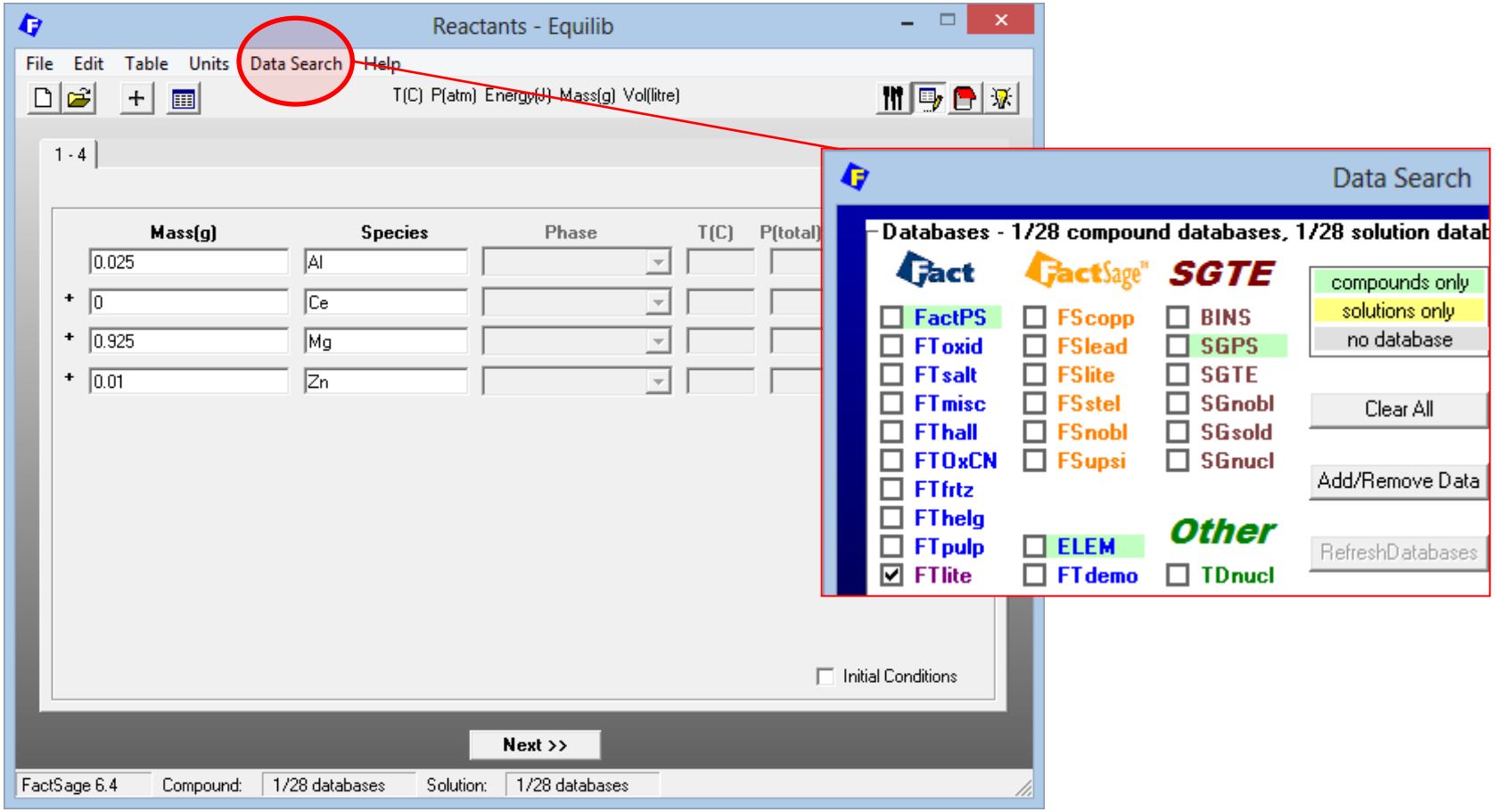
The adiabatic flame temperature in air is less than in $O_2$.



# Example 4 : Maximize the total mass of all precipitates in the hcp matrix for an (AZ31+Ce) Mg-based alloy after Scheil-Gulliver cooling and subsequent full annealing - 1

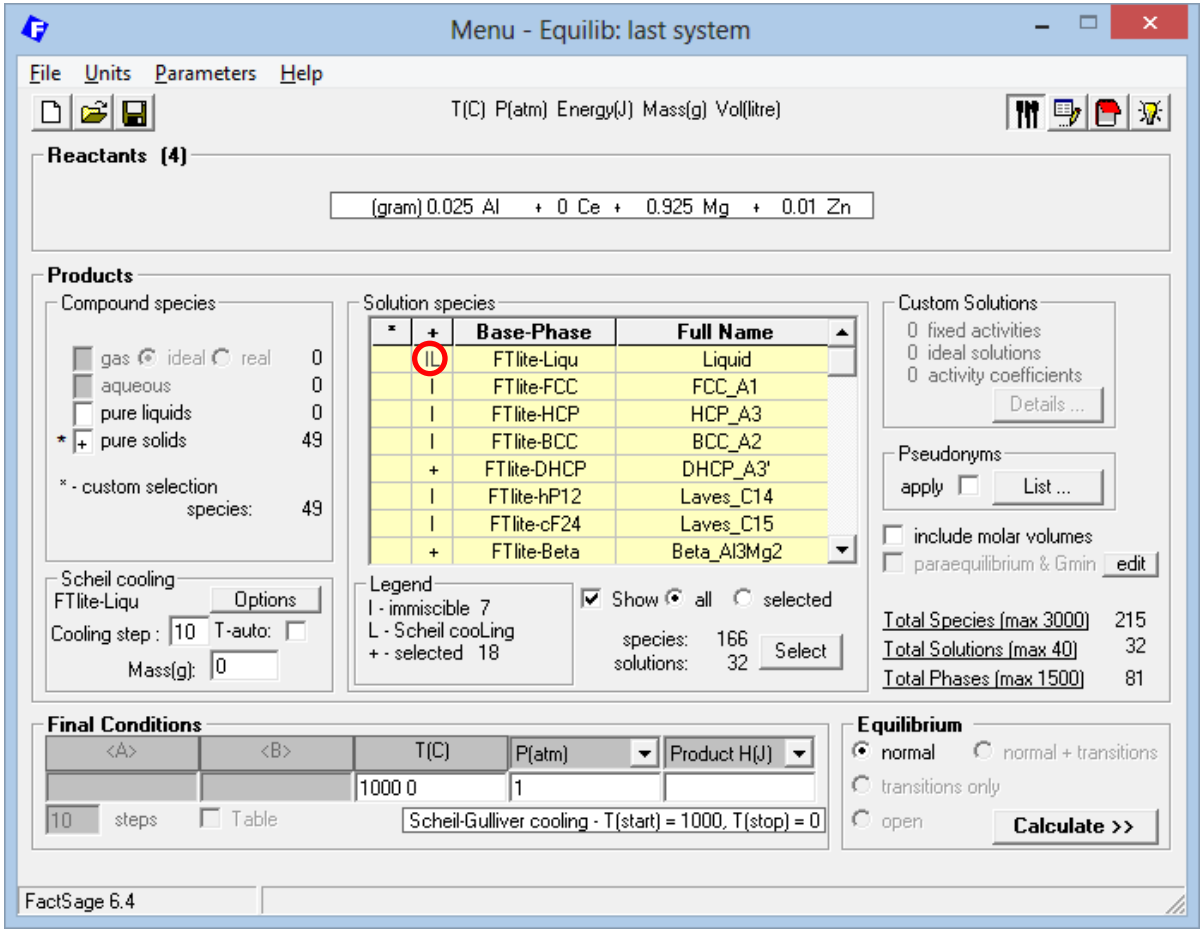
**System: Al-Ce-Mg-Zn**

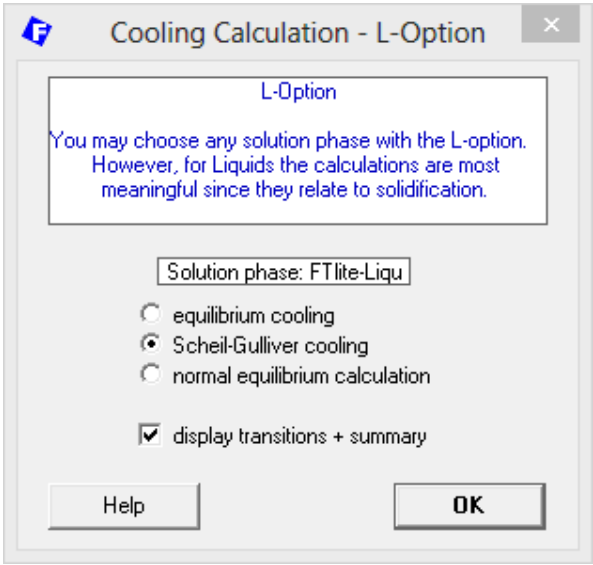
Step 1**:** Using **Equilib** we define the system and select the appropriate databases **FTlite**. The arbitrary composition corresponds to approximately the composition of AZ31 alloys.



# Example 4 : Maximize the total mass of all precipitates in the hcp matrix for an (AZ31+Ce) Mg-based alloy after Scheil-Gulliver cooling and subsequent full annealing - 2

Step 2: Perform a single **Equilib** calculation using the solidification software and choosing a *Scheil-Gulliver Cooling* type calculation (see *Equilib Advanced Slide Show*, slide 13.1)



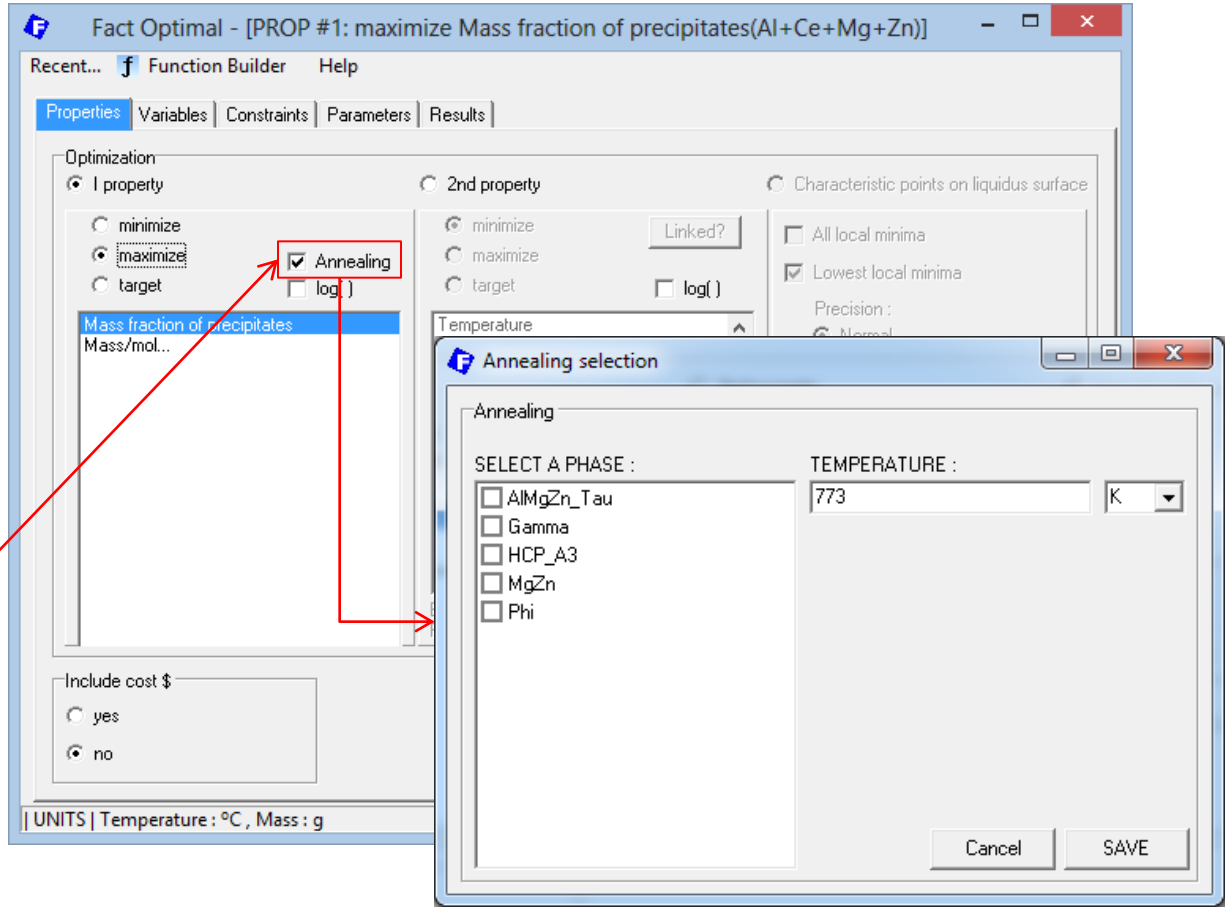



# Example 4 : Maximize the total mass of all precipitates in the hcp matrix for an (AZ31+Ce) Mg-based alloy after Scheil-Gulliver cooling and subsequent full annealing - 3

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 :

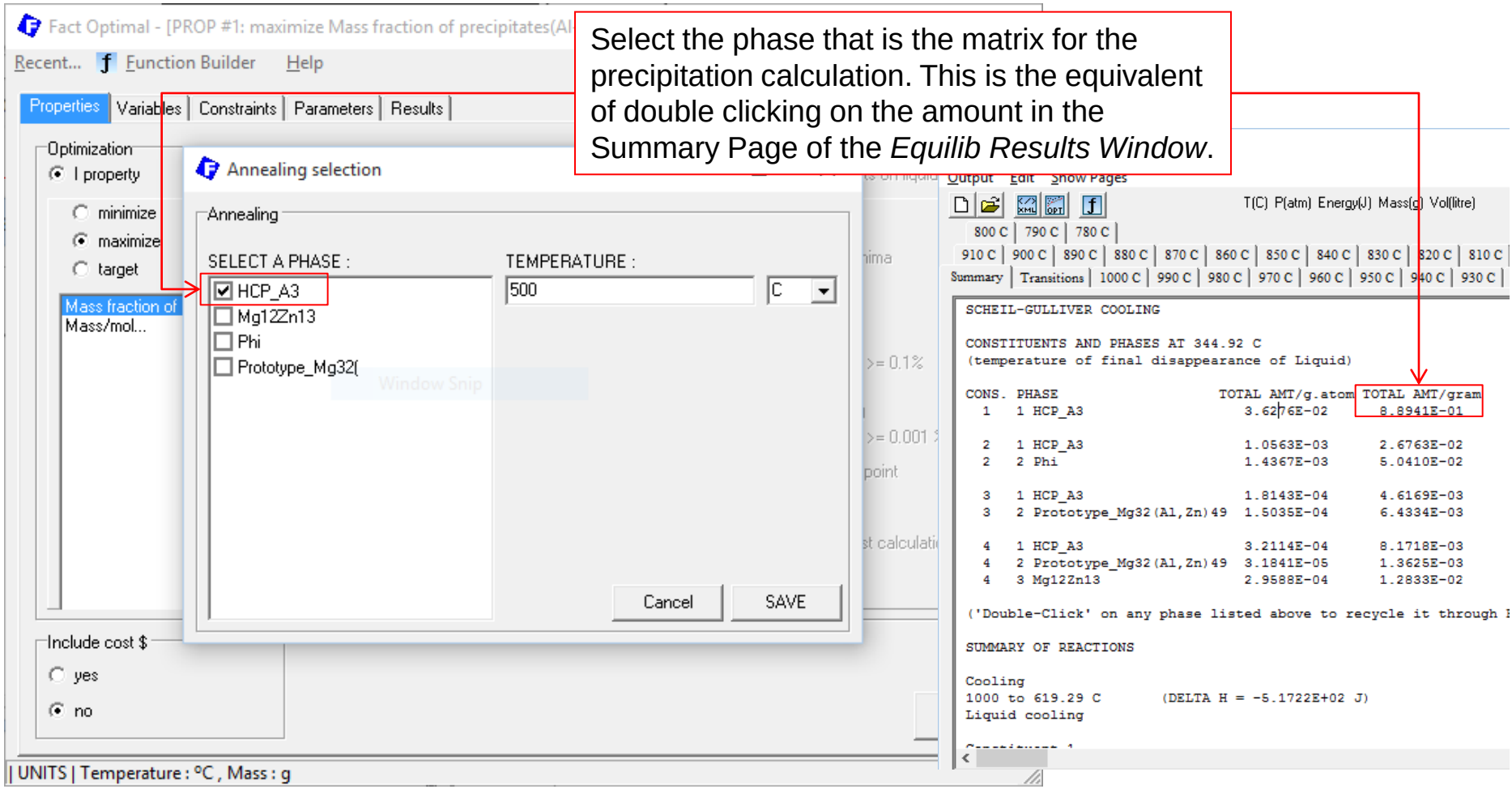
1. we consider **one property**
2. we want to **maximize this property**
3. the property that we consider is the total **mass of precipitates** after a subsequent annealing

Click on the Annealing box to activate the “mass of precipitate” option. The Anealing selection menu will pop-up



# Example 4 : Maximize the total mass of all precipitates in the hcp matrix for an (AZ31+Ce) Mg-based alloy after Scheil-Gulliver cooling and subsequent full annealing - 4

Step 4: Select the Annealing phase in the annealing selection window. Here we choose the primary phase (HCP) and define the annealing temperature (500 °C).



# Example 4 : Maximize the total mass of all precipitates in the hcp matrix for an (AZ31+Ce) Mg-based alloy after Scheil-Gulliver cooling and subsequent full annealing - 5

The *Mass fraction of precipitates* option can now be selected

In the variables tab, define the permissible composition ranges:

**96.5 > Wt.% Mg > 92.5**

**2 > Wt.% Ce**

**3.5 > Wt.% Al > 2.5**

**1 > Wt.% Zn > 2**

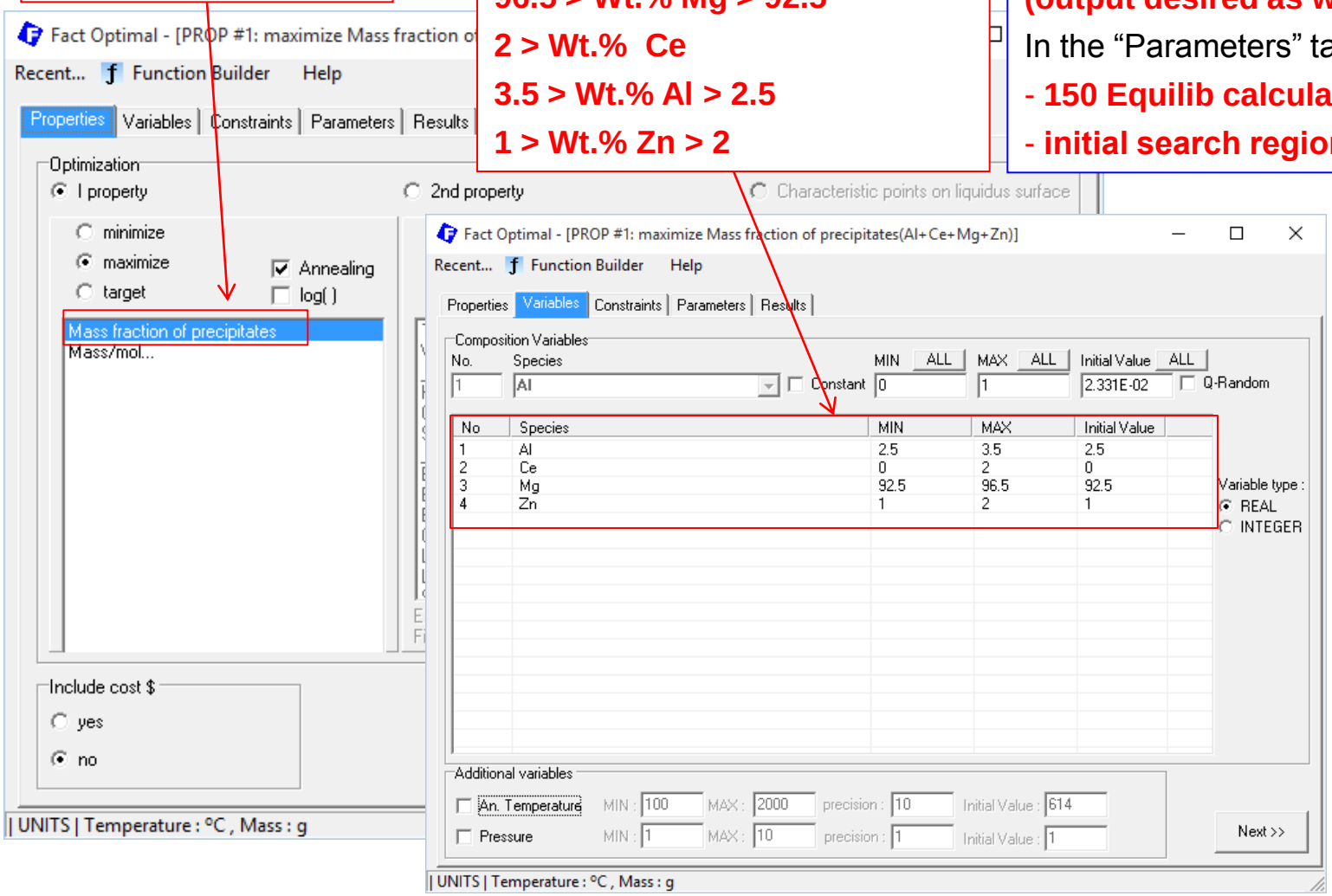
In the "Constraints" tab :

**- Sum(Comp. variables) = 100 (output desired as wt.%)**

In the "Parameters" tab :

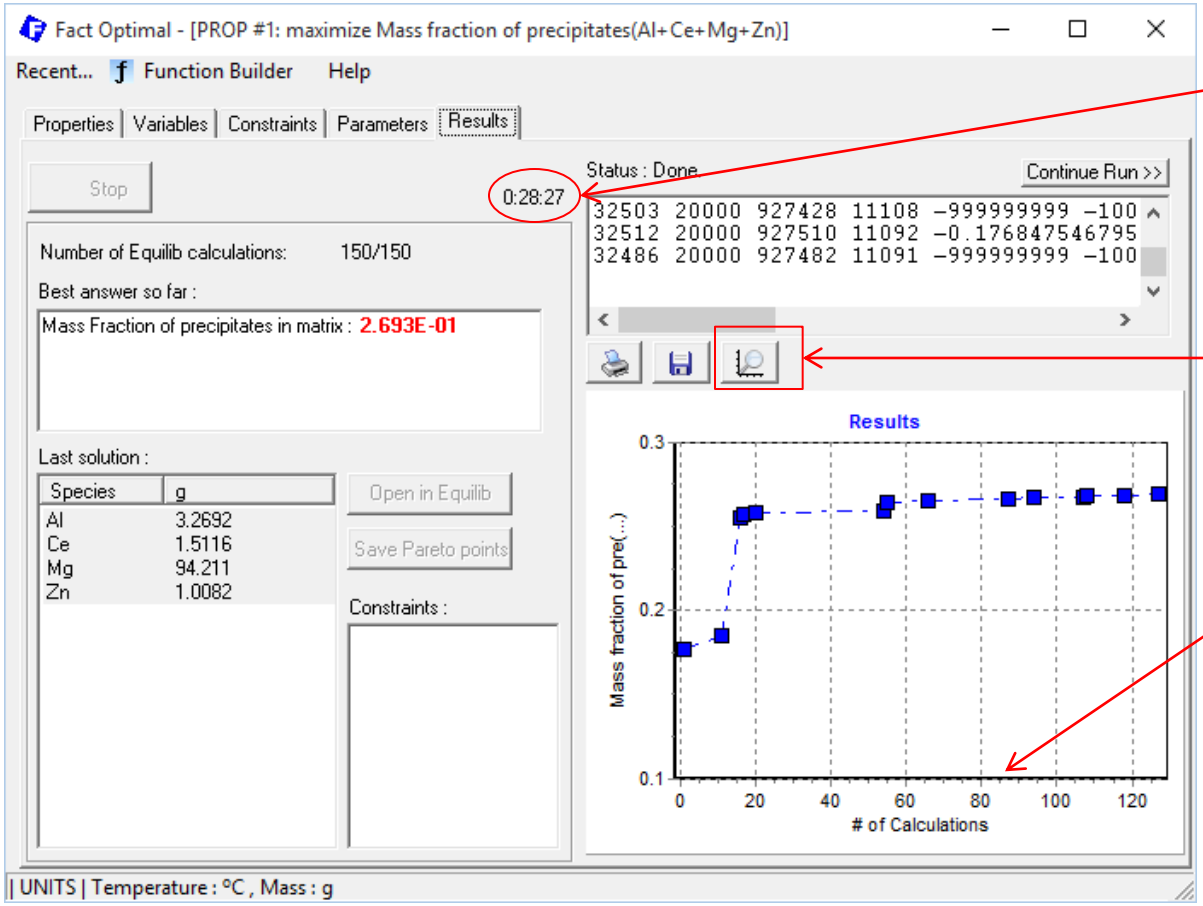
**- 150 Equilib calculations**

**- initial search region "large" (i.e. 1)**



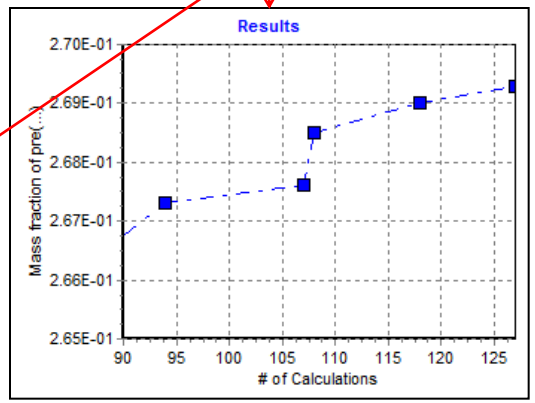
# Example 4 : Maximize the total mass of all precipitates in the hcp matrix for an (AZ31+Ce) Mg-based alloy after Scheil-Gulliver cooling and subsequent full annealing - 6

## *FactOptimal Results Window*

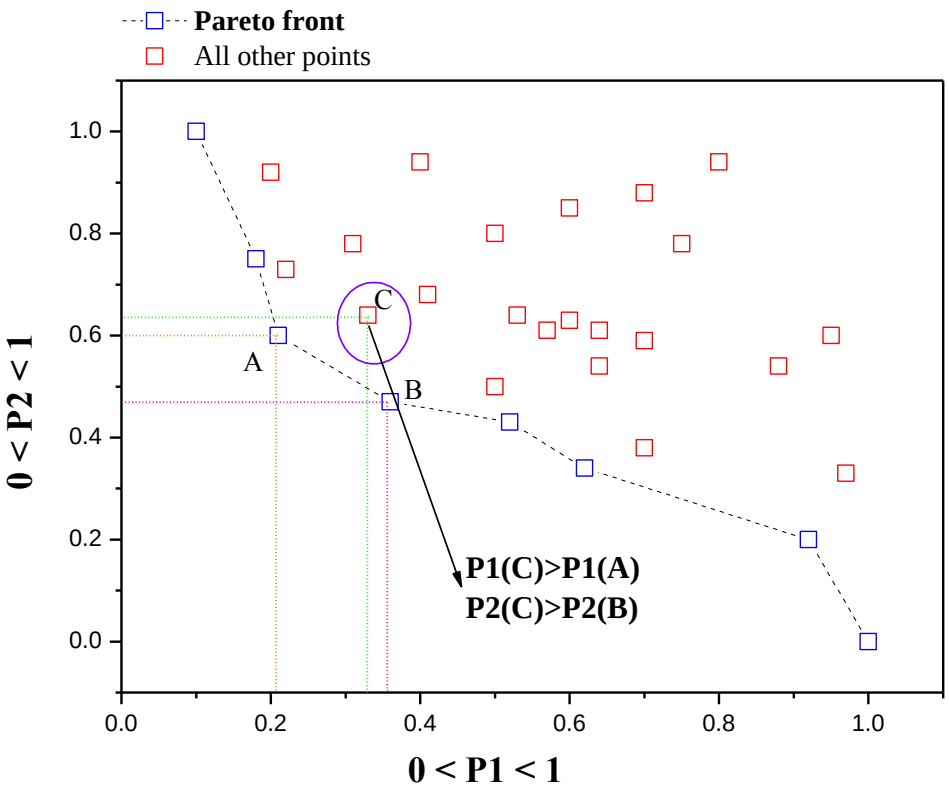



Total elapsed time

You can use the zoom icon to change the axis limits.



# **The Pareto Concept** - the simultaneous minimum and/or maximum of more than one function.




Example of a ***Pareto Front***.

We want to simultaneously minimize properties P1 and P2. All points shown are calculated. Blue points are on the Pareto front. For any point not on the Pareto Front (for example point C), "better" points can be found on the Pareto front. That is, for the same value of P1 as at point C there is a point on the Pareto front with a lower value of P2, and for the same value of P2 as at point C there is a point on the Pareto front with a lower value of P1.

**You must then select the optimal composition on the *Pareto Front* according to your requirements.**

# Example 5 : Minimize the density and maximize Cp under constraints on $T_{liq}$ - 1

*This example calculates a Pareto Front.*

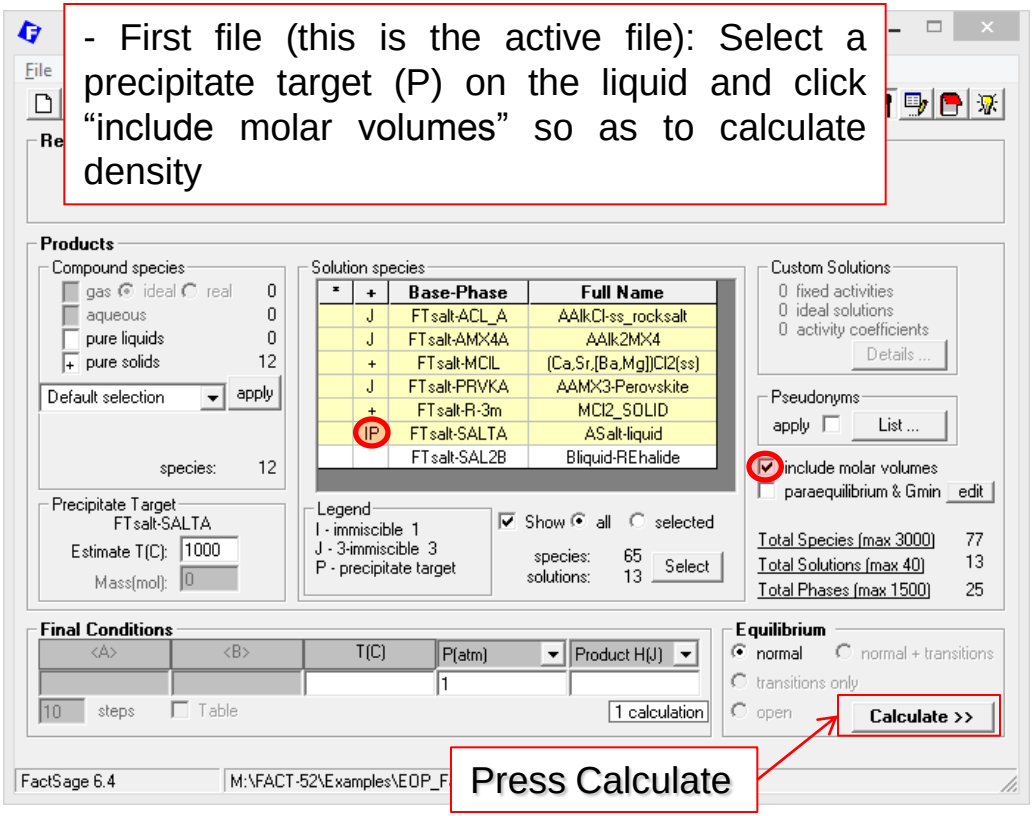
**System:** **$LiCl-NaCl-KCl-CaCl_2-MgCl_2$**

**Properties:** **Maximize density at $T_{liq}$ and minimize the heat capacity at ($T_{liq}$ + 20ºC).**

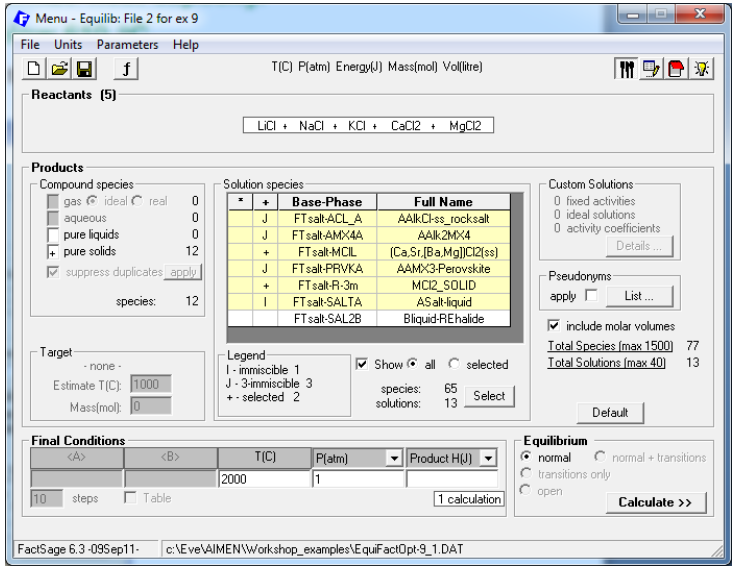
**Constraints:** **Liquidus temperature $T_{liq}$ below 610 ºC .**

Step 1: Define the system and select the appropriate database **FTSalt**. Two separate **Equilib** calculations are required, the first to calculate the liquidus temperature and density, and the 2nd to calculate Cp.

- First file (this is the active file): Select a precipitate target (P) on the liquid and click "include molar volumes" so as to calculate density




- Second file (this is a stored file that will be used later in the calculation): A normal calculation (without the P option) at an arbitrary temperature



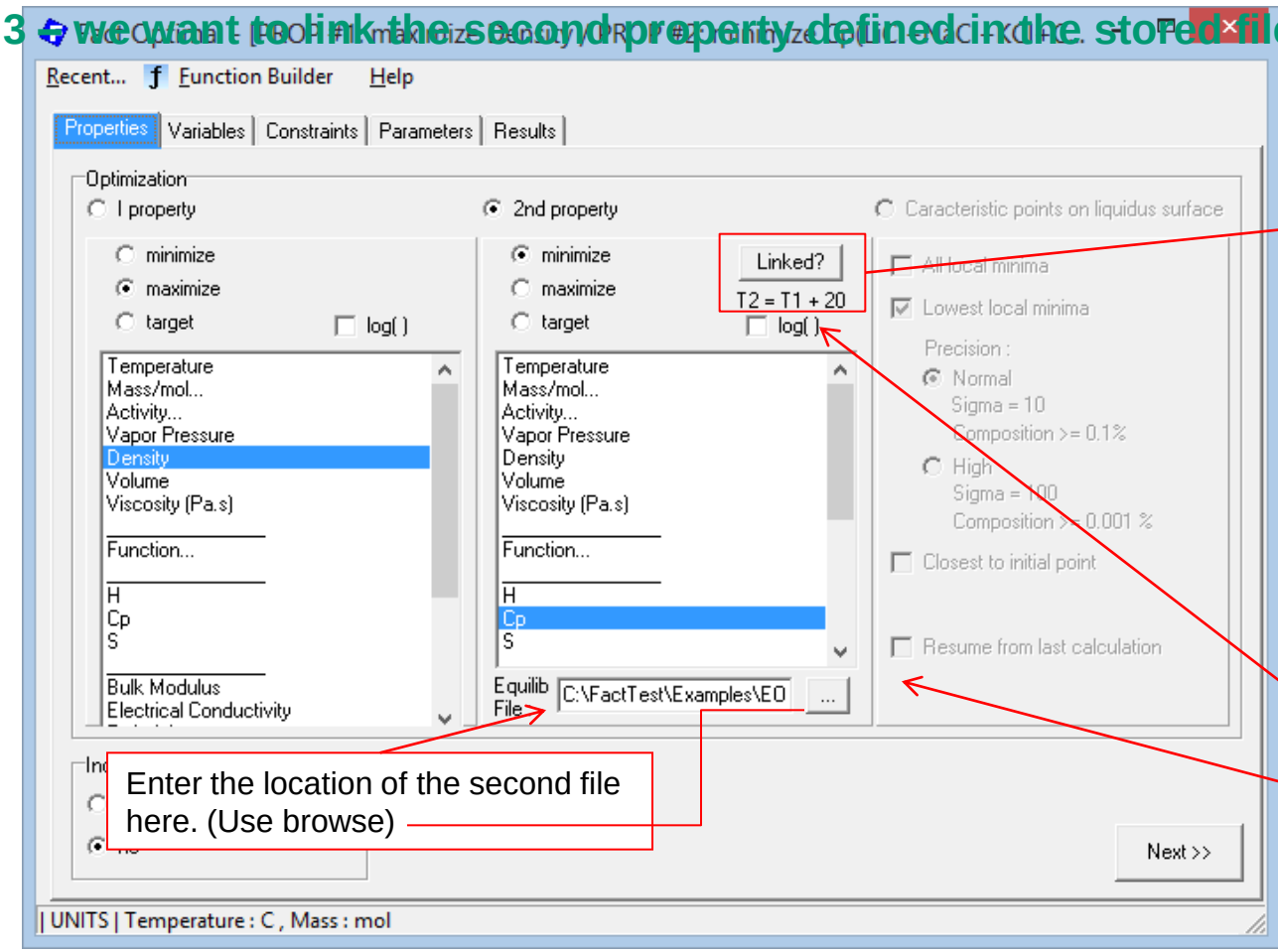
# Example 5 : Minimize the density and maximize Cp under constraints on $T_{liq}$ - 2

First file - Calculate and click the FactOptimal icon. If you are using the stored example files, click on "Recent..." to load the Fact Optimal file. In this example, we specify that :

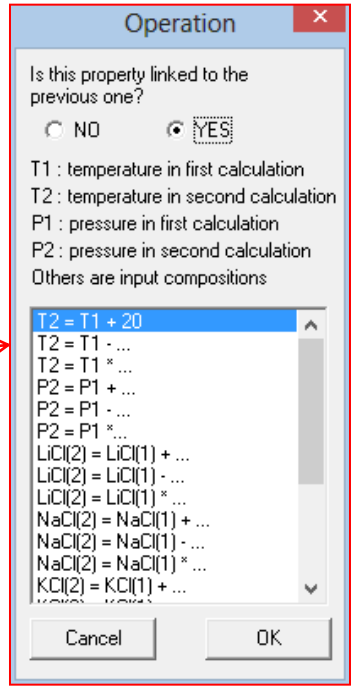
1- we consider **two properties, density and $C_p$**

2- we want to **maximize the first property and minimize the second**

3 - **we want to link the second property defined in the stored file**



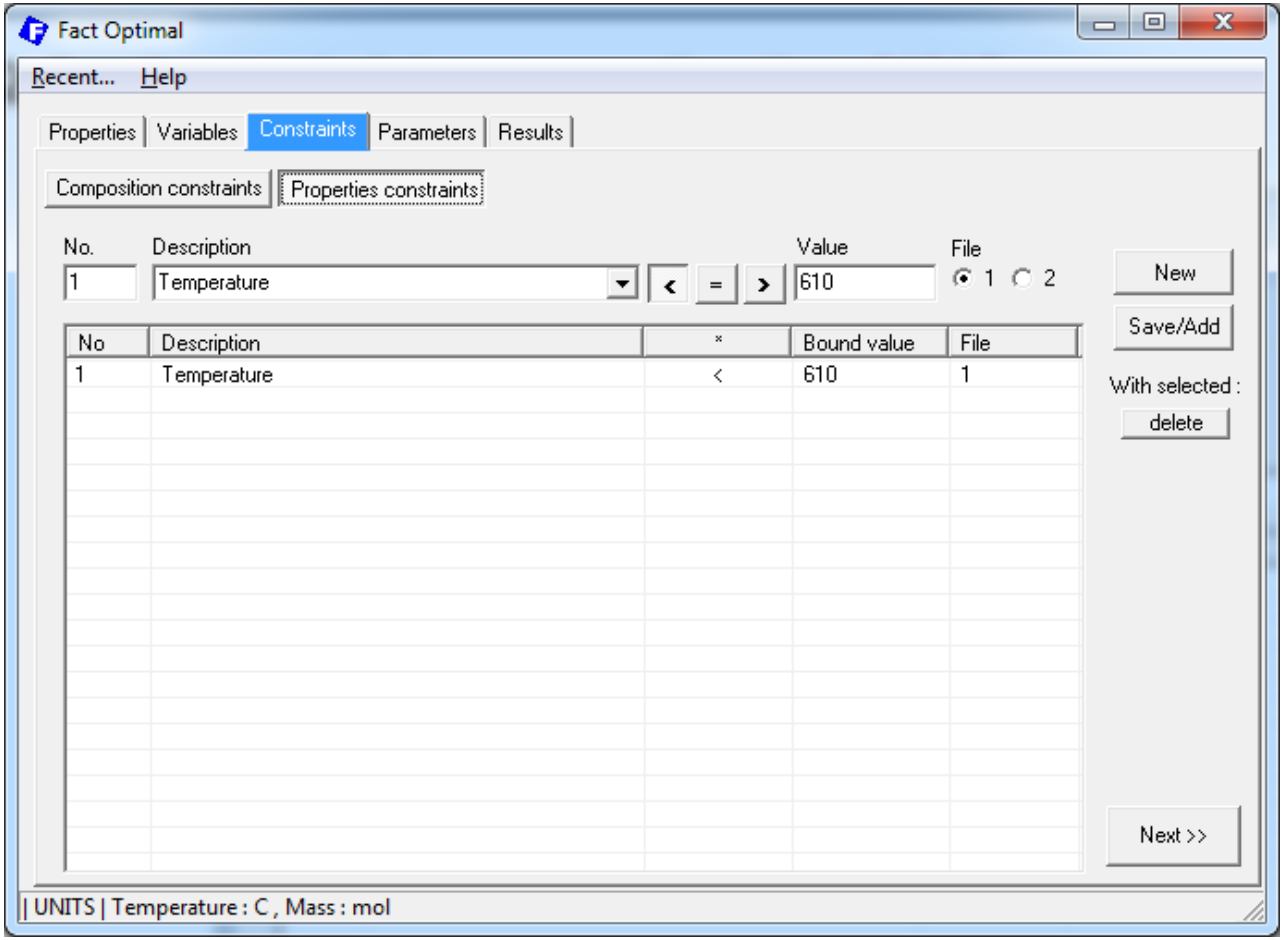

Enter the location of the second file here. (Use browse)




For the 2nd property, the calculation is performed using the precipitate (liquidus) temperature and adding 20ºC, using the stored second file.

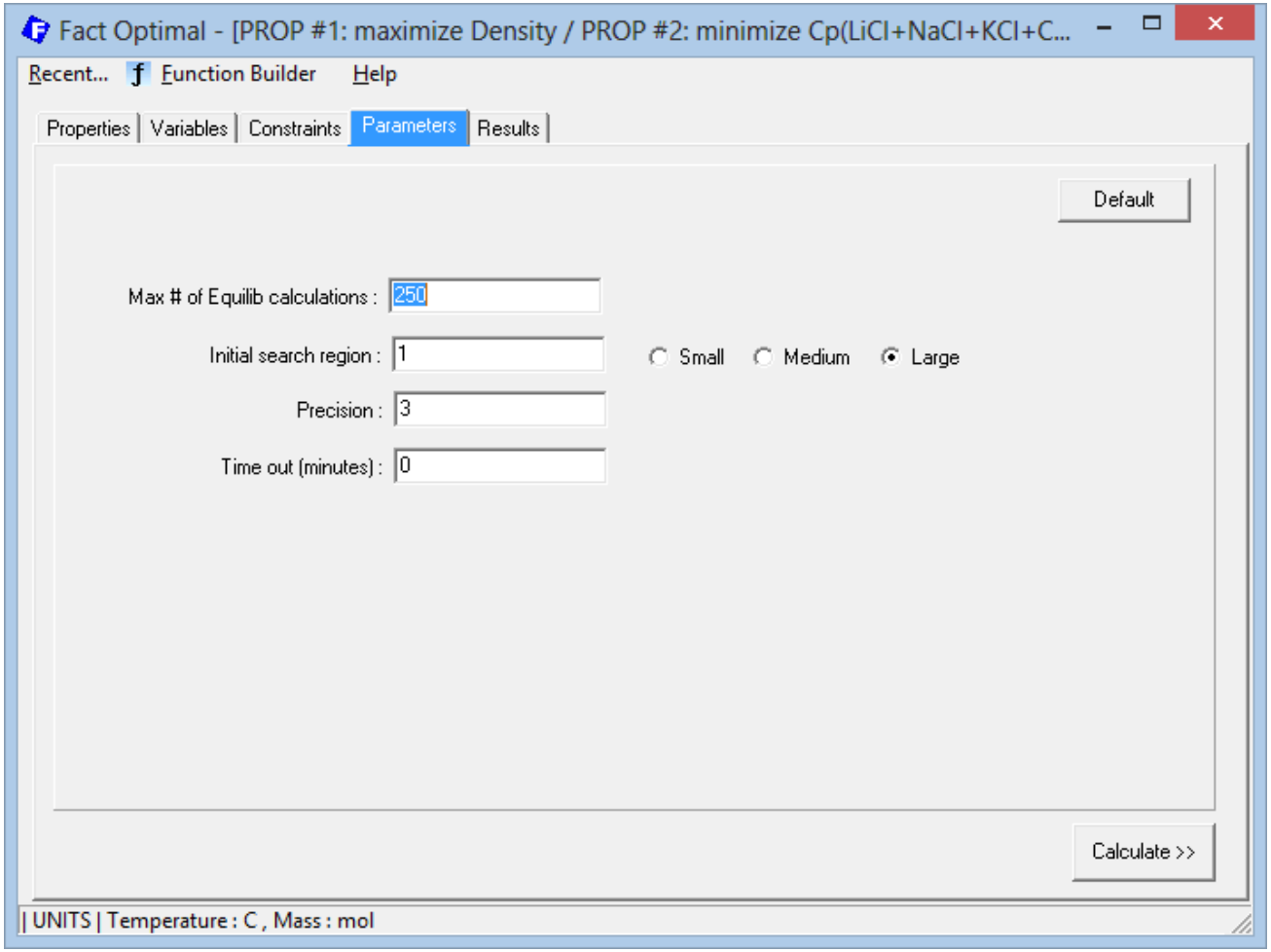
# Example 5 : Minimize the density and maximize Cp under constraints on $T_{liq}$ - 3

Define the constraints on properties: **$T_{liq}$ < 610 °C**



# Example 5 : Minimize the density and maximize Cp under constraints on $T_{liq}$ - 4

Set up the parameters:

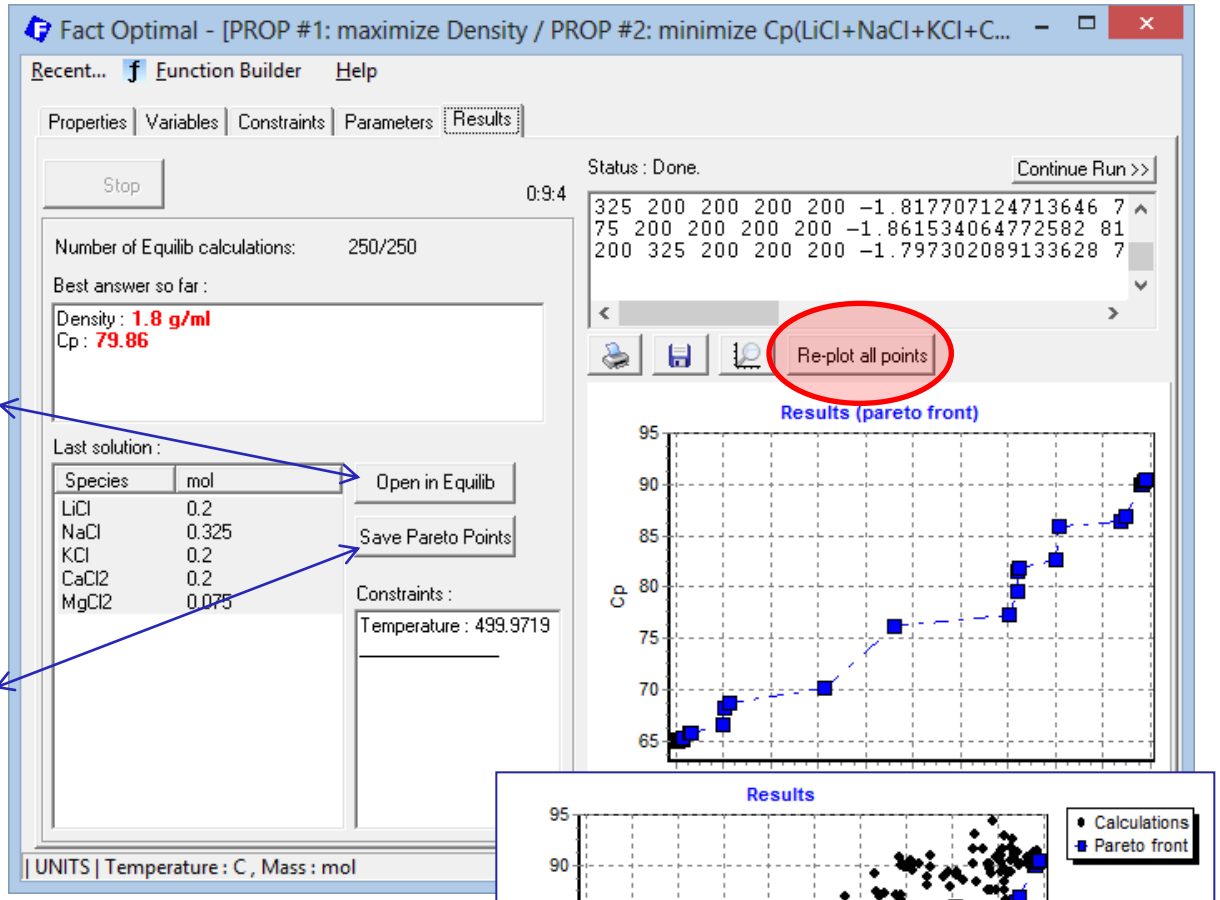


# Example 5 : Minimize the density and maximize Cp under constraints on $T_{liq}$ - 5

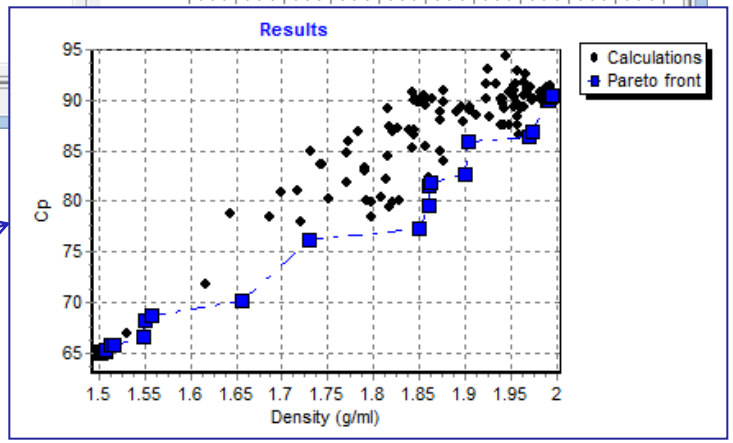
*FactOptimal Results Window*

One can perform an Equilib calculation at any point on the *Pareto Front* by clicking on it in the graph and and opening it in the **Equilib** module.

The compositions on the *Pareto Front* can be saved and opened in Text, Excel,.....

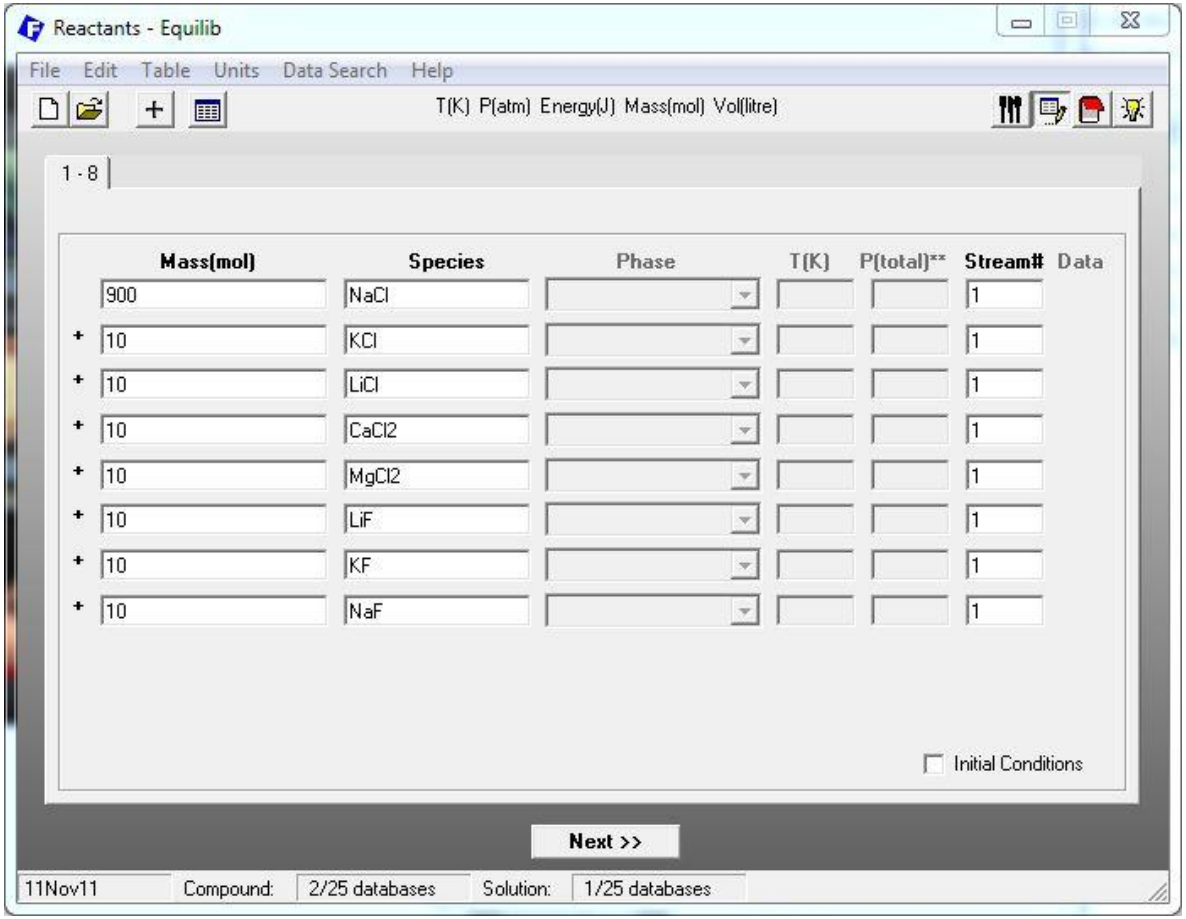



One can re-plot all calculated points or show only the *Pareto front.*



# Example 6 : Application using the cache option (Next Run) - 1

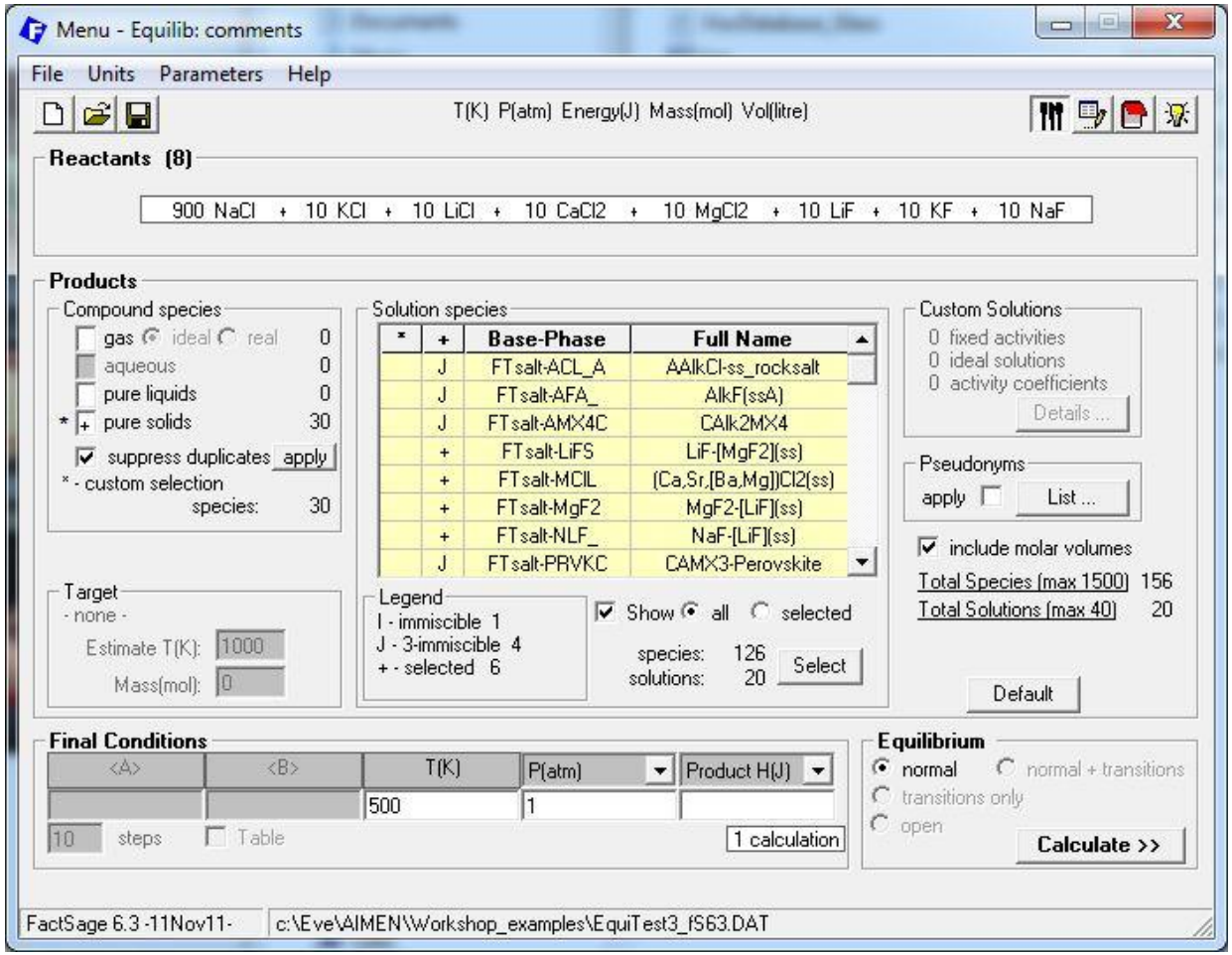
In some cases you may wish to stop a calculation before the convergence criterion has been met, or before the specified number of **Equilib** calculations has been reached. Alternatively, **Equilib** may fail to converge, especially for complex calculations. The cache option permits you to restart the optimization procedure and carry on from the last calculation.




In this example we use the **FTSalt** database with 8 reactants.

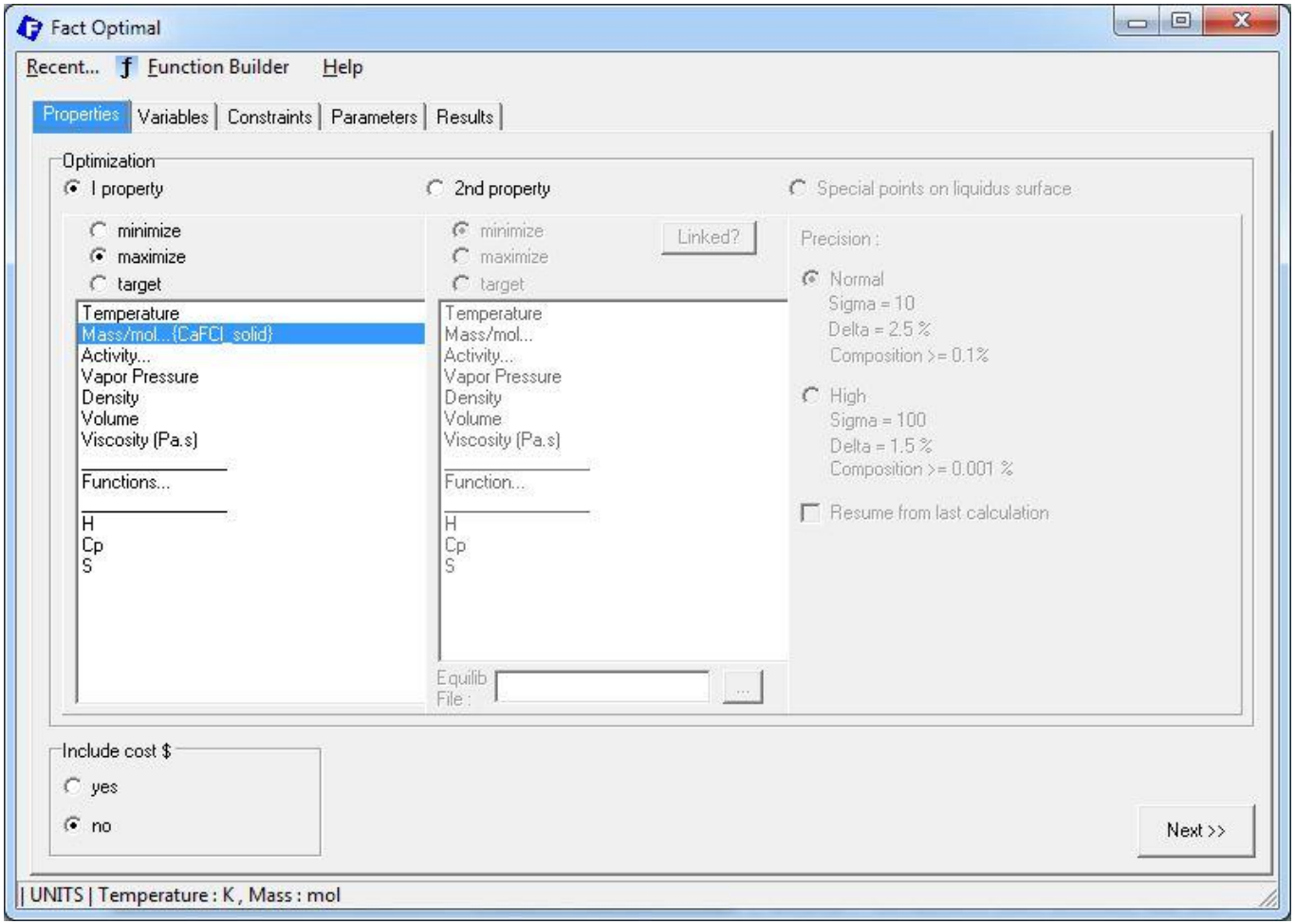
# Example 6 : Application using the cache option (Next Run) - 2

An **Equilib** calculation is first made at an arbitrary composition and temperature.

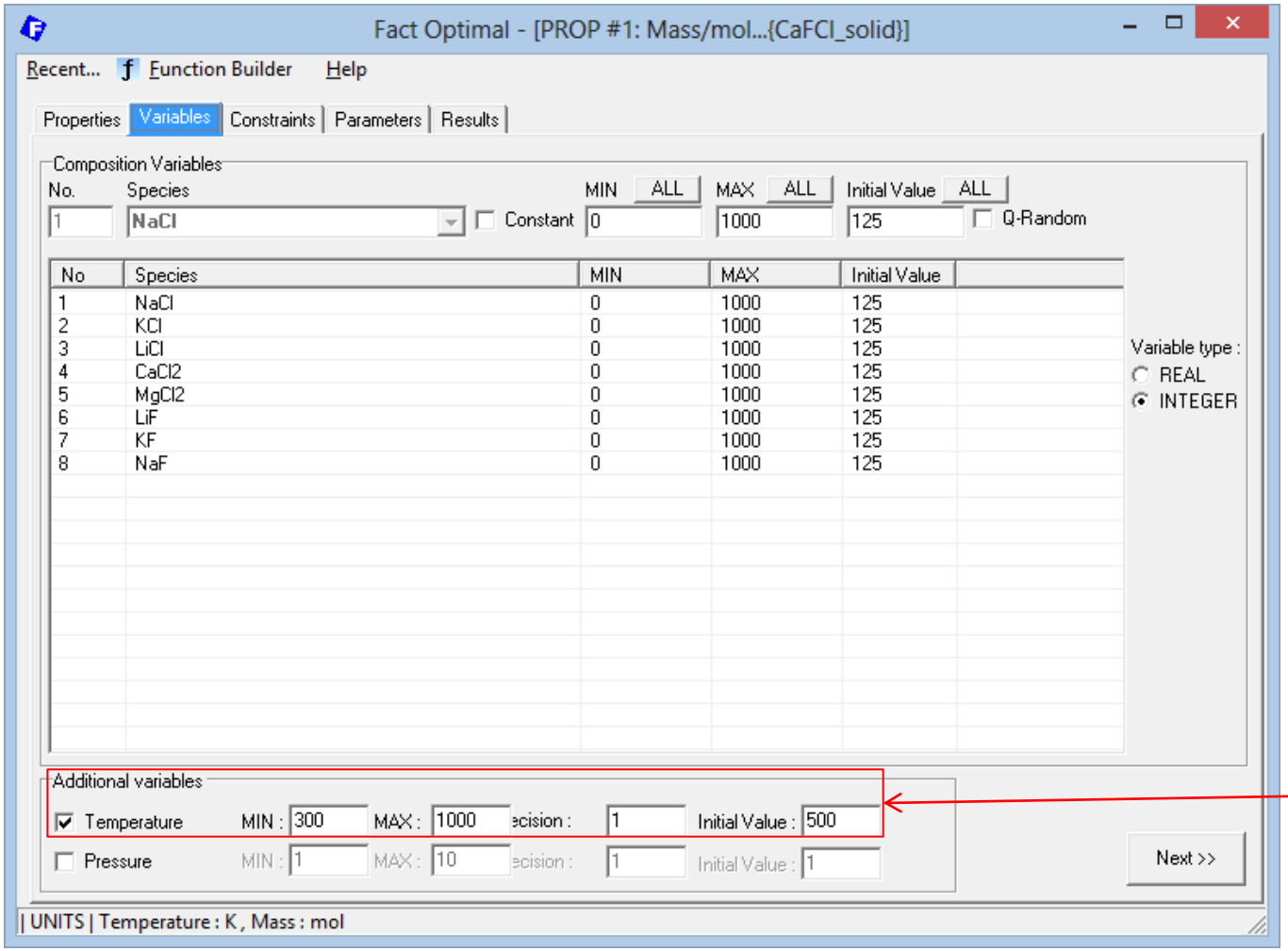


# Example 6 : Application using the cache option (Next Run) - 3

The objective is to optimize both composition and temperature in order to maximize the amount CaFCl (solid) at equilibrium.



# Example 6 : Application using the cache option (Next Run) - 4

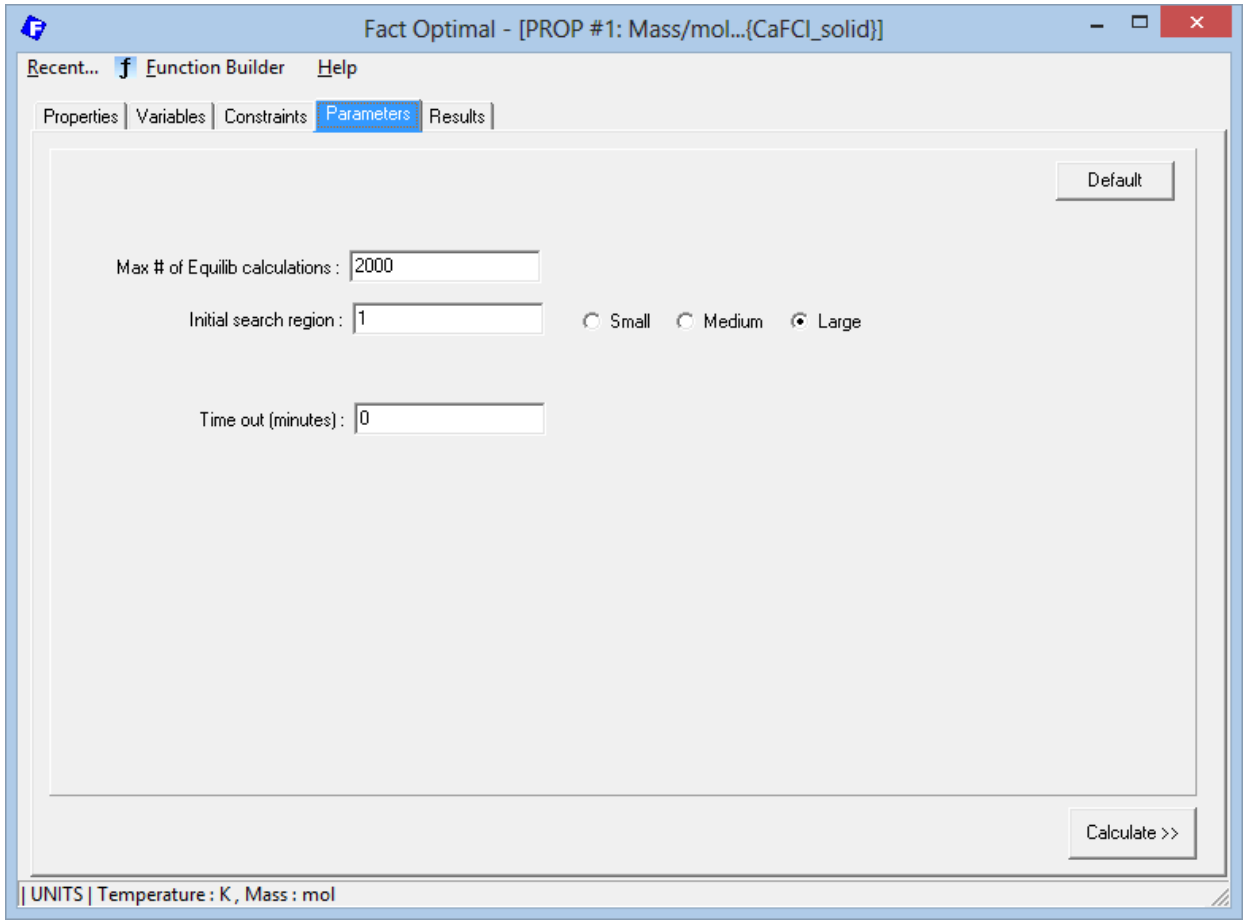



Each input constituent can vary between 0 and 1000 moles. We choose the INTEGER type of variable in order to reduce the precision and thus decrease the time to convergence.

We allow the temperaure to vary between 300K and 1000K every +/-1 degree (precision). Note that the temperature variable is of the INTEGER type.

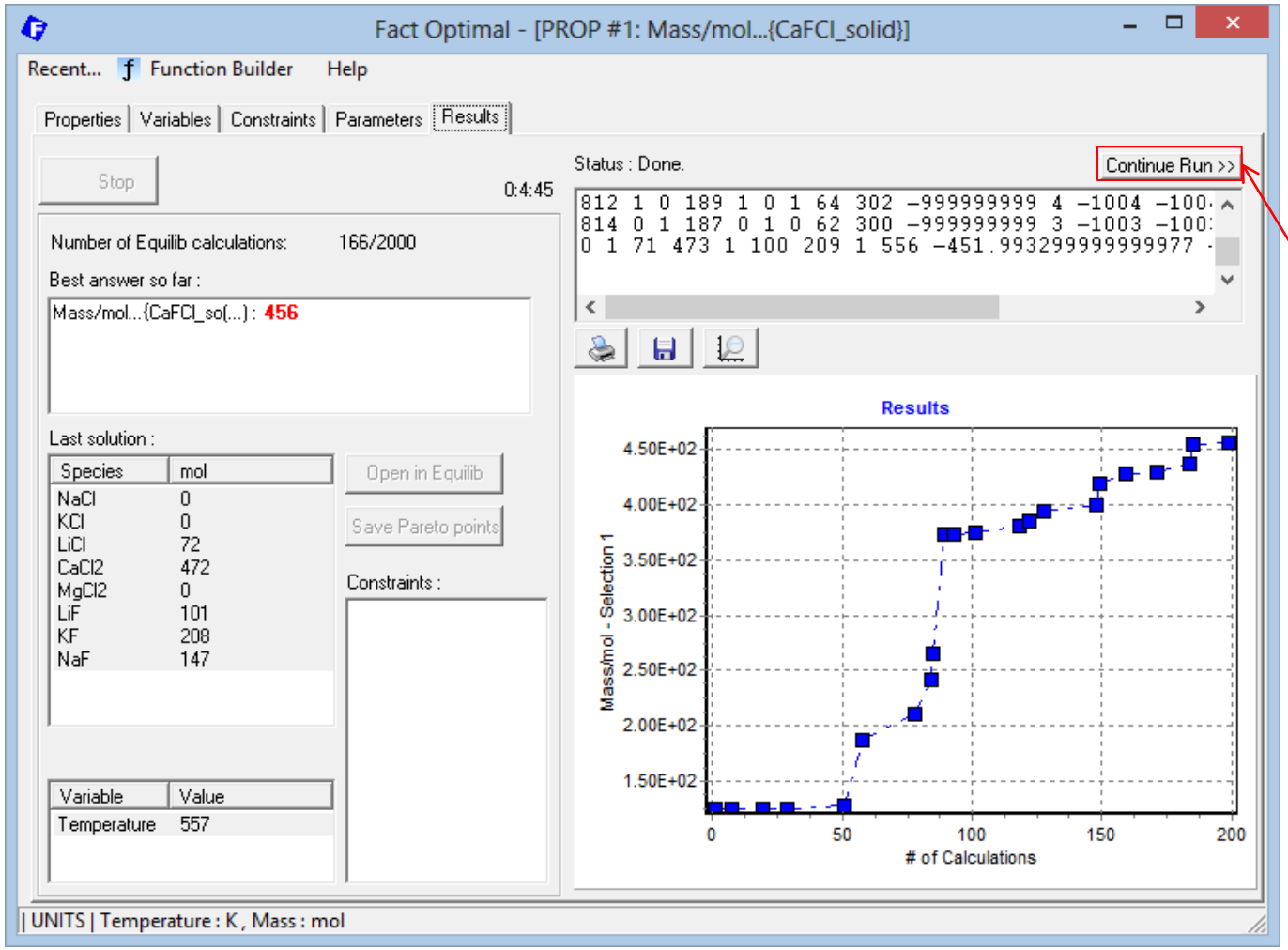
# Example 6 : Application using the cache option (Next Run) - 5

The maximum number of **Equilib** calculations is set to 2000.



# Example 6 : Application using the cache option (Next Run) - 6

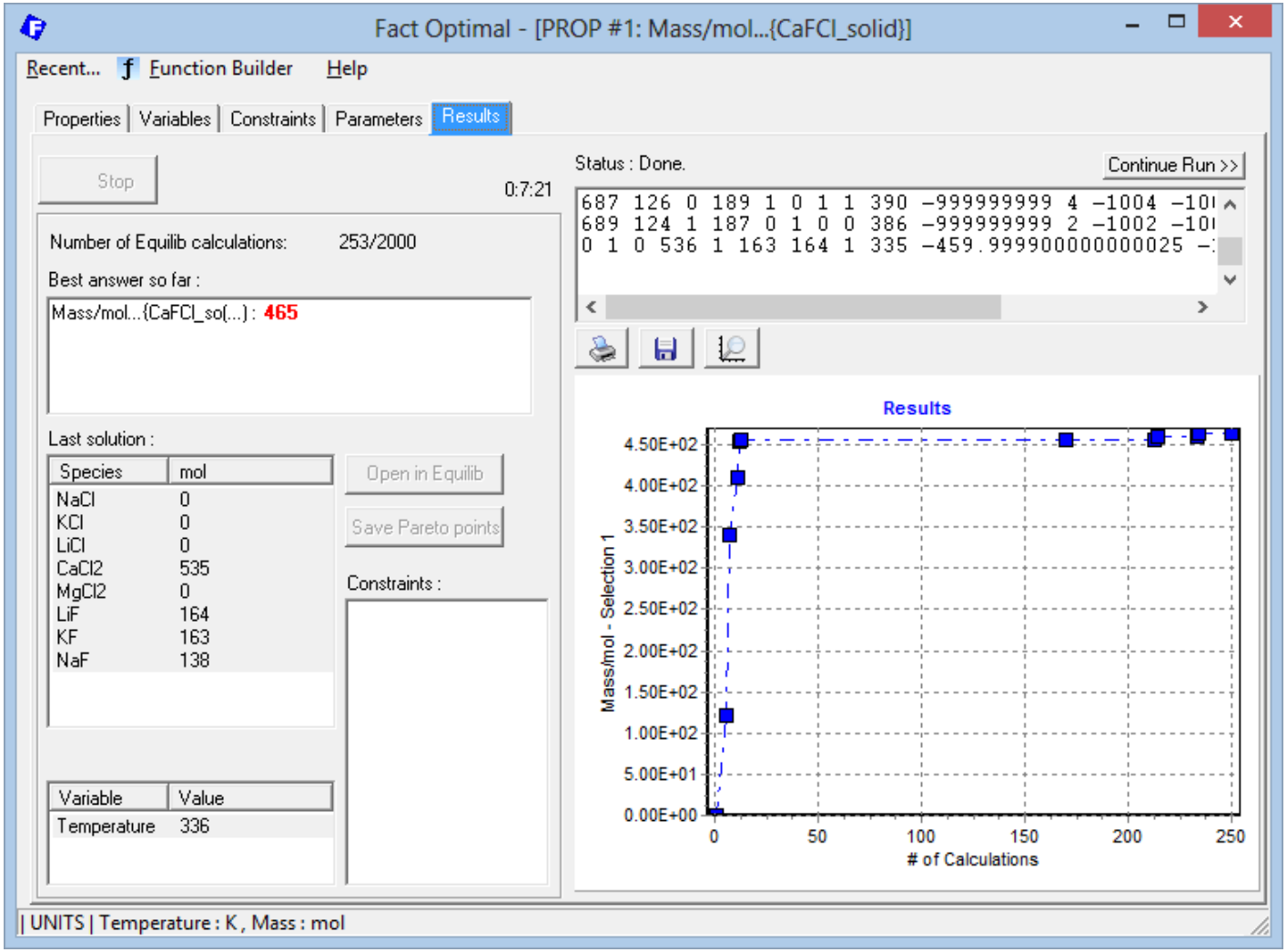
We stop the calculation after 166 calculations, at which point **FactOptimal** has obtained a value of 456 mol of CaFCl at 557K.




Click on the 'Continue Run' button to continue the optimization from the last point, using the previously saved calculations (cached).

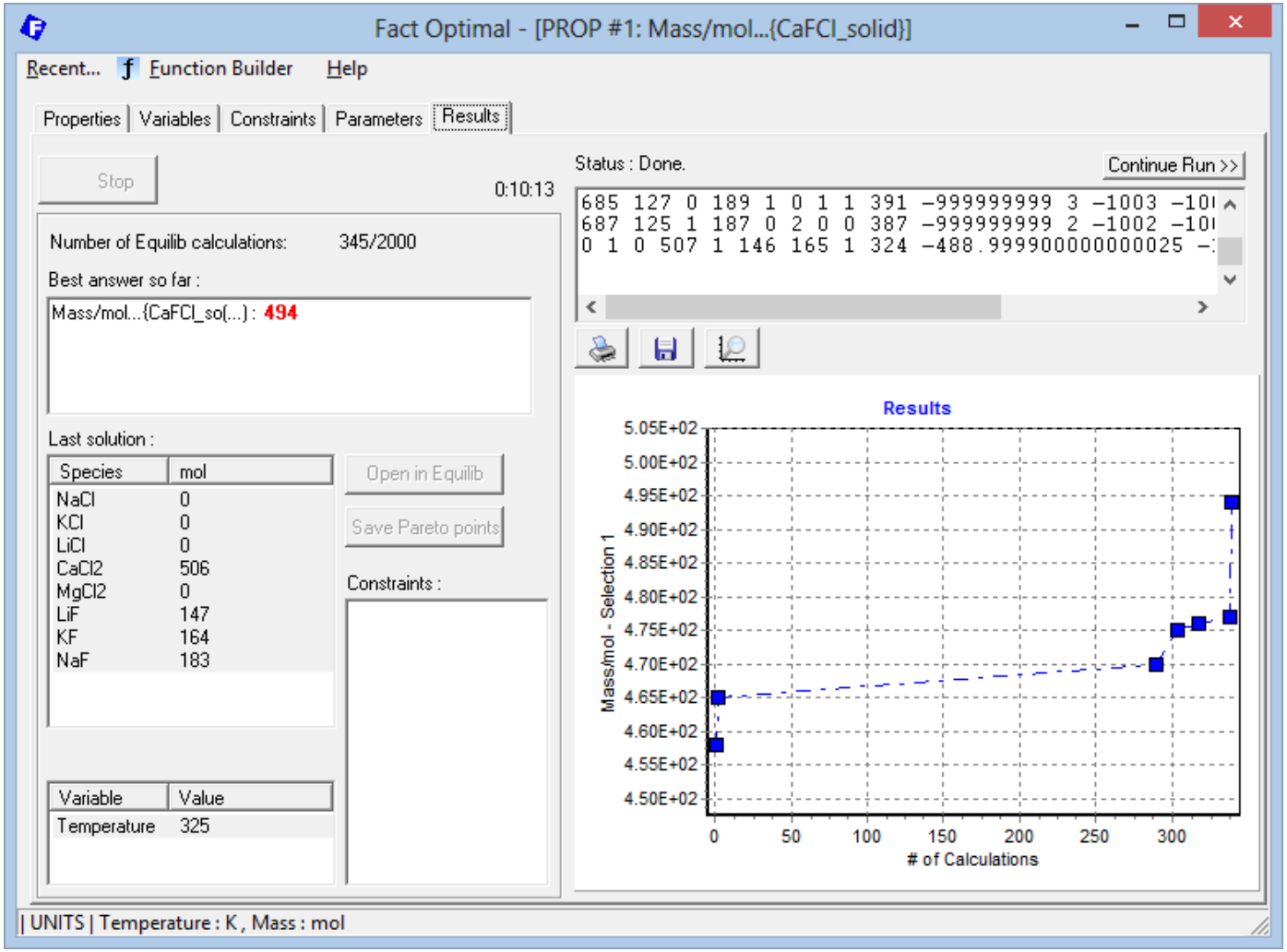
# Example 6 : Application using the cache option (Next Run) - 7

Next we stop the calculation after an additional 253 calculations, at which point **FactOptimal** has found a better value of 465 moles at 336K.



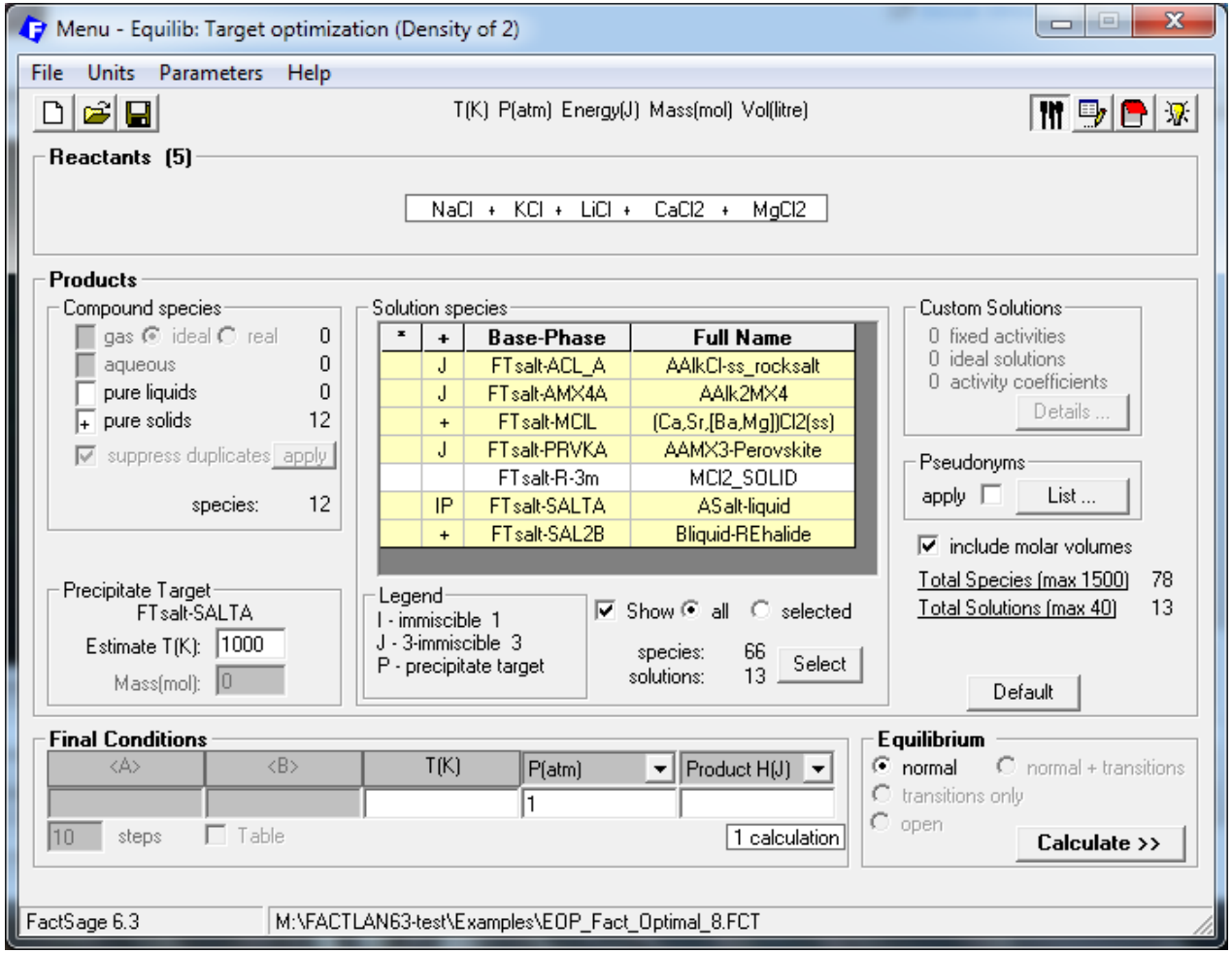
# Example 6 : Application using the cache option (Next Run) - 8

Next run FactOptimal for 345 more calculations, at which point **FactOptimal** has found a better value of 494 moles at 325K.



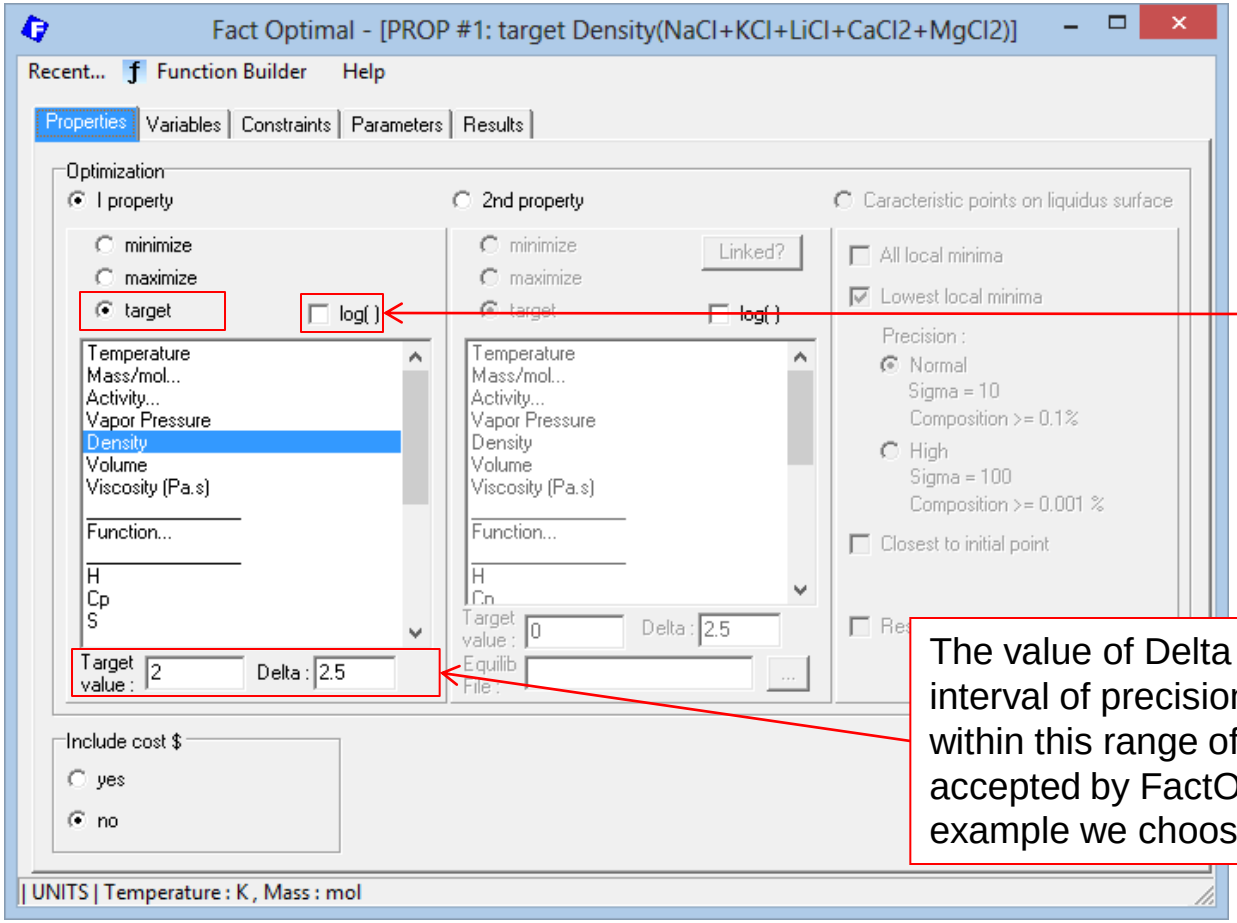
# Example 7 : Target Optimization - 1

Using the same system as Example 3 (slide 6.1) ($LiCl$-$NaCl$-$KCl$-$CaCl_2$-$MgCl_2$) let us perform a target calculation whereby we search for compositions where the density of the liquid at the liquidus temperature is 2.00 g/ml.



# Example 7 : Target Optimization - 2

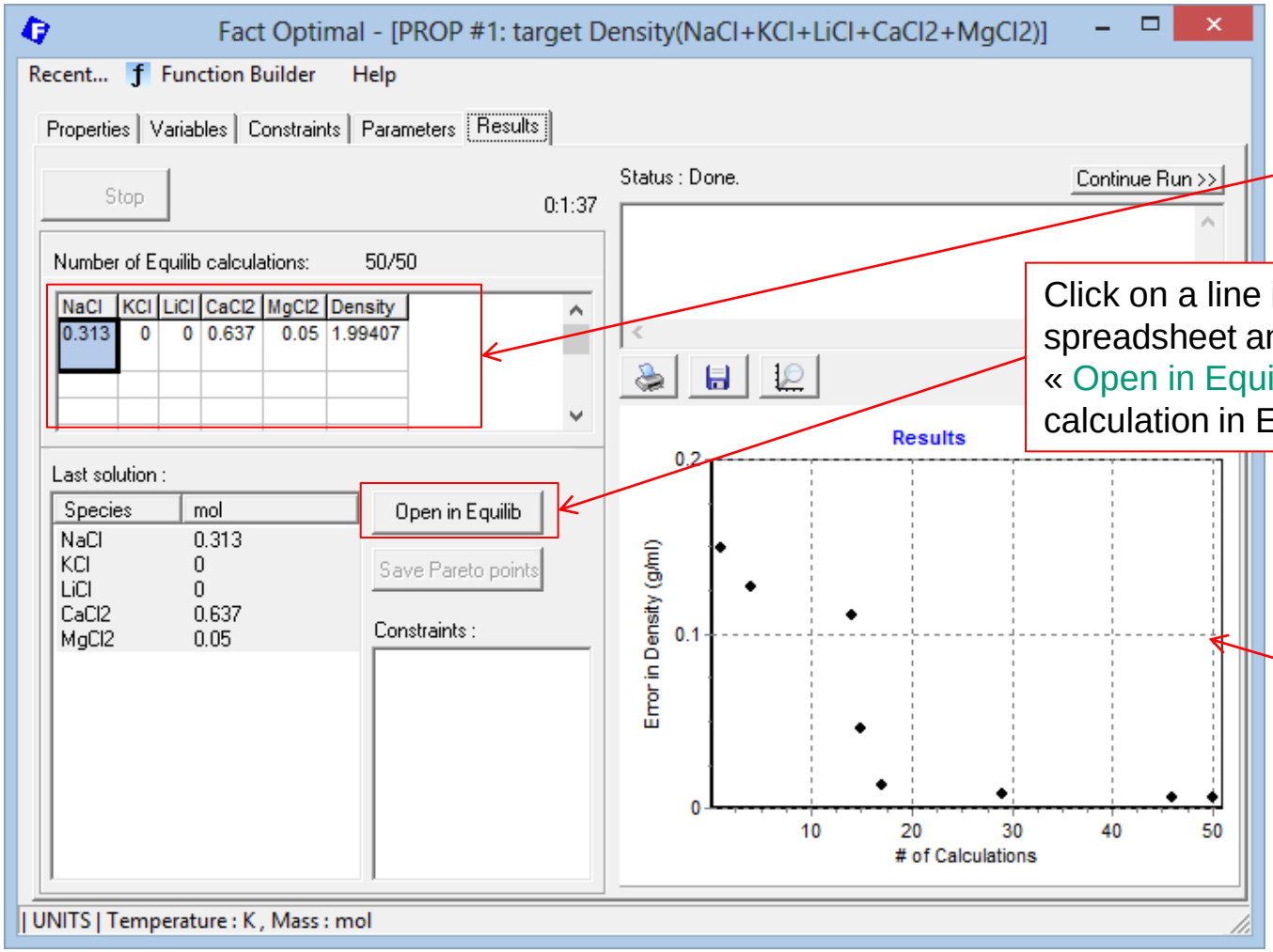
We are searching for compositions for which the density of the liquid at the liquidus temperature is **2.00 g/ml**.




Note: if you click here. the **logarithm** of the objective function will be optimized. This may present a numerical advantage, increasing the speed and precision of the calculation in some cases

The value of Delta is the normalized interval of precision. Any solution within this range of tolerance will be accepted by FactOptimal. In this example we choose an error of 2.5%.

# Example 7 : Target Optimization - 3

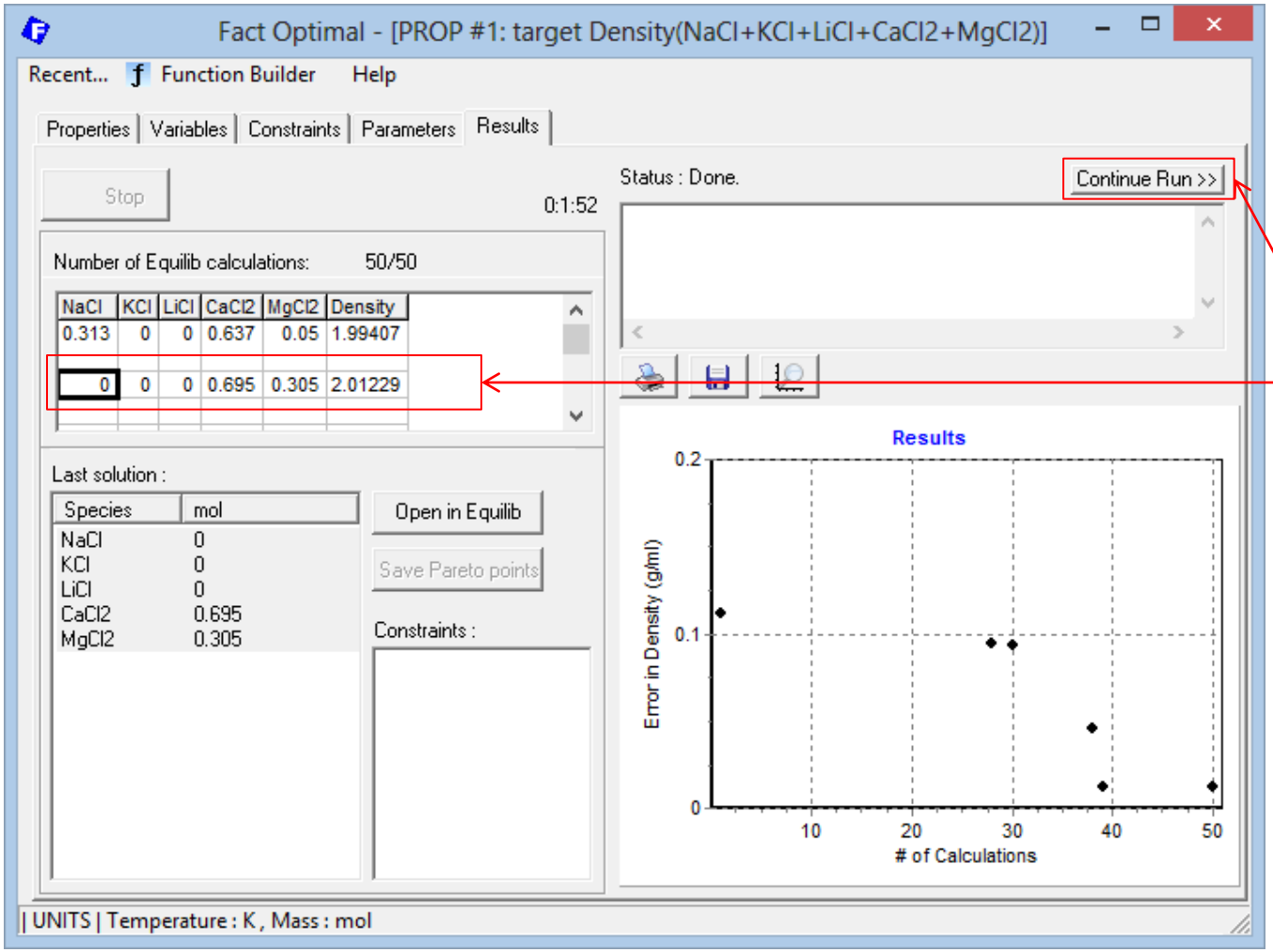



Here FactOptimal minimizes the error between the current calculated density and the targeted density. The best solution is displayed in the table at the end of the optimization.

Click on a line in the spreadsheet and then on « Open in Equilib » to load this calculation in Equilib.

The graph shows the error value versus the number of calculations.

# Example 7 : Target Optimization - 4




The user can click on **Continue Run >>** to perform another 50 calculations and get a different point targeting the same density.

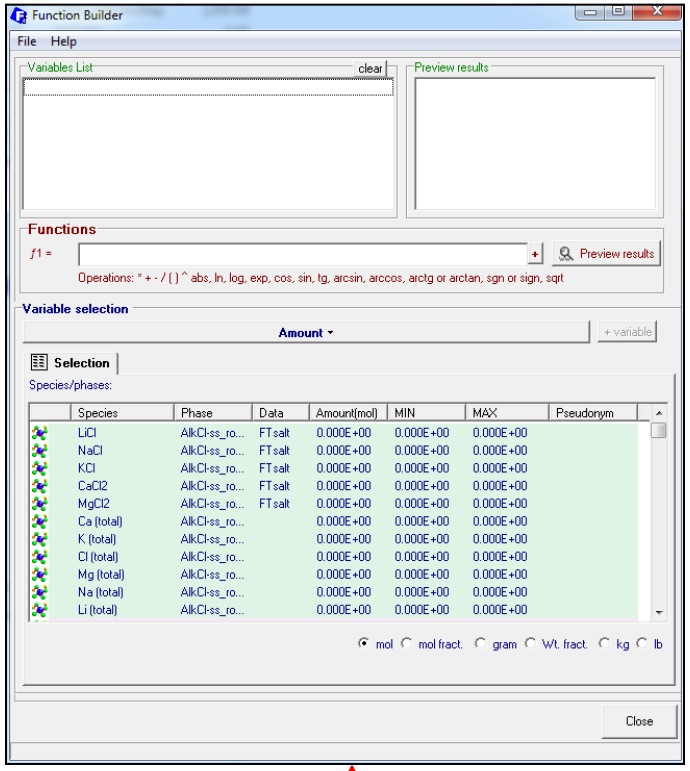
# Optimization using the Function Builder - 1

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.

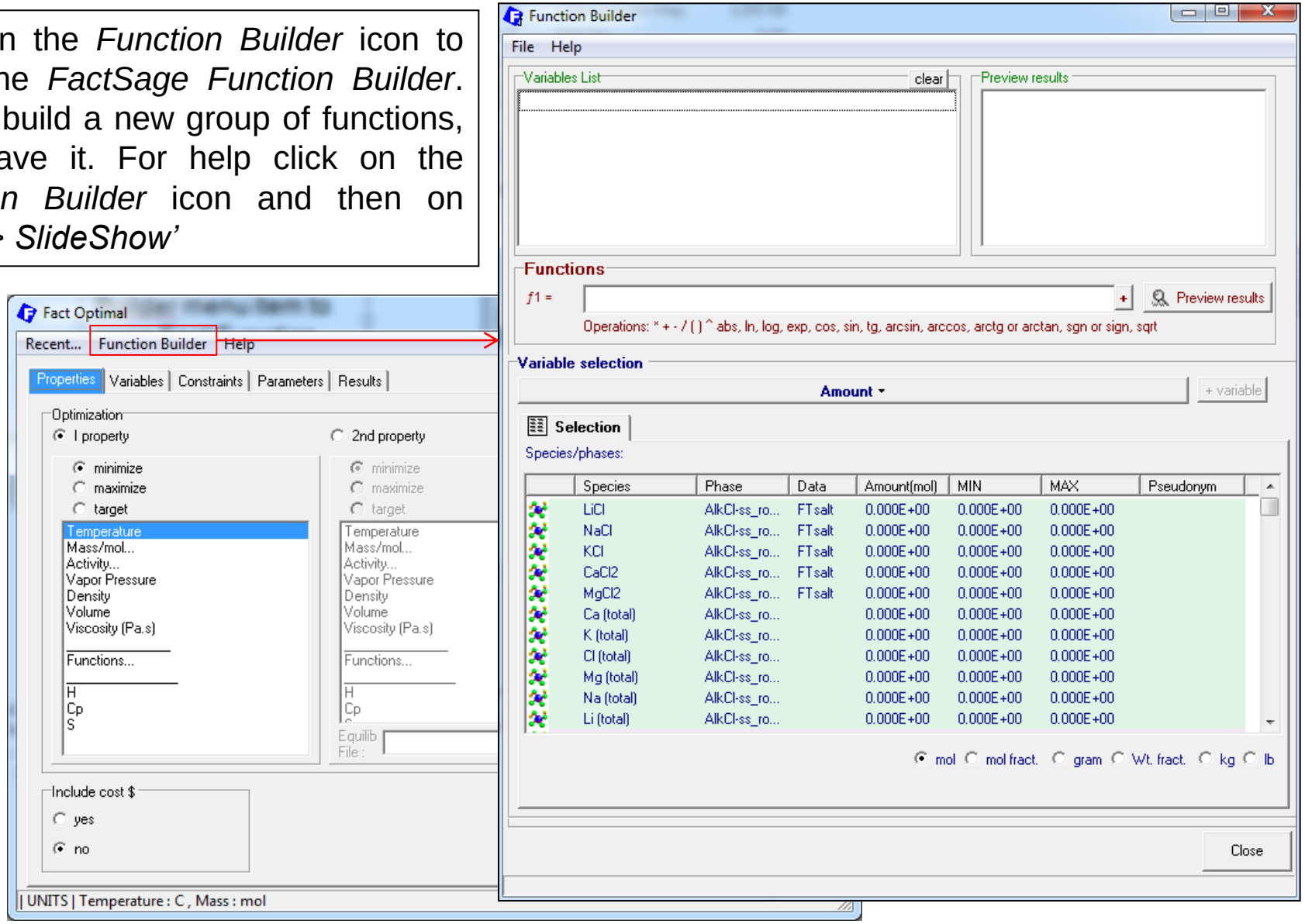



For examples of the use of Function Builder, see the Function Builder Slide Show.


[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

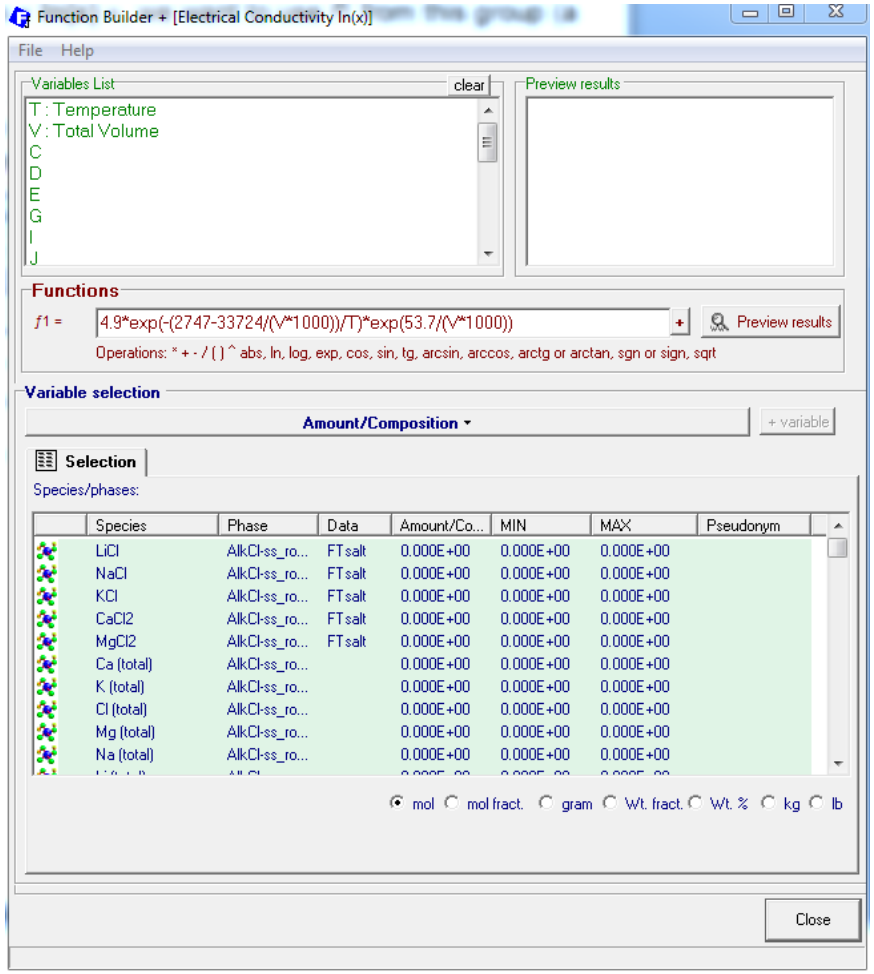
# Optimization using the Function Builder - 2

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 > SlideShow'*

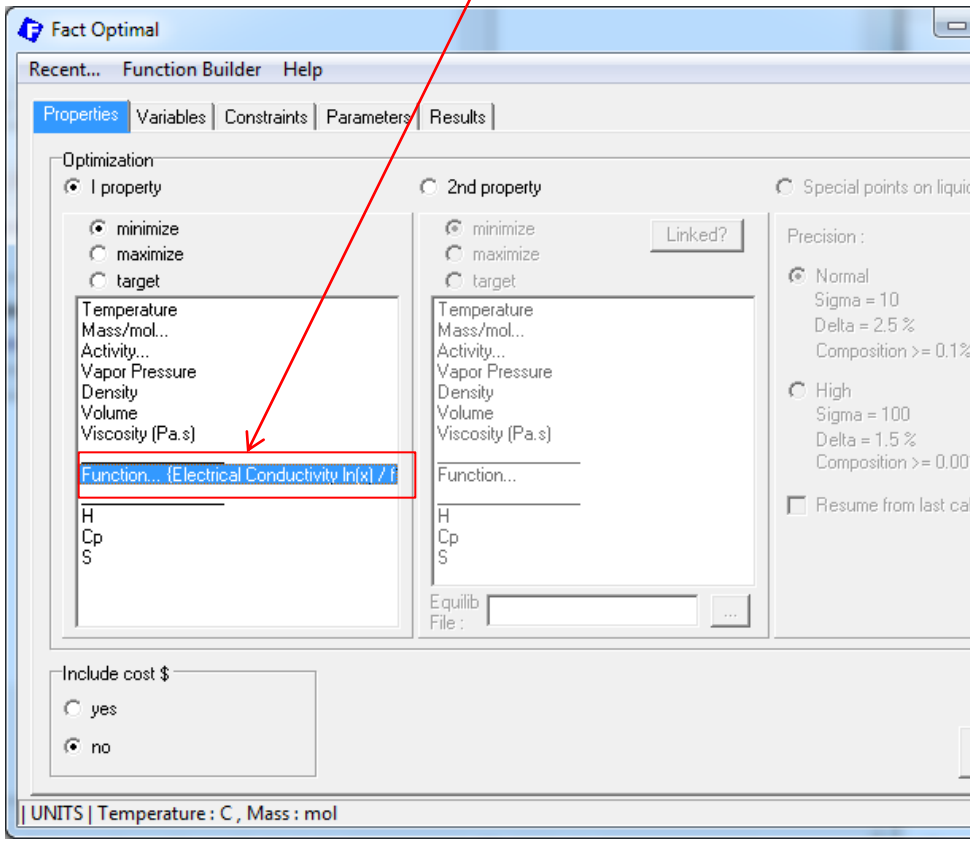


# Optimization using the Function Builder - 3

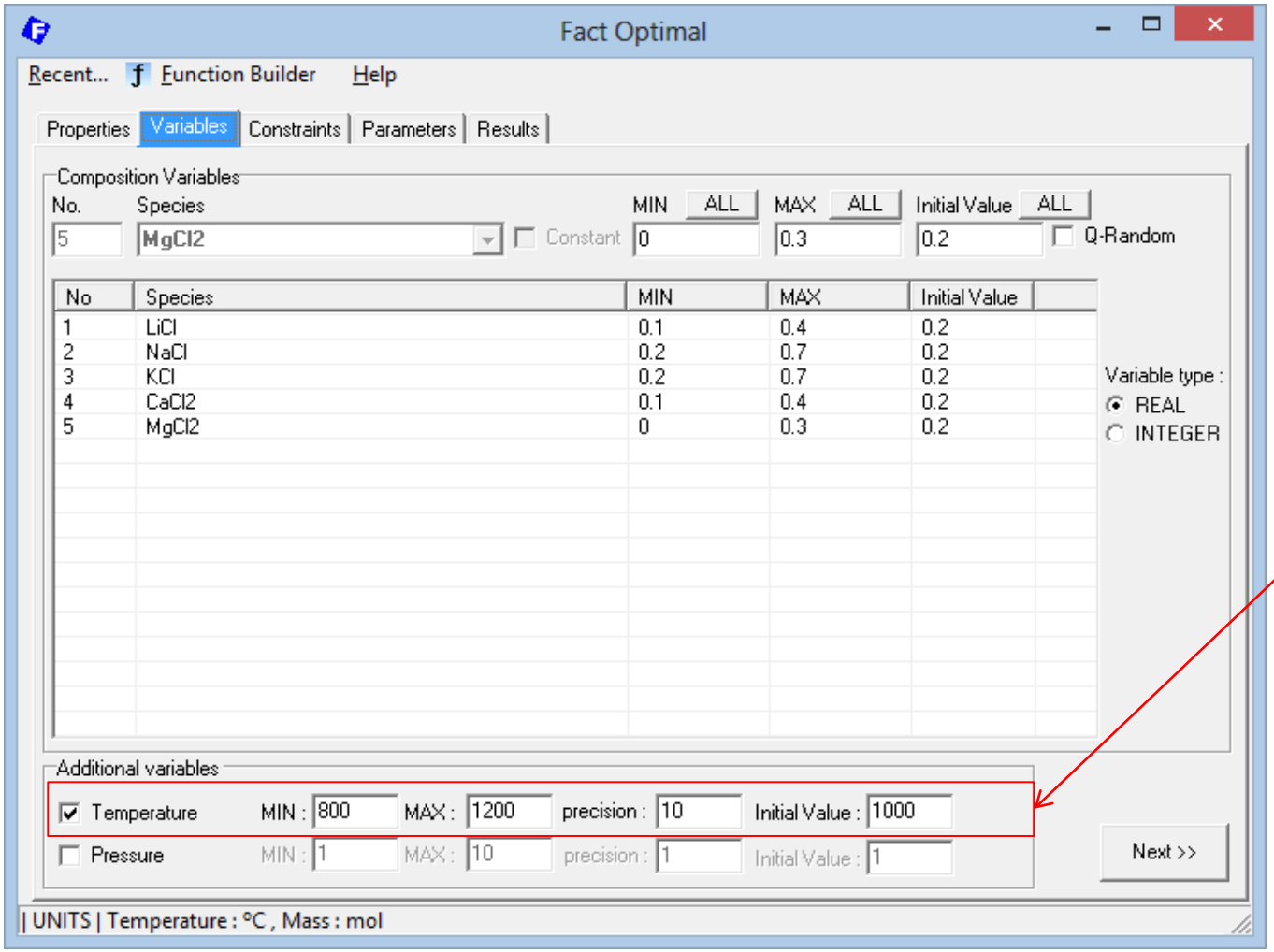
Here we enter the formula for electrical conductivity in the *Function Builder*. A group of functions is created in Function Builder, saved as « **Electrical Conductivity ln(x)** ». We want to use the fuction *f*1 from this group (a group can contain up to 10 functions *f*1, *f*2, *f*3, etc.)




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



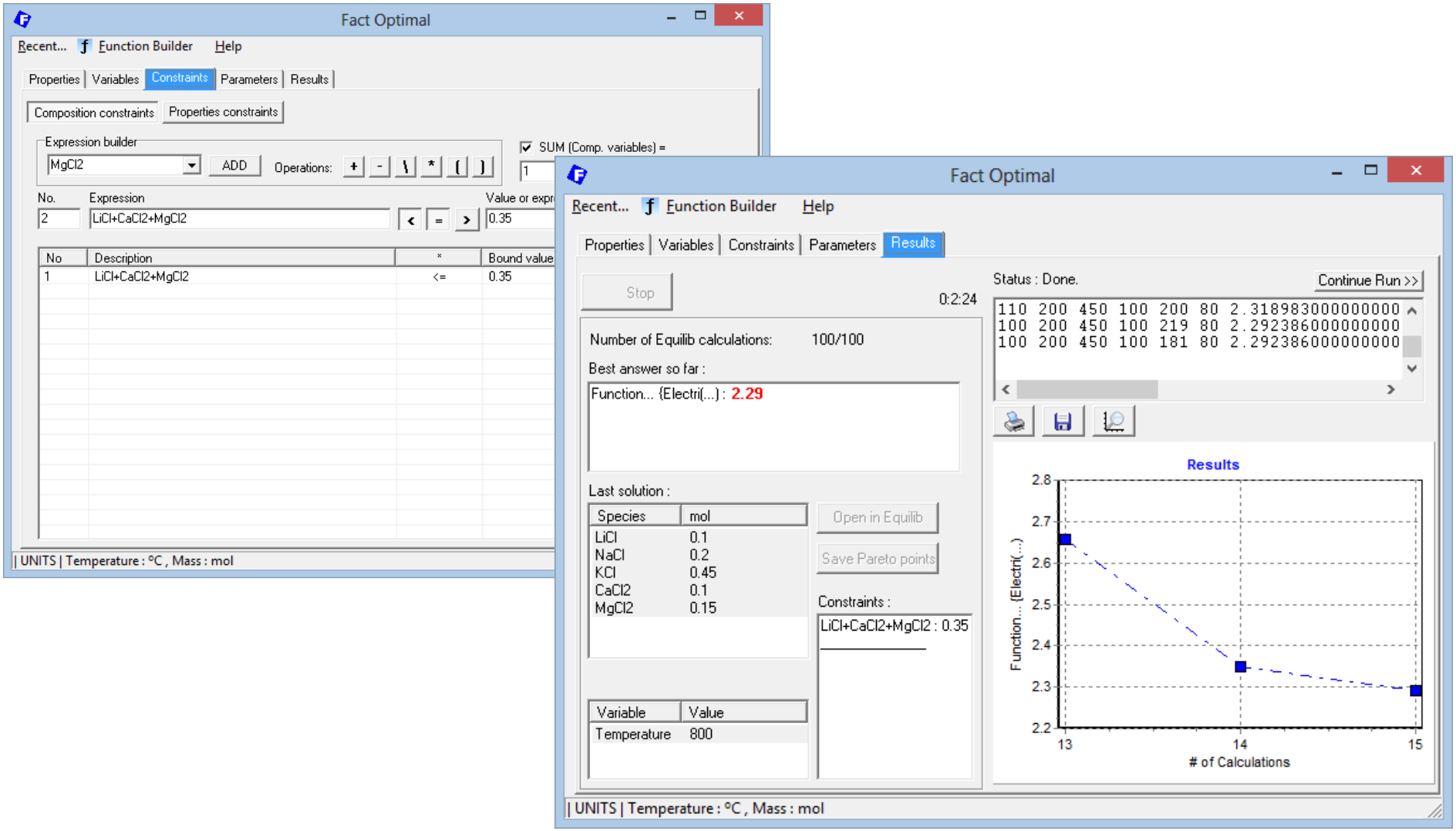
# Optimization using the Function Builder - 4




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

# Optimization using the Function Builder - 4

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

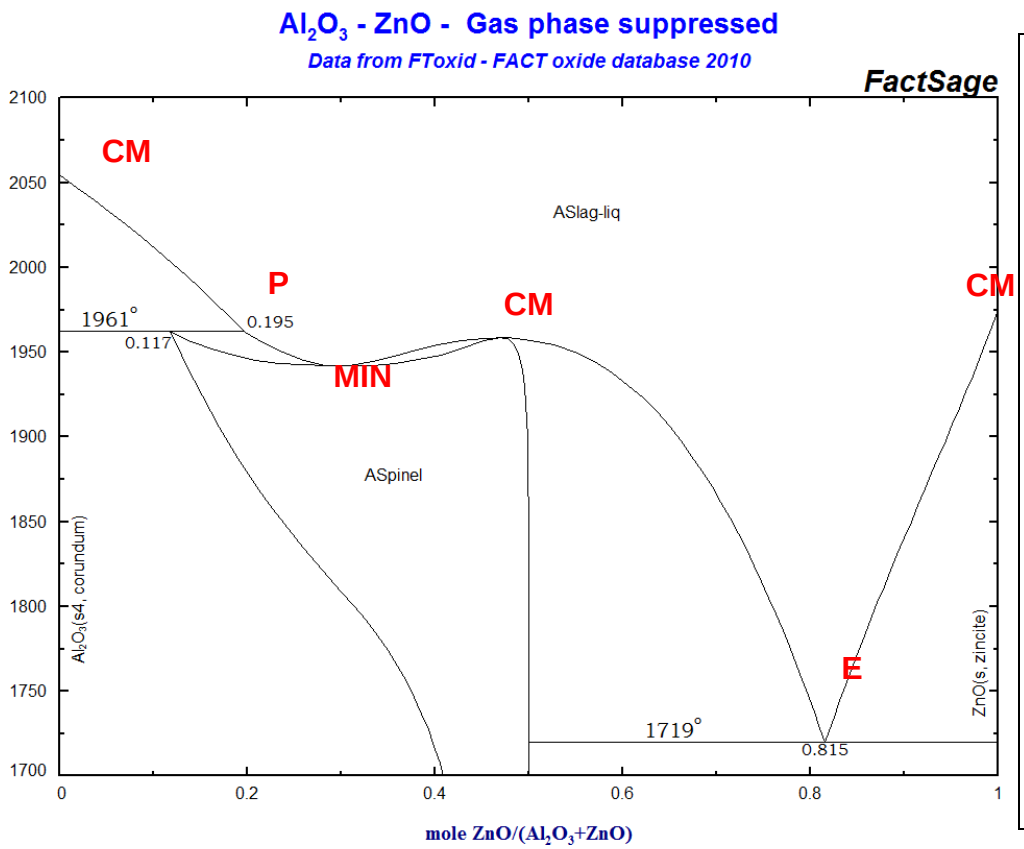


## *Characteristic points on the liquidus surface*

# What is a characteristic point on the liquidus surface

Eutectics, peritectics, monotectics, quasi-peritectics, minima and congruent melting points are <u>characteristic points</u> on the liquidus surface.

**FactOptimal** is able to calculate the compositions of eutectics, minima and congruent melting points.

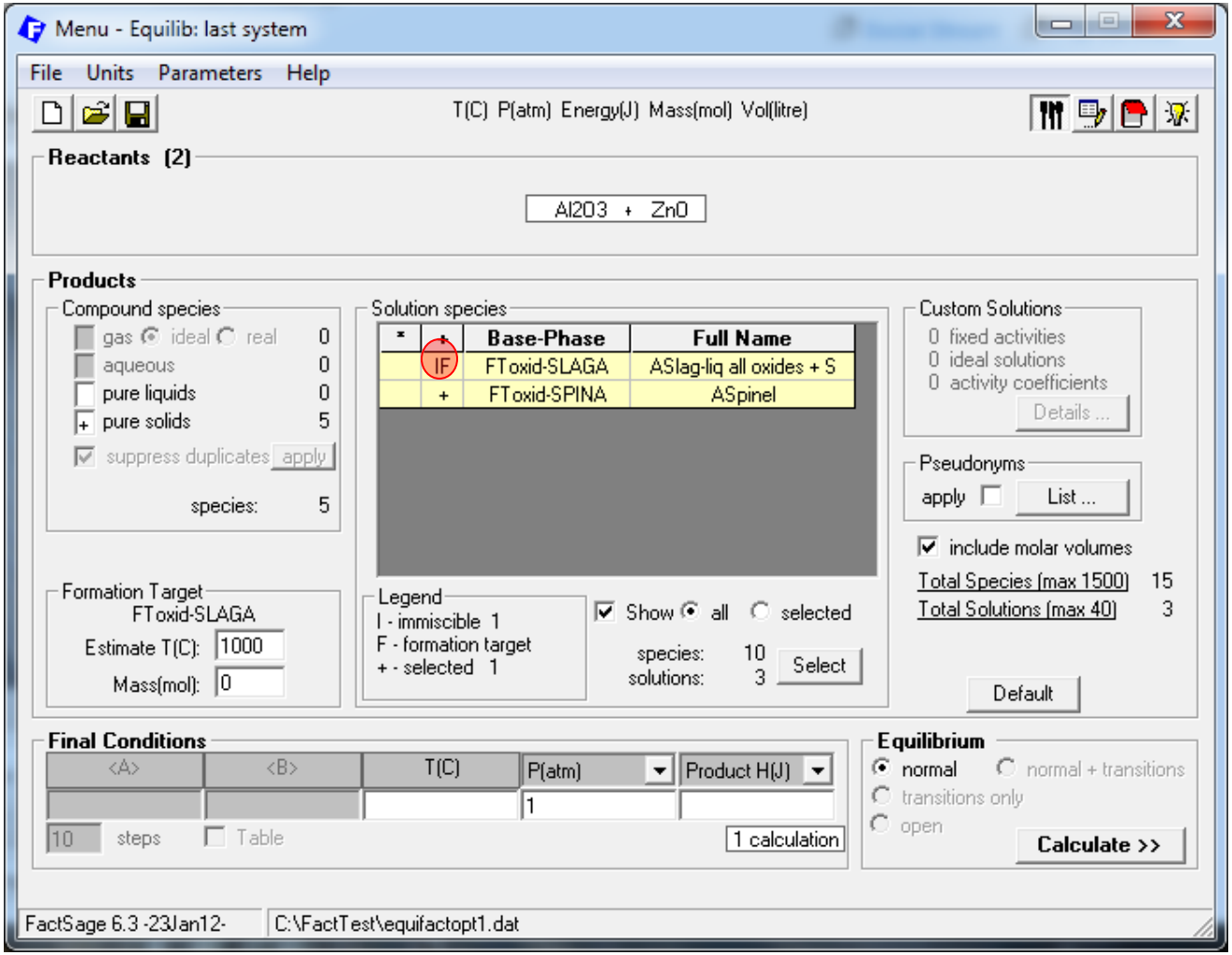



For example, within the $Al_2O_3$-ZnO system there is 1 eutectic (E), 1 minimum (MIN), 1 peritectic and 3 congruent melting points (CM).

We can calculate all these points with FactOptimal except for the peritectic. Clearly, for a <u>binary</u> system it is not necessary to use FactOptimal since the characteristic points are all given by the Phase Diagram module (or can be calculated with a Target option in the Equilib module). We use a binary example here simply to illustrate the input to FactOptimal.

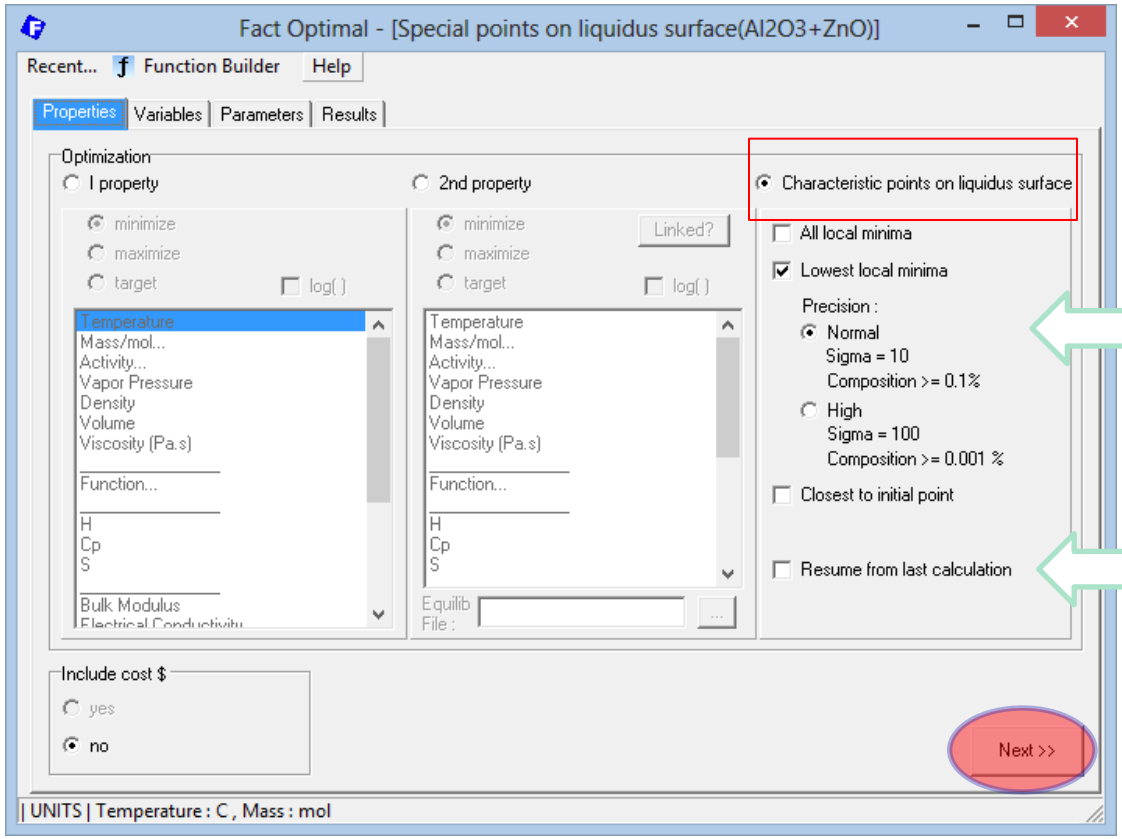
# Example 8 : How to calculate characteristic points with FactOptimal for the $Al_2O_3$-ZnO system -1

Step 1: define the system, select appropriate databases (in this case FTOxid), select a **formation** target (F) on the liquidus and perform a single calculation at an arbitrary composition.



# Example 8 : How to calculate characteristic points with FactOptimal for the $Al_2O_3$-ZnO system - 2

Step 2: Click on the **FactOptimal** icon, select “characteristic points on liquidus surface” and start the calculation. If you are using the stored example files, click on “Recent...” to load the **FactOptimal** file.




**Precision parameters.**
**The normal precision is recommended for multicomponent systems (N>4) in order to reduce computation time.**

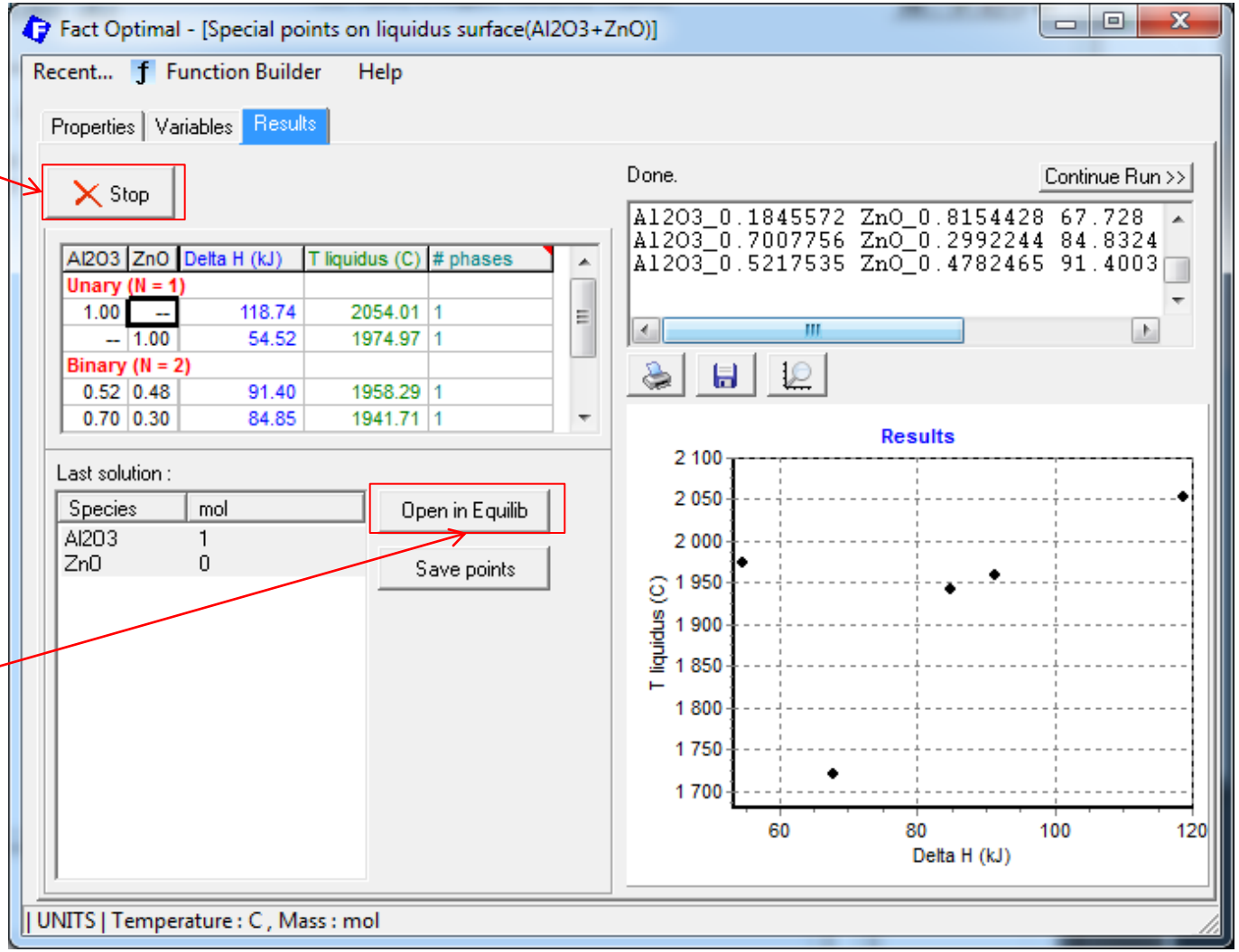
**For multicomponent systems the calculation of the characteristic points on the liquidus surface is usually lengthy . If the calculation should fail unexpectedly, the user can restart the calculation from the results of the previous calculation**

# Example 8 : How to calculate characteristic points with FactOptimal for the $Al_2O_3$-ZnO system - 3

*FactOptimal Results Window* : composition of the 5 characteristic points (MIN, E and CM) for $Al_2O_3$-ZnO, as well as the liquidus temperature and enthalpy of melting at each point.

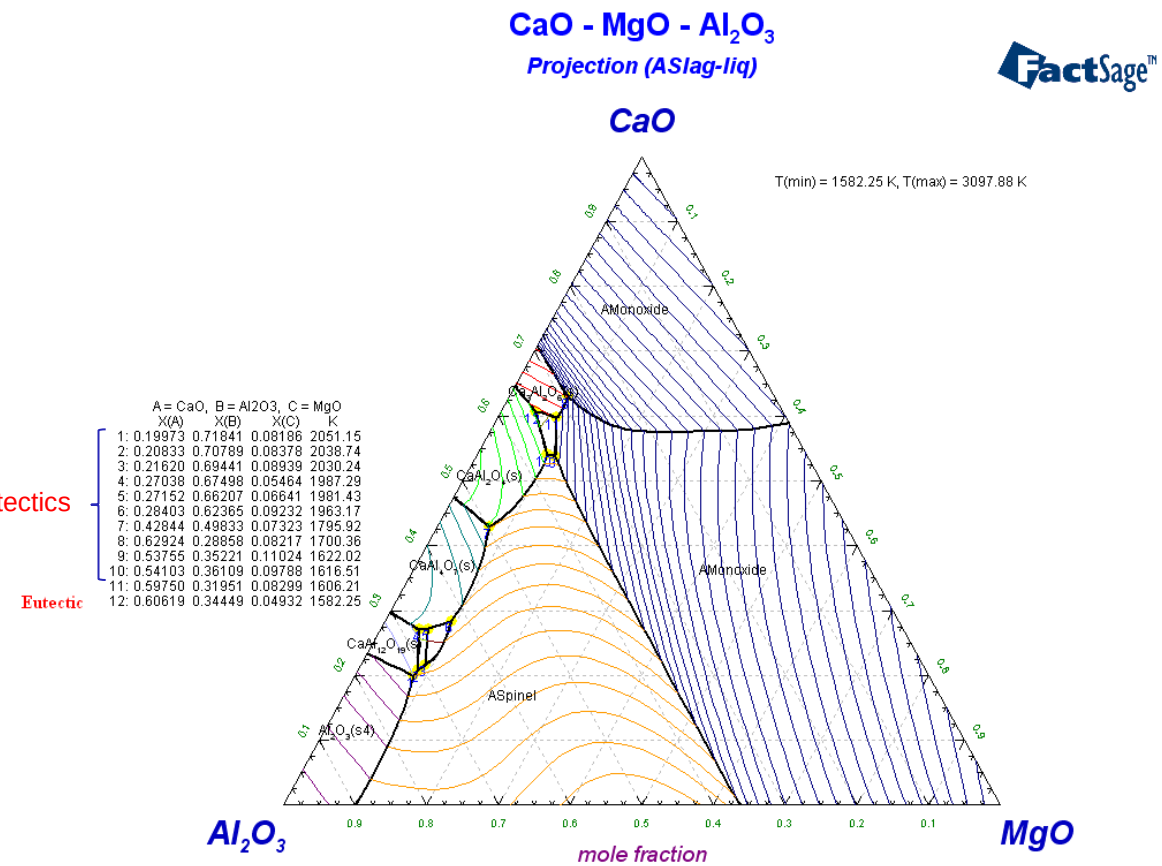
FactOptimal keeps searching for points until the user clicks on the Stop button.

Click on a point on the graph and then on "Open in Equilib" in order to see the output for that point



# And for higher order systems ?

Of course, for systems of 2 and 3 components, all the characteristic points can also be obtained with the **Phase Diagram** module: for binary systems a simple (T,X) calculation, and for ternary systems a liquidus projection.



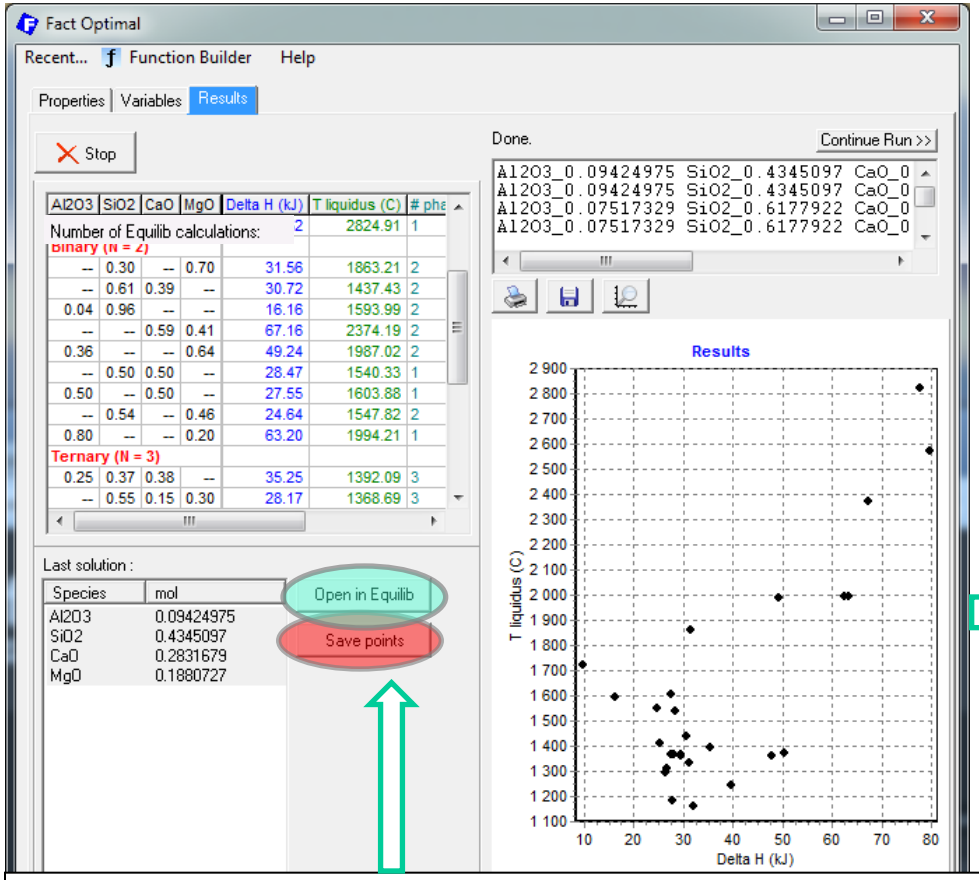

A = CaO, B = Al2O3, C = MgO

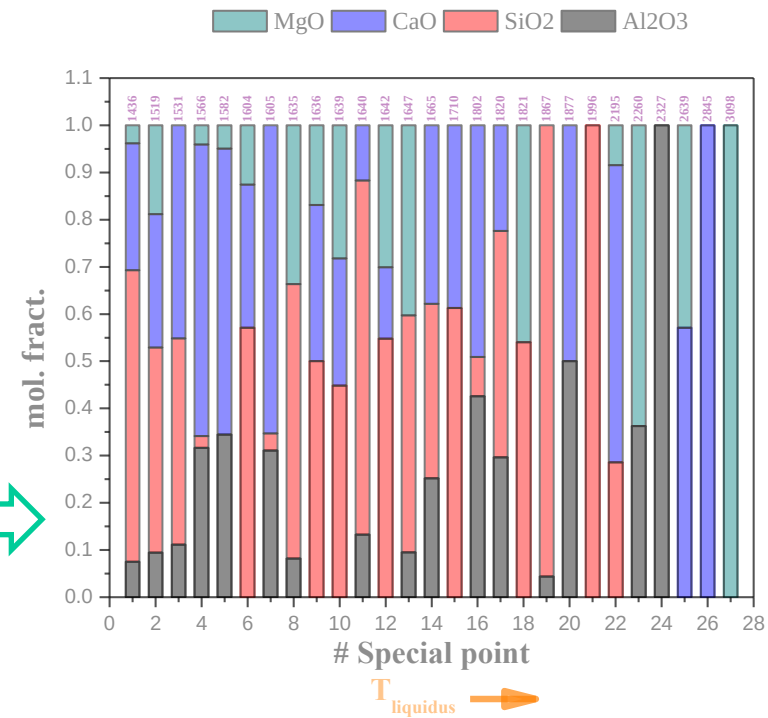
| | X(A) | X(B) | X(C) | K |
|---|---|---|---|---|
| 1: | 0.19973 | 0.71841 | 0.08186 | 2051.15 |
| 2: | 0.20833 | 0.70789 | 0.08378 | 2038.74 |
| 3: | 0.21620 | 0.69441 | 0.08939 | 2030.24 |
| 4: | 0.27038 | 0.67498 | 0.05464 | 1987.29 |
| 5: | 0.27152 | 0.66207 | 0.06641 | 1981.43 |
| 6: | 0.28403 | 0.62365 | 0.09232 | 1963.17 |
| 7: | 0.42844 | 0.49833 | 0.07323 | 1795.92 |
| 8: | 0.62924 | 0.28858 | 0.08217 | 1700.36 |
| 9: | 0.53755 | 0.35221 | 0.11024 | 1622.02 |
| 10: | 0.54103 | 0.36109 | 0.09788 | 1616.51 |
| 11: | 0.59750 | 0.31951 | 0.08299 | 1606.21 |
| 12: | 0.60619 | 0.34449 | 0.04932 | 1582.25 |

# Characteristic points on the $CaO$-$Al_2O_3$-$MgO$-$SiO_2$ liquidus

Applying the same procedure as previously one can calculate the characteristic points on the liquidus surface of the $CaO$-$Al_2O_3$-$MgO$-$SiO_2$ system.

By clicking on any point on the graph, you can obtain compositions of the characteristic points, the liquidus temperatures and the enthalpies of melting.

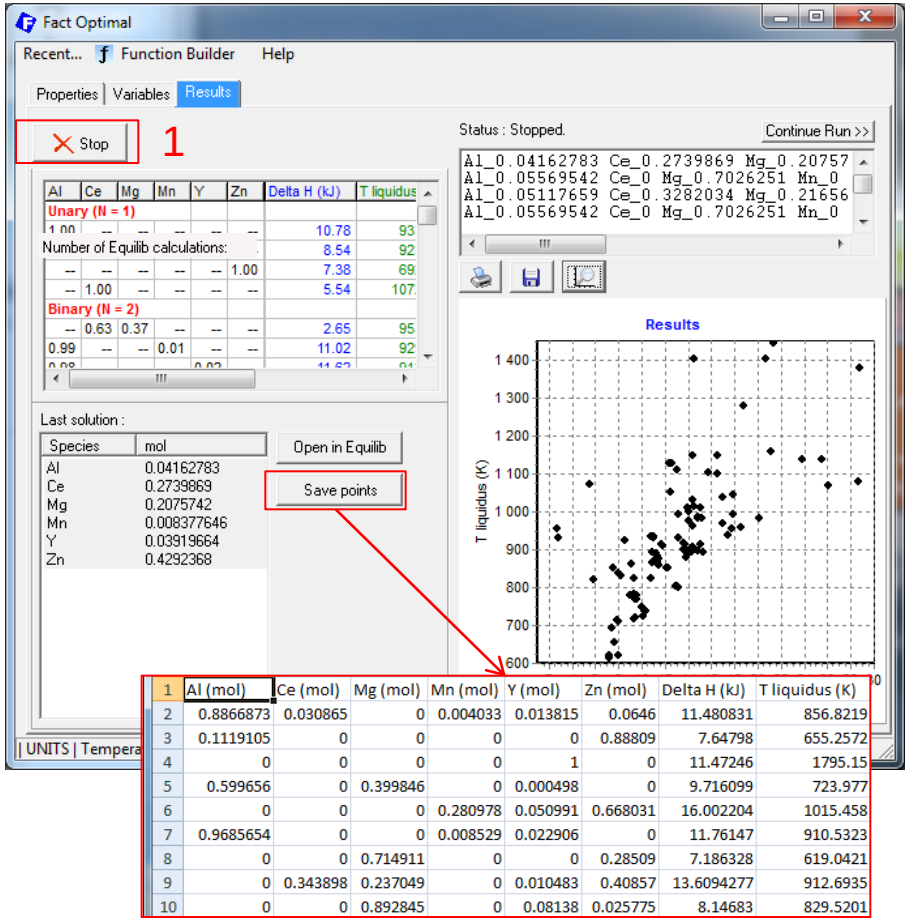



The points can be saved as a text file and opened in Excel for post treatment
The solid phases that precipitate at the minimum can be seen by opening **Equilib**

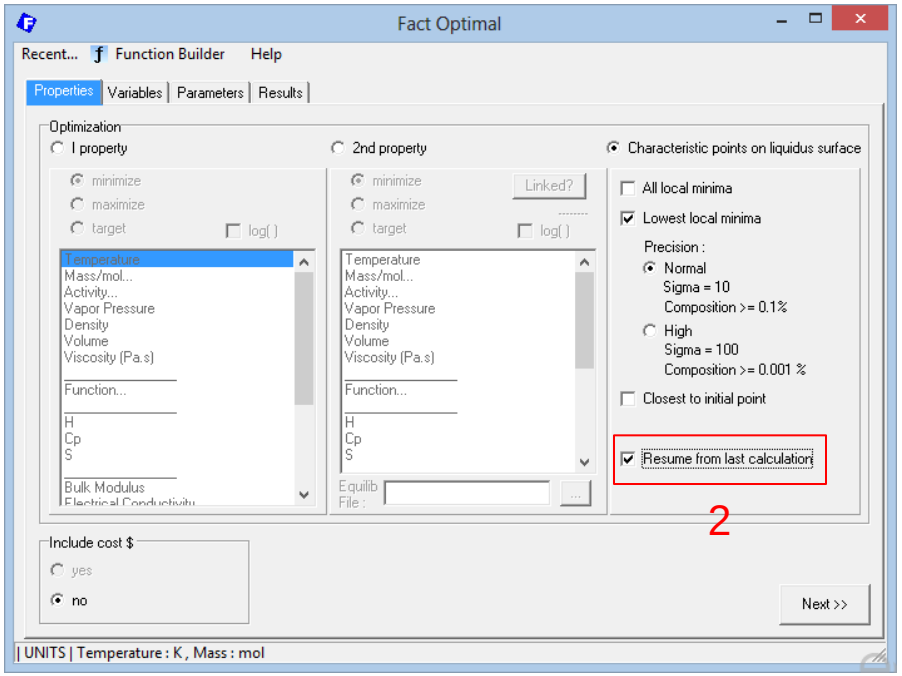
# Characteristic points on the Al-Mg-Ce-Mn-Y-Zn liquidus

Sometimes for large systems when many phases are involved, the calculations can be very time consuming. The user can stop (1) the calculations at any time. However the calculation can be restarted later without losing the previous results (2). The absolute minimum liquidus temperature will always be calculated relatively early in the calculation.



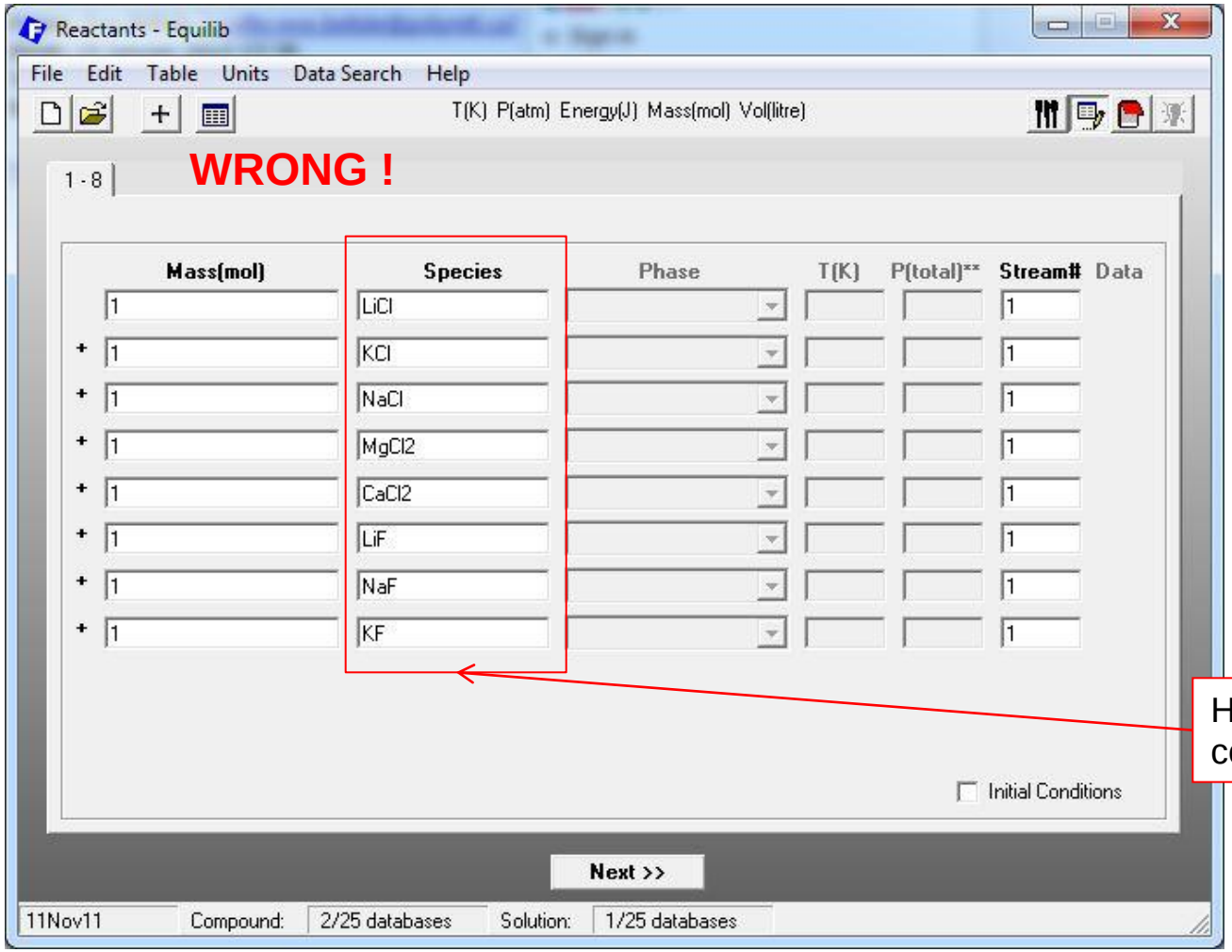

| 1 | Al (mol) | Ce (mol) | Mg (mol) | Mn (mol) | Y (mol) | Zn (mol) | Delta H (kJ) | T liquidus (K) |
|---|---|---|---|---|---|---|---|---|
| 2 | 0.8866873 | 0.030865 | 0 | 0.004033 | 0.013815 | 0.0646 | 11.480831 | 856.8219 |
| 3 | 0.1119105 | 0 | 0 | 0 | 0 | 0.88809 | 7.64798 | 655.2572 |
| 4 | 0 | 0 | 0 | 0 | 1 | 0 | 11.47246 | 1795.15 |
| 5 | 0.599656 | 0 | 0.399846 | 0 | 0.000498 | 0 | 9.716099 | 723.977 |
| 6 | 0 | 0 | 0 | 0.280978 | 0.050991 | 0.668031 | 16.002204 | 1015.458 |
| 7 | 0.9685654 | 0 | 0 | 0.008529 | 0.022906 | 0 | 11.76147 | 910.5323 |
| 8 | 0 | 0 | 0.714911 | 0 | 0 | 0.28509 | 7.186328 | 619.0421 |
| 9 | 0 | 0.343898 | 0.237049 | 0 | 0.010483 | 0.40857 | 13.6094277 | 912.6935 |
| 10 | 0 | 0 | 0.892845 | 0 | 0.08138 | 0.025775 | 8.14683 | 829.5201 |

In this example, we stopped the calculations after calculating the absolute minimum liquidus temperature and 70 other characteristic points.



# Characteristic points – reciprocal systems

In this example, we wish to calculate characteristic points on the liquidus of a reciprocal salt system (a system with 2 or more cations and 2 or more anions) : $Li^+$, $Na^+$, $K^+$, $Mg^{++}$, $Ca^{++}$ / $F^-$, $Cl^-$.

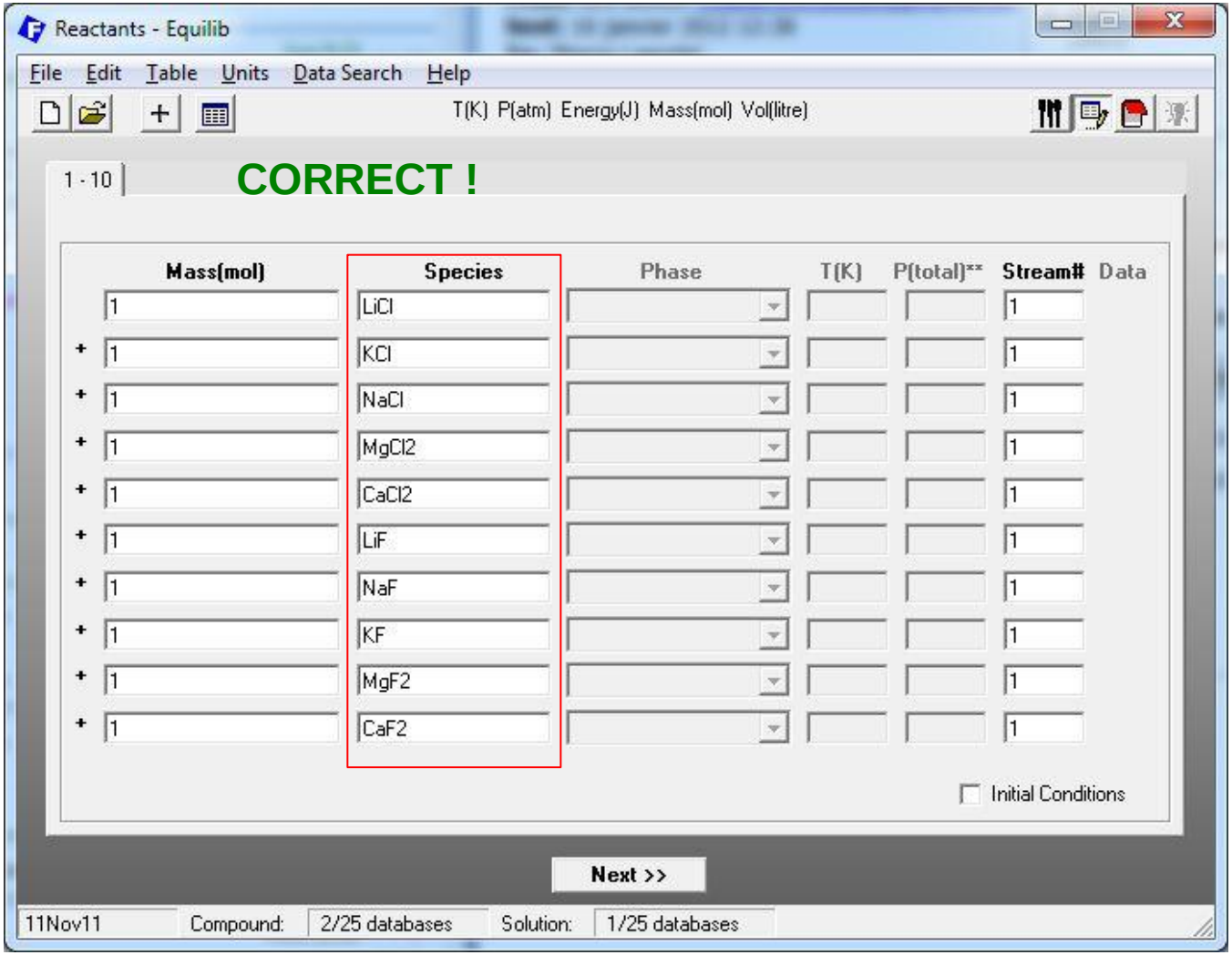



Make sure that the input components include all pairs of cations and anions (i.e. all possible end-members).

Here we are missing two components : CaF2 and MgF2.

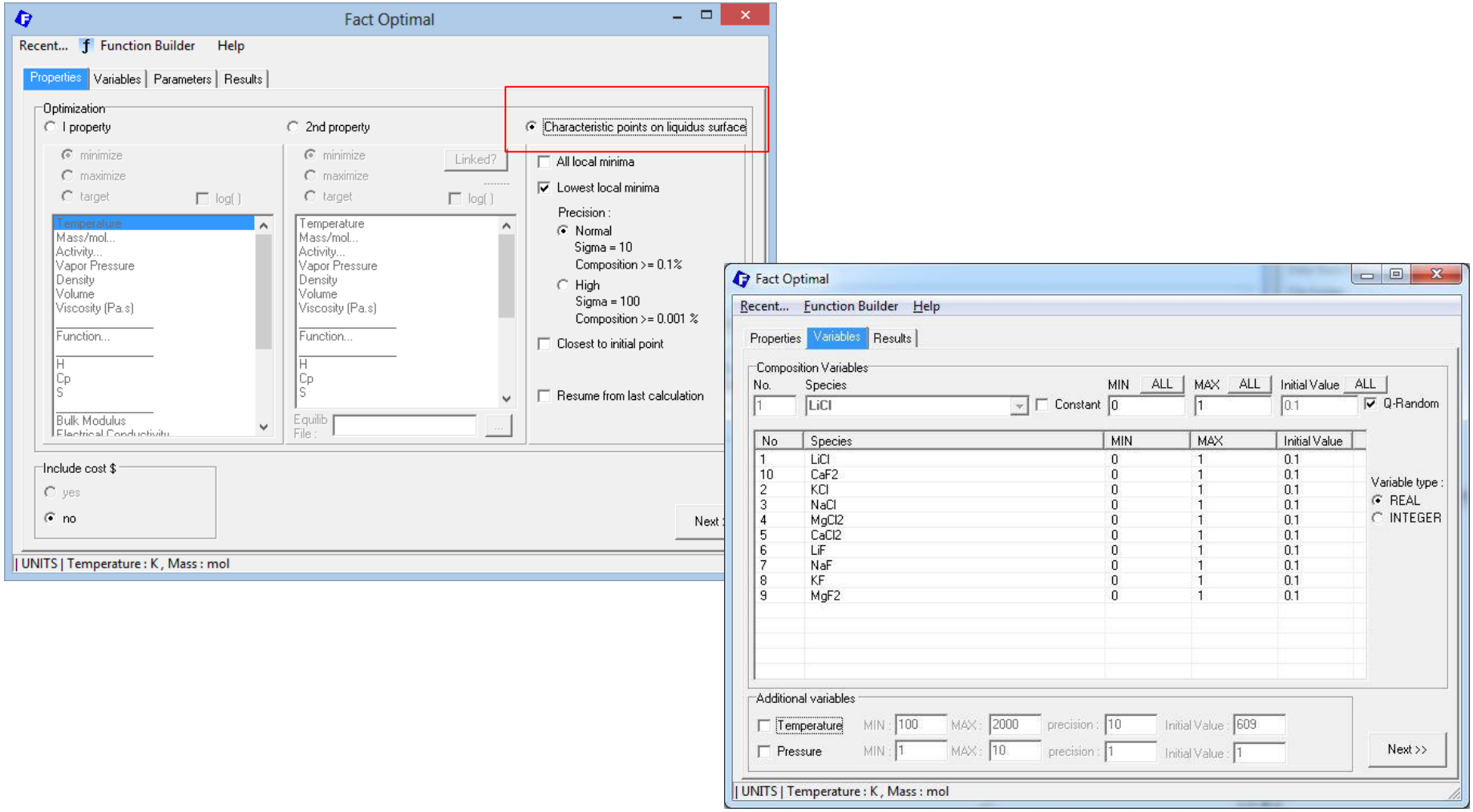
# Characteristic points – reciprocal systems

The correct input contains every end-member (cation-anion pair) in the liquid phase.



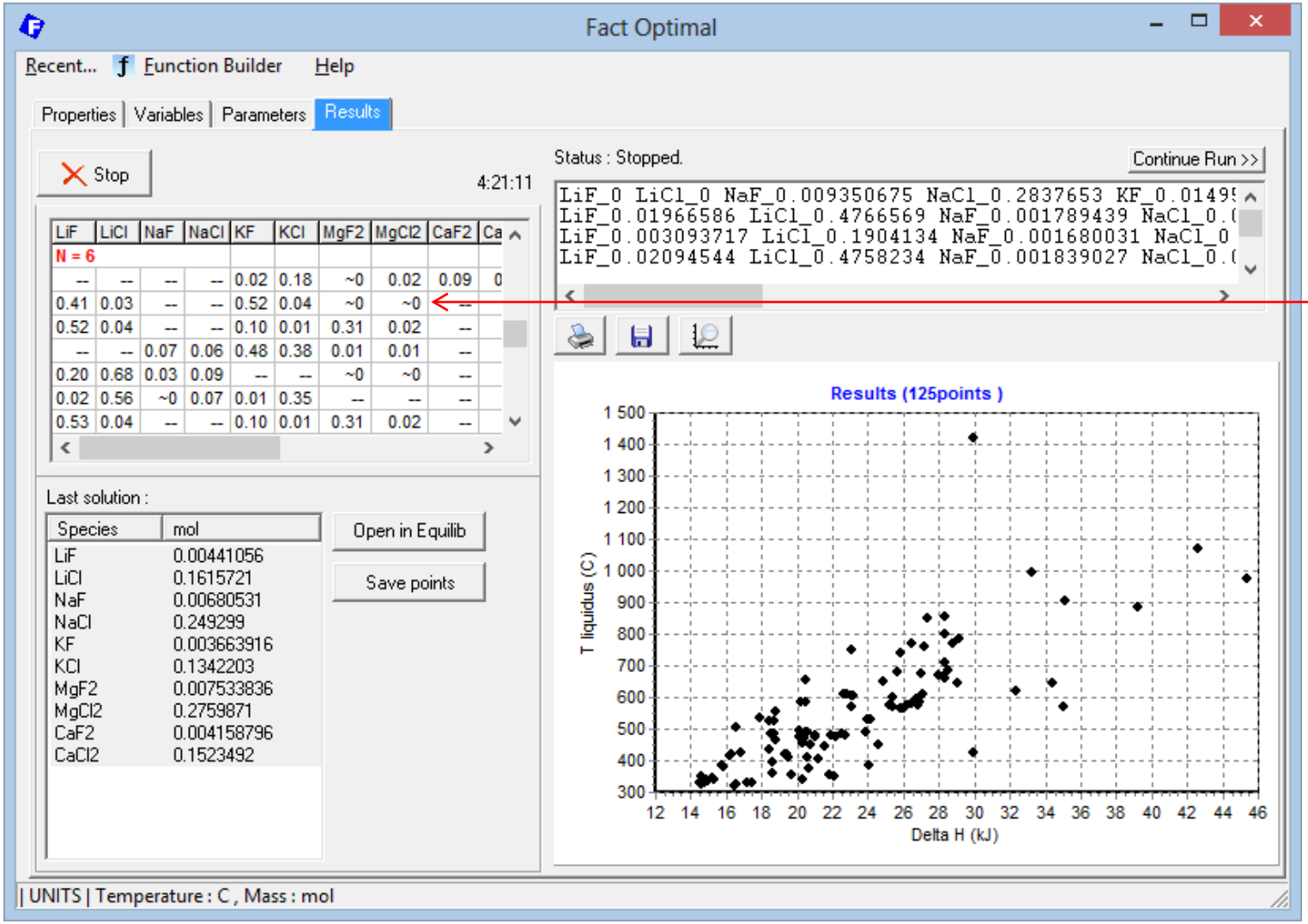
# Characteristic points – reciprocal systems

We choose the *Characteristic points on liquidus surface* option with the default settings.

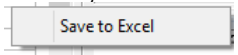


# Characteristic points – reciprocal systems

Calculated *Characteristic Points* in the $Li^+$, $Na^+$, $K^+$, $Mg^{++}$, $Ca^{++}$ / $F^-$, $Cl^-$ reciprocal system.




Right-click anywhere in the table to see this menu,




allowing you to save an Excel file.

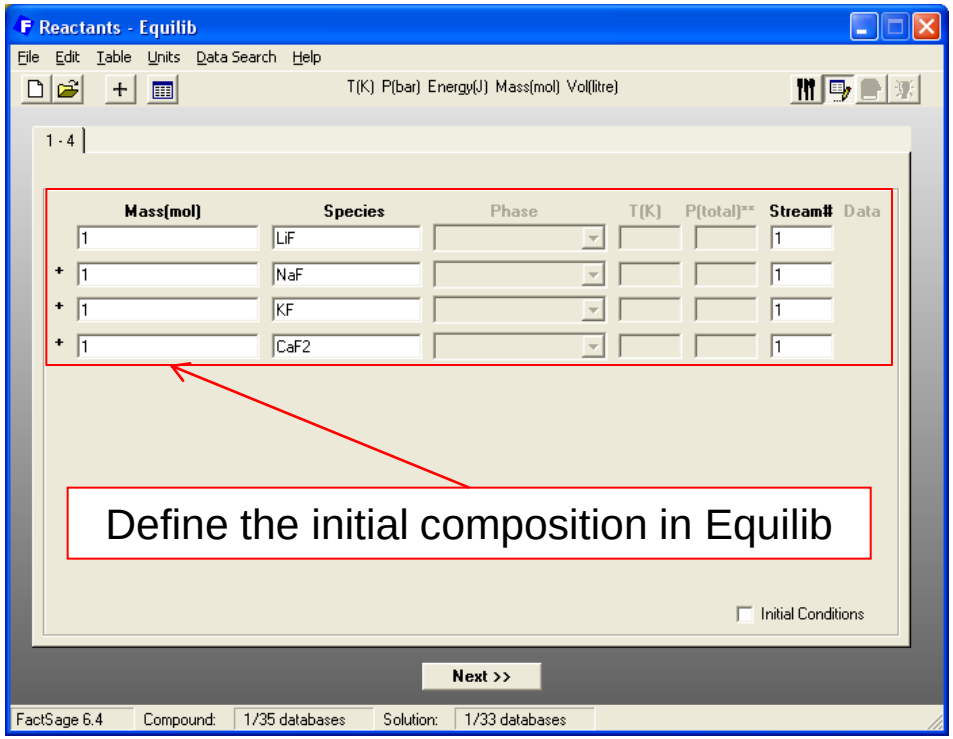
***Closest Characteristic point (to initial composition) on the liquidus surface***

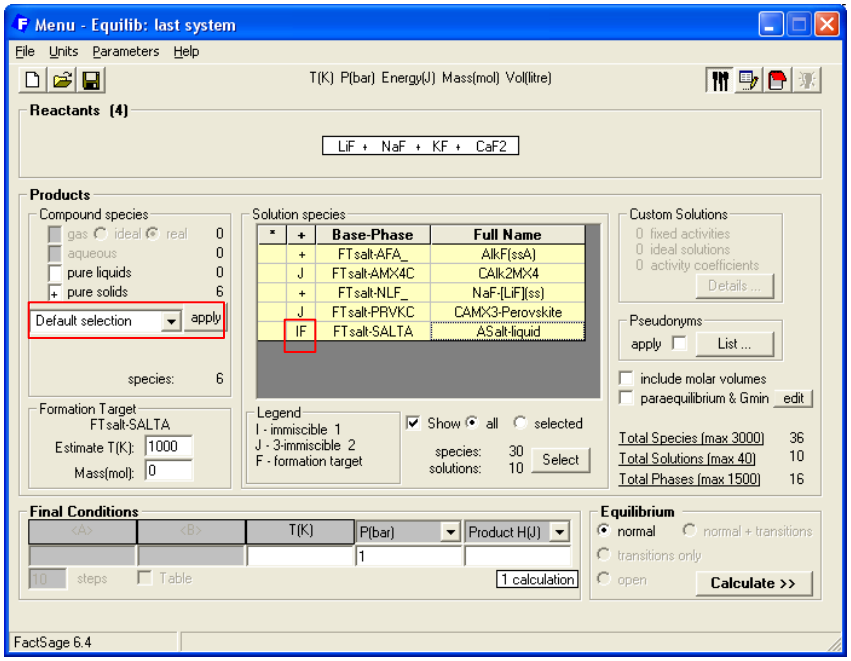
# Example 9: Characteristic points – closest characteristic point - 1

In this example, we wish to calculate **the** Characteristic point closest to the initial composition

Select the FTsalt database

Use Default selection option and **formation target** on the liquid



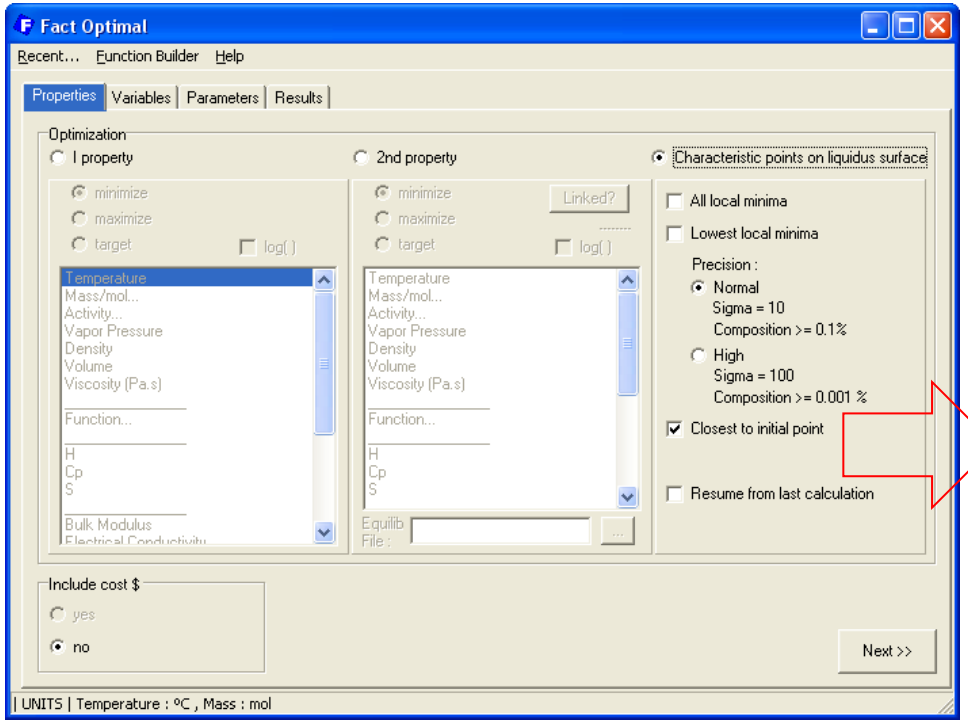



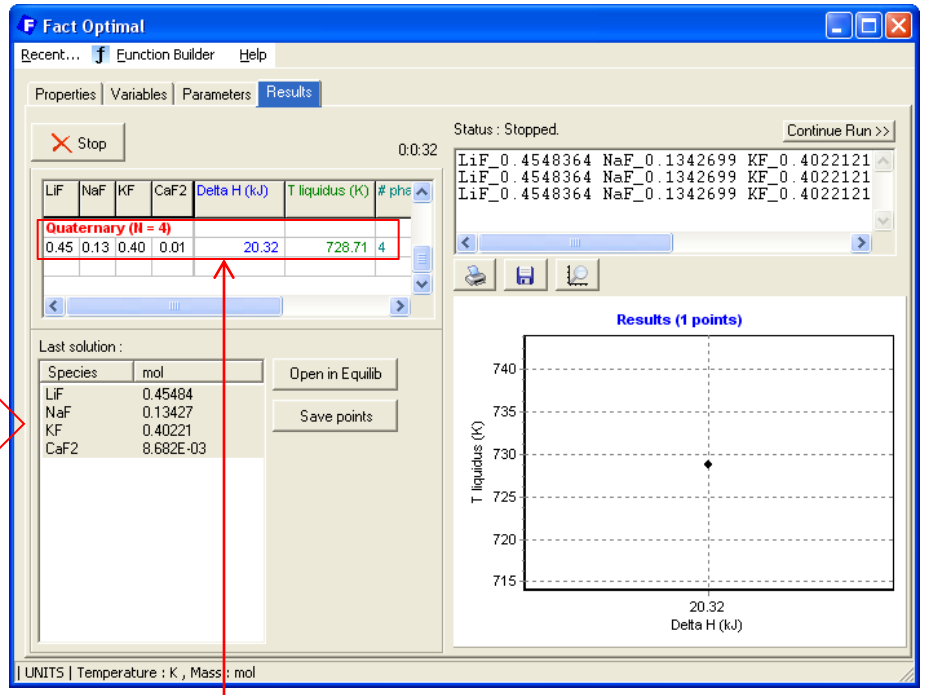
# Example 9: Characteristic points – closest characteristic point - 2

Calculate in Equilib and click on the FactOptmal icon in the Results window.

Select Characteristic points on liquidus surface and the closest to initial point option

Keep default values and click “calculate”




The composition, liquidus temperature, heat of melting and the number of solid phases precipitating at the minimum are given in the table.

# Example 9: Characteristic points – closest Characteristic point - 3

Once the optimization is complete, **Equilib** will automatically load the calculated point.

```
0.45484 LiF +  0.13427 NaF +  0.40221 KF +  8.680000E-03 CaF2 =

0.40065     mol   AlkF(ssA)#1
   (23.173 gram, 0.40065 mol)
           (728.71 K, 1 bar,     a=1.0000)
           ( 1.6027E-02      NaF
           + 0.98397         KF)

+ 0.13376   mol   NaF-[LiF](ss)
   (5.5216 gram, 0.13376 mol)
           (728.71 K, 1 bar,     a=1.0000)
           ( 4.4221E-02      LiF
           + 0.95578         NaF)

+ 8.68E-03  mol   CAMX3-Perovskite#1
   (1.1595 gram, 8.6800E-03 mol)
           (728.71 K, 1 bar,     a=1.0000)
           ( 8.0648E-02      LiCaF3
           + 4.1687E-10      NaCaF3
           + 0.91935         KCaF3)

0           mol   ASalt-liquid#1
           (728.71 K, 1 bar,     a=1.0000)
           ( 0.45484         LiF
           + 0.13427         NaF
           + 0.40221         KF
           + 8.6816E-03      CaF2)

+ 0.44822   mol   LiF_Griceite_(NaCl_rock_salt_structure)
   (11.627 gram, 0.44822 mol)
           (728.71 K, 1 bar, S1, a=1.0000)
```

In this example, the closest local minimum found by FactOptimal is a Eutectic since 4 phases are in equilibrium with the liquid.

FactOptimal found the closest local minimum on the liquidus surface of the quaternary system without trying to find a closer one in subsystems.

# *Advanced Examples*

*Simultaneous optimization of two masses of precipitate under constraints on composition, phases amount and density, with temperature as an optimized variable.*

# Improve the mechanical and corrosion properties of AZ91 by addition of Calcium and Rare Earth elements after a full anneal at 200°C<T<400°C

# Example 10: Improve the mechanical properties of AZ91 by addition of Ca and RE - 1

We consider an AZ91 base alloy (Mg-Al-Zn). We want to improve the mechanical properties by addition of Rare Earth elements (Ce,La) and calcium by simultaneously:

•**maximizing the amount of C15-$Al_2Ca$+$\alpha Al_{11}Re_3$**
– **$Al_2Ca$** can improve the tensile and elongation properties of AZ91 due to grain refinement. The formation of thermally stable $Al_{11}RE_3$ fine needle-shaped particles along the grain boundaries significantly improves the creep properties

**and**

•**maximizing the amount of $\gamma Al_{12}Mg_{17}$** in order to conserve AZ91 microstructure properties

Other constraints employed in this example:

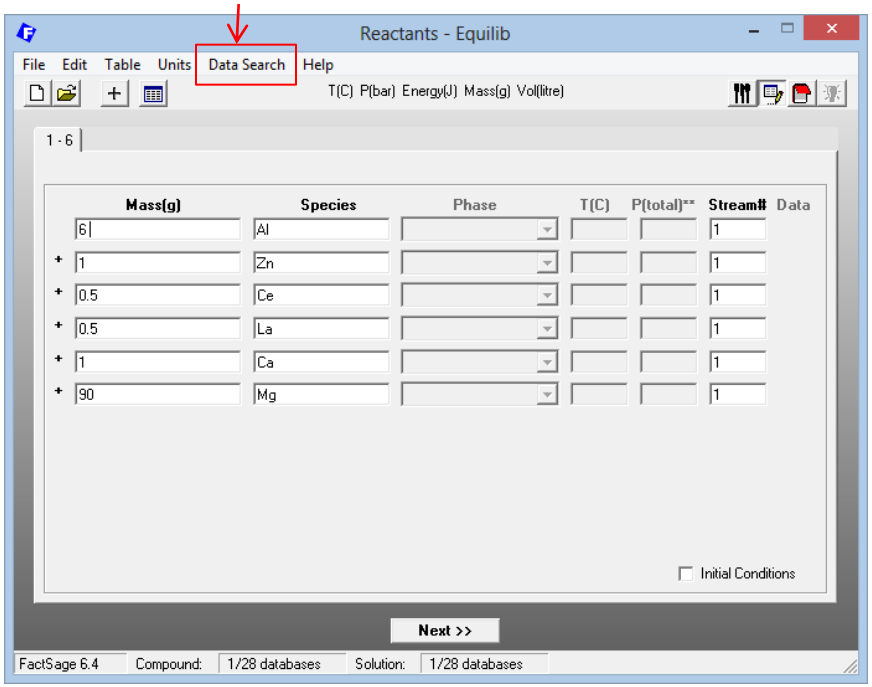
•Wt. %(Ce)+Wt. % (La) < 1 (to keep the price reasonable)
•density > 1.75 g/cm$^3$
•Wt. %(HCP phase)>90
•the HCP phase must be a single phase (i.e. no miscibility gap)

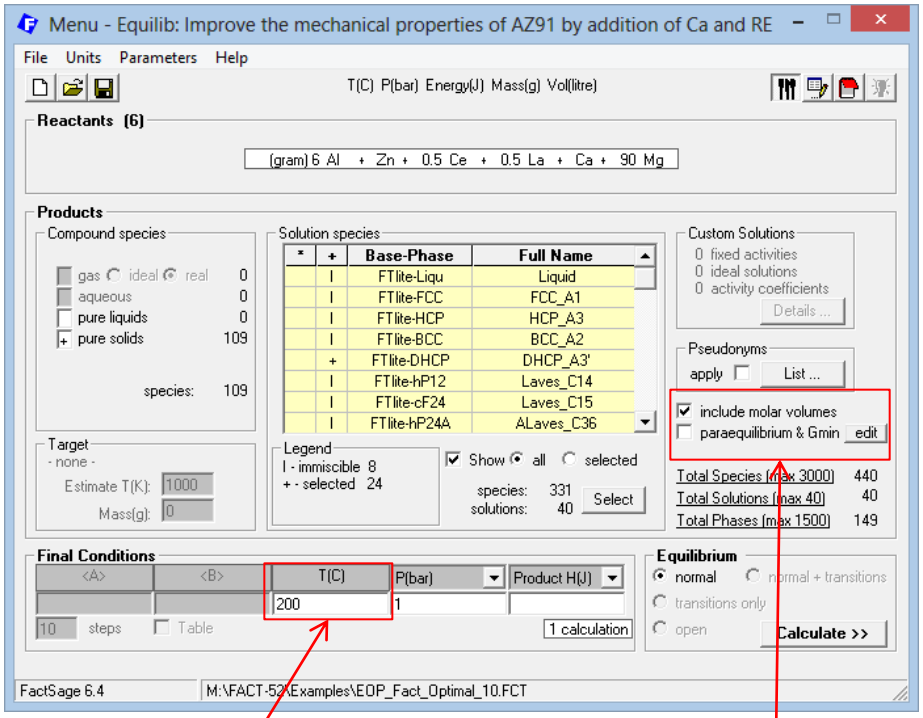
# Example 10: Improve the mechanical properties of AZ91 by addition of Ca and RE - 2

## System: AZ91+RE+Ca

<u>Step 1</u>**:** Using **Equilib** we define the system and select the appropriate database: **FTlite** and perform a single Equilb calculation.

Select only FTlite database



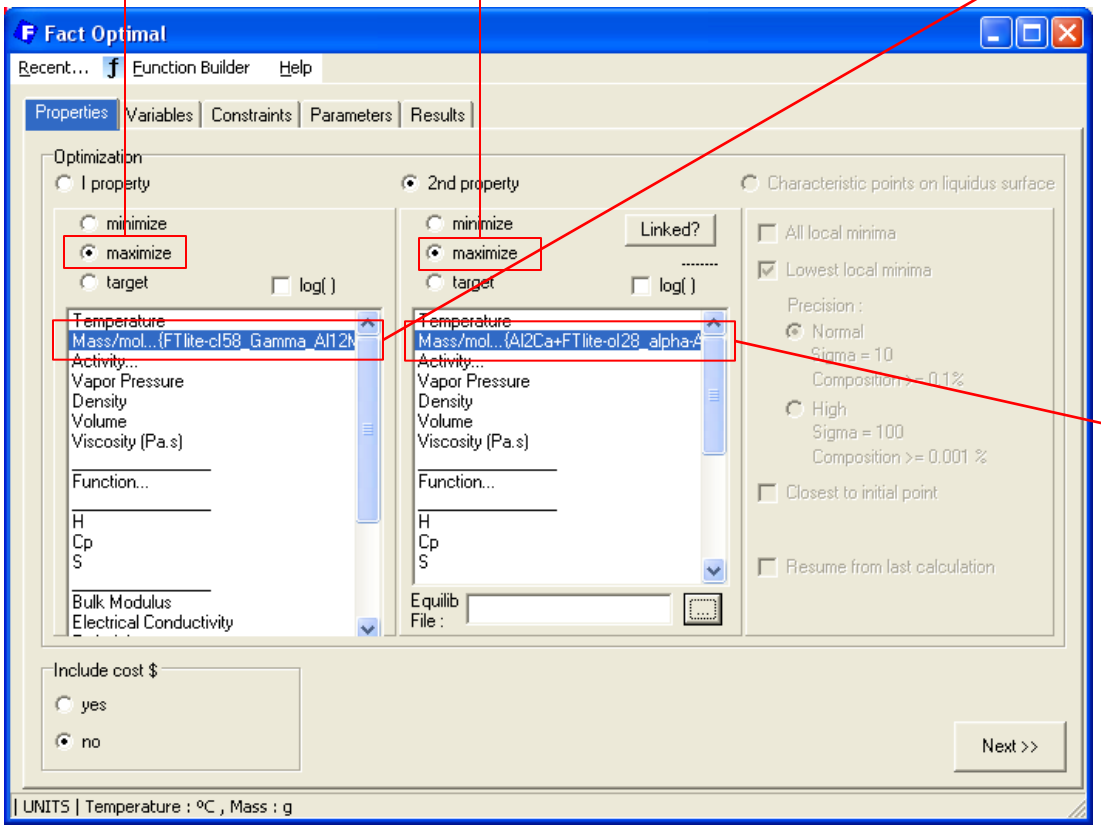

The temperature will be chosen as a variable, therefore it is irrelevant in the first Equilib calculation.

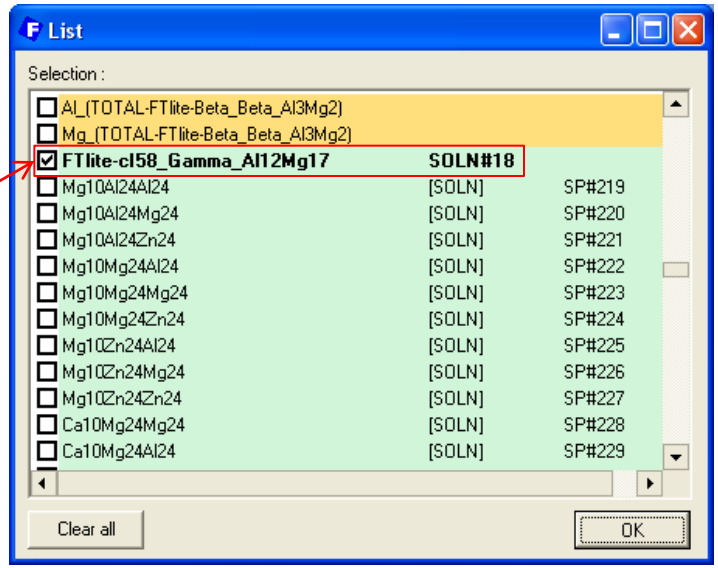
Include molar volumes in order to calculate the density

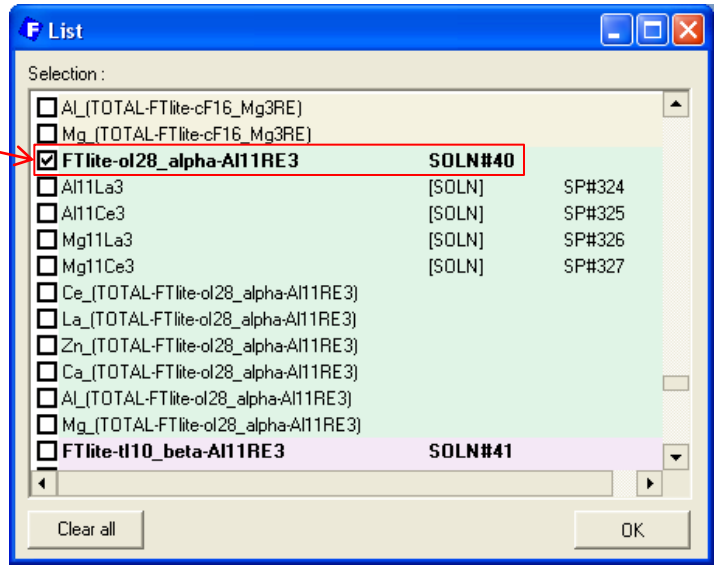
# Example 10: Improve the mechanical properties of AZ91 by addition of Ca and RE - 3

Step 2: after a single **Equilibrium** calculation, open FactOptimal and set up the objectives.

The two objectives are the maximum of the mass of two different phases



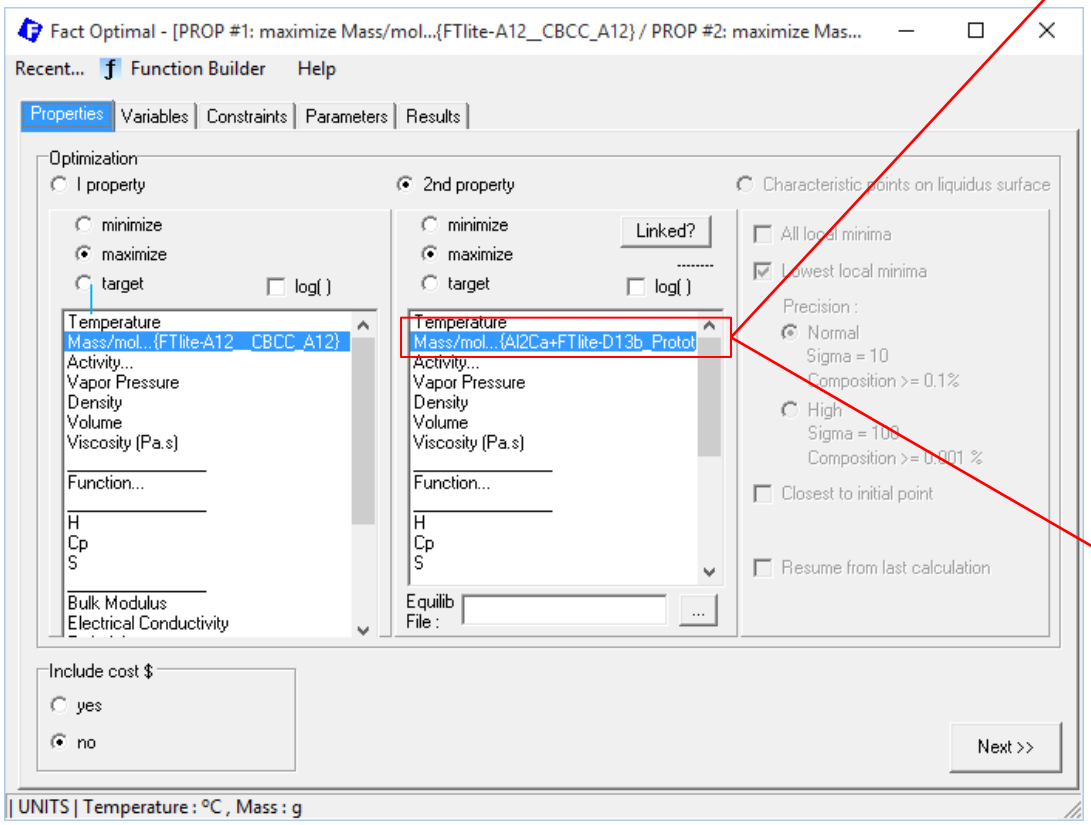



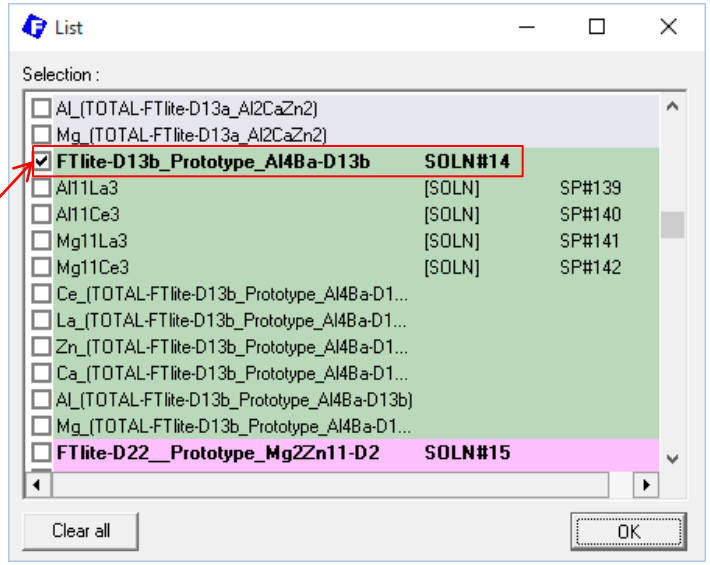



# Example 10: Improve the mechanical properties of AZ91 by addition of Ca and RE - 4

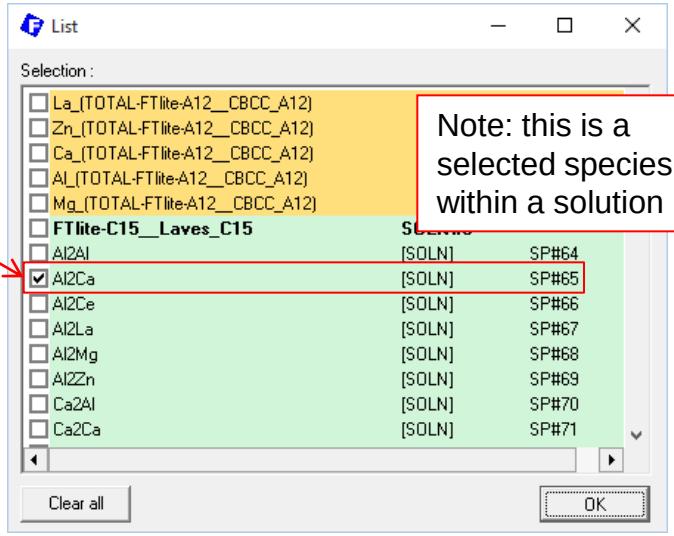
Step 2: after a single **Equilibrium** calculation, open FactOptimal and set up the objectives.

The second objective is a sum of the mass of two precipitates



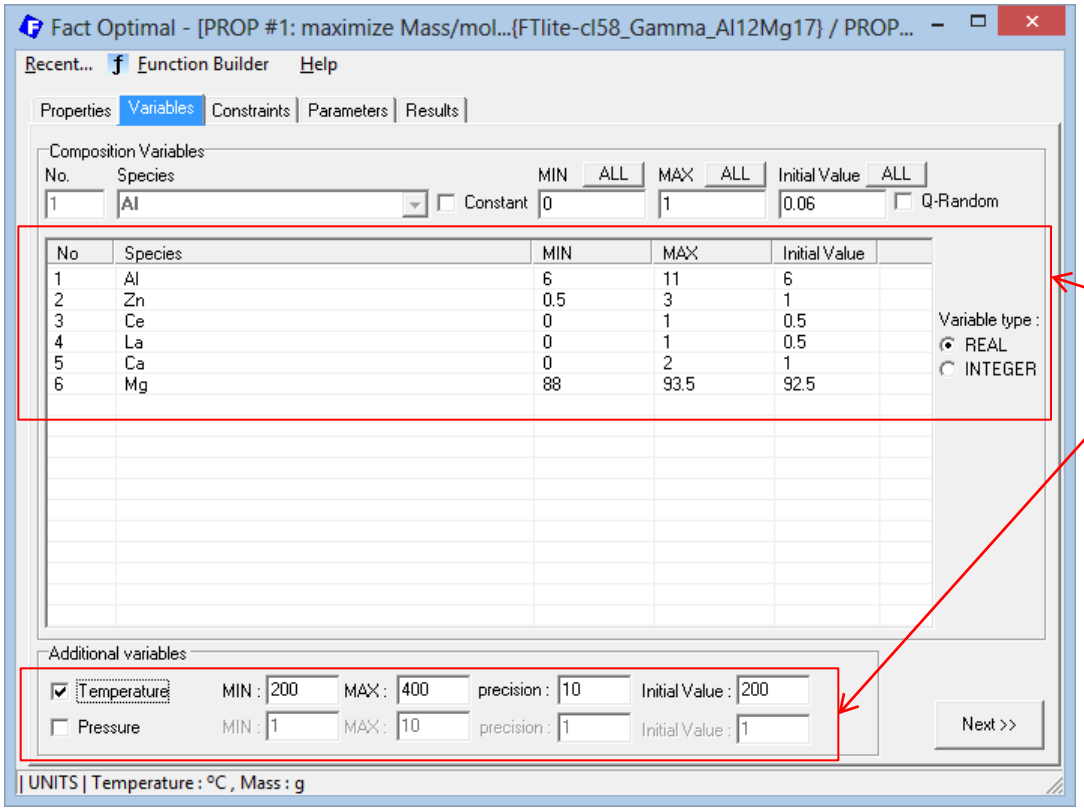

+




Note: this is a selected species within a solution

# Example 10: Improve the mechanical properties of AZ91 by addition of Ca and RE - 5

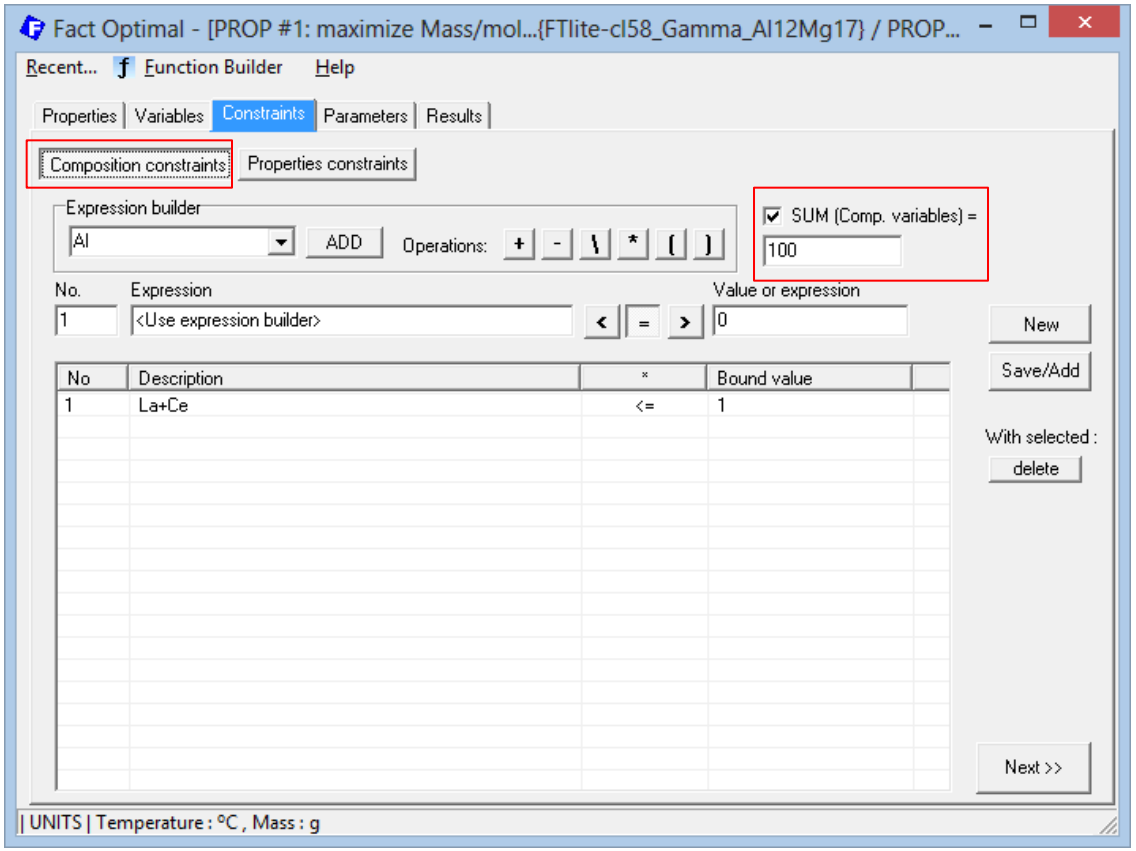
Step 3: Set up the range of compositions and temperature.




In the variables section, define range of compositions and temperature.

**The range of composition corresponds to approximately the composition of AZ91 alloys.**

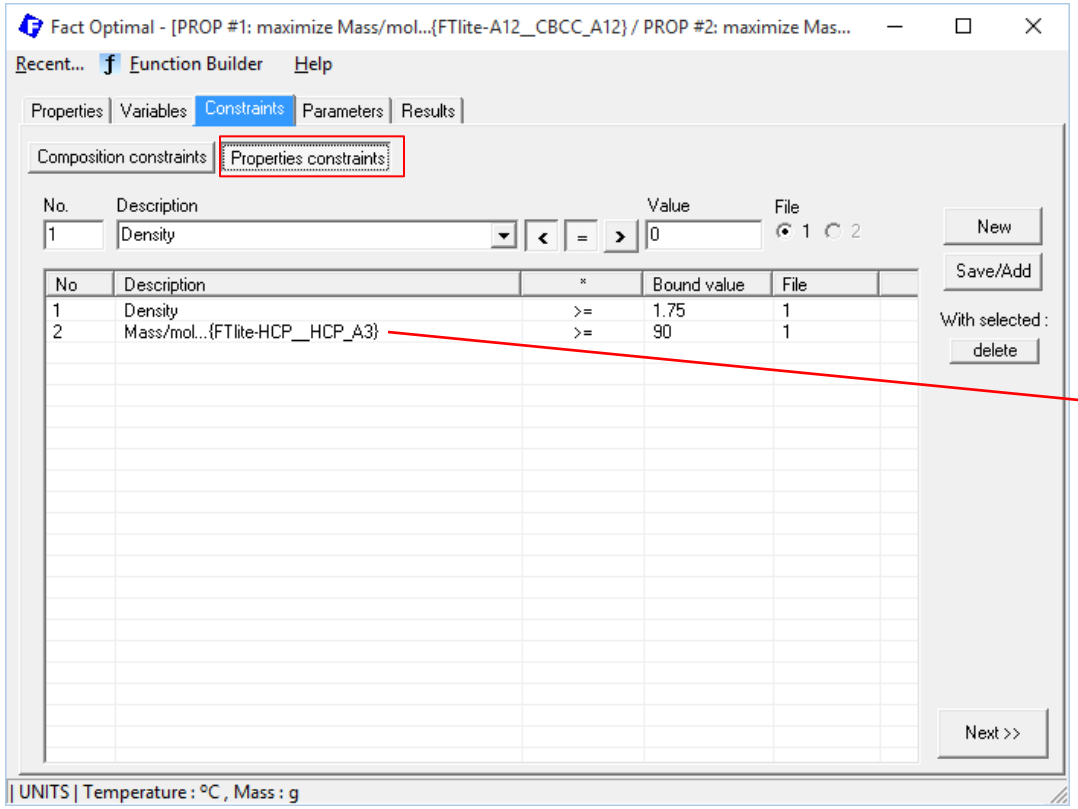
Step 4: Set up the composition constraints.

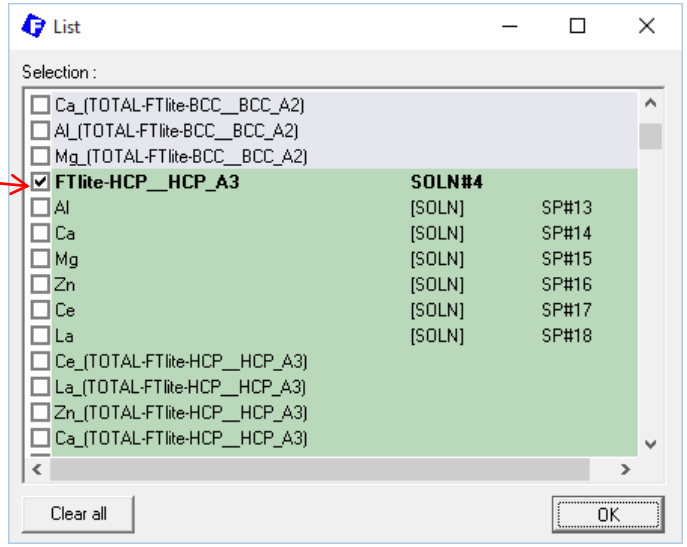



In the constraints section we click on Composition constraints and select a sum of 100 for all composition variables, and we specify that wt.% La + wt.% Ce ≤1

# Example 10: Improve the mechanical properties of AZ91 by addition of Ca and RE - 7

Step 5: Set up the properties constraints.

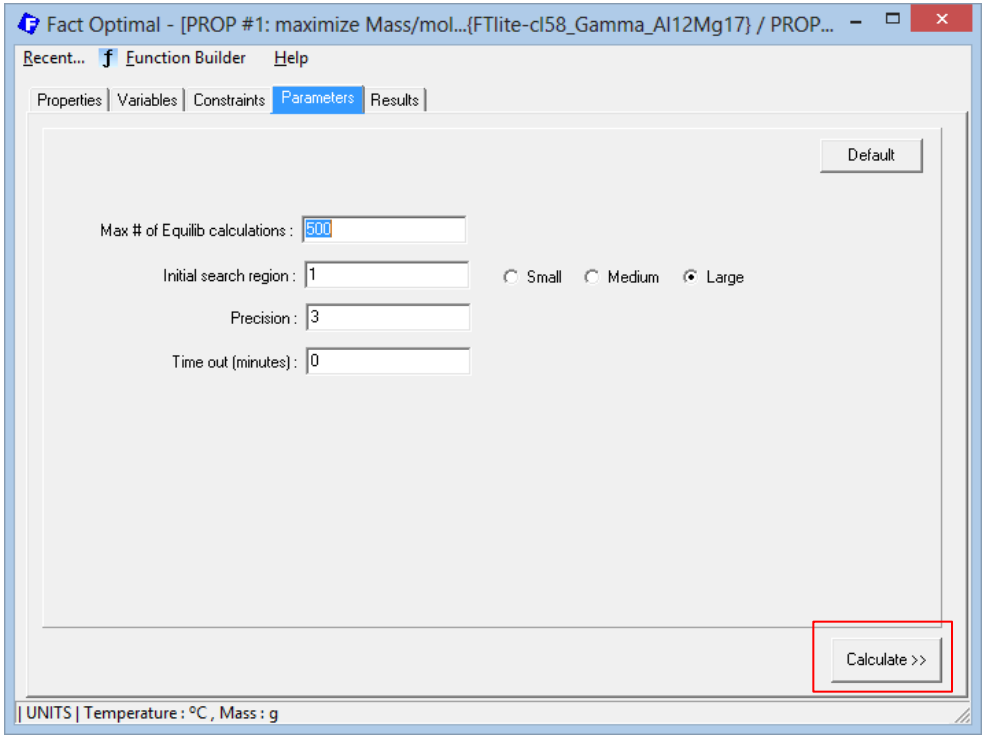


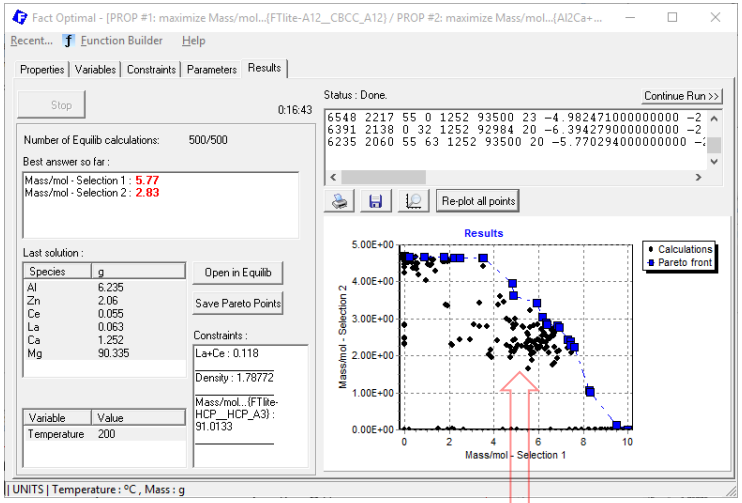

We select only HCP A3#1 so that HCP is a single phase (no miscibility gap possible)

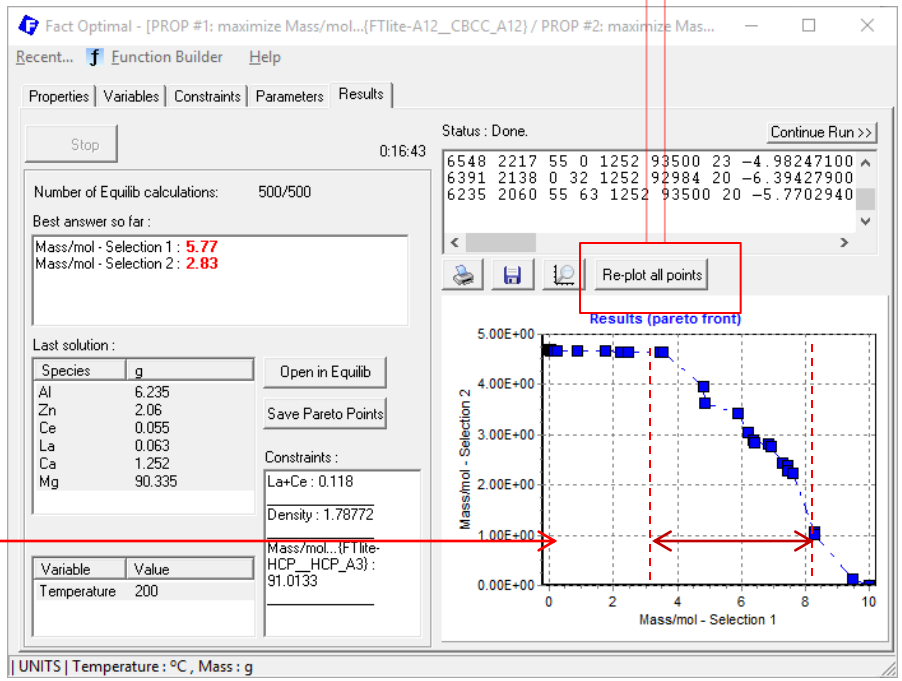
# Example 10: Improve the mechanical properties of AZ91 by addition of Ca and RE - 8

Step 6: Set up the parameters and calculate.



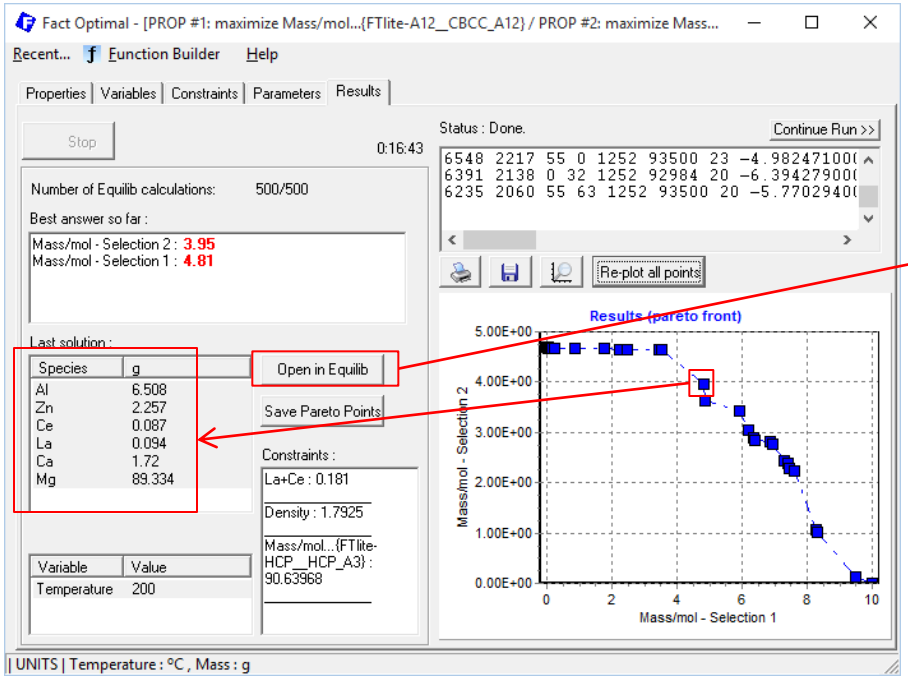

The region between the two dashed line, is the region with an acceptable amount of $\gamma Al_{12}Mg_{17}$ to conserve the typical microstructure of AZ91. Beyond this range the microstructure can be very different. The user has to choose a compositions within this range.



# Example 10: Improve the mechanical properties of AZ91 by addition of Ca and RE - 9

Step 7: Open a chosen point in Equilib and get the detailed results.




Summary of the Equilib file of the selected point on the Optimal Pareto

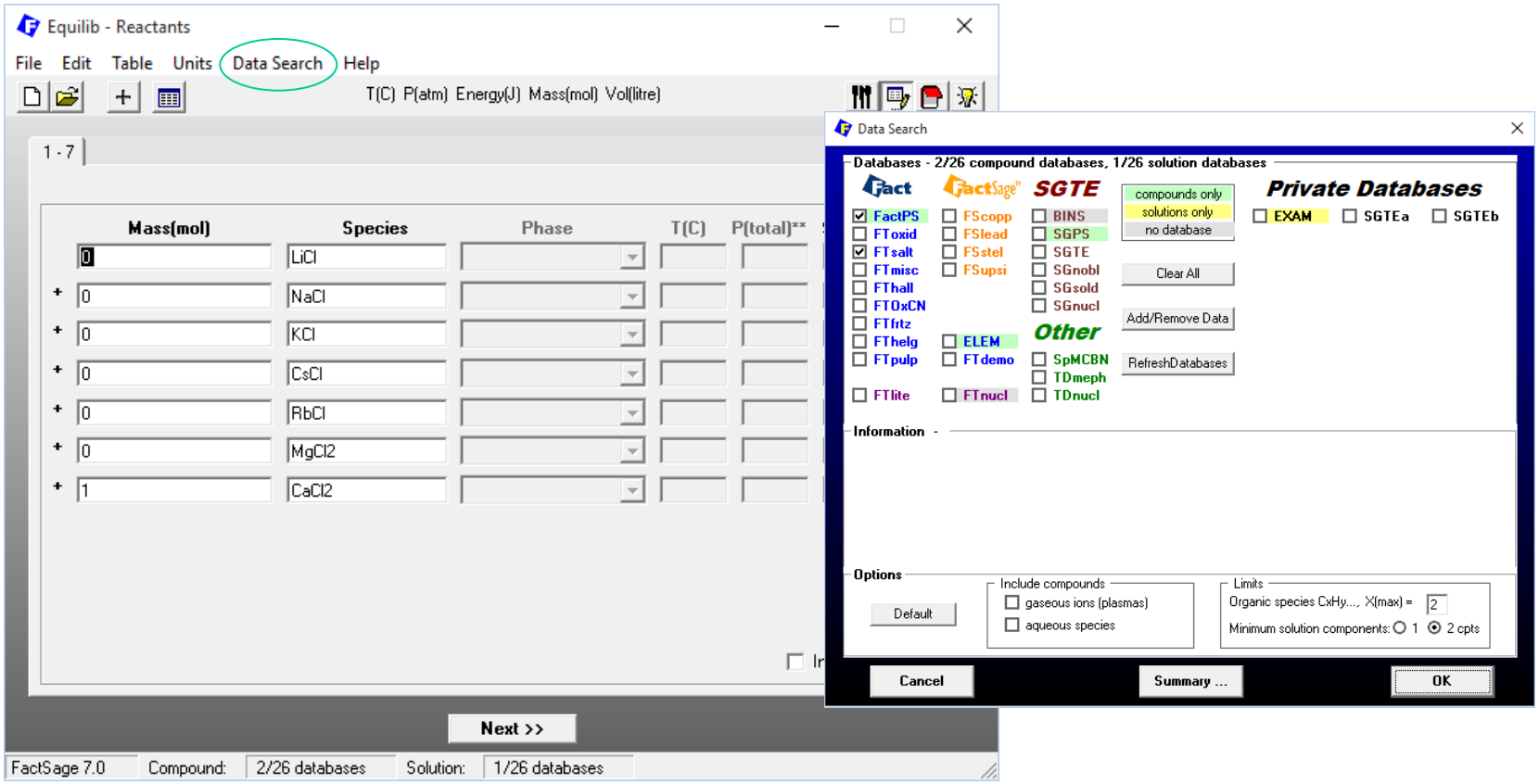
```
6.508 Al +  2.257 Zn +  0.087 Ce +  0.094 La + 1.72 Ca +  89.334 Mg =

   90.640     gram  HCP_A3
   (90.640 gram, 3.6767 mol, 5.1572E-02 litre, 1.7575 gram.cm-3)

+ 4.8067     gram  CBCC_A12
   (4.8067 gram, 3.1000E-03 mol, 2.2133E-03 litre, 2.1717 gram.cm-3)

+ 4.1029     gram  Laves_C15
   (4.1029 gram, 4.3895E-02 mol, 1.9969E-03 litre, 2.0547 gram.cm-3)

+ 0.43492    gram  Al2CaZn2
   (0.43492 gram, 1.3704E-03 mol)

+ 1.5809E-02 gram  Phi
   (1.5809E-02 gram, 4.2729E-05 mol, 5.8055E-06 litre, 2.7231 gram.cm-3)

*********************************************************************
       H            G        V(see note)        S            Cp
      (J)          (J)         (litre)        (J/K)        (J/K)
 *********************************************************************
  1.40373E+04  -7.22961E+04   5.57882E-02   1.82465E+02   1.21533E+02

 Total mass/gram = 100.00
 System density/gram.cm-3 = 1.7925 (see note)
```

# *Minimizing the total vapor pressure of a salt mixture - using the log option*

## System: LiCl-NaCl-KCl-CsCl-RbCl-MgCl2-CaCl2

Step 1:

- Using **Equilib** we define the system and select the suitable database **FTsalt**.
- The composition is arbitrary.

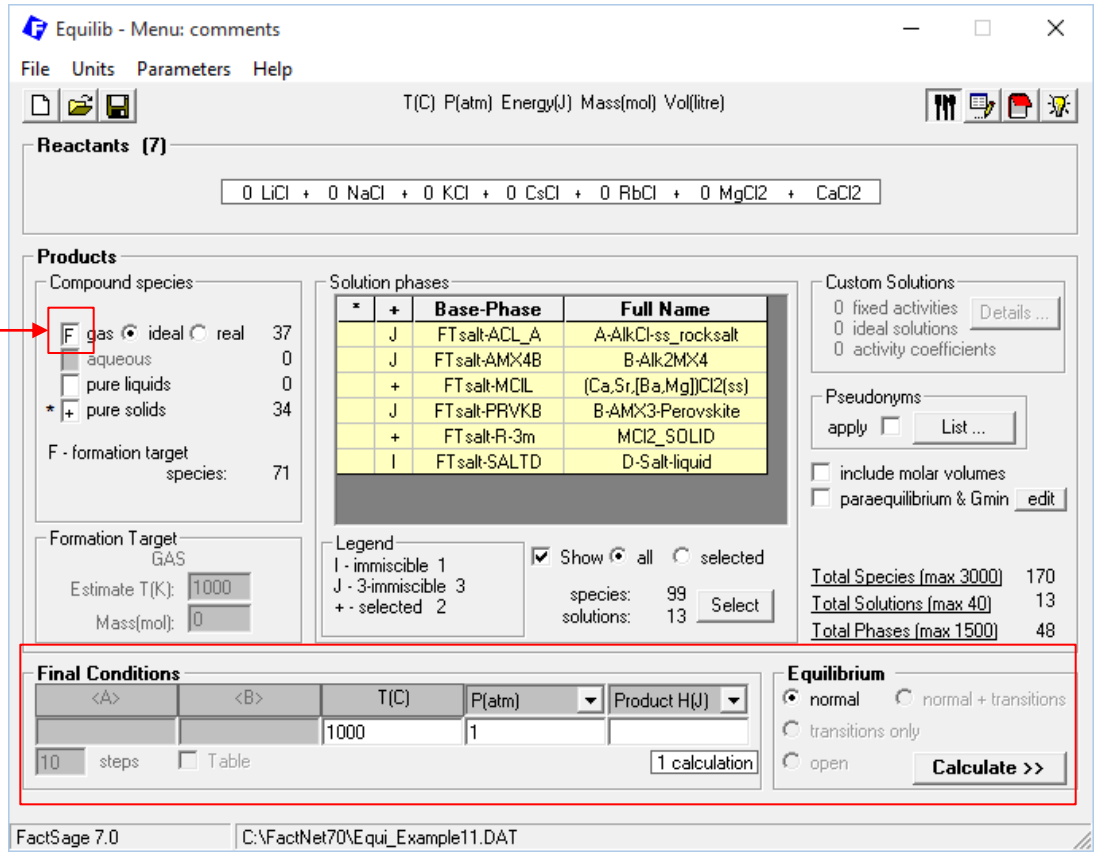


## System: LiCl-NaCl-KCl-CsCl-RbCl-MgCl2-CaCl2

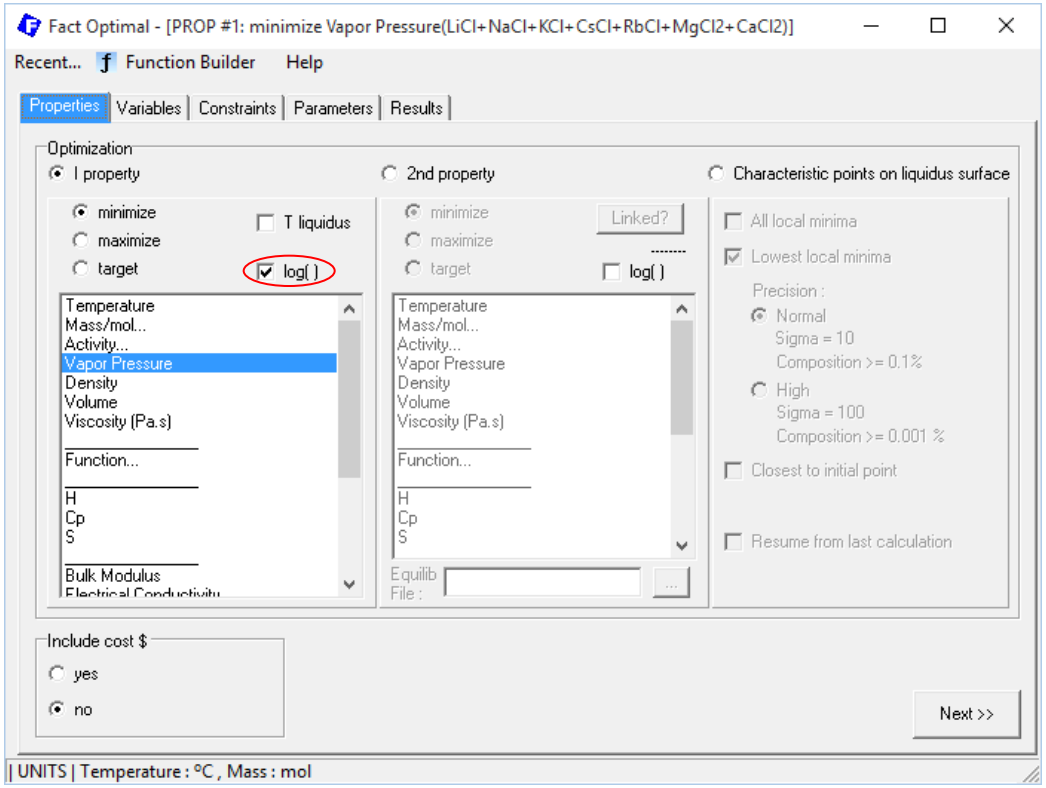
Step 2:

Define the species selection, final temperature and pressure and then calculate.

Make the gas phase formation target

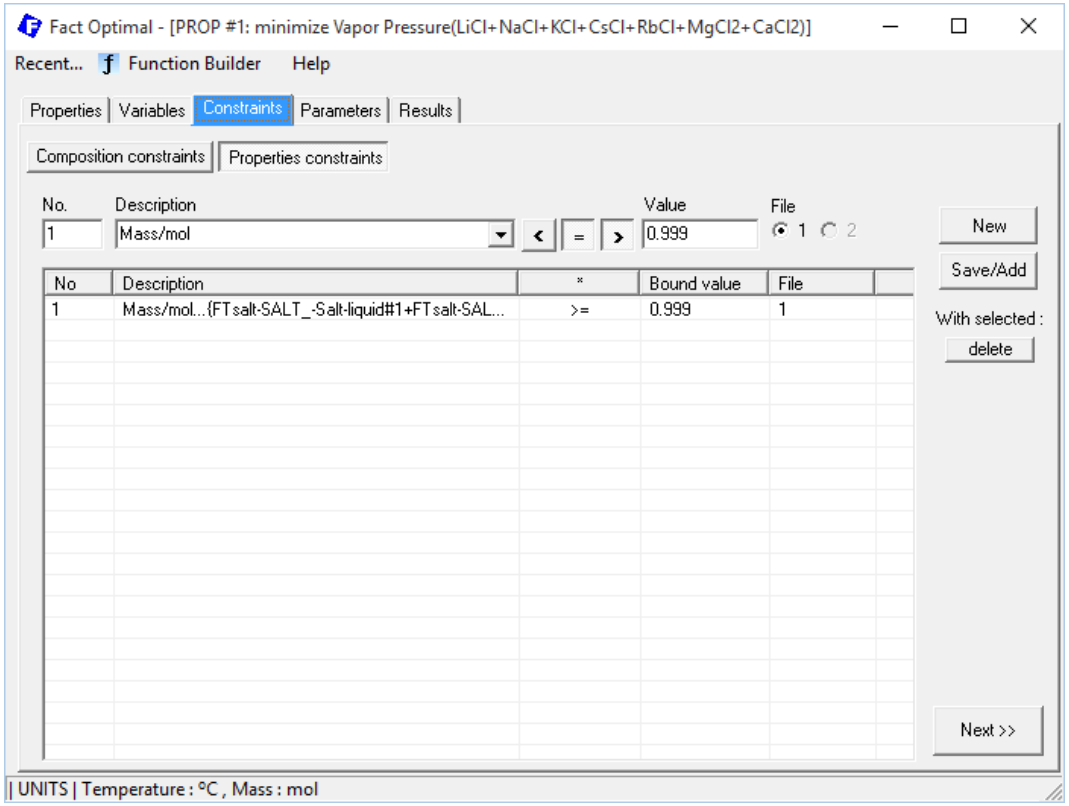


**Step 3:** Open FactOptimal and setup the problem.




1. we consider **one property, the vapor pressure**
2. we want to **minimize the <u>logarithm</u> of this property**

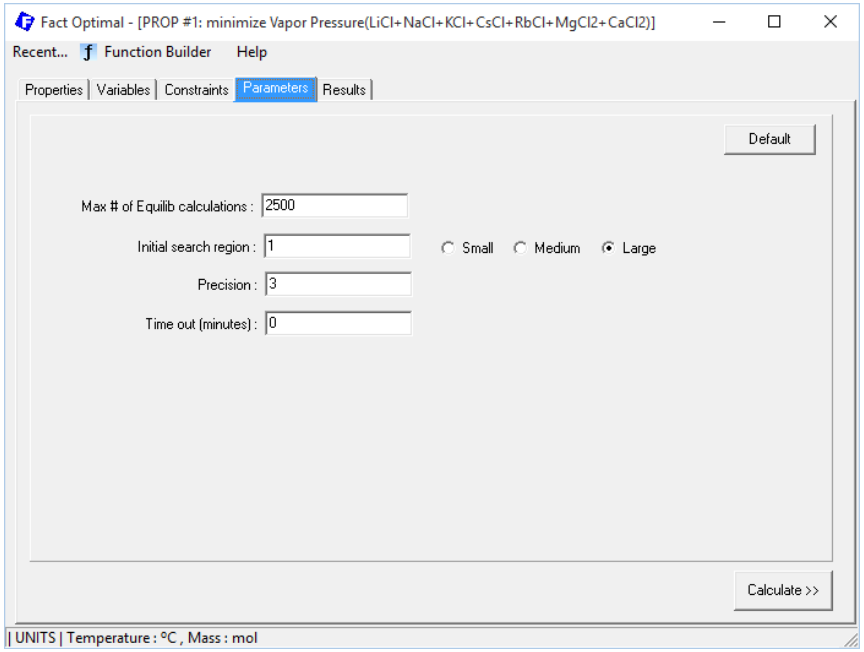
## Step 4: Add constraints



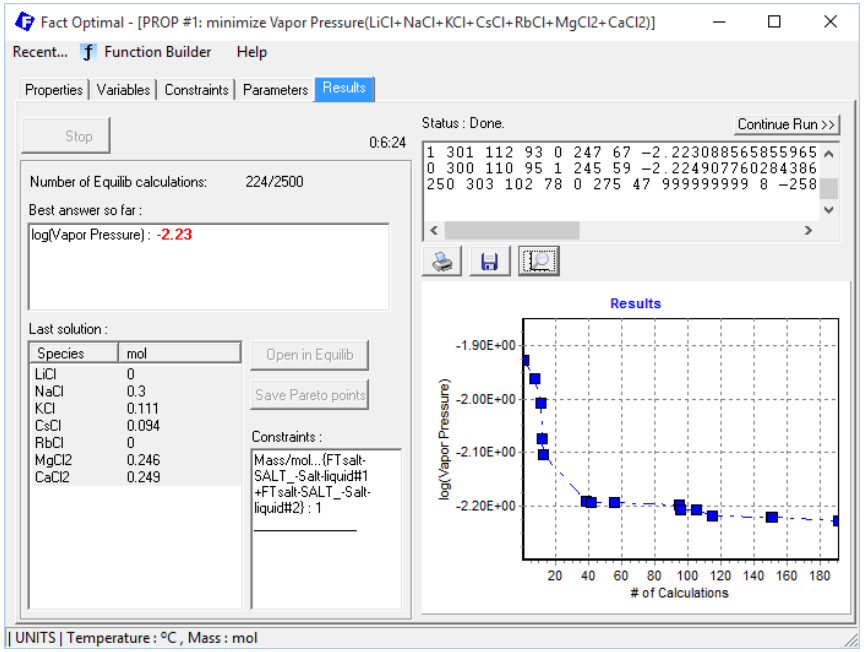

We add one constraint on the mass of the liquid phase

**Step 5**: Set up the parameters and press calculate

Parameters setup




Results, FactOptimal converged (stopped) after 224 calculations



***Maximizing the elemental solubility in a given phase under constraints of composition and amounts of phases.***

***Improvement of the texture and grain refinement***
**by maximizing the (molar) solubility of Rare Earths in a Mg matrix at T= 300 $^{o}$C**

# Example 12: Improve the texture and grain refinement properties at low temperature - 1

We consider a magnesium system with RE (Ce,La, Nd, Pr, Sm) additives.

The goal is to MAXIMIZE the solubility for a single HCP phase in order to improve the texture and the grain refinement properties.

OTHER CONSTRAINTS considered in this example :

•wt.%(Ce)+ wt.%(La) + wt.%(Nd) + wt.%(Pr) + wt.%(Sm) < 0.2
(in order to keep the cost of raw material reasonable)

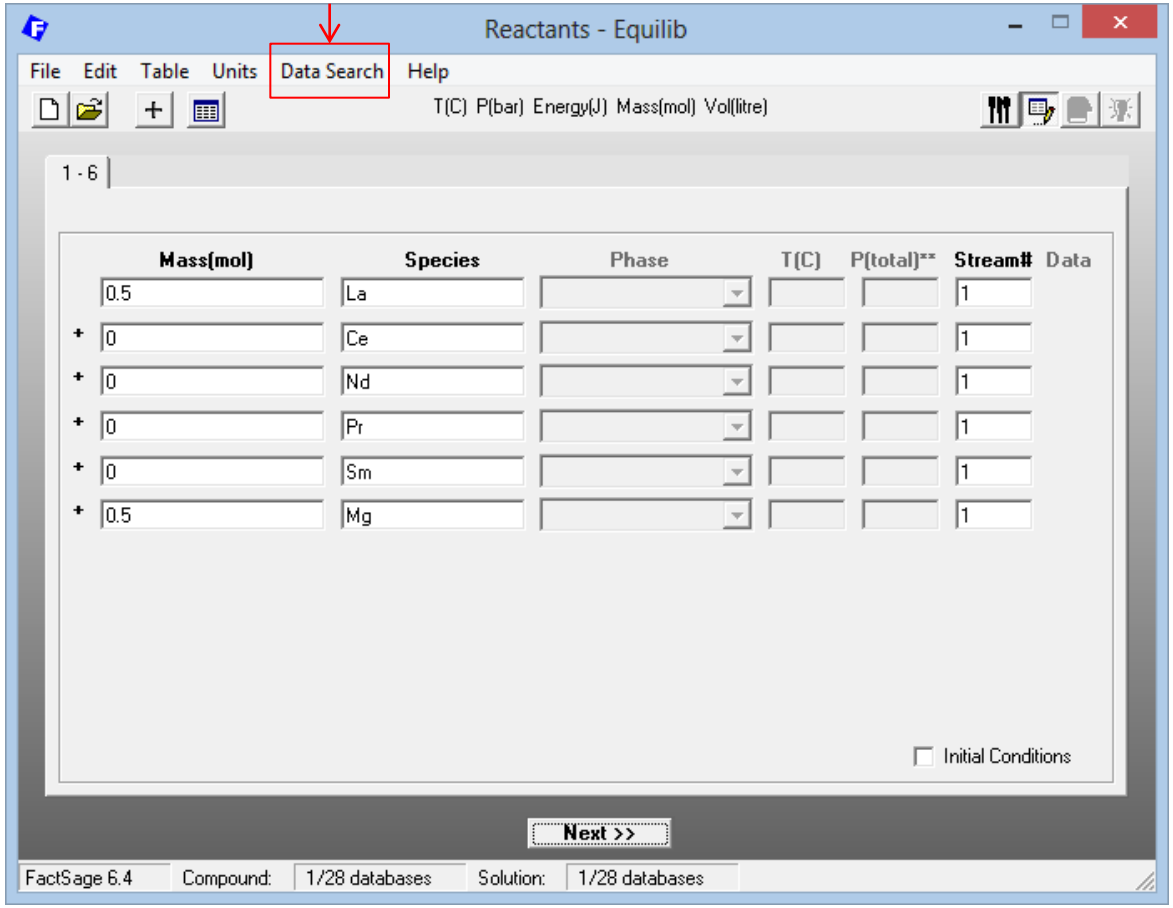
•%(HCP phase) = 100 (that is, no other phases)

•We want a single HCP phase (i.e. no miscibility gap)

# Example 12: Improve the texture and grain refinement properties at low temperature - 2

Step 1: Set up the system in Equilib.

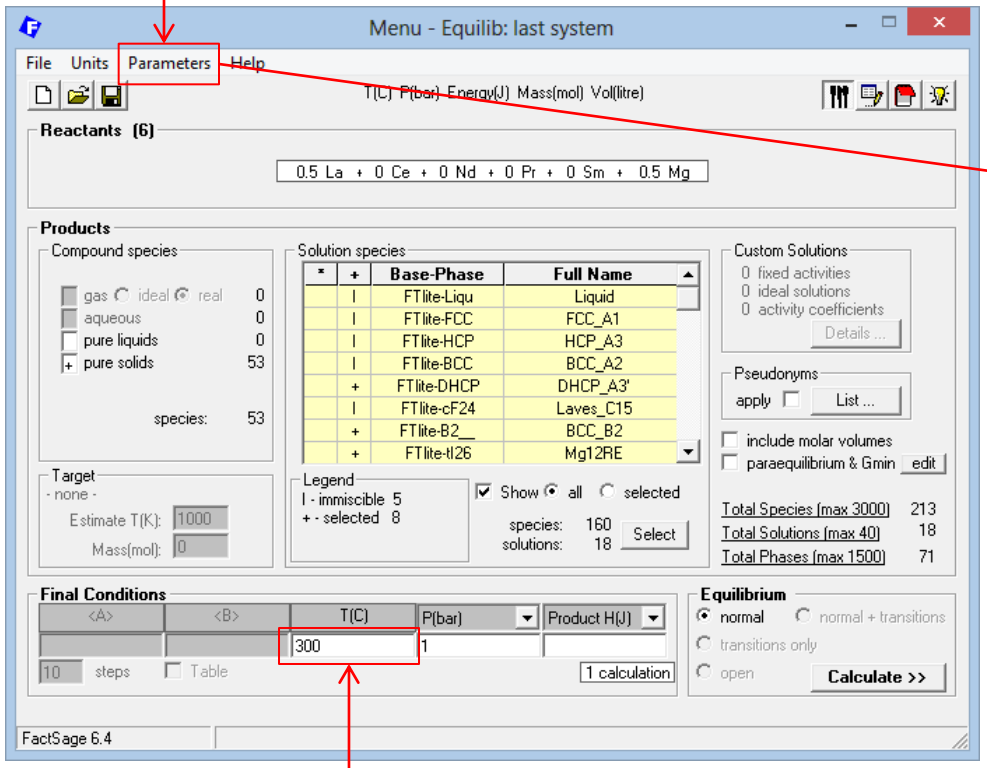
Select the FTlite database only

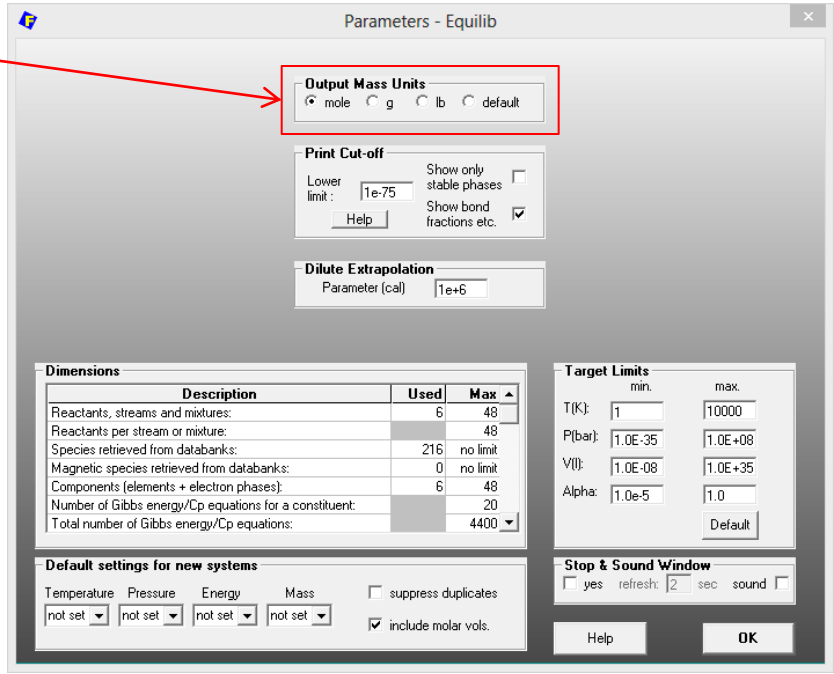


# Example 12: Improve the texture and grain refinement properties at low temperature - 3

Step 1: Set up the system in Equilib.

In the menu window, click on parameters and select output in mol, since the objective is to maximize the <u>molar solubility</u>

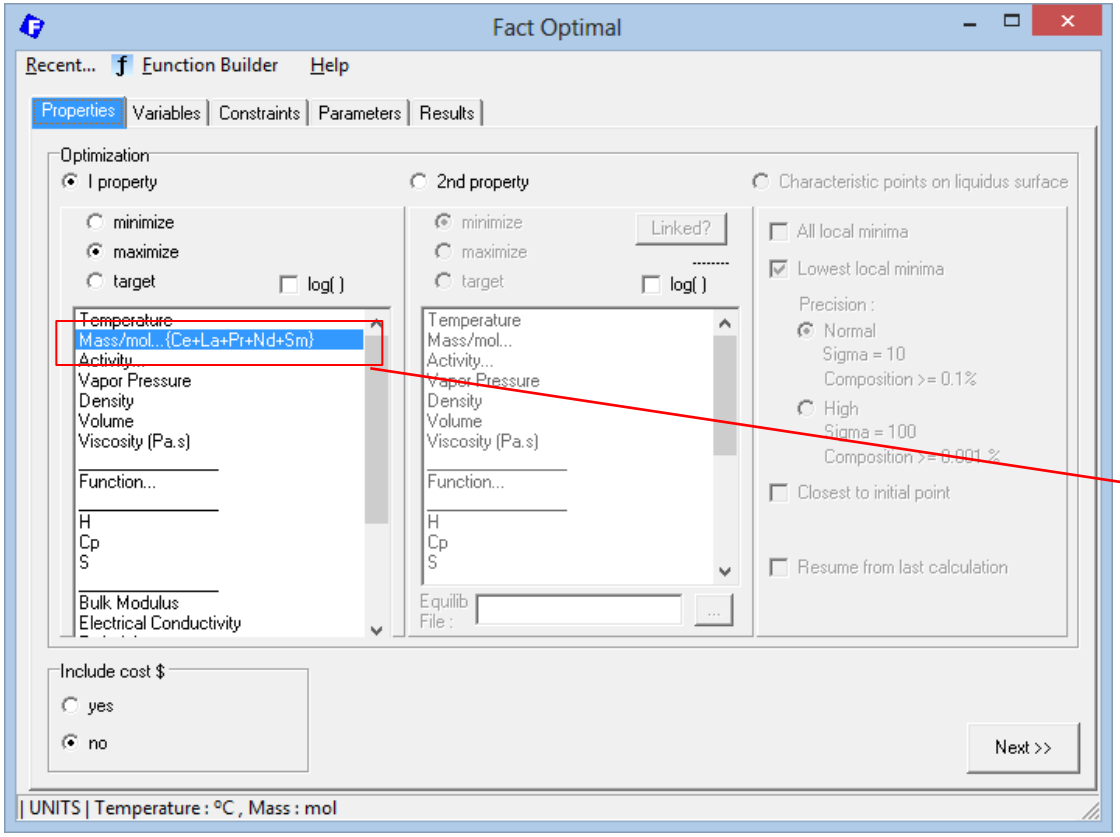


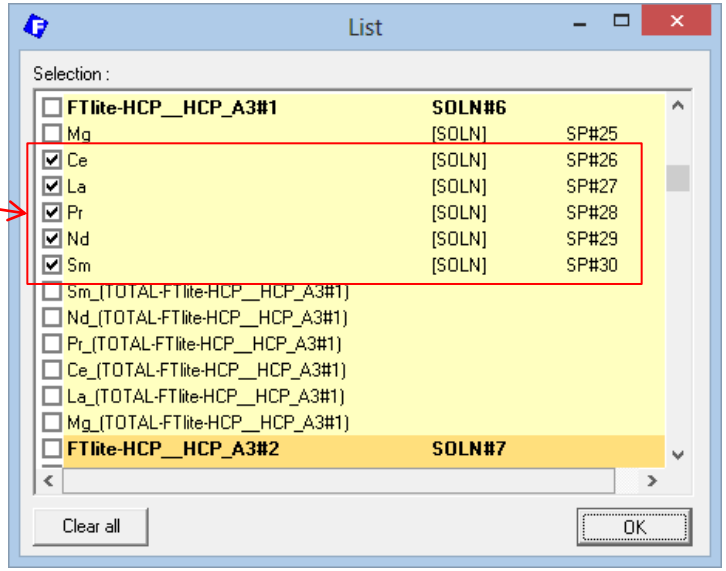

Set the temperature to 300ºC

# Example 12: Improve the texture and grain refinement properties at low temperature - 4

Step 2: after performing a single calculation, open FactOptimal and set up the problem.

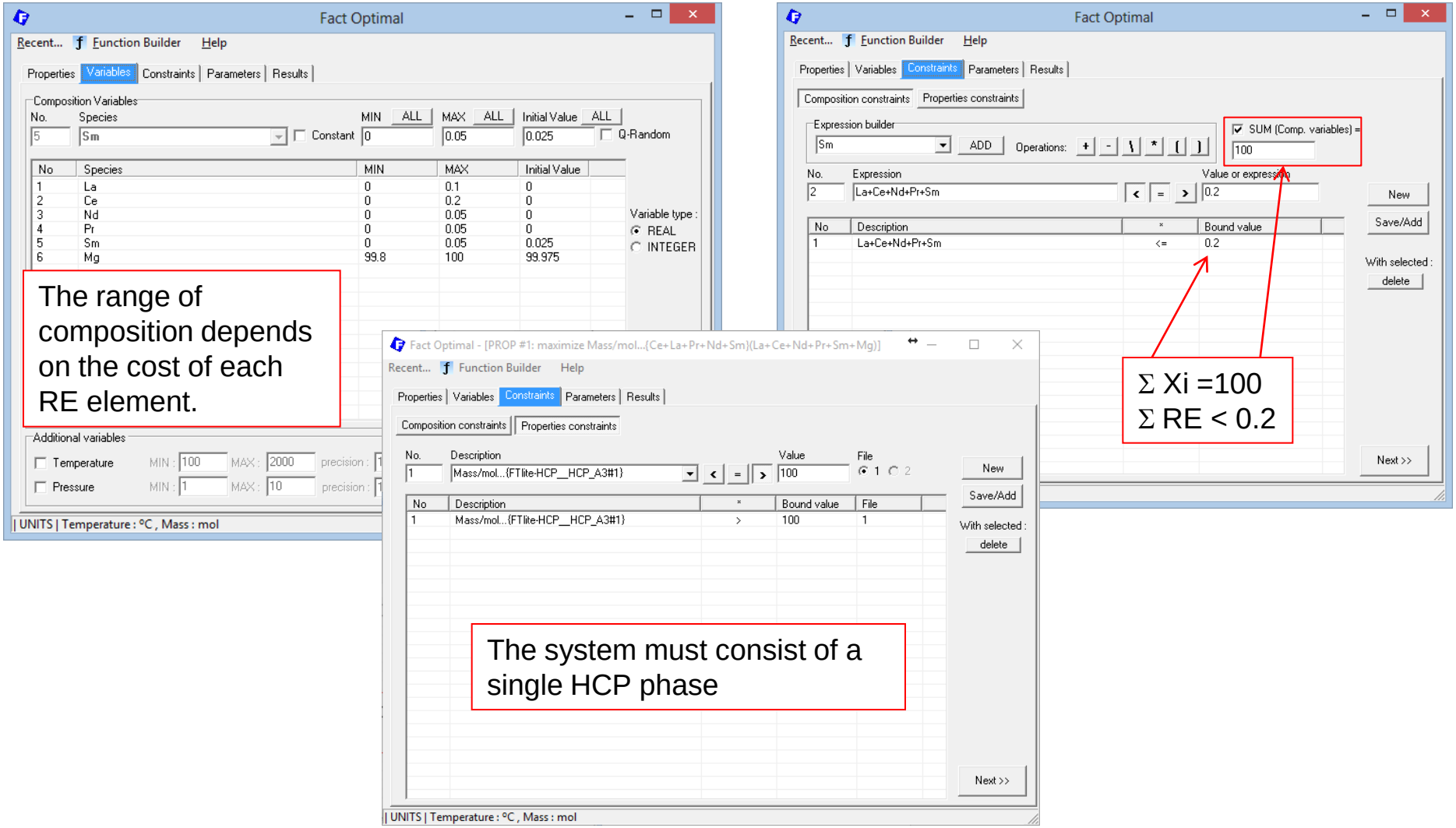



To maximize the molar solubility of RE elements in HCP matrix, select all the RE elements in HCP_A3#1 solution without selecting those in HCP_A3#2 since we want a single HCP phase



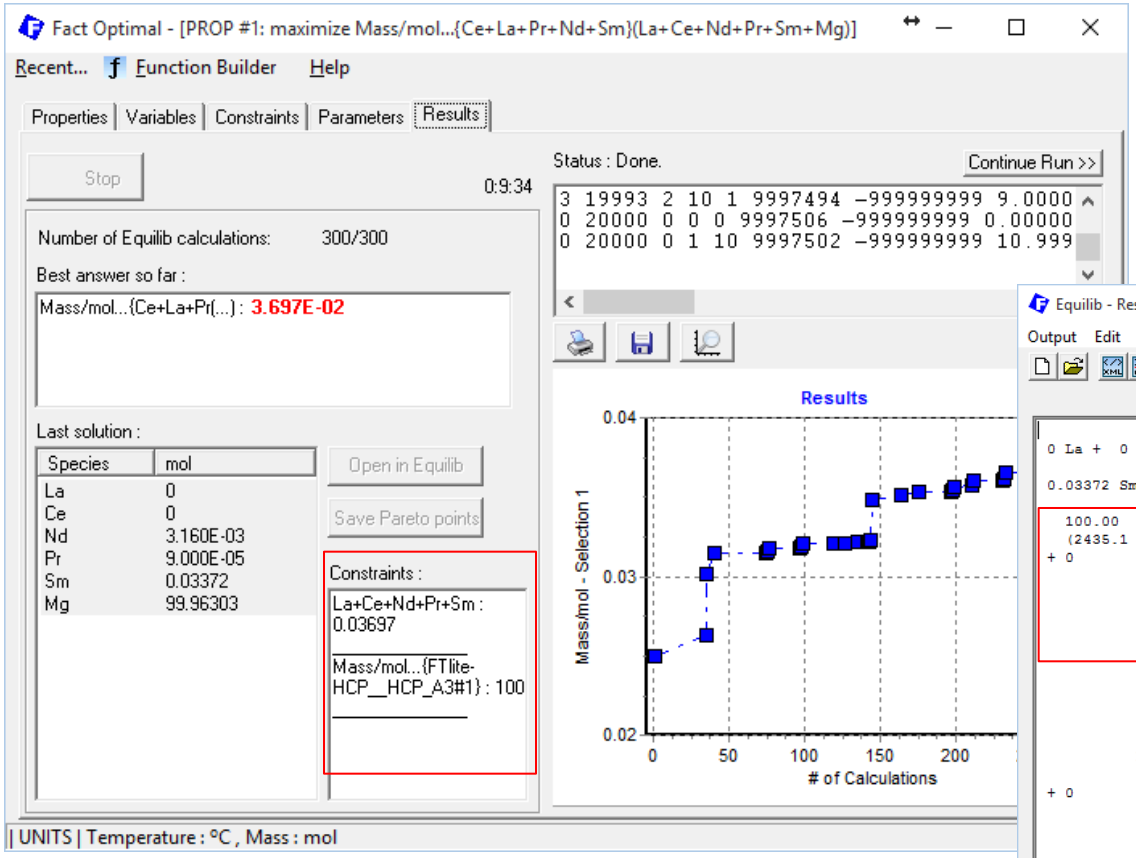
# Example 12: Improve the texture and grain refinement properties at low temperature - 5

Step 3: Set up the ranges of composition and constraints.

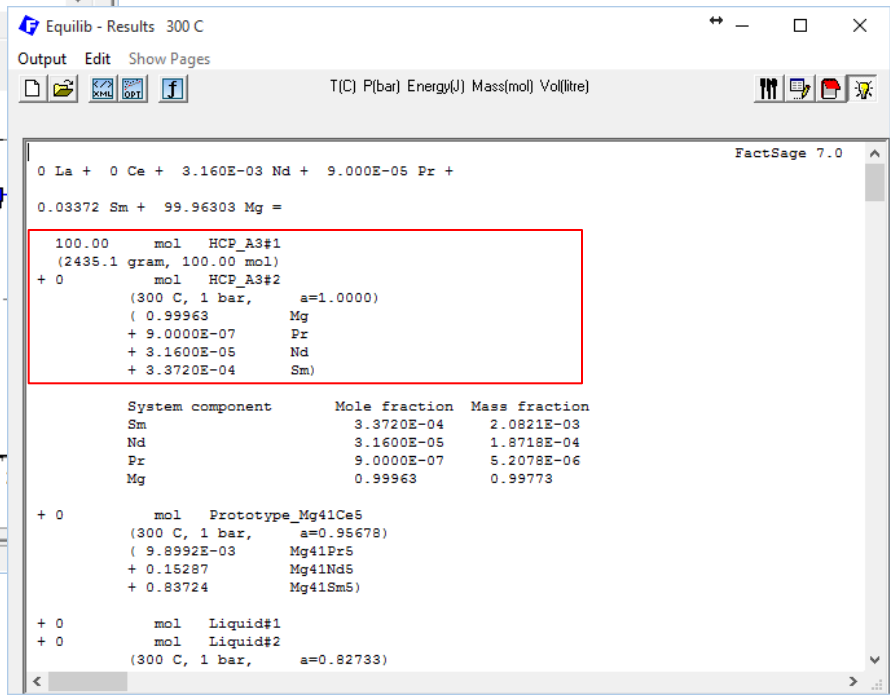


# Example 12: Improve the texture and grain refinement properties at low temperature - 6

Step 4: Set up the parameters (300 calculations with a large initial search region and a precision of 5) and calculate.




The Equilib file corresponding to the optimal value of the solubility is automatically given at the end of the calculation:



## *Optimize two linked properties*

*The properties are « linked » because the second calculation requires the calculation of the liquidus temperature.*

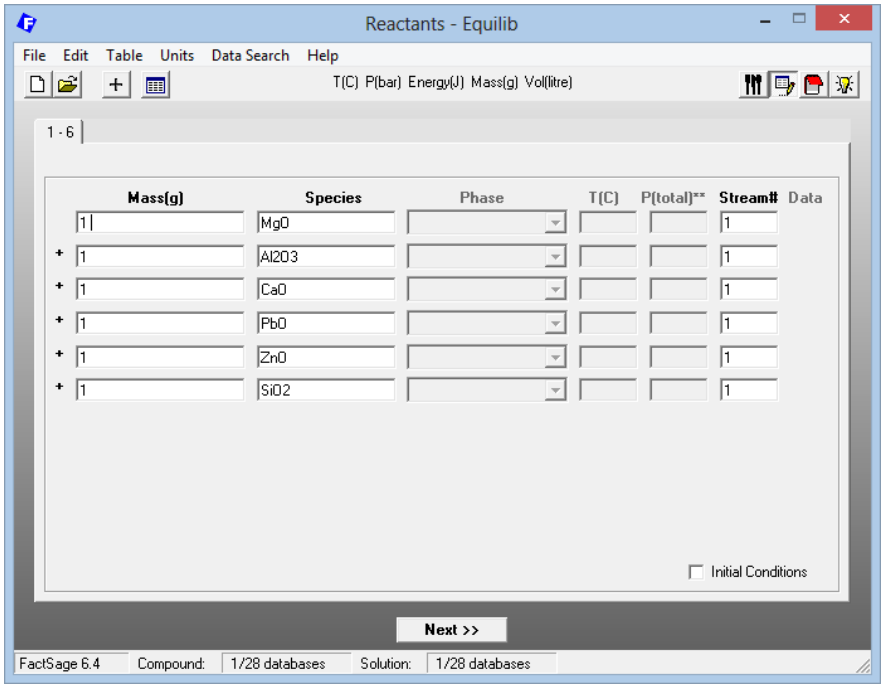
**Minimize the liquidus temperature and minimize the solid fraction 200 $^{o}$C below the liquidus**

# Example 13: Minimize the liquidus temperature and minimize the solid fraction 200 °C below the liquidus - 1

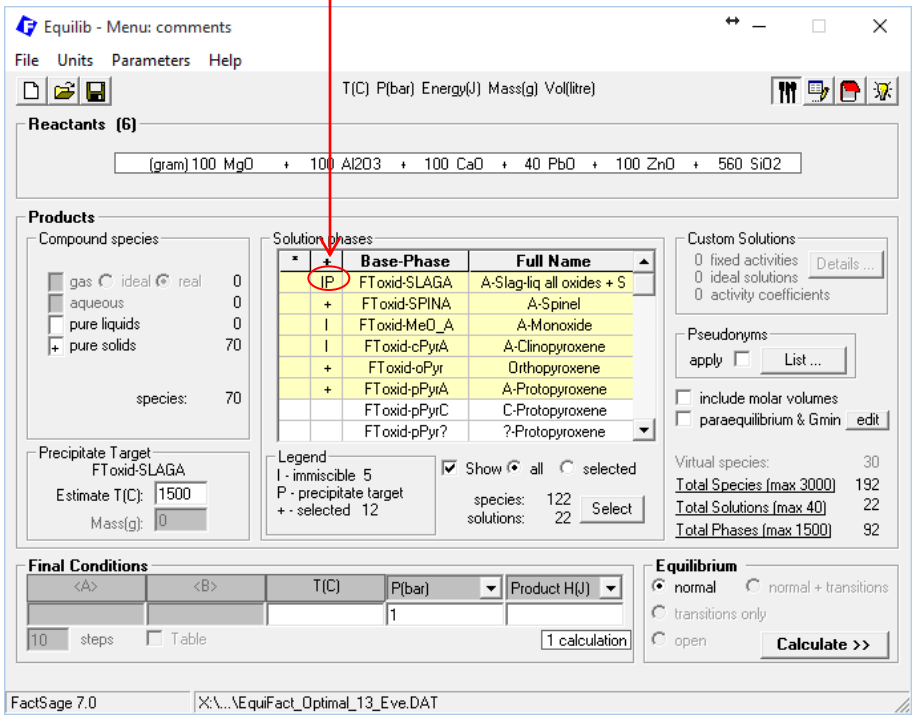
For the oxide system defined below, we want to minimize the liquidus temperature and minimize the solid fraction 200 °C below the liquidus

Step 1: Set up the system, select the database and perform a single Equilib calculation

Select only the FToxid database

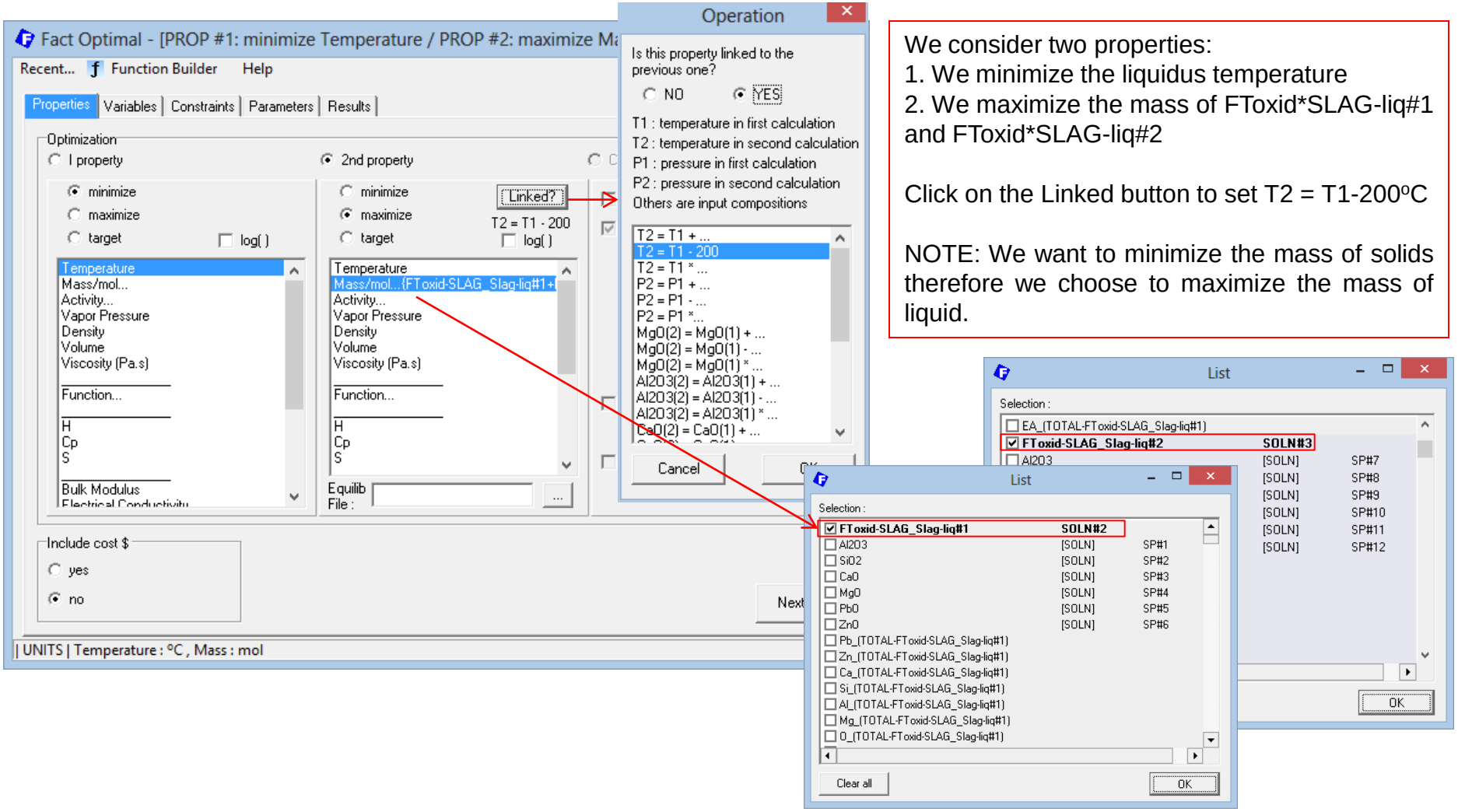



Select P option on the liquid in order to calculate the liquidus temperature



# Example 13: Minimize the liquidus temperature and minimize the solid fraction 200 °C below the liquidus - 2

Step 2: Perform a calculation and open FactOptimal. Then select two linked properties since the second temperature = ($T_{Liquidus}$-200°C).



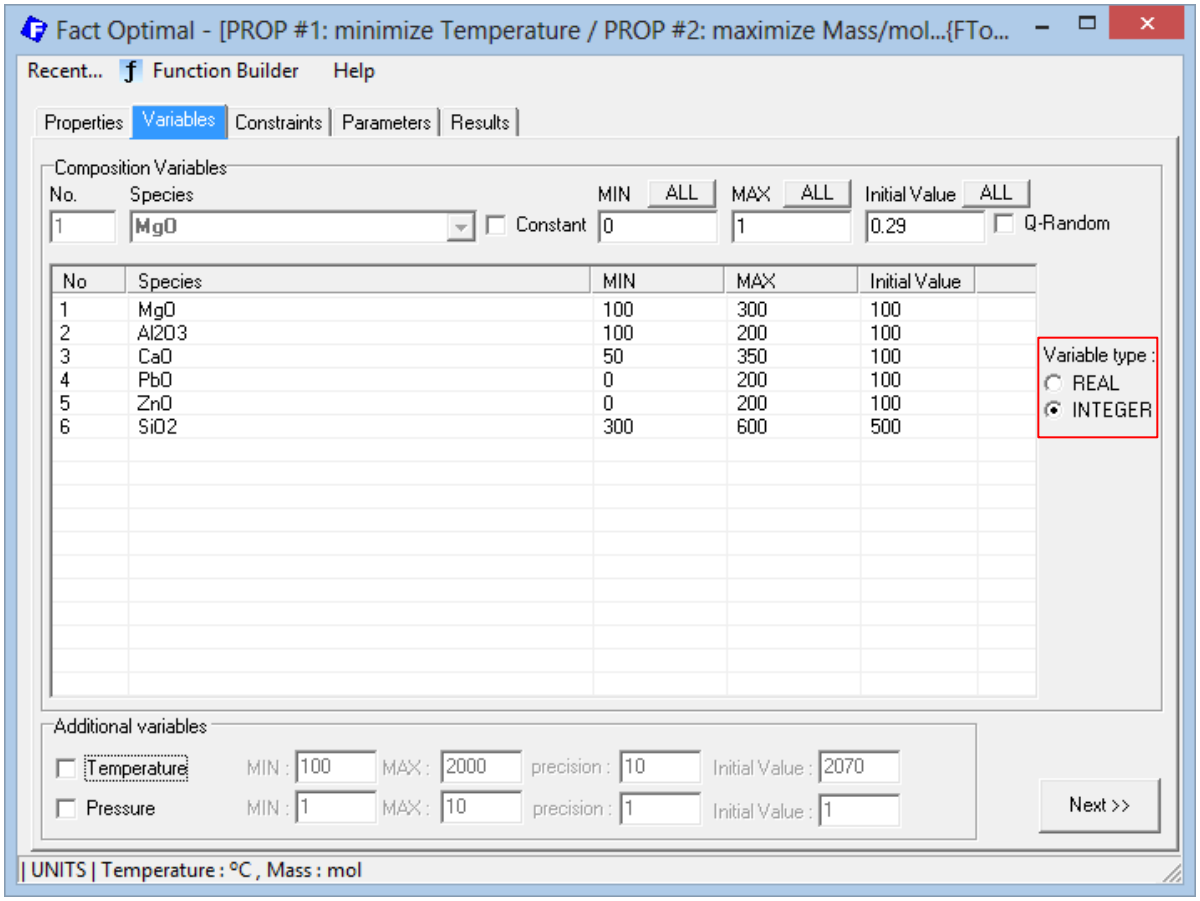

We consider two properties:
1. We minimize the liquidus temperature
2. We maximize the mass of FToxid*SLAG-liq#1 and FToxid*SLAG-liq#2

Click on the Linked button to set T2 = T1-200°C

NOTE: We want to minimize the mass of solids therefore we choose to maximize the mass of liquid.

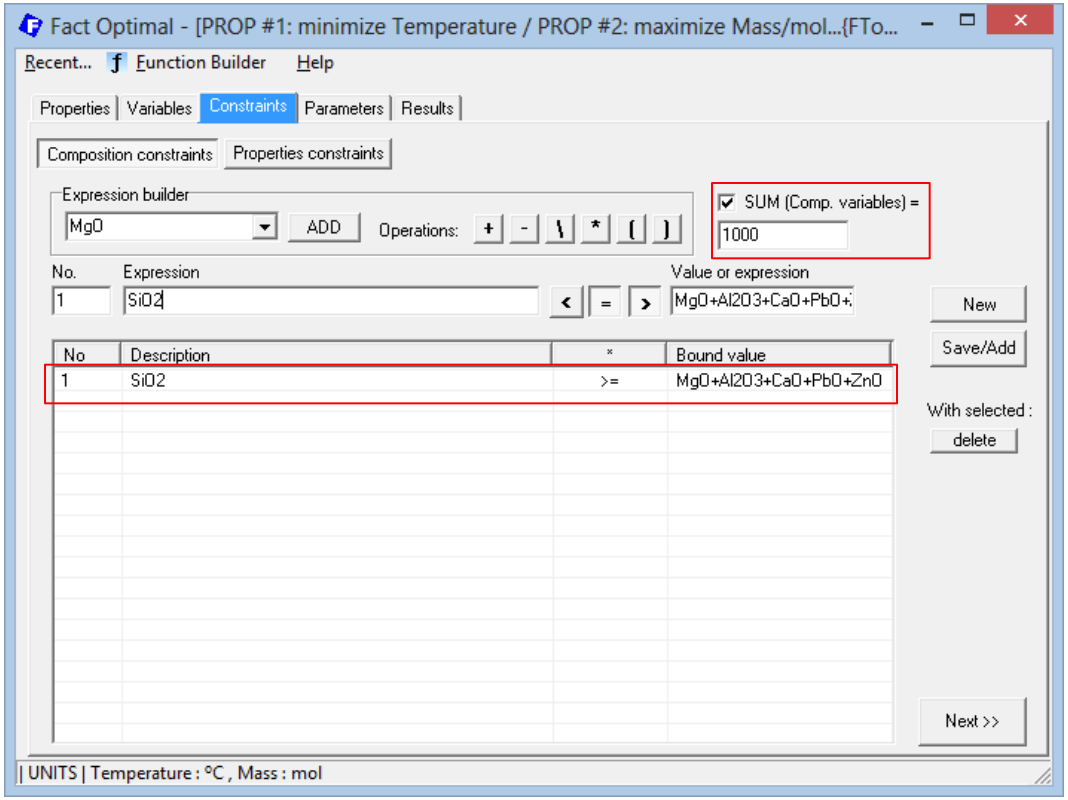
# Example 13: Minimize the liquidus temperature and minimize the solid fraction 200 °C below the liquidus - 3

Step 3: Define the range of compositions of each end-member. In this example we work with integer variables and a sum of 1000 in order to fix the precision to be exactly $1e^{-3}$.



# Example 13: Minimize the liquidus temperature and minimize the solid fraction 200 °C below the liquidus - 4

Step 4: define the two constraints (1 and 2) upon the compositions.



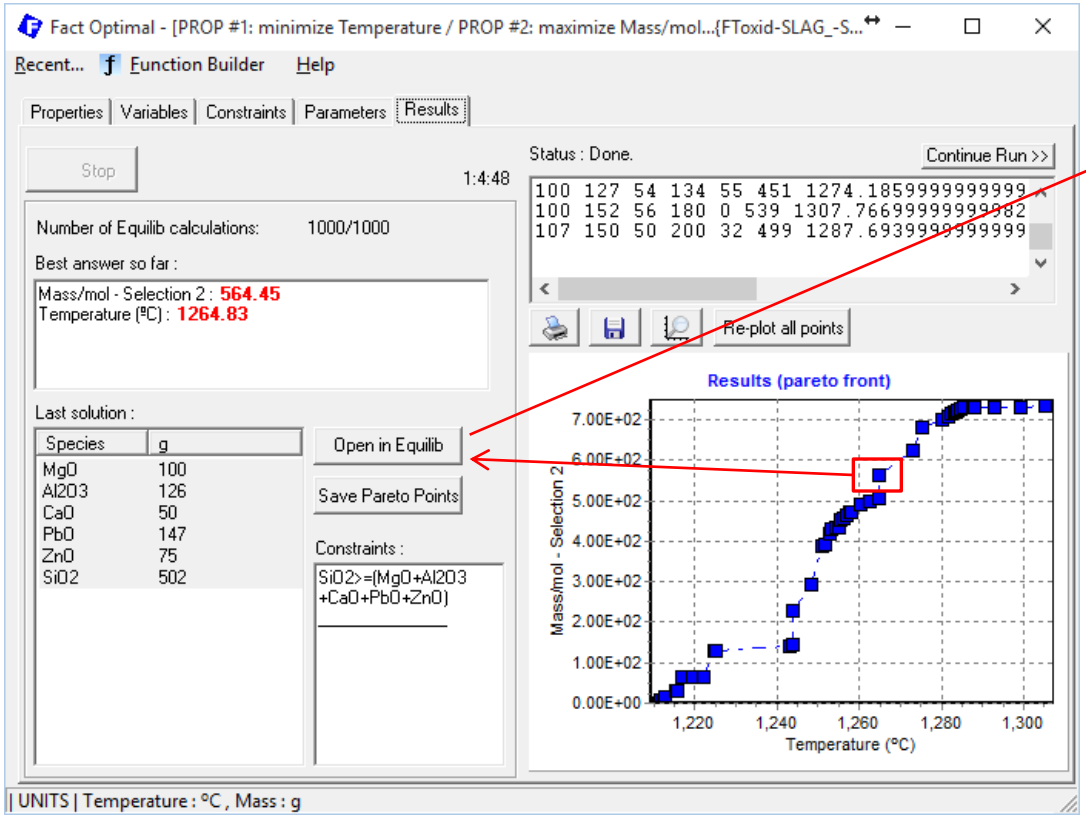

$\Sigma$ Compositions variables =1000

We make sure that SiO2 is the dominant species:

$SiO_2 \geq (MgO+Al_2O_3+CaO+PbO+ZnO)$

# Example 13: Minimize the liquidus temperature and minimize the solid fraction 200 ºC below the liquidus - 5

Step 5: Set up the parameters (1000 Equilib calculations, with small initial mesh region) and calculate.




Click on a point in the Pareto front, and click on Open in Equilib to calculate the phases which are in equilibrium at **$T_{liq}$-200 ºC**

```
(gram) 100 MgO +  126 Al2O3 +  50 CaO +  147 PbO +

(gram) 75 ZnO +  502 SiO2 =

561.38     gram  Slag-liq#1
  (561.38 gram, 7.0584 mol)

+ 186.05     gram  Protopyroxene
  (186.05 gram, 0.92555 mol)

+ 46.780     gram  Willemite
  (46.780 gram, 0.22952 mol)

+ 128.32     gram  Mg2Al4Si5O18_Cordierite
  (128.32 gram, 0.21937 mol)
          (1064 C, 1 bar, S1, a=1.0000)

+ 61.332     gram  CaAl2Si2O8_Anorthite
  (61.332 gram, 0.22045 mol)
          (1064 C, 1 bar, S2, a=1.0000)

+ 16.137     gram  SiO2_Tridymite(h)
  (16.137 gram, 0.26858 mol)
          (1064 C, 1 bar, S4, a=1.0000)
```

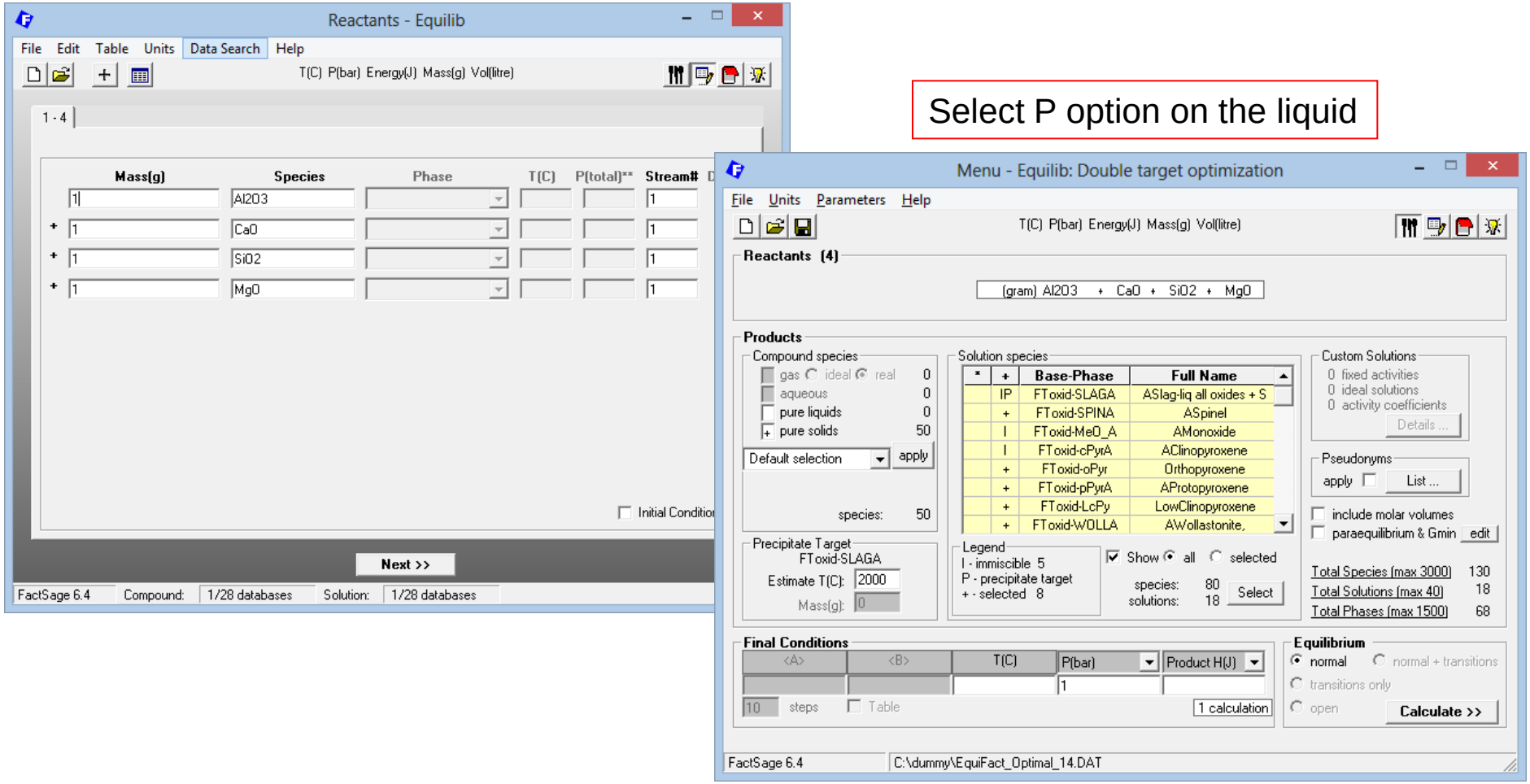
## *Example of double target optimization*

**Target simultaneously a liquidus temperature of 1500ºC and a solid fraction of 0.5 at 100ºC below the liquidus**

# Example 14: Double target optimization - 1

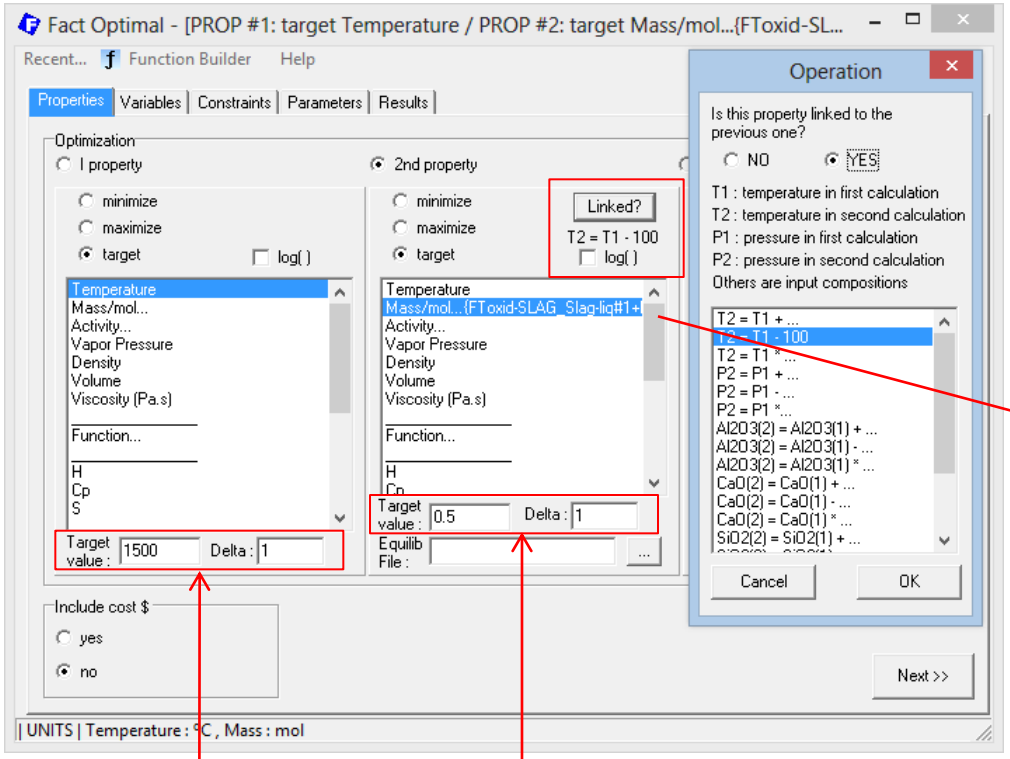
Set up the system: Al2O3-CaO-SiO2-MgO
Select only the FToxid database.

Select P option on the liquid



# Example 14: Double target optimization - 2

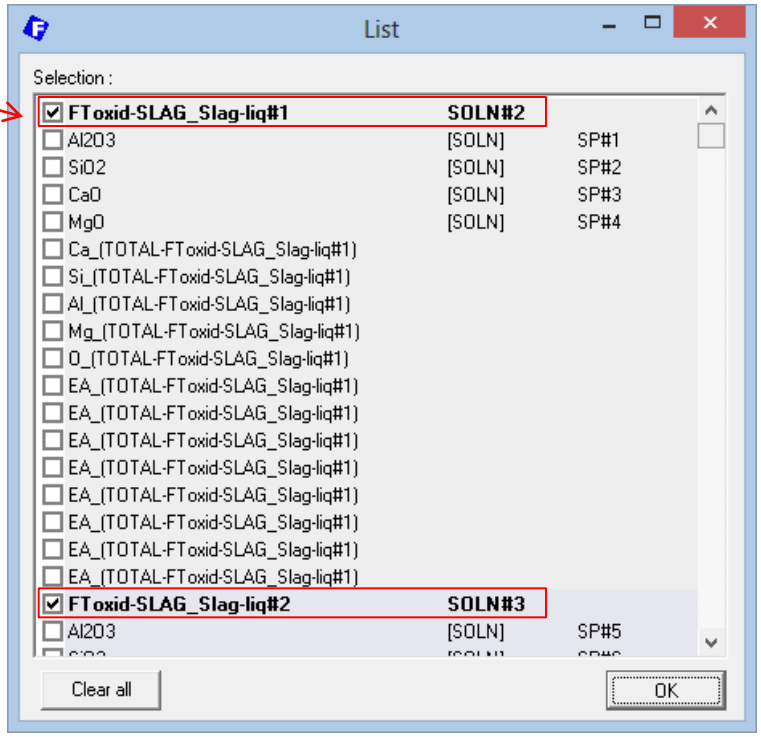
## Setup the problem




The first target is a liquidus temperature of **1500 °C** +/- **1%**

The second target is a **liquid mass fraction 100 °C below the liquidus of 0.5 +/- 1%**

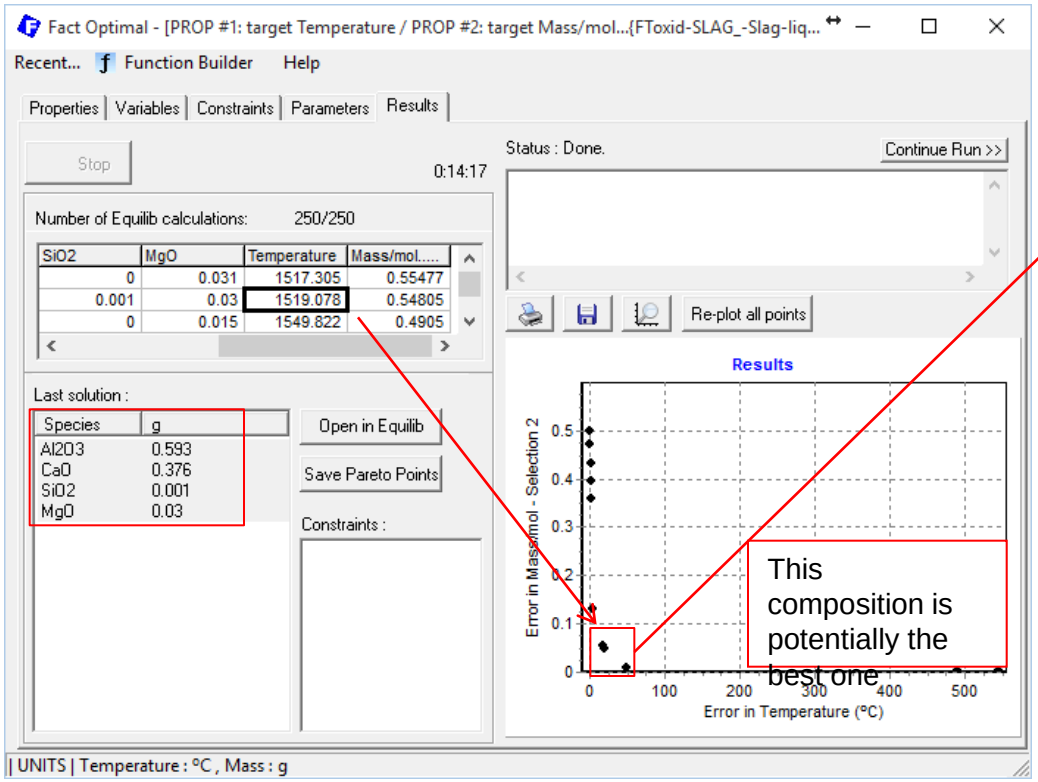
- The two properties are linked: click on the linked button and specify the second temperature to be 100 °C below the liquidus
- We target the solid fraction to be 0.5. This is equivalent to targeting the liquid fraction to be 0.5.
- We need to select both Slag-Liq#1 and Slag-Liq#2 since there is a possible miscibility gap



# Example 14: Double target optimization - 3

There are no constraints, except Σxi=1, setup 250 calculations with an initial mesh size of 1 and a precision of 3 then calculate.

The results show a Pareto front which minimizes simultaneously the error on both targets. The user then has to choose the better compromise according his own requirements.

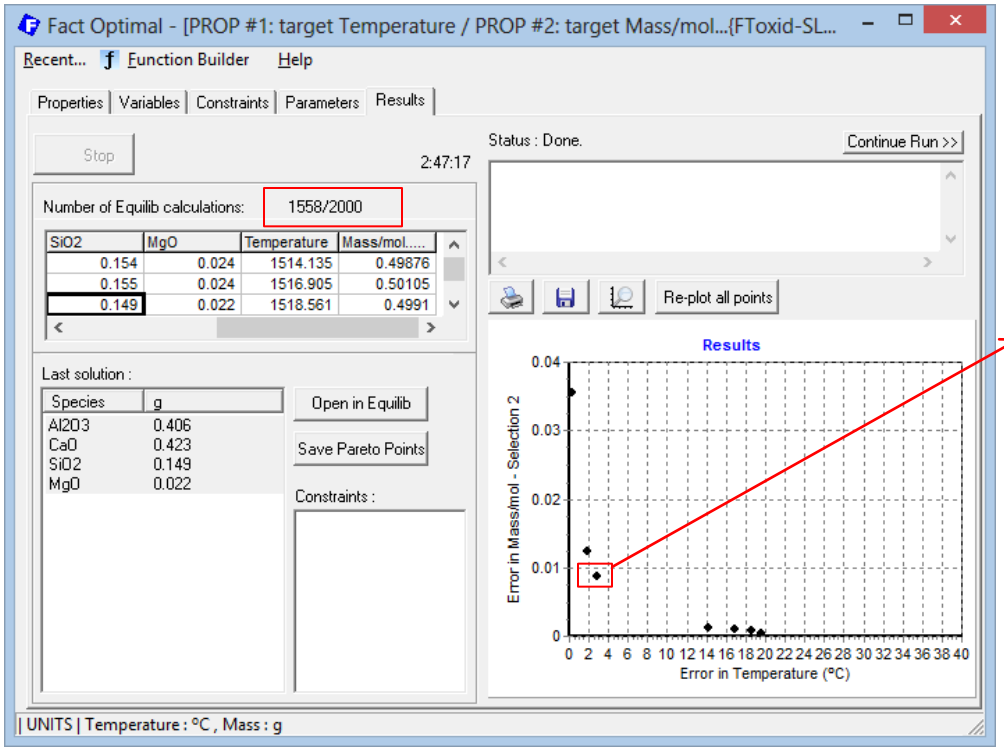



Open in Equilb and get the solids phases which precipitate at 100 °C below the liquidus

```
0.593 Al2O3 +  0.376 CaO +  0.001 SiO2 +
0.03 MgO =

 0.54788    gram  Slag-liq#1
   (0.54788 gram, 7.5602E-03 mol)

+ 0.45212    gram  CaAl2O4_solid
   (0.45212 gram, 2.8608E-03 mol)
```

# Example 14: Double target optimization - 4

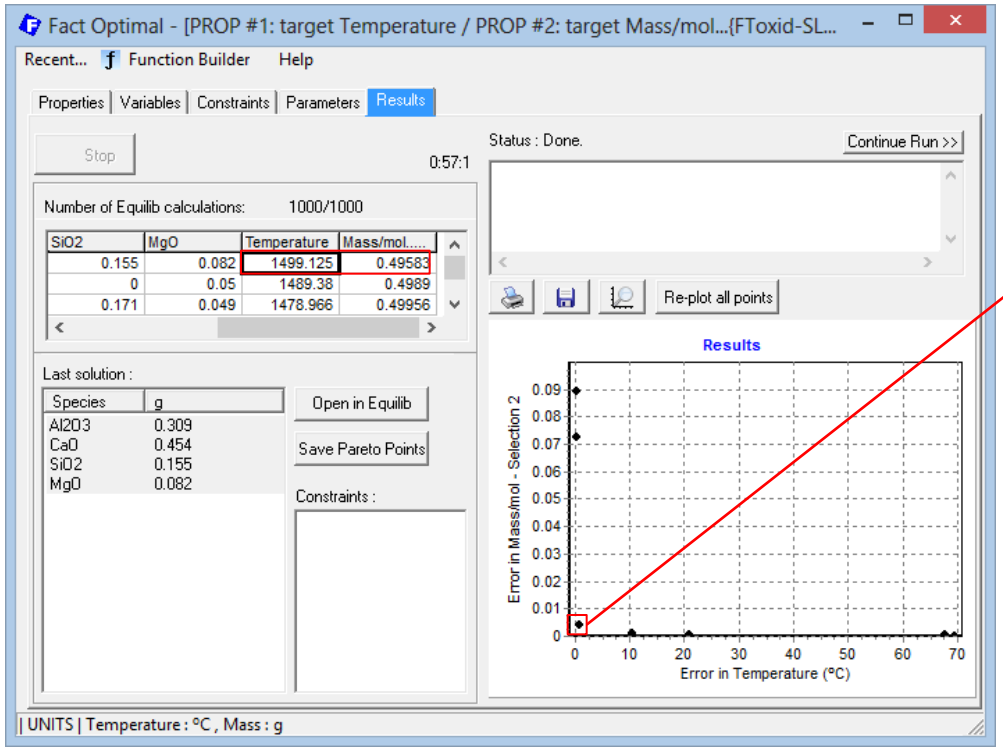
We ran the optimization for 2000 calculations. Fact Optimal stopped after 1558 calculations and found a solution with a very small error on both objectives.




```
0.49275    gram  ASlag-liq#1
   (0.49275 gram, 7.0244E-03 mol)

+ 0.43700    gram  Melilite
   (0.43700 gram, 1.5940E-03 mol)

+ 4.3242E-02 gram  a-Ca2SiO4
   (4.3242E-02 gram, 2.5248E-04 mol)

+ 2.7011E-02 gram  CaAl2O4_solid
   (2.7011E-02 gram, 1.7092E-04 mol)
```

# Example 14: Double target optimization - 5

For a difficult system or a system where the best starting point is unknown, using Quasi-Random calculations could actually provide better results than running a high number of optimization calculations. Here we did 500 Quasi-Random calculations and 500 optimization calculations and obtained a slightly better solution than in the previous slide.




We get almost the ideal solution:

```
0.49712      gram  ASlag-liq#1
+ 0.37811    gram  a'Ca2SiO4
+ 0.11655    gram  Aspinel
+ 8.2194E-03 gram  AMonoxide#1
```