Viscosity and *FactOptimal*

The ***Viscosity*** module calculates the **viscosity** of a glass or slag solution at a given temperature and composition.

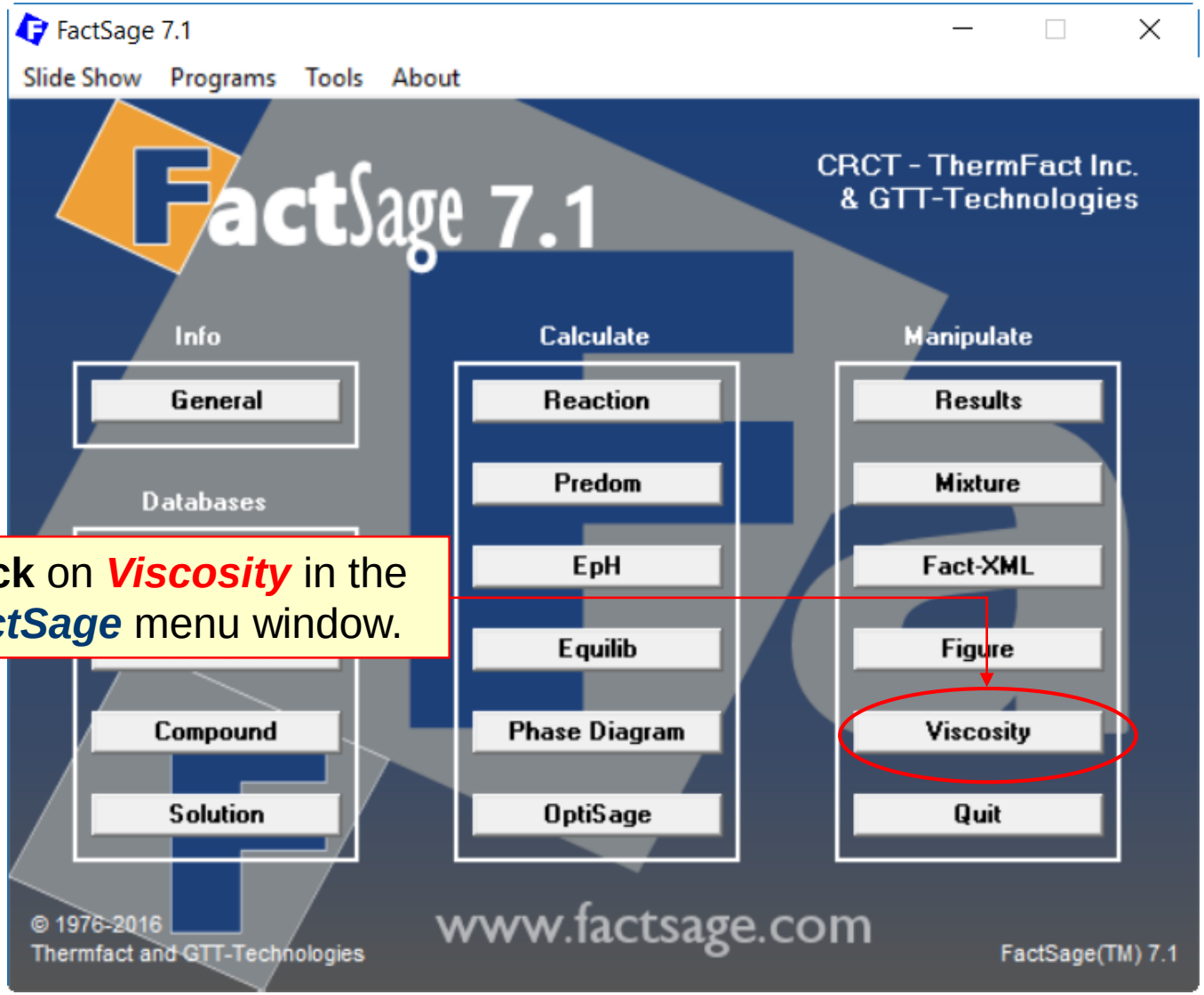
The ***FactOptimal*** module is programmed to identify the optimal conditions for alloy and process design using thermodynamic and property databases.

This slide show demonstrates how to call ***FactOptimal*** from within the ***Viscosity*** module and calculate the composition of a system that minimizes, maximizes or targets the viscosity within a set of constraints on temperature and composition.

In the example the system is SiO_2 - Al_2O_3 - CaO - MgO, the temperature range is 1400 ^oC - 1800 ^oC , and the composition constraints are $0.25 < X_{SiO2} < 0.5$ and $X_{CaO}+X_{MgO} < 0.5$

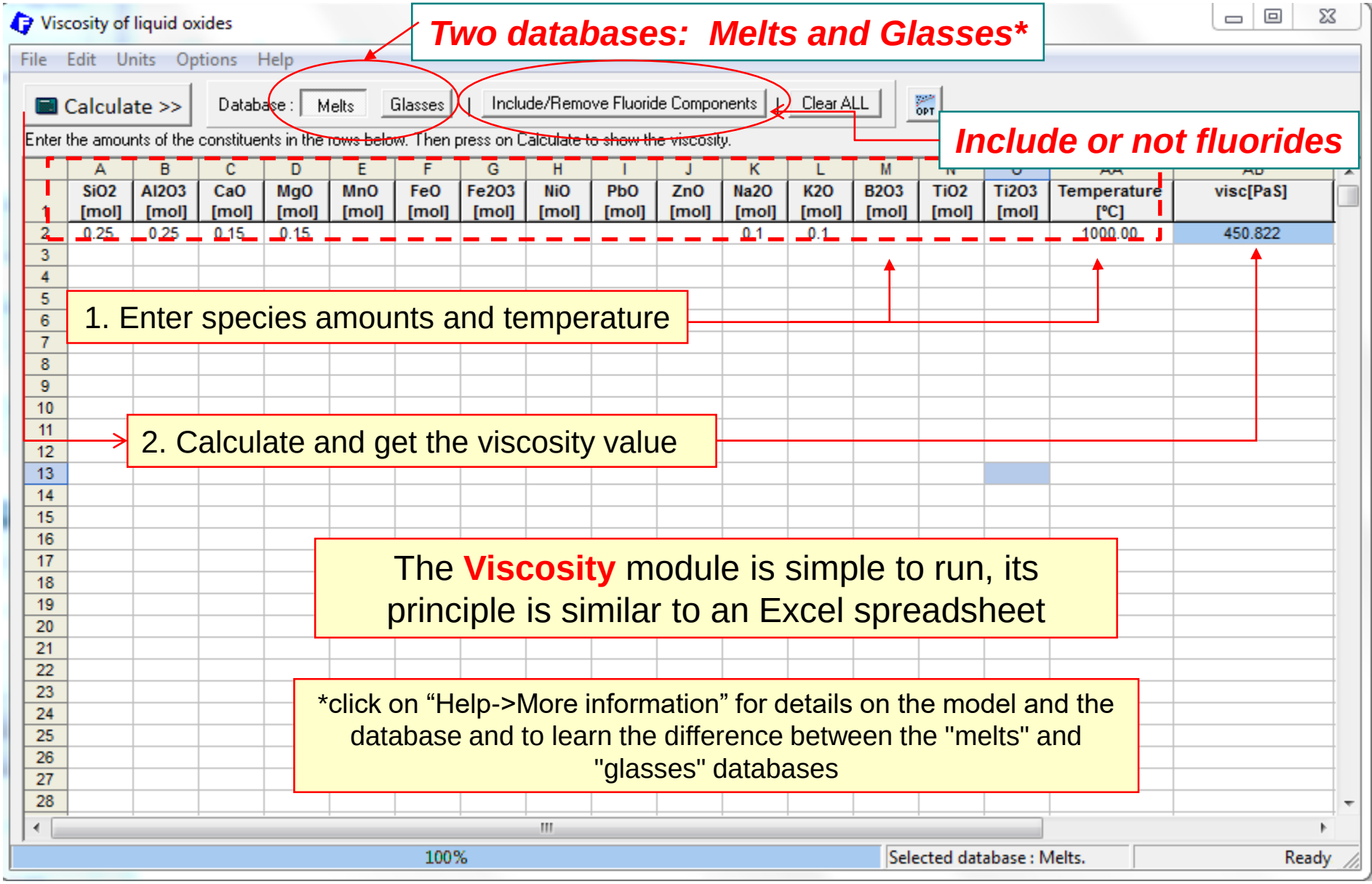
Note that ***FactOptimal*** has limited functionalities when called by ***Viscosity***.

The *Viscosity* module



Click on ***Viscosity*** in the ***FactSage*** menu window.

The *Viscosity* module



Optimization of the *Viscosity*

Viscosity of liquid oxides

File Edit Units Options Help

Calculate >> | Database : Melts | Glasses | Include/Remove Fluoride Components | Clear ALL | OPT

Enter the amounts of the constituents in the rows below. Then press on Calculate to show the viscosity.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	AA	AB
1	SiO2 [mol]	Al2O3 [mol]	CaO [mol]	MgO [mol]	MnO [mol]	FeO [mol]	Fe2O3 [mol]	NiO [mol]	PbO [mol]	ZnO [mol]	Na2O [mol]	K2O [mol]	B2O3 [mol]	TiO2 [mol]	Ti2O3 [mol]	Temperature [ºC]	visc[PaS]
2	0.25	0.25	0.15	0.15							0.1	0.1				1000.00	450.822

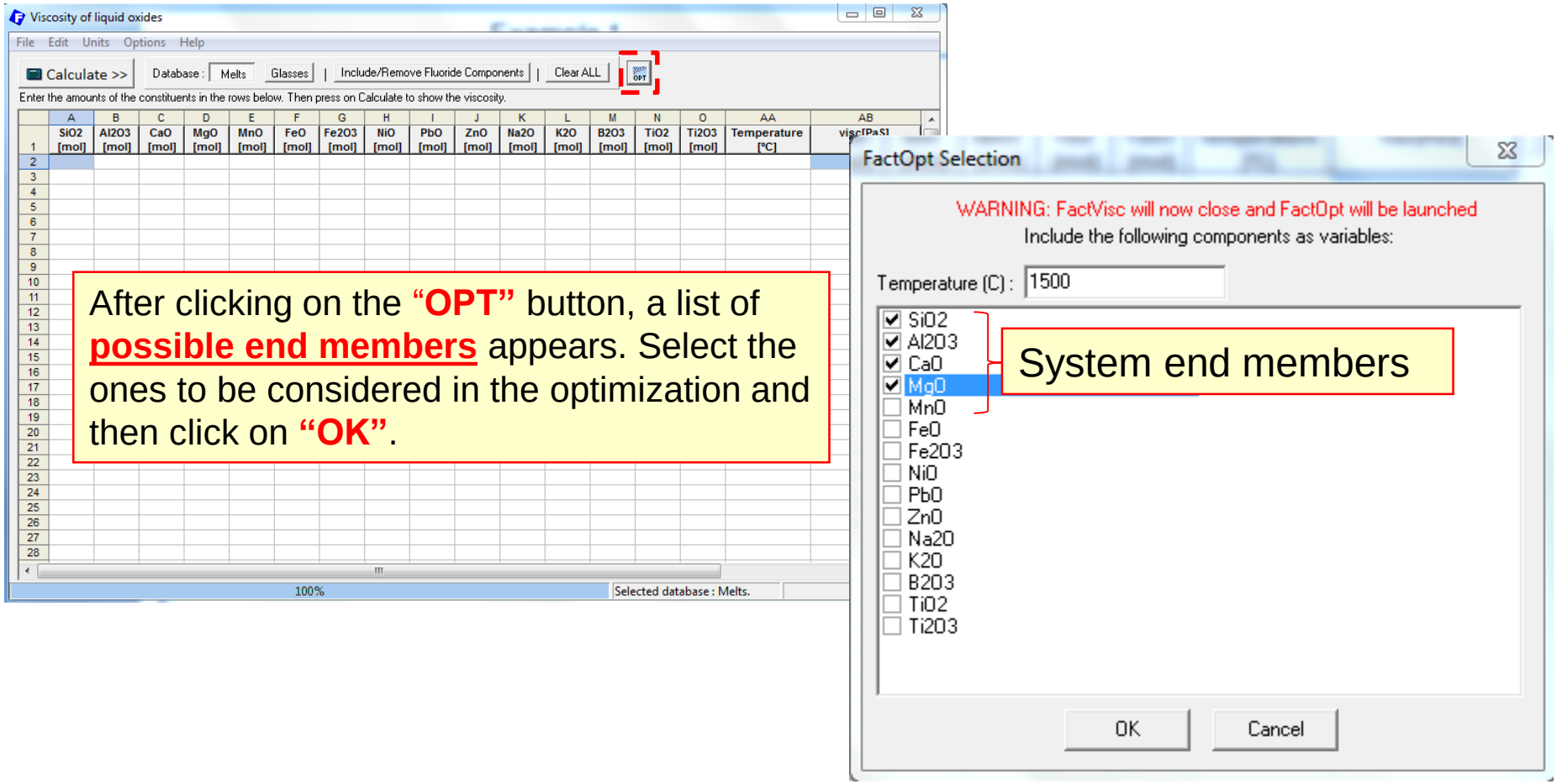
"**OPT**" – activates ***FactOptimal*** and allows you to calculate the **compositions and temperatures** that **minimize, maximize or target** the ***Viscosity*** under a set of **constraints**.

100% | Selected database : Melts. | Ready

FactOptimal and *Viscosity* - Example 1

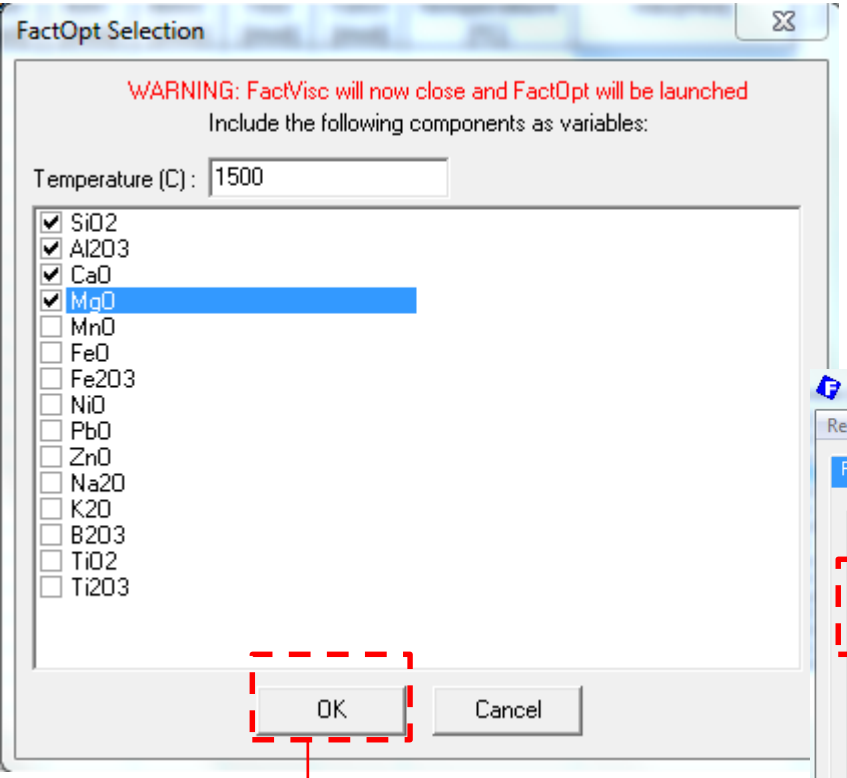
What is the composition of the system that has a minimum viscosity:

- within the temperature range 1400 °C - 1800 °C , and
- within the composition constraints $0.25 < X_{SiO2} < 0.5$ and $X_{CaO}+X_{MgO} < 0.5$?

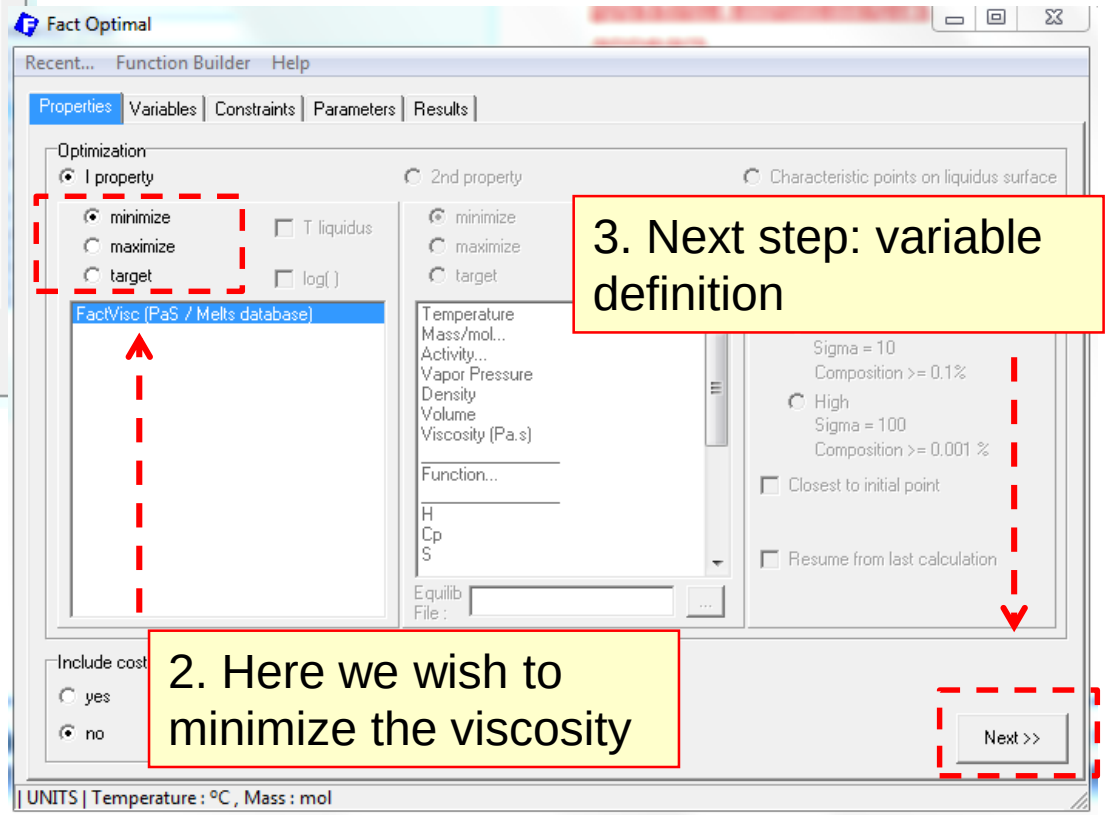


After clicking on the **"OPT"** button, a list of **possible end members** appears. Select the ones to be considered in the optimization and then click on **"OK"**.

FactOptimal and *Viscosity* - Example 1 (cont.)



The methodology of the optimization is explained in the FactOptimal module slide show.



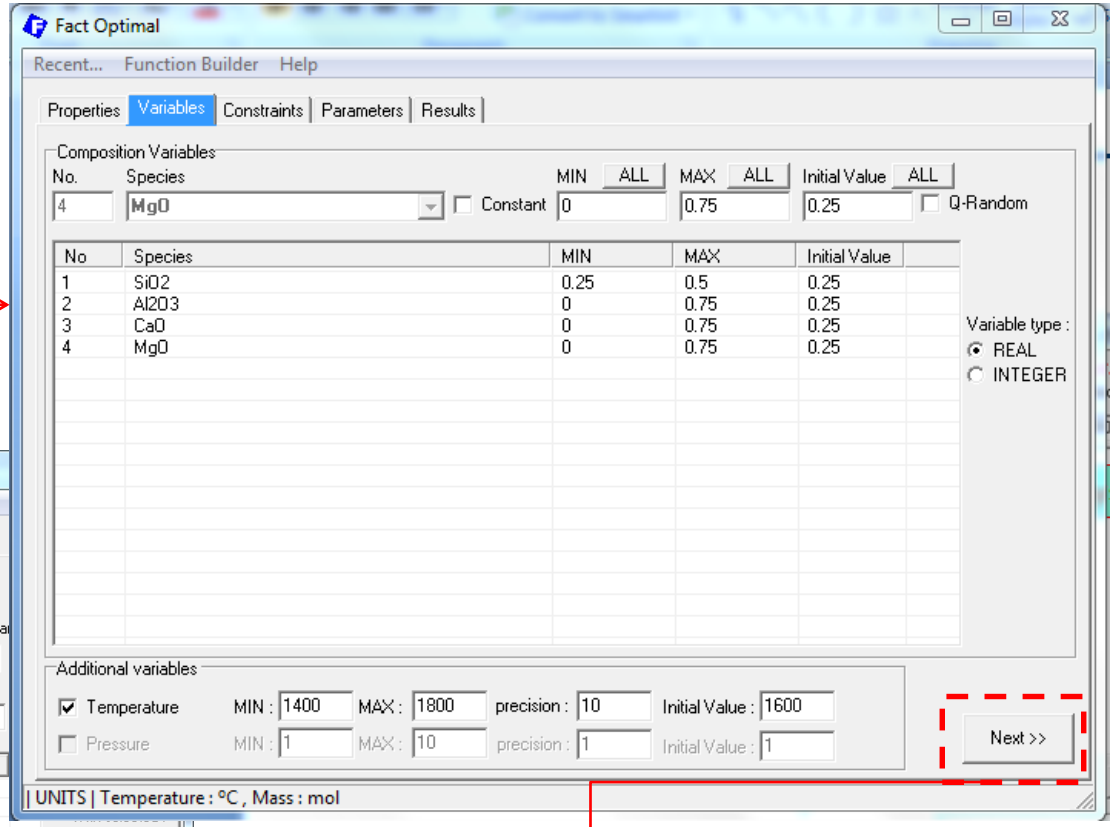
1. Activate FactOptimal

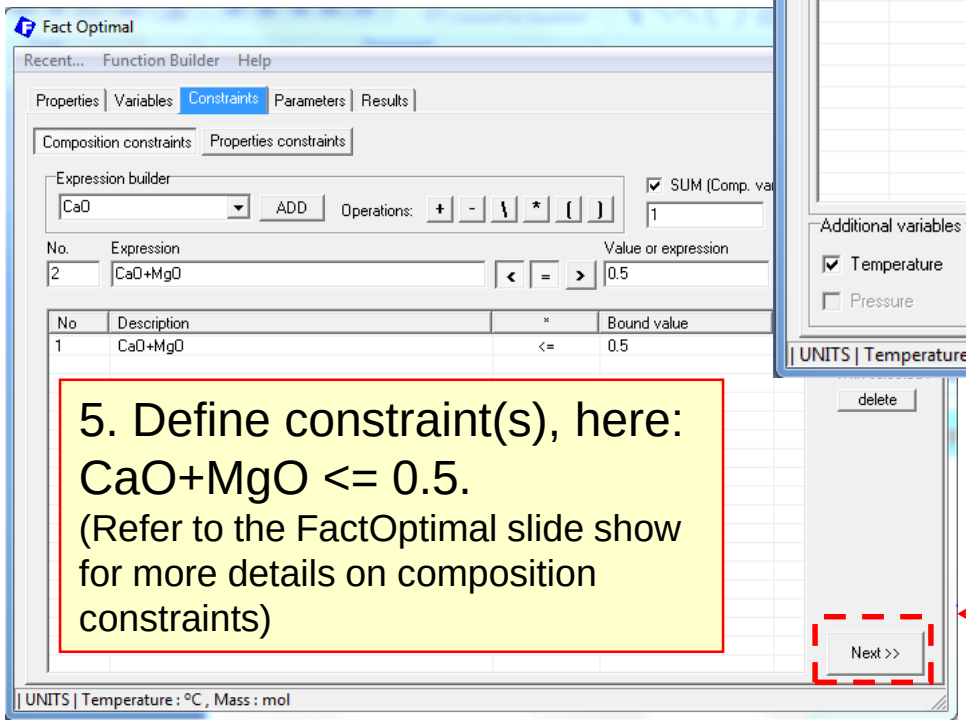
2. Here we wish to minimize the viscosity

3. Next step: variable definition

FactOptimal and *Viscosity* - Example 1 (cont.)

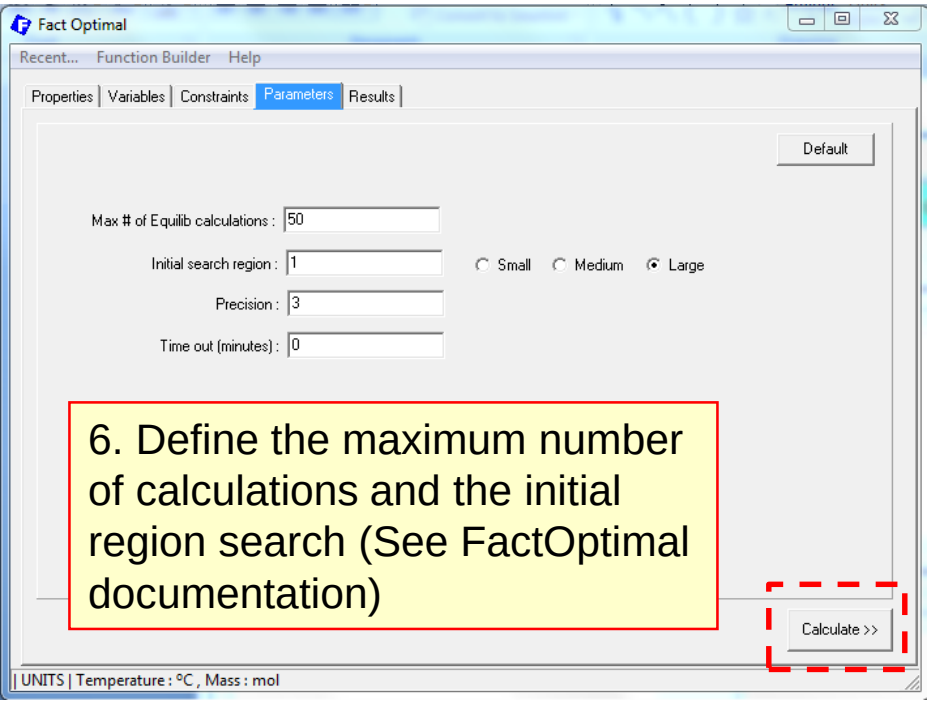
4. Define the range of composition and temperature.
(For a constant temperature, uncheck the temperature option under Additional variables)





5. Define constraint(s), here: CaO+MgO <= 0.5.
(Refer to the FactOptimal slide show for more details on composition constraints)

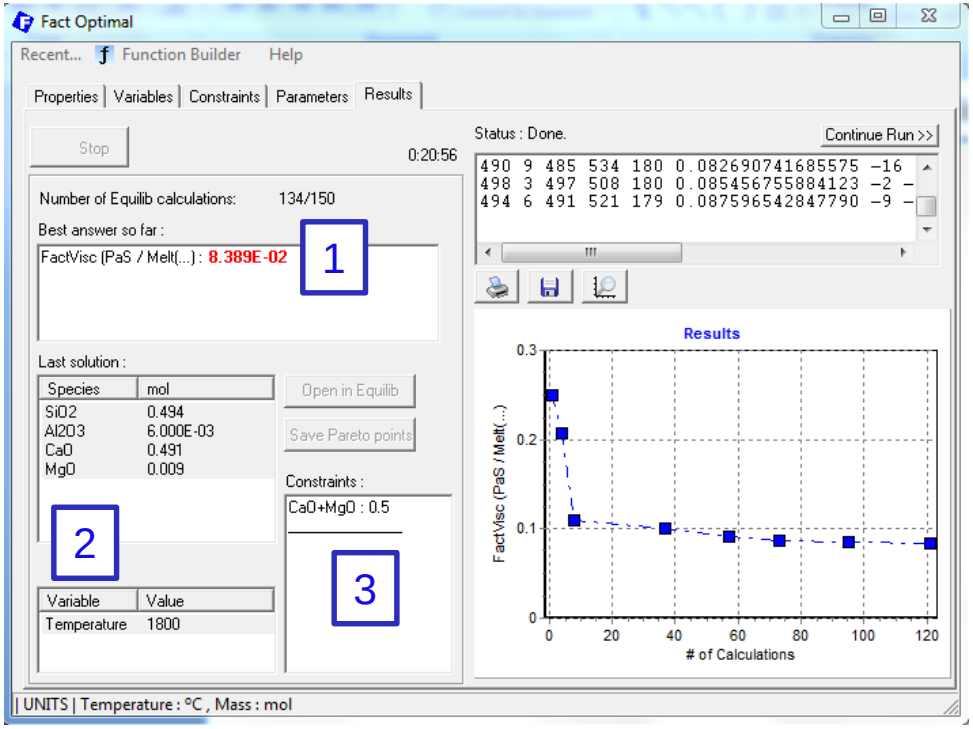
FactOptimal and *Viscosity* - Example 1 (cont.)



6. Define the maximum number of calculations and the initial region search (See FactOptimal documentation)

7. Calculate and display results

After 134 calculations FactOptimal converges to the minimum viscosity. It displays [1] the value of the minimum viscosity, [2] the composition and temperature and [3] the value of the constraint(s).



FactOptimal and *Viscosity* - Example 2

The same example can be performed, but instead of minimizing or maximizing the viscosity, one can target a viscosity value with a chosen accuracy.

FactOptimal returns the composition-temperature set for which the viscosity corresponds to the targeted value. "Continue Run" is for calculating another set of composition-temperature for the same target.