FactSage Practical
MSE302

Practical 5. Equilib Module

Advanced Applications

Acknowledgements

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Outline

Databases in FactSage for Steelmaking Applications

In this section, we will use the Equilb Module of FactSage to solve some real-world questions regularly faced in the steel industry. While here we present you the steelmaking applications, you should be aware that FactSage has also found wide applications in the fields of alloy design/development, extraction of base metals, etc. Please review the Documentation Module to find the applications of different FACT databases. The Help Files also include a number of advanced industrial examples.

First, let us review the FactSage databases which are particularly developed for **steelmaking** applications (pyrometallurgical extraction and solidification) as well as some key phase models.

Databases in FactSage for Steelmaking Applications

Database	Description
FactPS	All gaseous species, stoichiometric solids and liquids.
FToxid	Frequently updated **oxide** database containing (i) a large number of condensed solution phases (slag, spinel, monoxide, olivine, etc.); and (ii) pure solids and liquids, but no gaseous species.
FTmisc	FeLq solution which is the most reliable liquid steel database for steelmaking calculations, for example, slags/refractories/gases/**molten iron**.
FSStel	Solid and liquid steel phases (also includes small number of gases, oxides, sulfides, nitrides, etc.) and is used for: (i) steel solidifications and alloy design; and (ii) liquid steel: reasonable calculations for steelmaking applications.

Database priority for steelmaking calculations:

(a) FToxid > FTmisc > FactPS: without FSStel for pyrometallurgical calculations.

(b) FToxid > FSStel > FactPS: with FSStel for steel solidification related calculations.

FToxid Database: Main Solution Phases

Main solution phases when $T > 1550$ ℃ (steelmaking)

Note: these phases may still exist even when $T < 1550$ ℃.

Phase	Description
Slag [I]-option	**Major oxide components** Al_2O_3-CaO-FeO-Fe_2O_3-MgO-SiO_2 If the system contains other oxide components, for example, MnO, Mn_2O_3, CoO, NiO, PbO, ZnO, TiO_2, Ti_2O_3, etc. please consult Documentation for the limitations. Also, the gas solubility such as S (SO_2), P, H (OH), N, C, F, … is considered.
Spinel [I]-option	(SPIN) can be described as $(Mg, Fe, Mn, Co, Ni, Zn)[Al, Fe, Cr, Co, Mn, Va]_2SiO_4$, extensive solid solution containing $MgAl_2O_4$, $MgCr_2O_4$, $MgFe_2O_4$, $FeCr_2O_4$, Fe_3O_4, $FeAl_2O_4$, Cr_3O_4, $MnAl_2O_4$, $MnCr_2O_4$, $MnFe_2O_4$, etc.
Monoxide	(MeO_) can be described as CaO-MgO-FeO−Fe_2O_3-MnO-NiO-Al_2O_3-Cr_2O_3-etc. Covering most famously: lime (CaO), periclase (MgO) and wüstite (FeO). [I]-option should be considered especially when CaO and MgO exist together.

FToxid Database: Main Solution Phases

Main solution phases when $T > 1550$ ℃ (steelmaking)

Note: these phases may still exist even when $T < 1550$ ℃.

Phase	Description
α-, α'-Ca2SiO4	(aC2S, bC2S) Ca_2SiO_4 (CS2) rich solution with limited solubility of Mg_2SiO_4, Fe_2SiO_4, Mn_2SiO_4, etc.
Olivine	(Oliv) can be described as $(Mg, Fe, Ca, Mn, Ni, Zn, Co, Cr, etc.)_2SiO_4$, covering forsterite ($Mg_2SiO_4$), fayalite ($Fe_2SiO_4$), γ-$Ca_2SiO_4$, monticellite ($CaMgSiO_4$), tephroite ($Mn_2SiO_4$), [I]-option is used when Ca_2SiO_4, exists.
Corundum [I]-option	(CORU) can be described as $(Al, Cr, Fe, Mn)_2O_3$. Solid miscibility gaps exist between the constituents.
Mullite	(Mull) non-stoichiometric $Al_6Si_2O_{13}$ with possible solubility of B. (MulF) stoichiometric $Al_6Si_2O_{13}$ with dilute $Fe_6Si_2O_{13}$.

FToxid Database: Main Solution Phases

Main solution phases when $T > 1550$ ℃ (steelmaking)

Note: these phases may still exist even when $T < 1550$ ℃.

Phase	Description
Mn/Ti oxides	✓ ilmenite (ILME): $FeTiO_3$ (ilmenite)-Ti_2O_3-$MgTiO_3$-$MnTiO_3$ + Al_2O_3 ✓ pseudo-brookite (PSEU): Ti_3O_5-$FeTi_2O_5$-$MgTi_2O_5$-$MnTi_2O_5$ ✓ Ti-spinel (TiSp): $(Mg, Fe, Mn)[Mg, Fe, Mn, Ti, Al]_2O_4$ ✓ Rutile (TiO2): TiO_2 + Ti_2O_3-ZrO_2 solid solution

FToxid Database: Main Solution Phases

Main solution phases when $T < 1550$ °C (solidification of slag)

Phase	Description
Wollastonite	(Woll) can be described as $(Ca, Mg, Mn)SiO_3$ which is a $CaSiO_3$-rich phase stable below 1300 °C. Pseudo-wollastonite is stoichiometric $CaSiO_3$ stable below 1550 °C.
Pyroxene	(pPyr, oPyr, cPyr) $(Mg, Ca, Fe^{II})[Mg, Fe^{II}, Fe^{III}, Al]\{Al, Fe^{III}, Si\}SiO_6$, which is a $MgSiO_3$-rich phase stable below 1560 °C. proto-, ortho-, low-clino-pyroxene exist. Clino-pyroxene is a $CaMgSi_2O_6$-rich phase which is stable below 1390 °C.
Rhodonite	(Rhod) $(Mn, Ca)SiO_3$ which is a $MnSiO_3$-rich solid solution stable below 1300 °C.

FToxid Database: Main Solution Phases

Main solution phases when $T < 1550$ ℃ (mould flux, Na_2O-containing system)

Phase	Description
Nepheline	(Neph) $NaAlSiO_4$ with excess SiO_2.
Carnegeite	(Carn) $NaAlSiO_4$ with excess SiO_2.
NaAlO2	(NASl) low temperature-$NaAlO_2$ with excess $NaAlSiO_4$.
NaAlO2	(NASh) high temperature-$NaAlO_2$ with excess $NaAlSiO_4$.
Combeite	(NCSO) $Na_4CaSi_3O_9$ (bombeite) - $Na_2Ca_2Si_3O_9$ solid solution.
Feldspar	(Feld) complete solution between Anorthite ($CaAl_2Si_2O_8$) and Albite ($NaAlSi_3O_8$)
NCA2	The structure can be described as $(Na_2, Ca)O \cdot Na_2O \cdot 2Al_2O_3$.
C3A1	The structure can be described as $Ca_3Al_2O_6$ dissolving Na_2O.

FToxid Database: Main Solution Phases

Main solution phases in the CaO-Al_2O_3-SiO_2-FeO-Fe_2O_3 system with high oxygen partial pressure (e.g., Air)

Phase	Description
CAFS	The structure can be described as $Ca_2(Al, Fe^{III})_8SiO_{16}$.
CAF6	The structure can be described as $Ca(Al, Fe^{III})_{12}O_{19}$.
CAF3	The structure can be described as $Ca(Al, Fe^{III})_6O_{10}$.
CAF2	The structure can be described as $Ca(Al, Fe^{III})_4O_7$.
CAF1	The structure can be described as $Ca(Al, Fe^{III})_2O_4$.
C2AF	The structure can be described as $Ca_2(Al, Fe^{III})_2O_5$.
C3AF	The structure can be described as $Ca_3(Al, Fe^{III})_2O_6$.

FTmisc Database

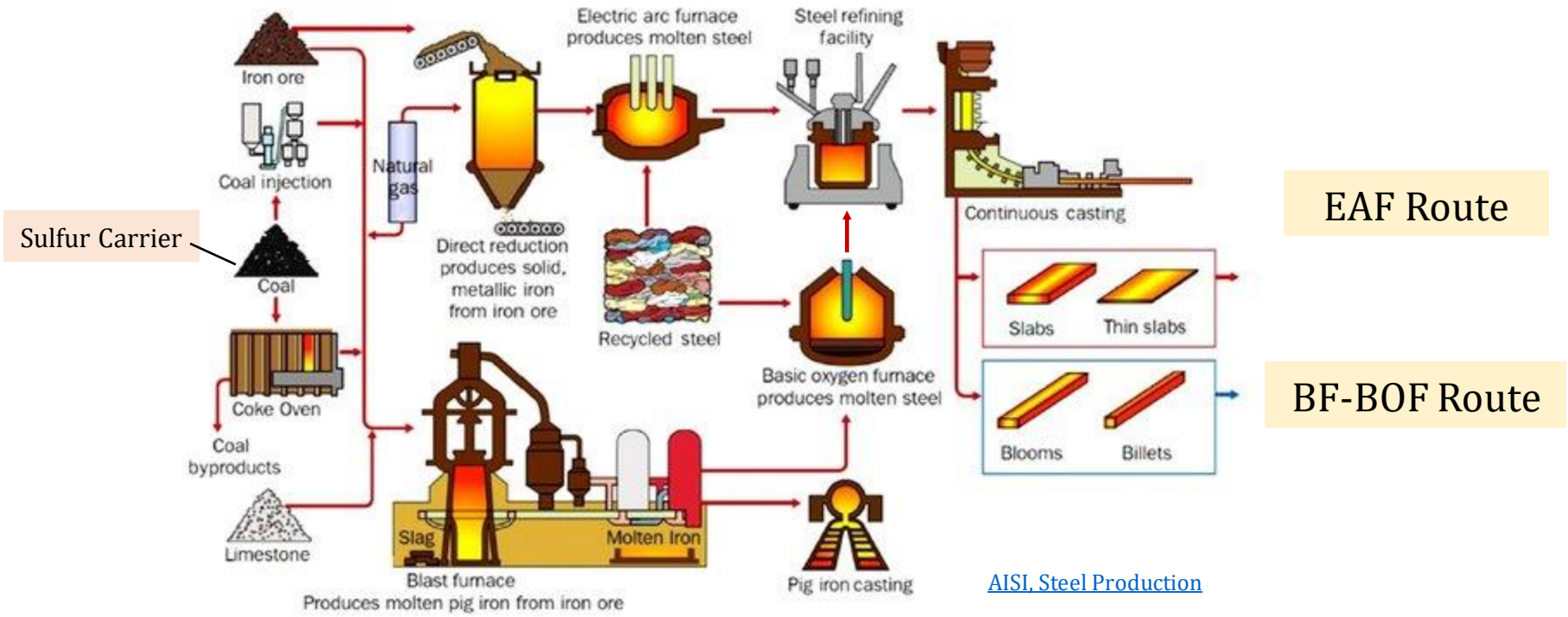
Phase	Description
FeLQ	Liquid Fe containing Ag, Al, B, Ba, C, Ca, Ce, Co, Cr, Cu, H, Hf, La, Mg, Mn, Mo, N, Nb, Nd, Ni, O, P, Pb, Pd, S, Si, Sn, Ta, Th, Ti, U, V, W, Zr. This phase is better suited for calculations involving iron and steelmaking processes (optimized for iron-rich solutions only).

FSStel Database

Phase	Description
FCC/BCC	Fe, Carbide, and Nitride are all treated as FCC phases. ✓ Fe with N and C: use [J]-option (3-miscibility gaps) ✓ Fe with N or C: use [I]-option (2-miscibility gaps) For BCC phase, [I]-option is recommended.
FCC ordered phase BCC ordered phase	(FCC_L12) and (BCC_B2) normally slow down the calculations significantly. If you are not really interested in order/disorder transitions, do not select these ordered phases.
Carbon	When the C content is lower than ~1%, metastable Fe_3C is normally formed instead of stable solid carbons. Therefore, in the selection of solid phases, "unselect" solid carbon phases to permit the appearance of metastable Fe_3C.

Example 1: Desulfurization (Background)

Background: How Steel is Made



For the BF-BOF Route, there are two "spots" for desulfurization:

(a) Hot Metal (Liquid Iron): after BF in torpedo car or desulfurization station

(b) Liquid Steel: during ladle treatment

Example 1: Desulfurization (Background)

Background: Desulfurization of Hot Metal

The hot metal tapped out of the BF typically contains 0.04~0.07 wt.%S; the BOF must be charged with de-sulfurized hot metal containing 0.01~0.001 wt.%S. The sulfur removal is performed at a desulfurization station, e.g., torpedo car.

Example 1: Desulfurization (Background)

Background: Desulfurization of <u>Hot Metal</u>

To remove sulfur from the hot metal, a suitable desulfurizing agent is added. The following agents are usually considered (highlighted in yellow):

$$\mathbf{Mg}(\mathbf{s}) + [\mathrm{S}] \rightarrow \mathrm{MgS(s)}$$

$$\mathbf{CaC_2}(\mathbf{s}) + [\mathrm{S}] \rightarrow \mathrm{CaS(s)} + 2[\mathrm{C}]$$

$$\mathbf{Mg}(\mathbf{s}) + \mathbf{CaO}(\mathbf{s}) + [\mathrm{S}] \rightarrow \mathrm{CaS(s)} + \mathrm{MgO(s)}$$

Note: [Element] represents the element dissolved in the hot metal.

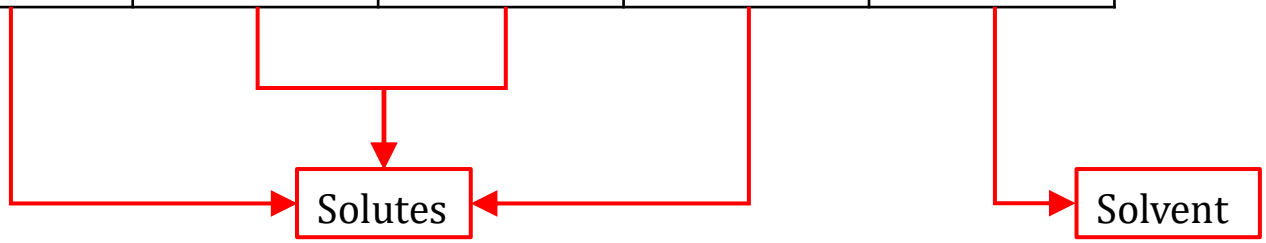
In the following pages, we will use the Equilib Module to compare the efficiency of these desulfurizing agents and to calculate the exact amount of desulfurizing agent that is required to achieve the desired sulfur content.

Example 1: Desulfurization (Basic Example)

Basic Example: Desulfurization of Hot Metal Using Mg

Let us assume the composition of hot metal (wt.%):

Element	C	Si	Mn	S	Fe
wt.%	4.50	0.50	0.60	0.065	94.335

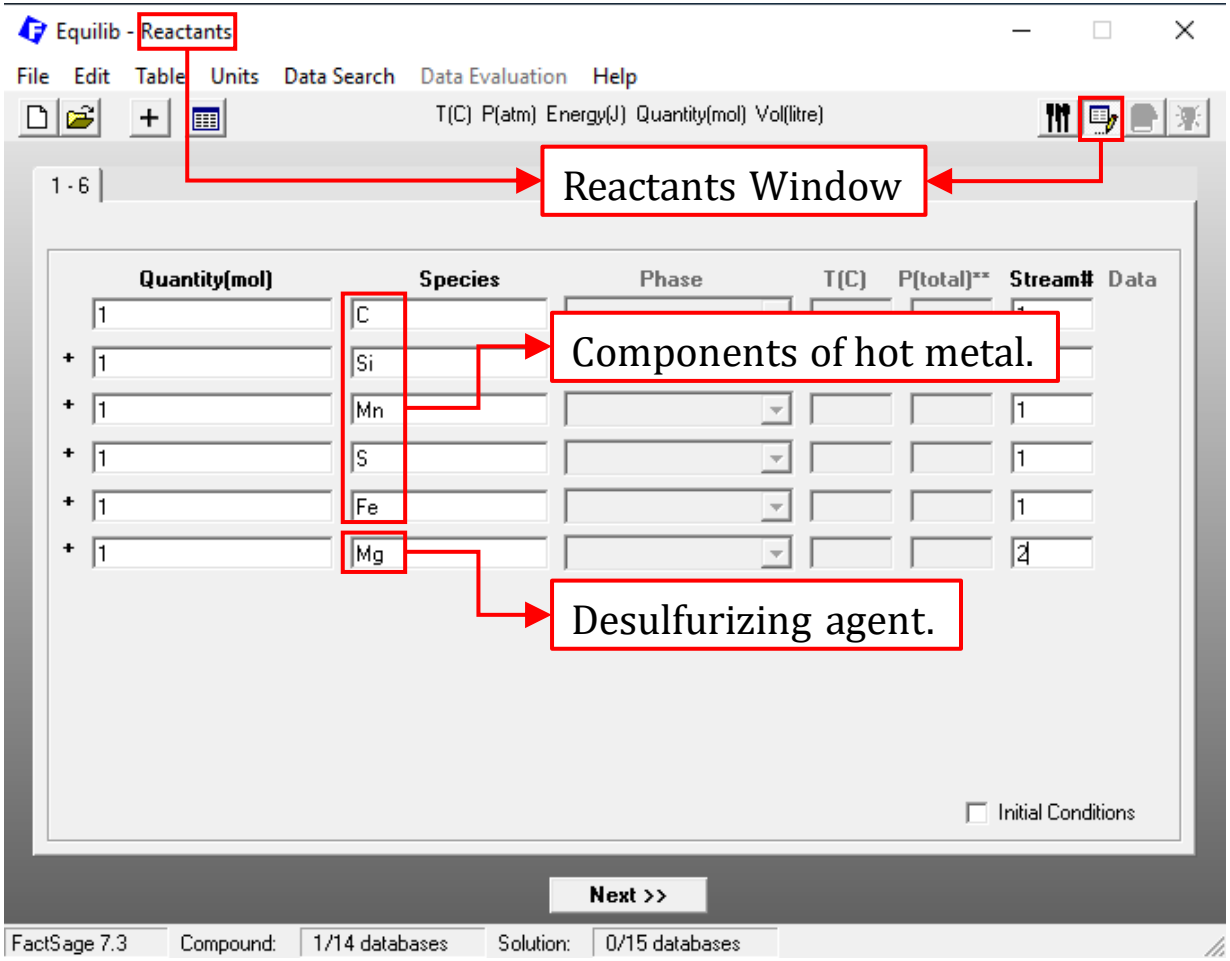


Note: the main difference between hot metal and liquid steel is the content of carbon.

Now, we will add varying amounts of Mg to this hot metal to remove S as solid MgS. Our calculation will be based on 100 g hot metal.

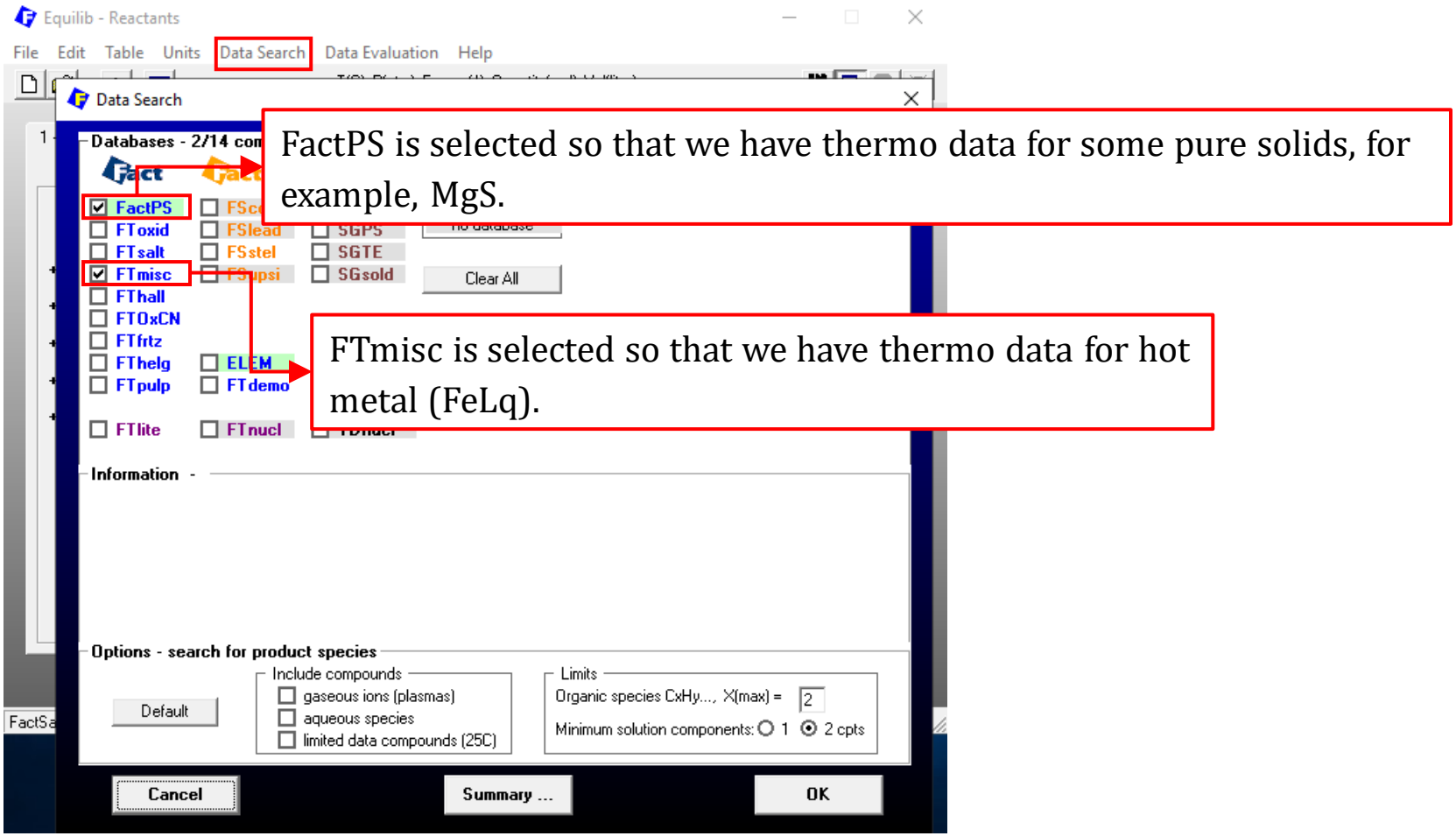
Example 1: Desulfurization (Basic Example)

Basic Example: Desulfurization of <u>Hot Metal</u> Using Mg



Example 1: Desulfurization (Basic Example)

Basic Example: Desulfurization of Hot Metal Using Mg

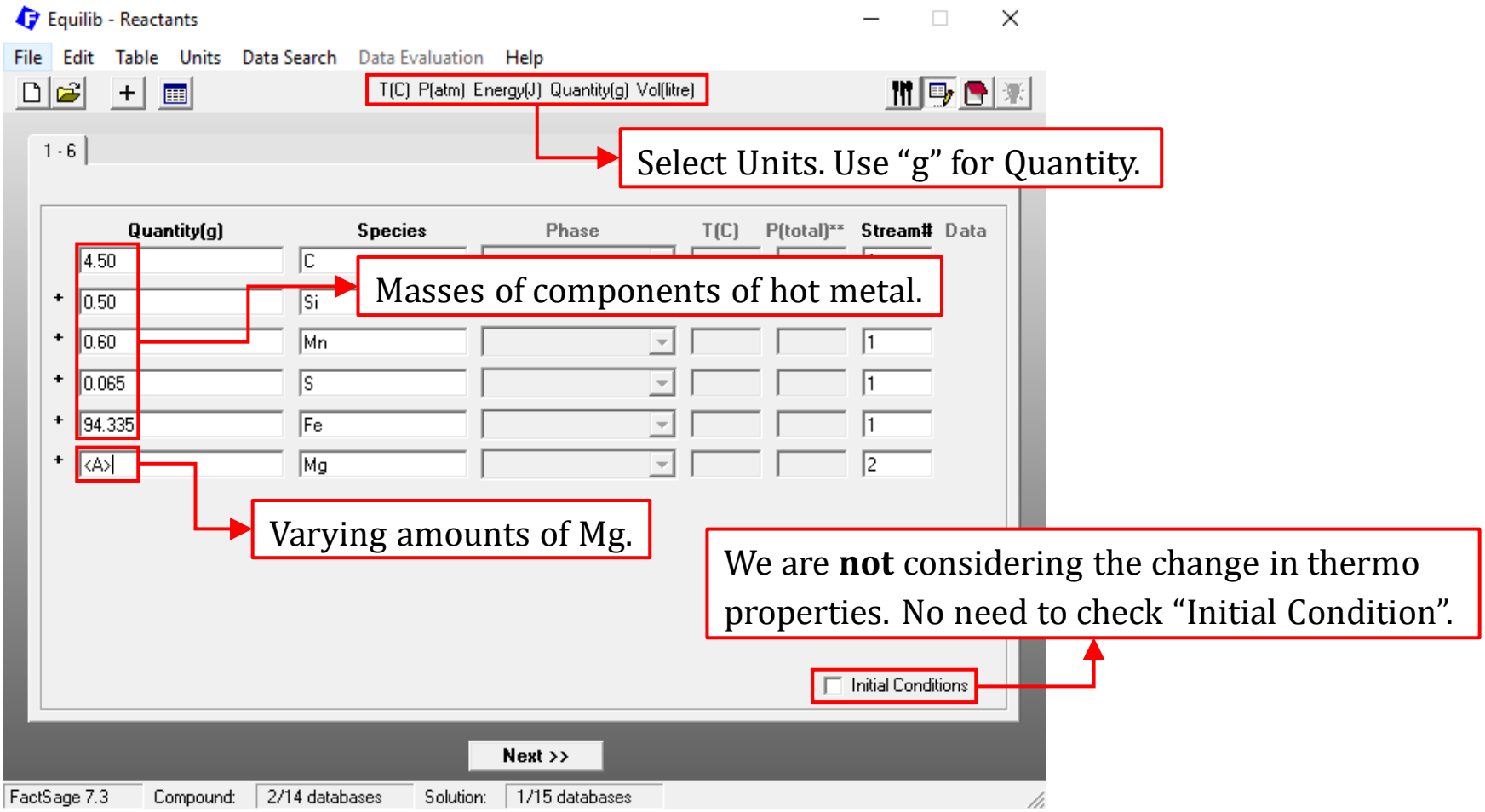


FactPS is selected so that we have thermo data for some pure solids, for example, MgS.

FTmisc is selected so that we have thermo data for hot metal (FeLq).

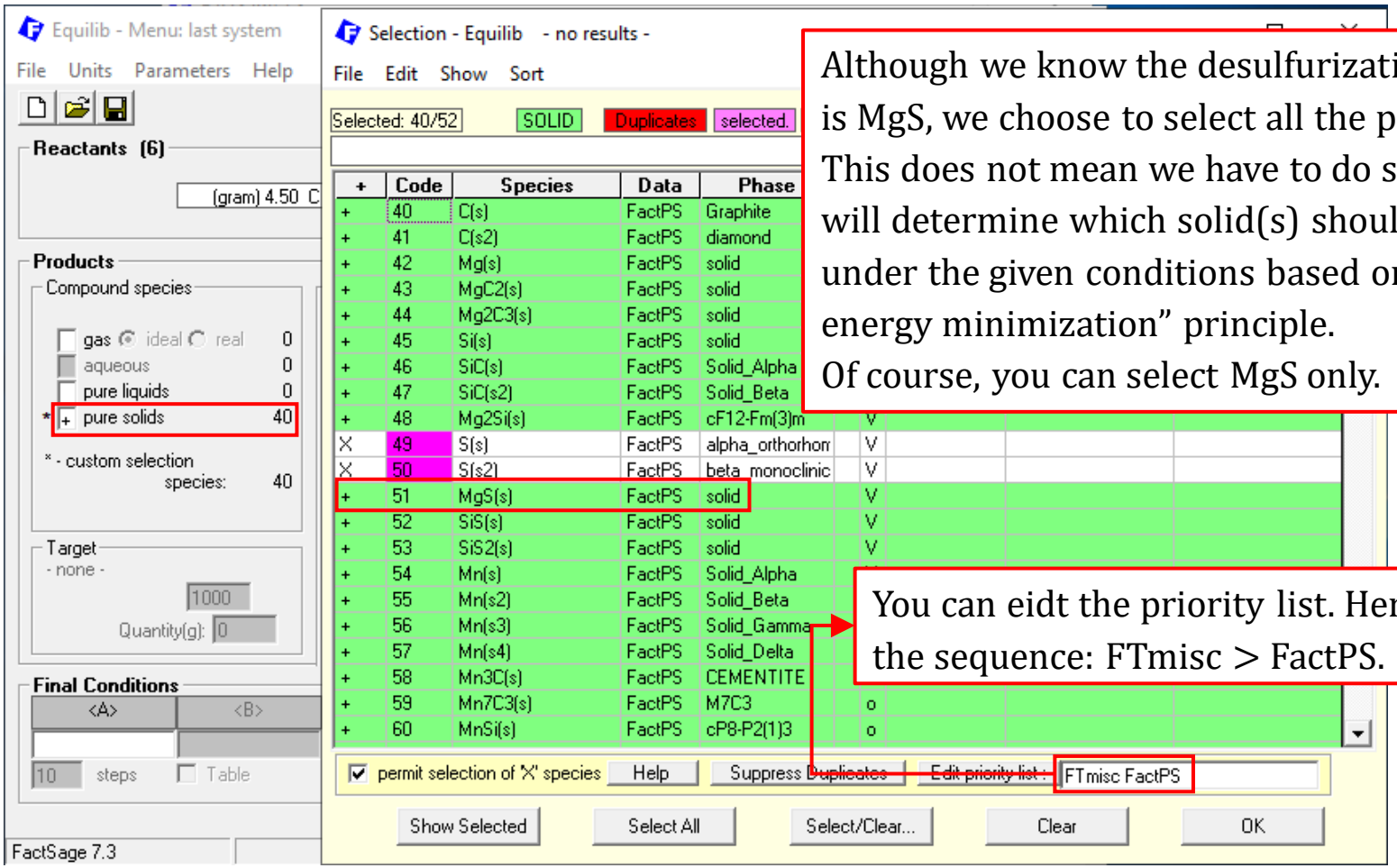
Example 1: Desulfurization (Basic Example)

Basic Example: Desulfurization of Hot Metal Using Mg



Example 1: Desulfurization (Basic Example)

Basic Example: Desulfurization of Hot Metal Using Mg

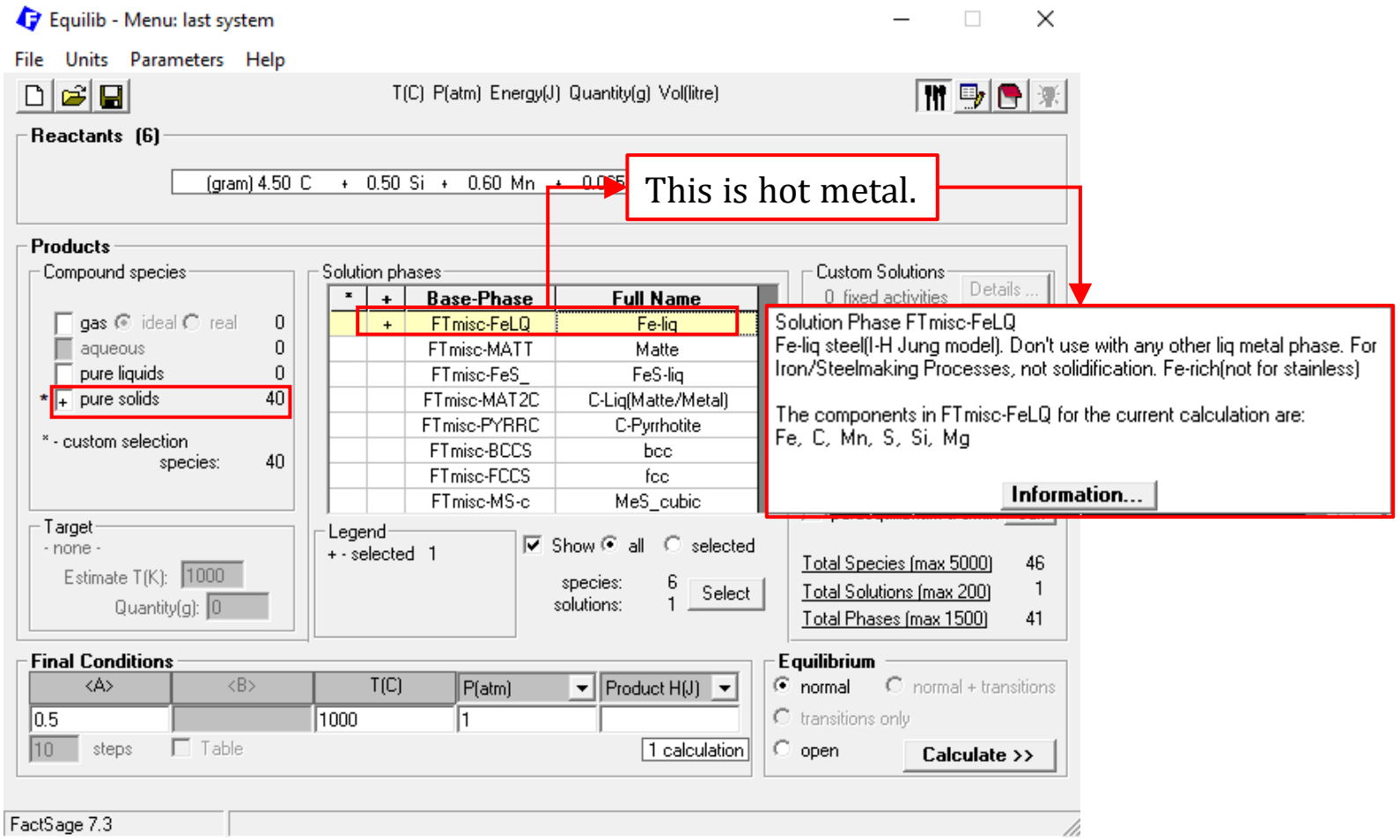


Although we know the desulfurization product is MgS, we choose to select all the pure solids. This does not mean we have to do so. FactSage will determine which solid(s) should exist under the given conditions based on the "Gibbs energy minimization" principle.
Of course, you can select MgS only.

You can eidt the priority list. Here, we follow the sequence: FTmisc > FactPS.

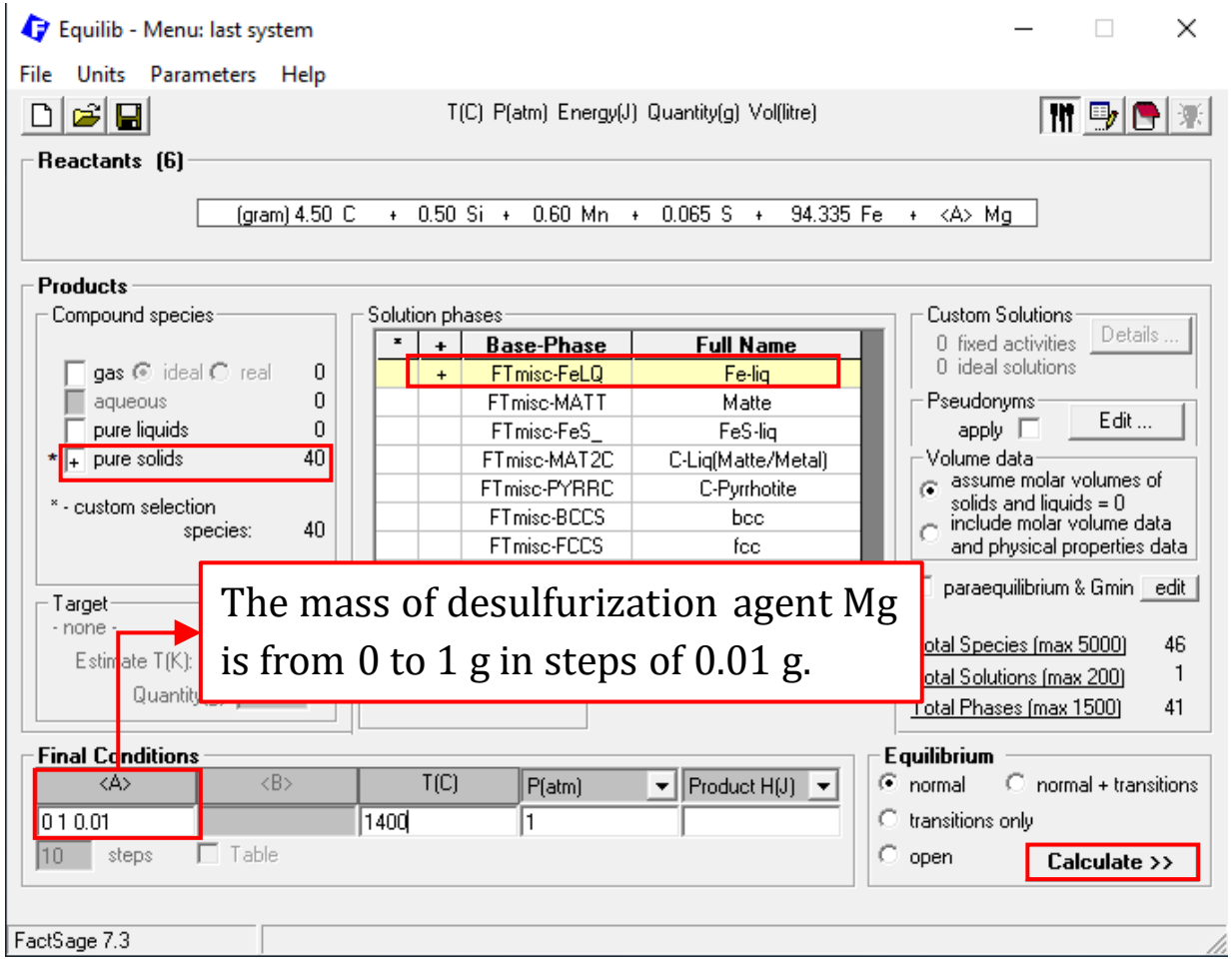
Example 1: Desulfurization (Basic Example)

Basic Example: Desulfurization of Hot Metal Using Mg



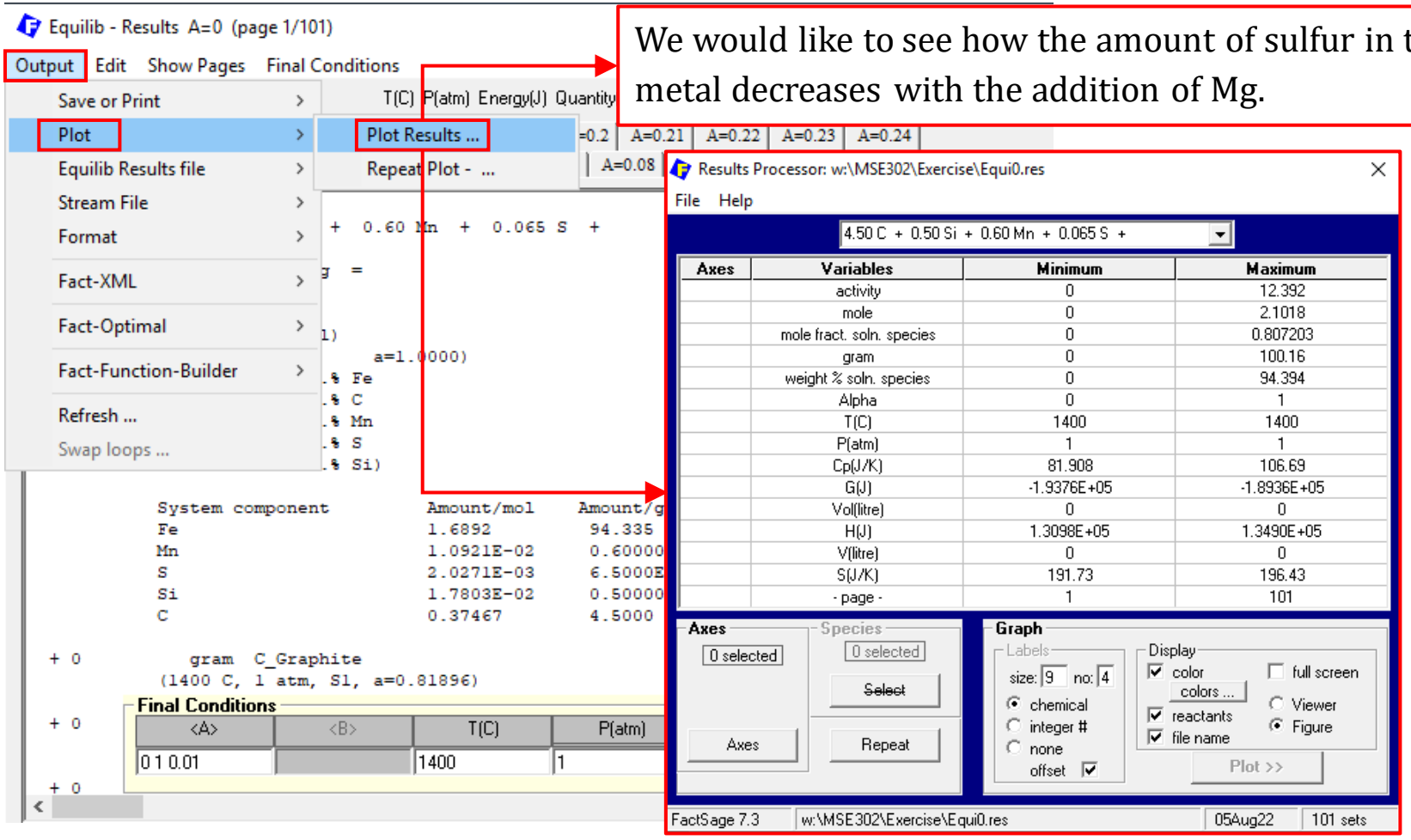
Example 1: Desulfurization (Basic Example)

Basic Example: Desulfurization of Hot Metal Using Mg



Example 1: Desulfurization (Basic Example)

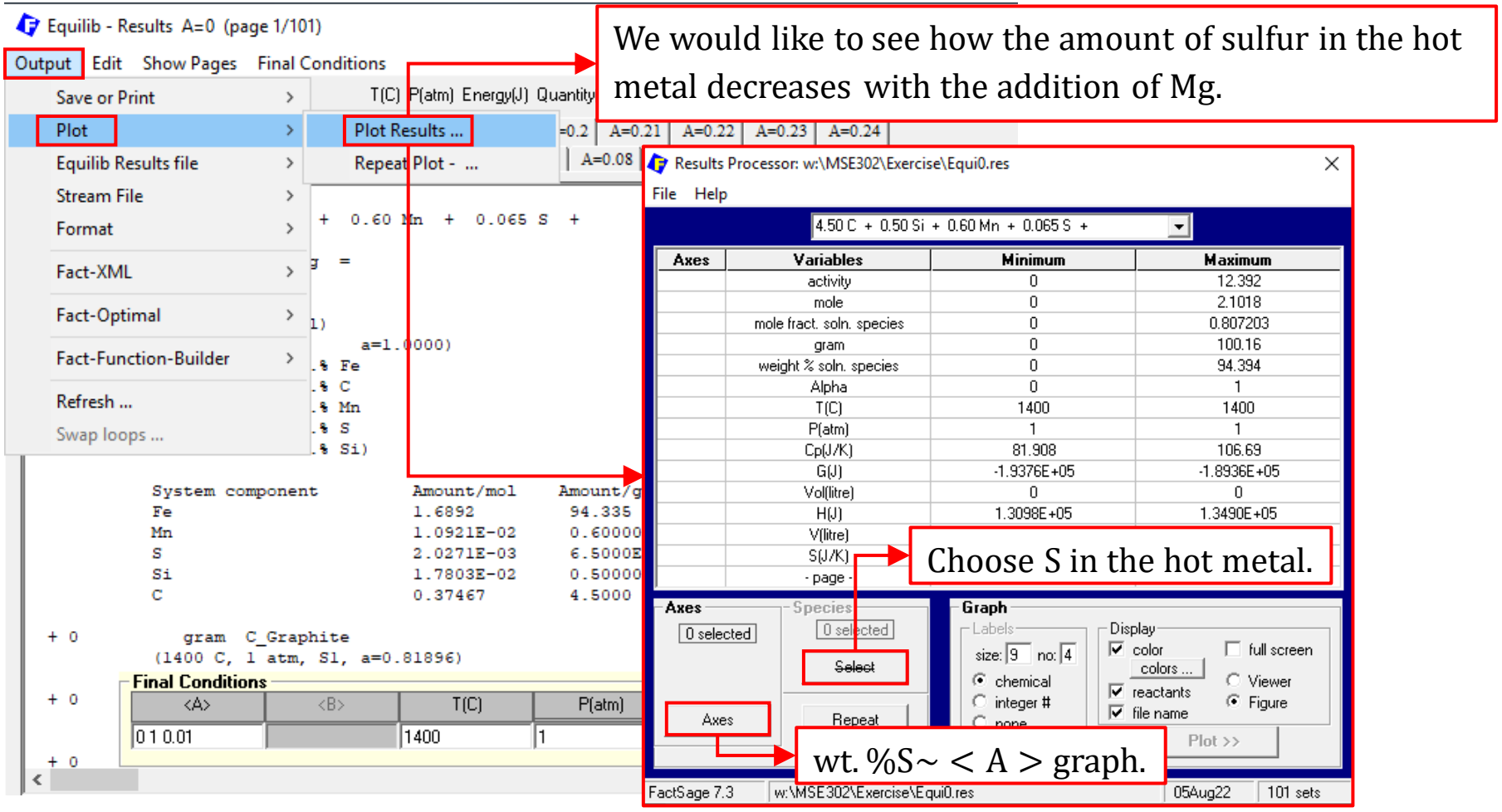
Basic Example: Desulfurization of Hot Metal Using Mg



We would like to see how the amount of sulfur in the hot metal decreases with the addition of Mg.

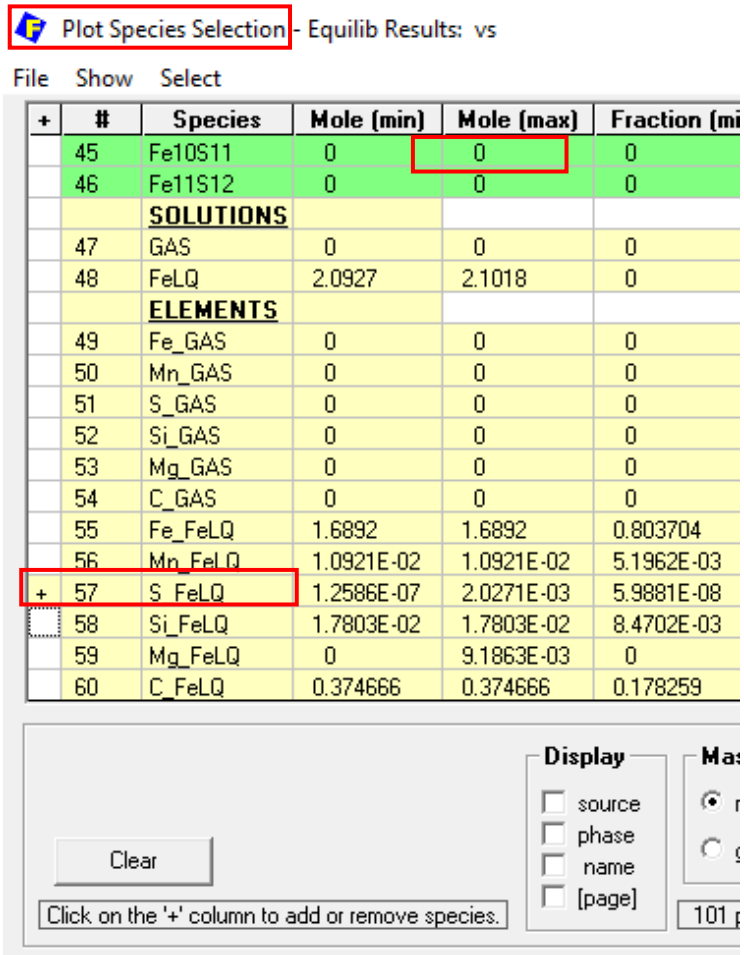
Example 1: Desulfurization (Basic Example)

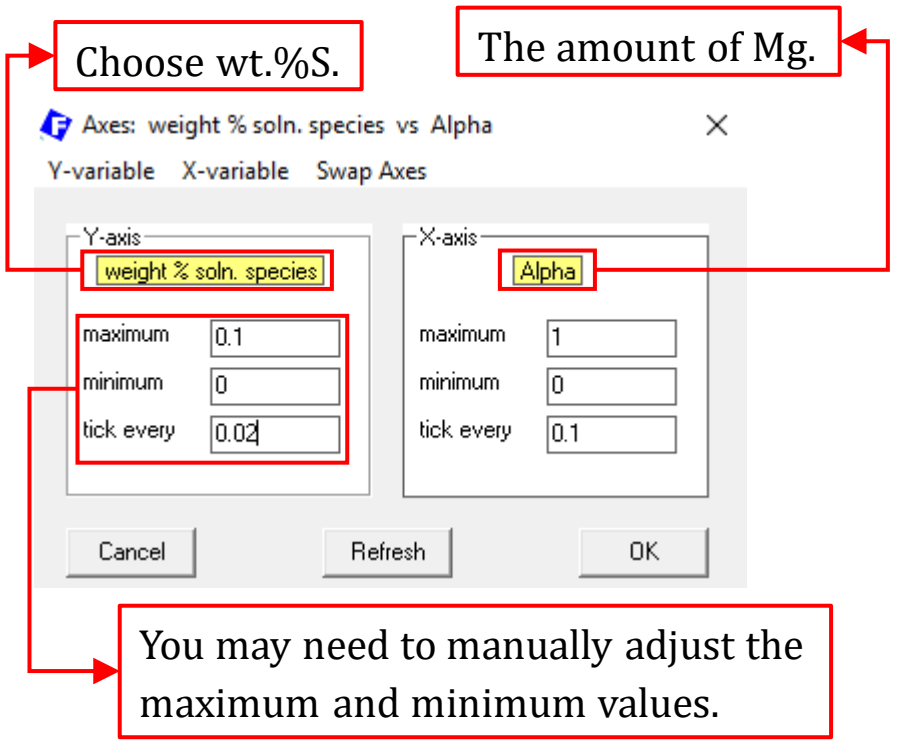
Basic Example: Desulfurization of Hot Metal Using Mg



Example 1: Desulfurization (Basic Example)

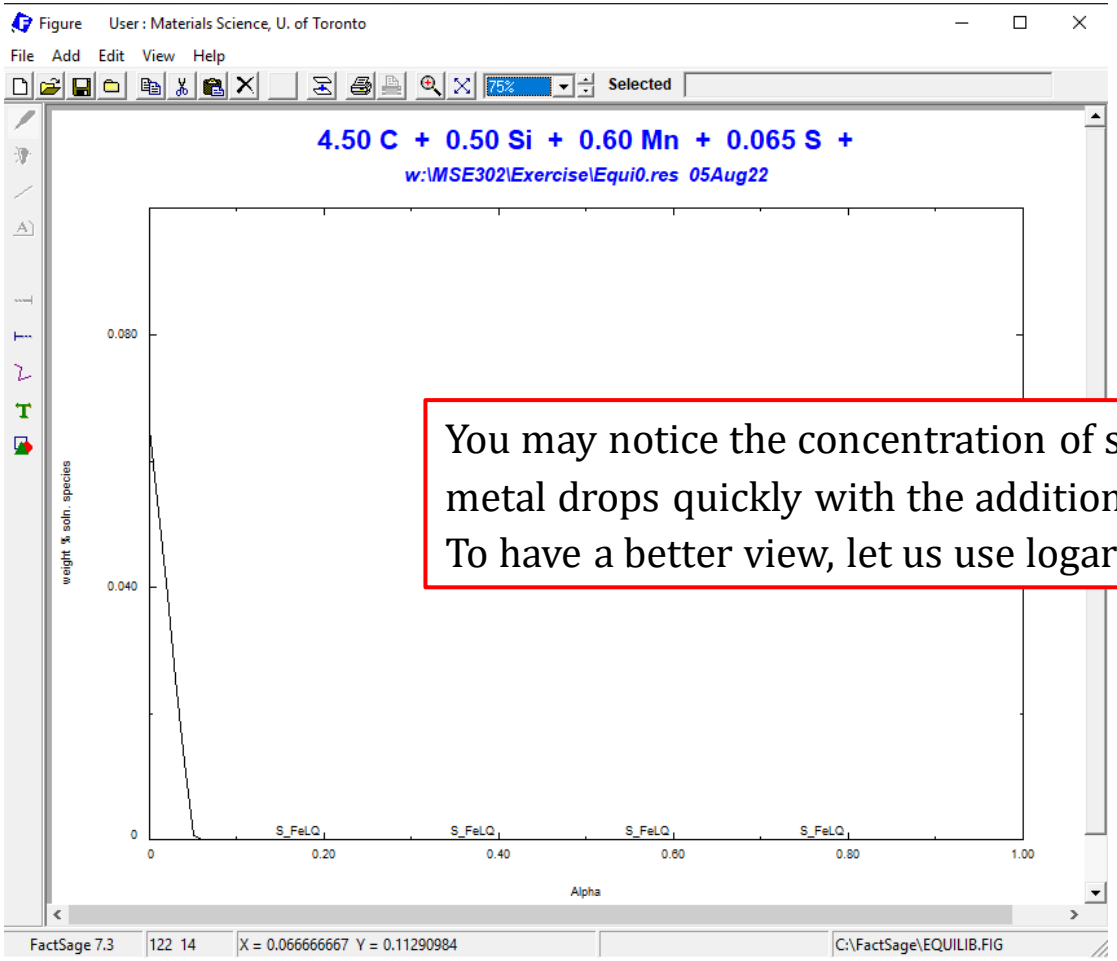
Basic Example: Desulfurization of Hot Metal Using Mg





Example 1: Desulfurization (Basic Example)

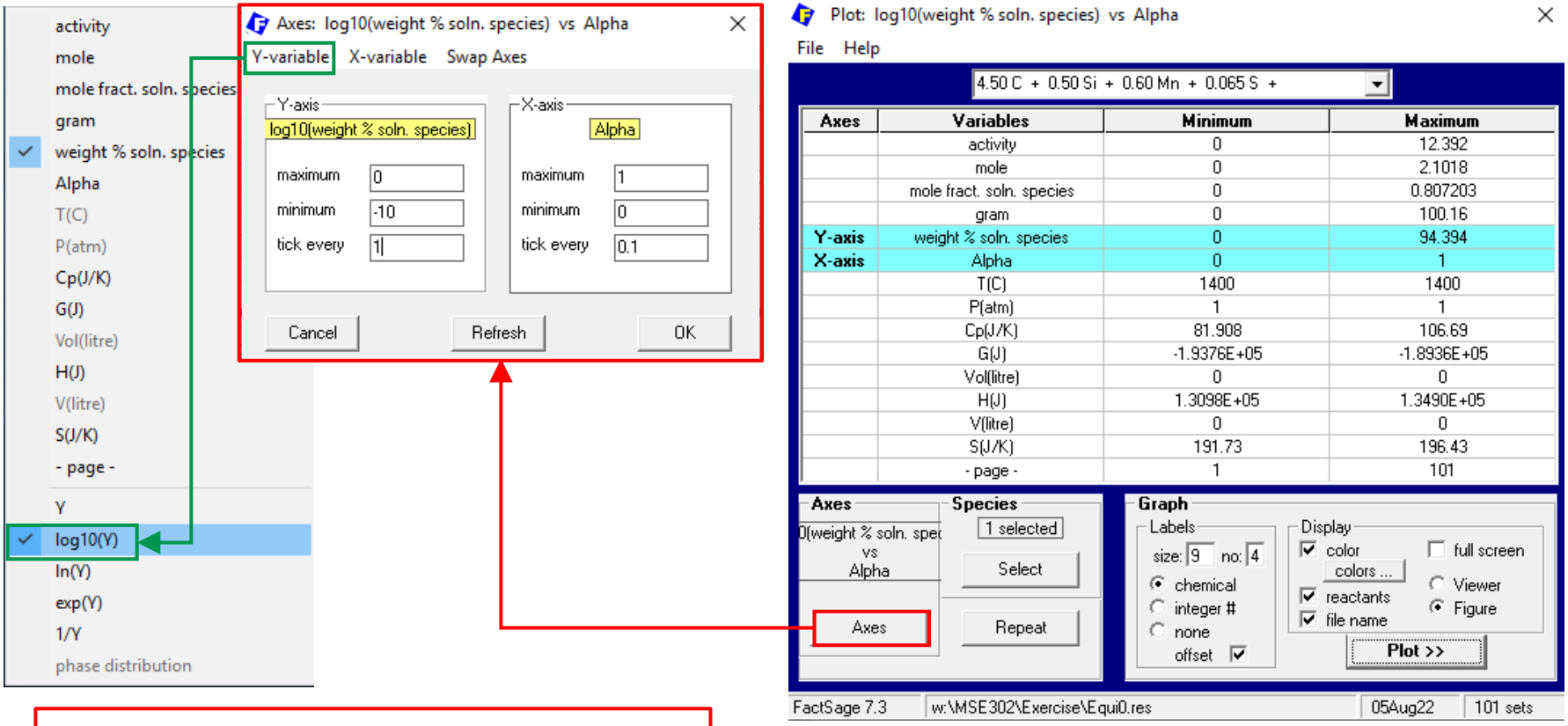
Basic Example: Desulfurization of Hot Metal Using Mg



You may notice the concentration of sulfur in the hot metal drops quickly with the addition of Mg.
To have a better view, let us use logarithm for Y-axis.

Example 1: Desulfurization (Basic Example)

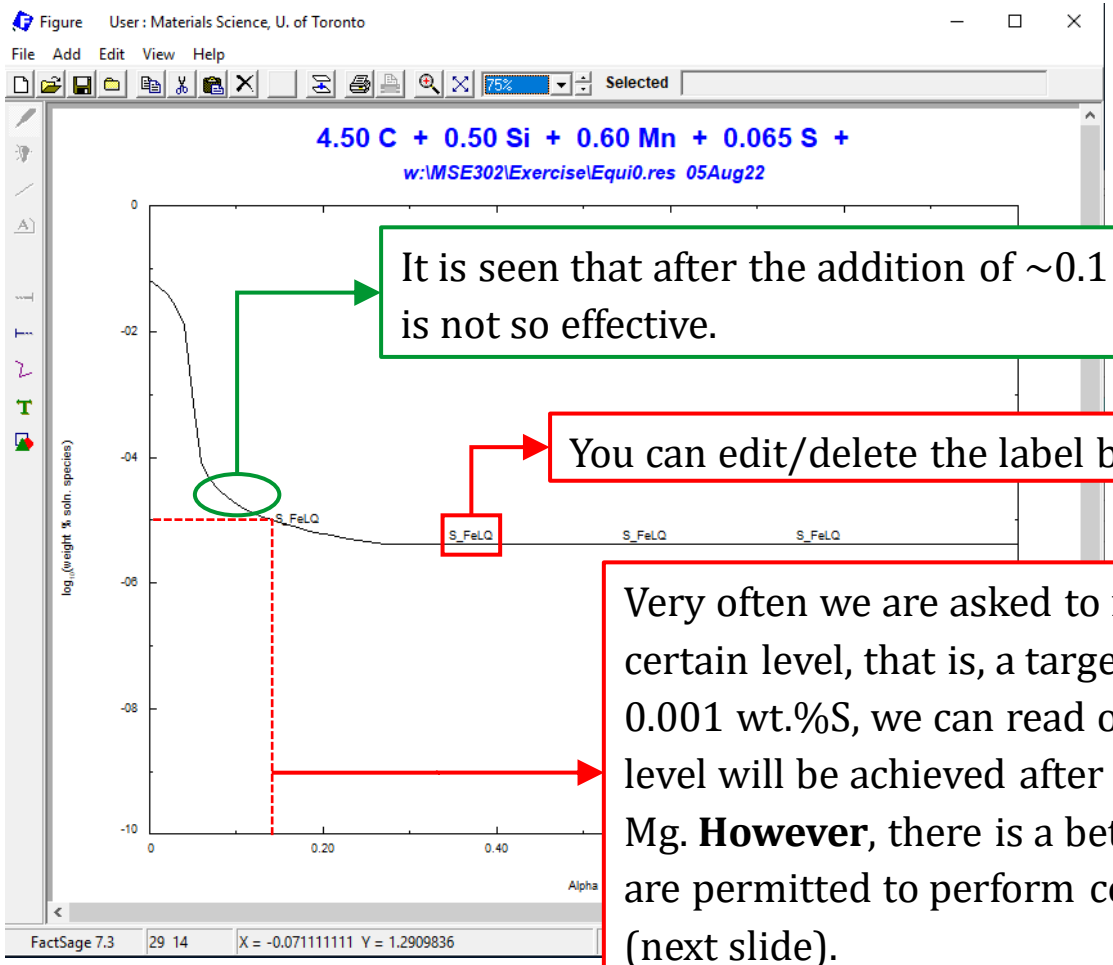
Basic Example: Desulfurization of Hot Metal Using Mg



Back to the Plot window. Click on “Axes”.

Example 1: Desulfurization (Basic Example)

Basic Example: Desulfurization of Hot Metal Using Mg



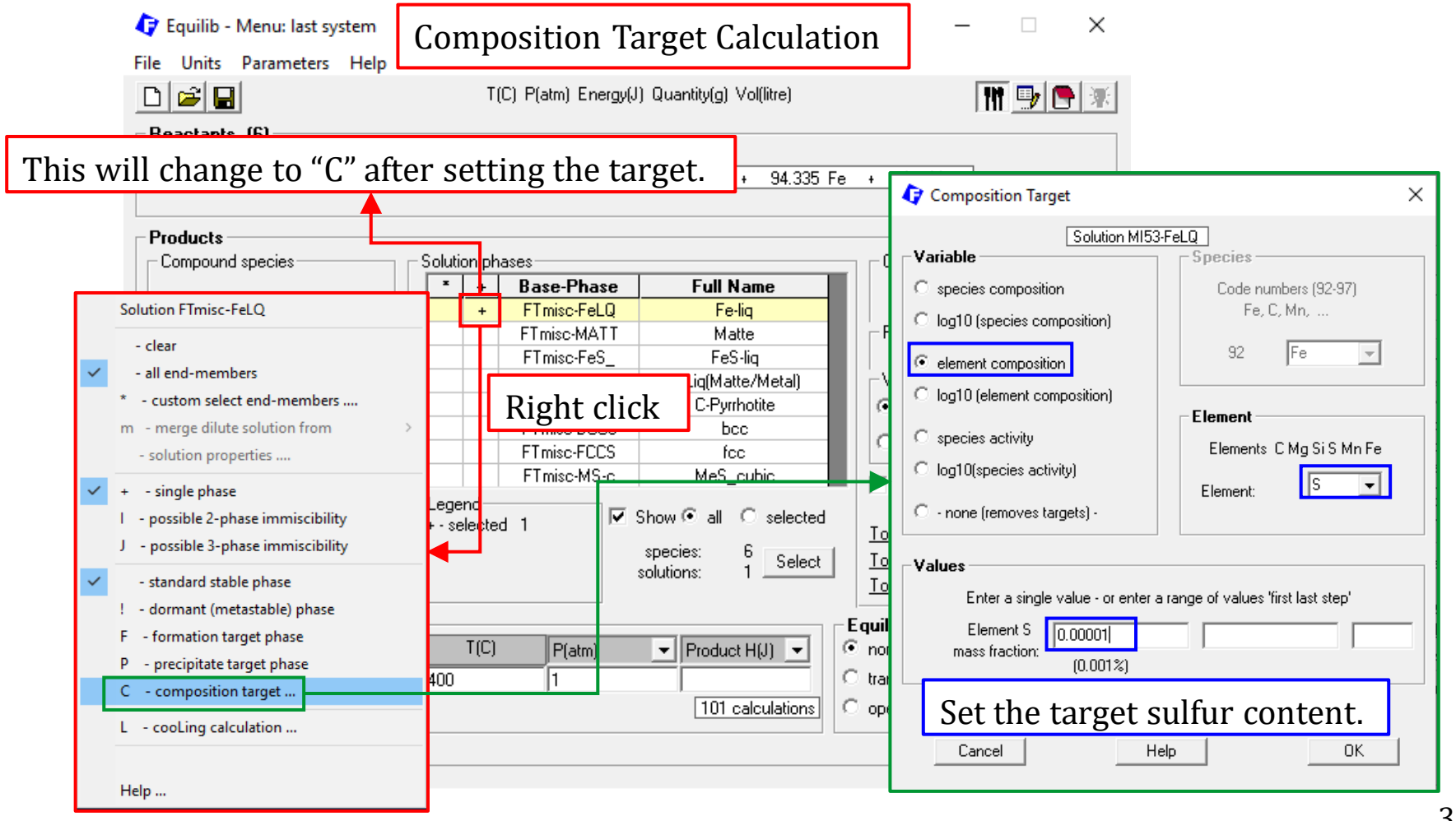
It is seen that after the addition of ~0.1 g Mg, the desulfurization is not so effective.

You can edit/delete the label by right clicking on it.

Very often we are asked to reduce the sulfur content to a certain level, that is, a target wt.%S. Say our target is 0.001 wt.%S, we can read off the graph that this sulfur level will be achieved after adding approximately 0.05 g Mg. **However**, there is a better way in FactSage and we are permitted to perform composition target calculation (next slide).

Example 1: Desulfurization (Basic Example)

Basic Example: Desulfurization of Hot Metal Using Mg



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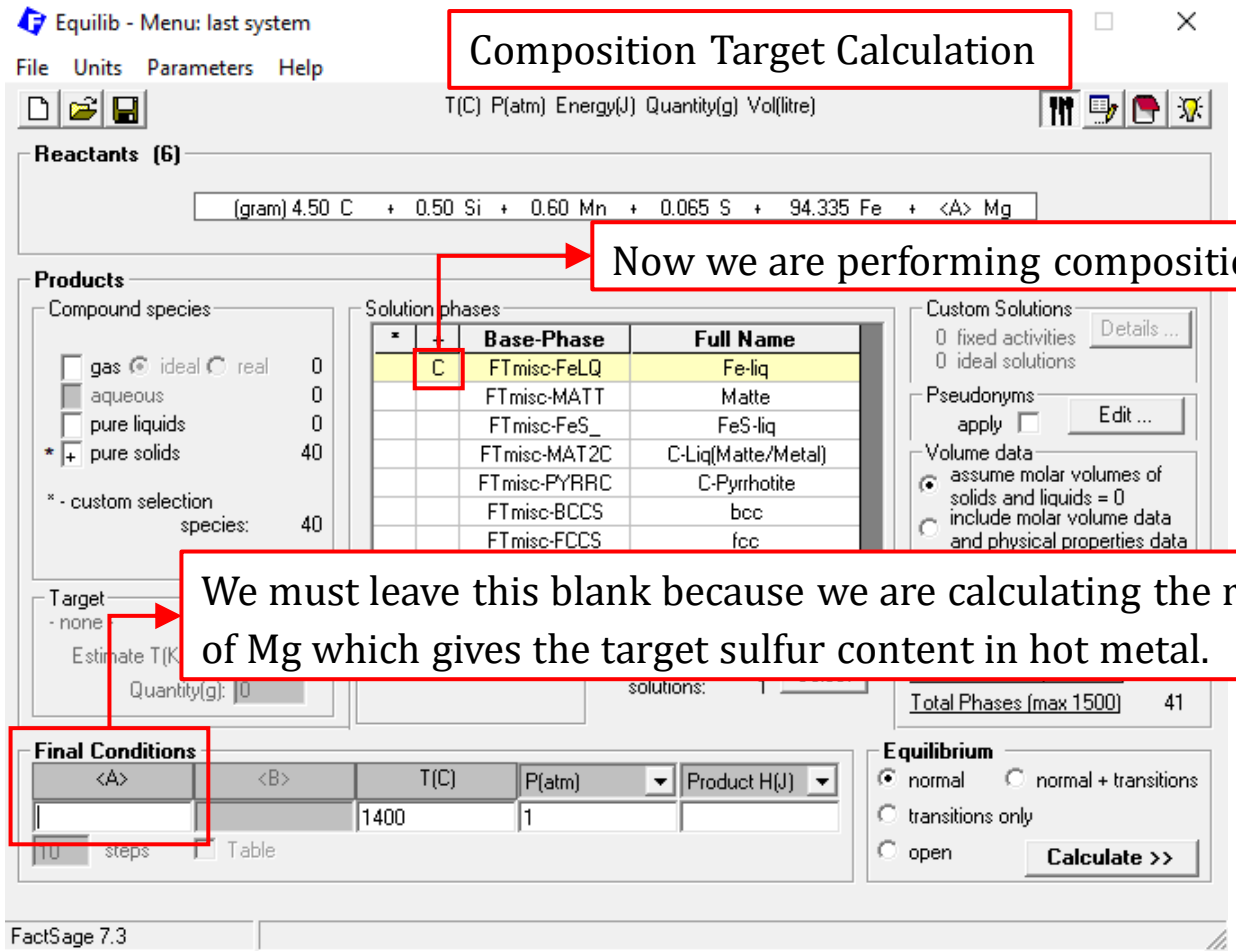
Basic Example: Desulfurization of Hot Metal Using Mg



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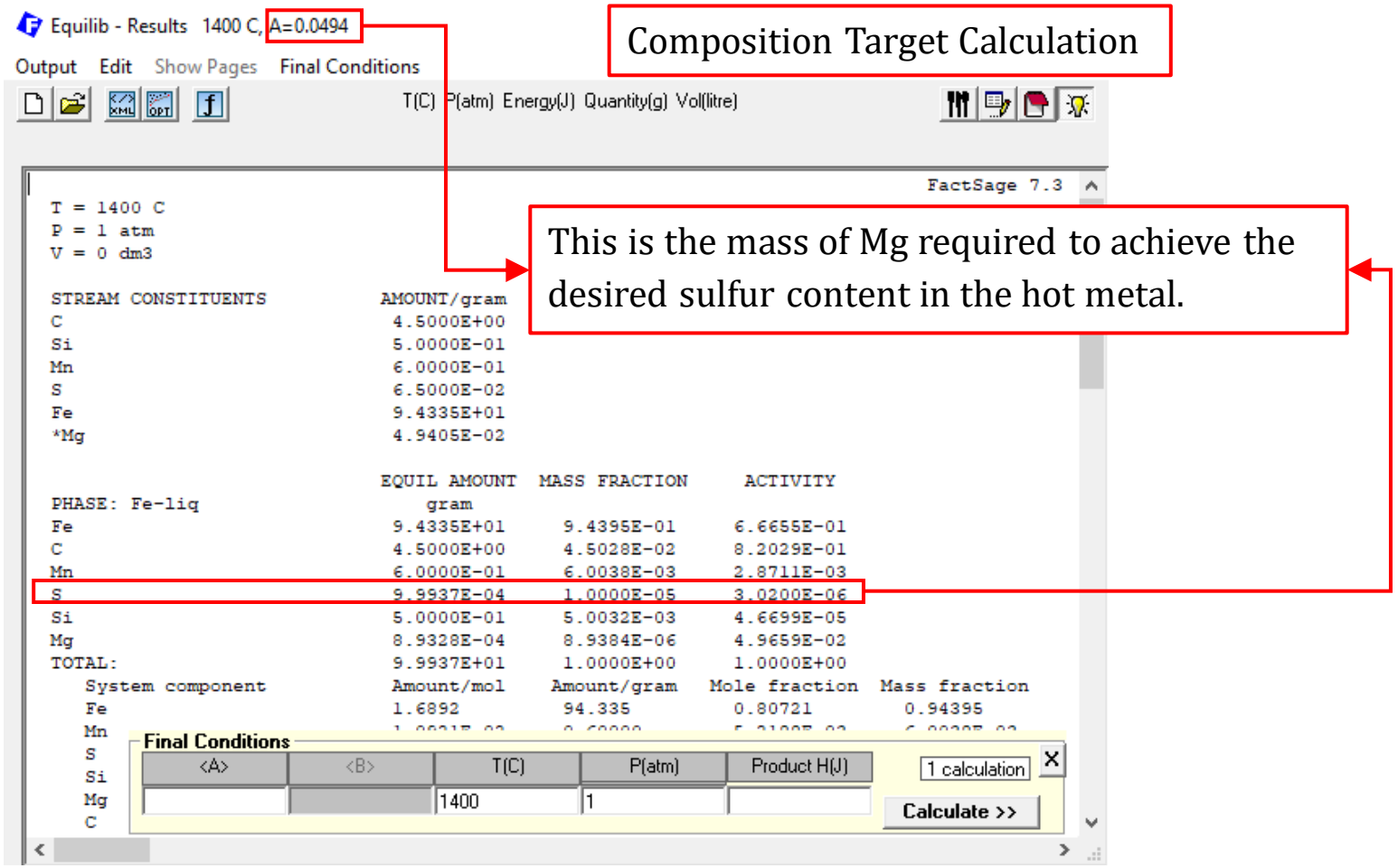
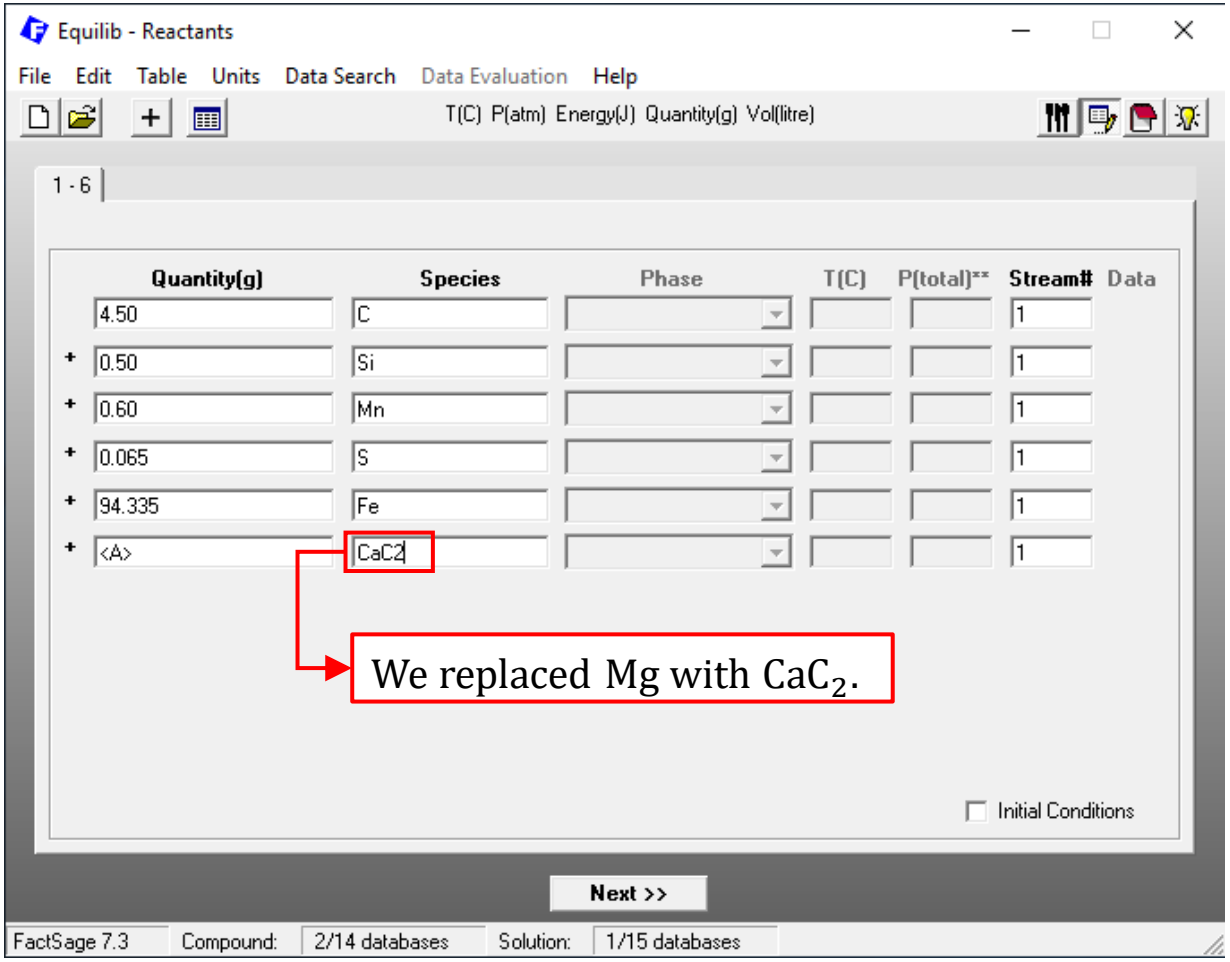
Basic Example: Desulfurization of Hot Metal Using Mg



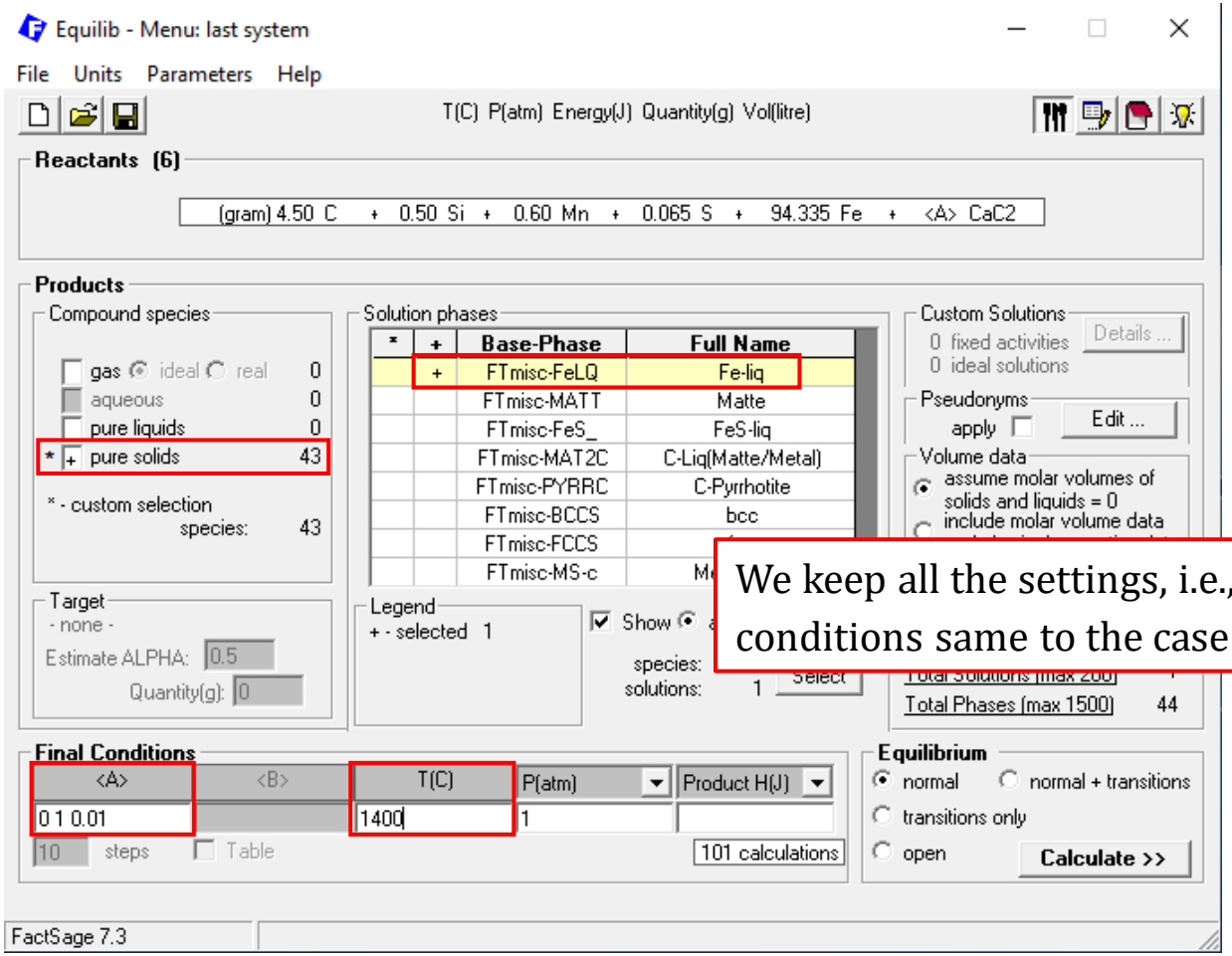
Example 1: Desulfurization (Basic Example)

Basic Example: Desulfurization of <u>Hot Metal</u> Using CaC_2



Example 1: Desulfurization (Basic Example)

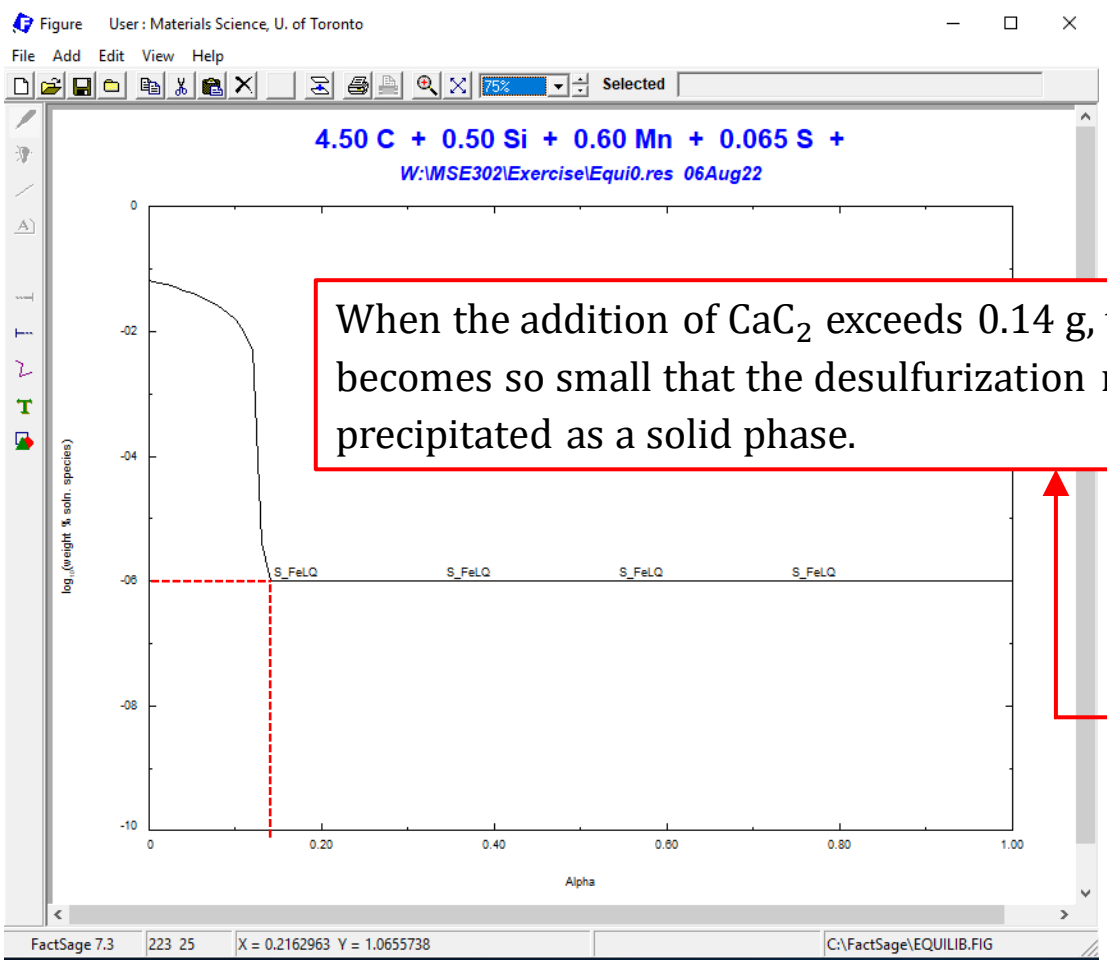
Basic Example: Desulfurization of Hot Metal Using CaC_2

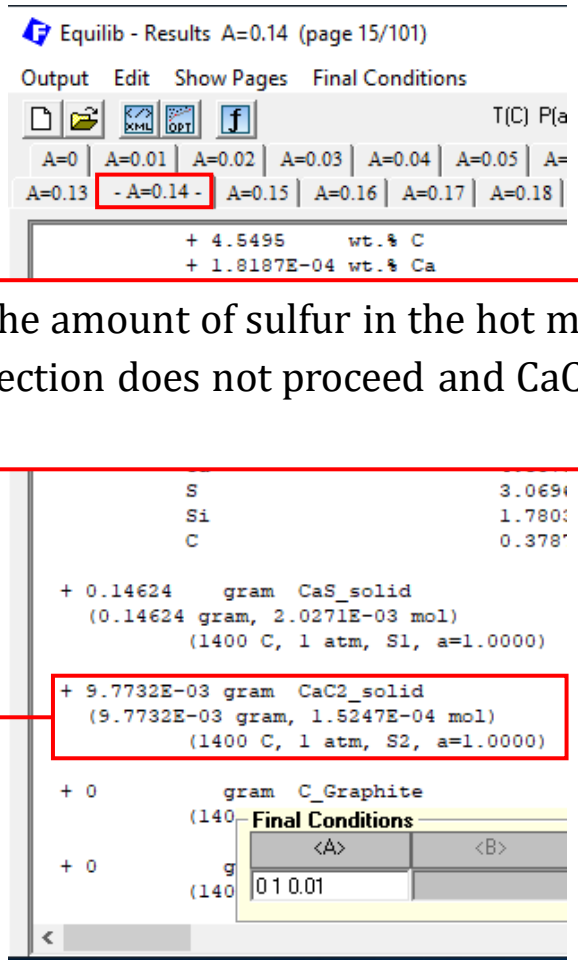


We keep all the settings, i.e., phase selection and final conditions same to the case where Mg was used.

Example 1: Desulfurization (Basic Example)

Basic Example: Desulfurization of Hot Metal Using CaC_2

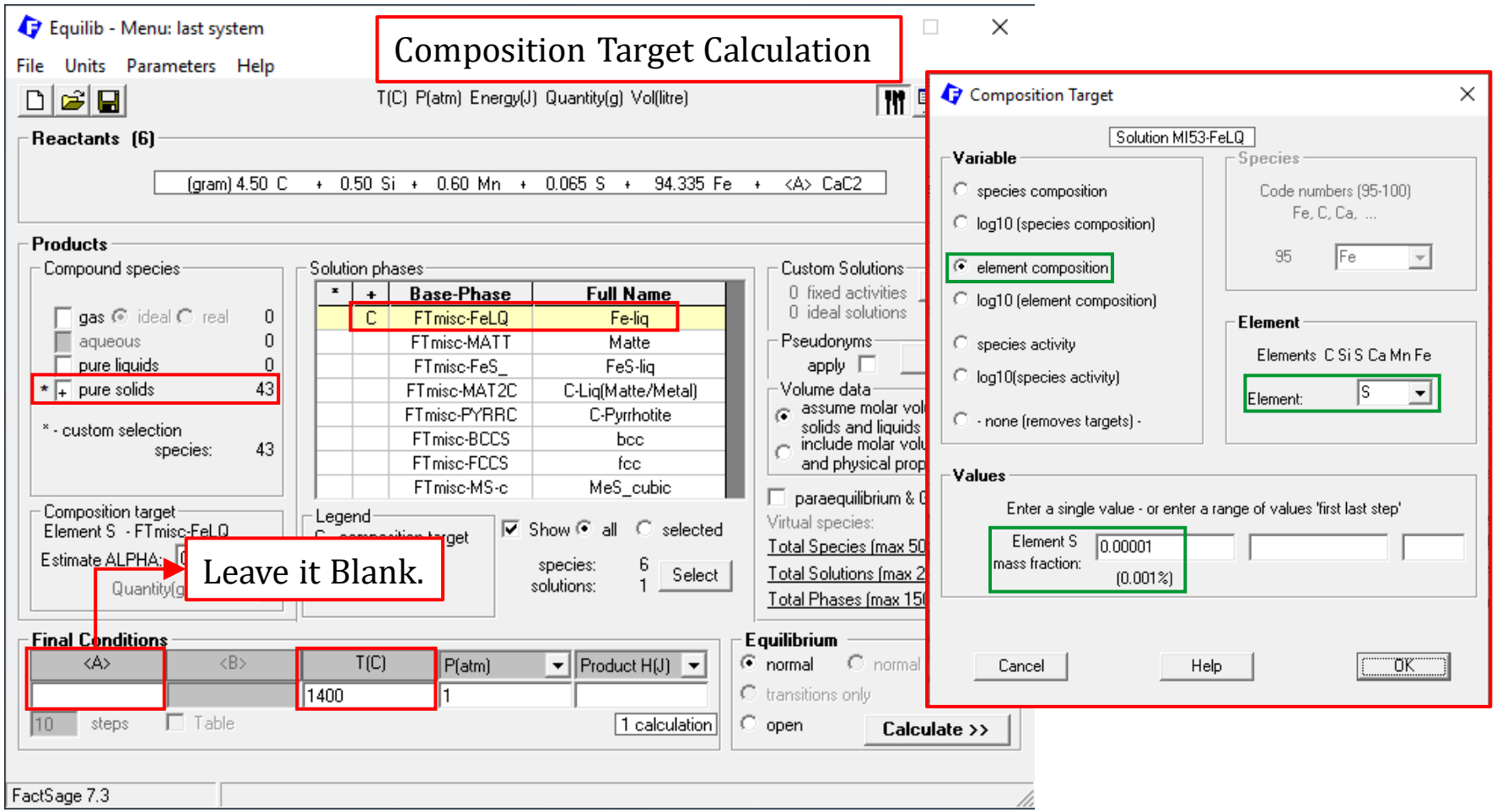




When the addition of CaC_2 exceeds 0.14 g, the amount of sulfur in the hot metal becomes so small that the desulfurization rection does not proceed and CaC_2 is precipitated as a solid phase.

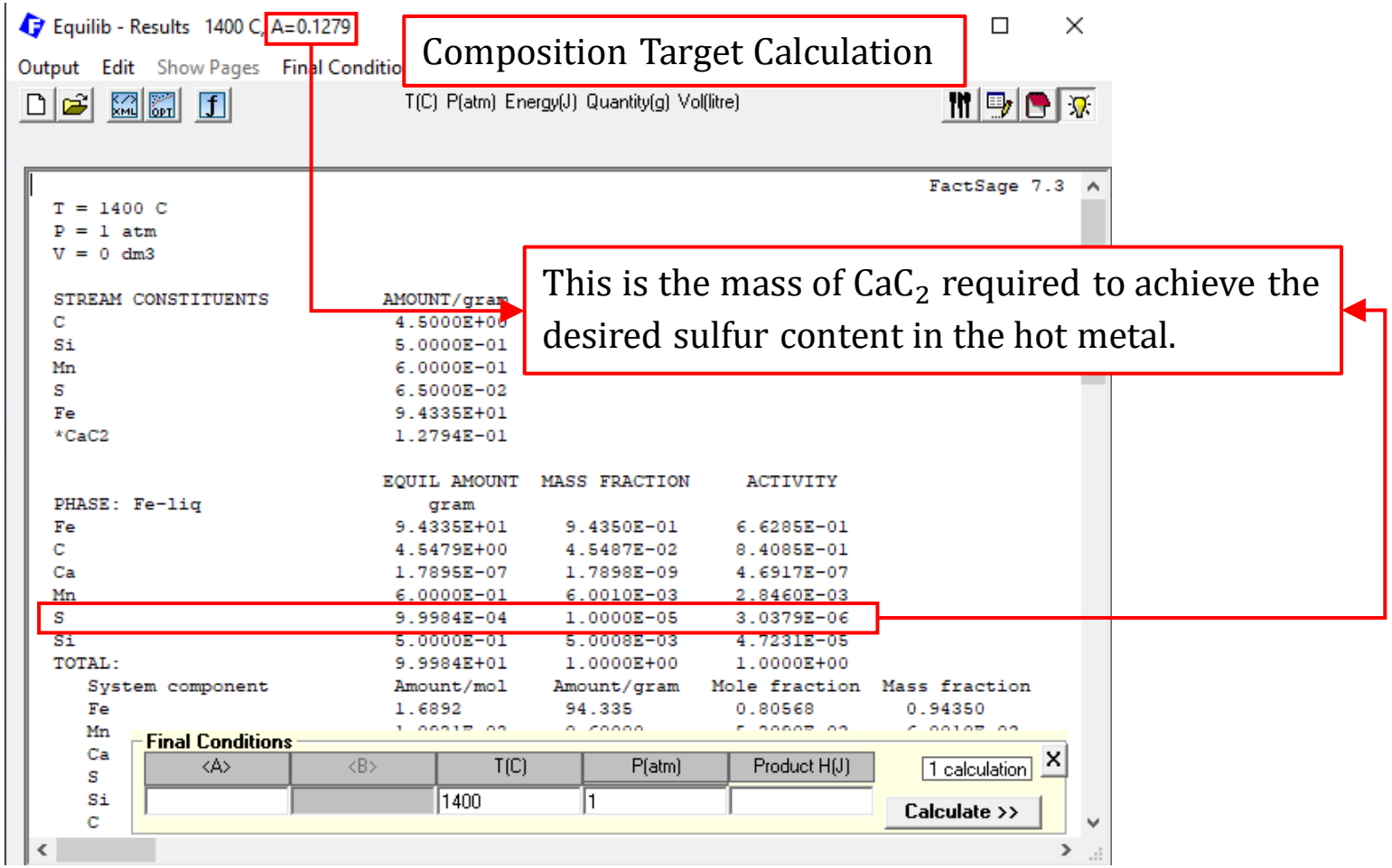
Example 1: Desulfurization (Basic Example)

Basic Example: Desulfurization of Hot Metal Using CaC_2



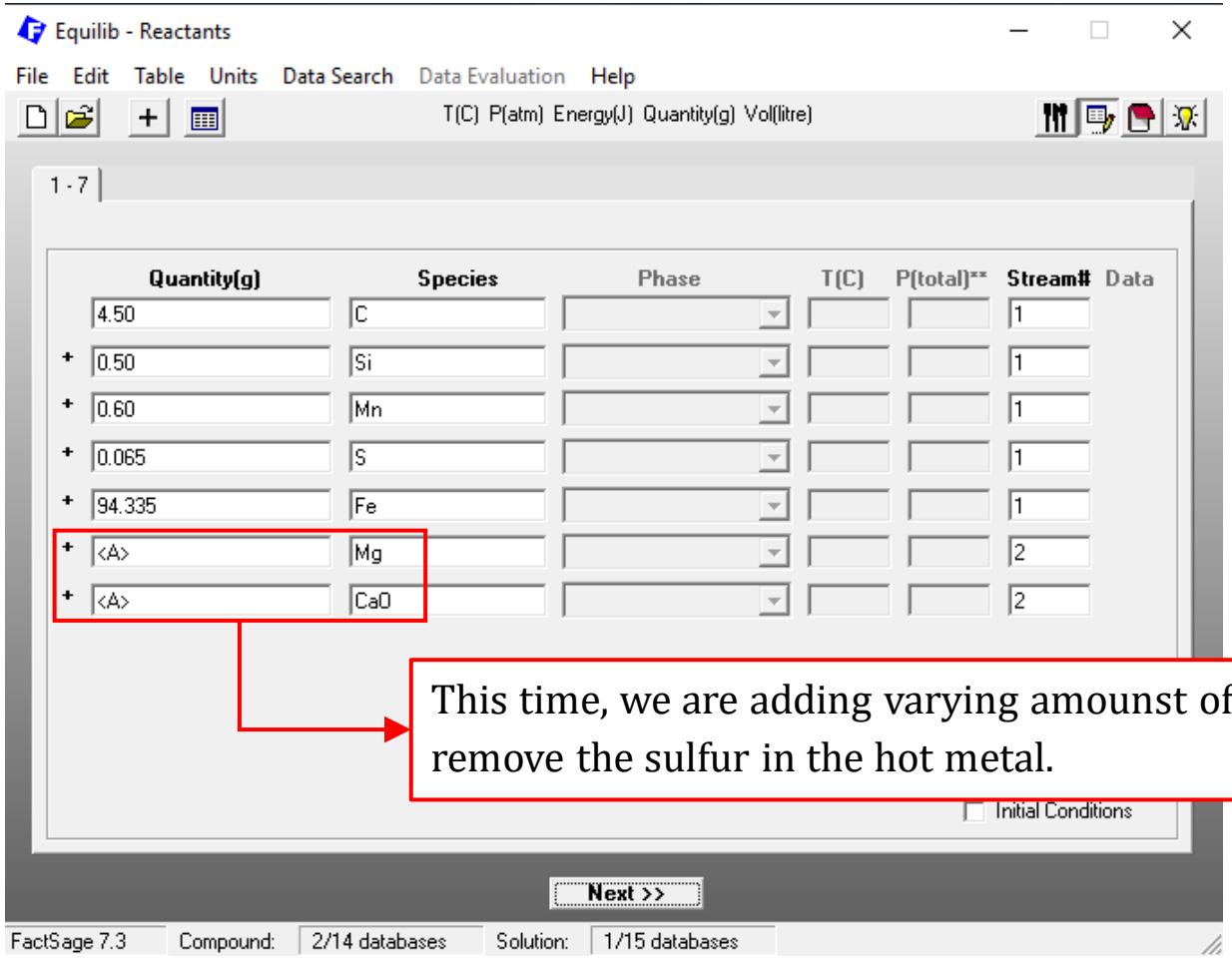
Example 1: Desulfurization (Basic Example)

Basic Example: Desulfurization of Hot Metal Using CaC_2



Example 1: Desulfurization (Basic Example)

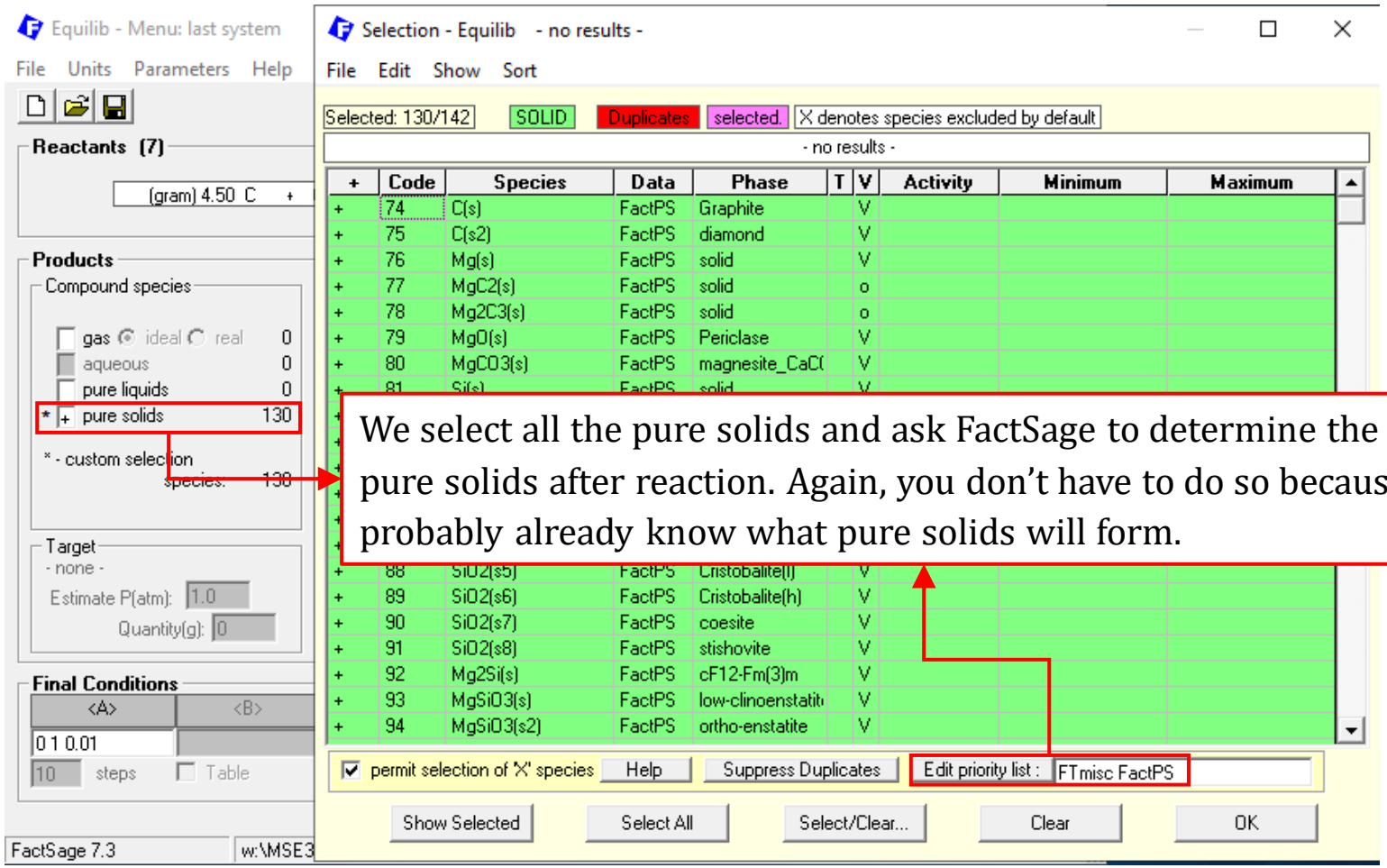
Basic Example: Desulfurization of <u>Hot Metal</u> Using CaO + Mg



This time, we are adding varying amounst of CaO and Mg to remove the sulfur in the hot metal.

Example 1: Desulfurization (Basic Example)

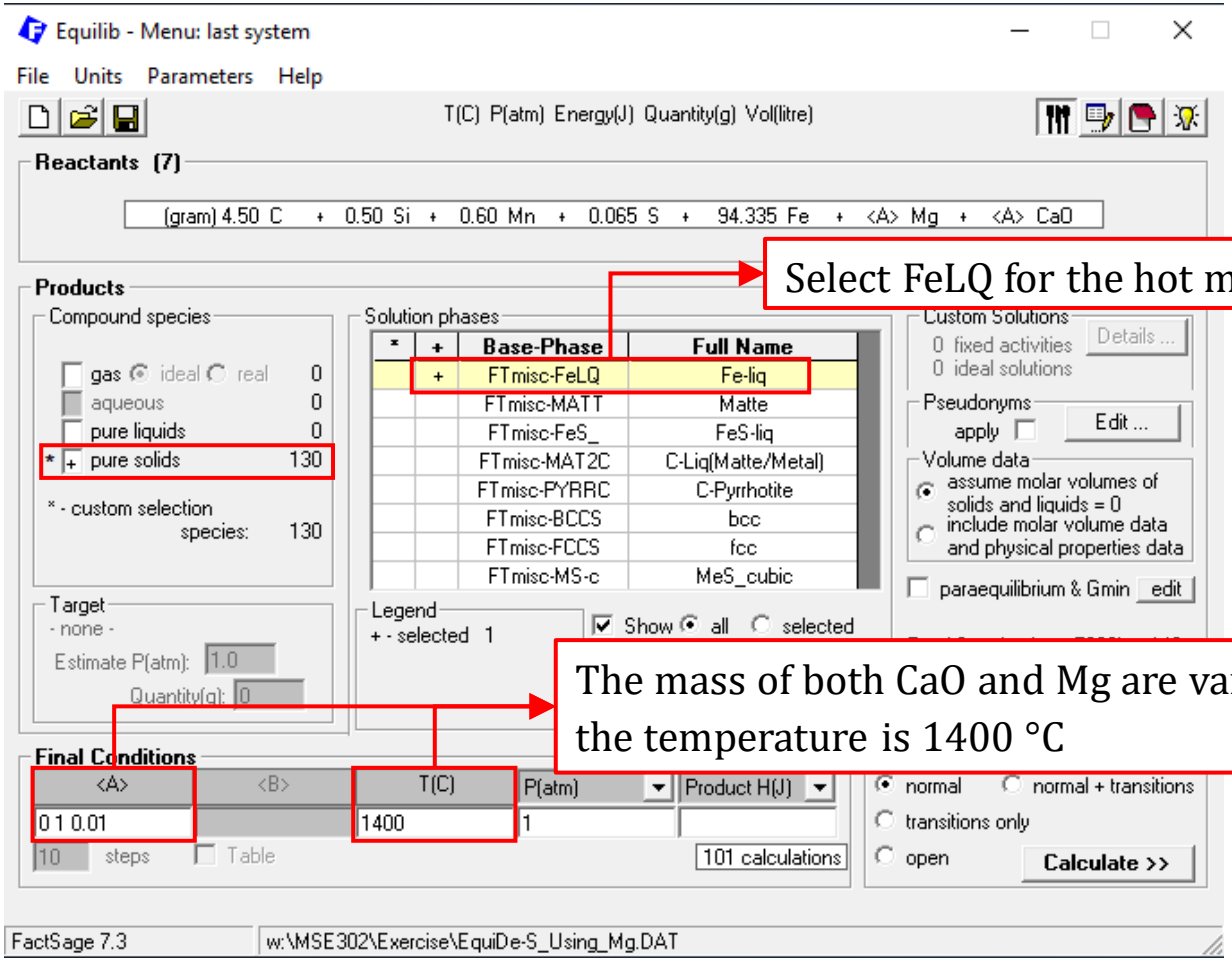
Basic Example: Desulfurization of Hot Metal Using CaO + Mg



We select all the pure solids and ask FactSage to determine the stable pure solids after reaction. Again, you don't have to do so because you probably already know what pure solids will form.

Example 1: Desulfurization (Basic Example)

Basic Example: Desulfurization of Hot Metal Using CaO + Mg

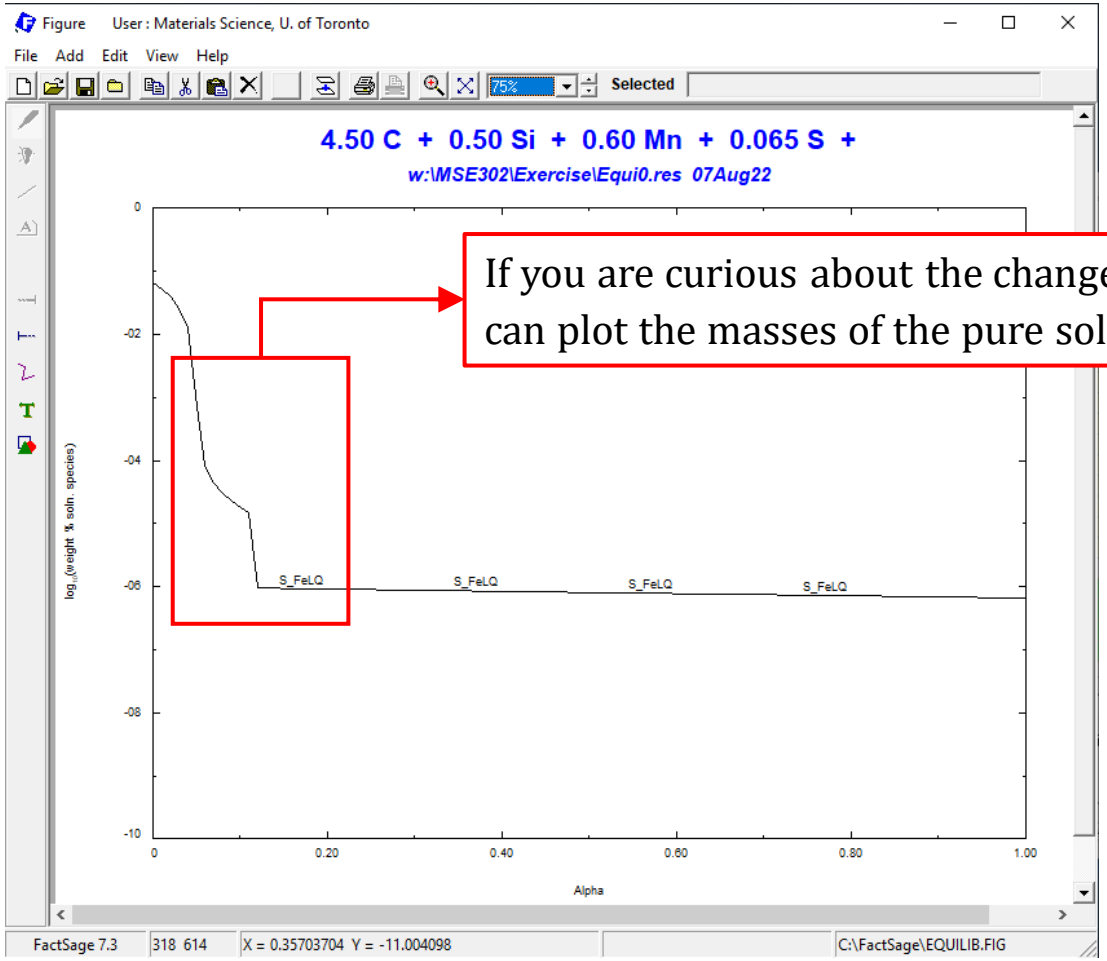


Select FeLQ for the hot metal.

The mass of both CaO and Mg are varied from 0 to 1.0 g, and the temperature is 1400 °C

Example 1: Desulfurization (Basic Example)

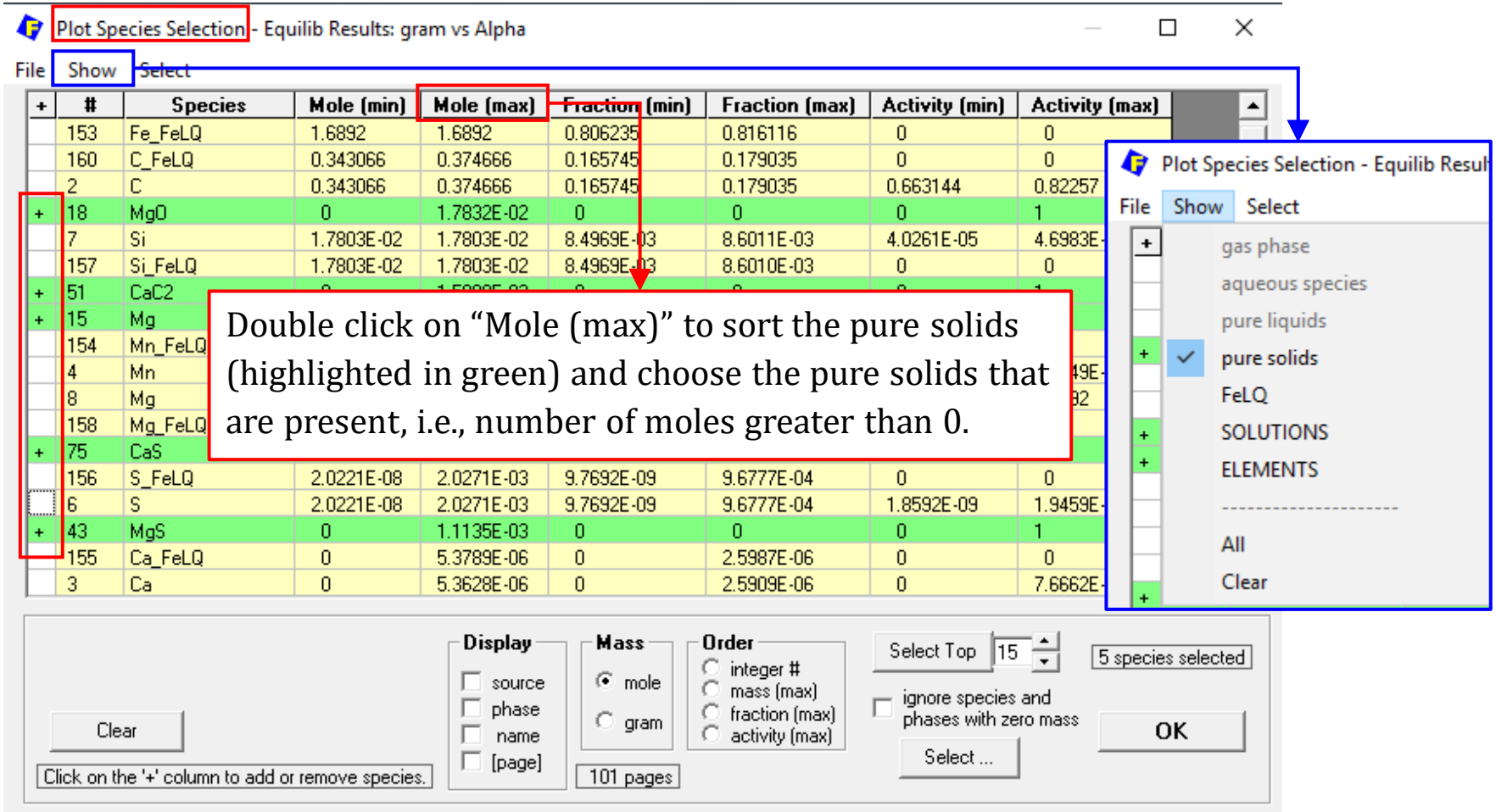
Basic Example: Desulfurization of <u>Hot Metal</u> Using CaO + Mg



If you are curious about the change in the slope of wt. %S~<A>, you can plot the masses of the pure solids against <A>.

Example 1: Desulfurization (Basic Example)

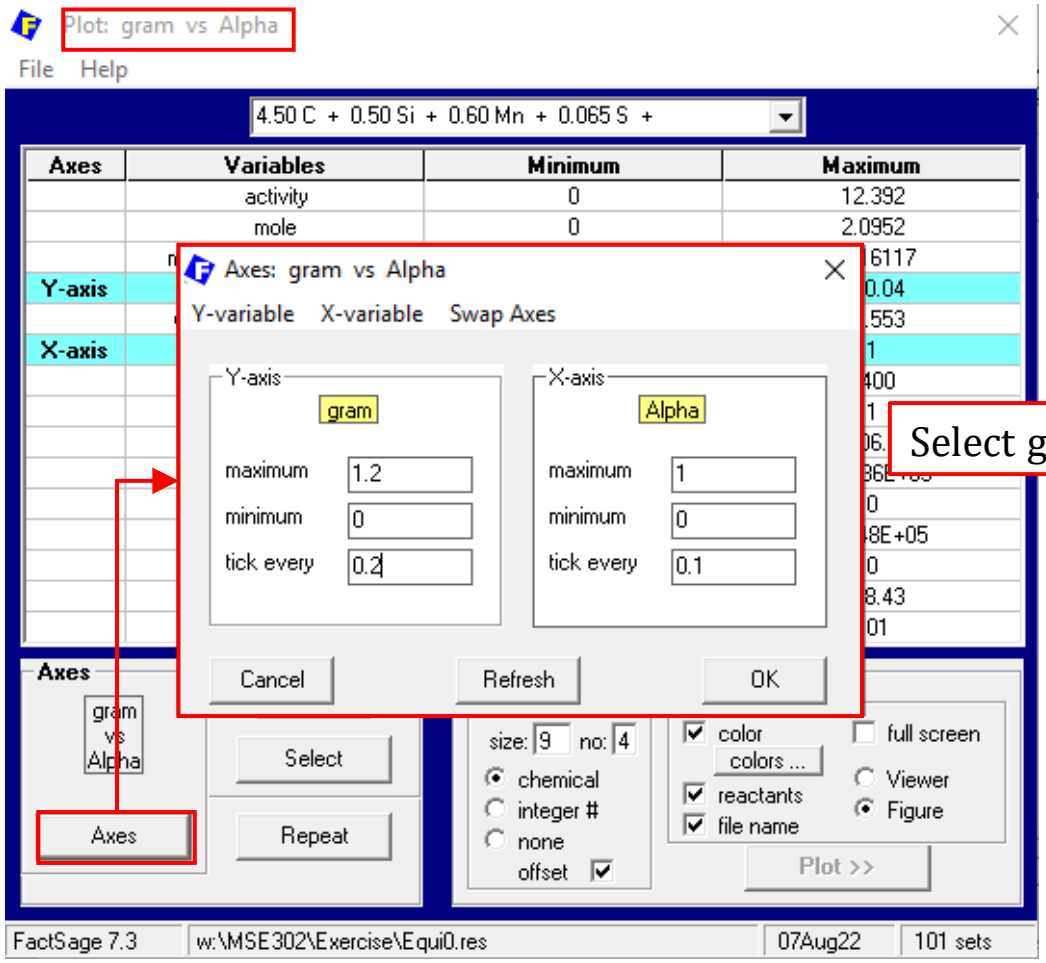
Basic Example: Desulfurization of Hot Metal Using CaO + Mg



+	#	Species	Mole (min)	Mole (max)	Fraction (min)	Fraction (max)	Activity (min)	Activity (max)
	153	Fe_FeLQ	1.6892	1.6892	0.806235	0.816116	0	0
	160	C_FeLQ	0.343066	0.374666	0.165745	0.179035	0	0
	2	C	0.343066	0.374666	0.165745	0.179035	0.663144	0.82257
+	18	MgO	0	1.7832E-02	0	0	0	1
	7	Si	1.7803E-02	1.7803E-02	8.4969E-03	8.6011E-03	4.0261E-05	4.6983E-
	157	Si_FeLQ	1.7803E-02	1.7803E-02	8.4969E-03	8.6010E-03	0	0
+	51	CaC2						
+	15	Mg						
	154	Mn_FeLQ						
	4	Mn						49E-
	8	Mg						82
	158	Mg_FeLQ						
+	75	CaS						
	156	S_FeLQ	2.0221E-08	2.0271E-03	9.7692E-09	9.6777E-04	0	0
	6	S	2.0221E-08	2.0271E-03	9.7692E-09	9.6777E-04	1.8592E-09	1.9459E-
+	43	MgS	0	1.1135E-03	0	0	0	1
	155	Ca_FeLQ	0	5.3789E-06	0	2.5987E-06	0	0
	3	Ca	0	5.3628E-06	0	2.5909E-06	0	7.6662E-

Example 1: Desulfurization (Basic Example)

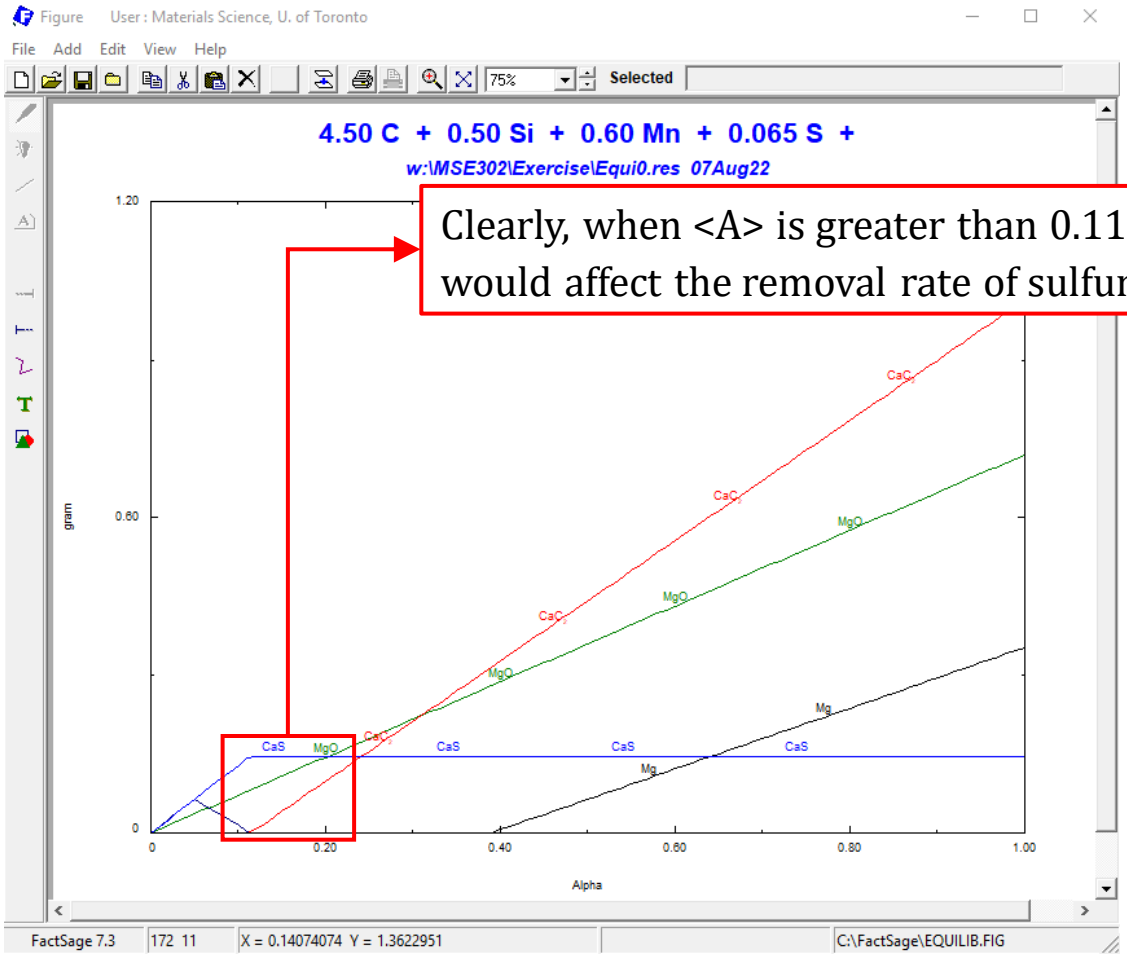
Basic Example: Desulfurization of <u>Hot Metal</u> Using CaO + Mg



Select gram for Y-axis and <A> for X-axis.

Example 1: Desulfurization (Basic Example)

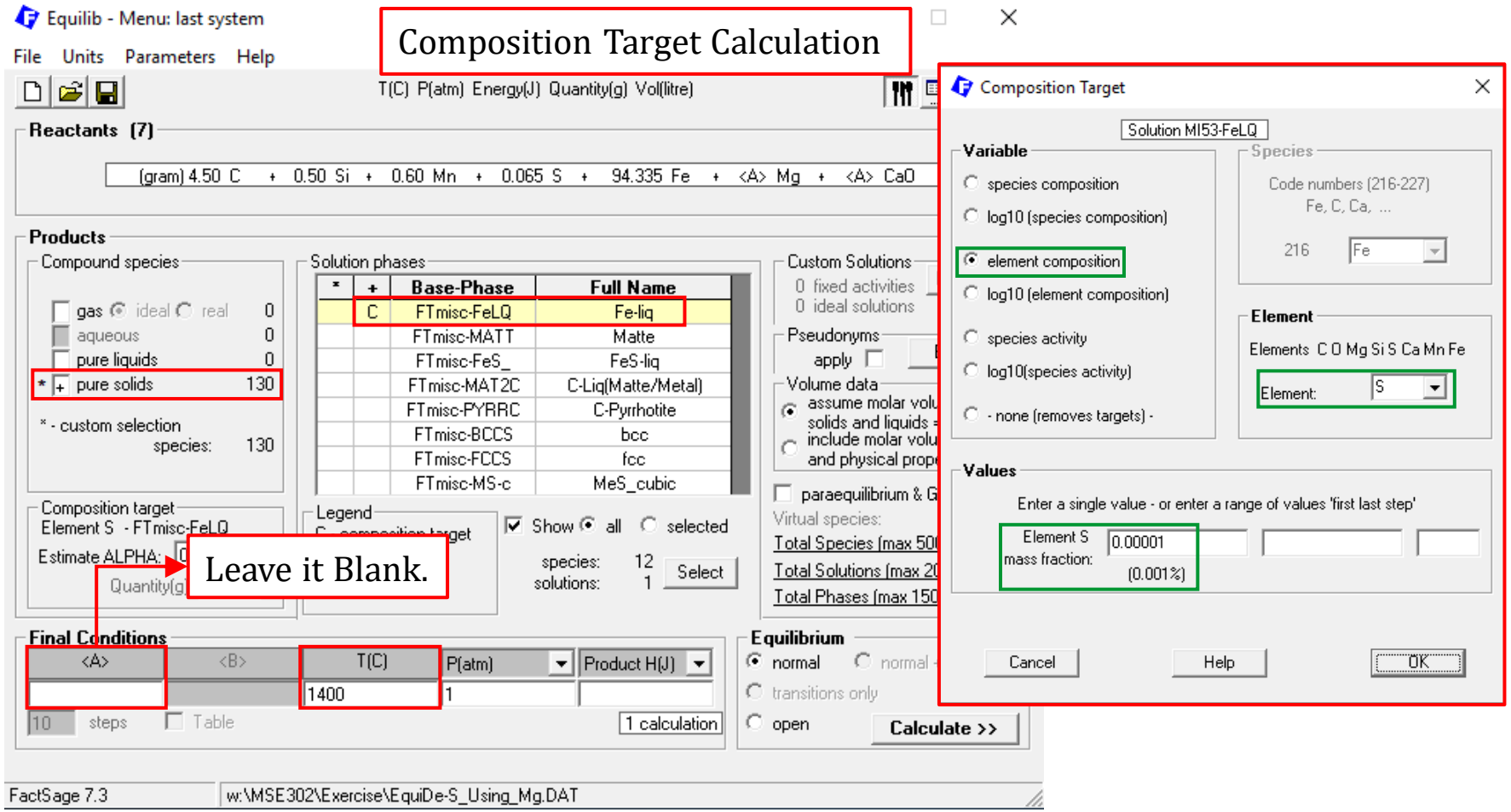
Basic Example: Desulfurization of Hot Metal Using CaO + Mg



Clearly, when <A> is greater than 0.11, CaC_2 starts to precipitate; this would affect the removal rate of sulfur from the hot metal.

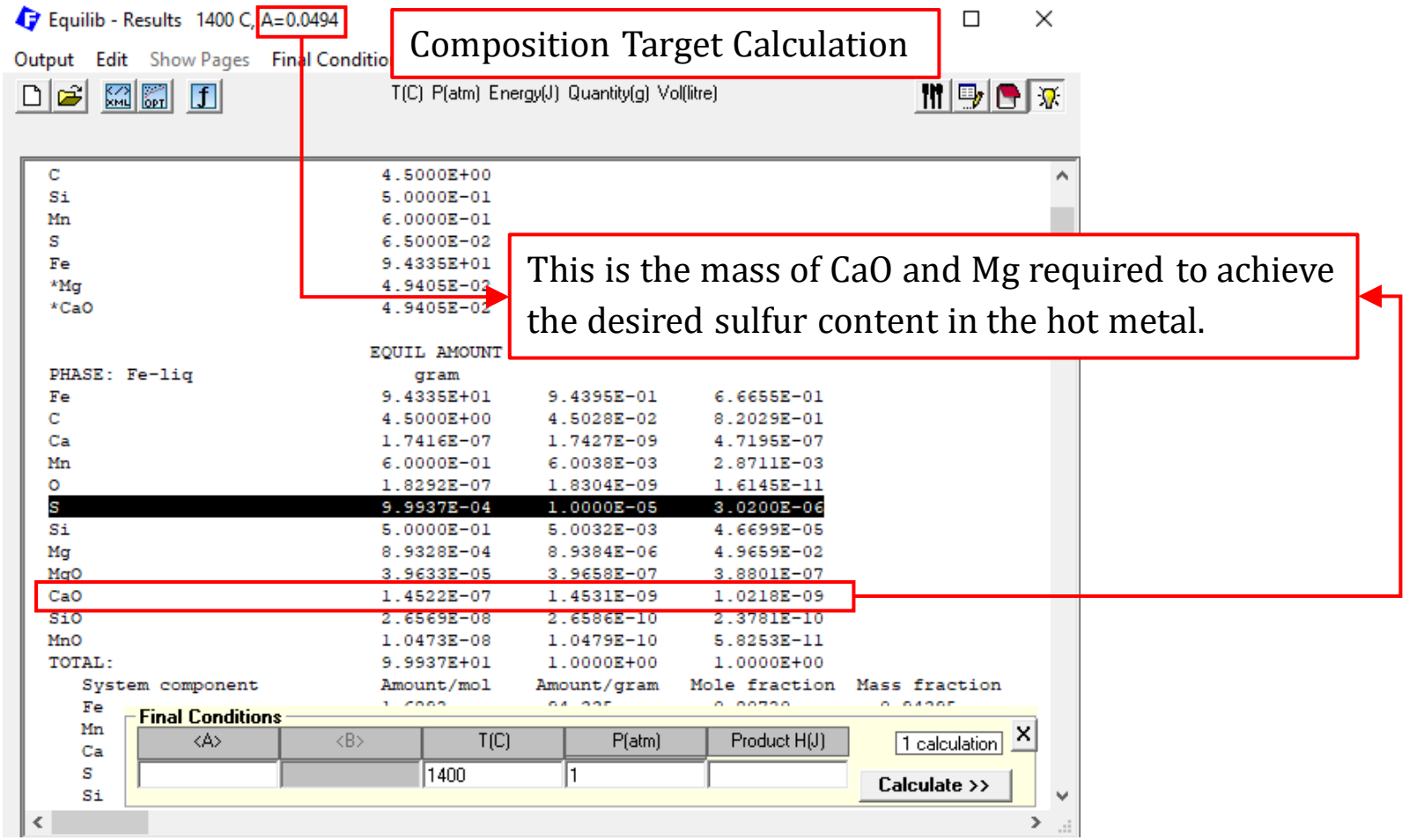
Example 1: Desulfurization (Basic Example)

Basic Example: Desulfurization of Hot Metal Using CaO + Mg



Example 1: Desulfurization (Basic Example)

Basic Example: Desulfurization of Hot Metal Using CaO + Mg



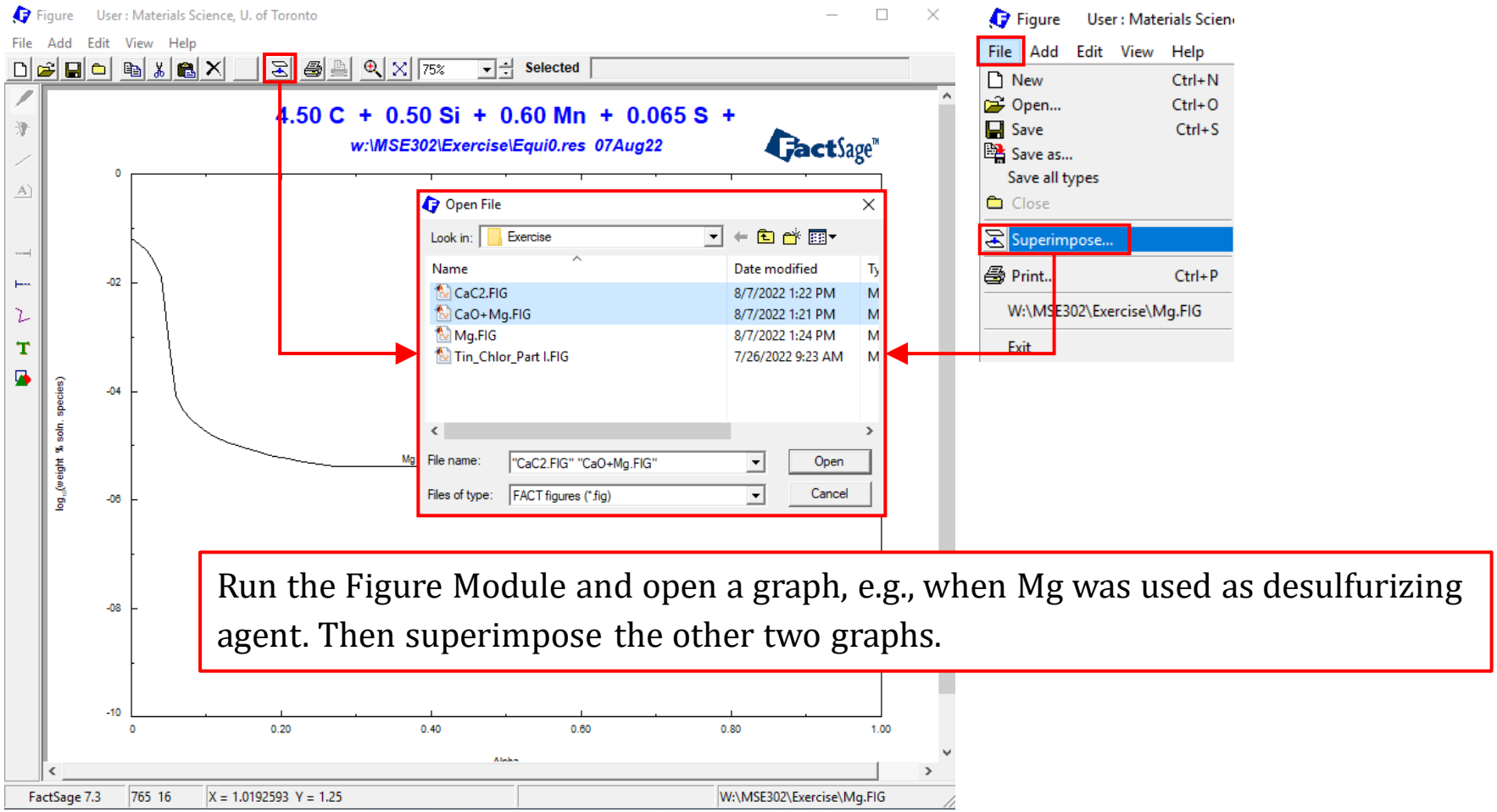
Example 1: Desulfurization (Basic Example)

Basic Example: Comparison of Desulfurizing Agents

To compare the efficiency of different desulfurizing agents, we can superimpose all the graphs, wt.%S~<A>, using the Figure Module.

Example 1: Desulfurization (Basic Example)

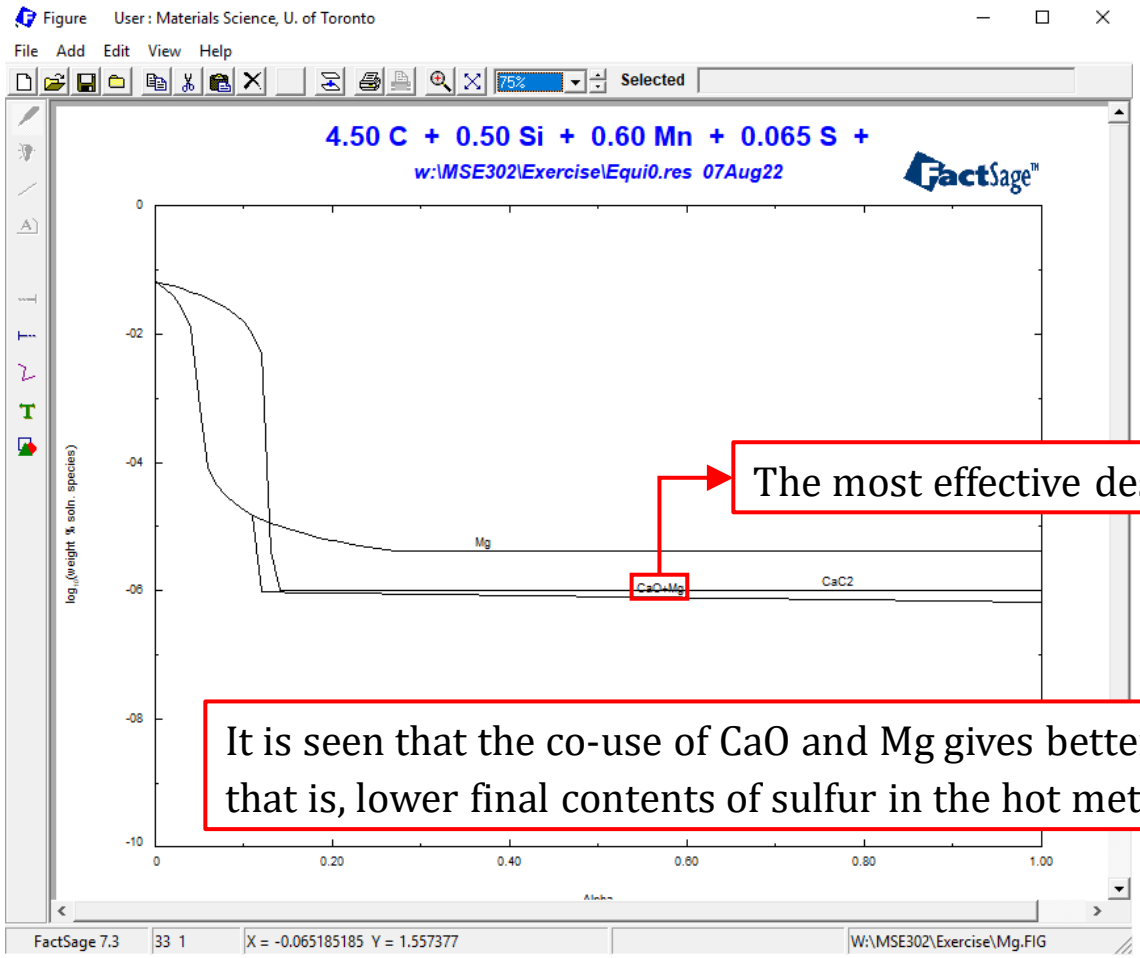
Basic Example: Comparison of Desulfurizing Agents



Run the Figure Module and open a graph, e.g., when Mg was used as desulfurizing agent. Then superimpose the other two graphs.

Example 1: Desulfurization (Basic Example)

Basic Example: Comparison of Desulfurizing Agents



The most effective desulfurizing agent for hot metal!

It is seen that the co-use of CaO and Mg gives better results of desulfurization, that is, lower final contents of sulfur in the hot metal.

Example 1: Desulfurization (Advanced Example)

Now, we know the "CaO + Mg" mixture can be used as an effective desulfurizing agent, and we would like to use this mixture for hot metal desulfurization in a torpedo car. It should be noted that **the commercial grade** "CaO + Mg" agent typically assaying 70 wt.% CaO and 30 wt.% Mg.

Background data: in a torpedo car, we assume the blast furnace slag carry over is 10 kg/tHM and the temperature is 1427 °C. The compositions of hot metal and slag are as follows:

Hot metal composition:

Element	C	Si	Mn	Ti	S	Fe
wt.%	4.50	0.80	1.00	0.05	0.06	93.59

Slag composition:

Component	CaO	SiO_2	MgO	Al_2O_3	MnO	TiO_2	CaS
wt.%	34.5	34.0	14.0	9.00	2.00	2.00	4.50

Example 1: Desulfurization (Advanced Example)

Also, the "CaO + Mg" agent is carried by the carrier argon gas at a rate of roughly 0.125 Nm^3/kg Mg.

For 1 Nm^3 argon (Nm^3 means normal cubic meter), the equivalent mass is calculated as follows:

$$\frac{1000 \text{ liter}}{1 \text{ Nm}^3} \times \frac{\frac{1}{22.4} \text{ mol}}{1 \text{ liter}} \times \frac{40 \text{ g}}{1 \text{ mol}} \times \frac{10^{-3} \text{ kg}}{1 \text{ g}} = 1.79 \text{ kg/Nm}^3 \text{ Ar}$$

Note: at standard temperature and pressure, i.e., 0 °C and 1 atm, 1 mole of any gas will occupy a volume of 22.4 liter.

Now, let us simulate the system consisting hot metal / slag / CaO-Mg agent / Ar using the Equilib Module.

Example 1: Desulfurization (Advanced Example)

Step 1. Define the Reactants (Type and Quantity)

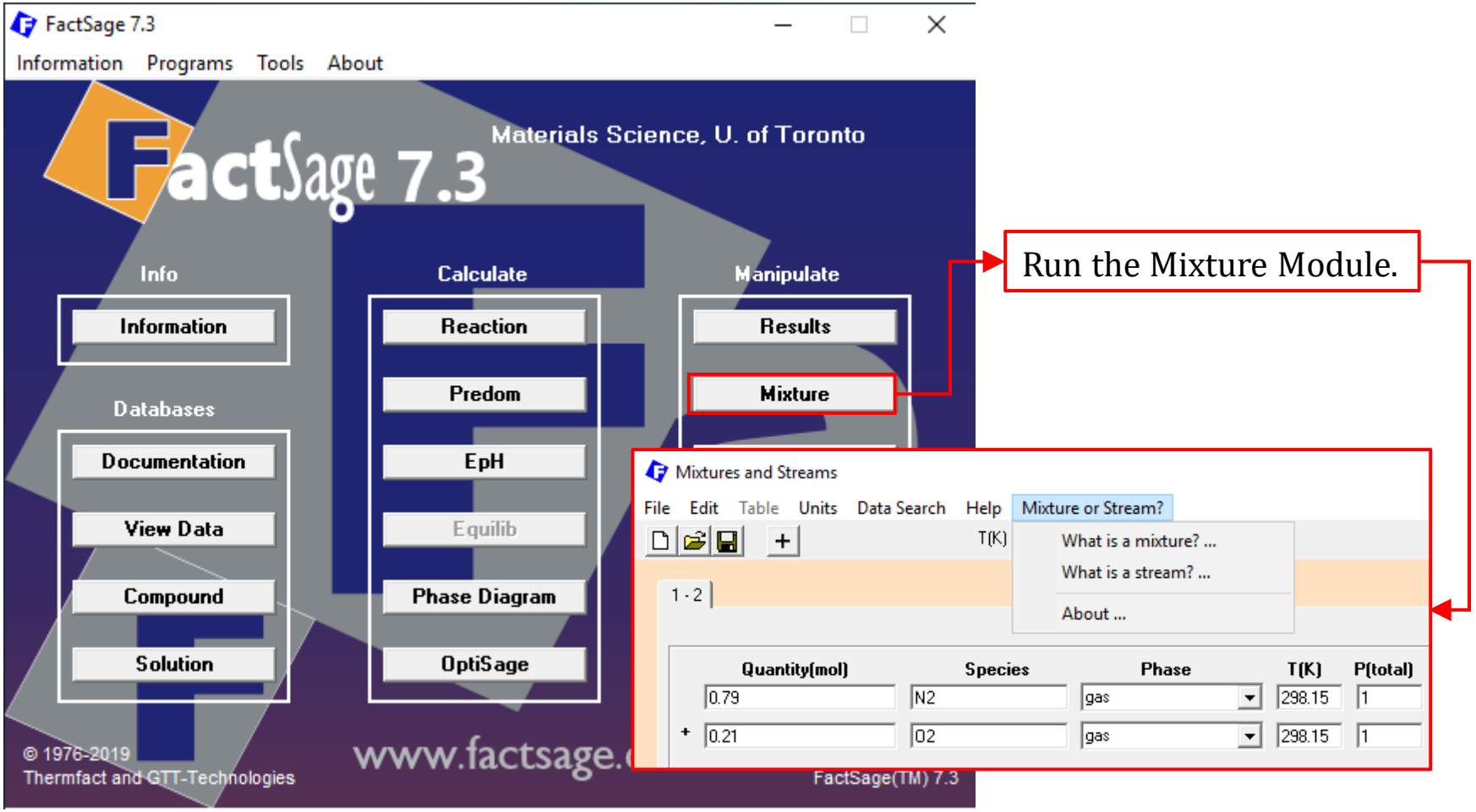
Since there are a quite number of species in this advanced example, we could either (a) calculate the quantities of all species and then enter all at once in the Reactants Window, or (b) define 2 separate streams for hot metal and slag which contain many species and then input these 2 streams together with the CaO-Mg agent and Ar in the Reactants Window.

We will choose the second approach because it avoids entering many species at the same time, and the input species will be more organized.

Note: our calculation will be based on 1 tonne (= 1000 kg) hot metal.

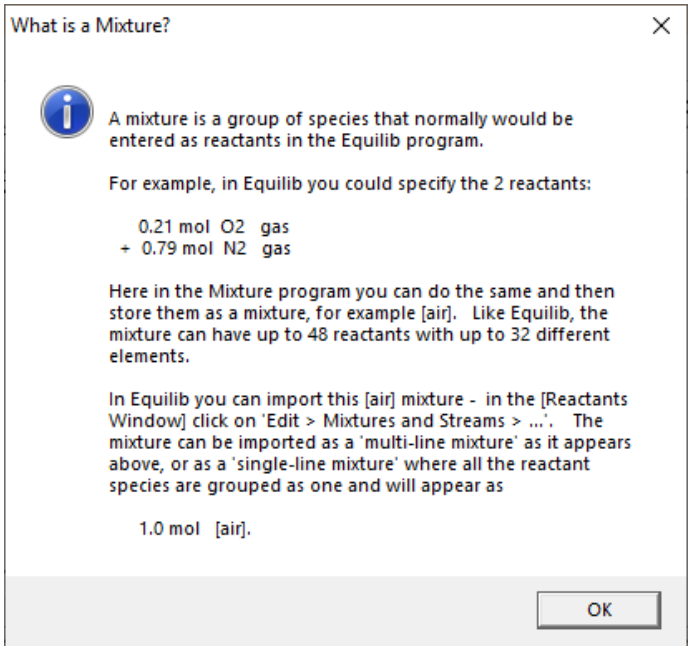
Example 1: Desulfurization (Advanced Example)

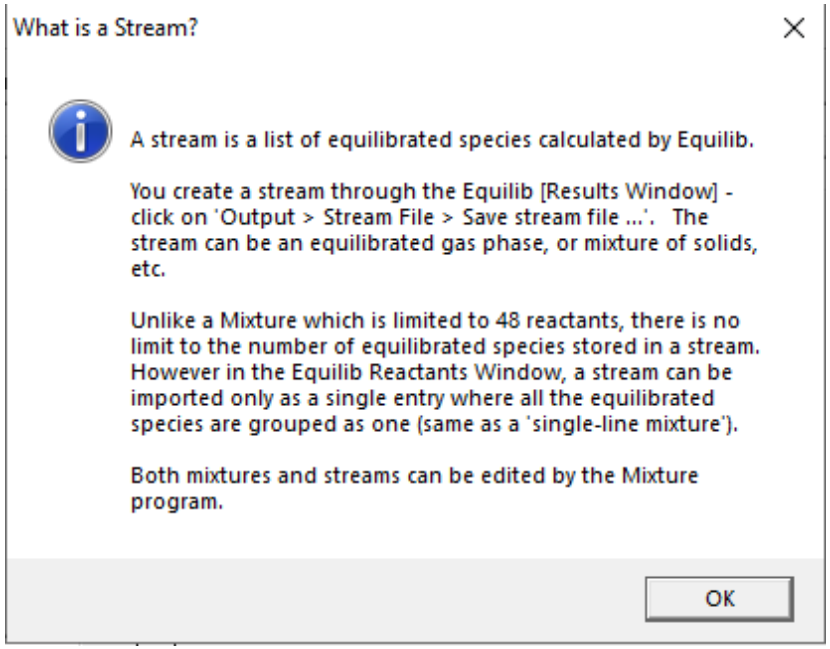
What is a Stream?



Example 1: Desulfurization (Advanced Example)

What is a Stream?



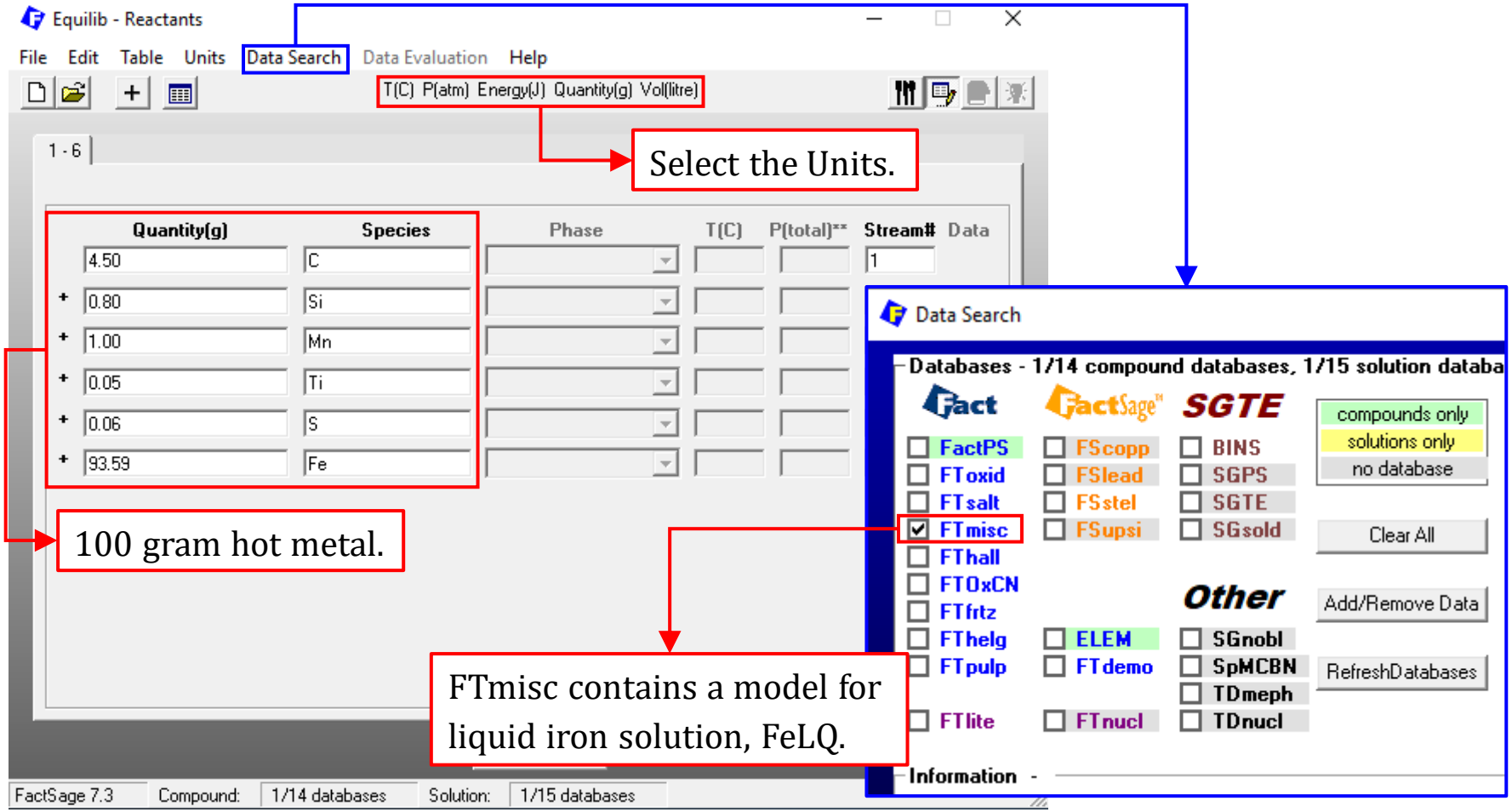


We will use the Equilb Module to define the streams, each of which simulate one of the following: hot metal / slag / CaO-Mg agent / Ar.

Note: defining a stream is a simple equilibrium calculation

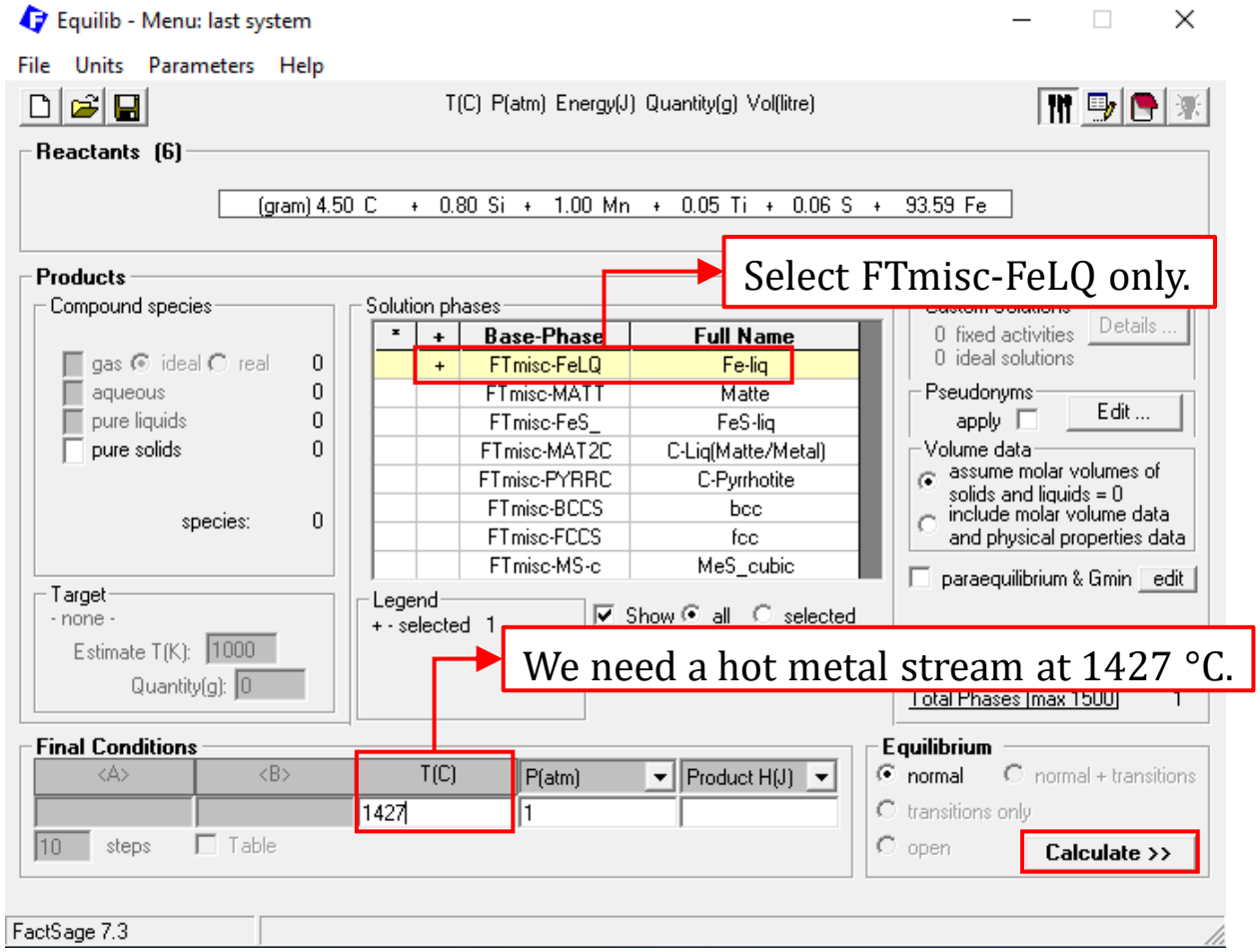
Example 1: Desulfurization (Advanced Example)

Stream 1: Hot Metal (FTmisc-FeLQ)



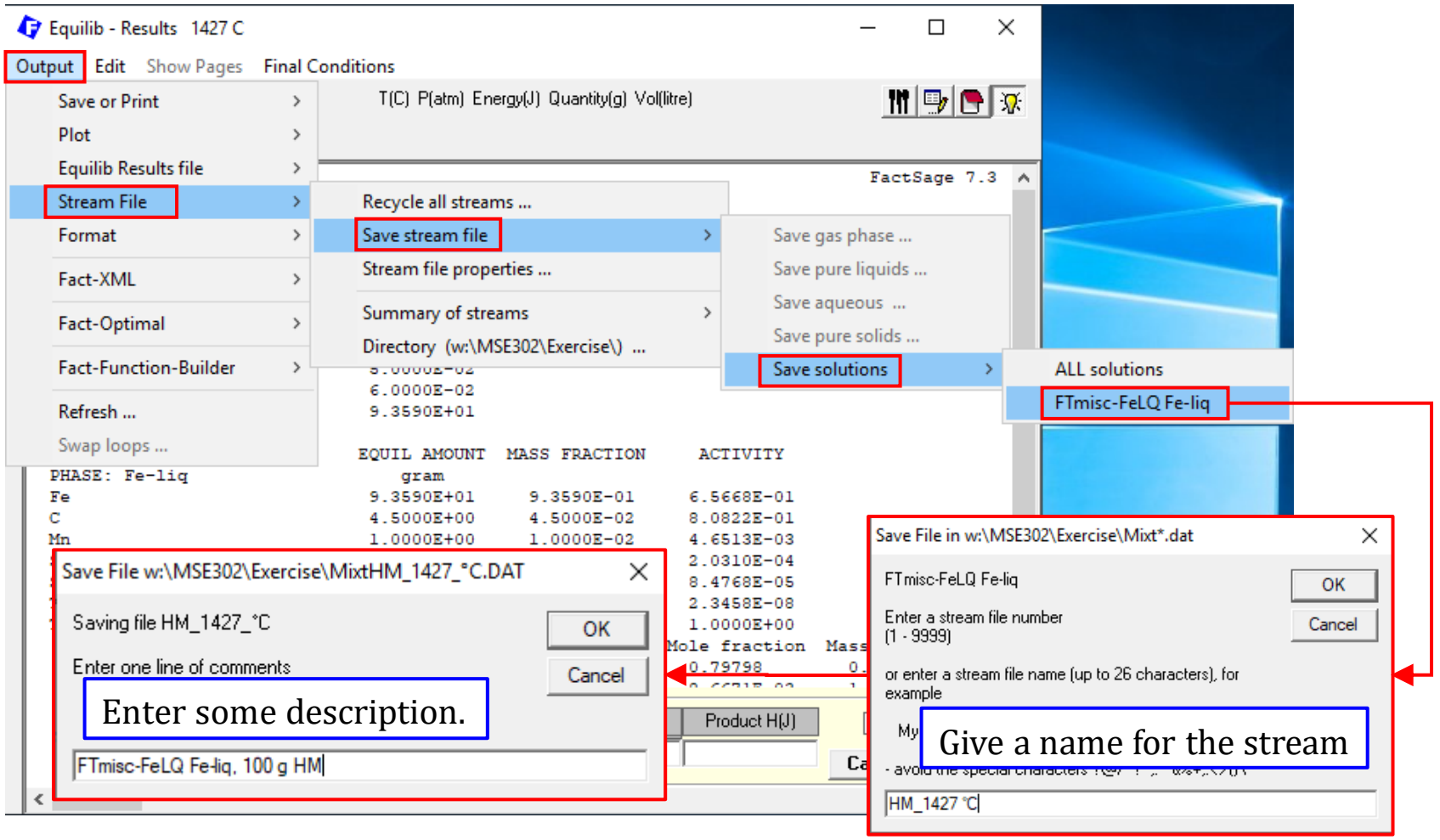
Example 1: Desulfurization (Advanced Example)

Stream 1: Hot Metal (FTmisc-FeLQ)



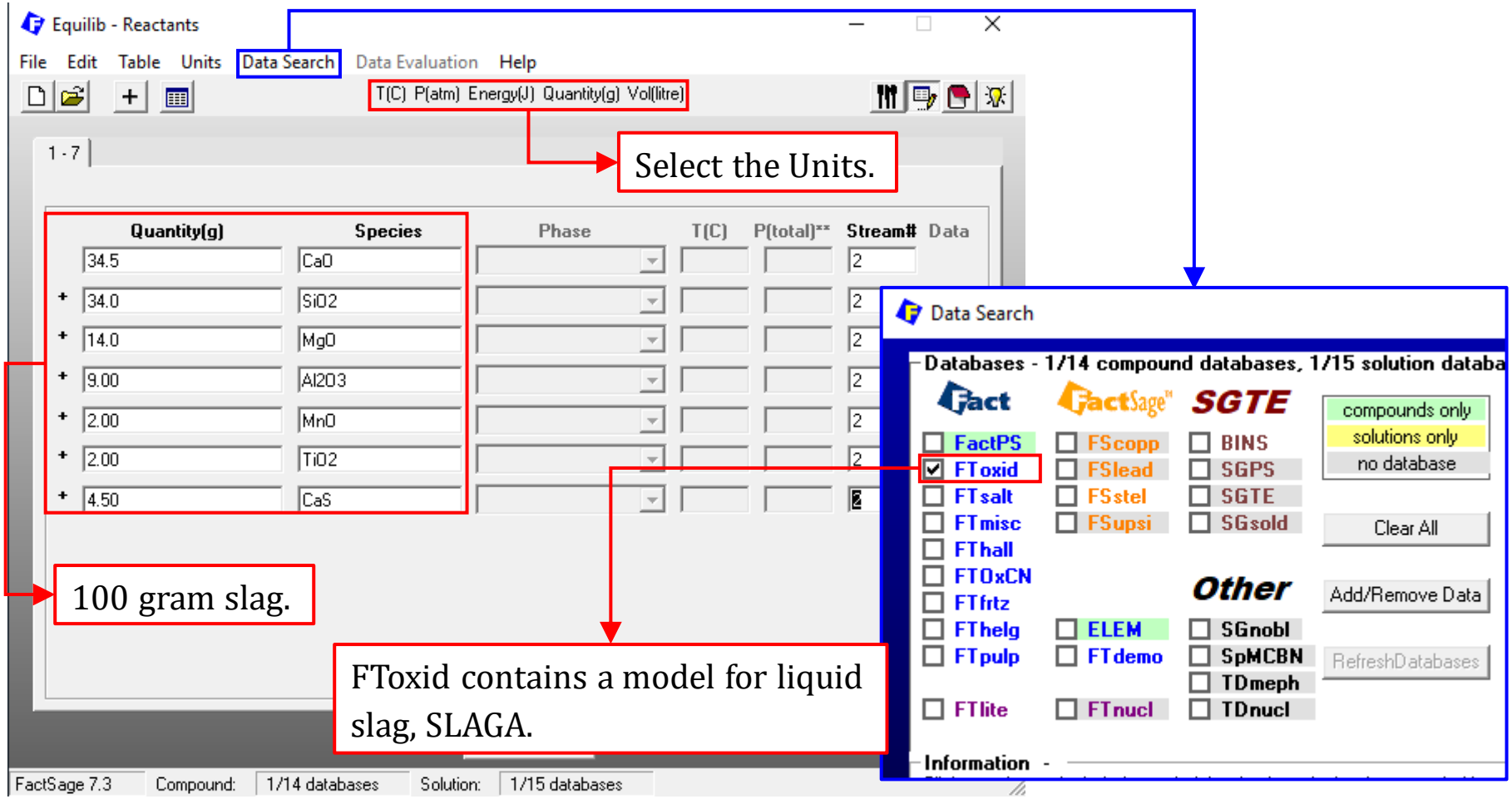
Example 1: Desulfurization (Advanced Example)

Stream 1: Hot Metal (FTmisc-FeLQ)



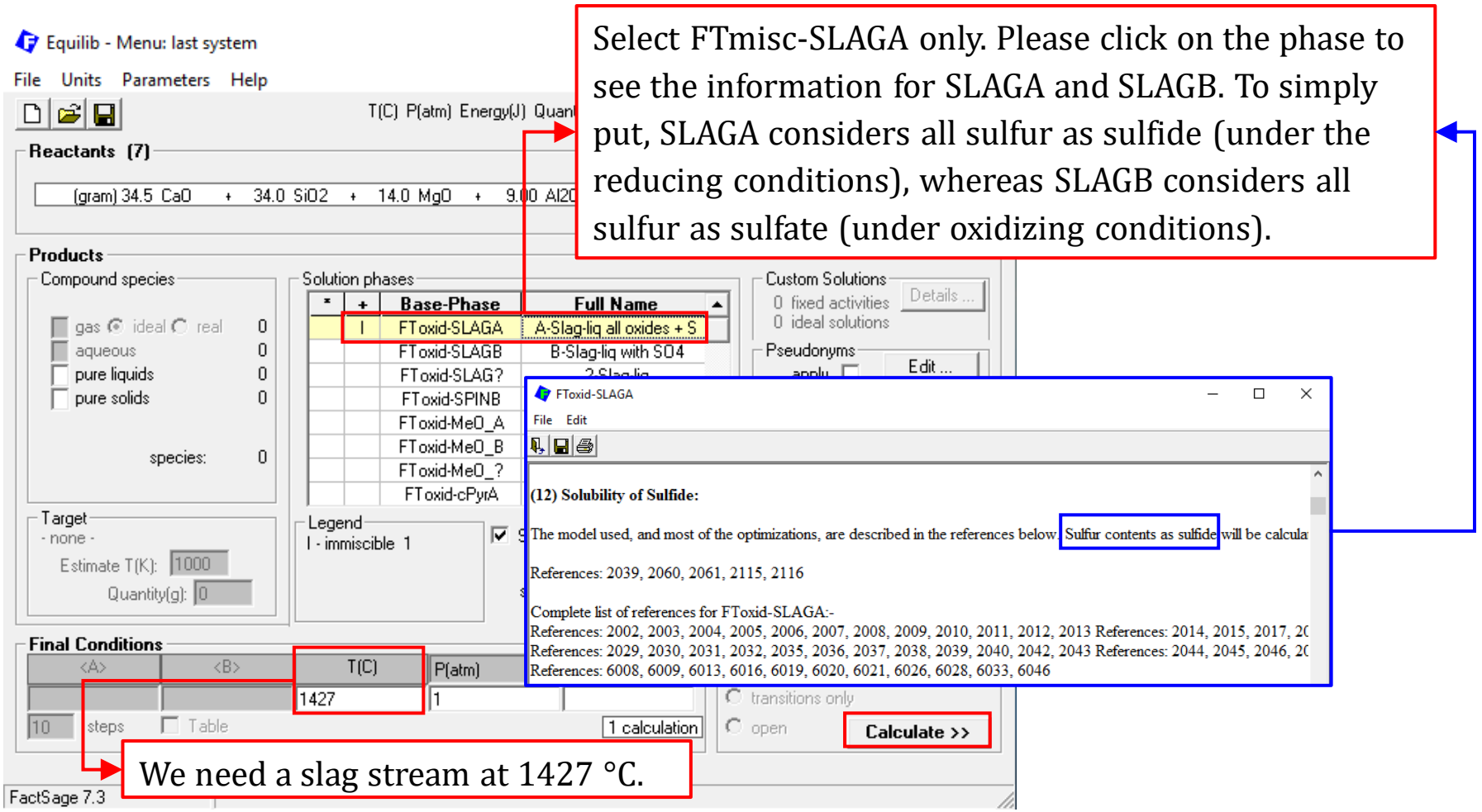
Example 1: Desulfurization (Advanced Example)

Stream 2: Slag (FToxid-Slag)



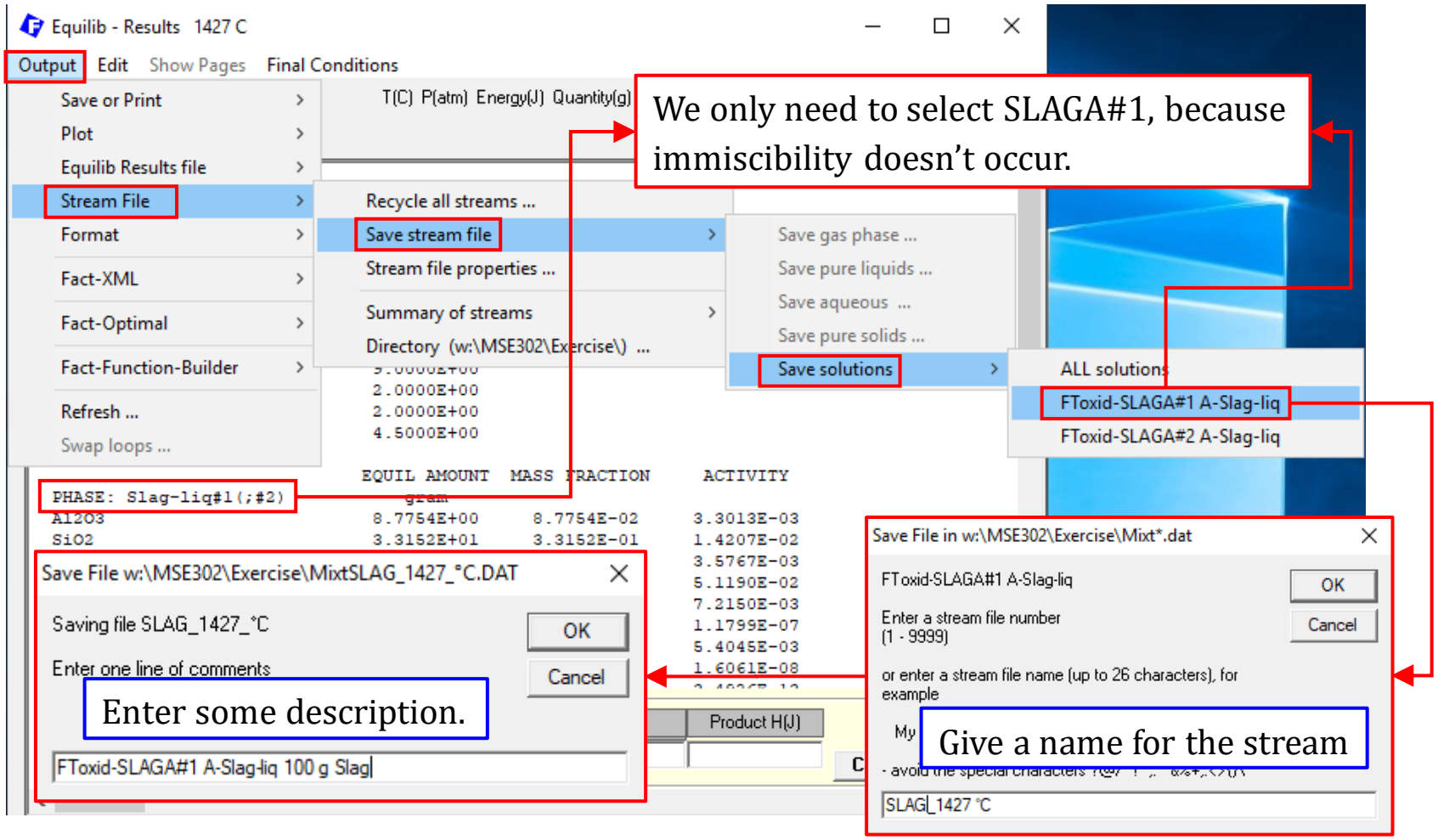
Example 1: Desulfurization (Advanced Example)

Stream 2: Slag (FToxid-Slag)



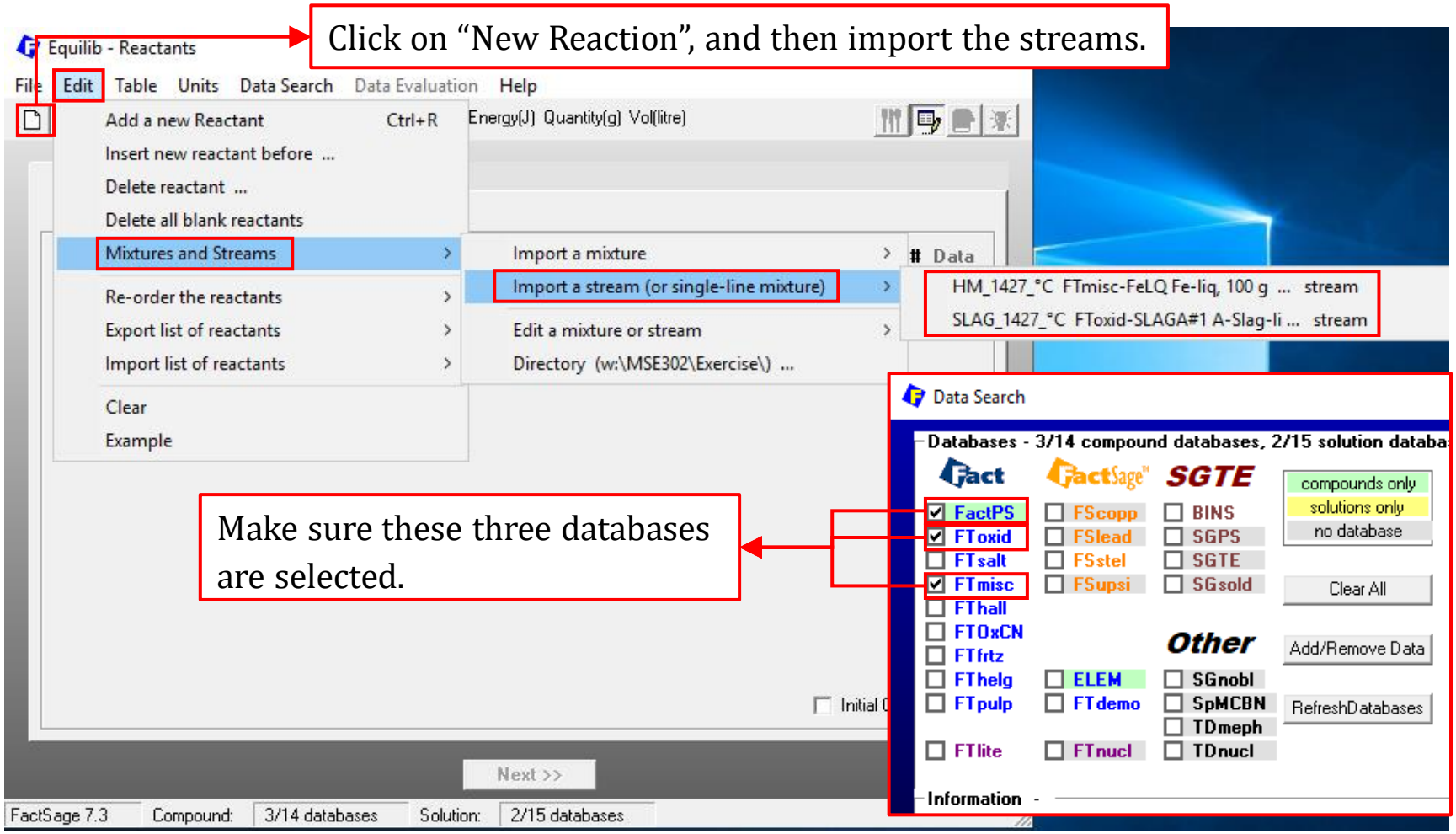
Example 1: Desulfurization (Advanced Example)

Stream 2: Slag (FToxid-Slag)



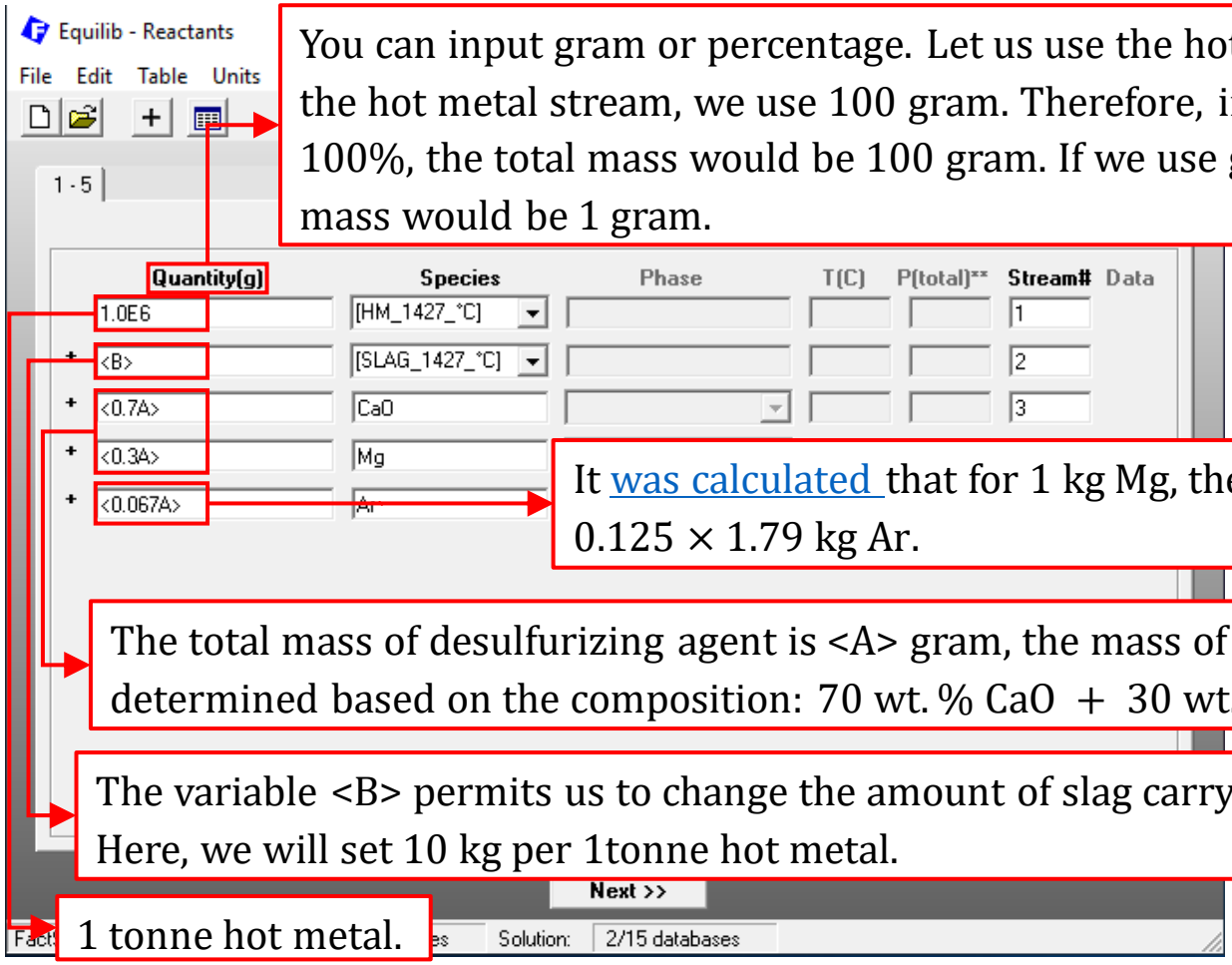
Example 1: Desulfurization (Advanced Example)

Import the streams: hot metal and slag



Example 1: Desulfurization (Advanced Example)

Import the streams, add desulfurizing agent and Ar



You can input gram or percentage. Let us use the hot metal stream. When defining the hot metal stream, we use 100 gram. Therefore, if we use percentage, e.g., 100%, the total mass would be 100 gram. If we use gram, e.g., 1 gram, the total mass would be 1 gram.

It was calculated that for 1 kg Mg, the mass of Ar was calculated as: 0.125×1.79 kg Ar.

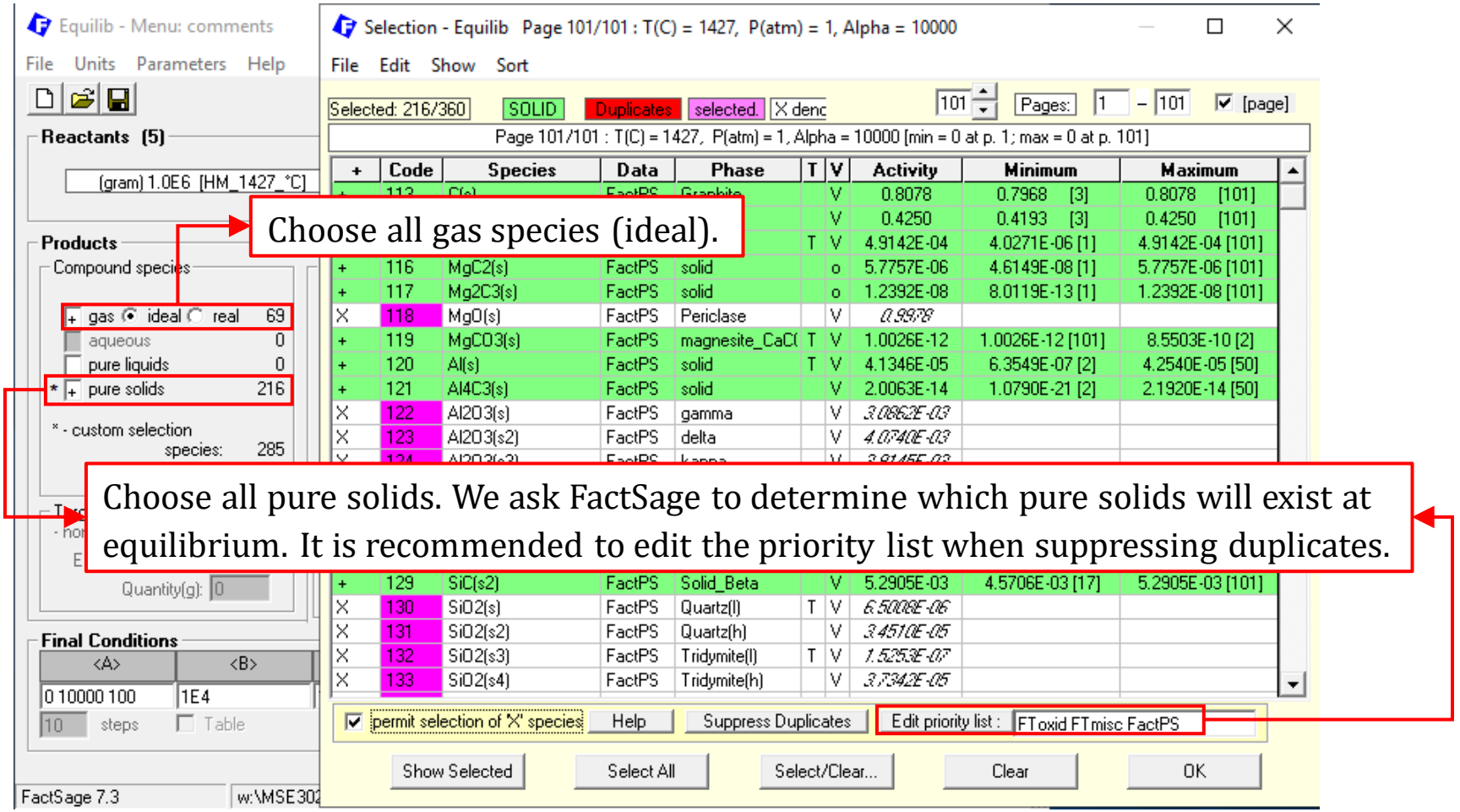
The total mass of desulfurizing agent is <A> gram, the mass of CaO and Mg can be determined based on the composition: 70 wt. % CaO + 30 wt. % Mg.

The variable <B> permits us to change the amount of slag carry-over. Here, we will set 10 kg per 1tonne hot metal.

1 tonne hot metal.

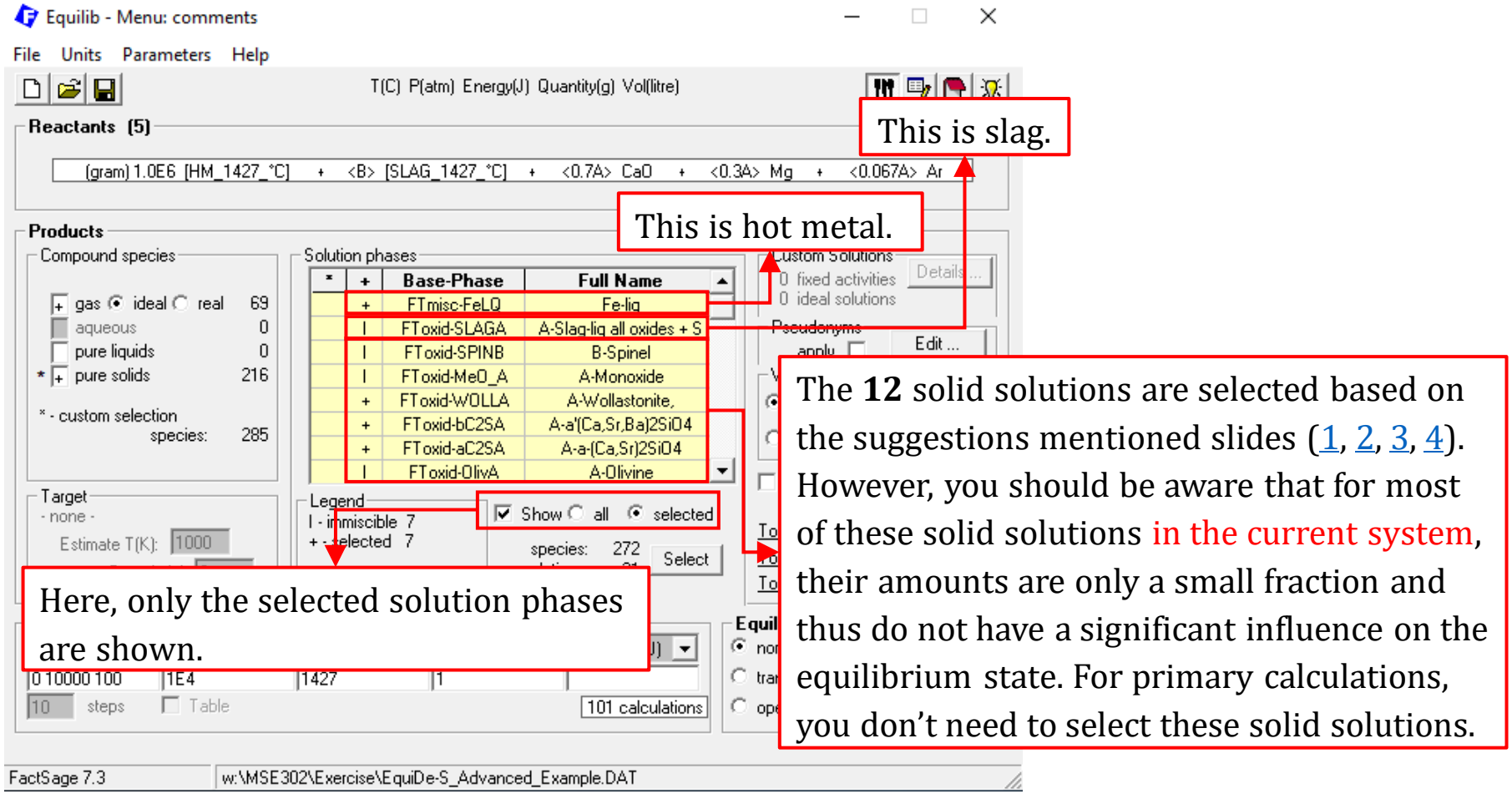
Example 1: Desulfurization (Advanced Example)

Selection of Compound Species



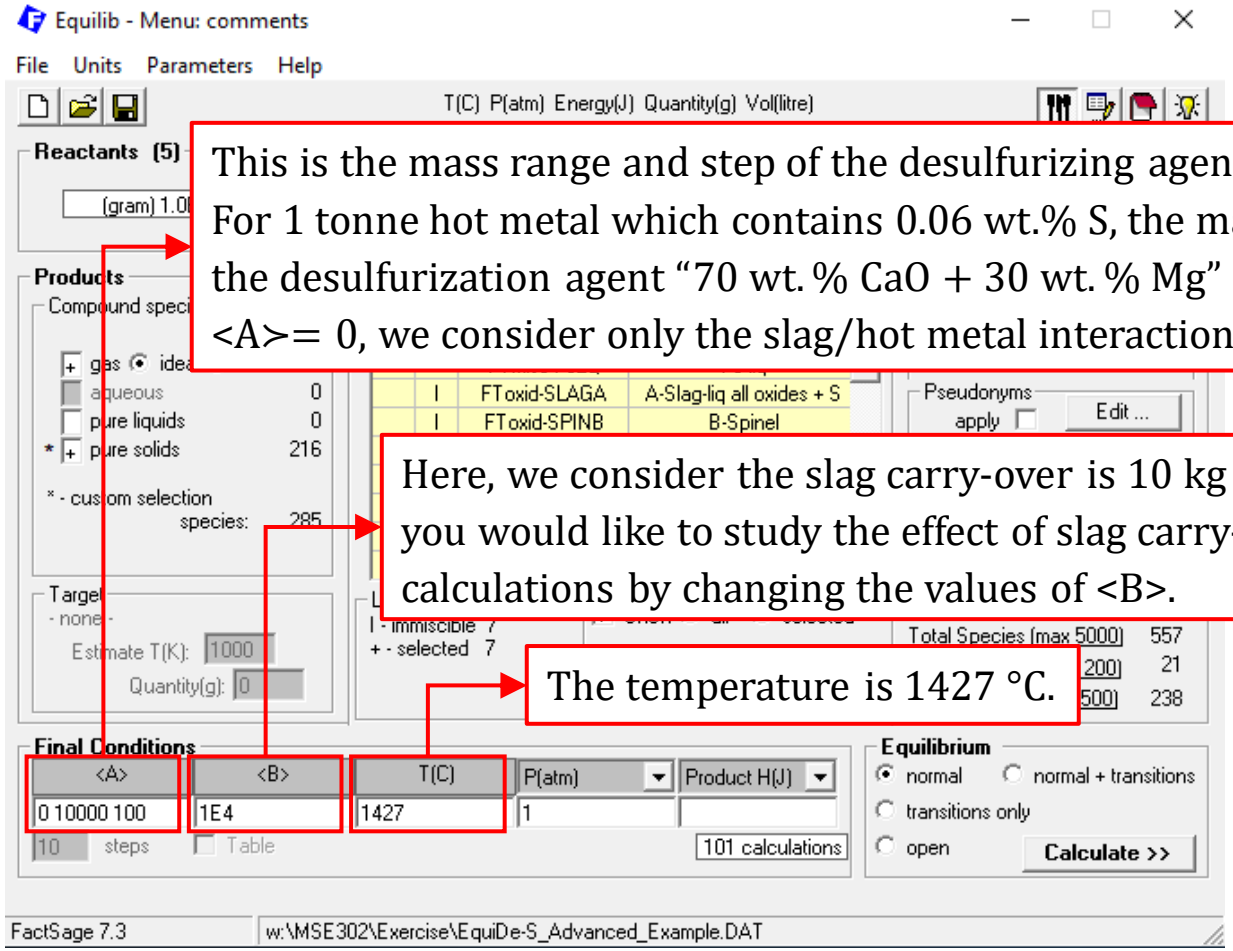
Example 1: Desulfurization (Advanced Example)

Selection of Compound Species



Example 1: Desulfurization (Advanced Example)

Setting Final Conditions

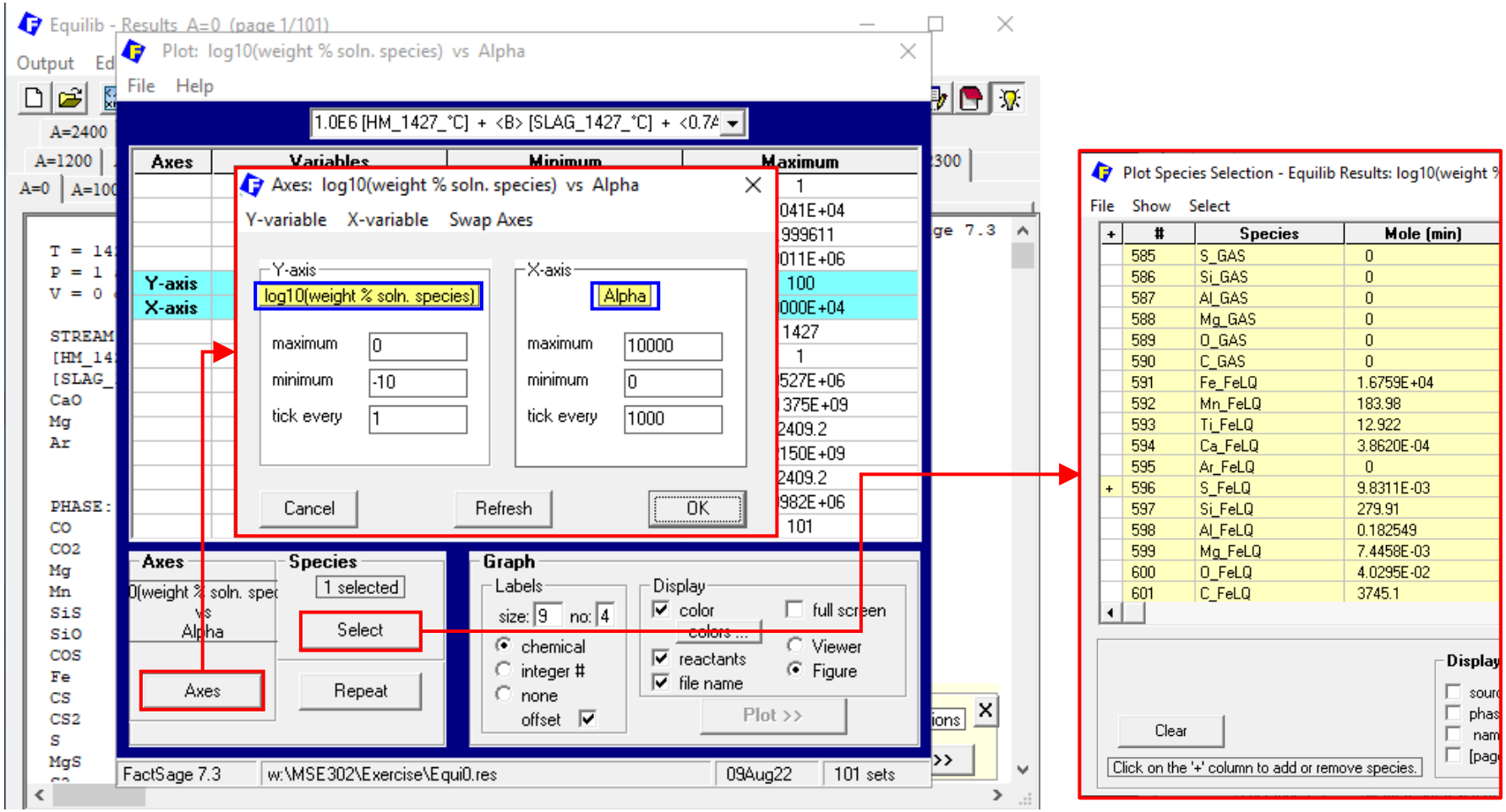


This is the mass range and step of the desulfurizing agent.
For 1 tonne hot metal which contains 0.06 wt.% S, the maximum mass of the desulfurization agent "70 wt. % CaO + 30 wt. % Mg" is 10 kg. When <A>= 0, we consider only the slag/hot metal interaction.

Here, we consider the slag carry-over is 10 kg per 1 tonne hot metal. If you would like to study the effect of slag carry-over, you can repeat the calculations by changing the values of <B>.

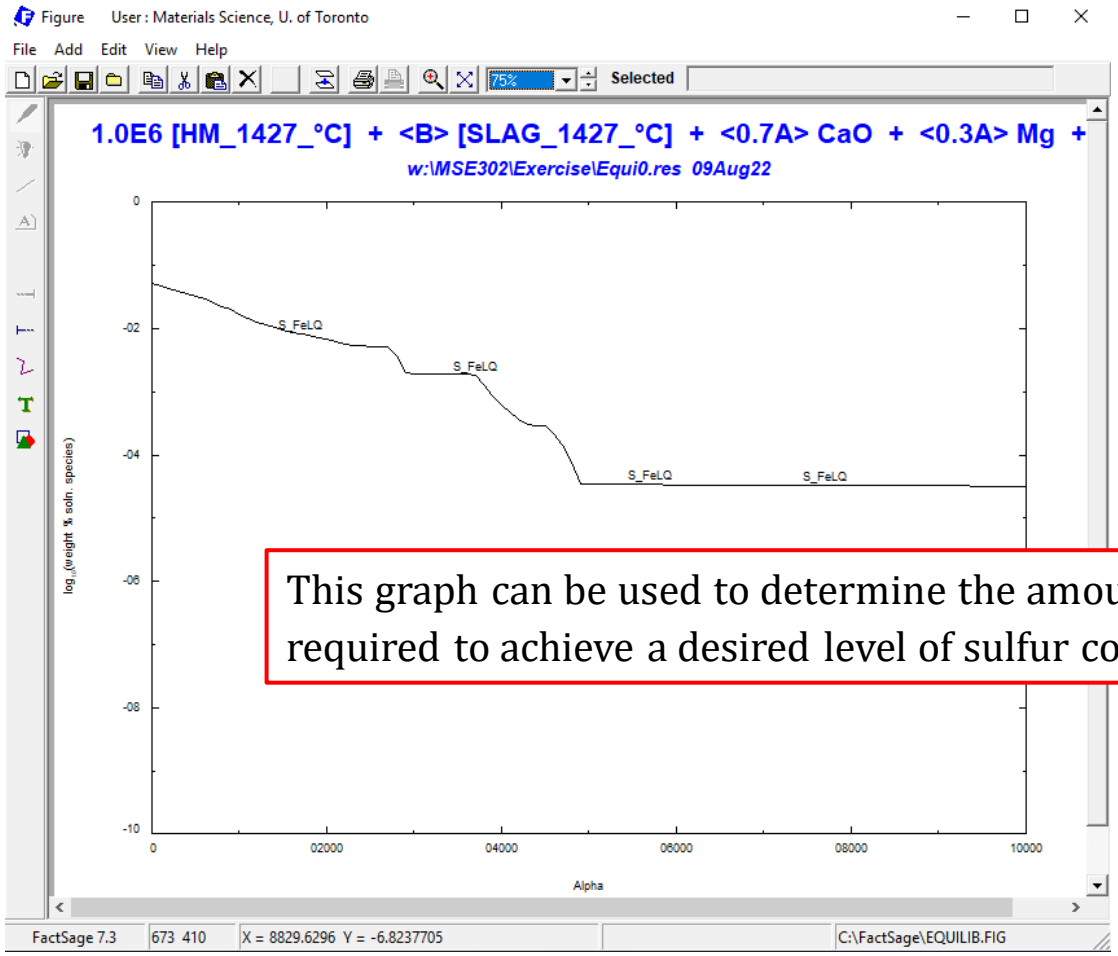
The temperature is 1427 °C.

Example 1: Desulfurization (Advanced Example)



Example 1: Desulfurization (Advanced Example)

Plot: wt.%S~<A>

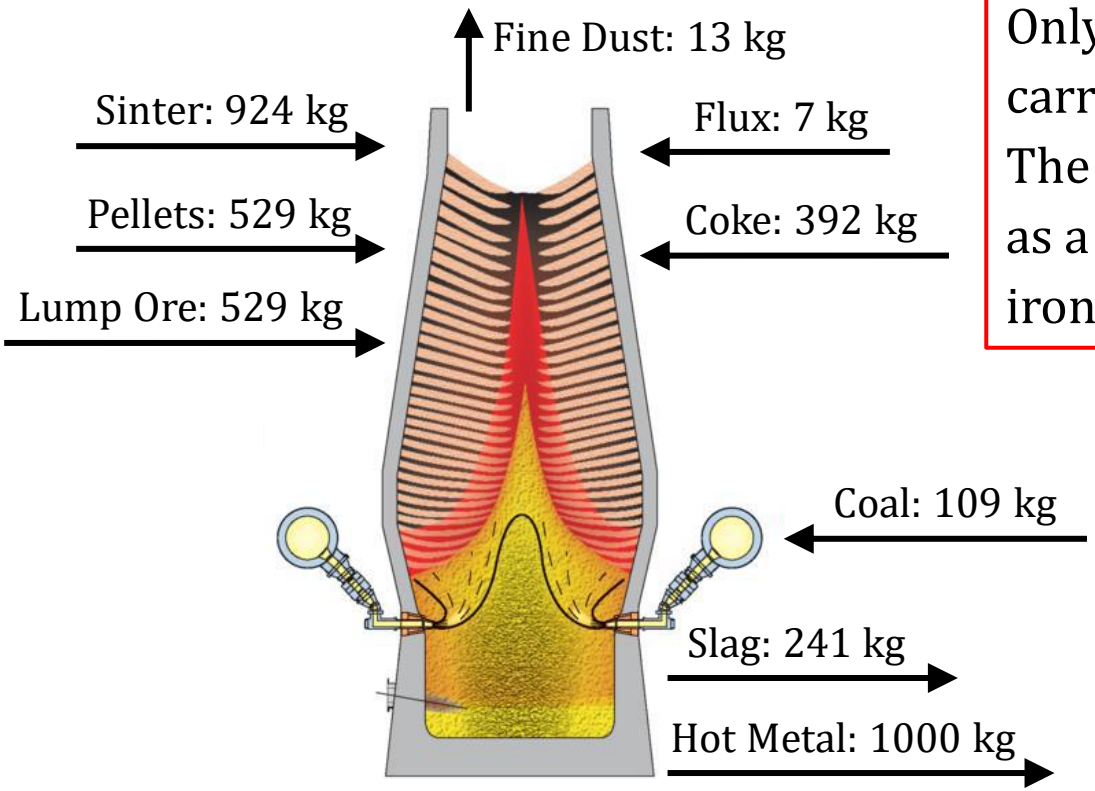


This graph can be used to determine the amount of desulfurizing agent required to achieve a desired level of sulfur content in the hot metal.

Example 2: Slag: Enthalpy, Melting Temperature

Background: Blast Furnace Slag

The following graph shows the mass balance for a typical ironmaking blast furnace.



Only a small fraction of slag is carried over to the torpedo car. The majority of slag will be tapped as a separate by-product of the ironmaking blast furnace process.

Babich et al. Ironmaking Text Book, RWTH Aachen University, Department of Ferrous Metallurgy, 2008

Example 2: Slag: Enthalpy, Melting Temperature

Background: Blast Furnace Slag

Each year, over 300 million tonnes of blast furnace slag are generated all over the world. The molten blast furnace slag, when tapped, has a temperature ~1500 °C, and thus the thermal energy contained is quite substantial. For the purpose of heat recovery from the molten blast furnace slag, its enthalpy and melting temperature data are required. We can use the Equilib Module in FactSage to calculate these data.

We will assume the molten blast furnace slag (1500 °C) has the following composition:

Oxide	CaO	SiO_2	Al_2O_3
wt.%	40.0	40.0	20.0

Barati and Jahanshahi, Journal of Sustainable Metallurgy (2020) 6: 191–206

Example 2: Slag: Enthalpy, Melting Temperature

Task 1: Calculating the Enthalpy of Slag and Recoverable Heat

The Enthalpy of molten slag at 1500 °C based on the SER state can be directly calculated in the Equilib Module.

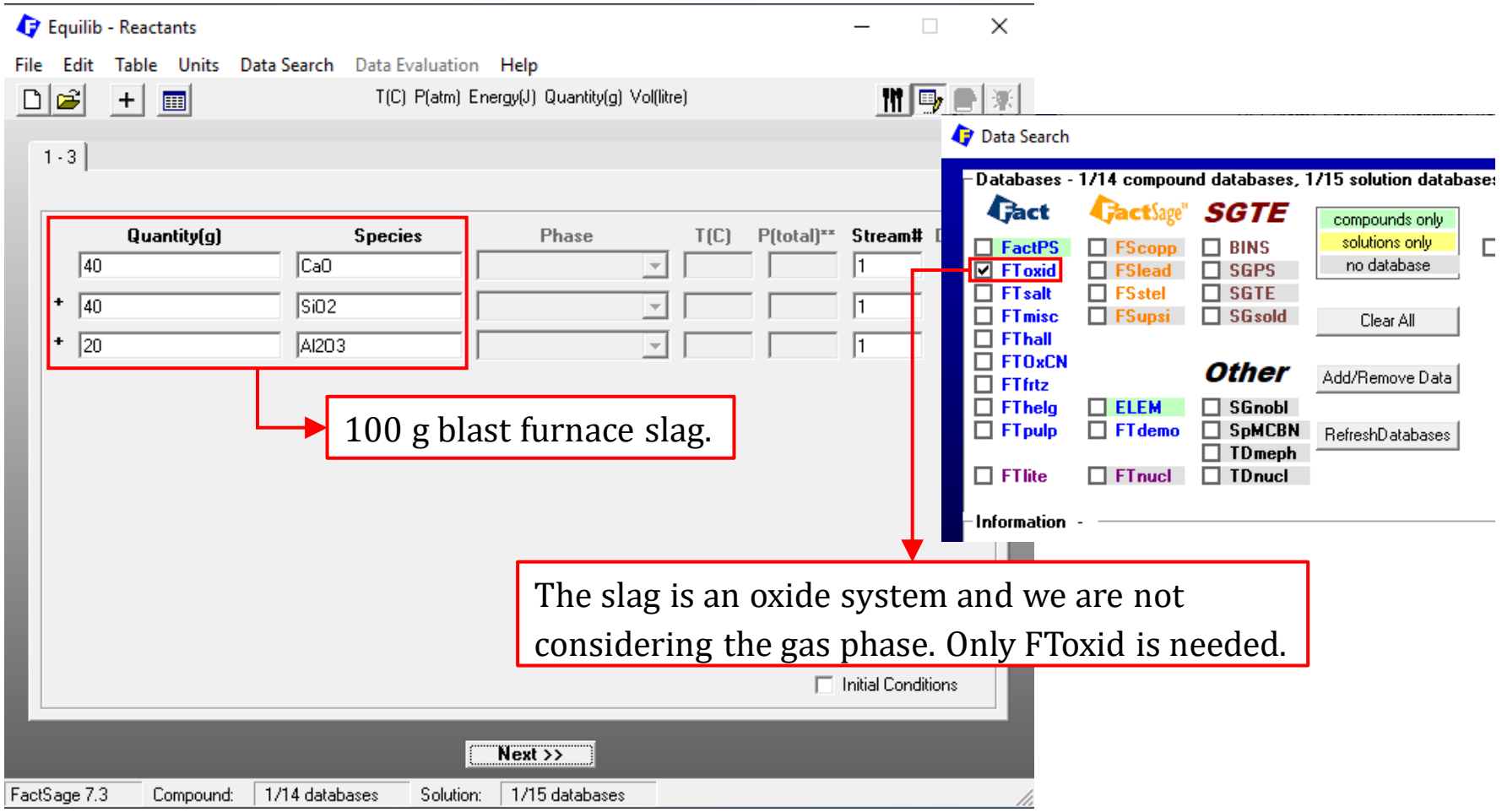
The maximum amount of heat (strictly speaking, the amount of thermal energy) that can be recovered corresponds to the Enthalpy change when the molten slag is cooled to room temperature. That is,

$$\left| H_{\text{slag,1500 °C}} - \sum n_i h^\circ_{i\text{(solid),25 °C}} \right|$$

Therefore, two equilibrium states are required: 25 °C and 1500 °C. The following slides present one approach to calculate the difference in the Enthalpy at these two temperatures.

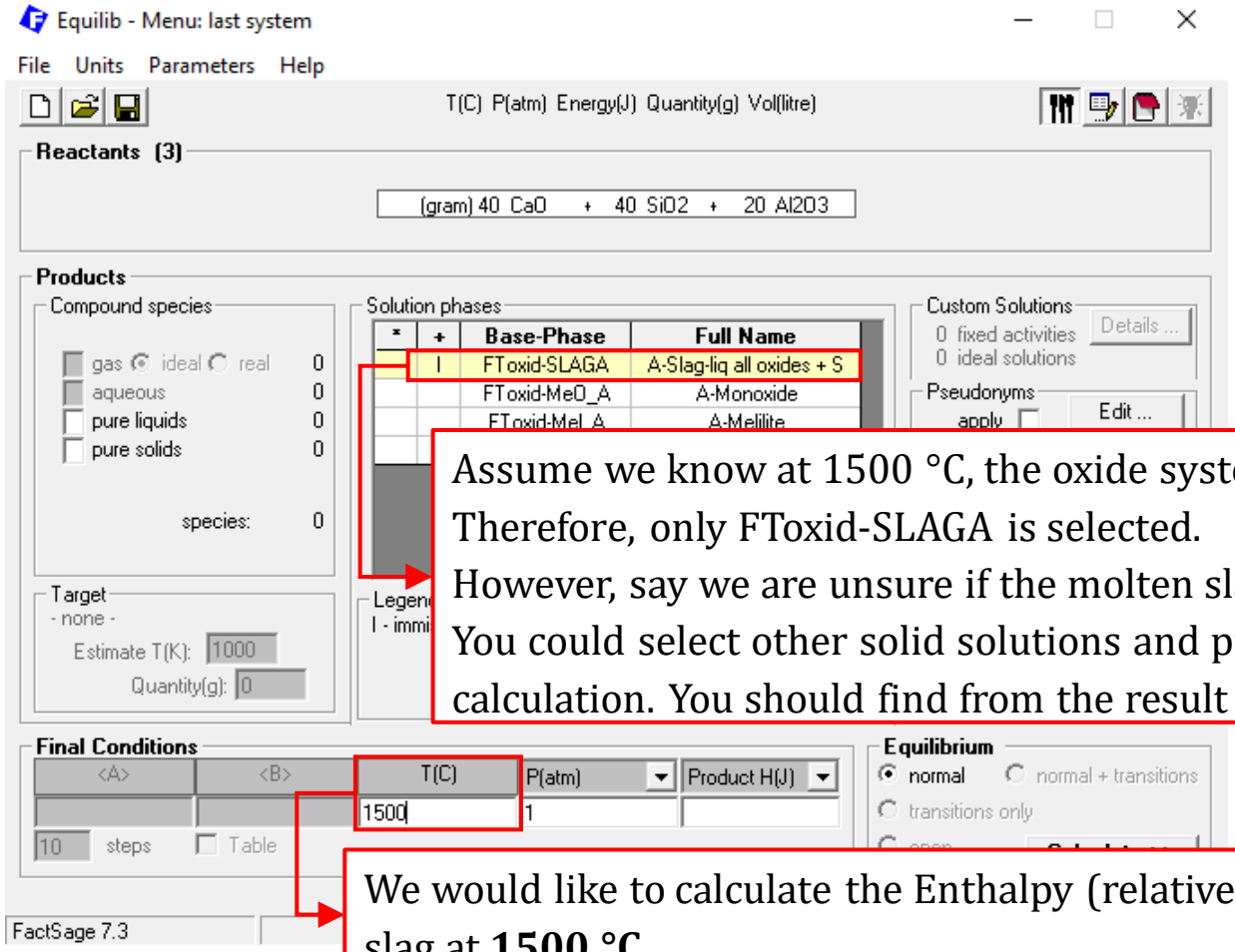
Example 2: Slag: Enthalpy, Melting Temperature

Task 1: Calculating the Enthalpy of Slag and Recoverable Heat



Example 2: Slag: Enthalpy, Melting Temperature

Task 1: Calculating the Enthalpy of Slag and Recoverable Heat



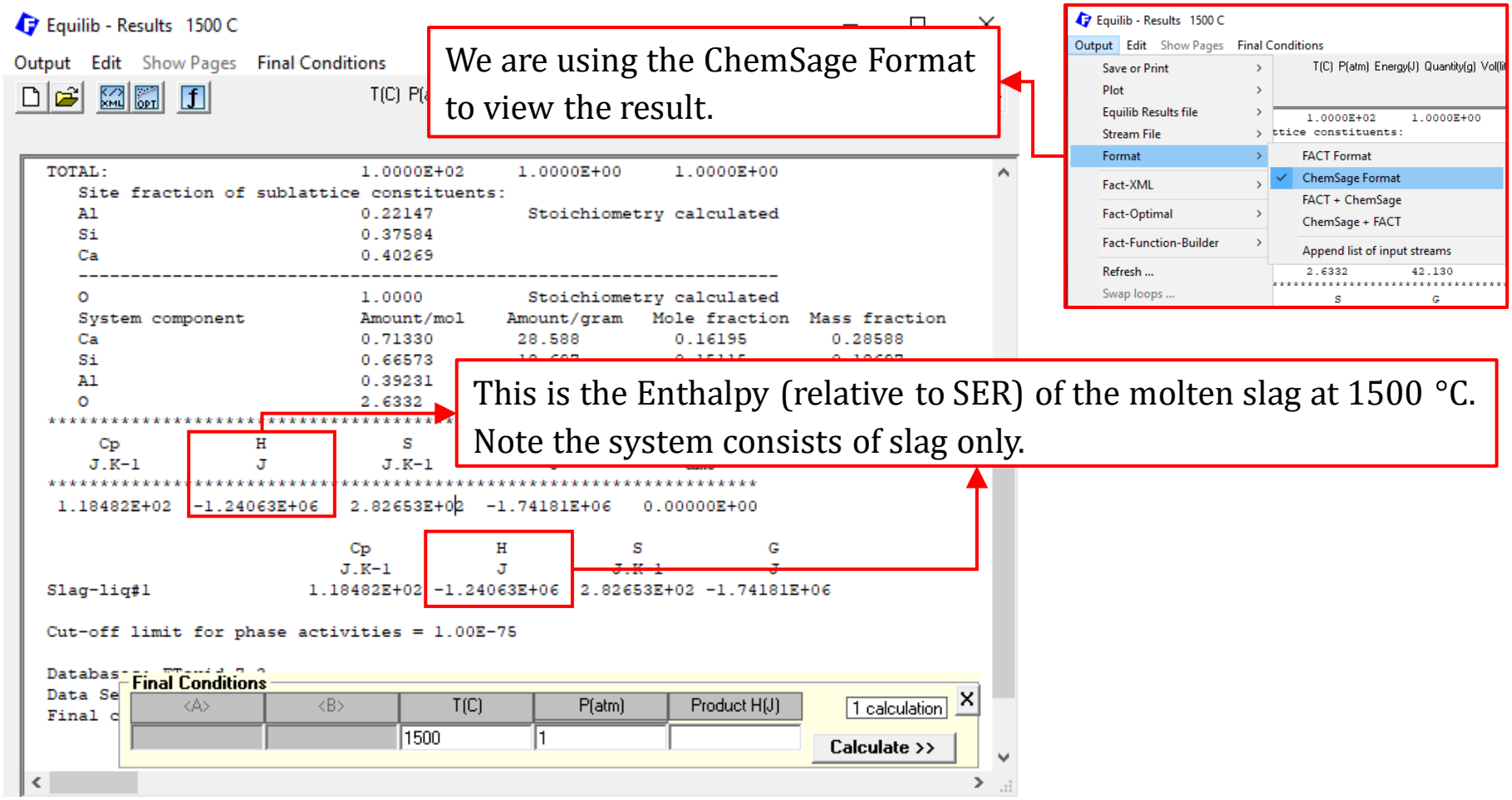
Assume we know at 1500 °C, the oxide system of interest is fully molten. Therefore, only FToxid-SLAGA is selected.

However, say we are unsure if the molten slag is the only phase at 1500 °C. You could select other solid solutions and pure solids and perform the calculation. You should find from the result that SLAGA is the only phase.

We would like to calculate the Enthalpy (relative to SER) of the molten slag at **1500 °C**.

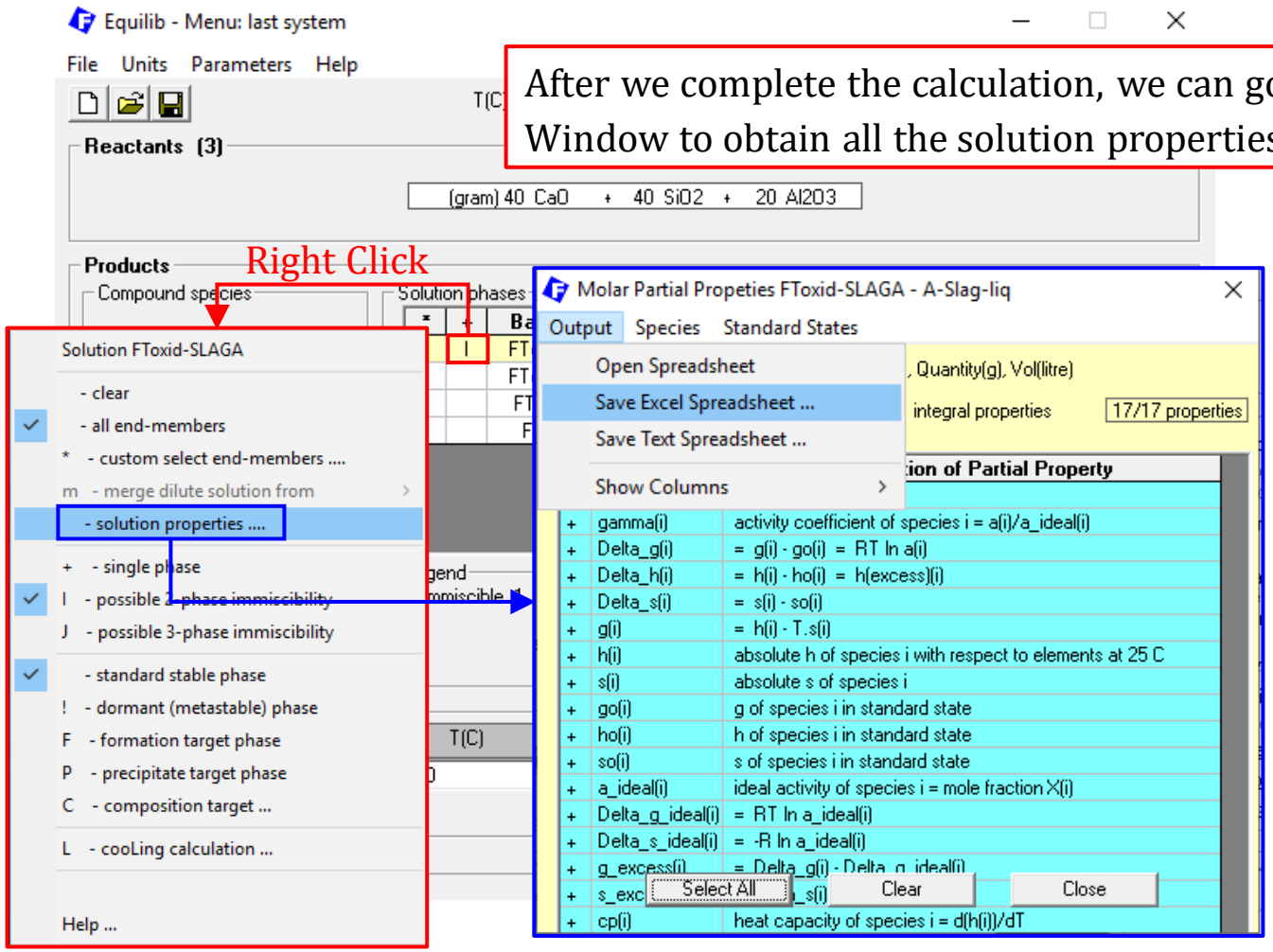
Example 2: Slag: Enthalpy, Melting Temperature

Task 1: Calculating the Enthalpy of Slag and Recoverable Heat



Example 2: Slag: Enthalpy, Melting Temperature

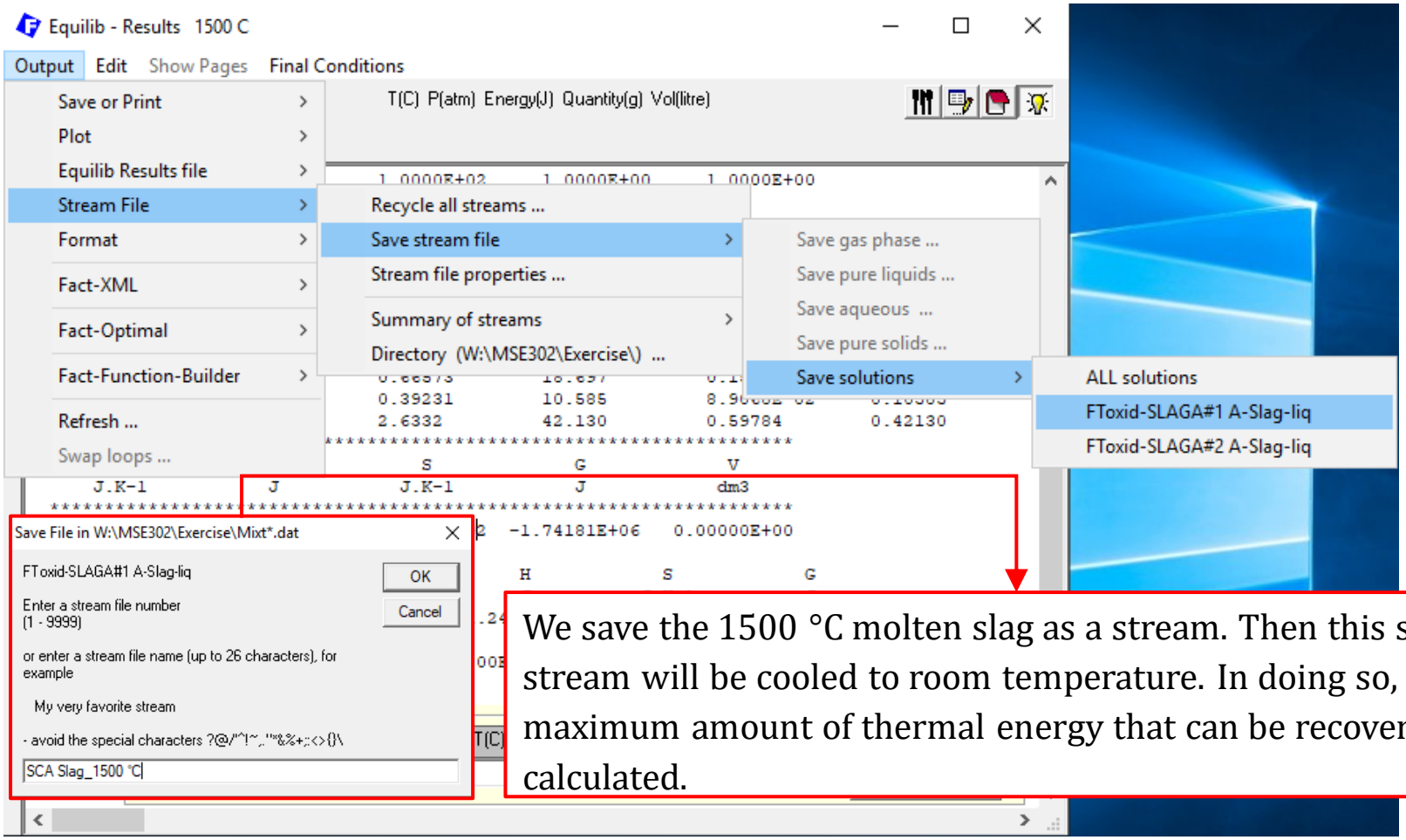
Task 1: Calculating the Enthalpy of Slag and Recoverable Heat



After we complete the calculation, we can go back to the Menu Window to obtain all the solution properties…. (see the list)

Example 2: Slag: Enthalpy, Melting Temperature

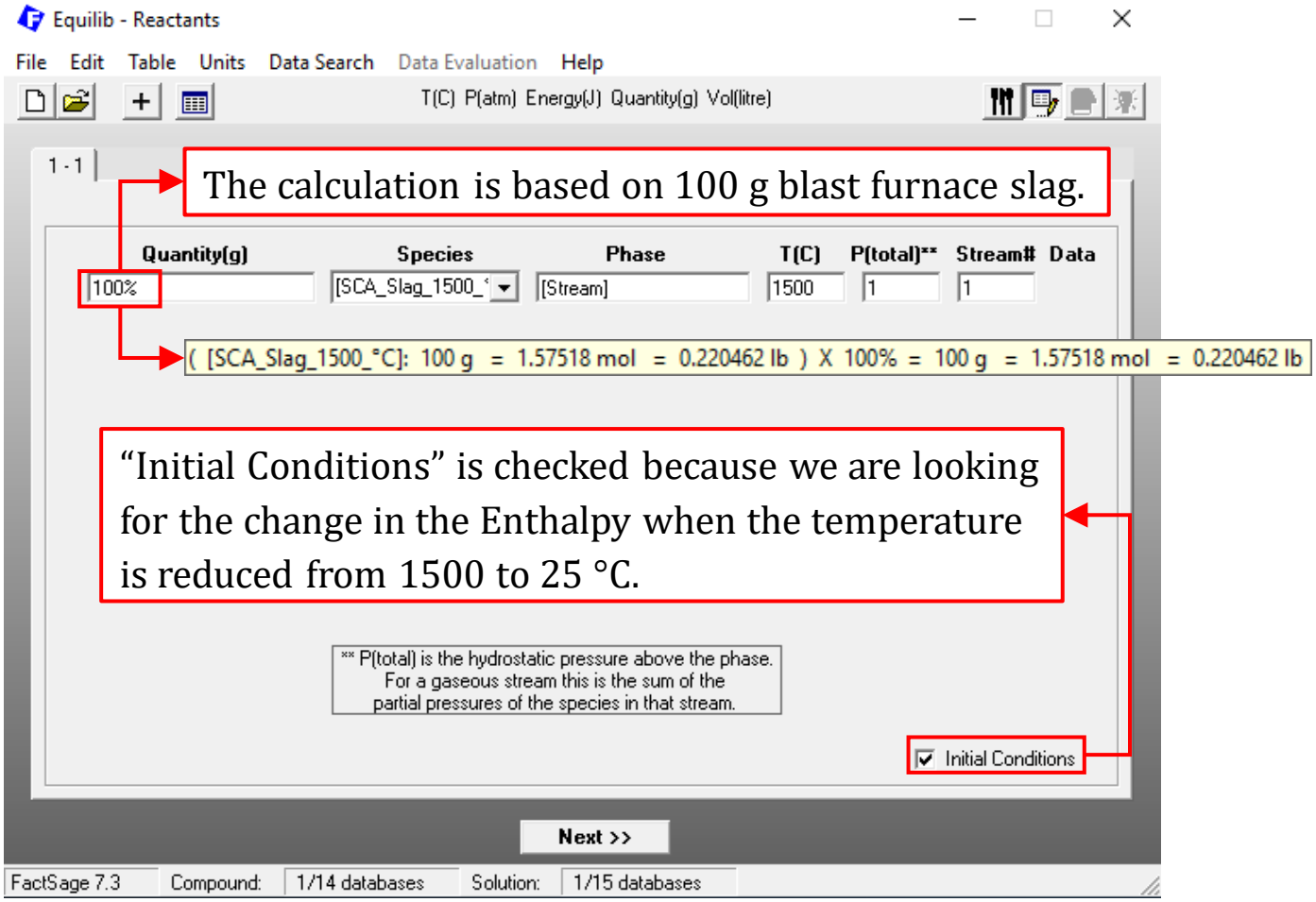
Task 1: Calculating the Enthalpy of Slag and Recoverable Heat



We save the 1500 °C molten slag as a stream. Then this slag stream will be cooled to room temperature. In doing so, the maximum amount of thermal energy that can be recovered is calculated.

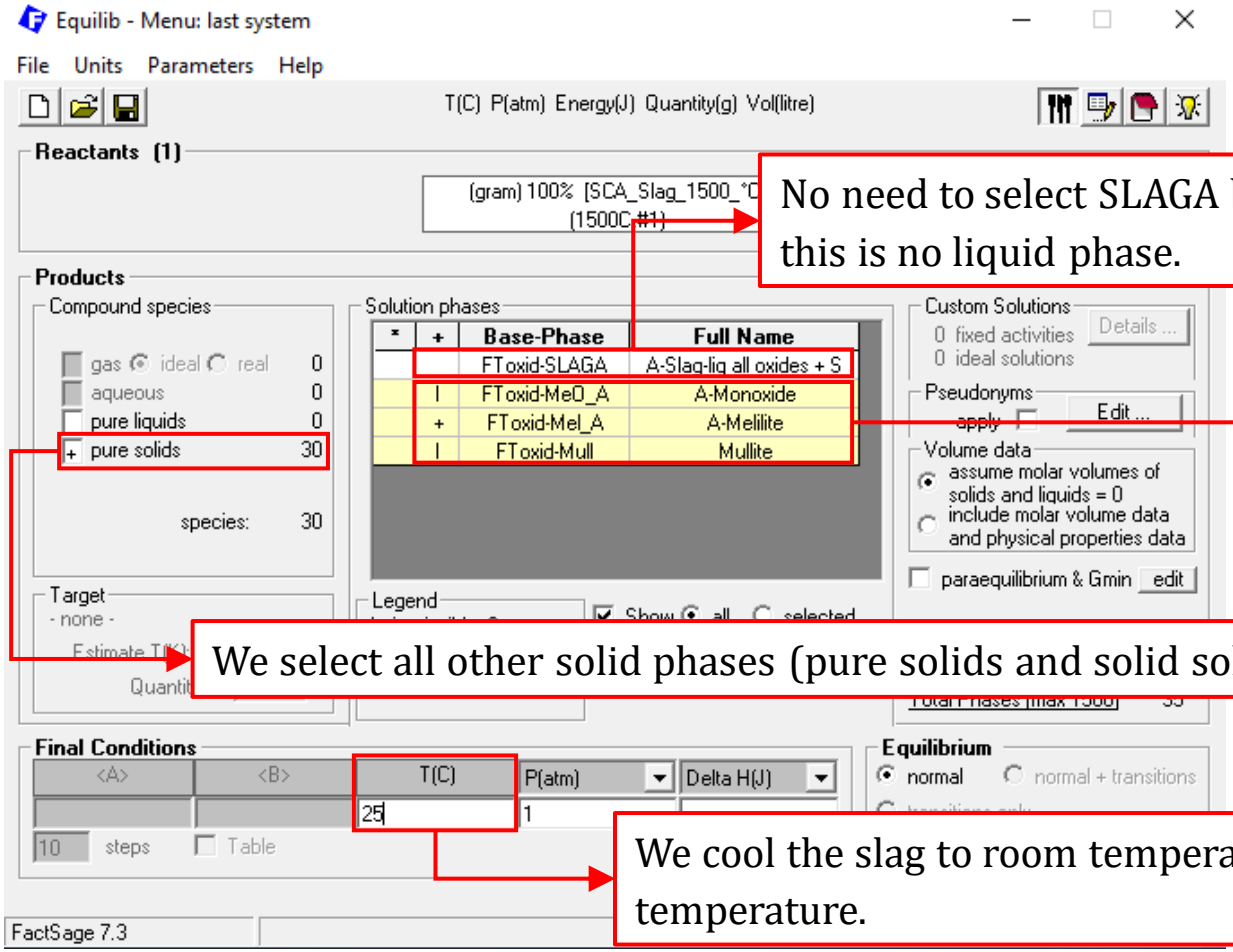
Example 2: Slag: Enthalpy, Melting Temperature

Task 1: Calculating the Enthalpy of Slag and Recoverable Heat



Example 2: Slag: Enthalpy, Melting Temperature

Task 1: Calculating the Enthalpy of Slag and Recoverable Heat



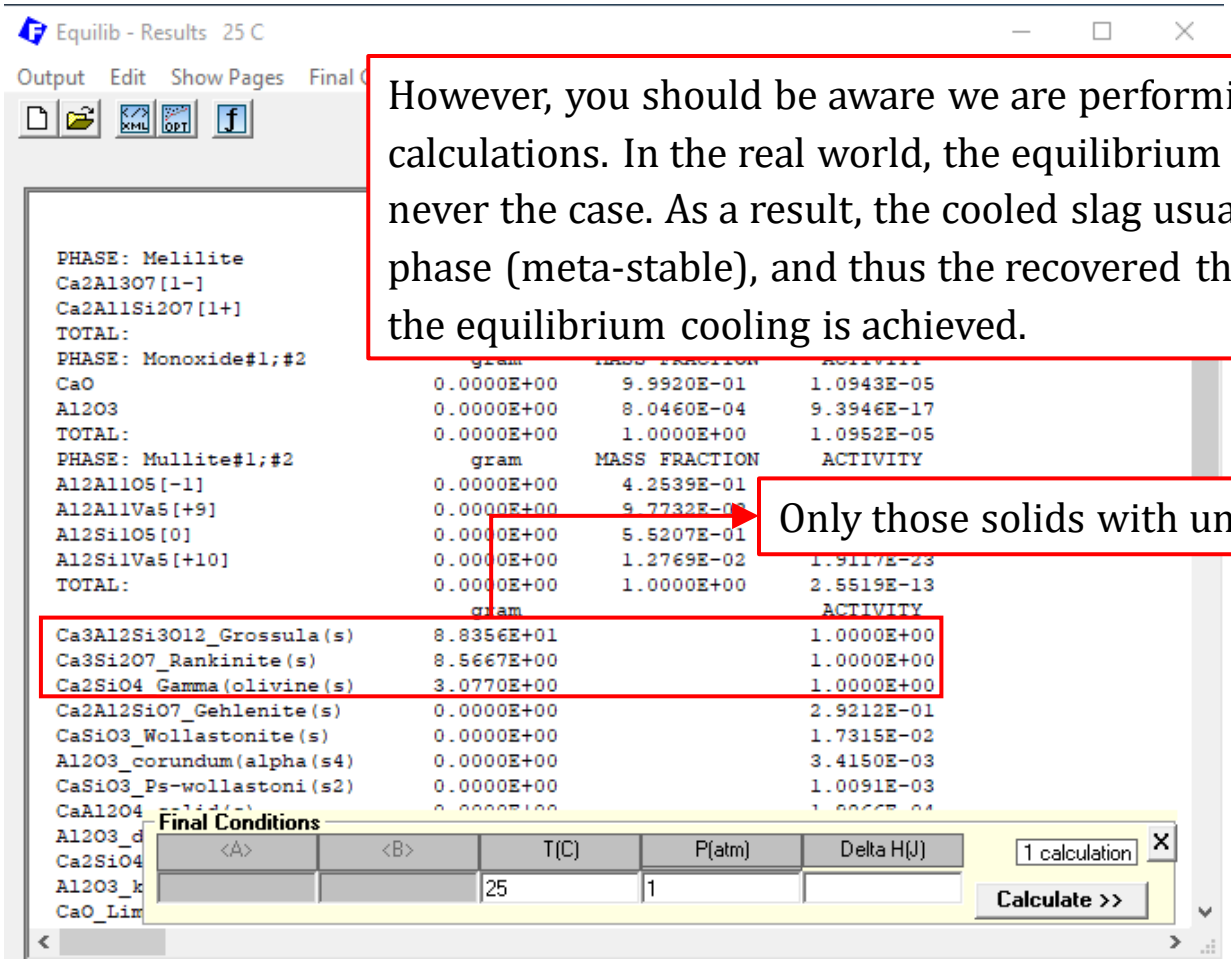
No need to select SLAGA because at 25 °C we are sure this is no liquid phase.

We select all other solid phases (pure solids and solid solutions).

We cool the slag to room temperature, which is the final temperature.

Example 2: Slag: Enthalpy, Melting Temperature

Task 1: Calculating the Enthalpy of Slag and Recoverable Heat

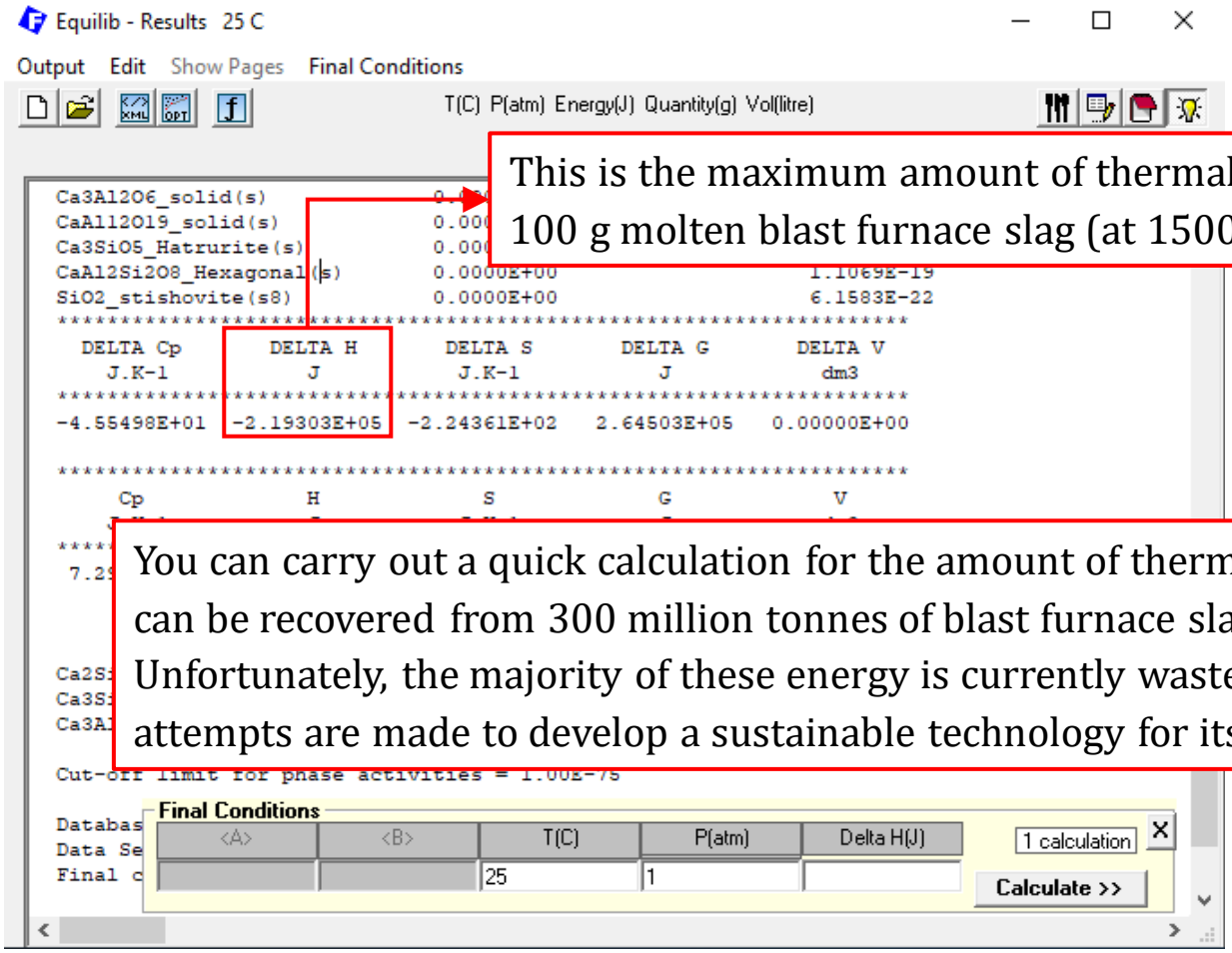


However, you should be aware we are performing equilibrium cooling calculations. In the real world, the equilibrium cooling of molten slag is never the case. As a result, the cooled slag usually contain a fraction of glass phase (meta-stable), and thus the recovered thermal energy is less than if the equilibrium cooling is achieved.

Only those solids with unity activity are stable.

Example 2: Slag: Enthalpy, Melting Temperature

Task 1: Calculating the Enthalpy of Slag and Recoverable Heat



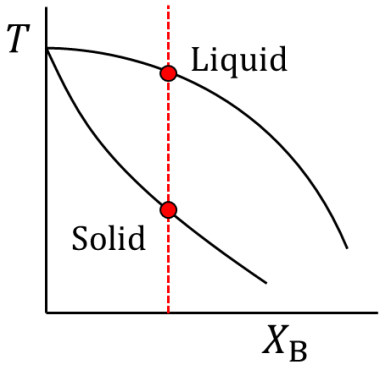
This is the maximum amount of thermal energy we can recover from 100 g molten blast furnace slag (at 1500 °C) that is considered.

You can carry out a quick calculation for the amount of thermal energy that can be recovered from 300 million tonnes of blast furnace slag. Unfortunately, the majority of these energy is currently wasted, and many attempts are made to develop a sustainable technology for its recovery.

Example 2: Slag: Enthalpy, Melting Temperature

Task 2: Calculating the Melting Temperature of Slag

First of all, you need to be aware that for pure substances, the melting or solidification process occurs at a fixed temperature (determined by the Gibbs phase rule). On the contrast, for solution phases, the melting or solidification process occurs within a certain temperature range, bounded by the liquidus temperature and solidus temperature. **The melting temperature of slag** refers to the liquidus temperature, that is, the temperature above which the system exists as 100% liquid. There are generally two approaches to calculating the melting temperature:

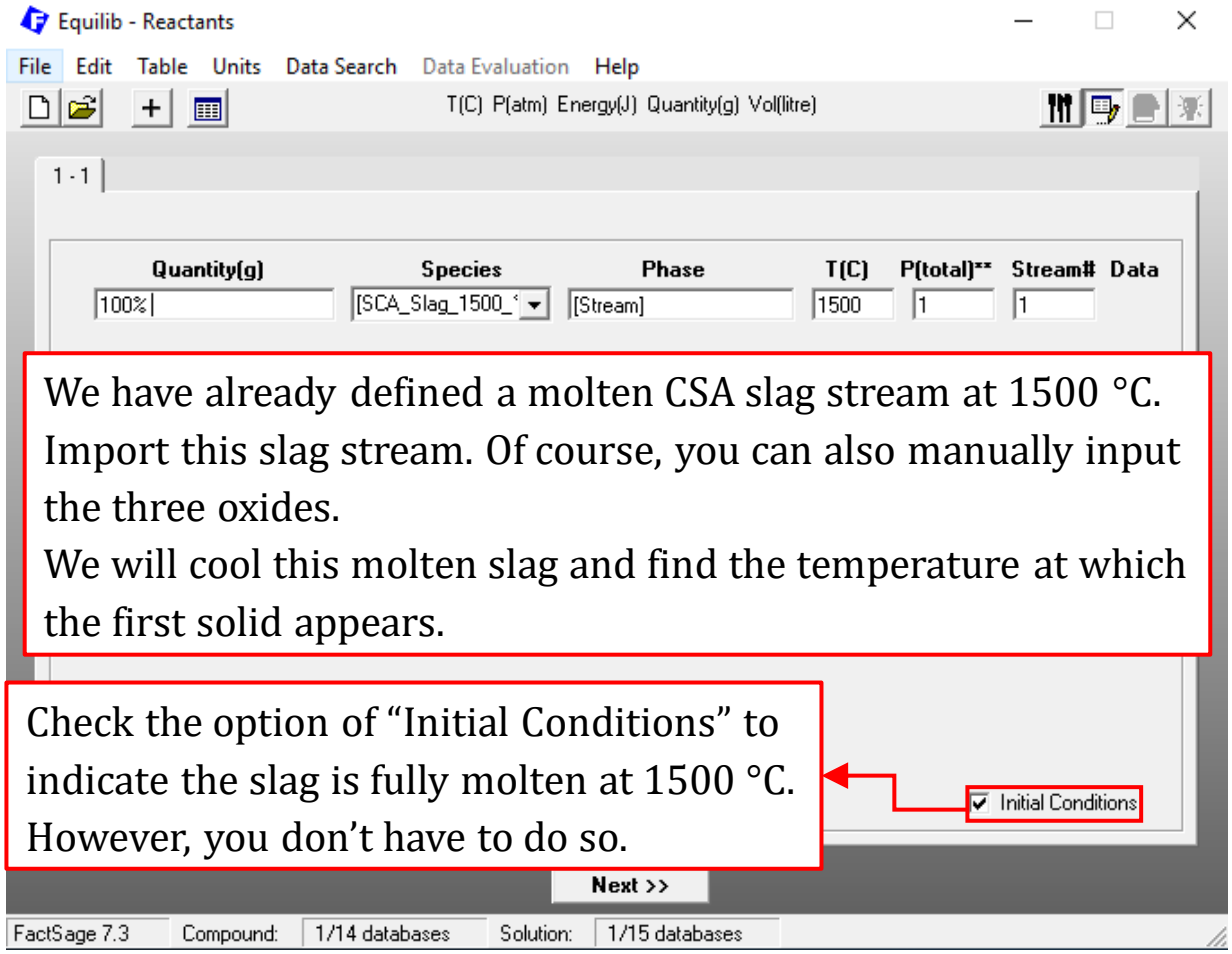


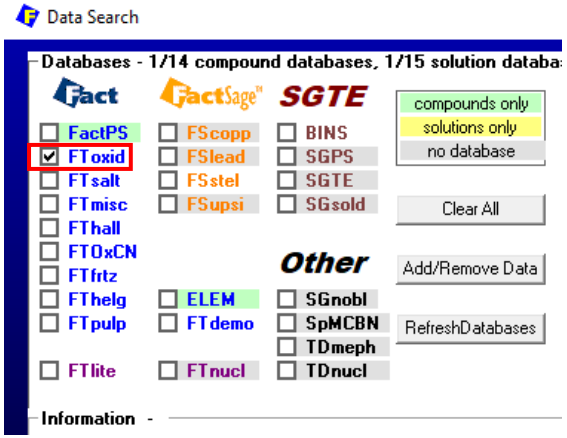
(a) Cooling Approach. Start with a temperature which is high enough so that the system is 100% liquid. Then cool the system to find the temperature when the first solid forms

(b) Heating Approach. Heat up the solid mixture and find the temperature when the last solid disappears.

Example 2: Slag: Enthalpy, Melting Temperature

Task 2: Calculating the Melting Temperature of Slag (Cooling Approach)





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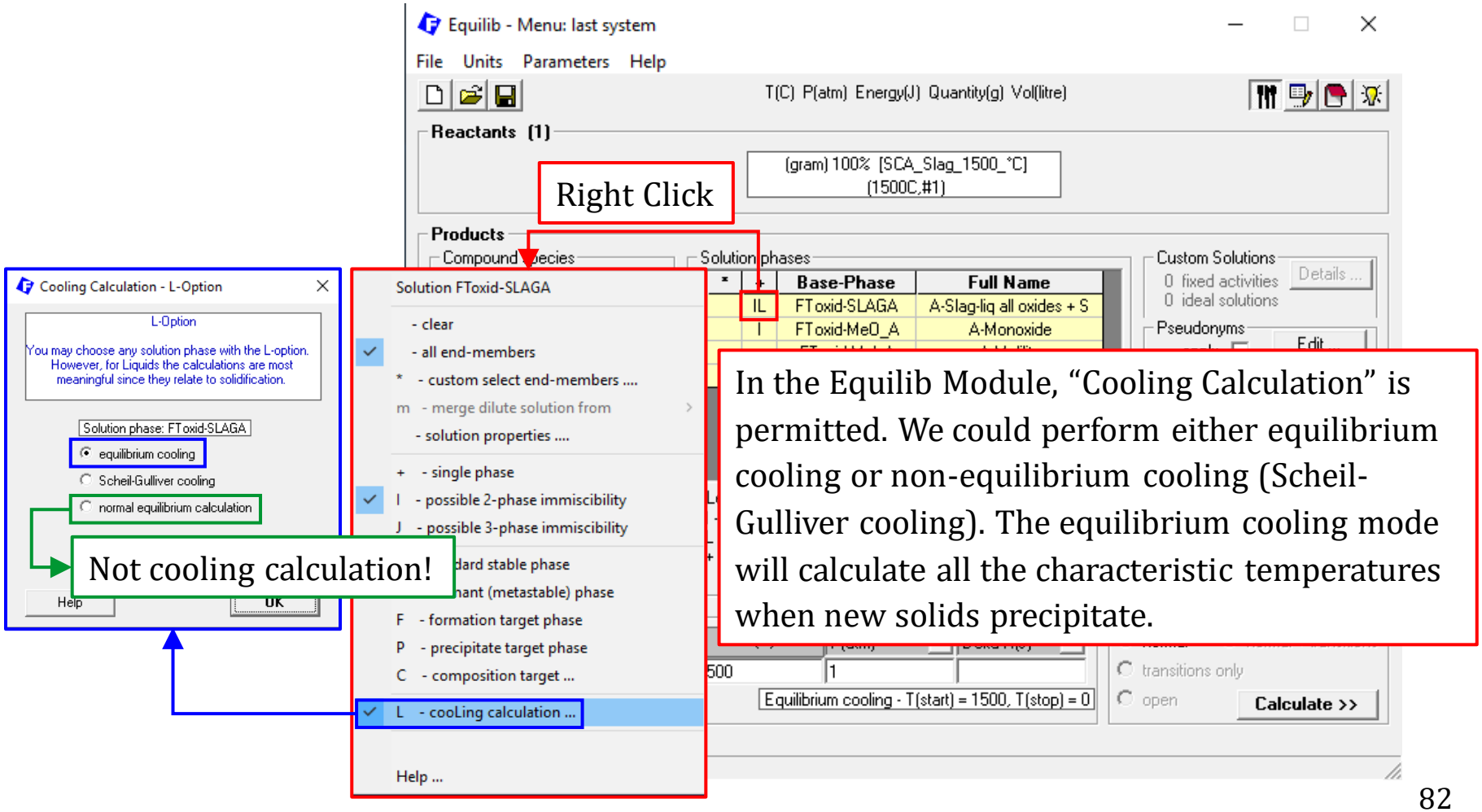
Task 2: Calculating the Melting Temperature of Slag (Cooling Approach)



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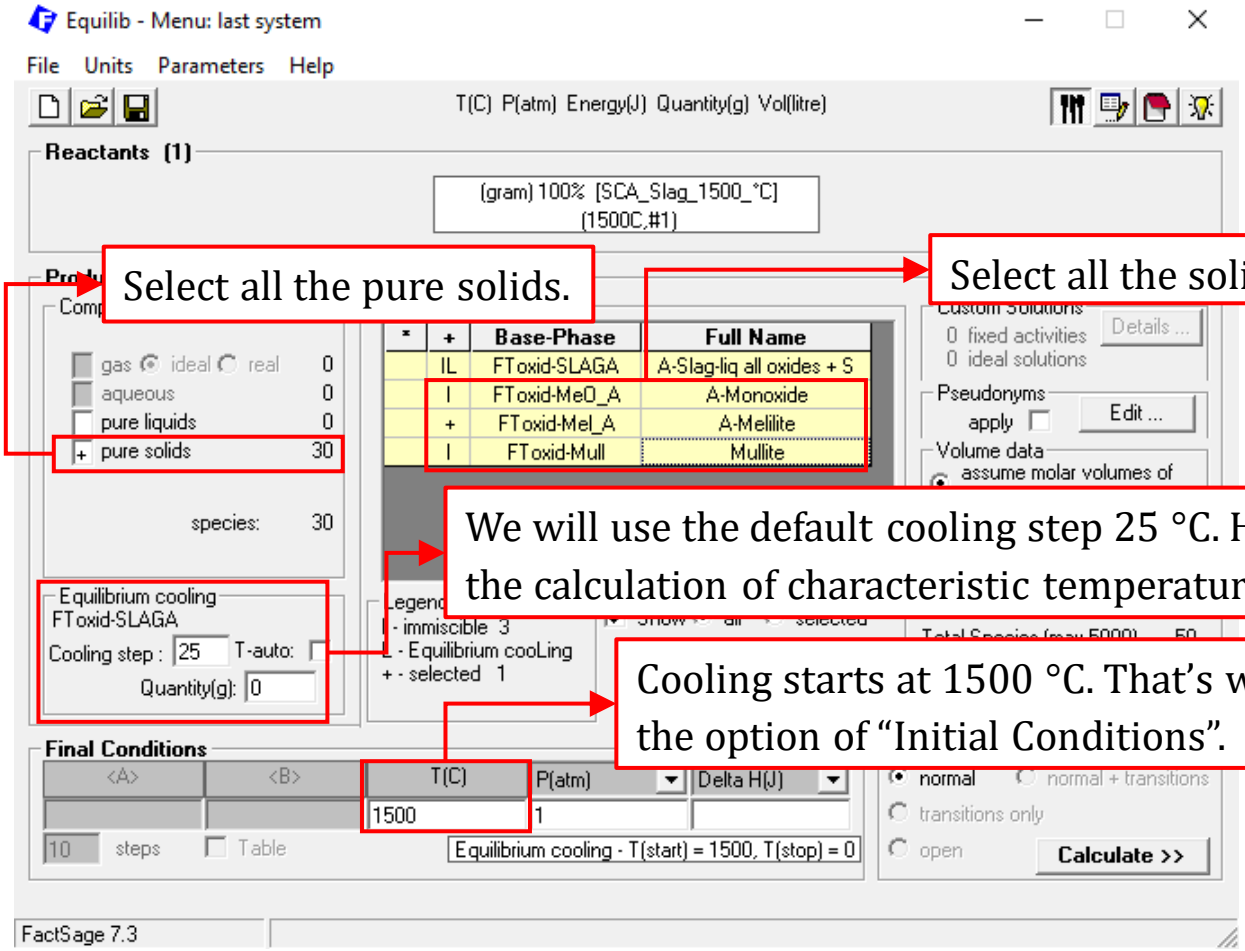
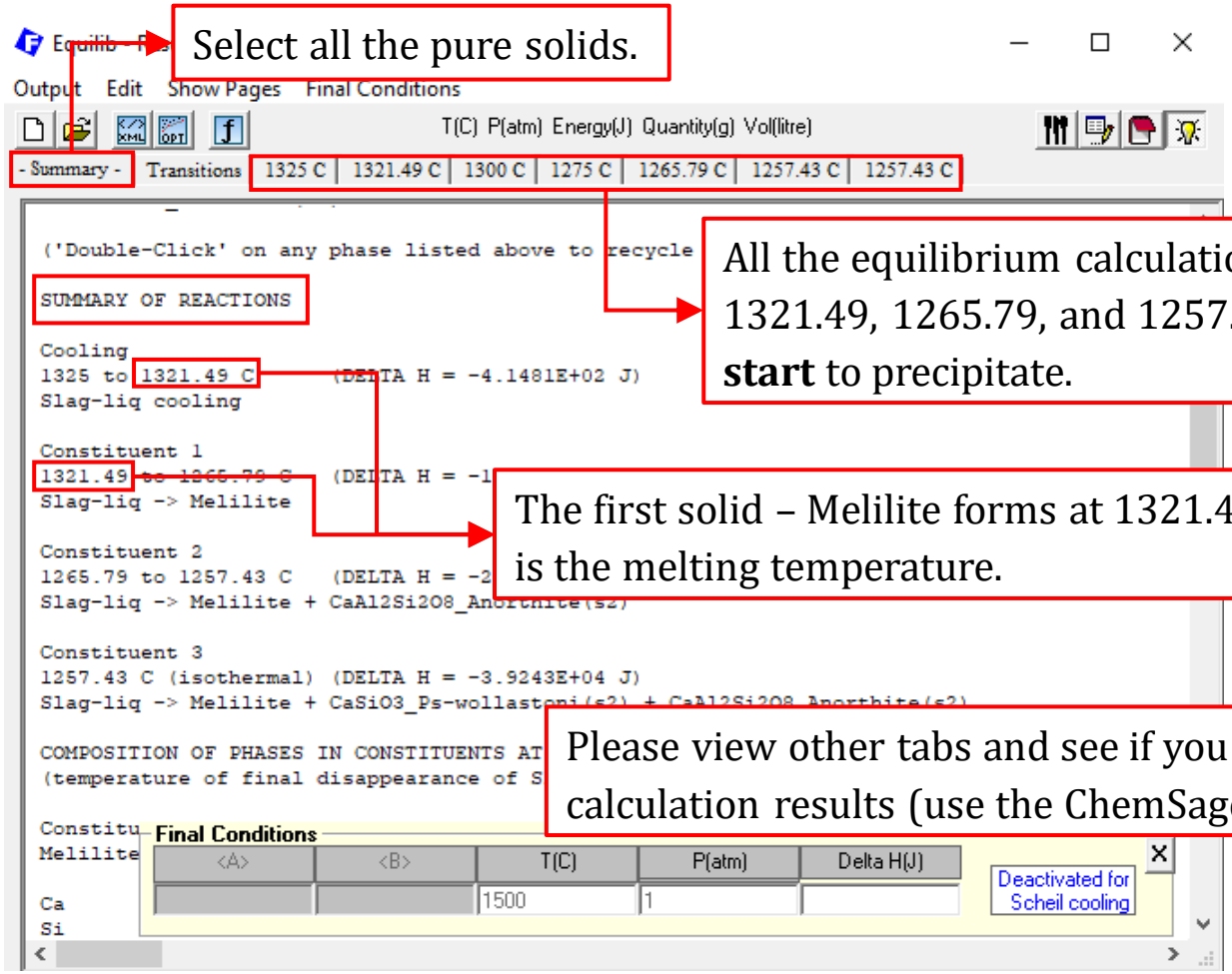


Example 2: Slag: Enthalpy, Melting Temperature

Task 2: Calculating the Melting Temperature of Slag (Cooling Approach)

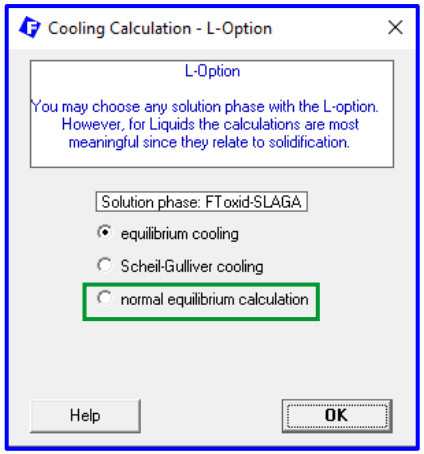


Example 2: Slag: Enthalpy, Melting Temperature

Task 2: Calculating the Melting Temperature of Slag (Cooling Approach)

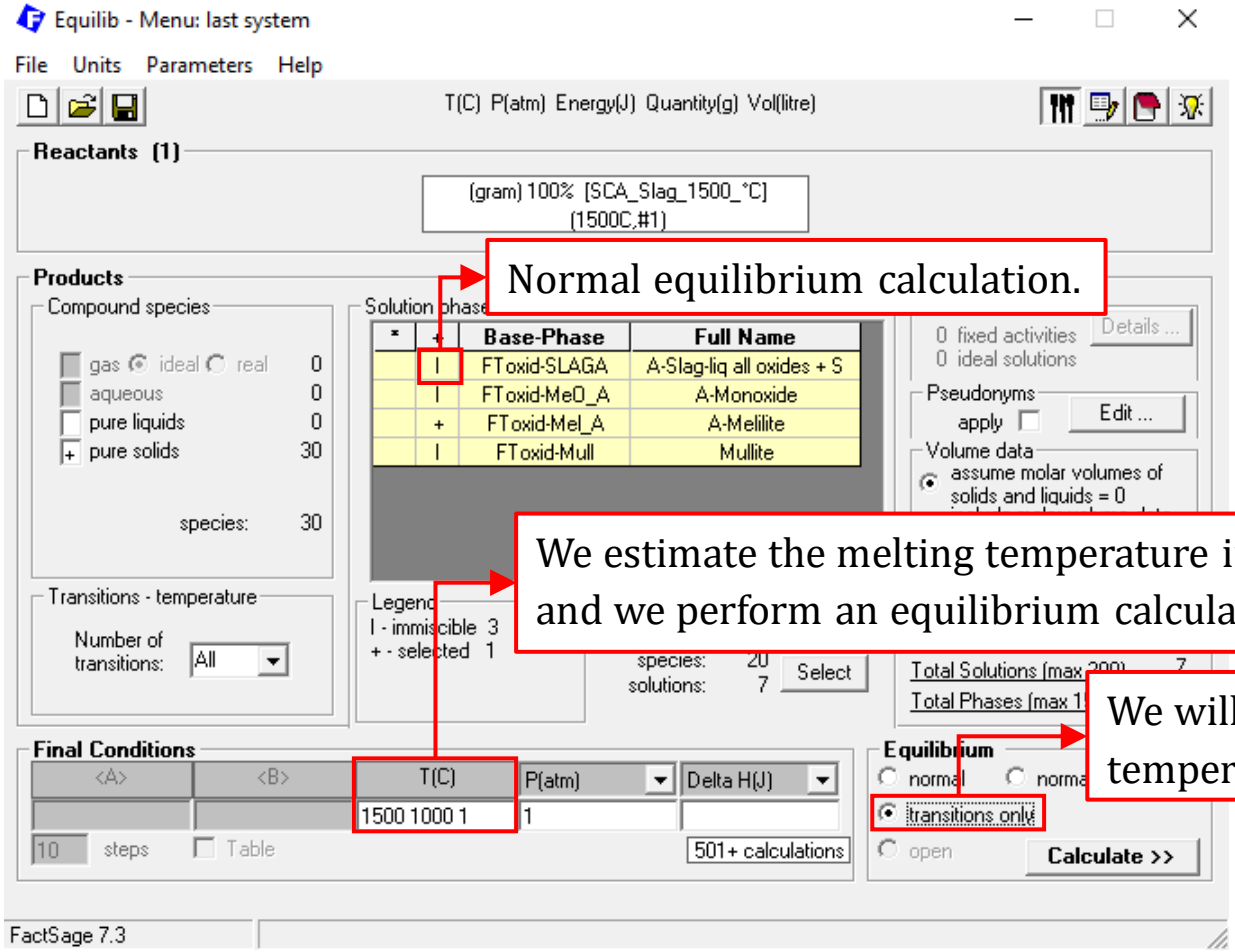
A Note on "Normal Equilibrium Calculation":

You can also use the mode of "normal equilibrium calculation" to calculate the melting temperature (Next Page).



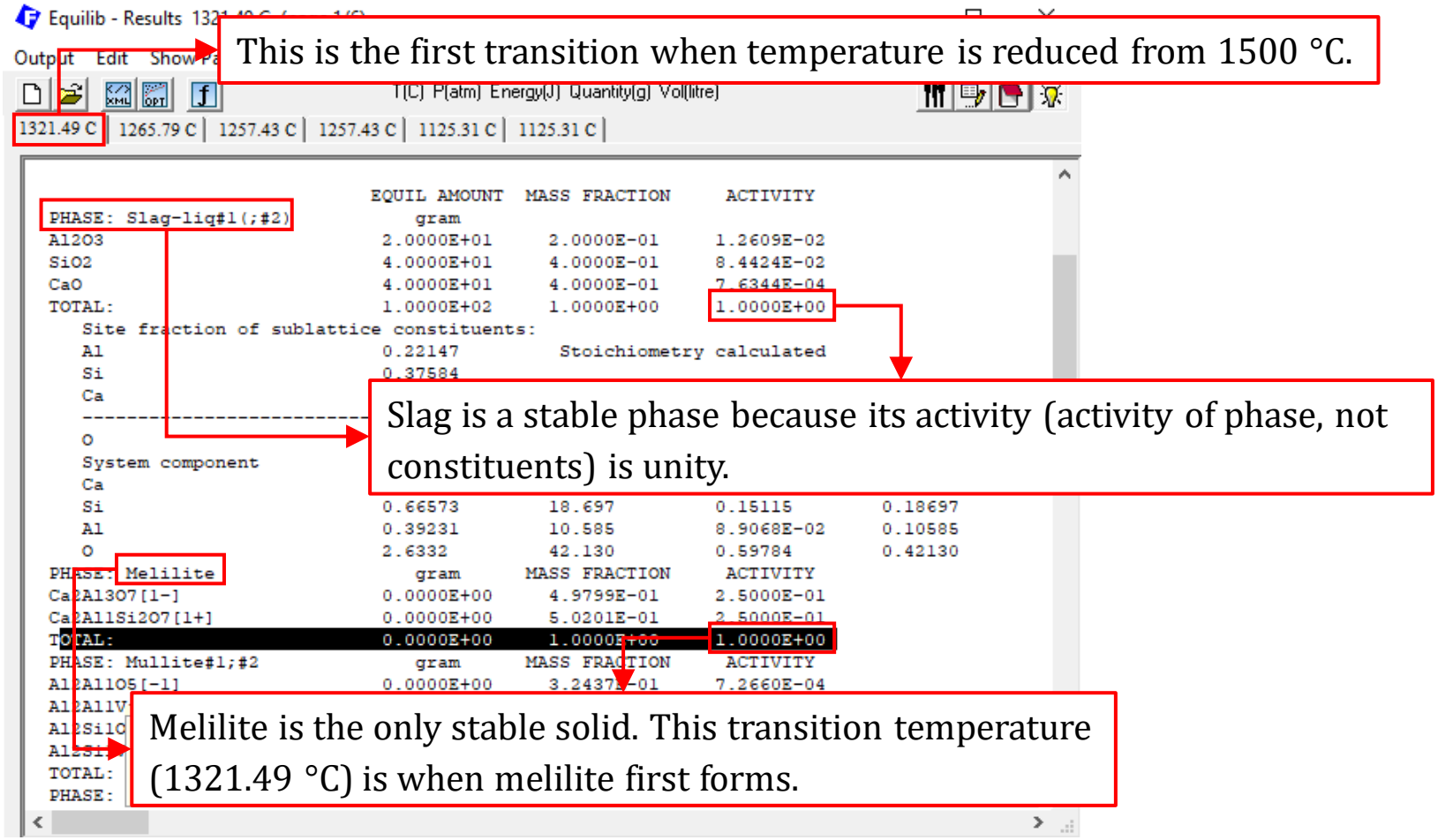
Example 2: Slag: Enthalpy, Melting Temperature

Task 2: Calculating the Melting Temperature of Slag (Cooling Approach)



Example 2: Slag: Enthalpy, Melting Temperature

Task 2: Calculating the Melting Temperature of Slag (Cooling Approach)



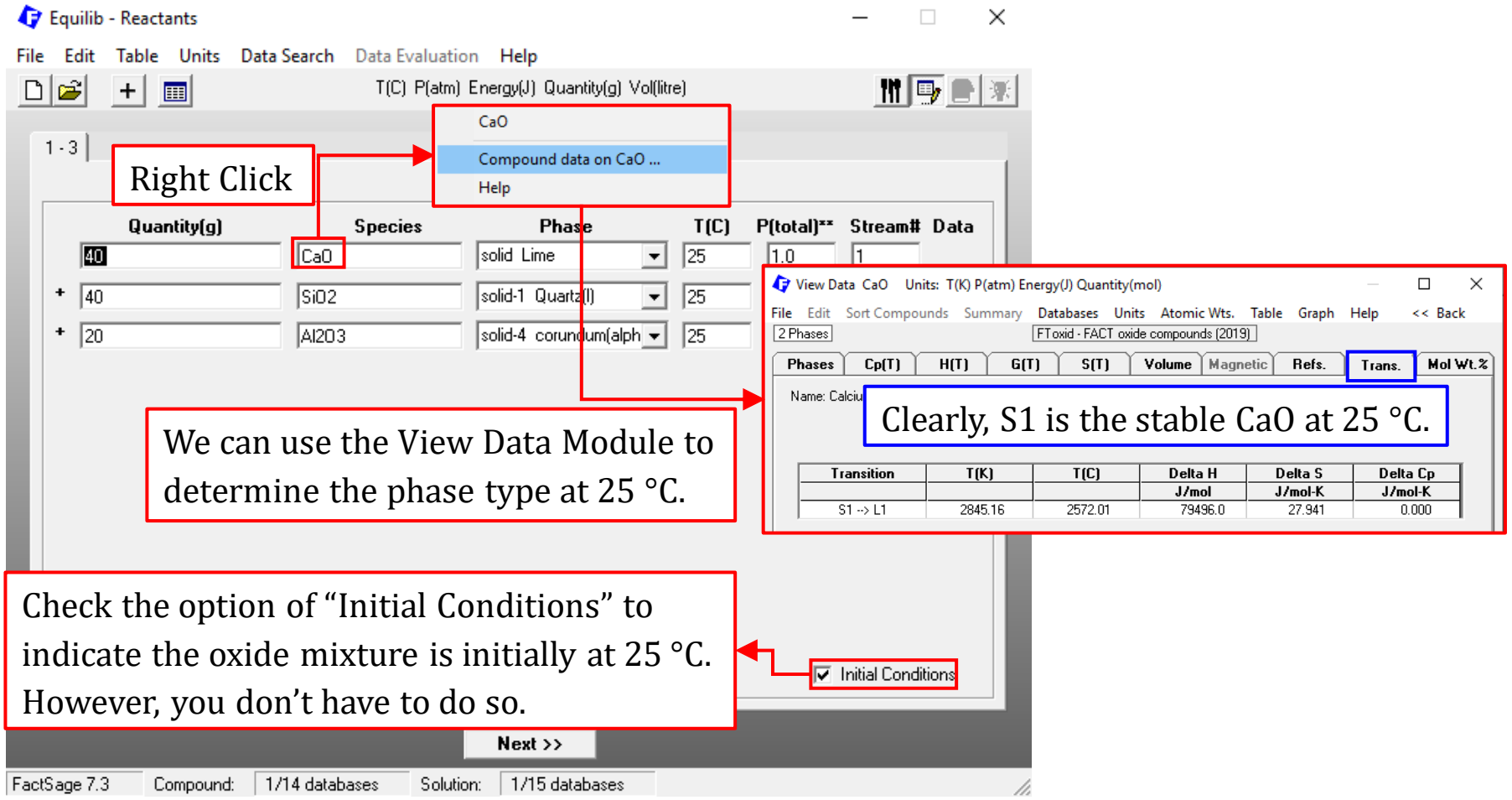
Example 2: Slag: Enthalpy, Melting Temperature

Task 2: Calculating the Melting Temperature of Slag (Heating Approach)

In the heating approach, we will manually input the oxides at 25 °C, and then perform higher-temperature calculations. The following slides show the calculation details.

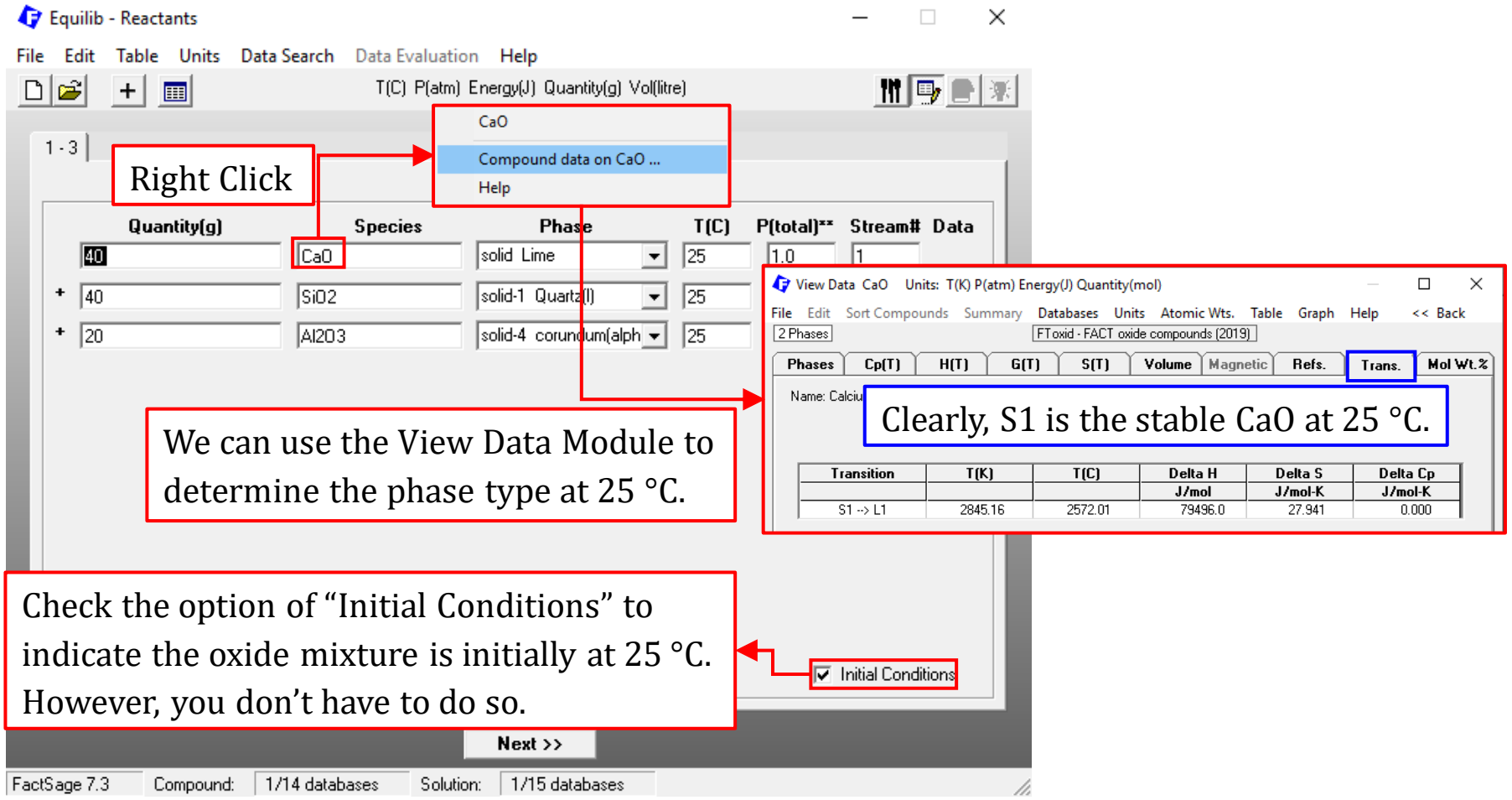
Example 2: Slag: Enthalpy, Melting Temperature

Task 2: Calculating the Melting Temperature of Slag (Heating Approach)



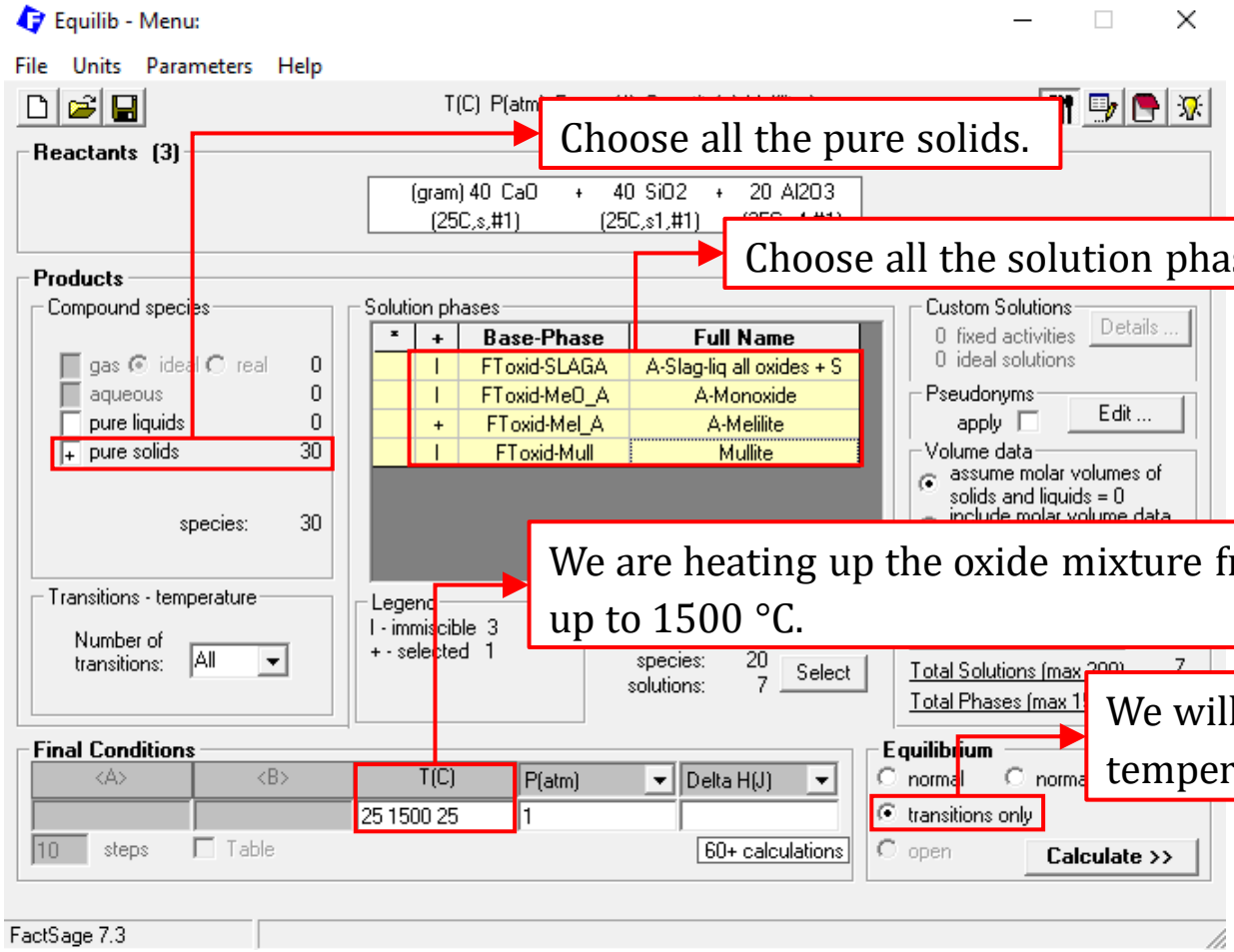
Example 2: Slag: Enthalpy, Melting Temperature

Task 2: Calculating the Melting Temperature of Slag (Heating Approach)



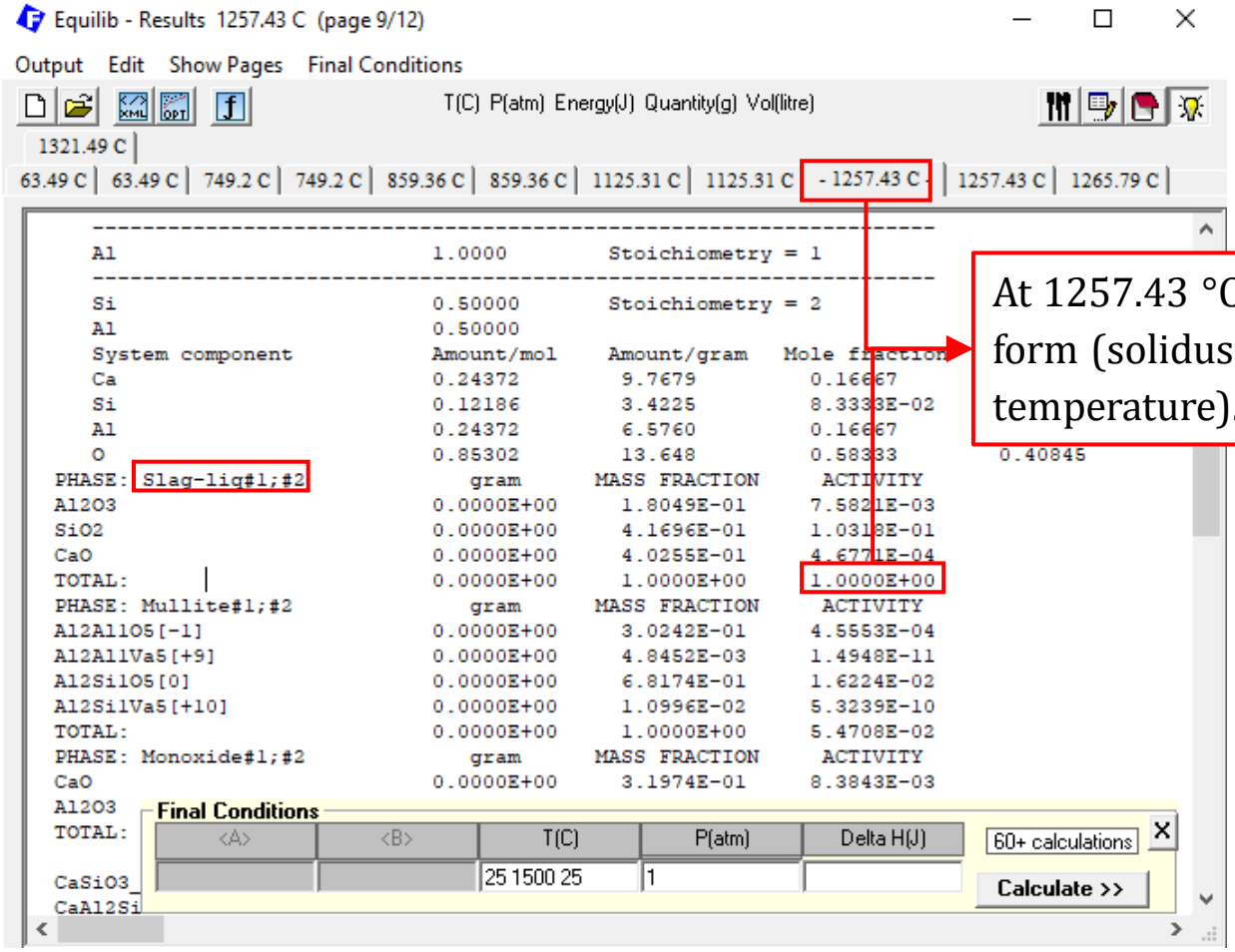
Example 2: Slag: Enthalpy, Melting Temperature

Task 2: Calculating the Melting Temperature of Slag (Heating Approach)



Example 2: Slag: Enthalpy, Melting Temperature

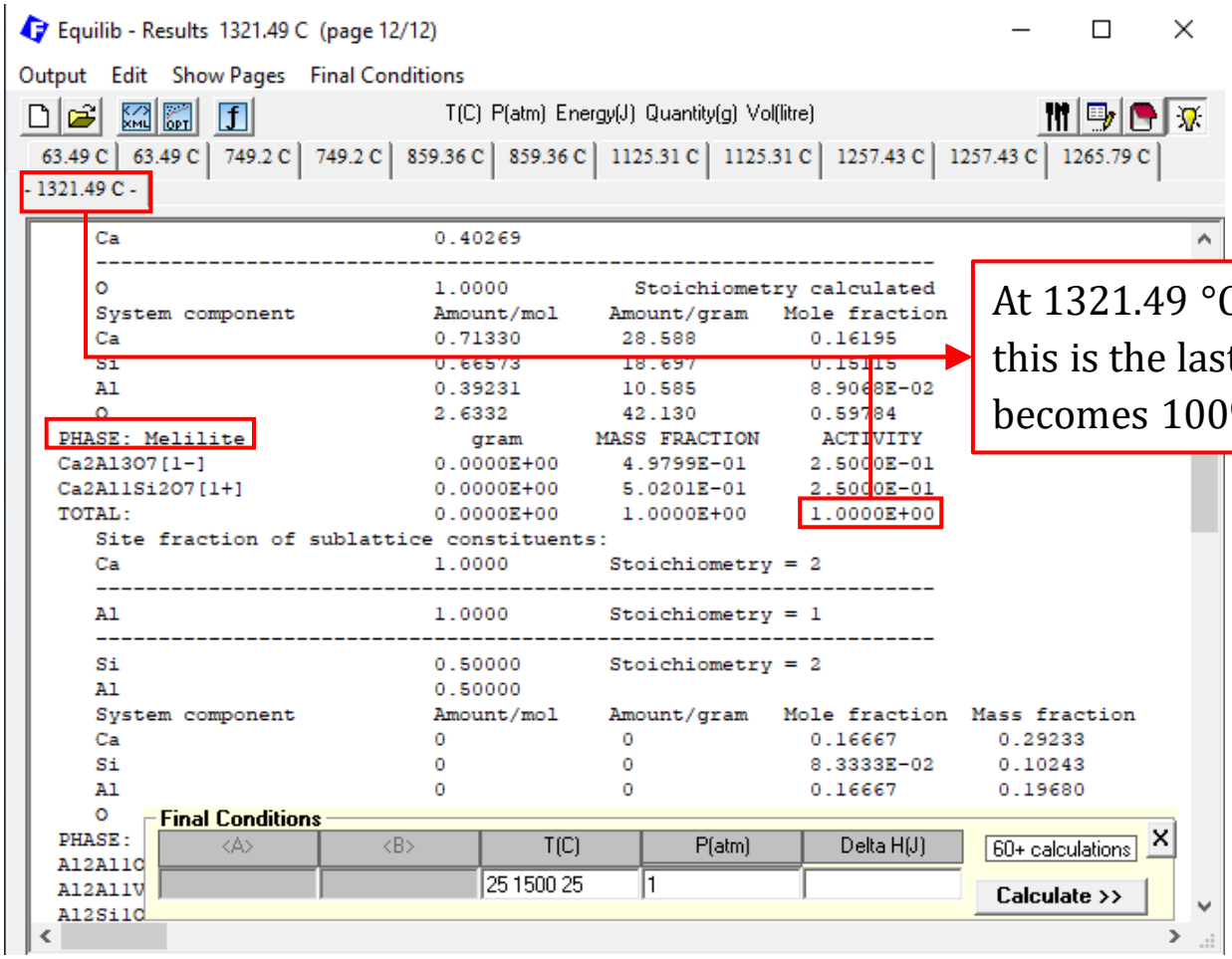
Task 2: Calculating the Melting Temperature of Slag (Heating Approach)



At 1257.43 °C, the liquid slag starts to form (solidus temperature or first melting temperature).

Example 2: Slag: Enthalpy, Melting Temperature

Task 2: Calculating the Melting Temperature of Slag (Heating Approach)



At 1321.49 °C, only melilite is present, but this is the last solid before the system becomes 100% liquid.

In-Class Exercise

Question 1. The typical composition of copper slag is shown below.

Oxide	FeO	SiO_2	CaO	Al_2O_3
wt.%	40.0	40.0	10.0	10.0

Calculate the equilibrium when this copper slag is heated between 1000 and 1800 °C in air (i.e., $P_{O_2} = 0.21$ atm).

Tip: (1) perform the calculation based on 100 gram of copper slag; (2) plot the masses of all stable phases against temperature.

In-Class Exercise

Question 2. Desulfurization of Liquid Steel

We have studied the desulfurization of hot metal using different desulfurizing agents. The hot metal after desulfurization is transferred to a basic oxygen furnace (BOF) for decarbonation. The resulting metal product is referred to as liquid steel.

Another spot of desulfurization is during ladle refining of liquid steel. Say we choose Mg as the desulfurization agent. Use the Equilib Module to find the required Mg if the sulfur content is reduced from 0.01 to 0.001 wt.%S. You may need the data shown on the next slide.

In-Class Exercise

Question 2. Desulfurization of Liquid Steel

Liquid Steel Composition.

Element	C	Mn	S	Fe
wt.%	0.05	0.10	0.01	99.84

Ladle Furnace Slag Composition.

Component	CaO	SiO_2	MgO	Al_2O_3
wt.%	40.0	10.0	10.0	40.0

The slag carry-over is 100 kg/tonne steel, and the temperature is 1600 °C.

Note: you don't have to consider the gas phase.

In-Class Exercise

Question 3. Preparation of Synthetic Slags

Use the Equilib Module to solve the following questions

As a summer student, your professor asked you to prepare a synthetic blast furnace slag. You have the following available chemical reagents, including solid quartz (low-temperature, SiO_2), solid lime (CaO), solid alpha corundom (Al_2O_3), and solid periclase (MgO).

(1) If the composition of the blast furnace slag is 32 wt.% SiO_2, 40 wt.% CaO, 17 wt.% Al_2O_3 and 11 wt.% MgO, what is the melting temperature?

(2) If all the chemical reagents which are initially at room temperature (25 °C) are fed into the furnace, calculate the minimum energy requirement when forming 100 g slag with the temperature determined in (1).