Case 3: Ilmenite ($FeTiO_3$) Smelting

Ilmenite Smelting

Ilmenite is a mixture of FeO and TiO_2. Canada currently has one of the largest ilmenite deposits. This ilmenite is processed by Rio Tinto Iron and Titanium (QIT) in Sorel, Quebec.

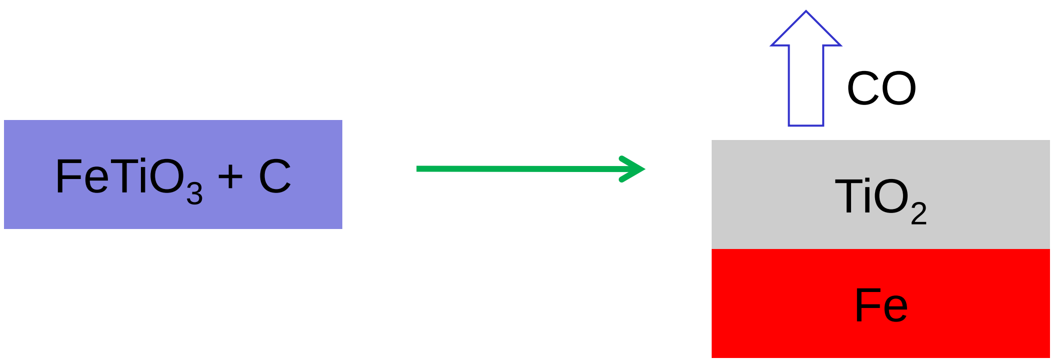
The main reactions occurring during ilmenite smelting is the reduction of FeO from slag to metal:

$$FeO(l)+C(s) \rightarrow Fe(l)+CO(g)$$

and the partial reduction of TiO_2 in the slag:

$$TiO_2(l)+0.5C(s) \rightarrow TiO_{1.5}(l)+0.5CO(g)$$

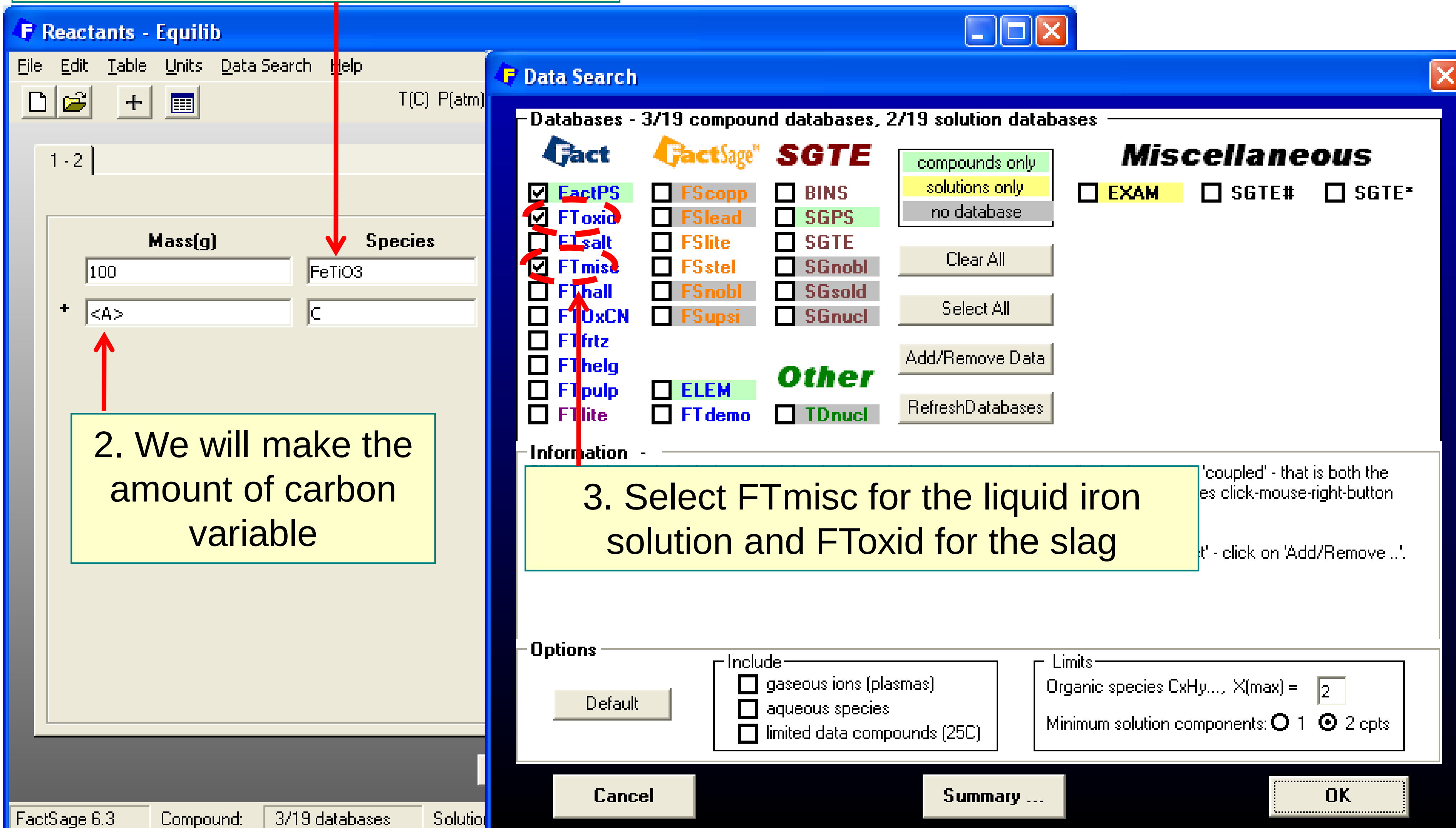
The ideal product would be a pure TiO2 slag and pure Fe metal.



In the following slides, we will study this reaction and analyze the smelting products.

Ilmenite Smelting

1. We will assume that the ore is composed of pure ilmenite



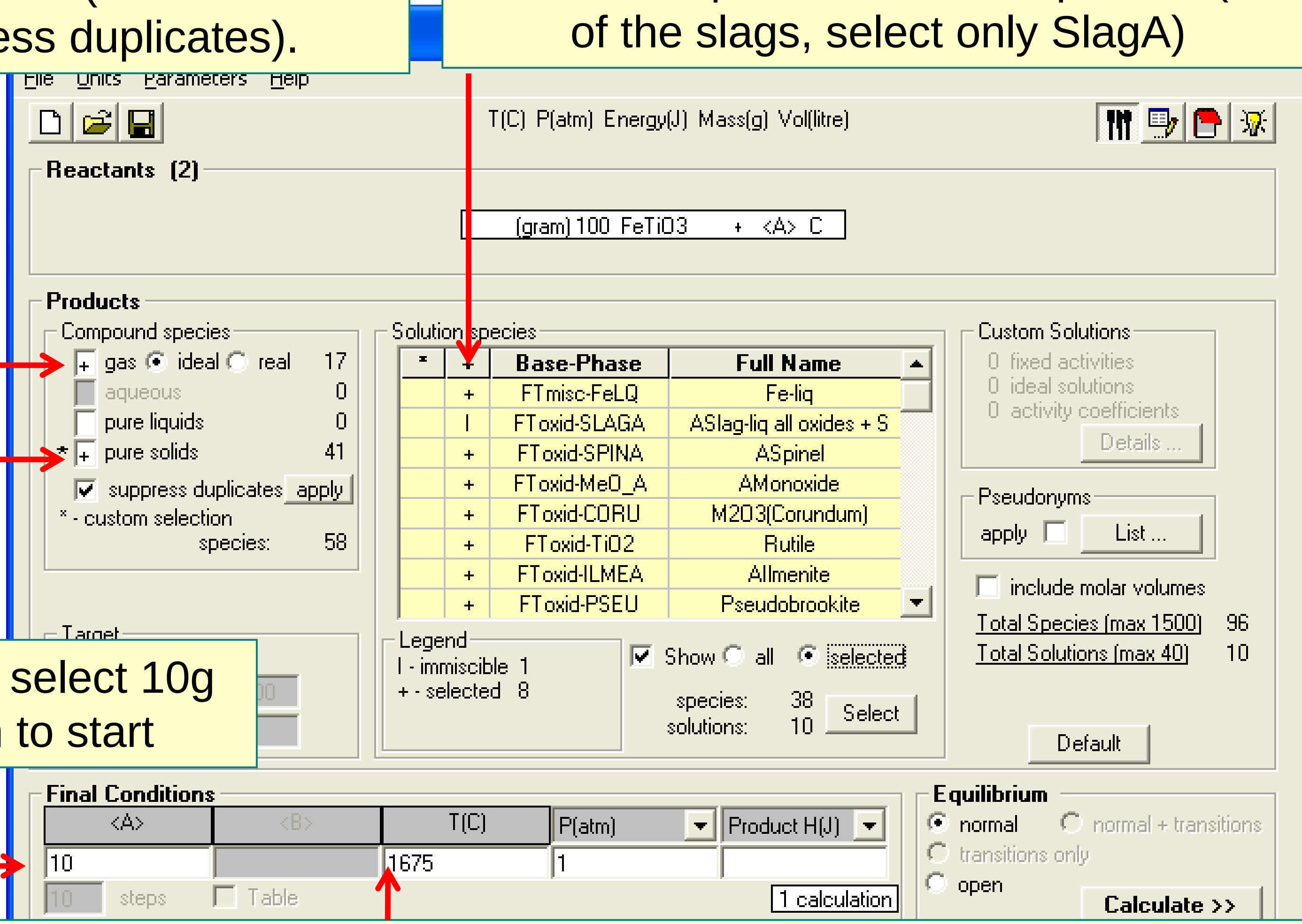
2. We will make the amount of carbon variable

3. Select FTmisc for the liquid iron solution and FToxid for the slag

Ilmenite Smelting

1. Select all gas and pure solid phases (remember to suppress duplicates).

2. Select all possible solution phases (out of the slags, select only SlagA)



3. We will select 10g carbon to start

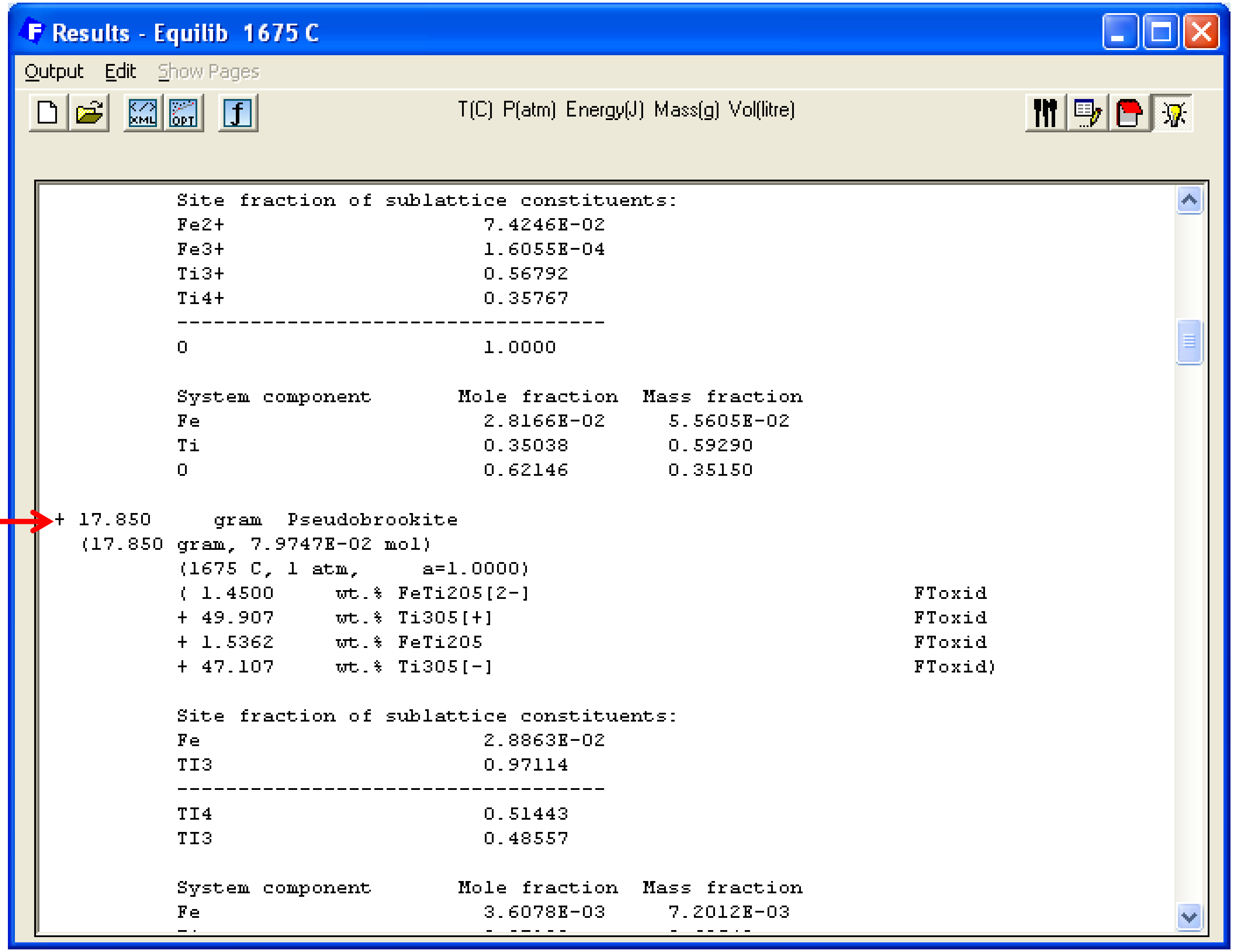
4. The average temperature of an ilmenite smelter is 1650-1700C, so we will select 1675 as the final temperature.

Ilmenite Smelting

1. After calculation, it is found that solid pseudobrookite is precipitated.

2. It is necessary to select the right amount of carbon to avoid precipitation of pseudobrookite

3. This can be done using “Formation target”



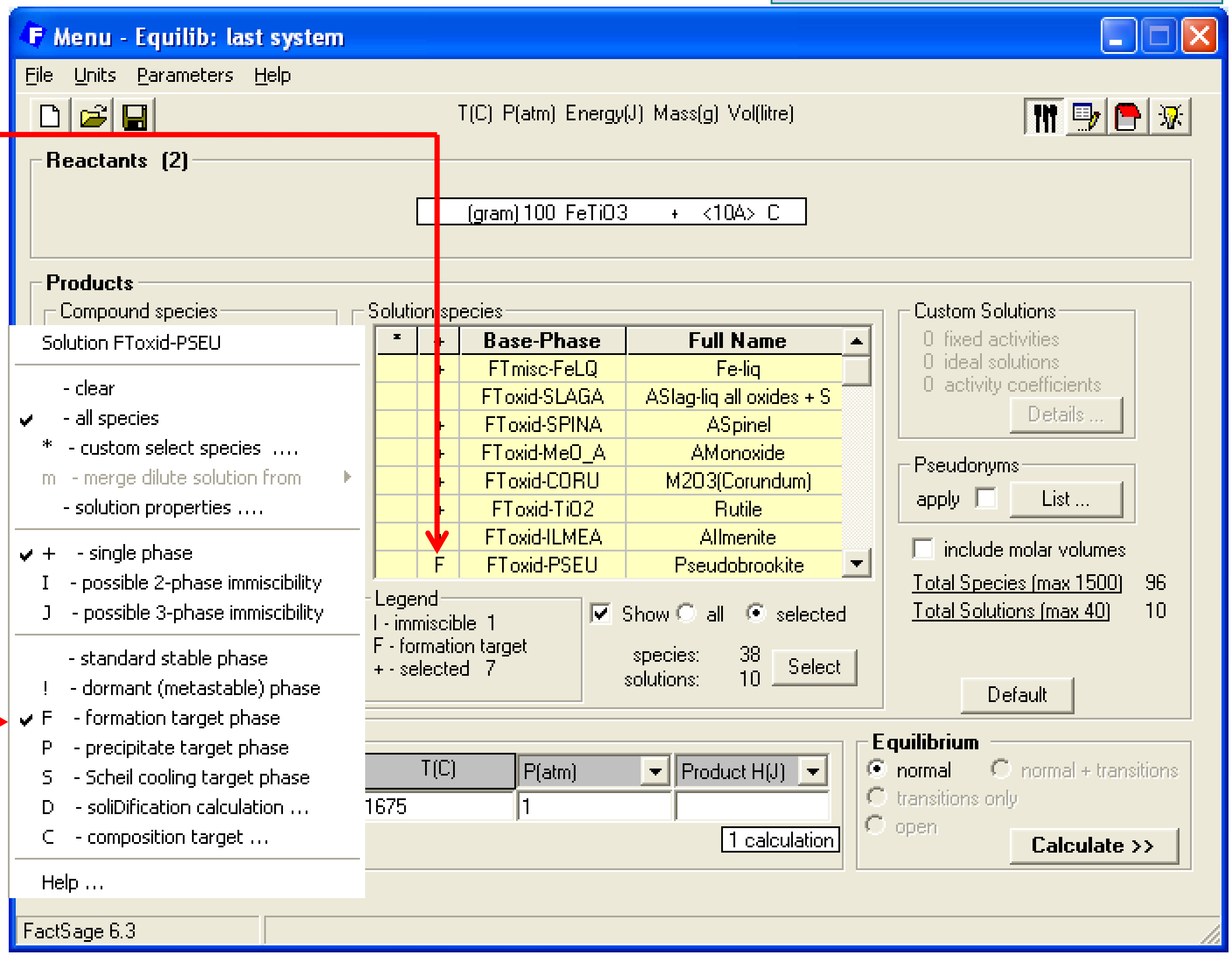
Calculating the optimum amount of carbon addition: Pseudobrookite formation target

Ilmenite Smelting

1. Right-click on the pseudobrookite selection

2. Select “Formation target phase”

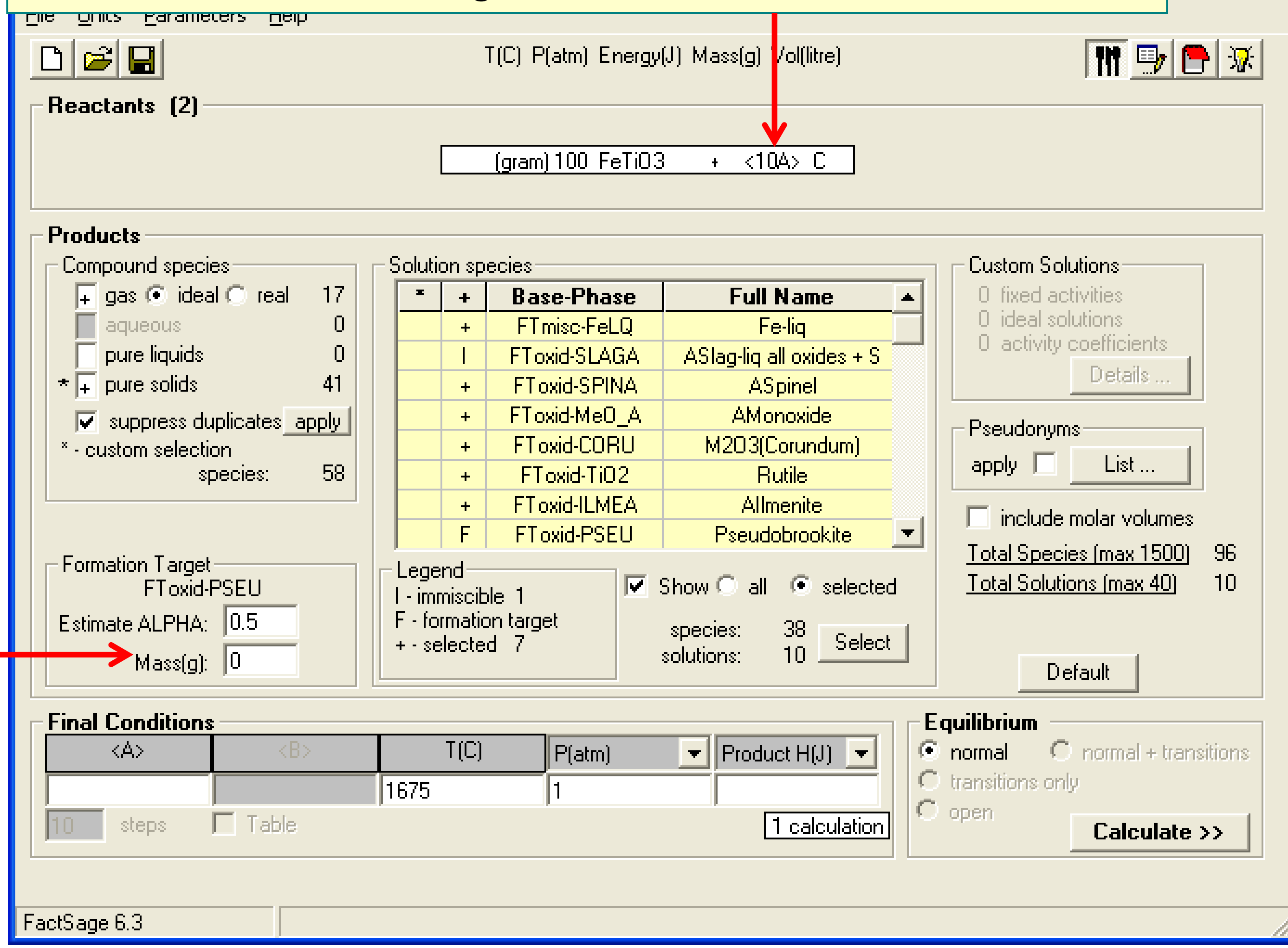
This example can be found in EquiCase3-1.dat



Ilmenite Smelting

1. Leaving <A> blank, a solution will be found for the value of <A>, where the activity of pseudobrookite will be 1, but its amount will be 0.

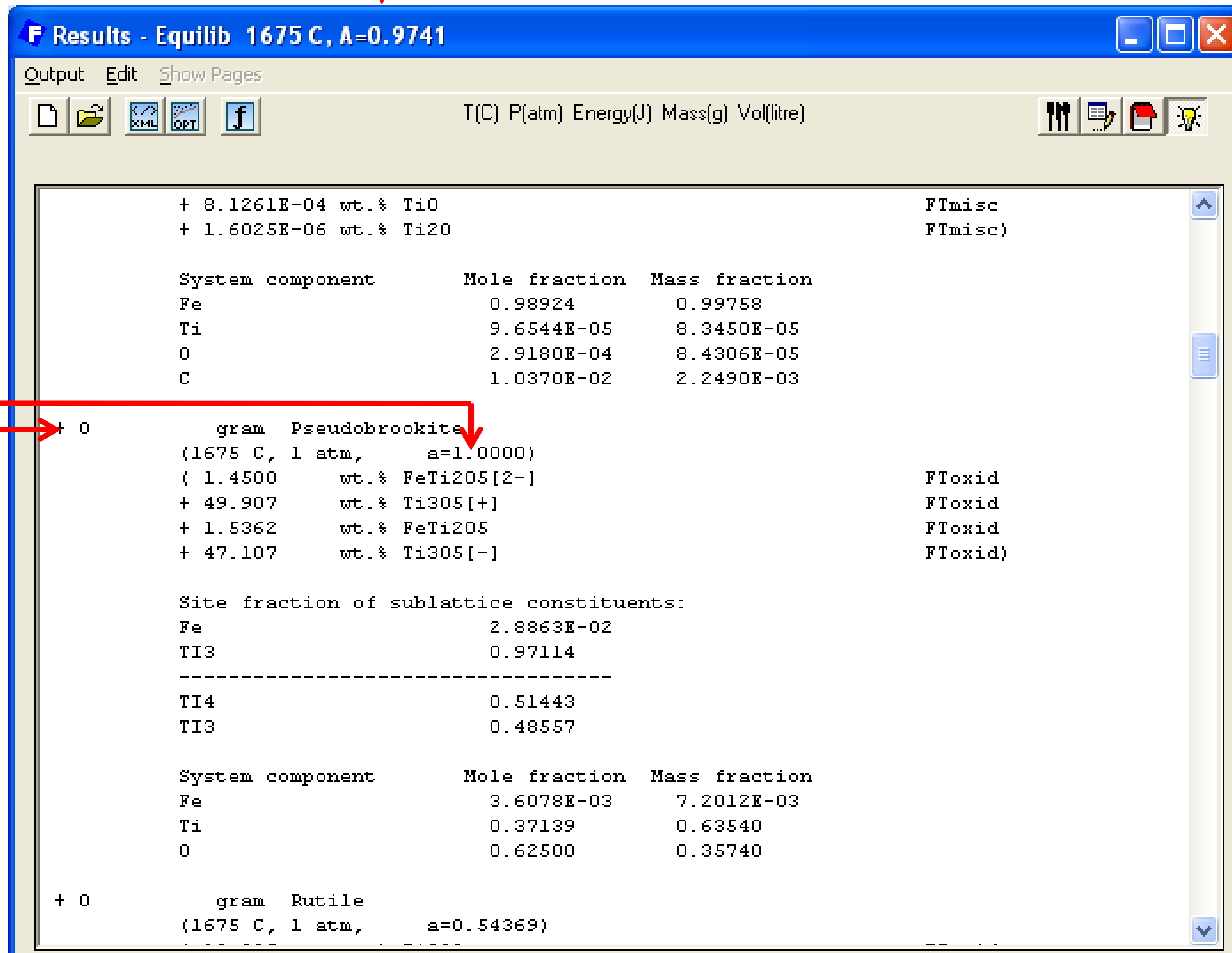
2. Note that the amount of carbon was changed to <10A> to allow carbon amount to change from 0 to 10g during the calculation.



Ilmenite Smelting

1. The solution is 9.741g carbon

2. Note that the amount of pseudobrookite is 0g, but its activity is 1. So it is ready to form as soon as we add just a little more carbon



Ilmenite Smelting

1. Looking at the slag composition, it can be noted that the slag contains about 7% FeO

Results - Equilib 1675 C, A=0.9741

Output Edit Show Pages

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

PHASE	gram	MASS FRACTION	ACTIVITY
PHASE: ASlag-liq#1	gram	MASS FRACTION	ACTIVITY
FeO	3.7983E+00	7.1382E-02	2.6445E-02
Fe2O3	9.1279E-03	1.7154E-04	3.1829E-08
Ti2O3	2.9063E+01	5.4618E-01	2.2613E-01
TiO2	2.0341E+01	3.8227E-01	3.3919E-01
TOTAL:	5.3211E+01	1.0000E+00	1.0000E+00
PHASE: ASlag-liq#2	gram	MASS FRACTION	ACTIVITY
FeO	0.0000E+00	7.1382E-02	2.6445E-02
Fe2O3	0.0000E+00	1.7154E-04	3.1829E-08
Ti2O3	0.0000E+00	5.4618E-01	2.2613E-01
TiO2	0.0000E+00	3.8227E-01	3.3919E-01
TOTAL:	0.0000E+00	1.0000E+00	1.0000E+00
PHASE: Fe-liq	gram	MASS FRACTION	ACTIVITY
Fe	3.3842E+01	9.9758E-01	9.8884E-01
C	7.6297E-02	2.2490E-03	7.5501E-03
O	2.7909E-03	8.2268E-05	3.6983E-06
Ti	2.6239E-03	7.7345E-05	3.1673E-06
TiO	2.7567E-04	8.1261E-06	7.0432E-06
Ti2O	5.4362E-07	1.6025E-08	7.9390E-09
TOTAL:	3.3924E+01	1.0000E+00	1.0000E+00
PHASE: Pseudobrookite	gram	MASS FRACTION	ACTIVITY
FeTi2O5[2-]	0.0000E+00	1.4500E-02	2.6757E-03
Ti3O5[+]	0.0000E+00	4.9907E-01	2.5036E-01
FeTi2O5	0.0000E+00	1.5362E-02	1.8435E-02
Ti3O5[-]	0.0000E+00	4.7107E-01	2.3541E-01
TOTAL:	0.0000E+00	1.0000E+00	1.0000E+00
PHASE: Rutile	gram	MASS FRACTION	ACTIVITY
Ti2O3	0.0000E+00	1.8825E-01	3.7713E-01
TiO2	0.0000E+00	8.1175E-01	4.3228E-01
TOTAL:	0.0000E+00	1.0000E+00	5.4369E-01

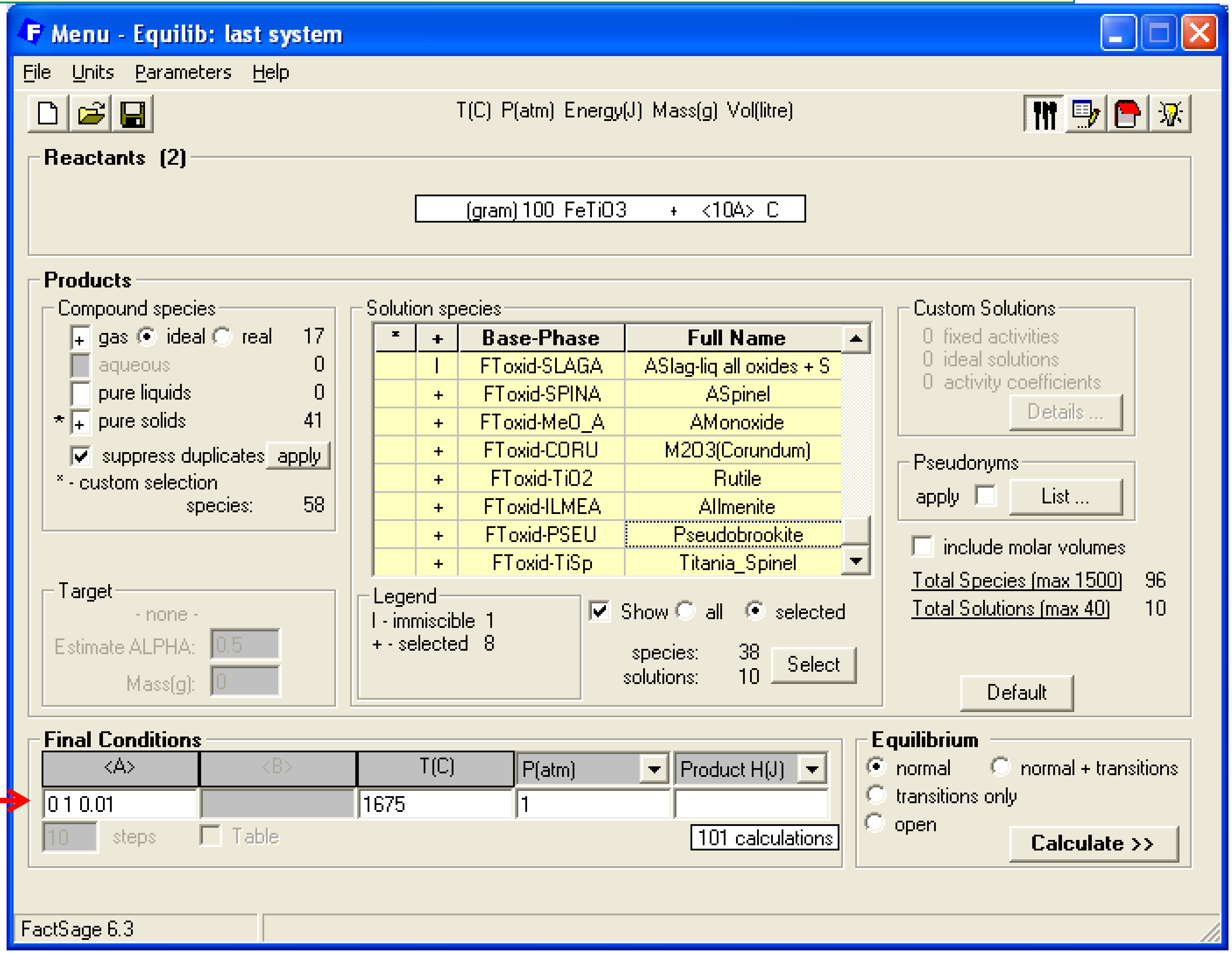
2. The iron phase, however, is composed of 99.8% Fe

3. It would be interesting to see how the slag and metal composition changes with carbon addition

Visualizing the change in metal and slag composition with carbon addition

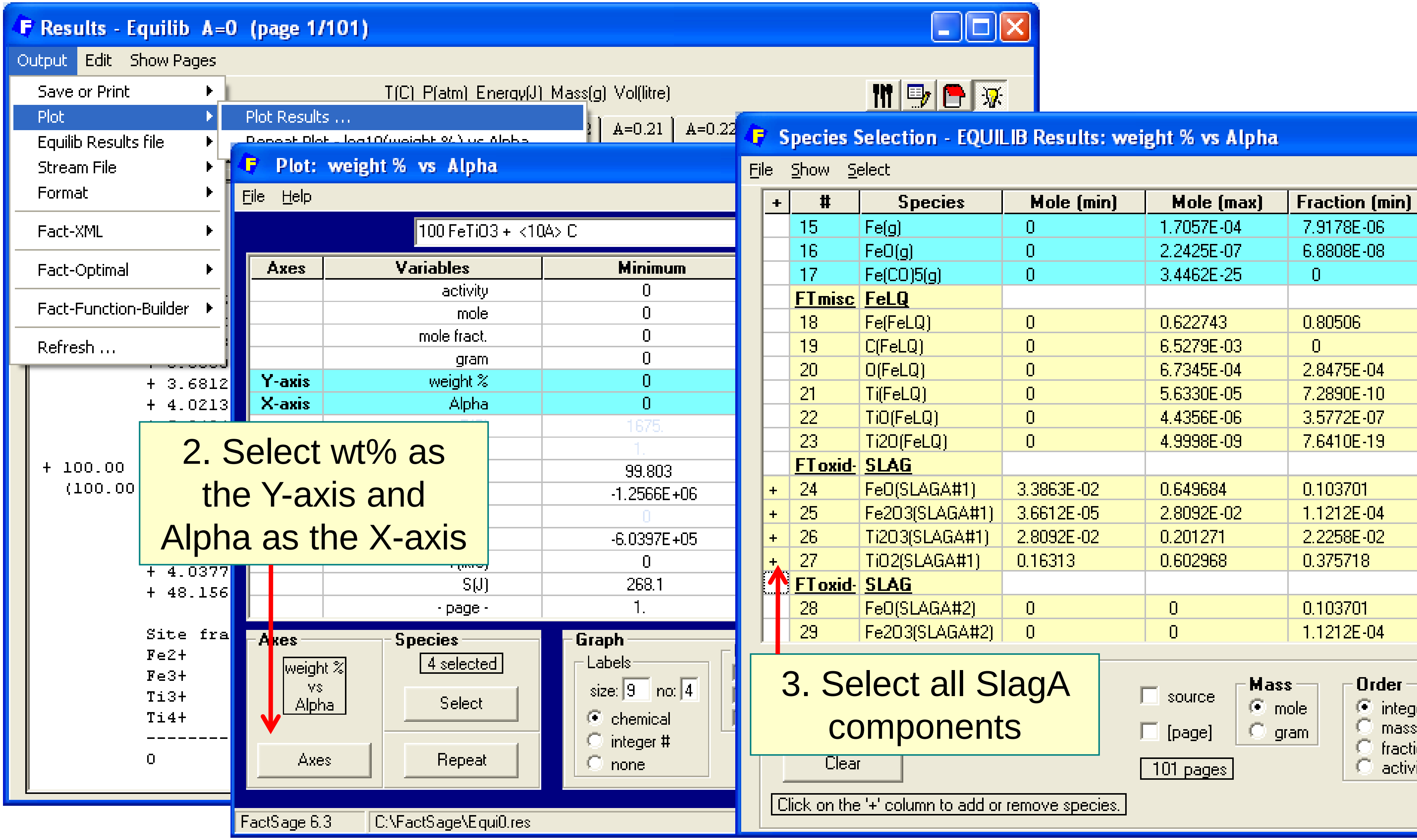
Ilmenite Smelting

A series of calculations at different carbon addition is performed to see how carbon content affects the composition of metal and slag.

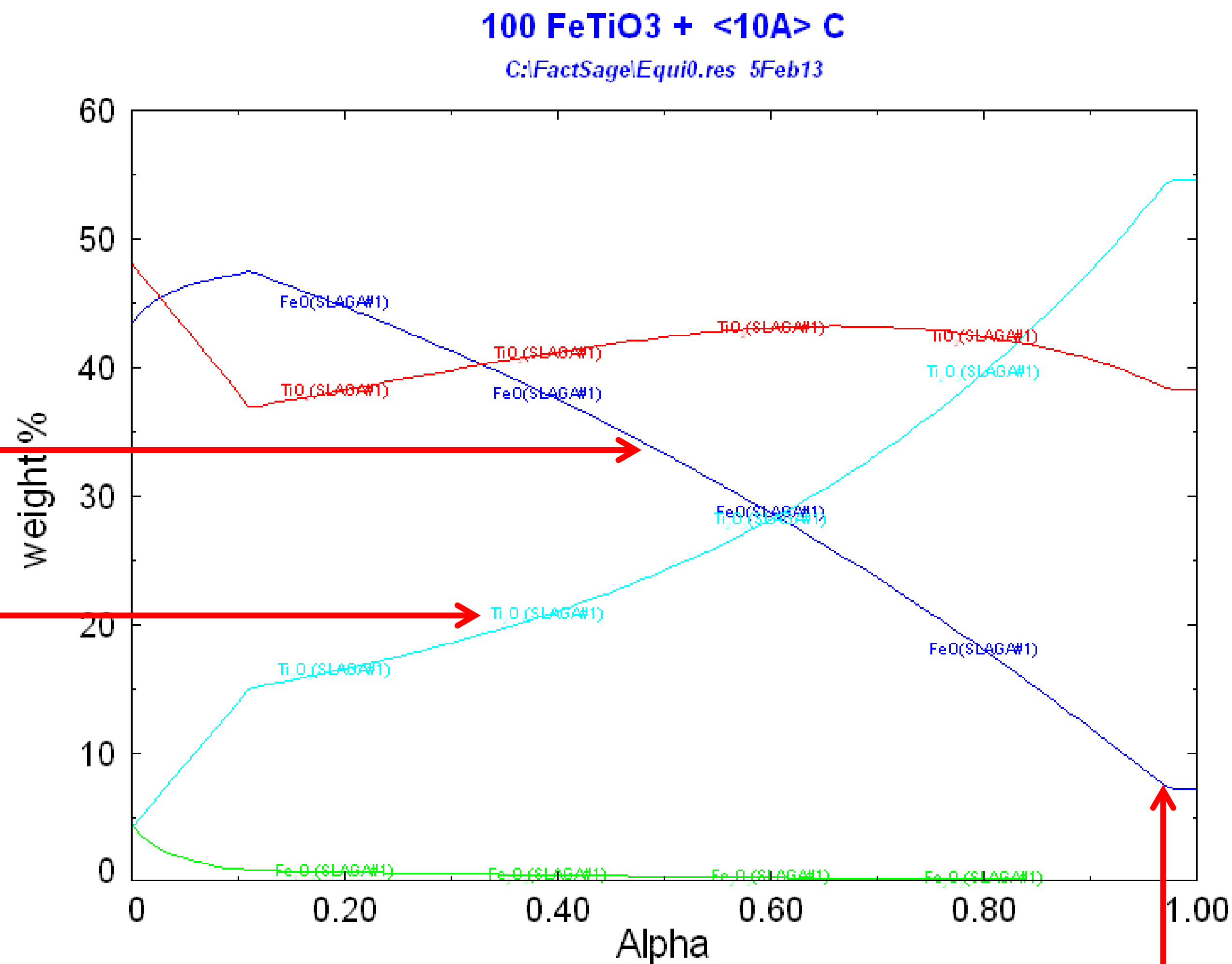


Ilmenite Smelting

1. For a graphical representation, we will plot the results



Ilmenite Smelting

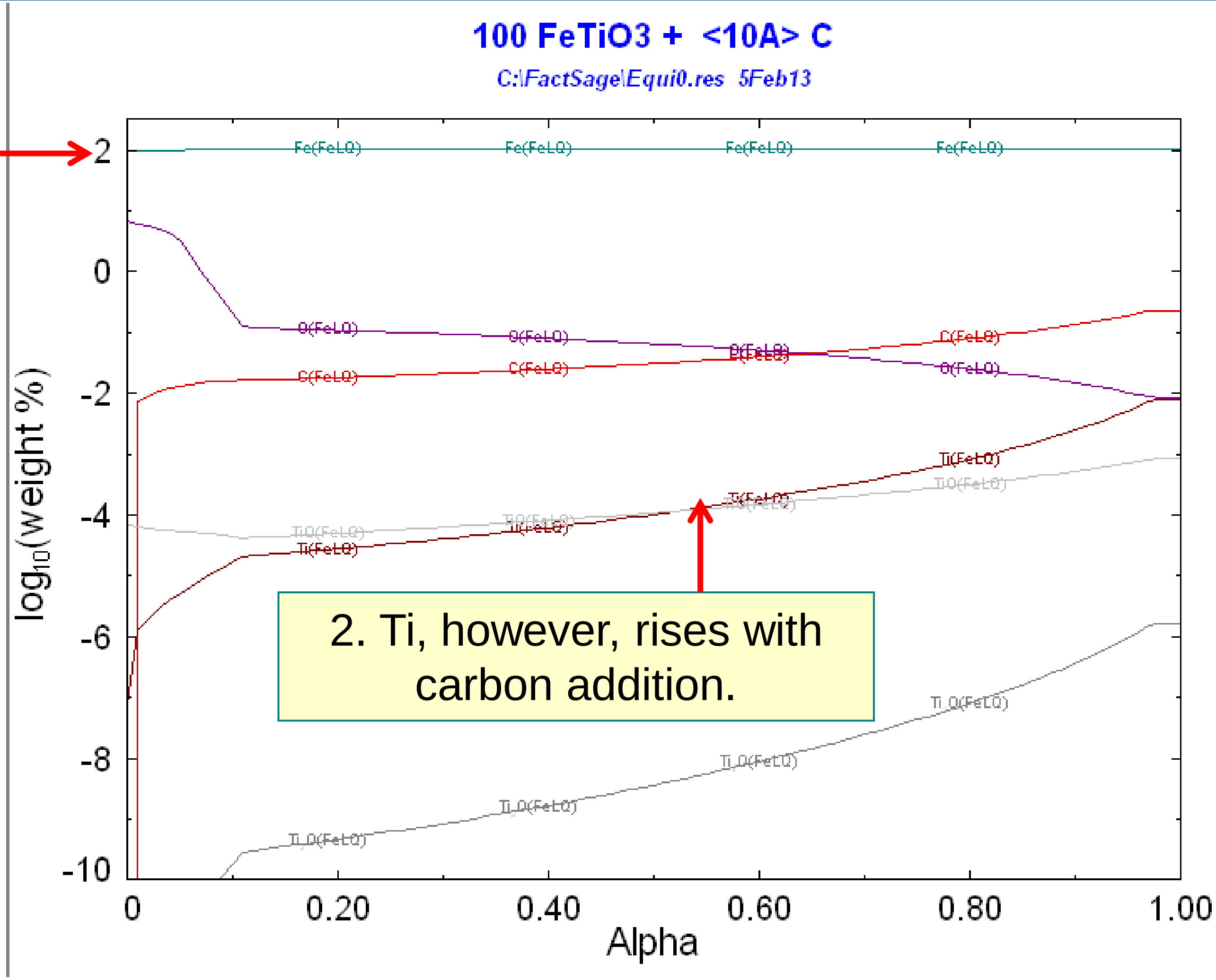


1. FeO content is decreased as carbon is added. Ti_2O_3 increases at almost the same rate.

2. The compositions remain constant after a certain point. This is when pseudobrookite precipitates.

Ilmenite Smelting

1. In the liquid metal, the percentage of iron remains close to 100%

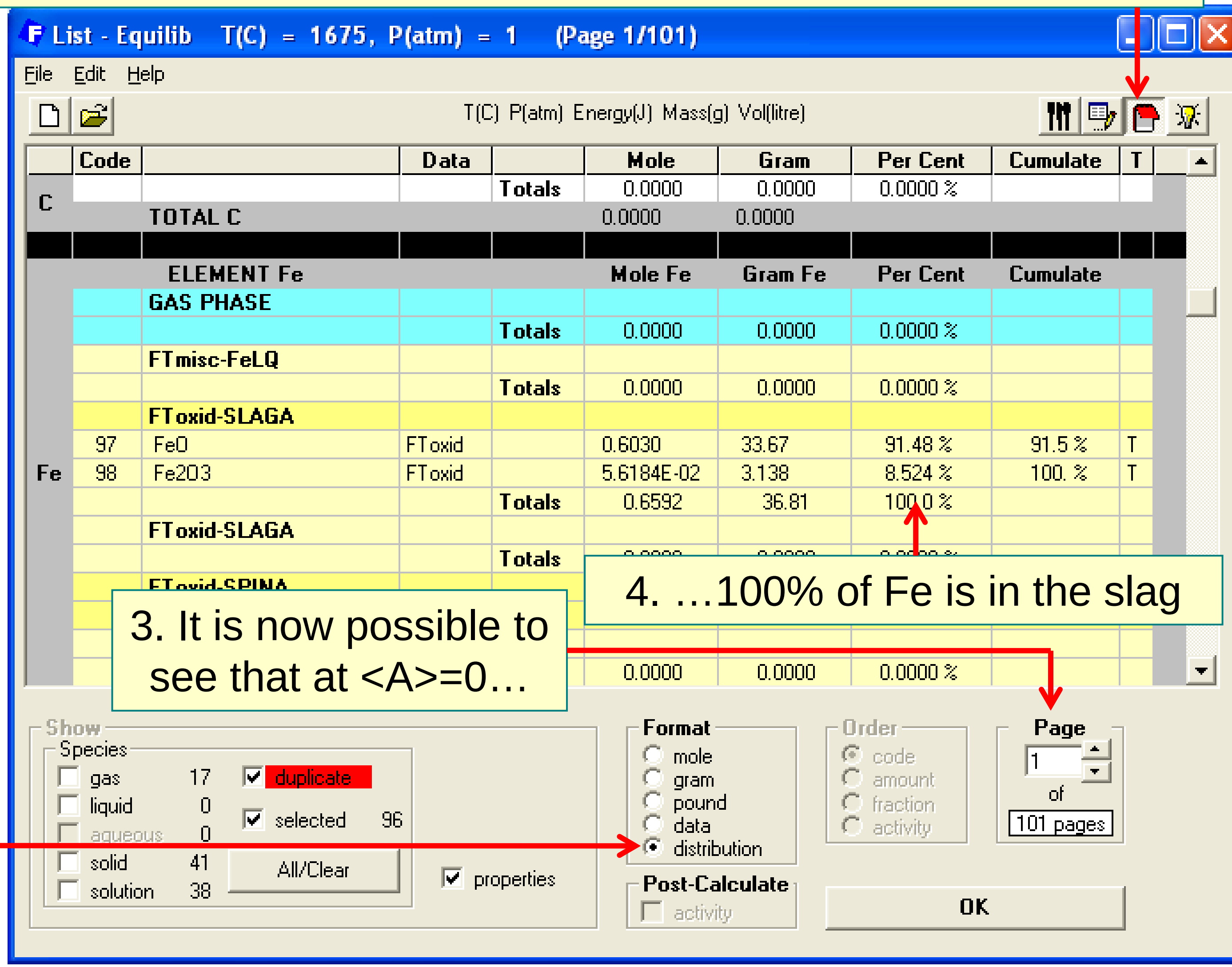


2. Ti, however, rises with carbon addition.

3. Because TiO_2 slag is the more important product of ilmenite smelting, we will select the amount of carbon to be 9.7g to keep wt%FeO at a minimum

Visualizing the distribution of elements between phases:
The “List” window

1. A good way of seeing the distribution of the elements between phases is by clicking on the “List” button…



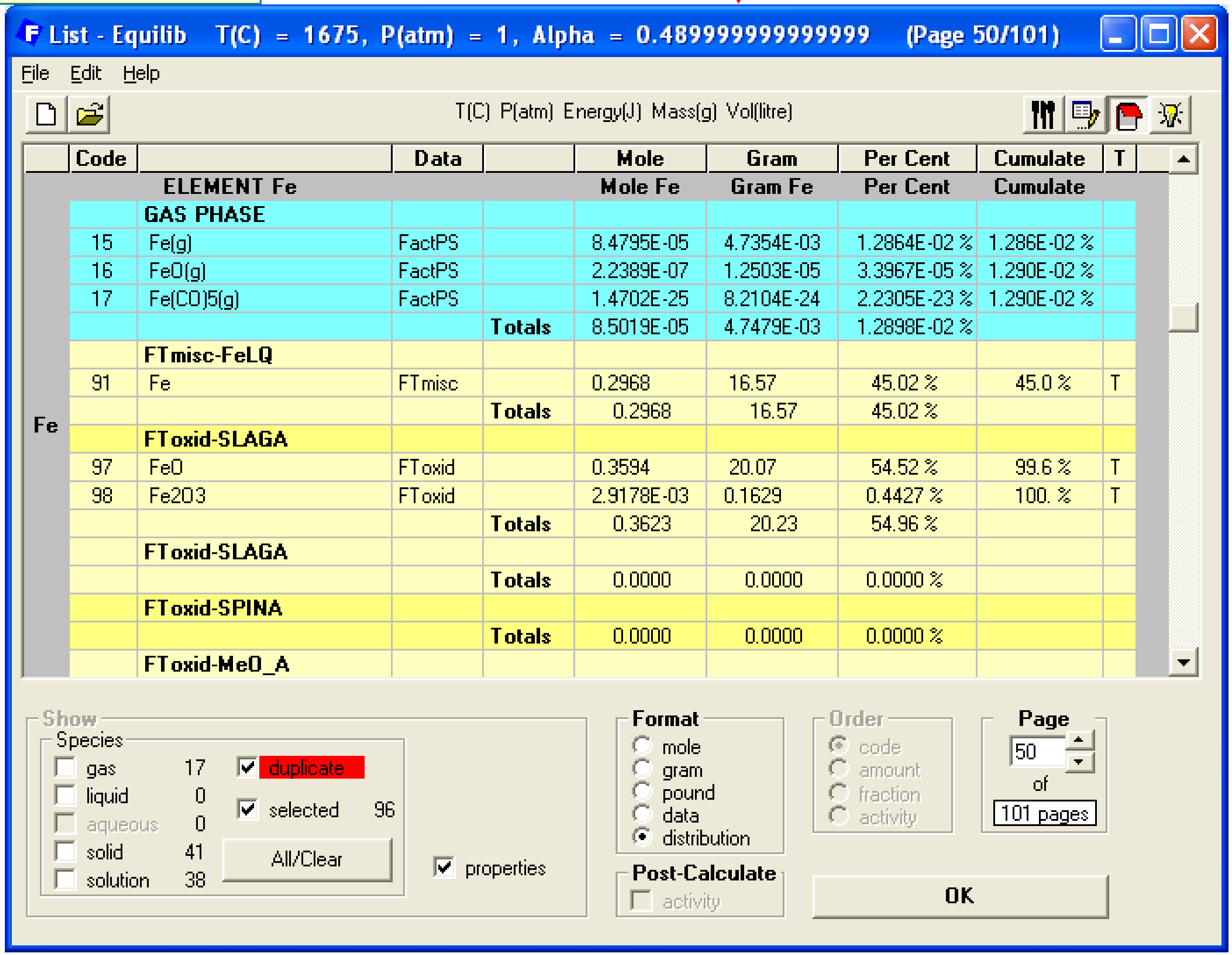
3. It is now possible to see that at <A>=0…

4. …100% of Fe is in the slag

2. …and selecting “distribution”

Ilmenite Smelting

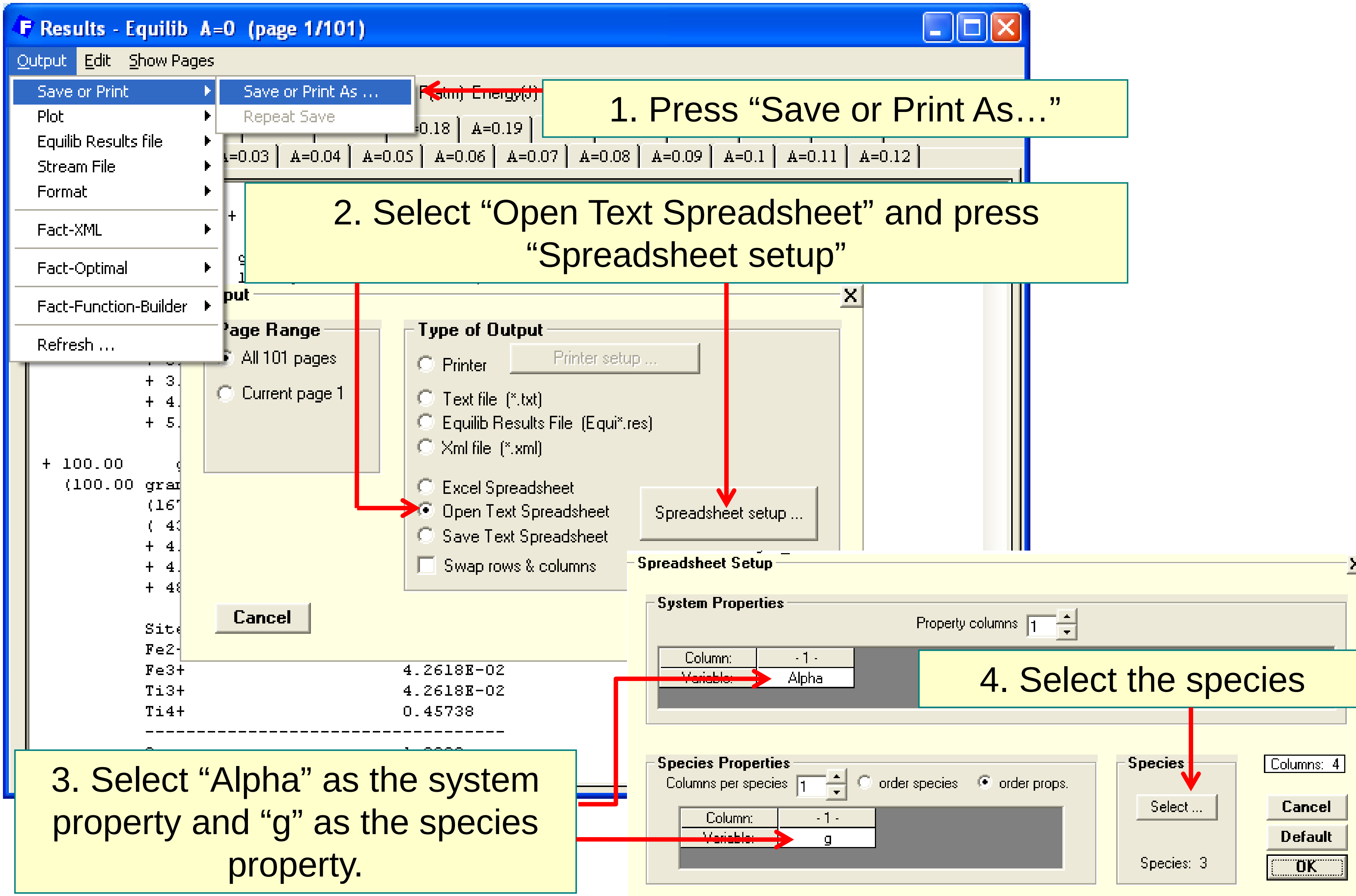
1. And this is the distribution at <A>=0.49



	Code		Data		Mole	Gram	Per Cent	Cumulate	T
		ELEMENT Fe			Mole Fe	Gram Fe	Per Cent	Cumulate	
		GAS PHASE							
	15	Fe(g)	FactPS		8.4795E-05	4.7354E-03	1.2864E-02 %	1.286E-02 %	
	16	FeO(g)	FactPS		2.2389E-07	1.2503E-05	3.3967E-05 %	1.290E-02 %	
	17	Fe(CO)5(g)	FactPS		1.4702E-25	8.2104E-24	2.2305E-23 %	1.290E-02 %	
				Totals	8.5019E-05	4.7479E-03	1.2898E-02 %		
		FTmisc-FeLQ							
	91	Fe	FTmisc		0.2968	16.57	45.02 %	45.0 %	T
Fe				Totals	0.2968	16.57	45.02 %		
		FToxid-SLAGA							
	97	FeO	FToxid		0.3594	20.07	54.52 %	99.6 %	T
	98	Fe2O3	FToxid		2.9178E-03	0.1629	0.4427 %	100. %	T
				Totals	0.3623	20.23	54.96 %		
		FToxid-SLAGA							
				Totals	0.0000	0.0000	0.0000 %		
		FToxid-SPINA							
				Totals	0.0000	0.0000	0.0000 %		
		FToxid-MeO_A							

2. A convenient way to see the distribution of Fe for all values of <A> is to export the data into an Excel file

Ilmenite Smelting



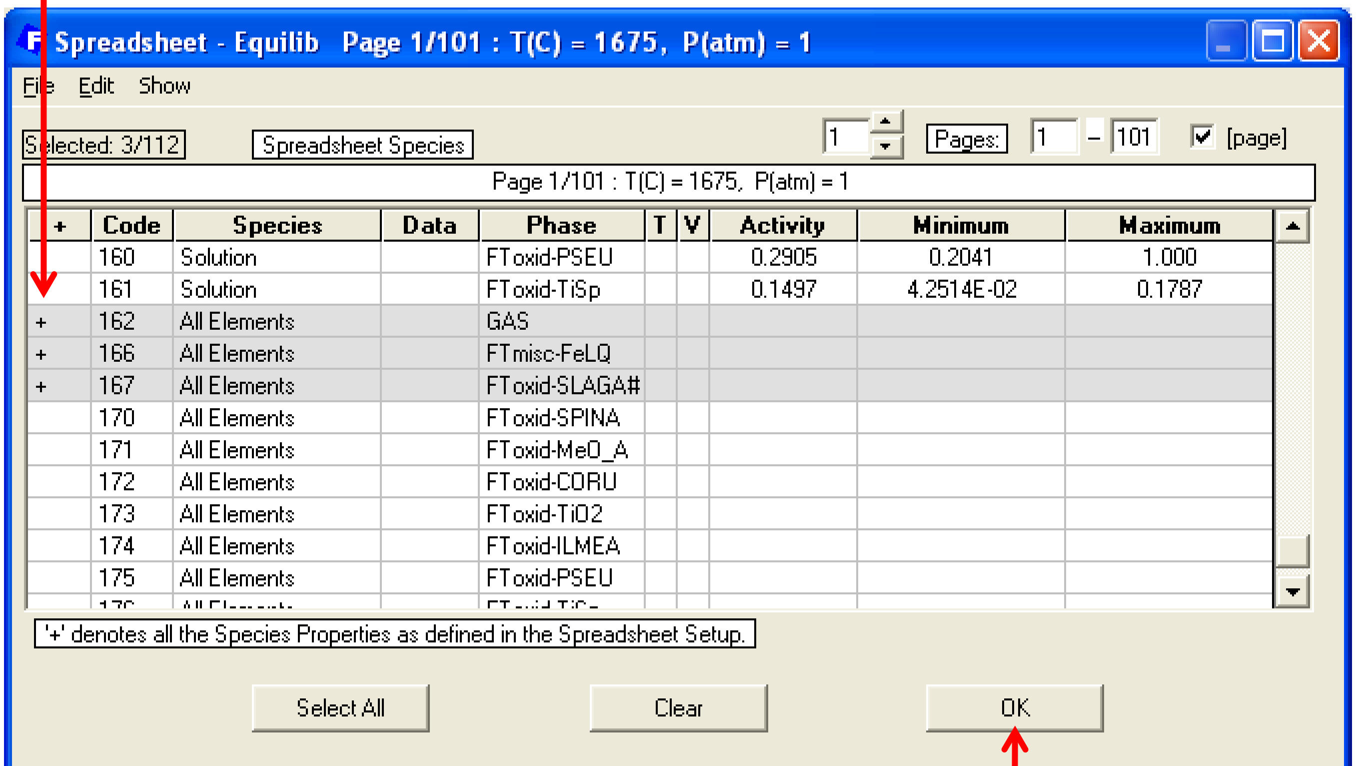
1. Press “Save or Print As…”

2. Select “Open Text Spreadsheet” and press “Spreadsheet setup”

3. Select “Alpha” as the system property and “g” as the species property.

4. Select the species

1. Because Fe gets distributed in the gas, metal and slag phases, all elements from these phases must be selected.



2. Press “OK” in all windows

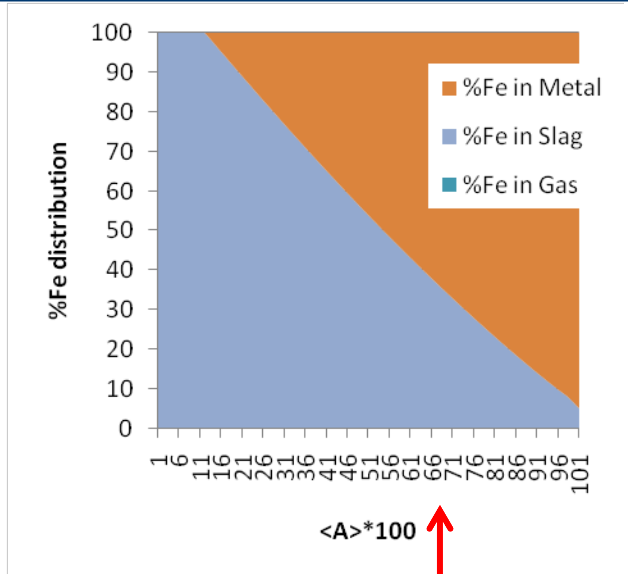
Ilmenite Smelting

1. The window with the amount of all elements in each phase will appear.

Equilib Results

File   Edit   Swap rows and columns

Alpha	g-Fe_GAS	g-Ti_GAS	g-O_GAS	g-C_GAS
0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00
1.0000000E-02	4.0964224E-06	2.4064555E-11	2.1365509E-01	1.0000000E-01
2.0000000E-02	1.2742725E-05	7.3638352E-11	3.9713850E-01	2.0000000E-01
3.0000000E-02	2.8197135E-05	1.5878802E-10	5.5682909E-01	3.0000000E-01
4.0000000E-02	5.3171052E-05	2.9045652E-10	7.0012011E-01	4.0000000E-01
5.0000000E-02	9.1190691E-05	4.8186466E-10	8.3272130E-01	5.0000000E-01
6.0000000E-02	1.4703239E-04	7.4978548E-10	9.5858400E-01	6.0000000E-01
7.0000000E-02	2.2727793E-04	1.1158442E-09	1.0803894E+00	7.0000000E-01



2. Copy all the values in Excel and keep only the columns with Fe

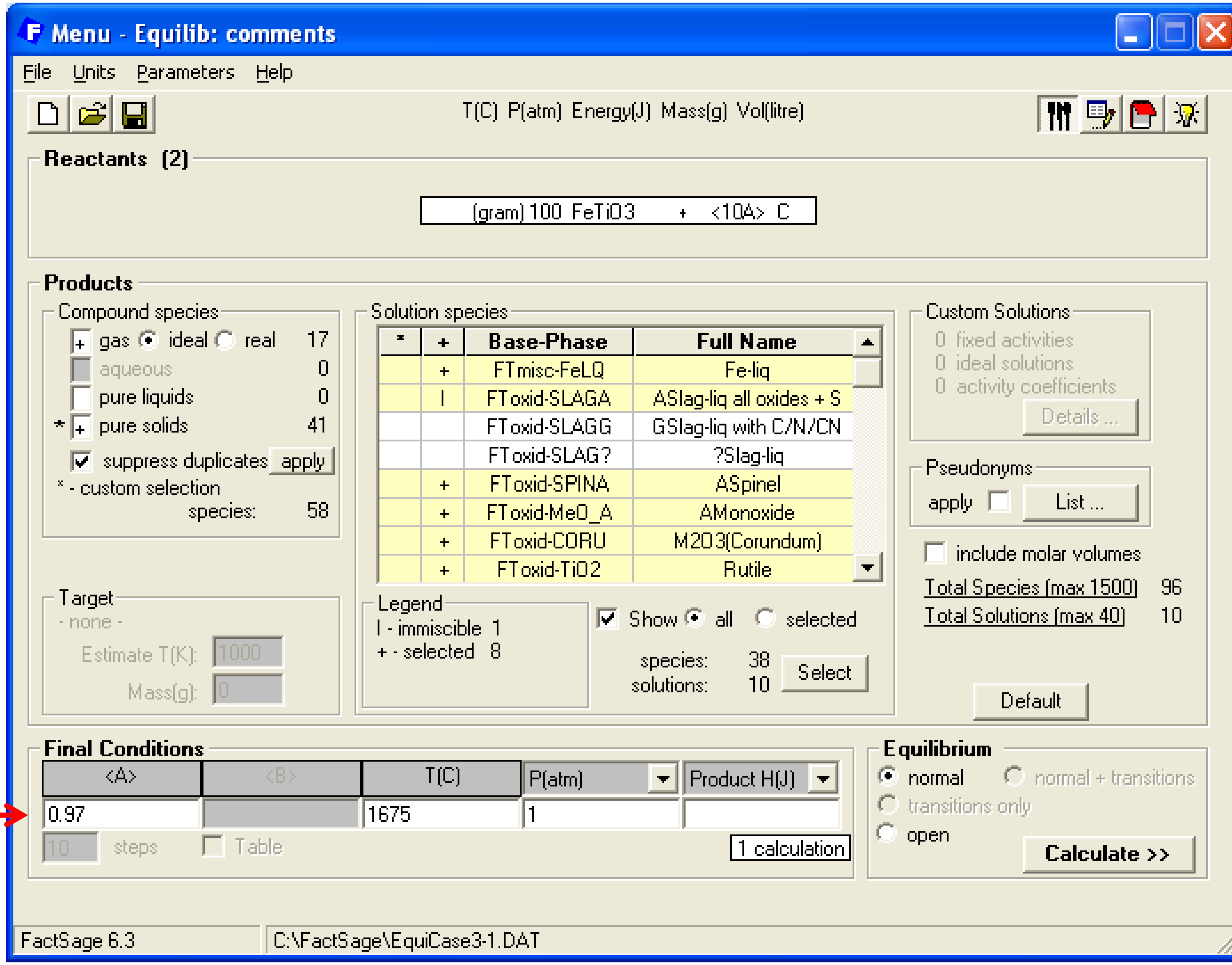
	A	B	C	D	E	F	G
1	Alpha	g-Fe_GAS	g-Fe_FTmisc-FeLQ	g-Fe_FToxid-SLAGA#1	%Fe in Gas	%Fe in Metal	%Fe in Slag
2	0.00E+00	0.00E+00	0.00E+00	3.68E+01	0.00E+00	0.00E+00	1.00E+02
3	1.00E-02	4.10E-06	0.00E+00	3.68E+01	1.11E-05	0.00E+00	1.00E+02
4	2.00E-02	1.27E-05	0.00E+00	3.68E+01	3.46E-05	0.00E+00	1.00E+02
5	3.00E-02	2.82E-05	0.00E+00	3.68E+01	7.66E-05	0.00E+00	1.00E+02
6	4.00E-02	5.32E-05	0.00E+00	3.	=100*B6/($B6+$C6+$D6)		1.00E+02
7	5.00E-02	9.12E-05	0.00E+00	3.68E+01	2.48E-04	0.00E+00	1.00E+02

3. Add columns to calculate the %Fe in each phase

4. It is now convenient to plot the Fe distribution as an area plot. It can be seen that Fe in the slag is reduced as carbon is added

Calculating the liquidus of slag and metal:
"Precipitate target" calculation

1. As mentioned in slide 13, we will now calculate the equilibrium at 9.7g addition to reduce as much as possible the FeO content in the slag, but avoid pseudobrookite precipitation.



Ilmenite Smelting

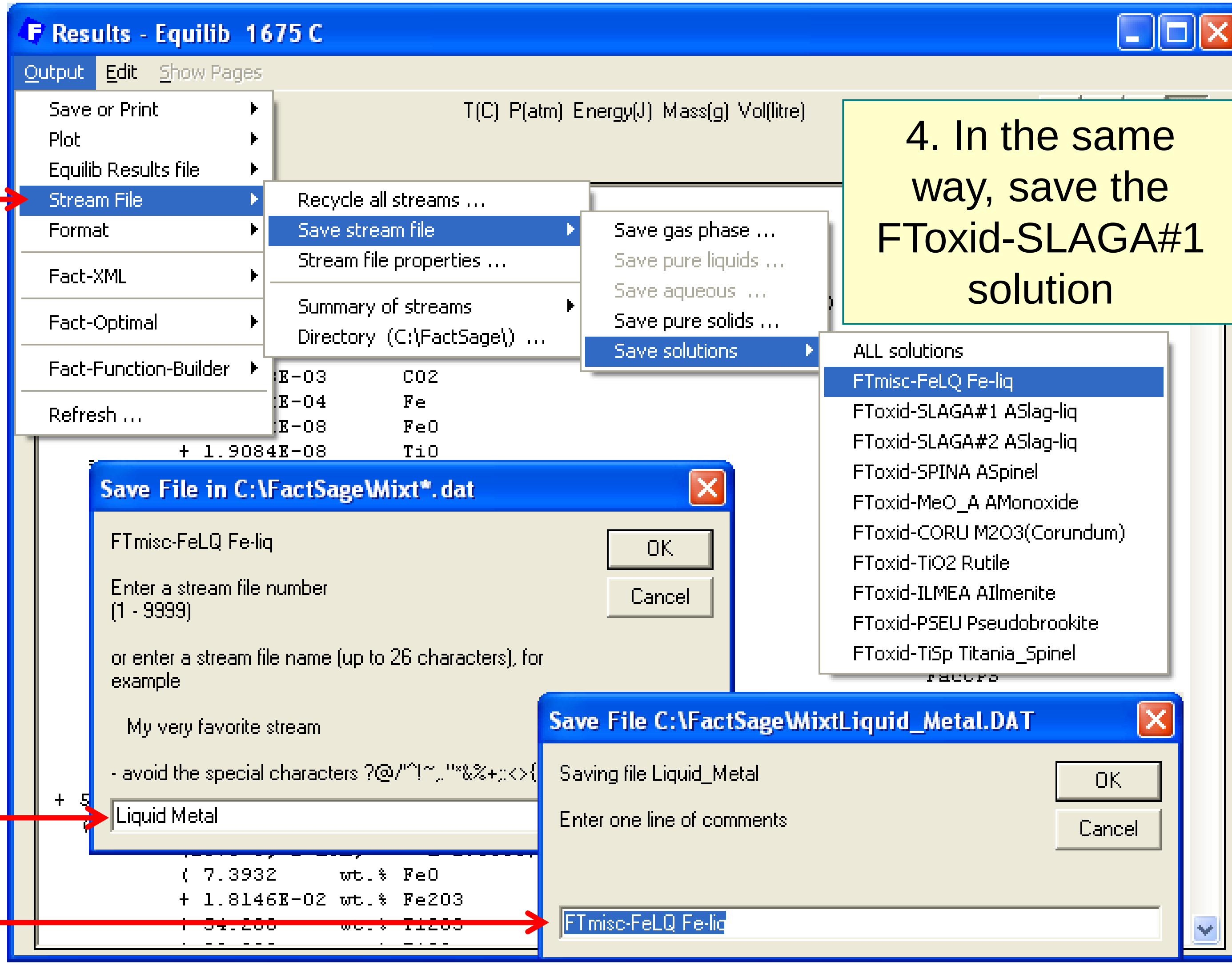
We would now like to see if our temperature is well chosen. For this, we want to see what is the liquidus temperature of the slag and the metal.

1. Press “Output” → “Stream File” → “Save solutions” and select the solution you would like to save. In this case, we want to save the metal and slag solutions.

2. In the pop-up window, enter the name of stream file

3. In the next window, enter any comments you might have.

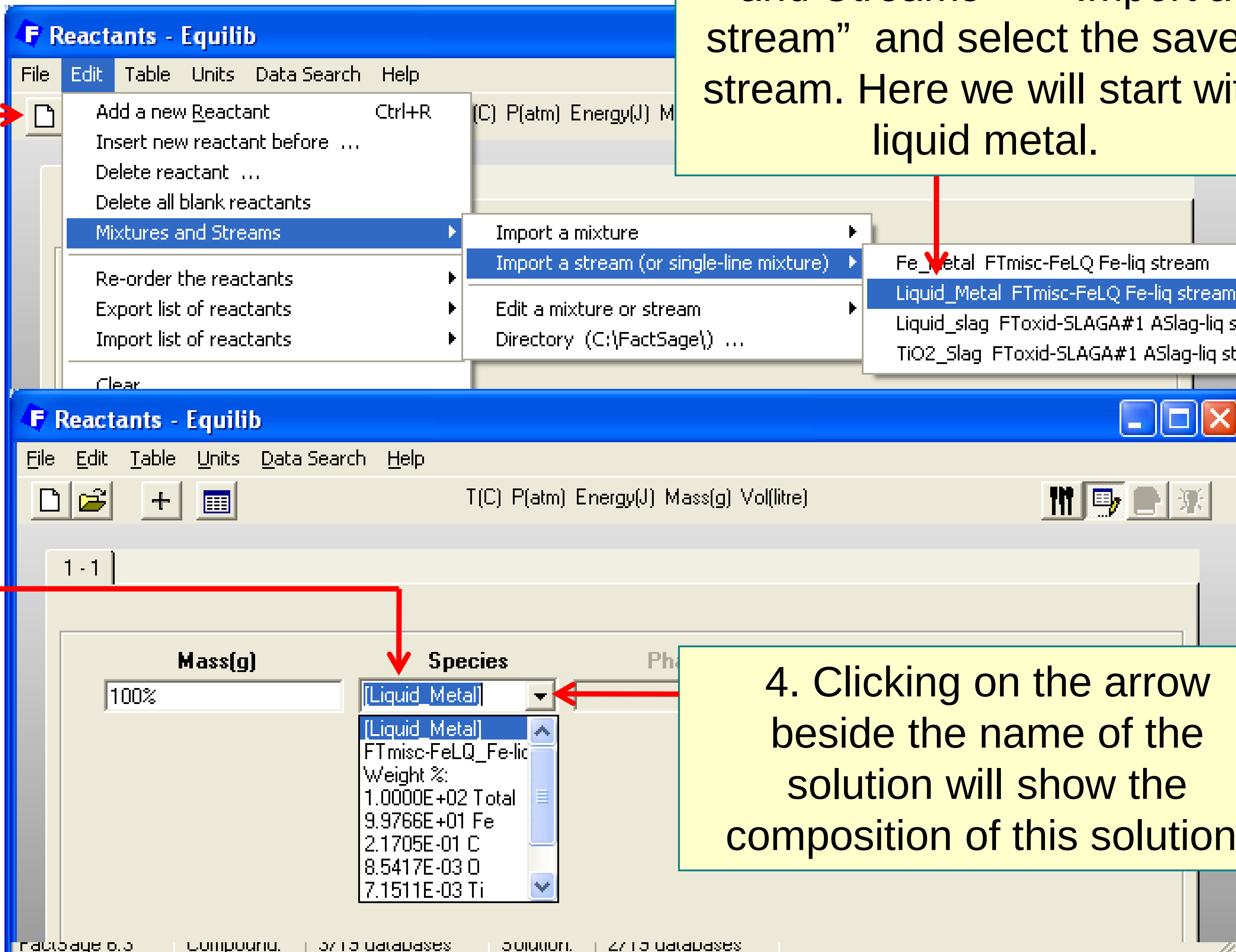
4. In the same way, save the FToxid-SLAGA#1 solution



Ilmenite Smelting

1. Set up a new reaction in the reactants window by pressing the “new reaction” button.

2. Press “Edit” → “Mixtures and Streams” → “Import a stream” and select the saved stream. Here we will start with liquid metal.



3. The “Liquid Metal” solution will be selected as one of the reactants.

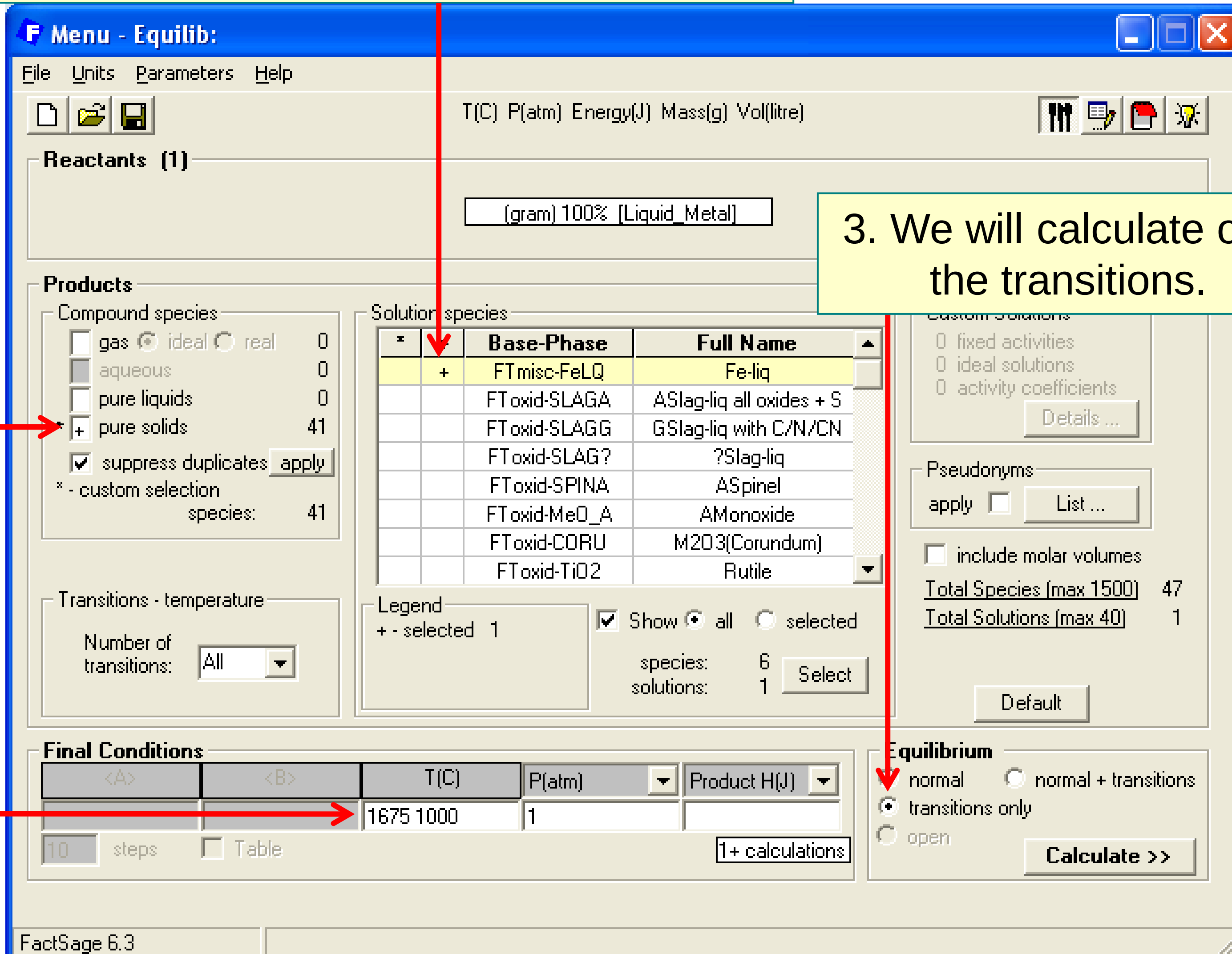
4. Clicking on the arrow beside the name of the solution will show the composition of this solution.

Ilmenite Smelting

1. In the “Menu” window, we will select the liquid metal solution and all the solids as possible products.

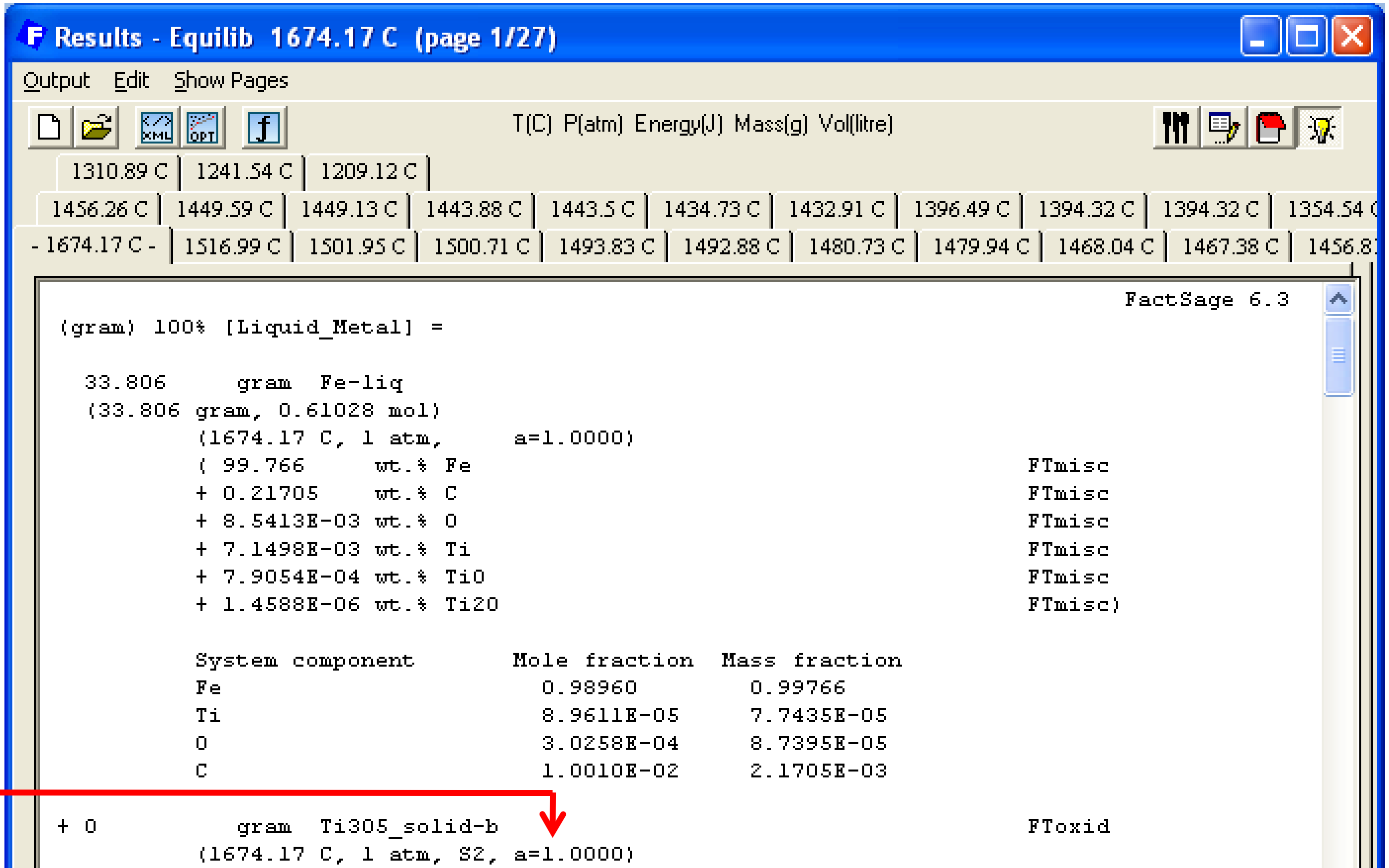
2. To make a “cooling” calculation, we will select 1675C as the starting temperature and 1000C as the final temperature.

3. We will calculate only the transitions.

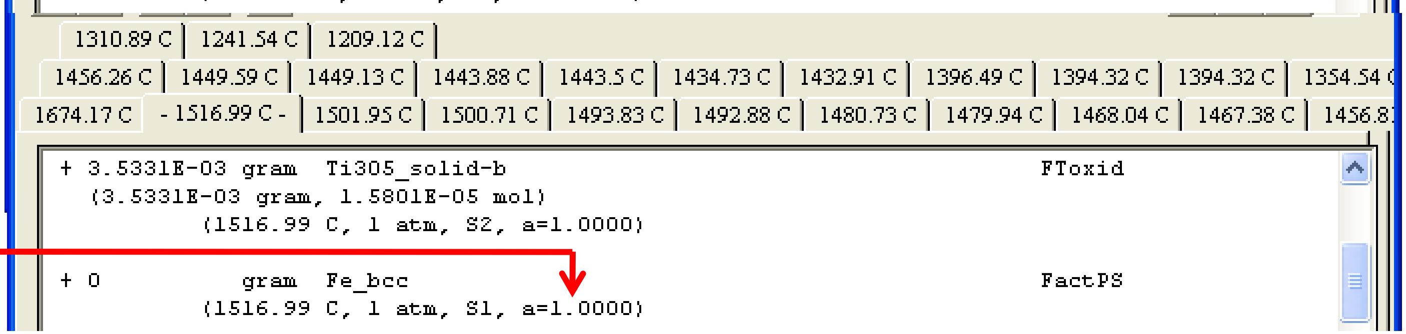


Ilmenite Smelting

1. In the "Results" window, it is seen that Ti_3O_5 is ready to precipitate at 1674.17C (its activity is 1). So this is the liquidus temperature of our liquid metal.



2. At 1516.99C, solid iron starts to precipitate.

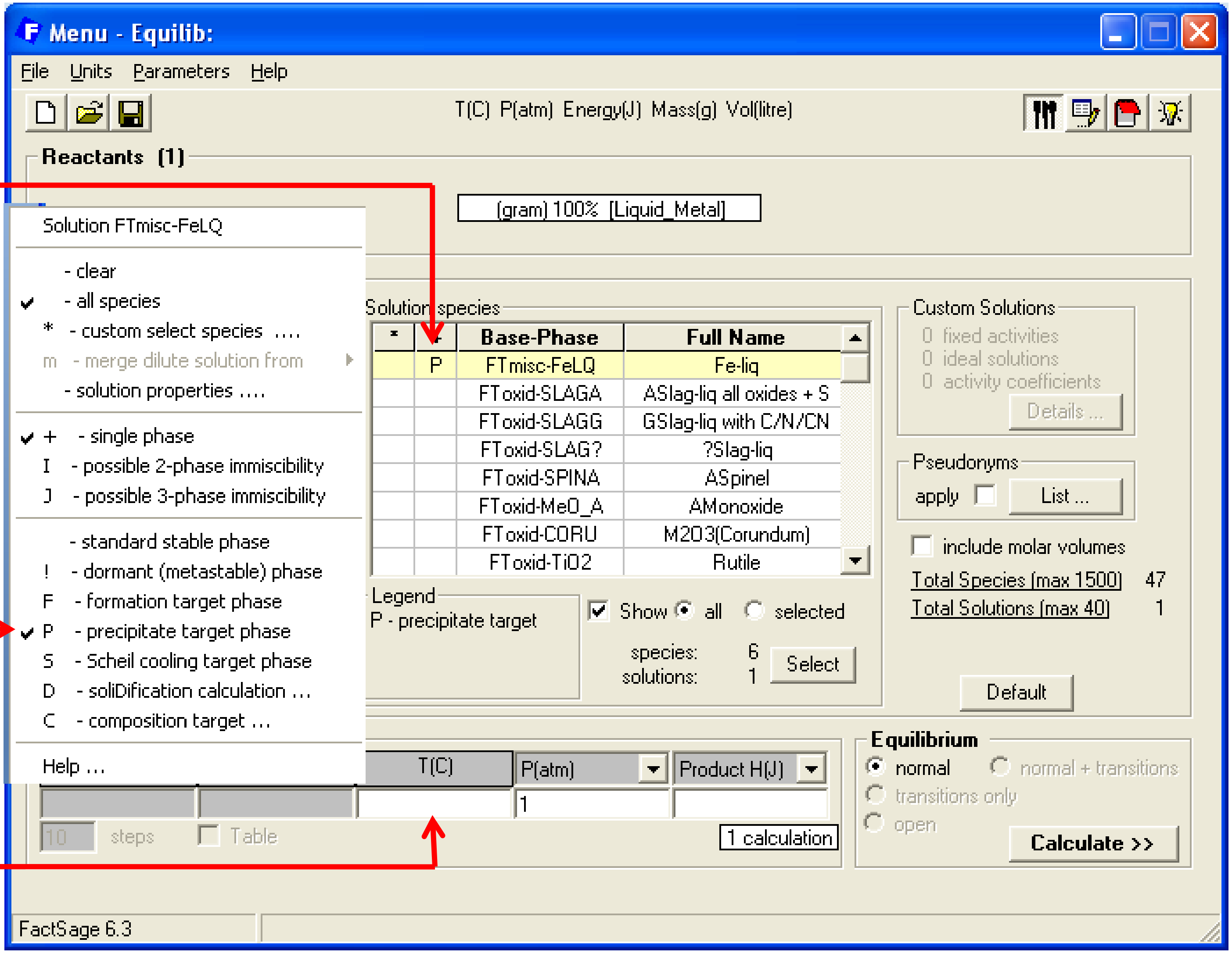


Ilmenite Smelting

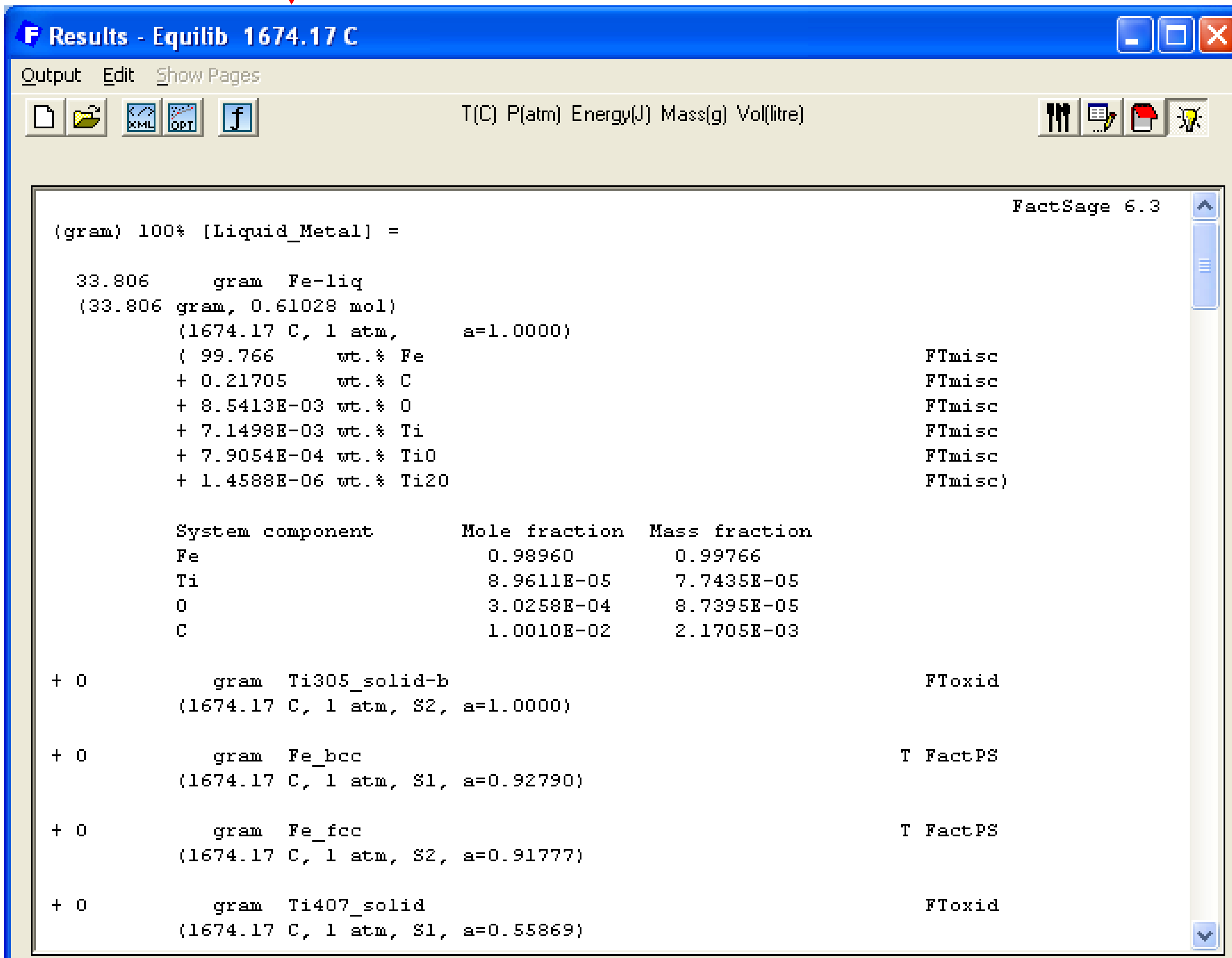
1. An easier way to find the liquidus of the liquid metal solution is by using the "Precipitate target" calculation.

2. Right-click on the Fe-liq selection and select "precipitate target phase"

3. Leave the temperature field blank. This calculation will find the temperature at which the first solid will precipitate from the Fe-liq solution



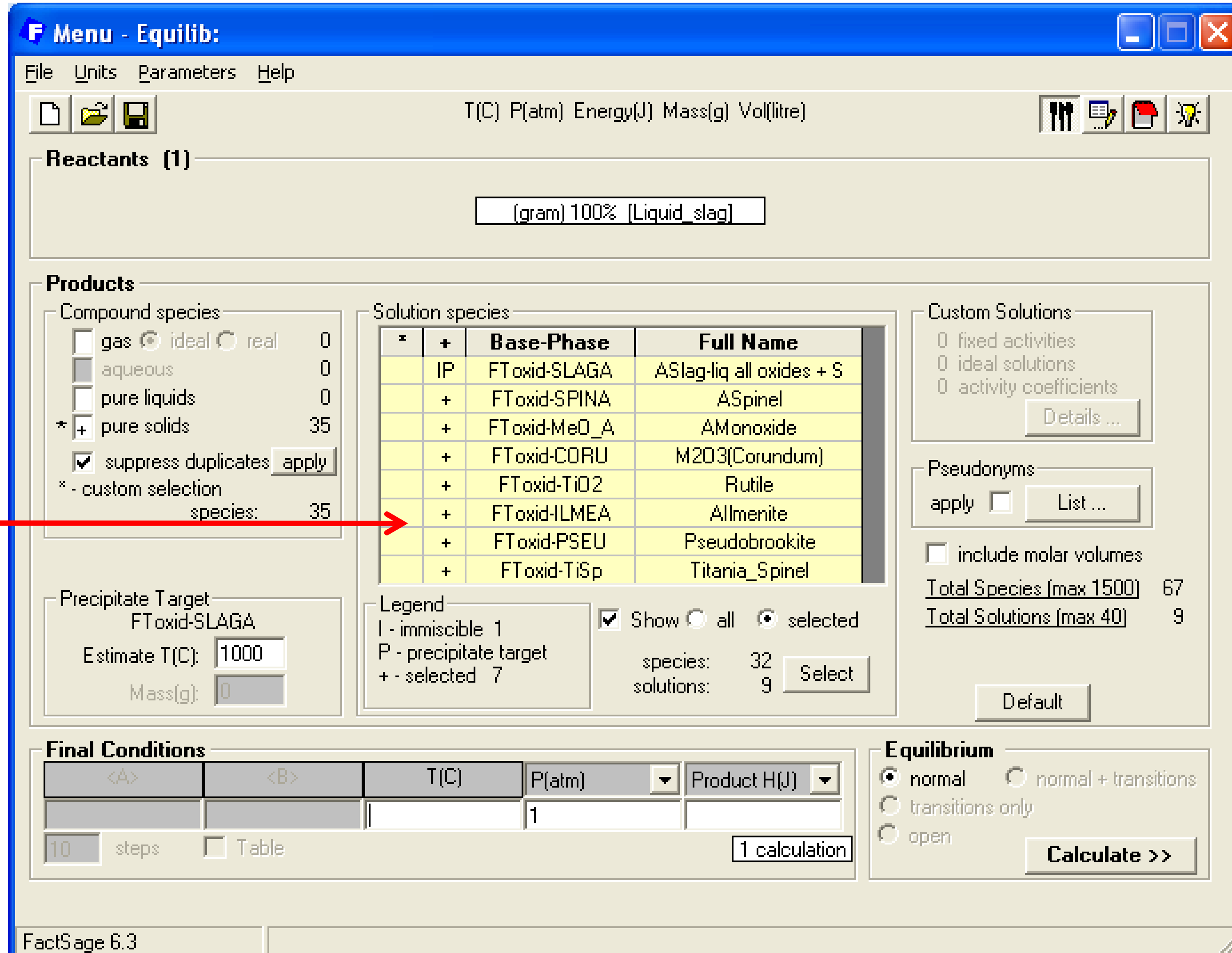
1. The liquidus temperature found is the same as in slide 23, but only one calculation had to be performed.



Ilmenite Smelting

1. The same calculation can be performed on the liquid slag to find its liquidus temperature.

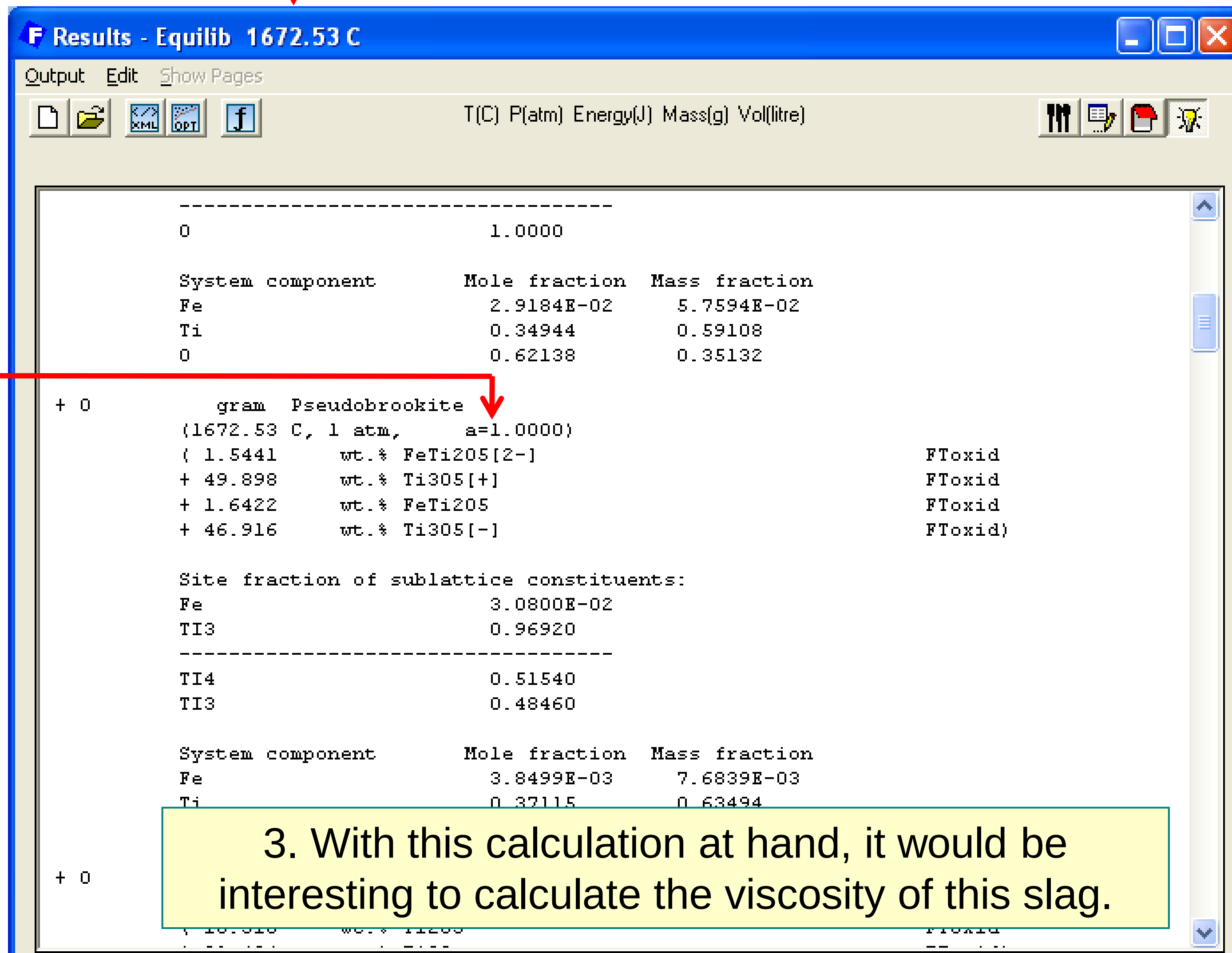
2. Select all the solids and FToxid solutions, because they can all precipitate out of the slag phase



Ilmenite Smelting

1. The results show that pseudobrookite will precipitate out at 1672.53C

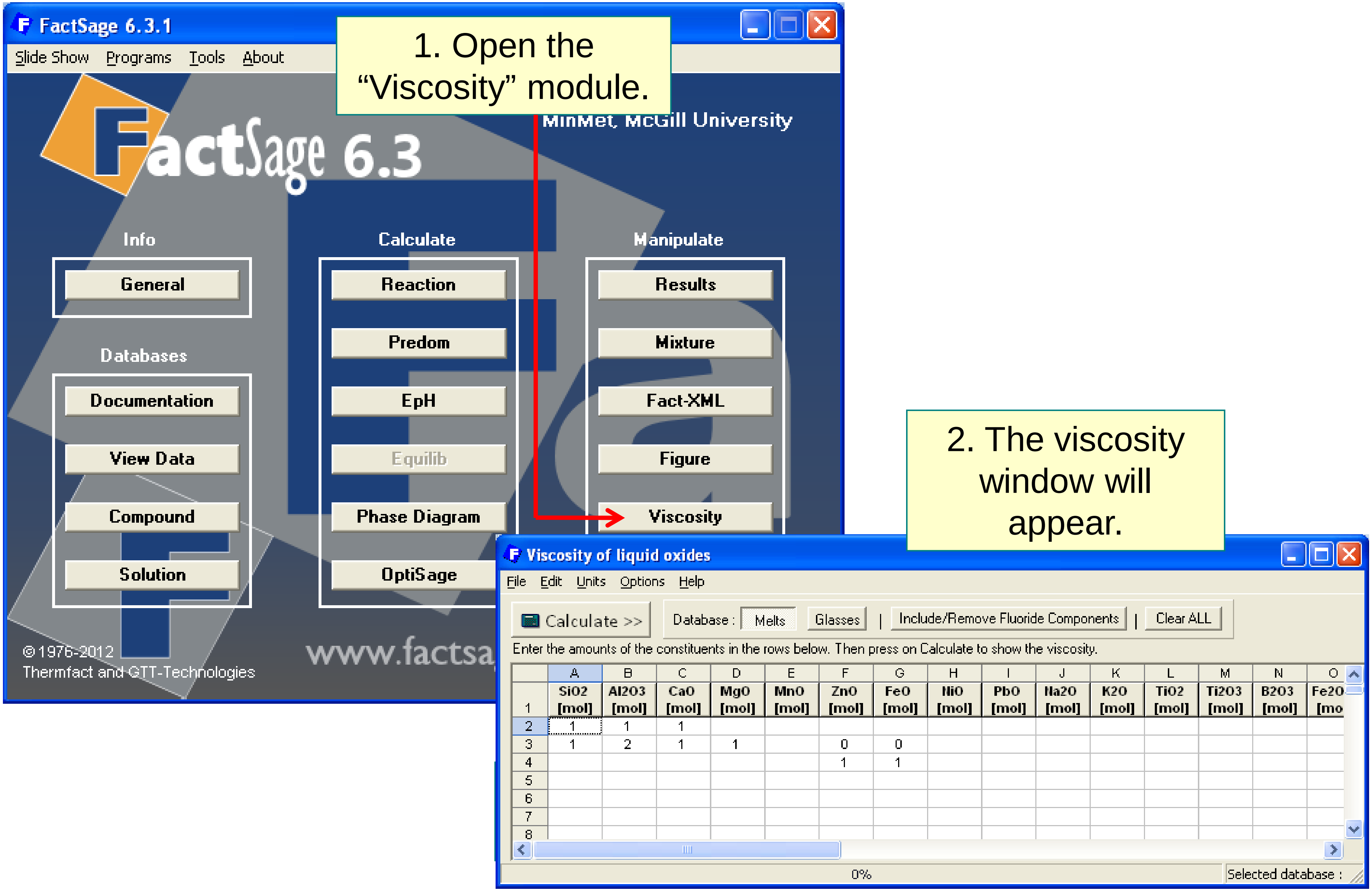
2. The last two results show that our smelting temperature is quite close to both the metal and the slag liquidus temperatures. It would thus be wise to increase the smelting temperature, to avoid precipitation of solid phases.



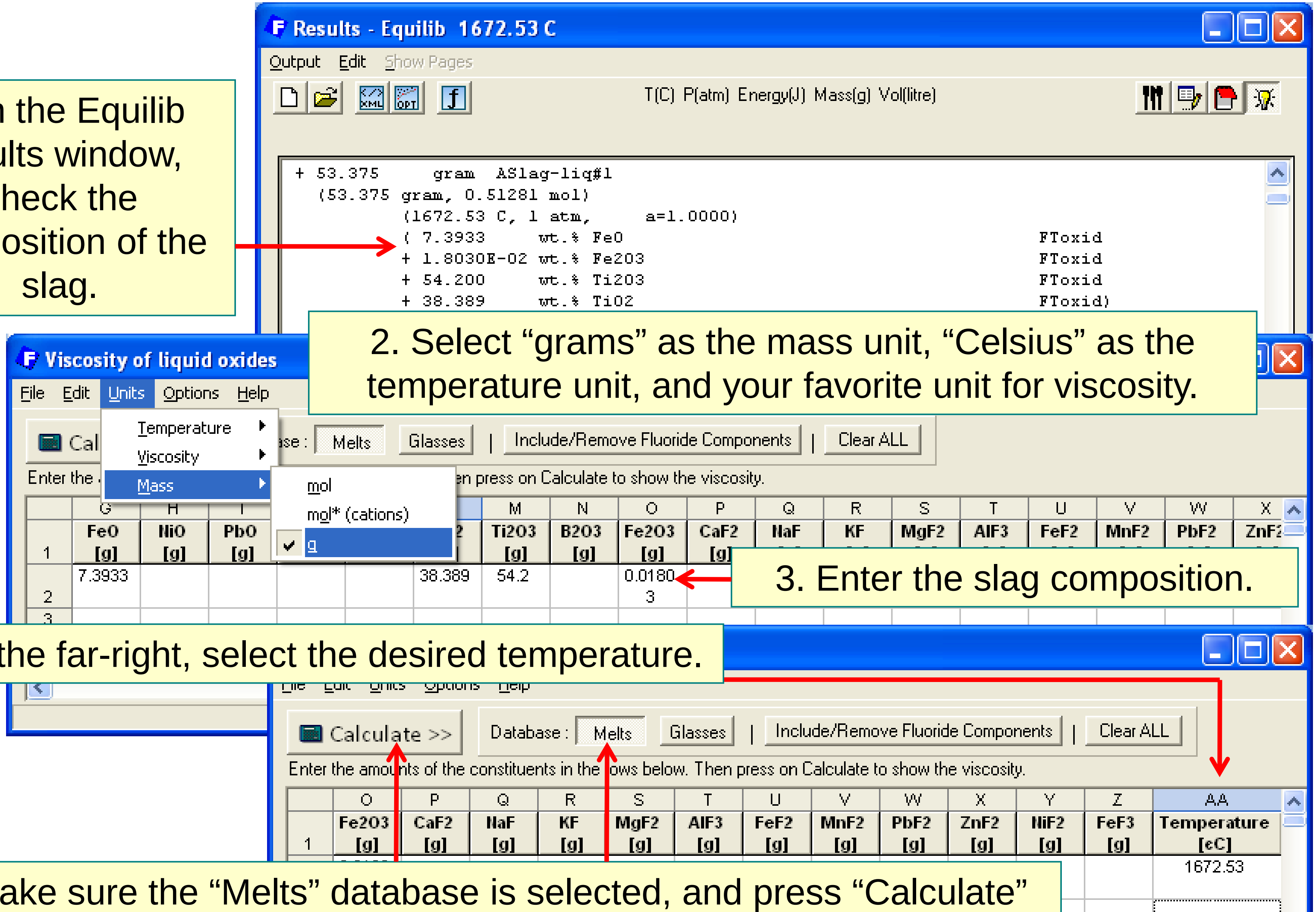
3. With this calculation at hand, it would be interesting to calculate the viscosity of this slag.

Calculating the viscosity of the slag:
“Viscosity” calculation

Ilmenite Smelting



Ilmenite Smelting



1. In the Equilib results window, check the composition of the slag.

2. Select “grams” as the mass unit, “Celsius” as the temperature unit, and your favorite unit for viscosity.

3. Enter the slag composition.

4. On the far-right, select the desired temperature.

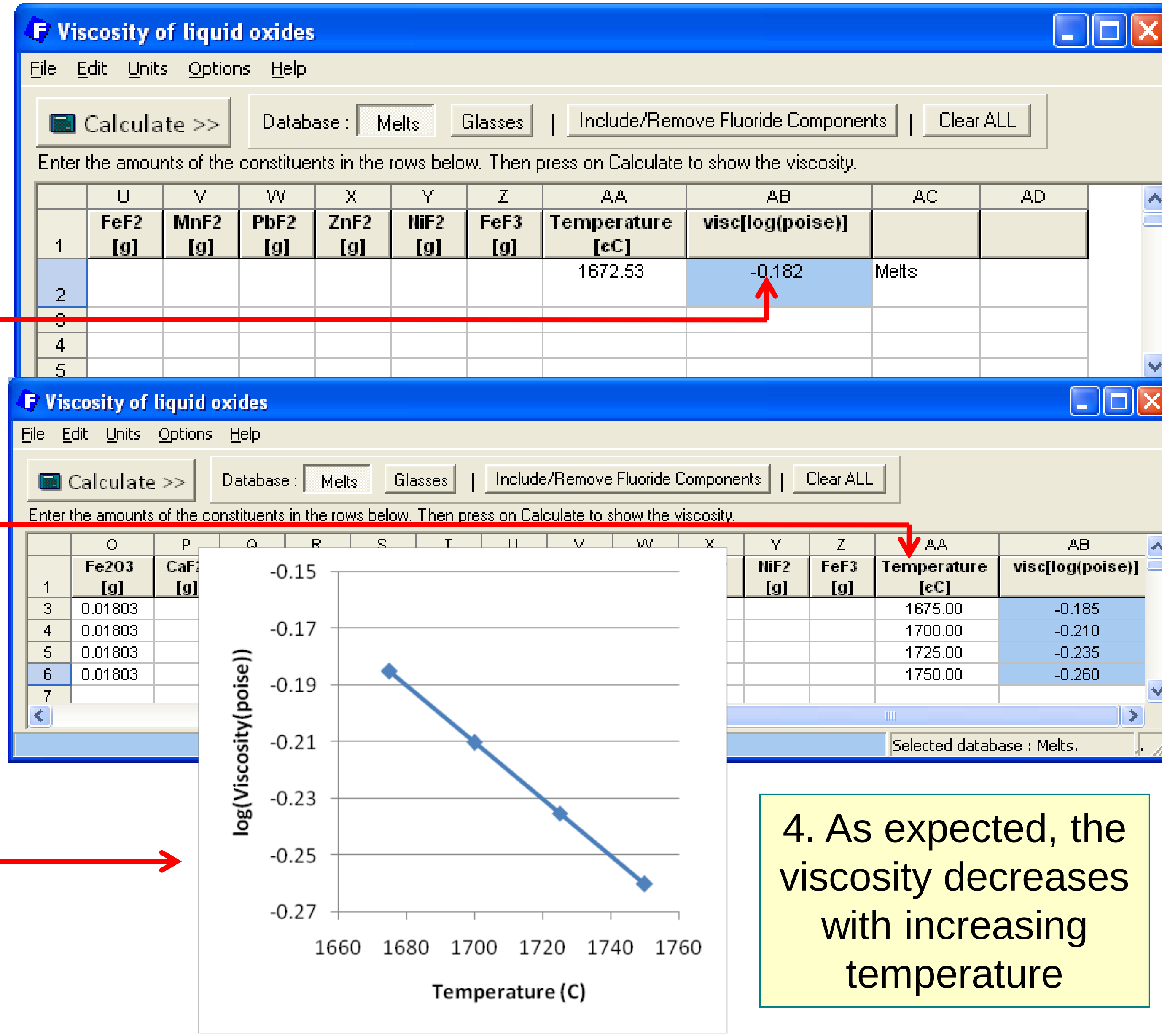
5. Make sure the “Melts” database is selected, and press “Calculate”

Ilmenite Smelting

1. The result will be given on the far right.

2. To calculate the viscosity at different temperatures, enter the same composition several times and use a different temperature for each calculation.

3. Copying the results to Excel, it is possible to plot these results



4. As expected, the viscosity decreases with increasing temperature

Temperature-Pressure relationship at fixed slag composition:
"Composition target" calculation

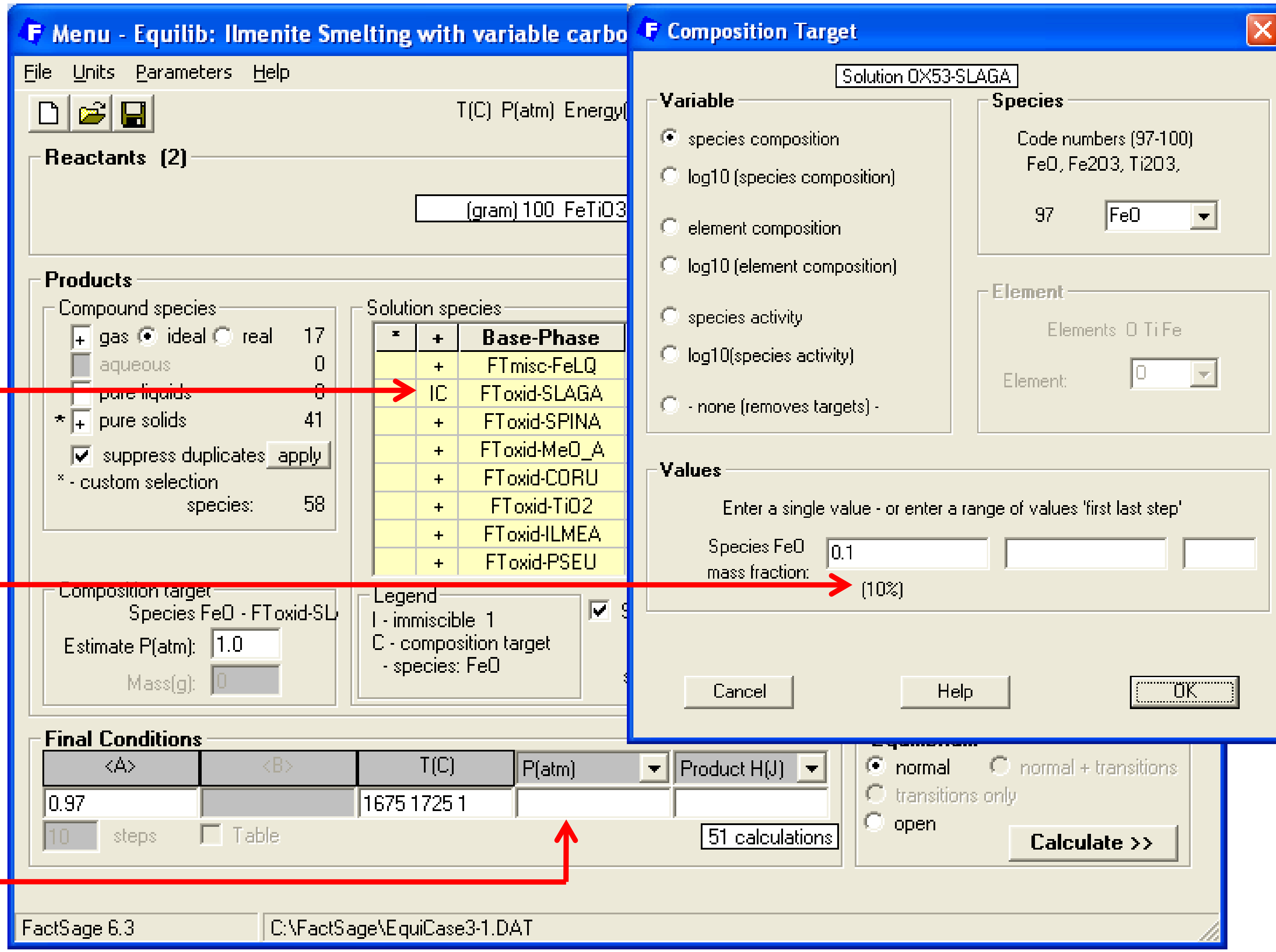
Ilmenite Smelting

Next, we would like to calculate the relationship between Temperature and partial pressure of oxygen at a constant slag composition.

1. Select "composition target" for the slag phase.

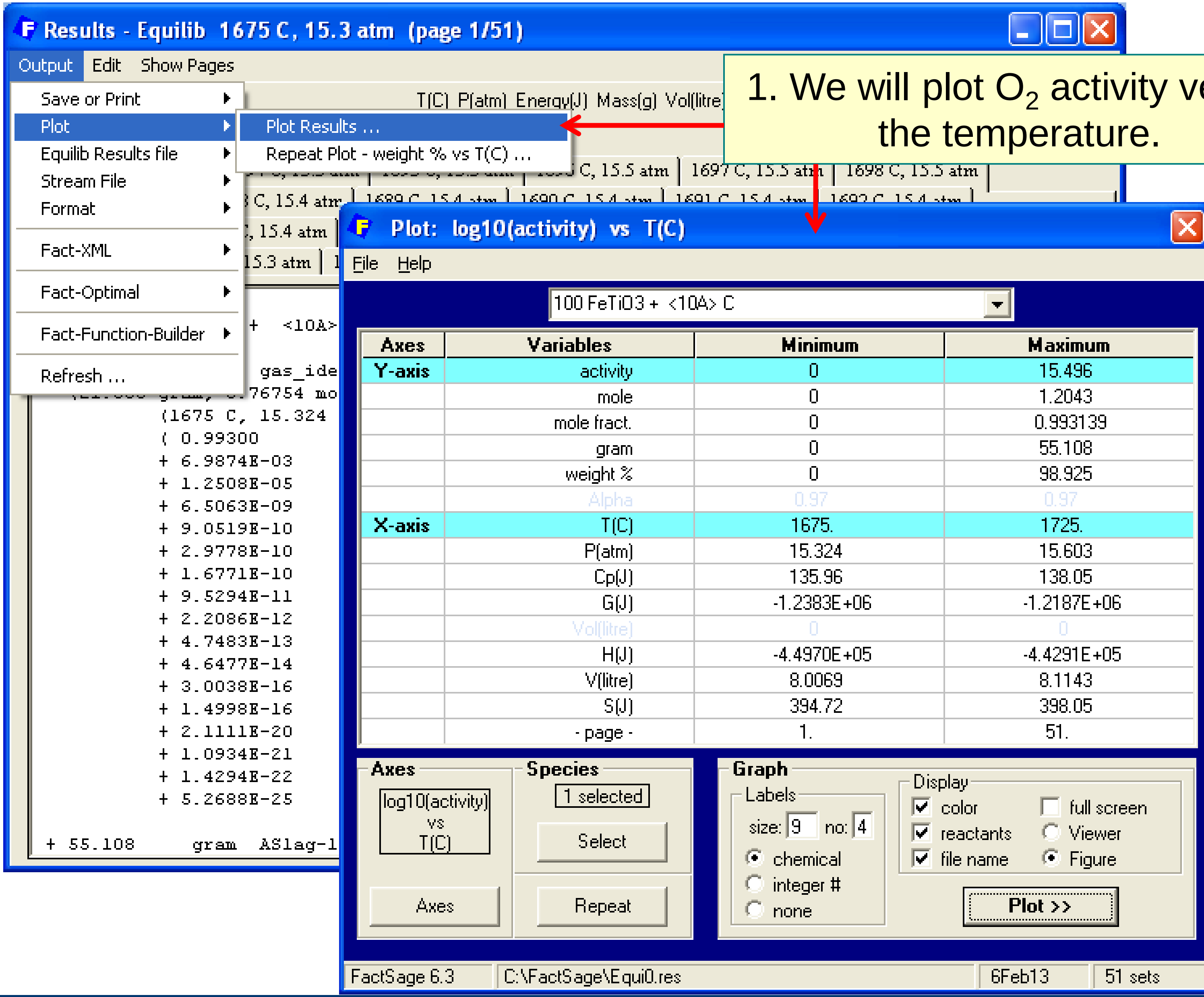
2. We will select 10% FeO as our composition target.

3. Leave the Pressure field blank.



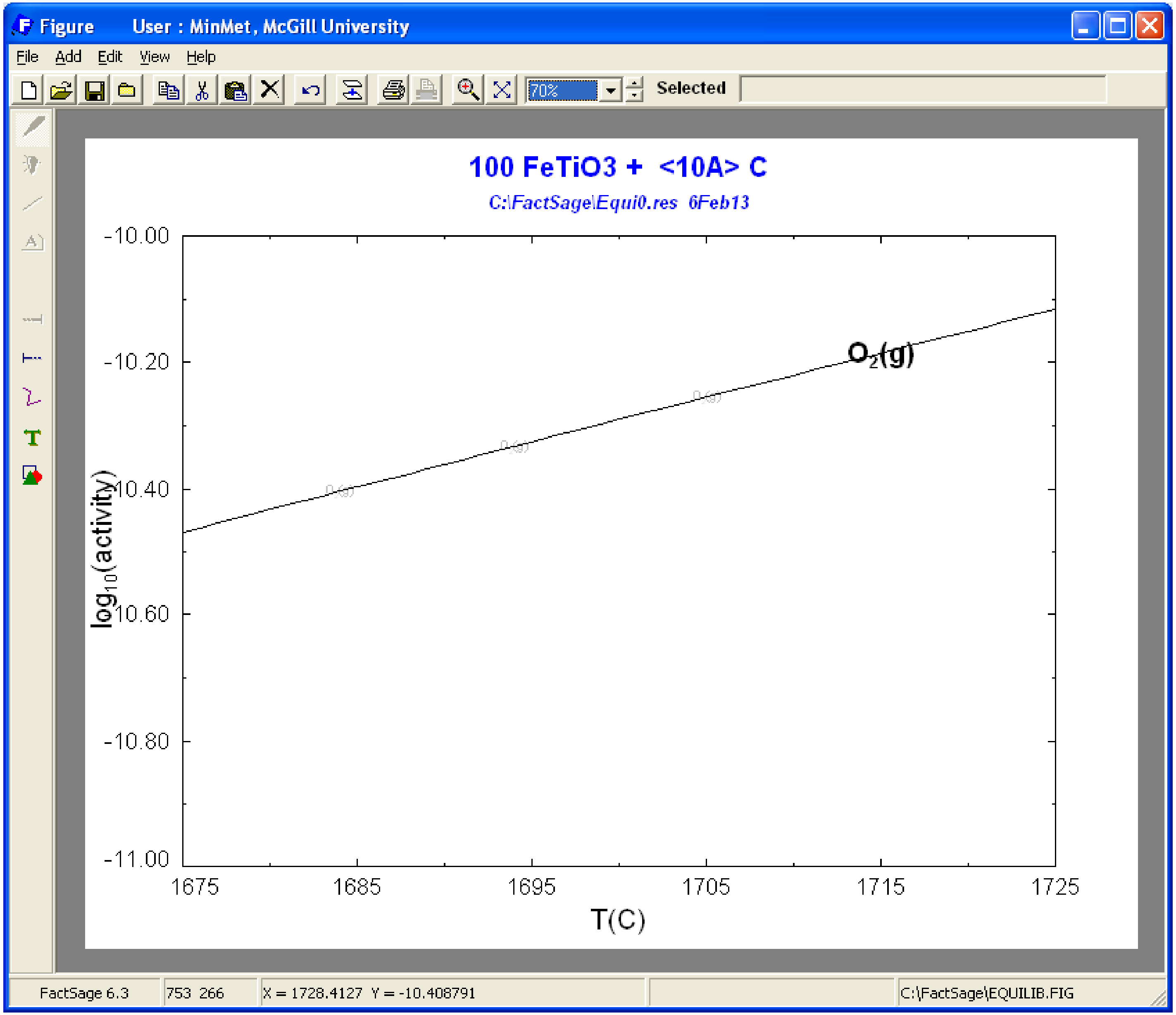
Ilmenite Smelting

1. We will plot O_2 activity versus the temperature.



Ilmenite Smelting

The graph shows that at lower temperatures, the oxygen pressure must be kept lower to keep the FeO content in the slag constant.



Ilmenite Smelting

Summarizing our findings:

9.7g C per 100g ilmenite seems to be ideal to reduce the amount of FeO in the slag while preventing the precipitation of pseudobrookite

The liquidus temperature of the resulting slag is 1672°C and the liquidus of the metal is 1674°C, so smelting at 1700°C would be better to avoid the precipitation of undesired phases