Ferrous Applications
Use of macros in process simulation

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Please see manual and more examples in:
http://in-ho-group.mcgill.ca/publicfiles.php

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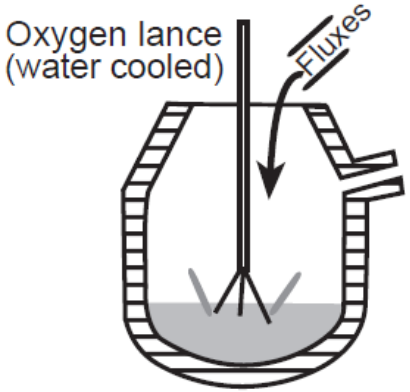
- Application I: Secondary steelmaking (slide #3)
- Application II: Simplified BOF process (slide #27)
- Application III: Slag/Steel/Inclusion interaction (slide #59)

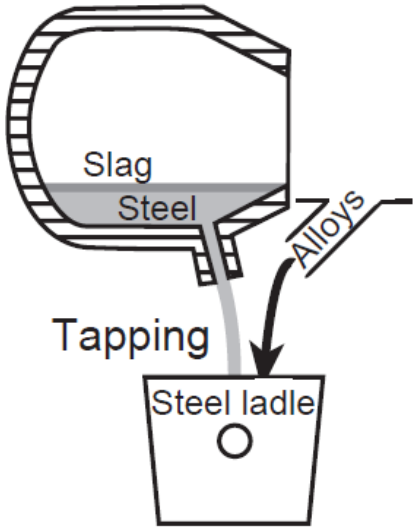
Application I

SECONDARY STEELMAKING

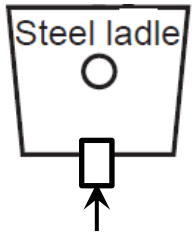
Secondary steelmaking



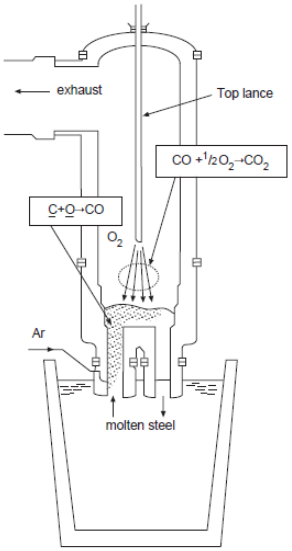
BOF



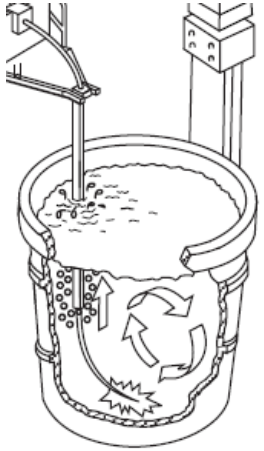
1. Tapping and alloy/flux addition



2. Stirring



3. degassing

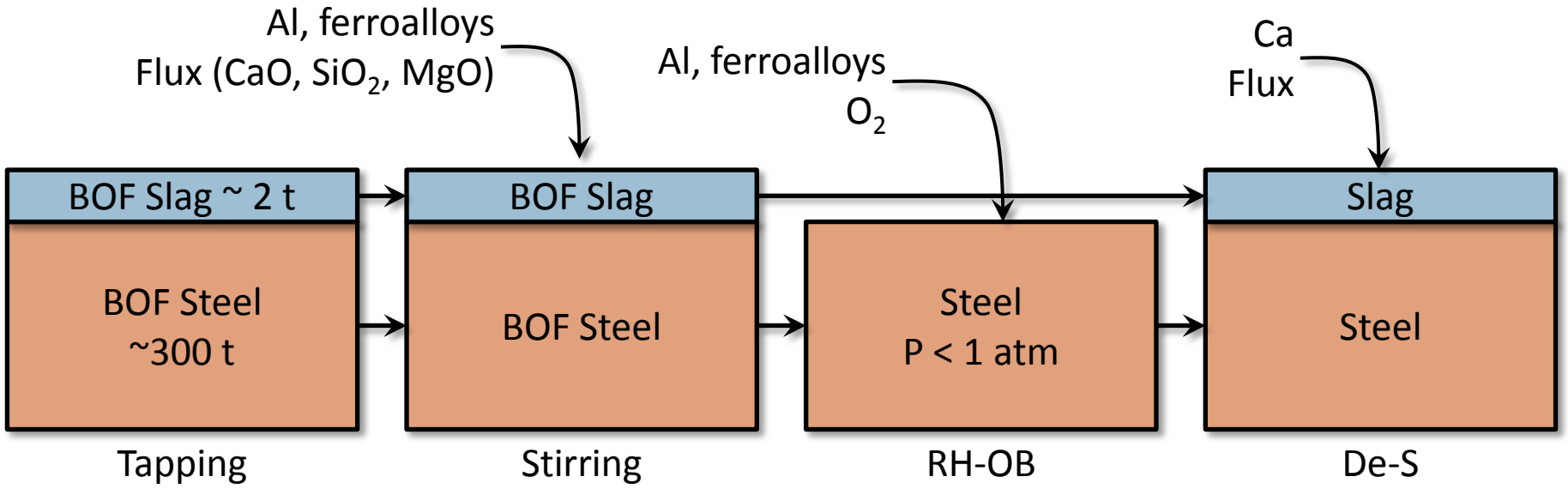


4. Wire feeding powder injection (De-S)

Procedure

1. Draw flowsheet
2. Prepare Excel file with input data
3. Prepare Equilib files for initialisation and save the streams. Write the associated macro commands
4. Prepare Equilib files for reactions and save the streams. Write the associated macro commands
5. Organise the Excel file to print the outputs. Write the associated macro commands

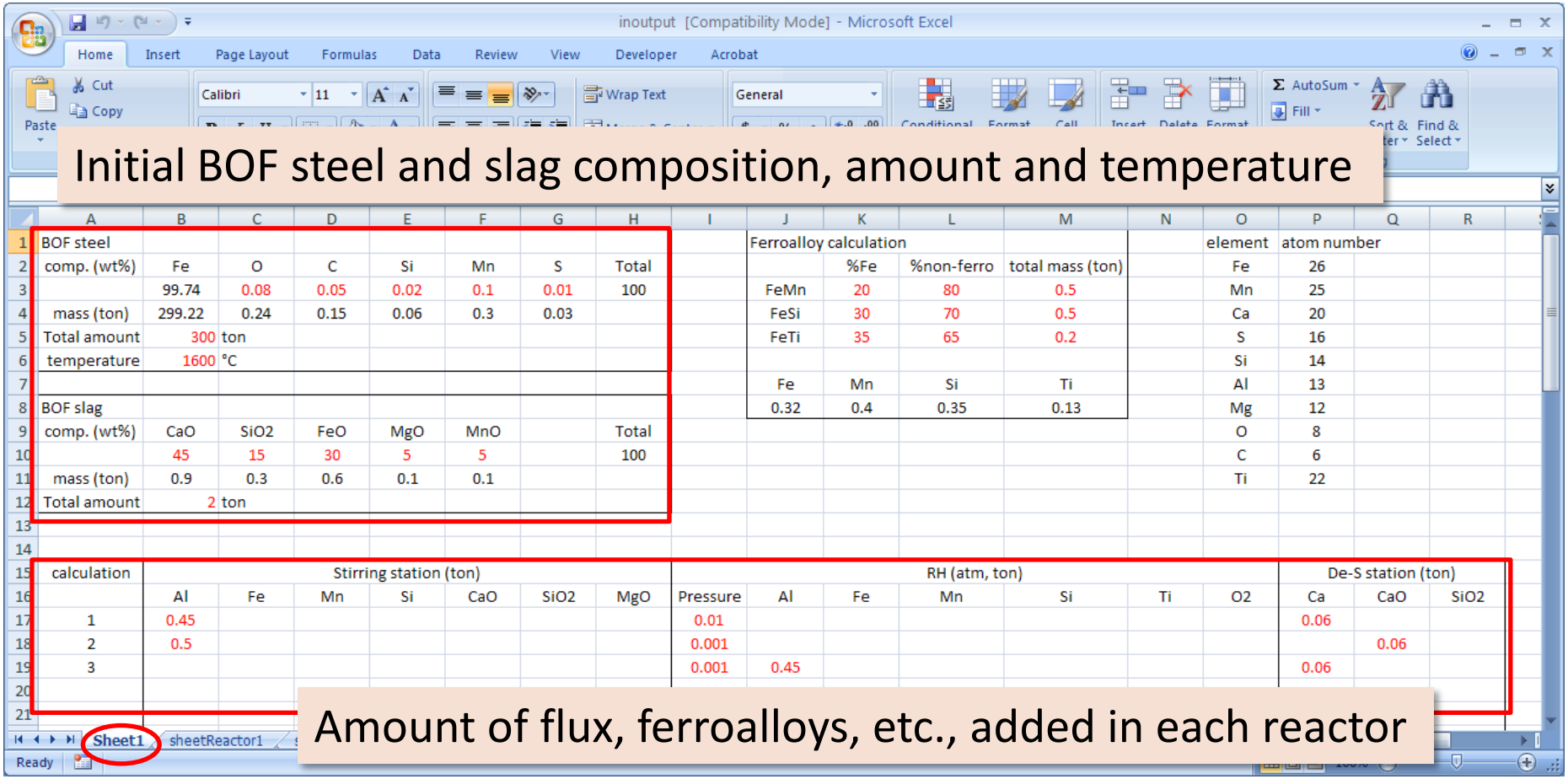
1. Secondary steelmaking – flow sheet



Initialisation **Reactor 1** **Reactor 2** **Reactor 3**

Simplifications:
- No kinetic factors
- Isothermal conditions

2. Input data in *inoutput.xls* - sheet 1



	A	B	C	D	E	F	G	H
1	BOF steel							
2	comp. (wt%)	Fe	O	C	Si	Mn	S	Total
3		99.74	0.08	0.05	0.02	0.1	0.01	100
4	mass (ton)	299.22	0.24	0.15	0.06	0.3	0.03	
5	Total amount	300	ton					
6	temperature	1600	°C					
7								
8	BOF slag							
9	comp. (wt%)	CaO	SiO2	FeO	MgO	MnO		Total
10		45	15	30	5	5		100
11	mass (ton)	0.9	0.3	0.6	0.1	0.1		
12	Total amount	2	ton					

	J	K	L	M
	Ferroalloy calculation			
		%Fe	%non-ferro	total mass (ton)
	FeMn	20	80	0.5
	FeSi	30	70	0.5
	FeTi	35	65	0.2
	Fe	Mn	Si	Ti
	0.32	0.4	0.35	0.13

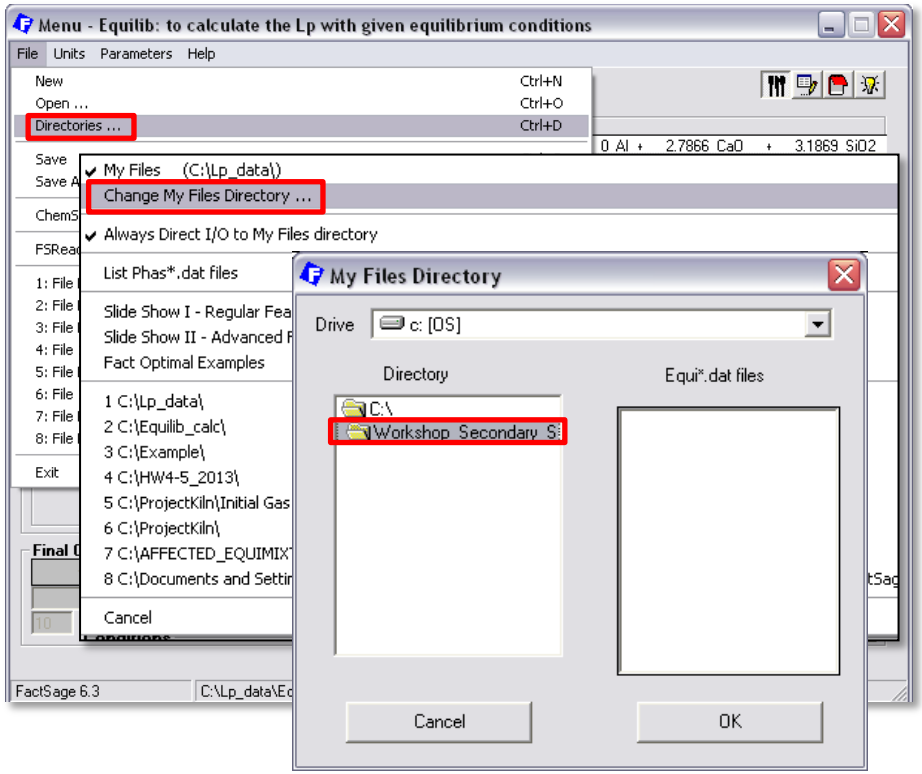
	N	O	P
		element	atom number
		Fe	26
		Mn	25
		Ca	20
		S	16
		Si	14
		Al	13
		Mg	12
		O	8
		C	6
		Ti	22

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
15	calculation	Stirring station (ton)							RH (atm, ton)							De-S station (ton)		
16		Al	Fe	Mn	Si	CaO	SiO2	MgO	Pressure	Al	Fe	Mn	Si	Ti	O2	Ca	CaO	SiO2
17	1	0.45							0.01							0.06		
18	2	0.5							0.001								0.06	
19	3								0.001	0.45						0.06		

Save as inoutput.xls in the folder C:\ Workshop_Secondary_Steelmaking\

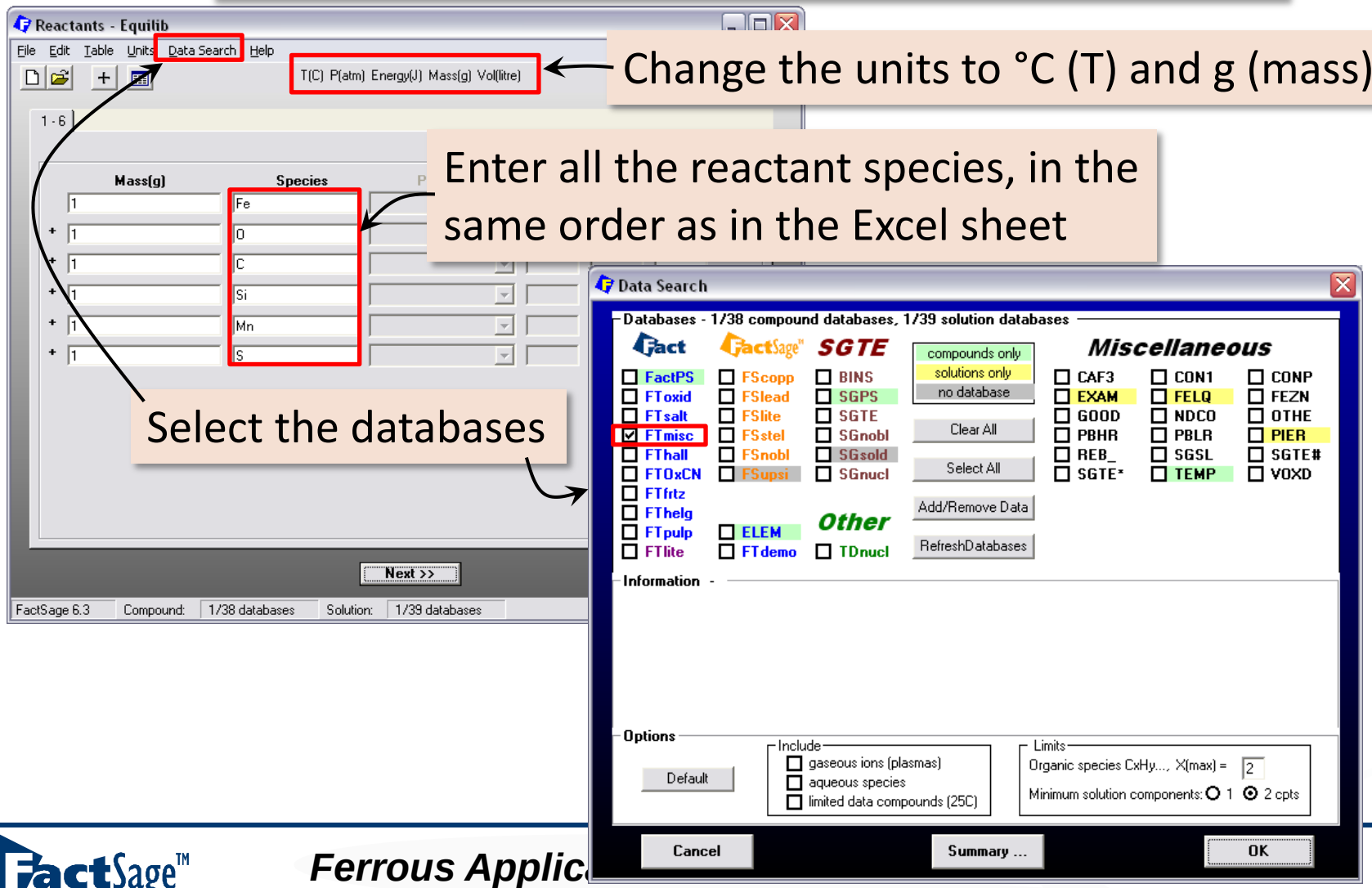
3. Streams initialization

Change Directory to C:\Workshop_Secondary_Steelmaking\



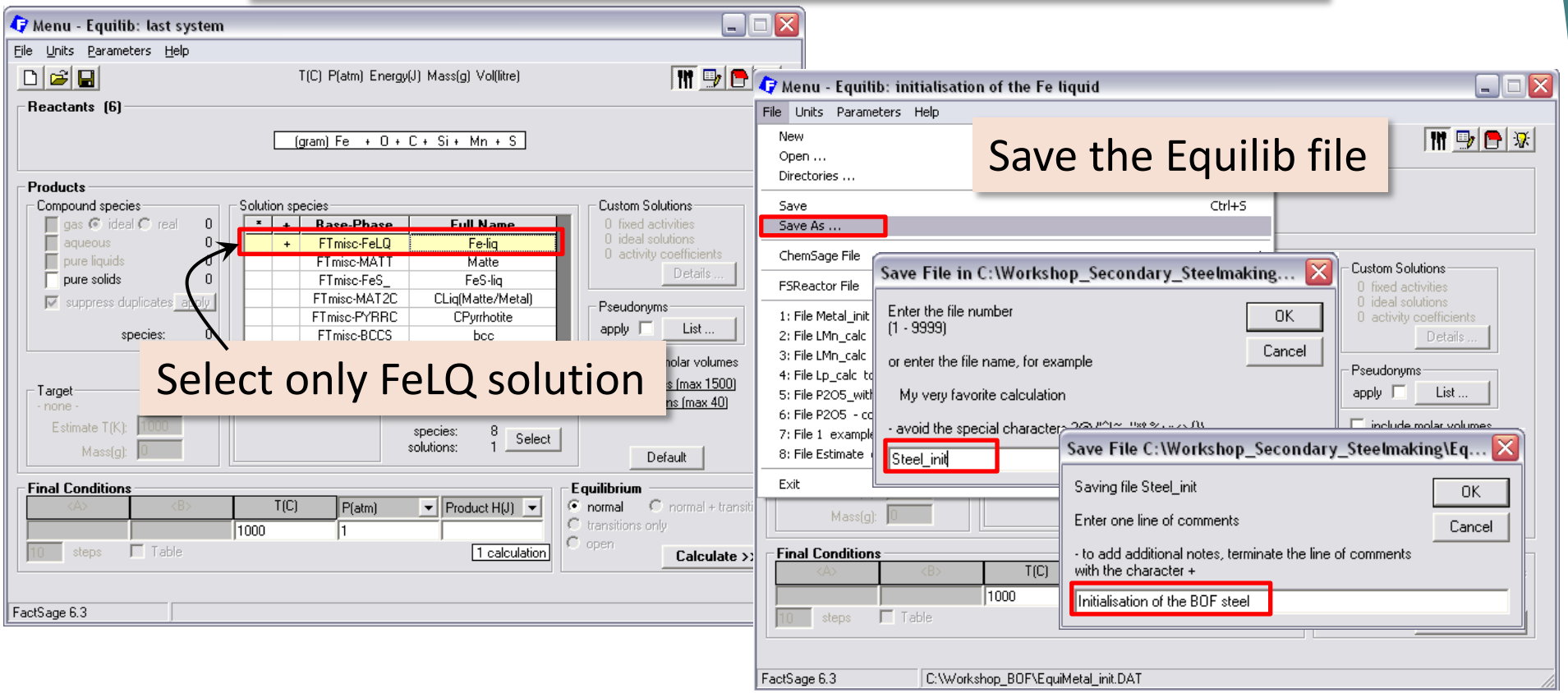
3. Streams initialization – BOF steel

Initialization of the BOF steel – EquiSteel_init.dat



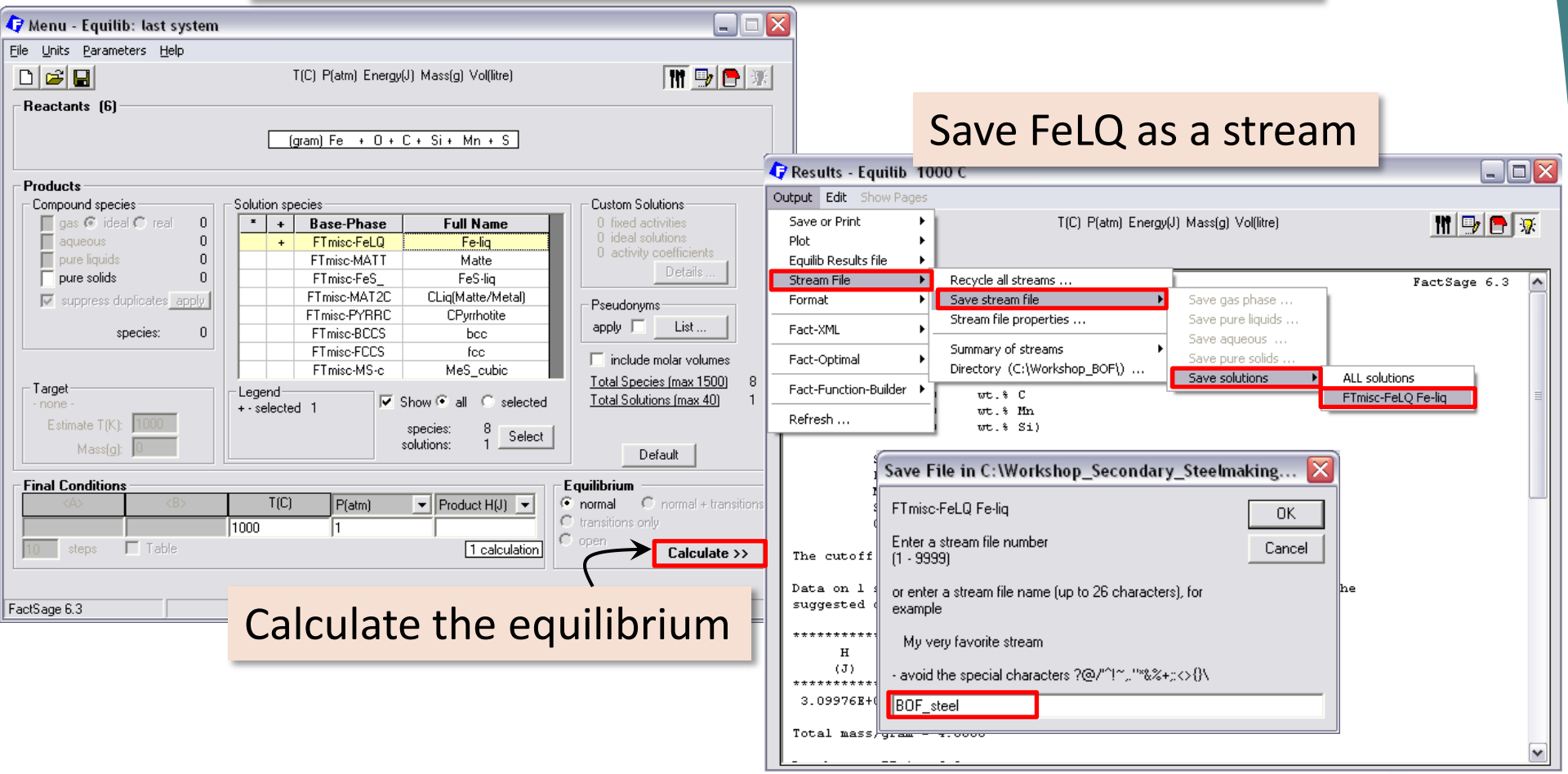
3. Streams initialization – BOF steel

Initialization of the BOF steel – EquiSteel_init.dat



3. Streams initialization – BOF steel

Initialization of the BOF steel – EquiSteel_init.dat

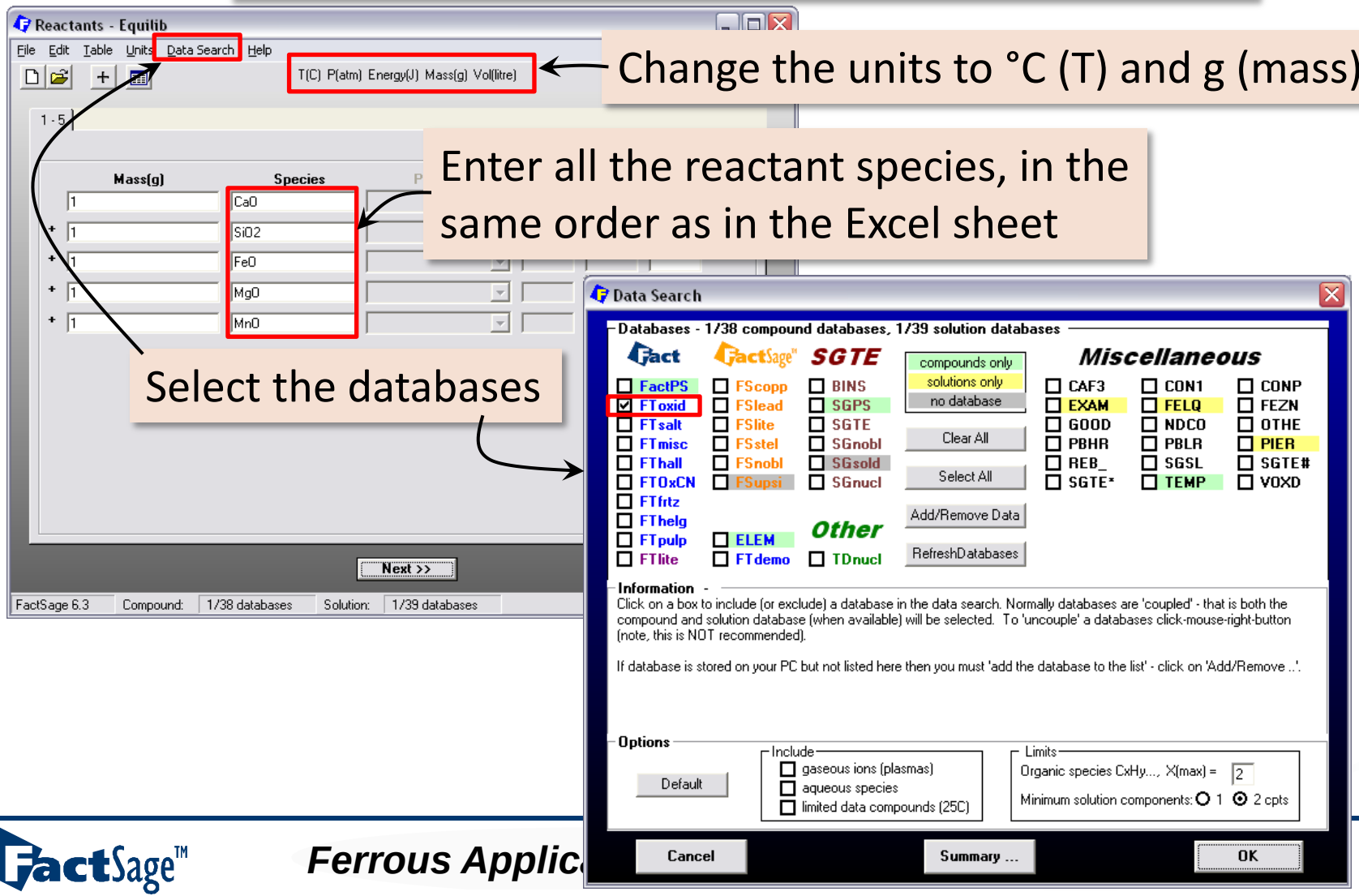


Save FeLQ as a stream

Calculate the equilibrium

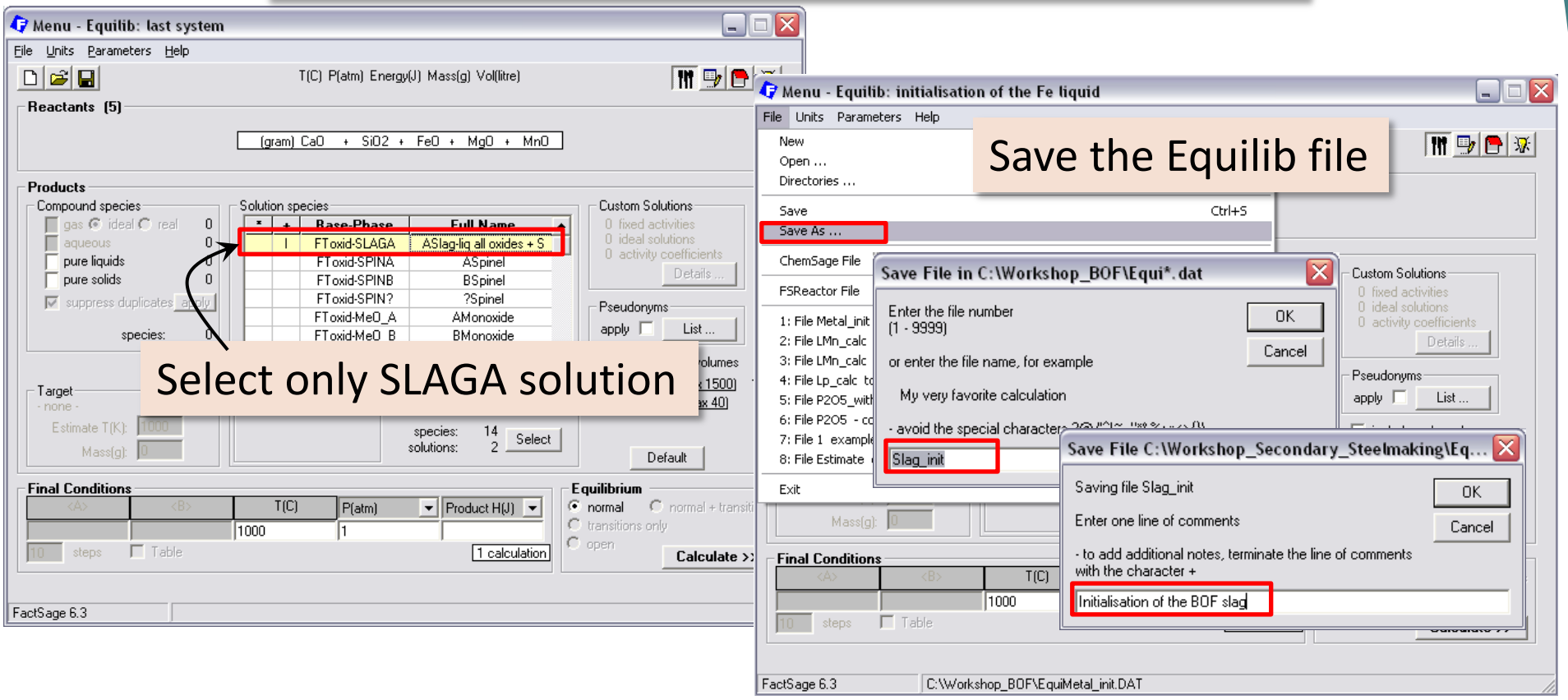
3. Streams initialization – BOF slag

Initialization of the BOF slag – EquiSlag_init.dat



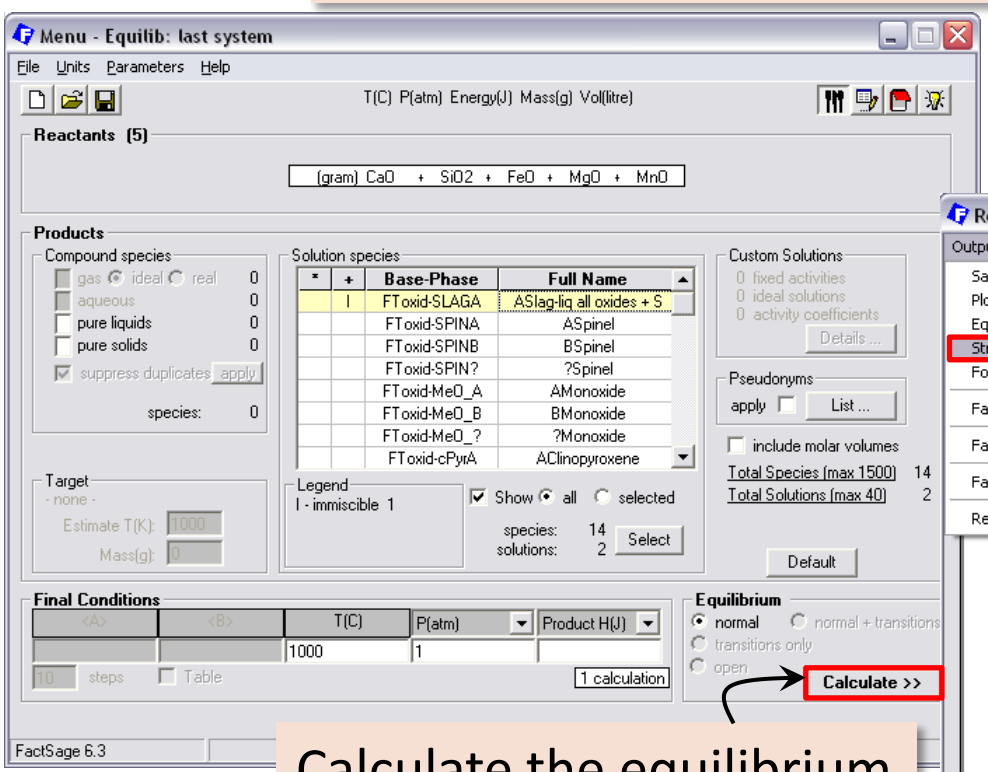
3. Streams initialization – BOF slag

Initialization of the BOF slag – EquiSlag_init.dat



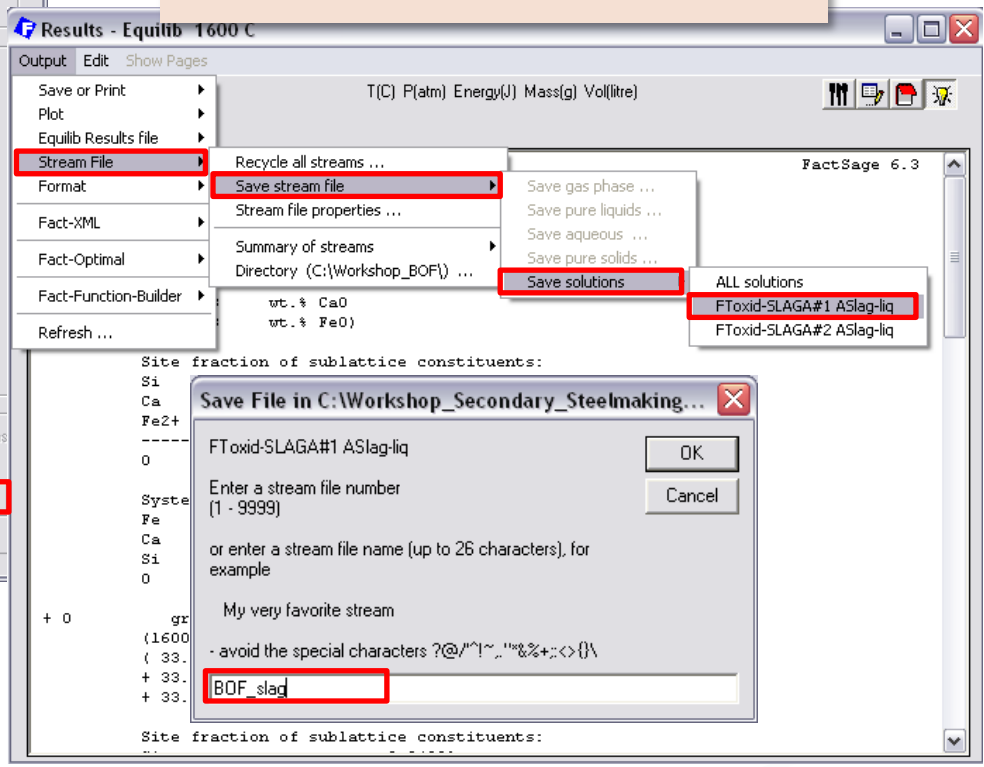
3. Streams initialization – BOF slag

Initialization of the BOF slag – MixtBOF_slag.dat



Calculate the equilibrium

Save SLAGA#1 as a stream

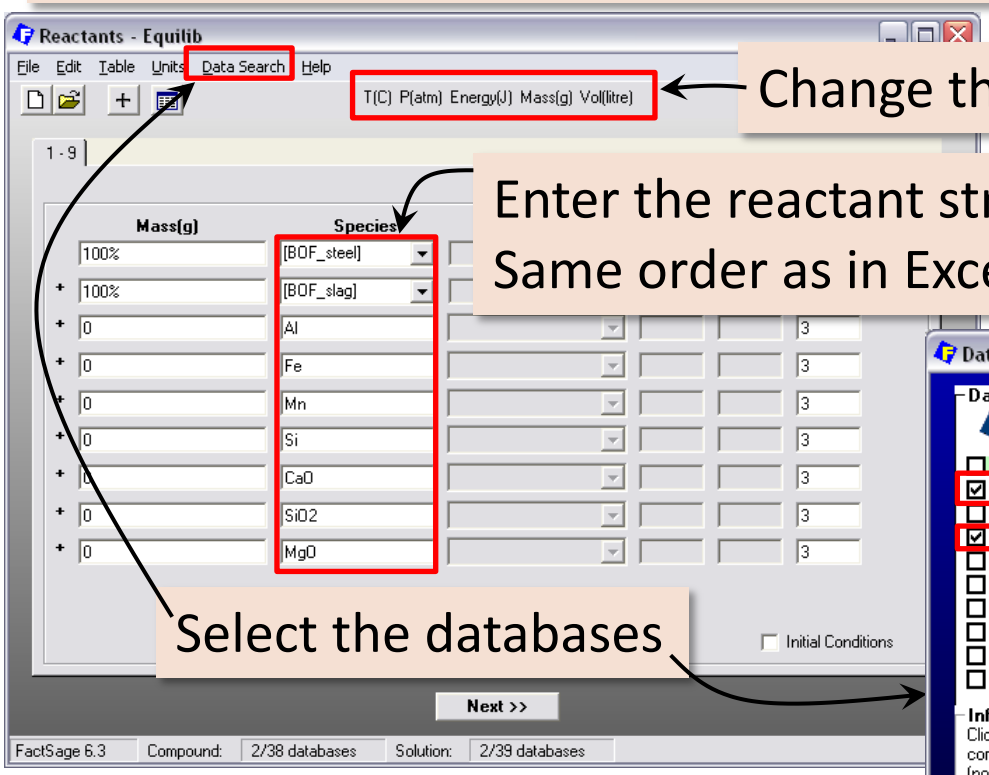


3. Streams initialization – macro

```
HIDE                                                    // Hide the equilib window

// Declaration of variables:
VARIABLE %MyDir. %temperature %Metal_input(6) %Slag_input(5)

%MyDir. = C:\Workshop_Secondary_Steelmaking\            // path definition

OLE1 %MyDir.inoutput.xls sheet1                         // creation of OLE link

%Metal_input OLE1 READ B4:G4                            // reading and storing initial steel
%Slag_input OLE1 READ B11:F11                           // reading and storing initial slag
%temperature OLE1 READ B6                               // reading and storing temperature

// ****************************** Initialisation ******************************

OPEN %MyDir.EquiSteel_init.dat                          // open the equilib file
%1 = 1 TO 6                                             // loop on the equilib reactants
    SET REACTANT %1 MASS %Metal_input(%1)               // overwrite the reactant amounts
%1 LOOP                                                 // end of loop
SET FINAL T %temperature                                // overwrite the temperature in Equilib
CALC                                                    // calculate the equilibrium
SAVE %MyDir.MixtBOF_steel.dat FTmisc-FeLQ               // save FeLQ as a stream

OPEN %MyDir.EquiSlag_init.dat                           // open the equilib file
%1 = 1 TO 5                                             // loop on the equilib reactants
    SET REACTANT %1 MASS %Slag_input(%1)                // overwrite the reactant amounts
%1 LOOP                                                 // end of loop
SET FINAL T %temperature                                // overwrite the temperature in Equilib
CALC                                                    // calculate the equilibrium
SAVE %MyDir.MixtBOF_slag.dat FToxid-SLAGA#1             // save SLAGA#1 as a stream

END                                                     // end of macro
```

4. Equilib file for Reactor 1 - stirring

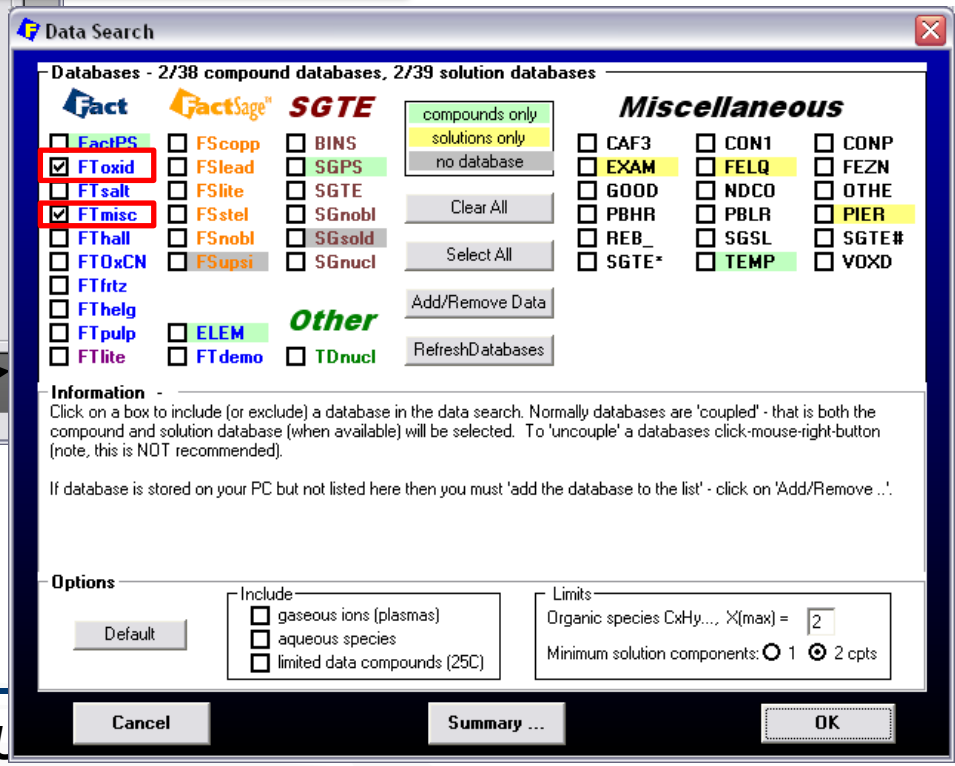
Reaction between BOF steel, slag, Al, ferroalloys, flux – EquiR1.dat



Change the units to °C (T) and g (mass)

Enter the reactant streams for R1, Same order as in Excel file

Select the databases



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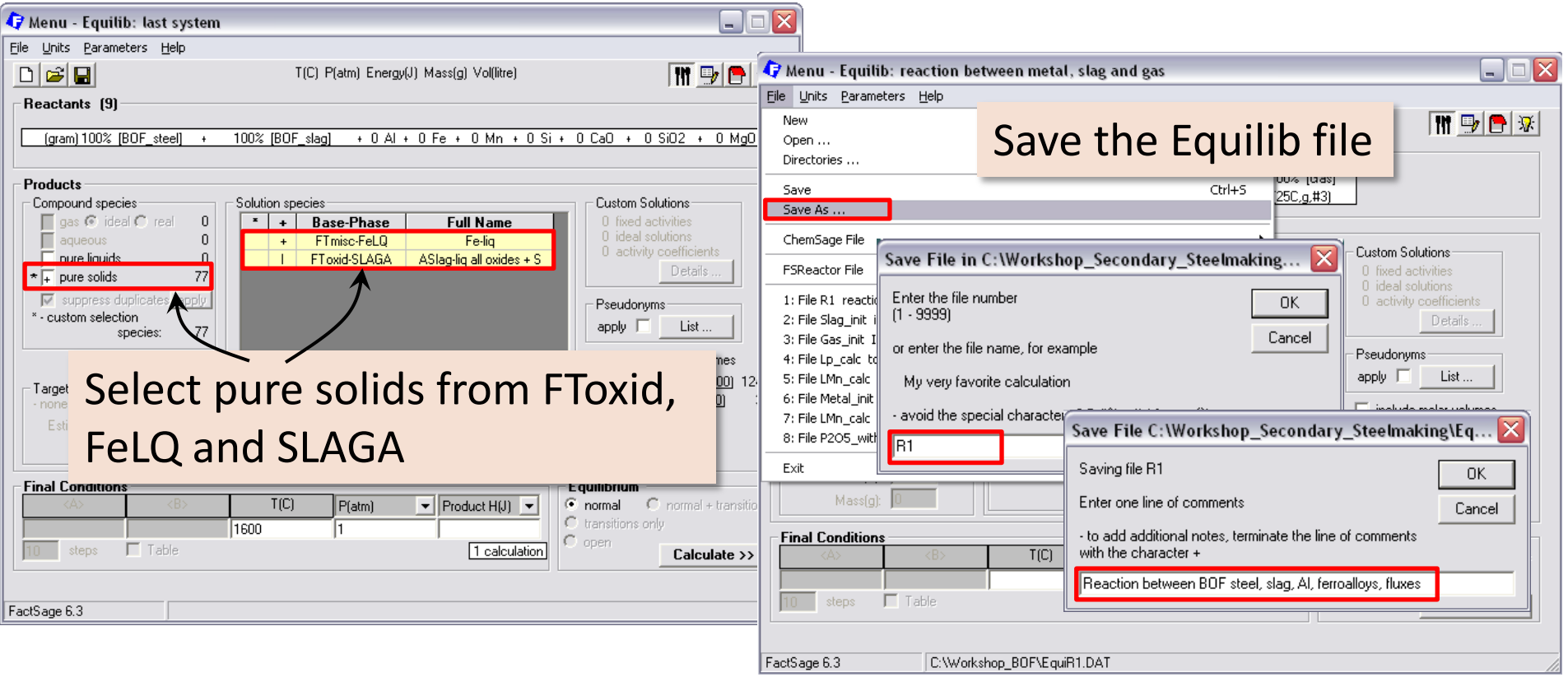
Reaction between BOF steel, slag, Al, ferroalloys, flux – EquiR1.dat



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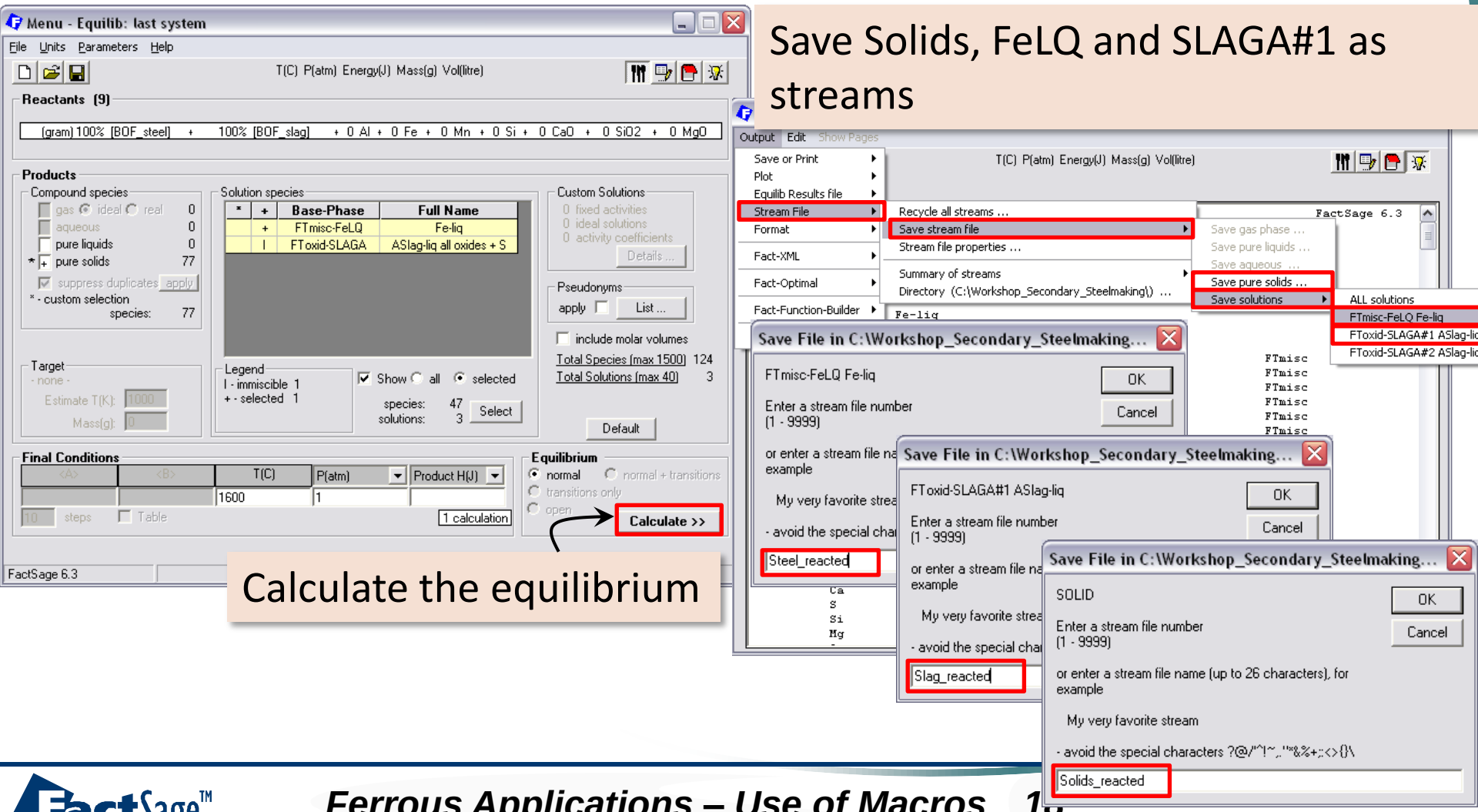
Reaction between BOF steel, slag, Al, ferroalloys, flux – EquiR1.dat

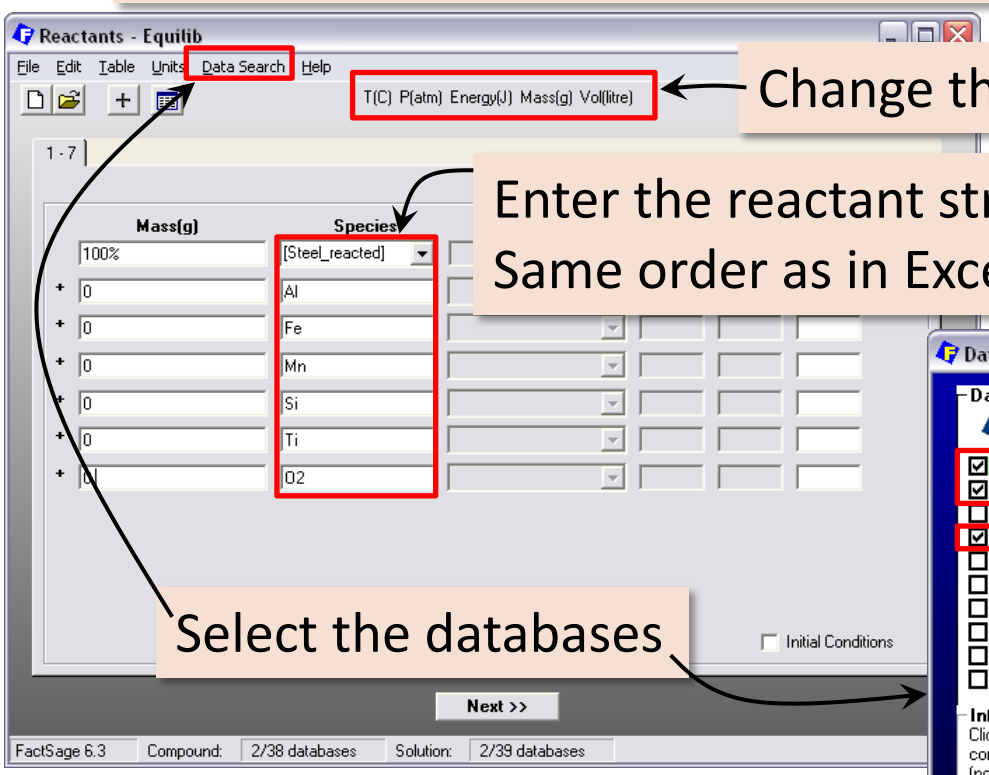


Save Solids, FeLQ and SLAGA#1 as streams

Calculate the equilibrium

4. Equilib file for Reactor 2 - RH

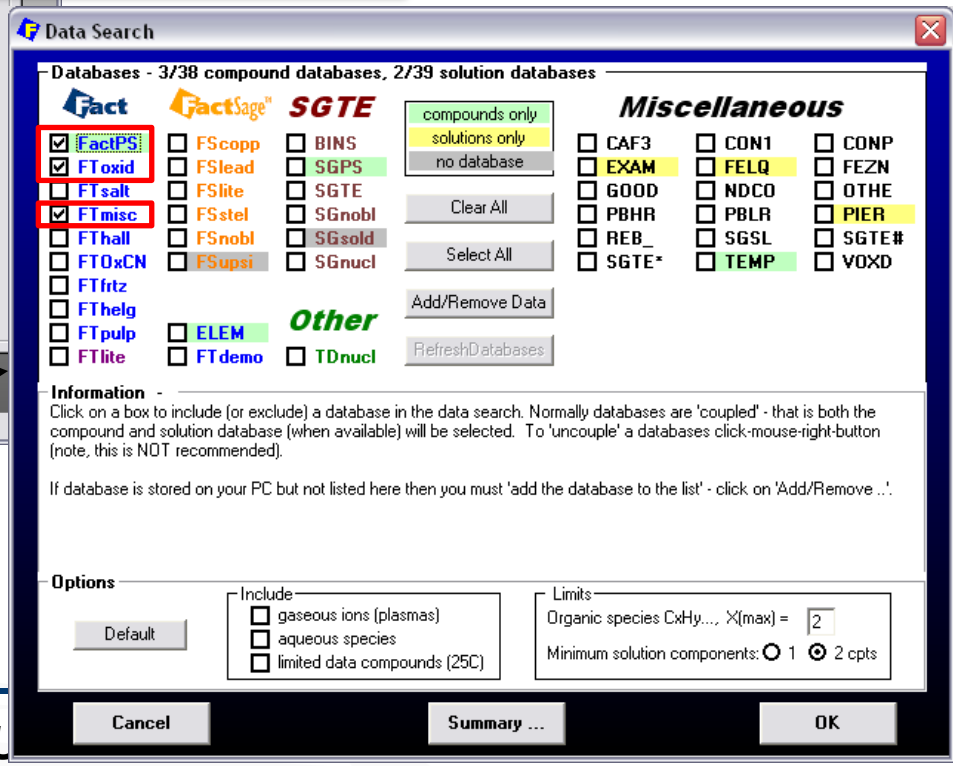
Reaction between steel, Al, ferroalloys at low P – EquiR2.dat



Change the units to °C (T) and g (mass)

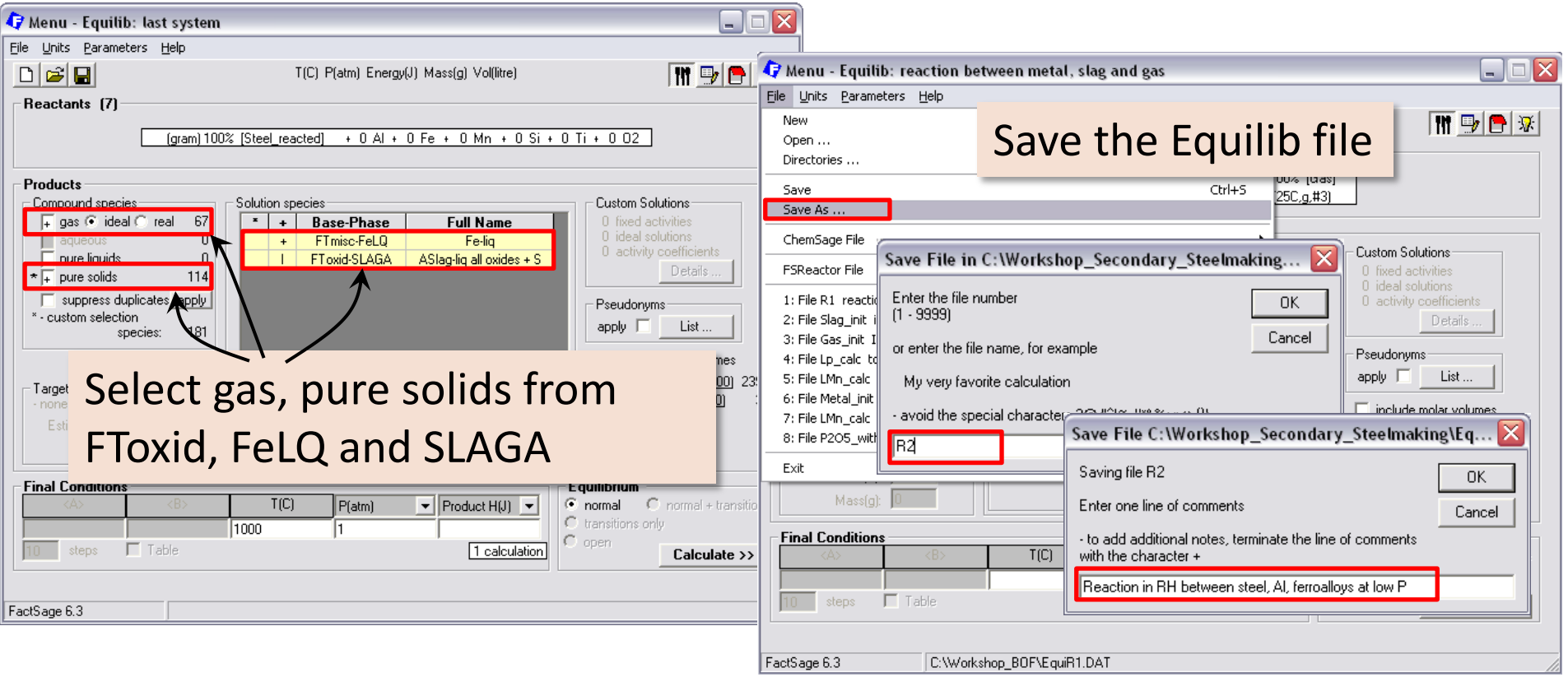
Enter the reactant streams for R2, Same order as in Excel file

Select the databases



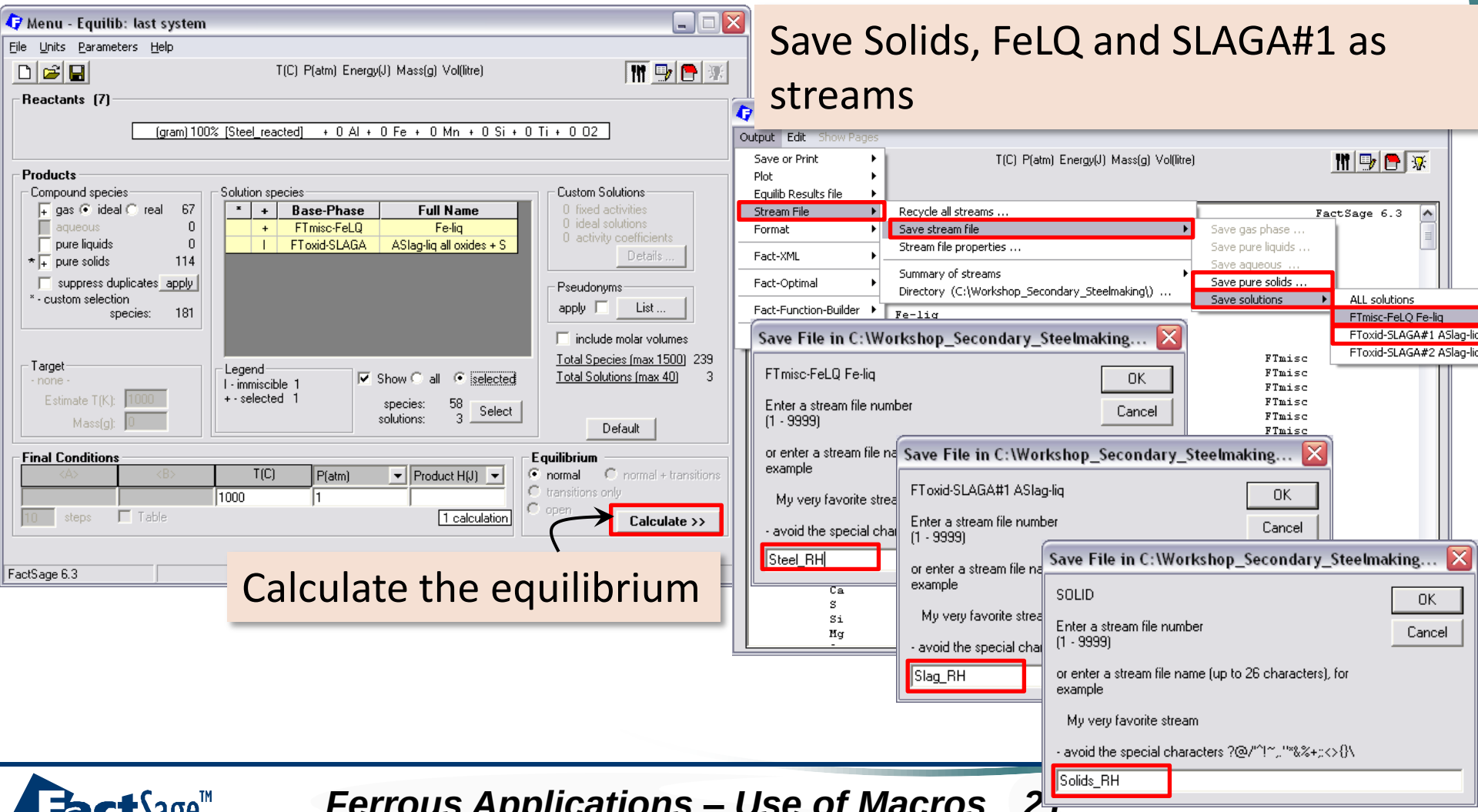
4. Equilib file for Reactor 2 - RH

Reaction between steel, Al, ferroalloys at low P – EquiR2.dat



4. Equilib file for Reactor 2 - RH

Reaction between steel, Al, ferroalloys at low P – EquiR2.dat

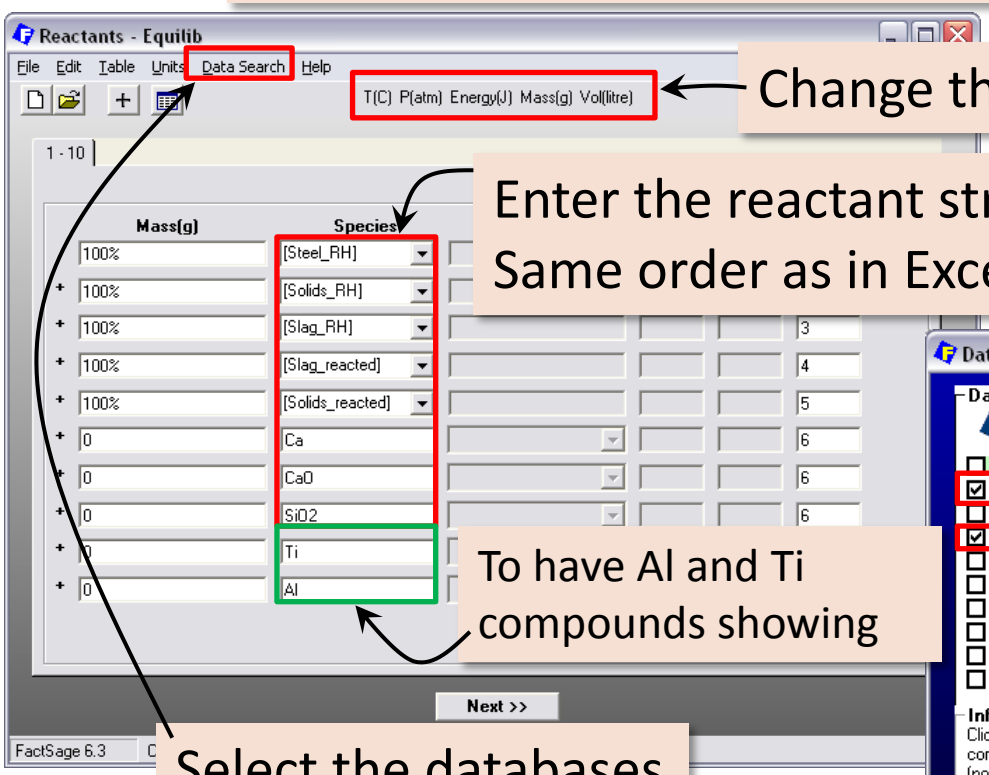


Save Solids, FeLQ and SLAGA#1 as streams

Calculate the equilibrium

4. Equilib file for Reactor 3 – De-S

Reaction between steel, slag and flux – EquiR3.dat

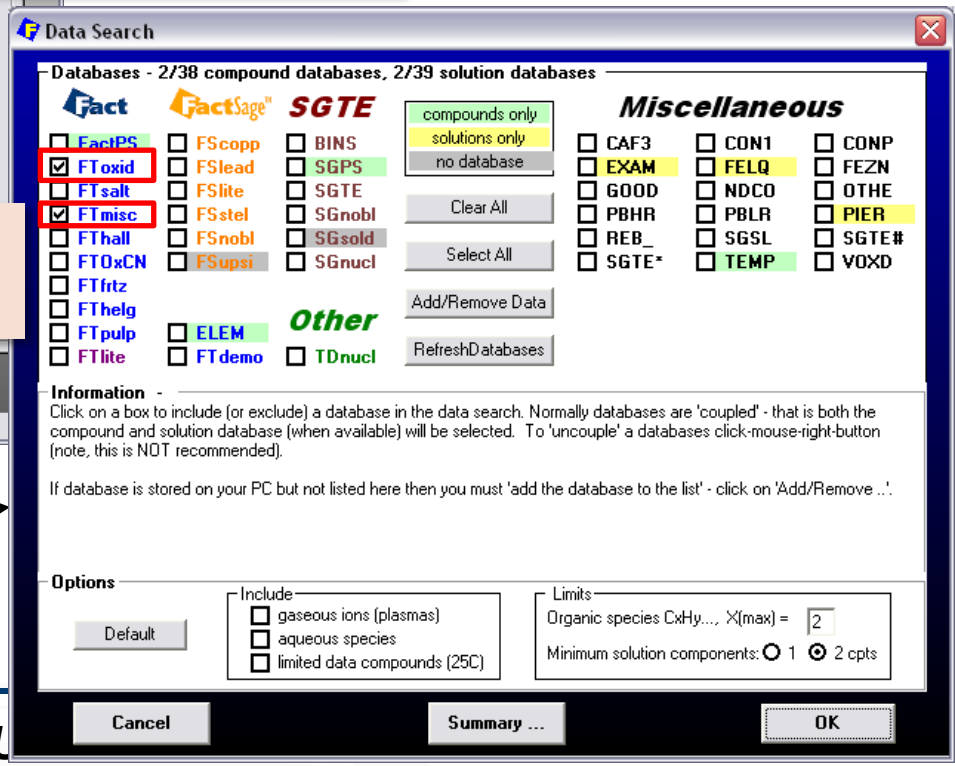


Change the units to °C (T) and g (mass)

Enter the reactant streams for R3, Same order as in Excel file

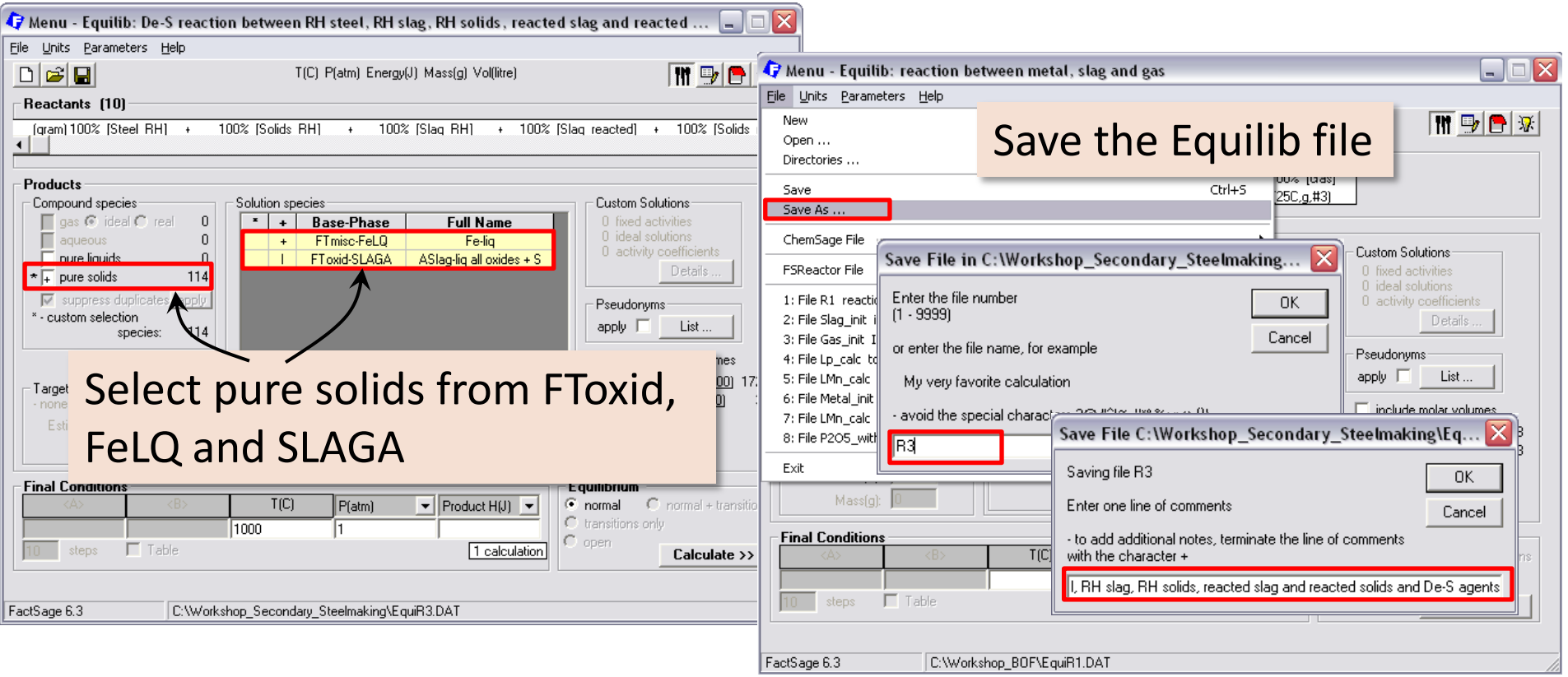
To have Al and Ti compounds showing

Select the databases



4. Equilib file for Reactor 3 – De-S

Reaction between steel, slag and flux – EquiR3.dat



4. Main reactions – macro

```
// ****************************** START OF PROCESS ******************************

// Declaration of variables:
VARIABLE %R1_flux(7) %R2_flux(6) %R3_flux(3) %RH_pressure %pos %num_calc %check %react

%pos = 17                                          // position of row to read in excel file

%num_calc = 1 TO 65536                             // loop over the max amount of rows in excel
    %check OLE1 READ R%posC1                       // read the calculation number
    IF %check = 0 GOTO END                         // if cell is empty, stop the macro
    %R1_flux OLE1 READ R%posC2:R%posC8             // reading and storing flux R1
    %RH_pressure OLE1 READ R%posC9                 // reading and storing RH pressure
    %R2_flux OLE1 READ R%posC10:R%posC15           // reading and storing flux R2
    %R3_flux OLE1 READ R%posC16:R%posC18           // reading and storing flux R3

    OPEN %MyDir.EquiR1.dat                         // open the equilib file - reactor 1
    %react = 3                                     // position of first reactant to overwrite mass
    %1 = 1 TO 7                                    // loop over the size of %R1_flux
        SET REACTANT %react MASS %R1_flux(%1)      // overwrite the reactant mass
        %react STEP                                // move to the next reactant
    %1 LOOP                                        // end of loop
    SET FINAL T %temperature                       // overwrite the temperature in Equilib
    CALC                                           // calculate the equilibrium
    SAVE %MyDir.MixtSteel_reacted.dat FTmisc-FeLQ      // save FeLQ as a stream
    SAVE %MyDir.MixtSlag_reacted.dat FToxid-SLAGA#1    // save SLAGA#1 as a stream
    SAVE %MyDir.MixtSolids_reacted.dat SOLIDS          // save solids as as stream

    OPEN %MyDir.EquiR2.dat                         // open the equilib file - reactor 2
    %react = 2                                     // position of first reactant to overwrite mass
    %1 = 1 TO 6                                    // loop over the size of %R2_flux
        SET REACTANT %react MASS %R2_flux(%1)      // overwrite the reactant mass
        %react STEP                                // move to the next reactant
    %1 LOOP                                        // end of loop
    SET FINAL T %temperature                       // overwrite the temperature in Equilib
    CALC                                           // calculate the equilibrium
    SAVE %MyDir.MixtSteel_RH.dat FTmisc-FeLQ       // save FeLQ as a stream
    SAVE %MyDir.MixtSlag_RH.dat FToxid-SLAGA#1     // save SLAGA#1 as a stream
    SAVE %MyDir.MixtSolids_RH.dat SOLIDS           // save solids as as stream

    OPEN %MyDir.EquiR3.dat                         // open the equilib file - reactor 3
    %react = 6                                     // position of first reactant to overwrite mass
    %1 = 1 TO 3                                    // loop over the size of %R3_flux
        SET REACTANT %react MASS %R3_flux(%1)      // overwrite the reactant mass
        %react STEP                                // move to the next reactant
    %1 LOOP                                        // end of loop
    SET FINAL T %temperature                       // overwrite the temperature in Equilib
    CALC                                           // calculate the equilibrium

    %pos STEP                                      // move to the next row in Excel (new process)
%num_calc LOOP                                     // end of loop
END                                                // end of macro
```

FactSage™

5. Organise the outputs in Excel

- 3 Excel sheets to print out all the calculation results for each reactor
- For each reactor, print out the mass of each phase, the mass of each element in steel, mass of each slag species and mass of each solid species

5. Macro for printing in Excel

```
VARIABLE %atom_num(10) %Inc %row %results

OLE2 %MyDir.inoutput.xls sheetReactor1          // creation of OLE link
OLE3 %MyDir.inoutput.xls sheetReactor2          // creation of OLE link
OLE4 %MyDir.inoutput.xls sheetReactor3          // creation of OLE link
OLE2 CELLS ALL CLEAR                            // clear the worksheet
OLE3 CELLS ALL CLEAR                            // clear the worksheet
OLE4 CELLS ALL CLEAR                            // clear the worksheet
%atom_num OLE1 READ P2:P11                      // read and store the atomic number
%row = 2                                        // position of row to write in excel file
```

```
// PRINTING:
    IF %num_calc = 1 THEN                       // if first loop, print the names in first row
        %Inc = 1                                // start from first column
        %results = calculation                  // column title
        %results OLE2 WRITE R1C%Inc             // write in first row
        %Inc STEP                               // move to next column
        %1 = 2 TO 4                             // loop on the mixture number
            %results = $E_mN%1$                 // store the name of mixture
            %results OLE2 WRITE R1C%Inc         // write in first row
            %Inc STEP                           // move to next column
        %1 LOOP                                 // end of loop
        %1 = 1 TO 9                             // loop on element atomic number
            %results = $E_e%atom_num(%1)_N$_steel   // name of element
            %results OLE2 WRITE R1C%Inc         // write in first row
            %Inc STEP                           // move to next column
        %1 LOOP                                 // end of loop
        %1 = 16 TO 31                           // loop on the species code number (SLAGA#1)
            %results = $E_sN%1$                 // store the name of the species
            %results OLE2 WRITE R1C%Inc         // write in first row
            %Inc STEP                           // move to next column
        %1 LOOP                                 // end of loop
        %1 = 48 TO 124                          // loop on the species code number (solids)
            %results = $E_sN%1$                 // store the name of the species
            %results OLE2 WRITE R1C%Inc         // write in first row
            %Inc STEP                           // move to next column
        %1 LOOP                                 // end of loop
    ENDIF                                       // end of IF
```

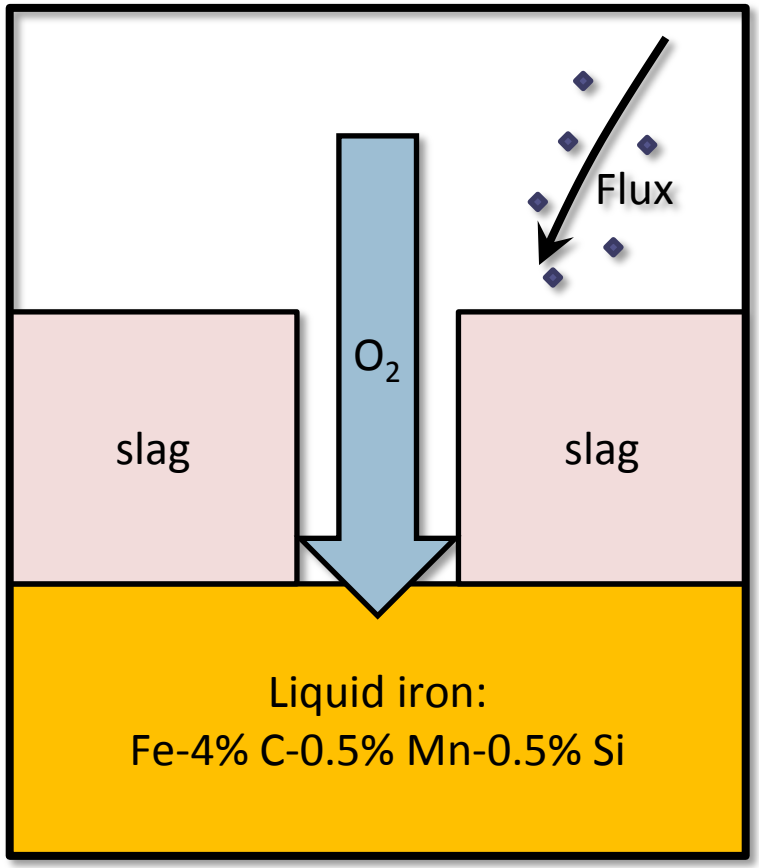
Macro commands for printing the Equilib results of Reactor 1

```
        %Inc = 1                                // start from first column
        %num_calc OLE2 WRITE R%rowC%Inc         // write calculation number
        %Inc STEP                               // move to next column
        %1 = 2 TO 4                             // loop on the mixture number
            %results = $E_mg%1$                 // store the mass of mixture
            %results OLE2 WRITE R%rowC%Inc      // write in excel
            %Inc STEP                           // move to next column
        %1 LOOP                                 // end of loop
        %1 = 1 TO 9                             // loop on element atomic number
            %results = $E_e%atom_num(%1)_mg2$   // mass of element in mixture 2 (steel)
            %results OLE2 WRITE R%rowC%Inc      // write in excel
            %Inc STEP                           // move to next column
        %1 LOOP                                 // end of loop
        %1 = 16 TO 31                           // loop on the species code number (SLAGA#1)
            %results = $E_sg%1$                 // store the mass of species
            %results OLE2 WRITE R%rowC%Inc      // write in excel
            %Inc STEP                           // move to next column
        %1 LOOP                                 // end of loop
        %1 = 48 TO 124                          // loop on the species code number (solids)
            %results = $E_sg%1$                 // store the mass of species
            %results OLE2 WRITE R%rowC%Inc      // write in excel
            %Inc STEP                           // move to next column
        %1 LOOP                                 // end of loop
// end of PRINTING
```

Application II

SIMPLIFIED BOF PROCESS

Process simulation of the BOF process



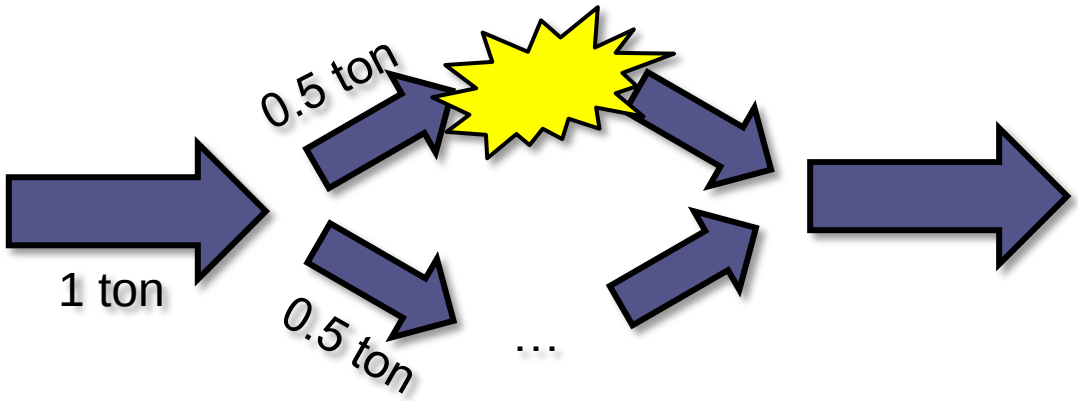
Phase	Amount	Composition	Temperature
Metal	100 ton	95% Fe 4% C 0.5% Mn 0.5% Si	1300 °C
Slag	2 ton	55% CaO 25% FeO 20% SiO_2	1300 °C
Gas	0.4 ton/min	100% O_2	25 °C
Flux	0.25 ton/min 1 to 5 min	100% CaO	25 °C

Process duration : 15 min

All reactions under adiabatic conditions

Kinetics vs. equilibrium

- Real process is dictated by kinetics
- Kinetics can be simulated with FactSage by allowing only a portion of the feeds to react

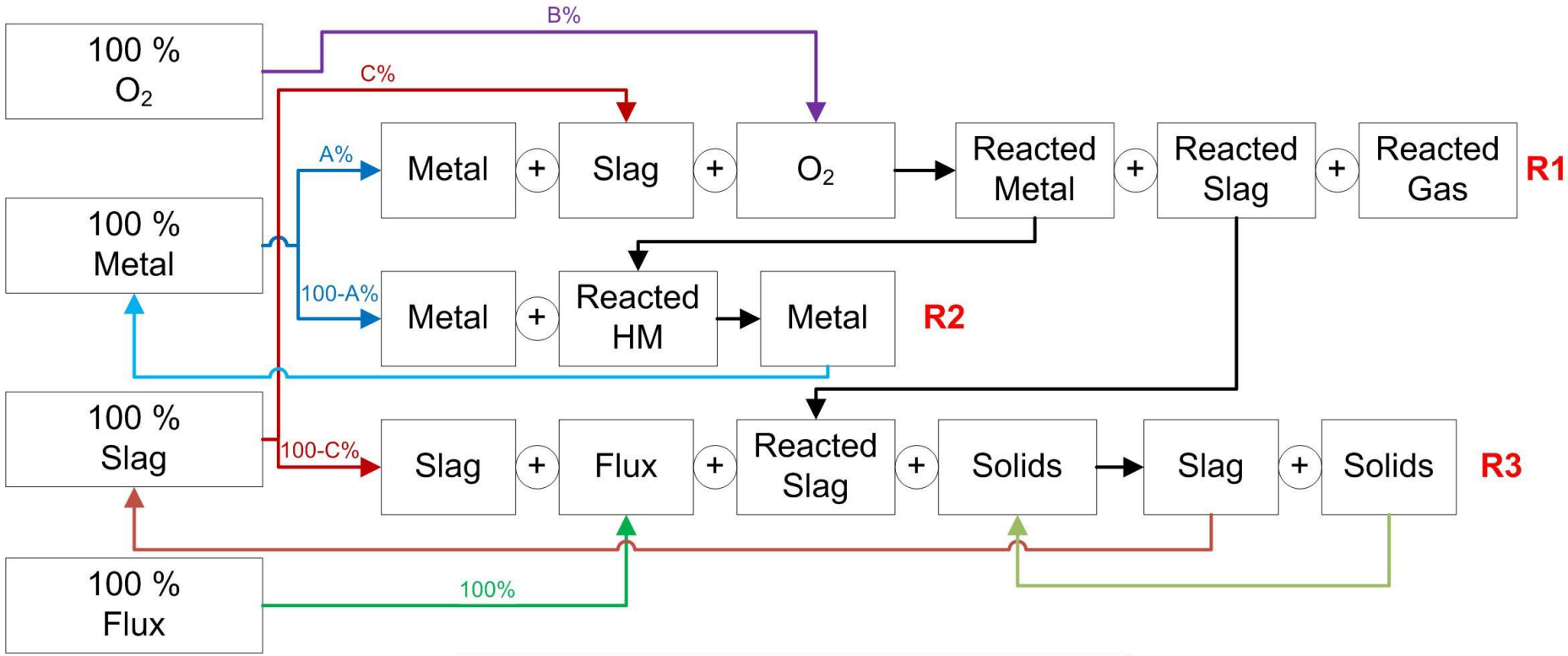


- Finding the suitable proportion of material reacting and non-reacting

Procedure

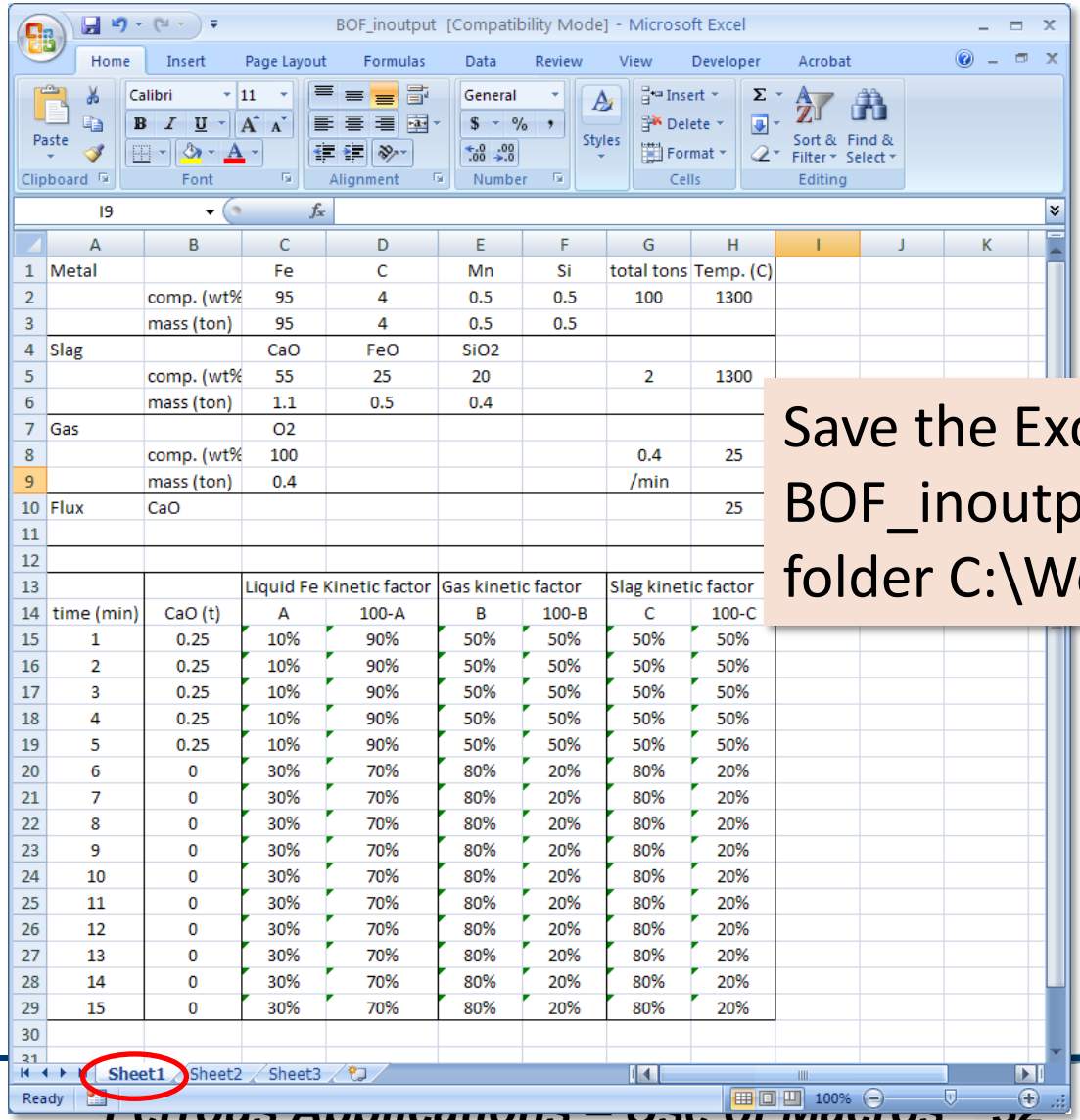
1. Draw flowsheet
2. Prepare Excel file with input data
3. Prepare Equilib files for initialisation and save the streams. Write the associated macro commands
4. Prepare Equilib files for reactions and save the streams. Write the associated macro commands
5. Organise the Excel file to print the outputs. Write the associated macro commands

1. Flow sheet of the process



Kinetic factor	1 ~ 5 min	6 ~ 15 min
A	10%	30%
B	50%	80%
C	50%	80%

2. Process inputs in Excel file

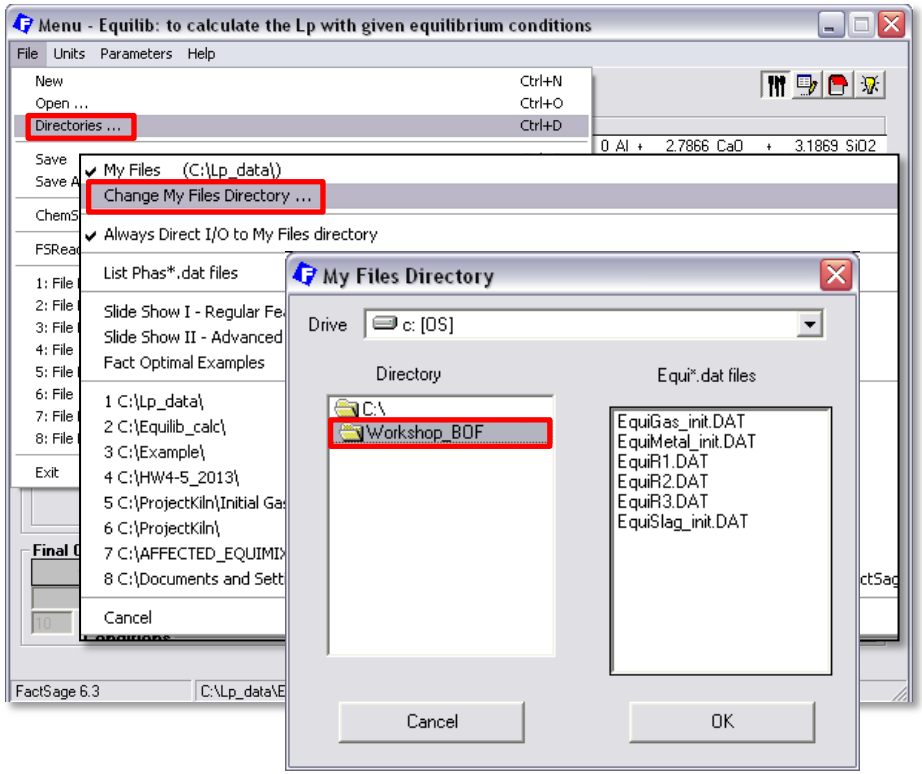


	A	B	C	D	E	F	G	H
1	Metal		Fe	C	Mn	Si	total tons	Temp. (C)
2		comp. (wt%	95	4	0.5	0.5	100	1300
3		mass (ton)	95	4	0.5	0.5		
4	Slag		CaO	FeO	SiO2			
5		comp. (wt%	55	25	20		2	1300
6		mass (ton)	1.1	0.5	0.4			
7	Gas		O2					
8		comp. (wt%	100				0.4	25
9		mass (ton)	0.4				/min	
10	Flux	CaO						25
11								
12								
13			Liquid Fe Kinetic factor		Gas kinetic factor		Slag kinetic factor	
14	time (min)	CaO (t)	A	100-A	B	100-B	C	100-C
15	1	0.25	10%	90%	50%	50%	50%	50%
16	2	0.25	10%	90%	50%	50%	50%	50%
17	3	0.25	10%	90%	50%	50%	50%	50%
18	4	0.25	10%	90%	50%	50%	50%	50%
19	5	0.25	10%	90%	50%	50%	50%	50%
20	6	0	30%	70%	80%	20%	80%	20%
21	7	0	30%	70%	80%	20%	80%	20%
22	8	0	30%	70%	80%	20%	80%	20%
23	9	0	30%	70%	80%	20%	80%	20%
24	10	0	30%	70%	80%	20%	80%	20%
25	11	0	30%	70%	80%	20%	80%	20%
26	12	0	30%	70%	80%	20%	80%	20%
27	13	0	30%	70%	80%	20%	80%	20%
28	14	0	30%	70%	80%	20%	80%	20%
29	15	0	30%	70%	80%	20%	80%	20%
30								

Save the Excel file as BOF_inoutput.xls in the folder C:\Workshop_BOF\

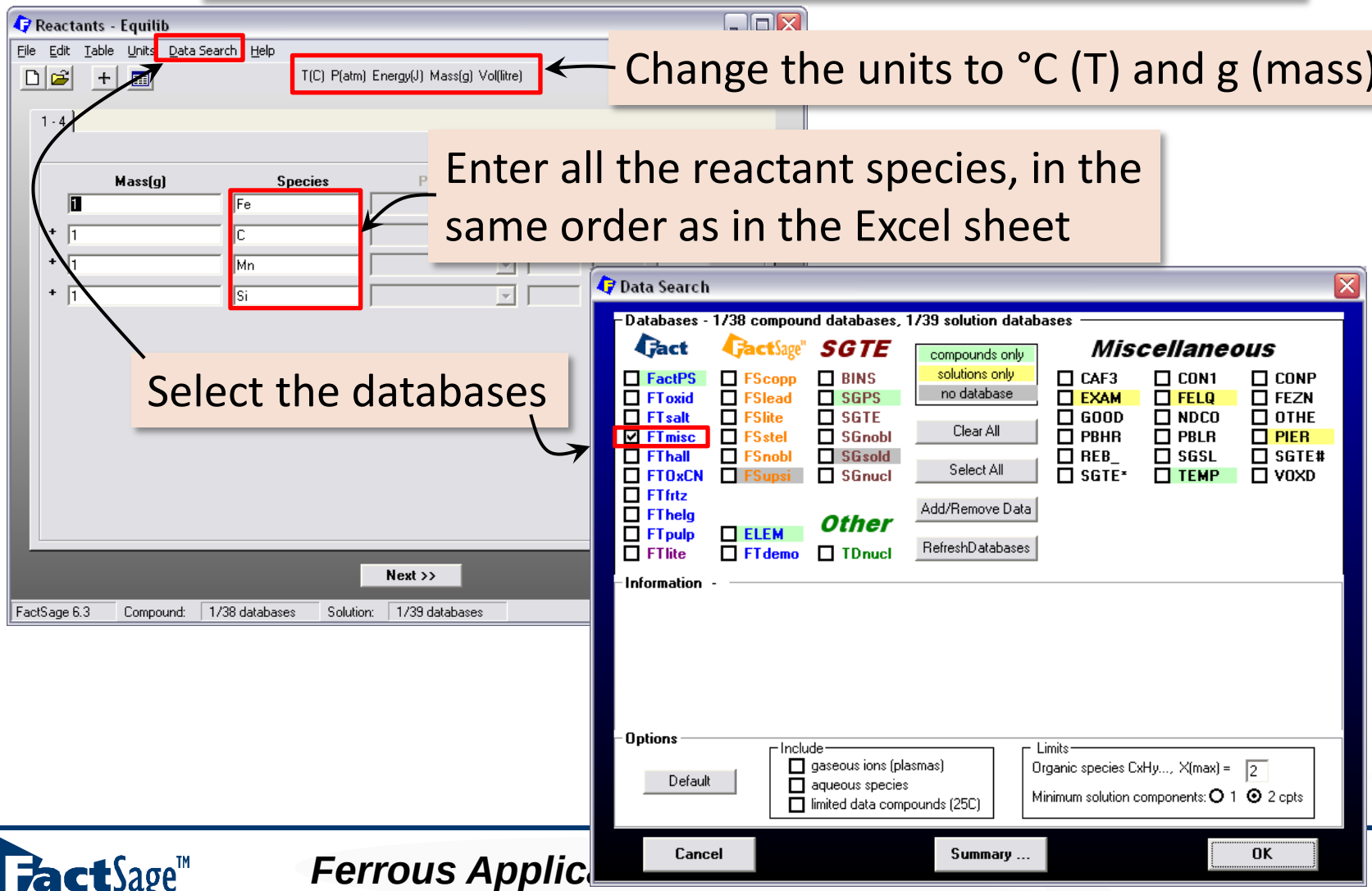
3. Streams initialization

Change Directory to C:\Workshop_BOF\



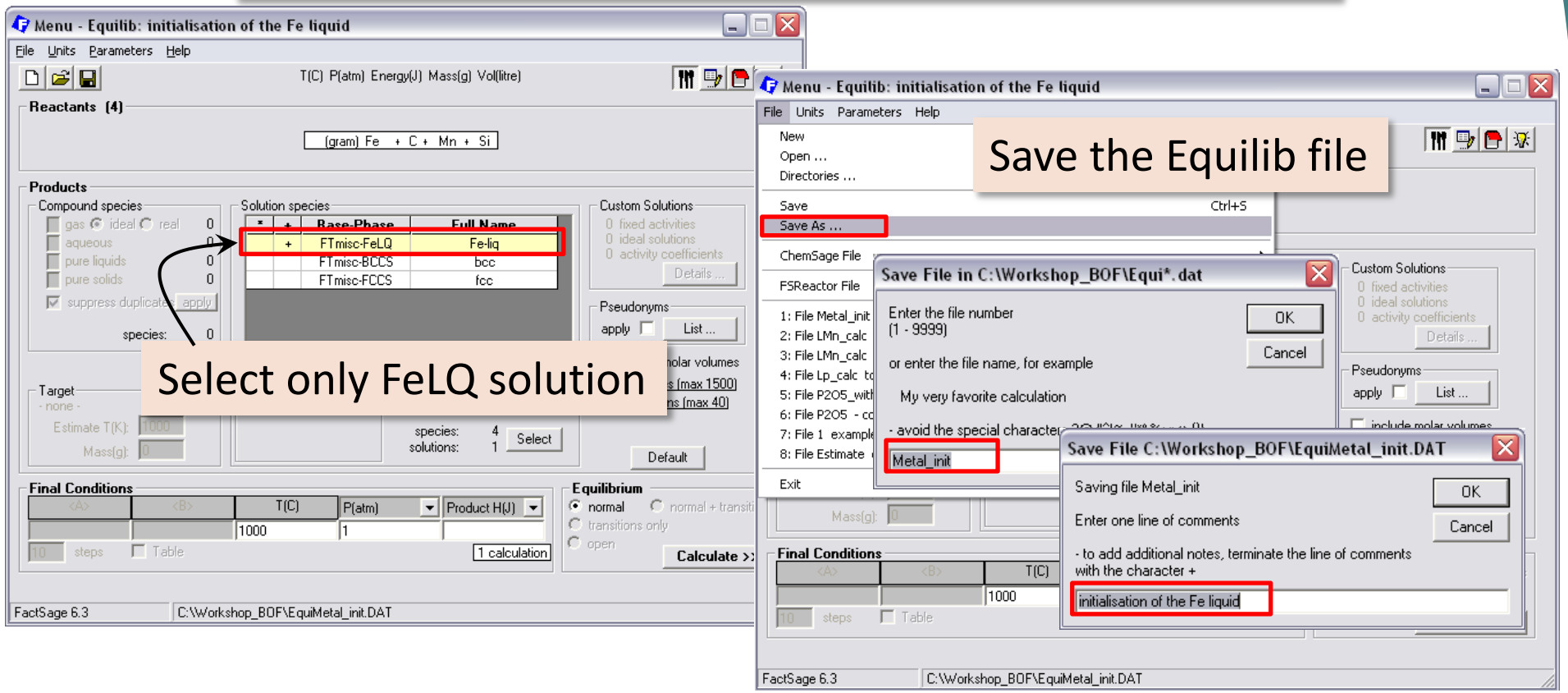
3. Streams initialization – Metal

Initialization of the hot metal – EquiMetal_init.dat



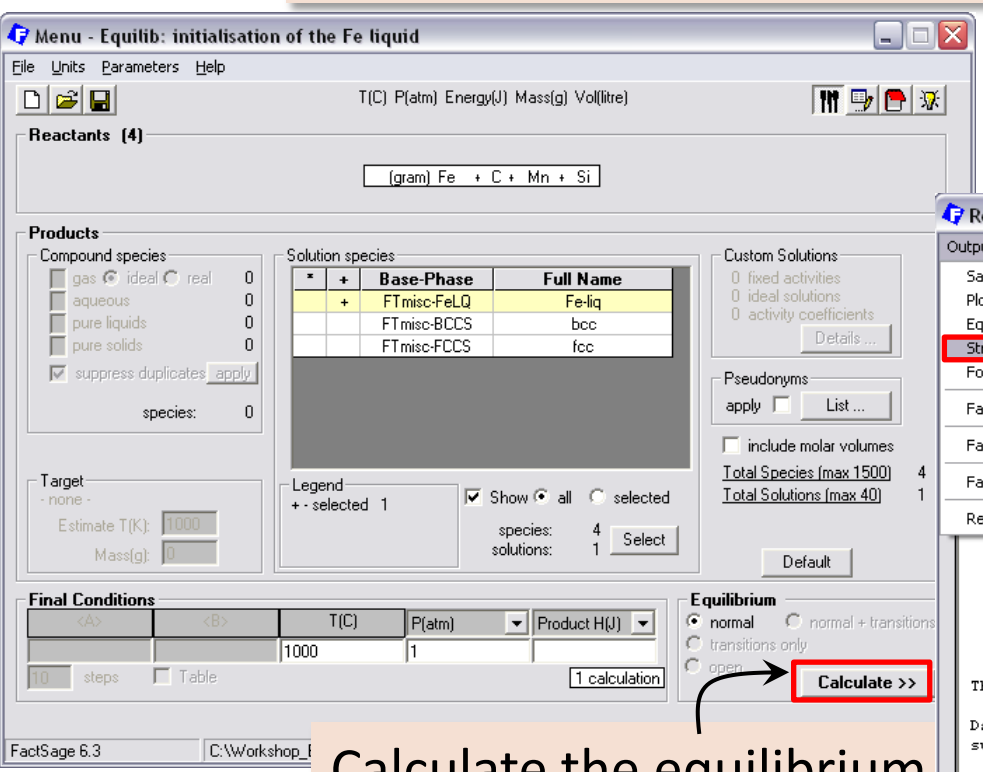
3. Streams initialization – Metal

Initialization of the hot metal – EquiMetal_init.dat



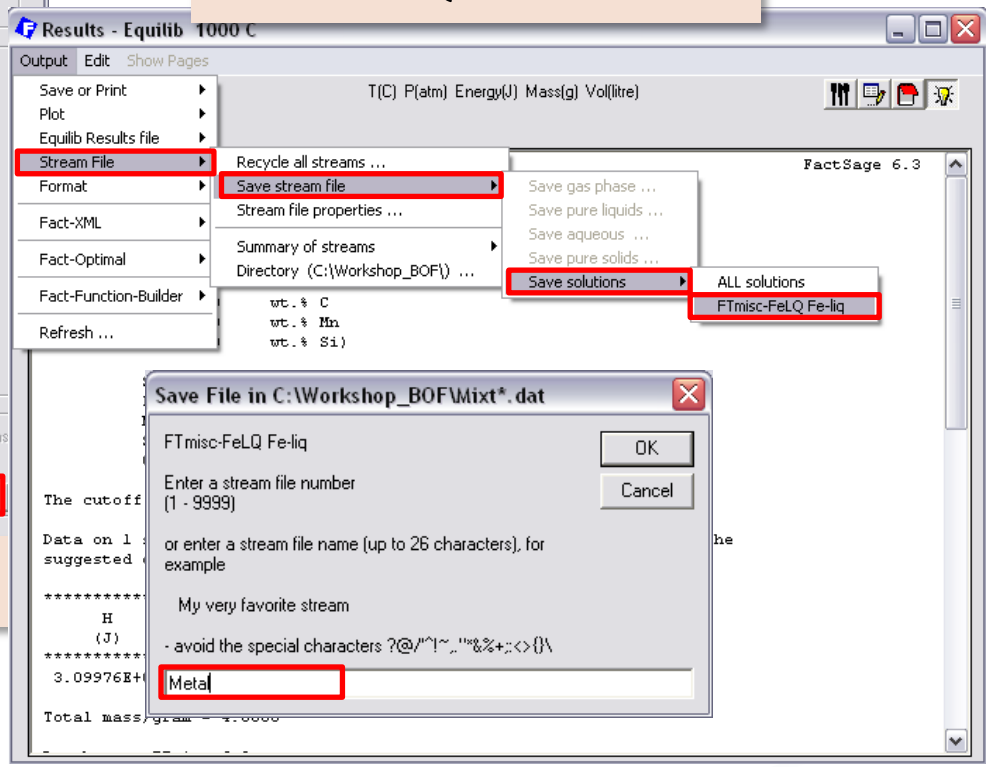
3. Streams initialization – Metal

Initialization of the hot metal – EquiMetal_init.dat



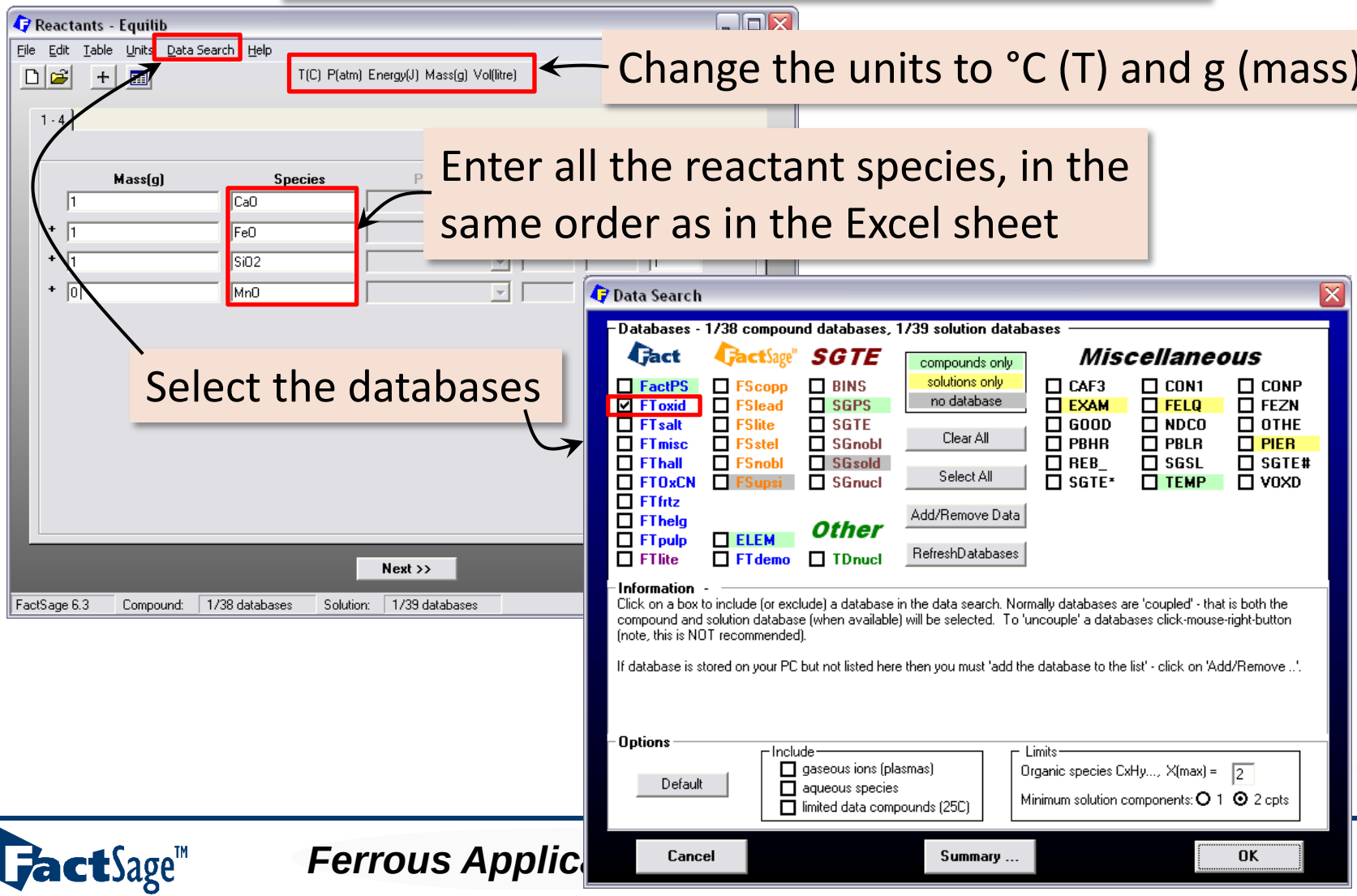
Calculate the equilibrium

Save FeLQ as a stream



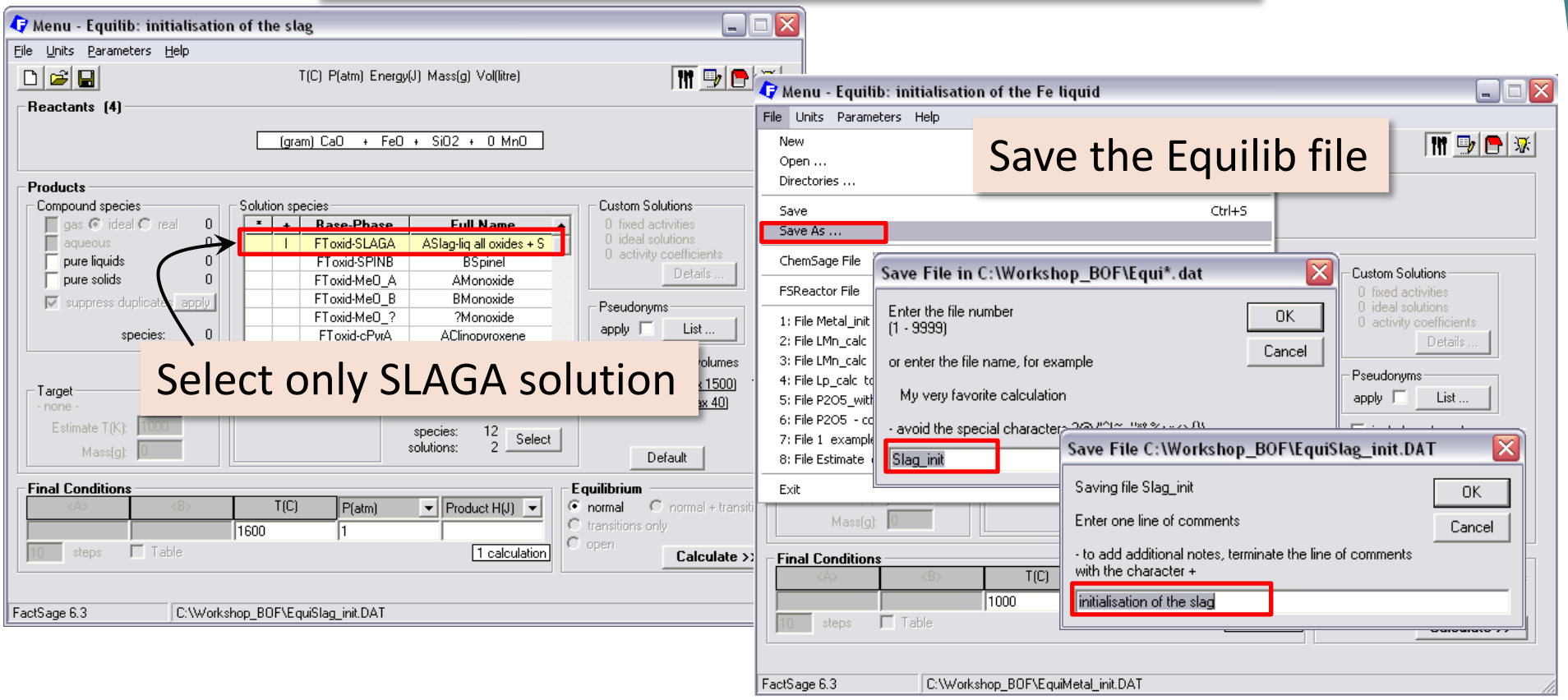
3. Streams initialization – Slag

Initialization of the slag – EquiSlag_init.dat



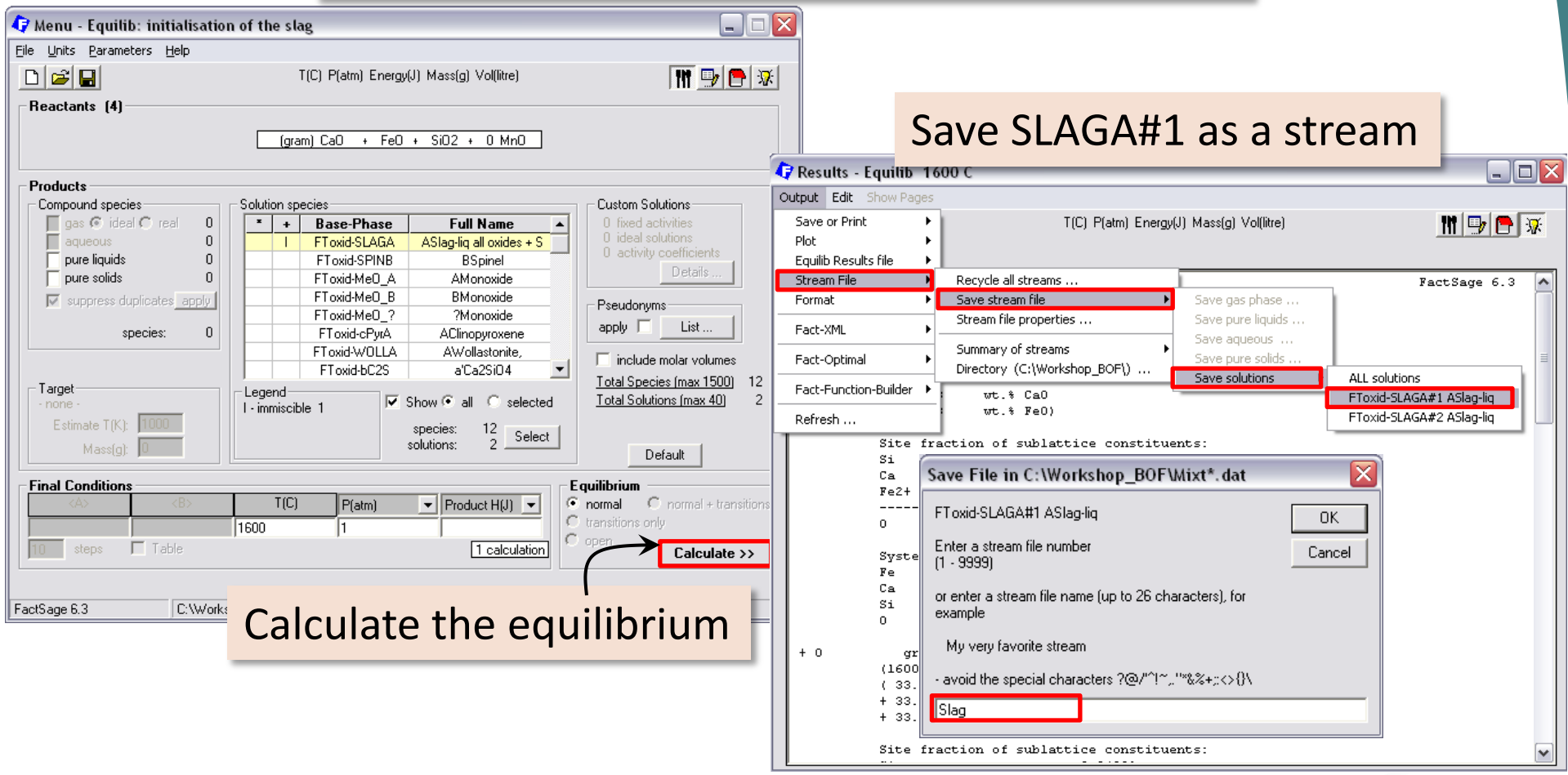
3. Streams initialization – Slag

Initialization of the slag – EquiSlag_init.dat



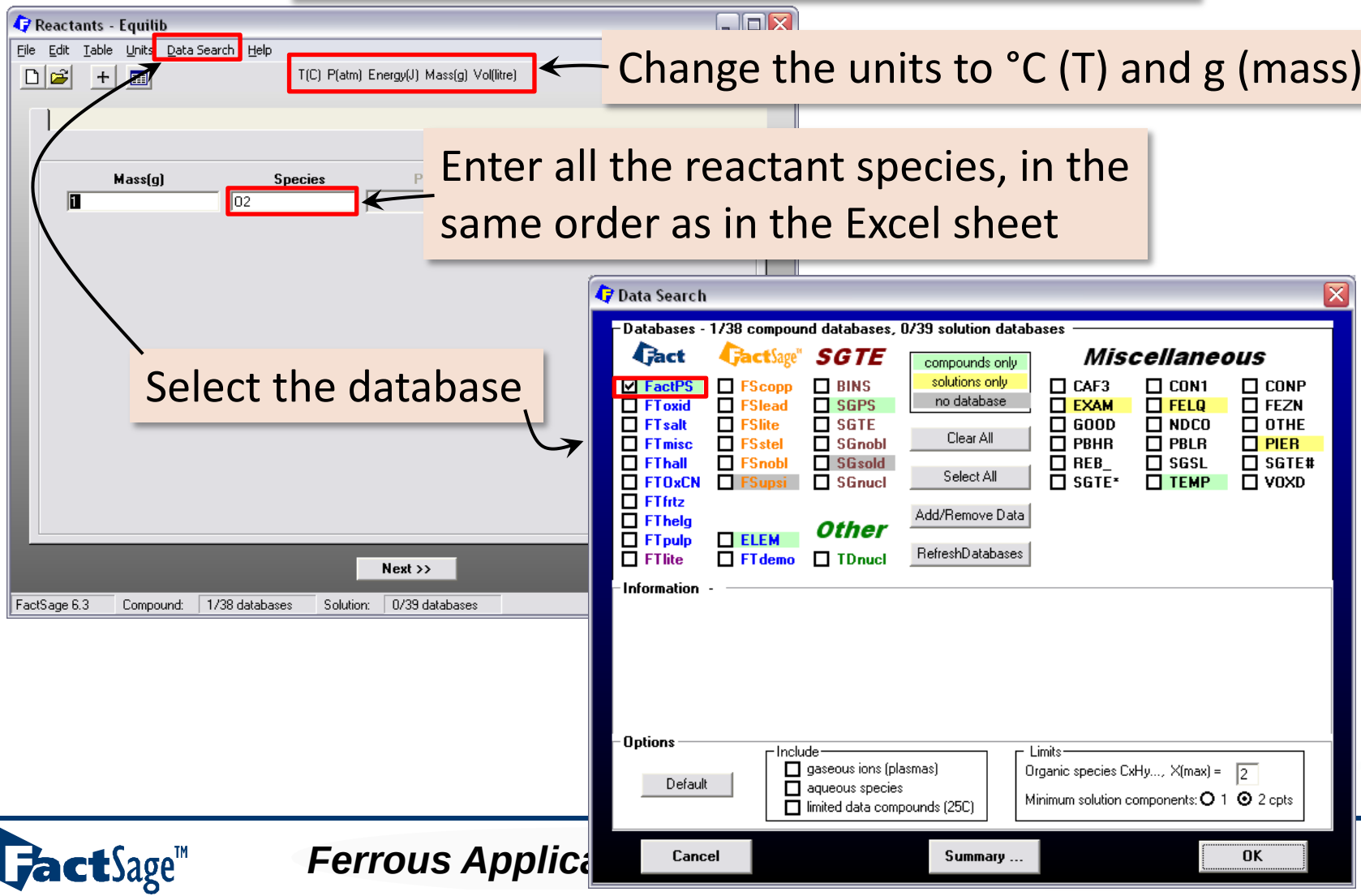
3. Streams initialization – Slag

Initialization of the slag – EquiSlag_init.dat



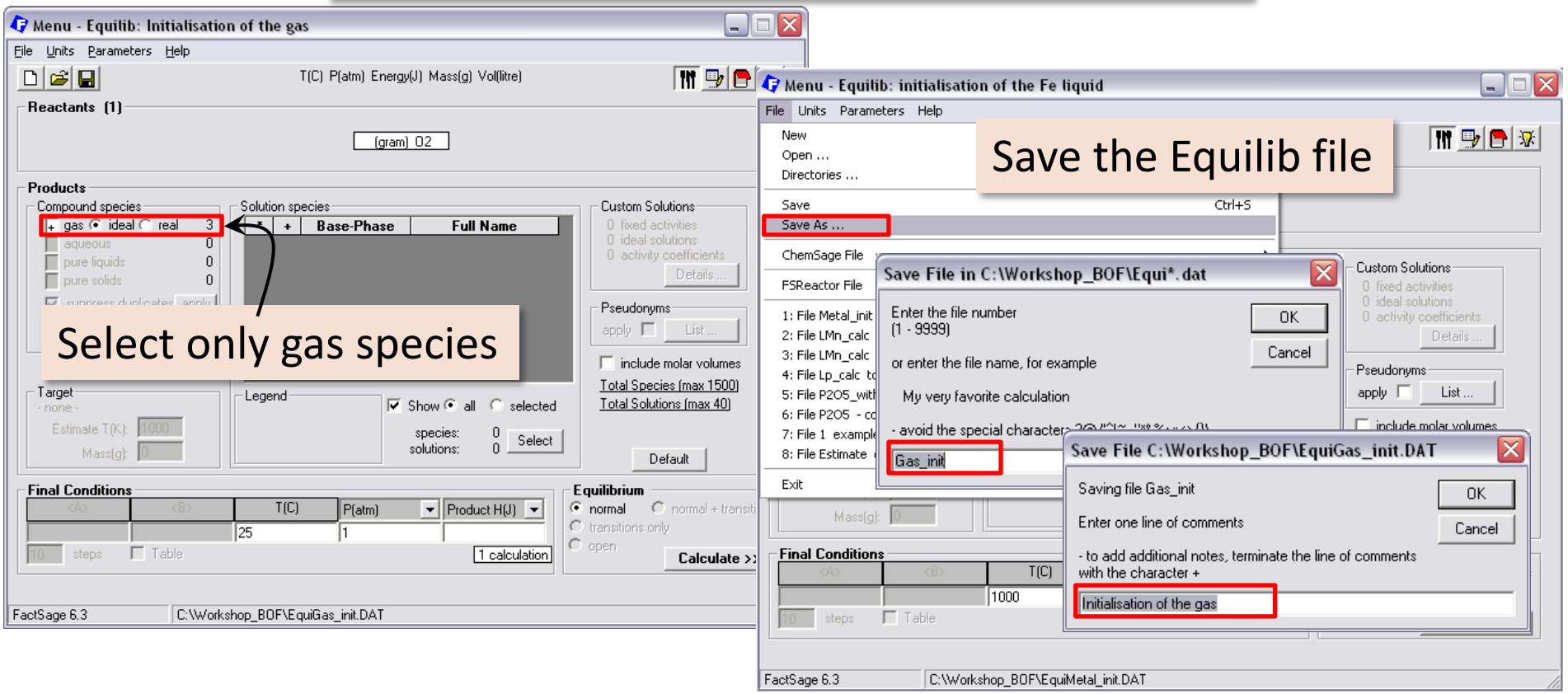
3. Streams initialization – Gas

Initialization of the gas – EquiGas_init.dat



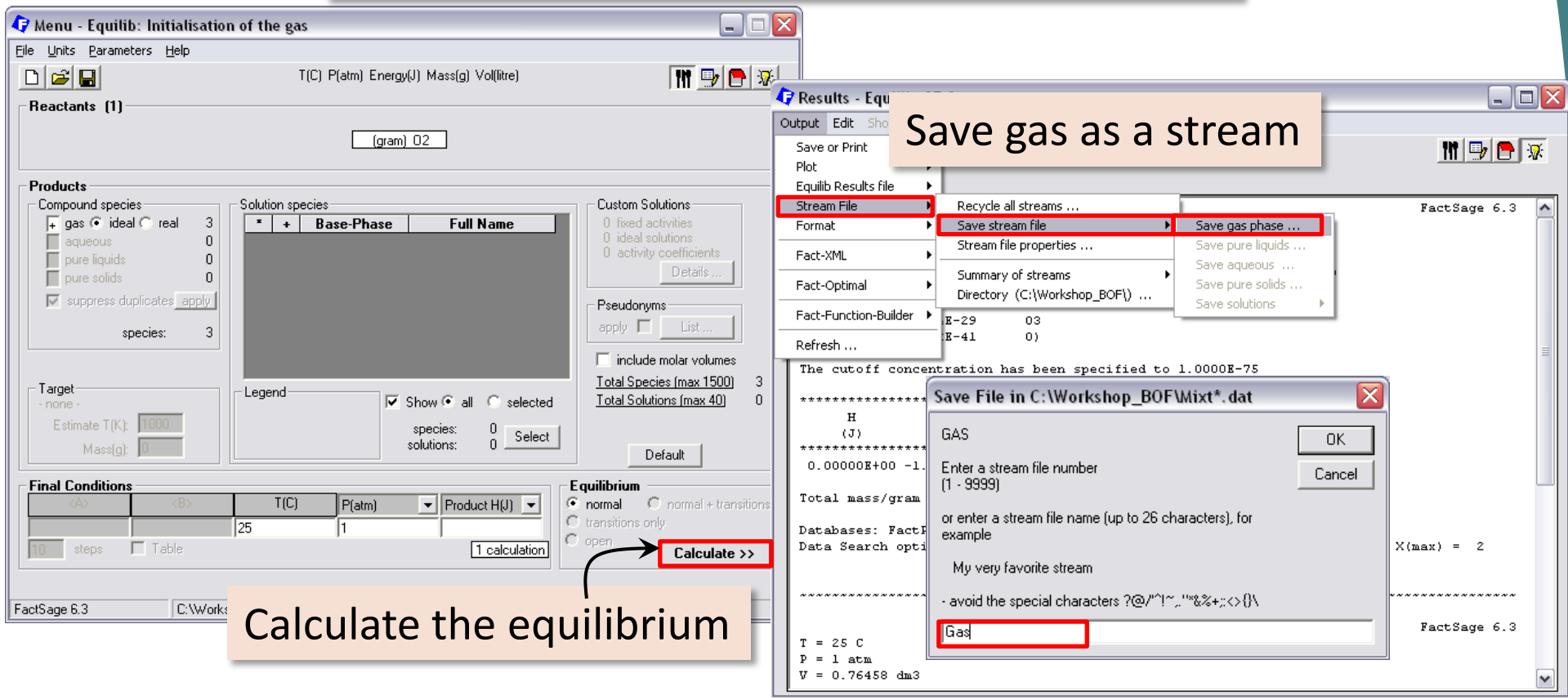
3. Streams initialization – Gas

Initialization of the gas – EquiGas_init.dat



3. Streams initialization – Gas

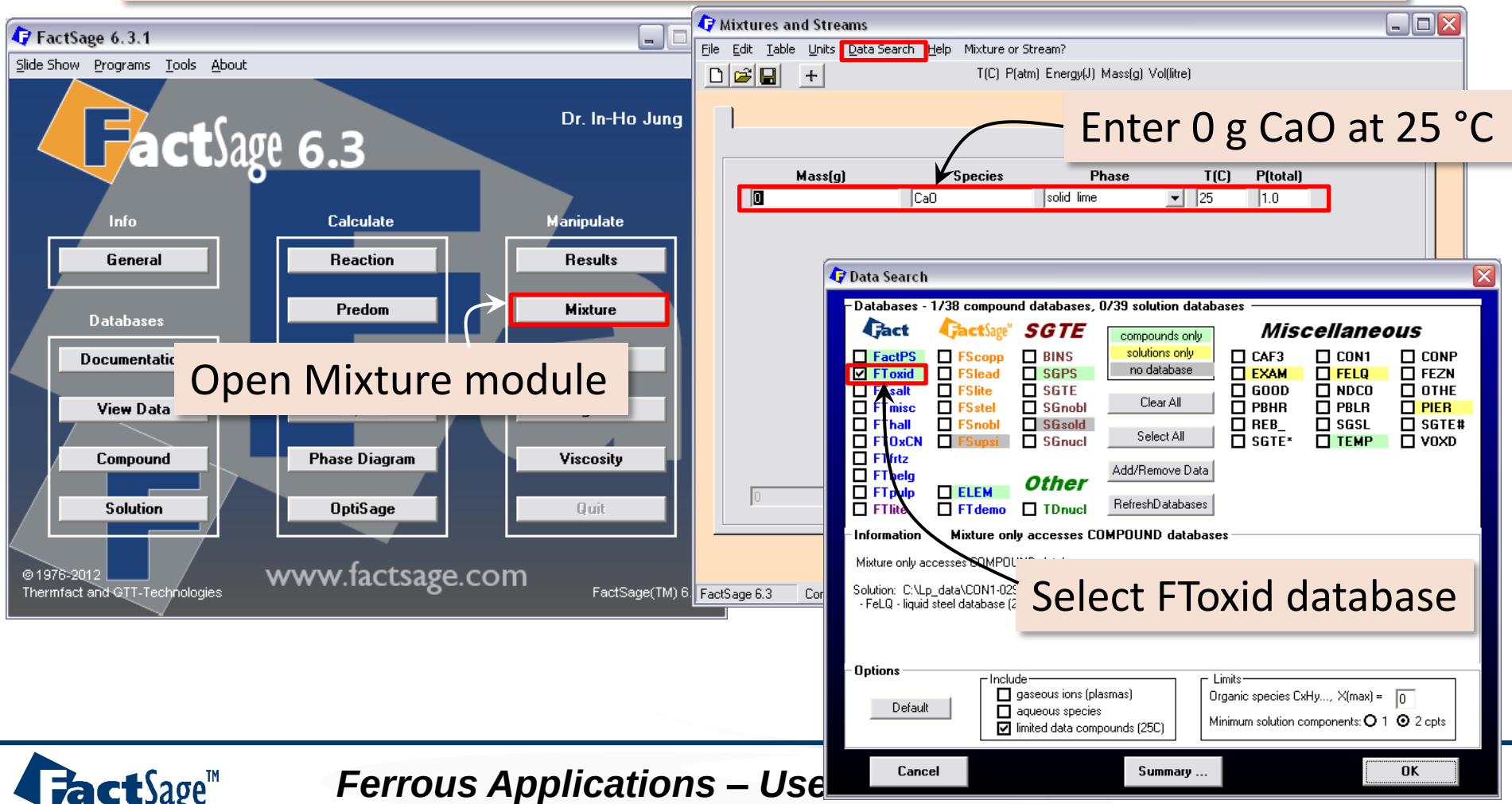
Initialization of the gas – EquiGas_init.dat



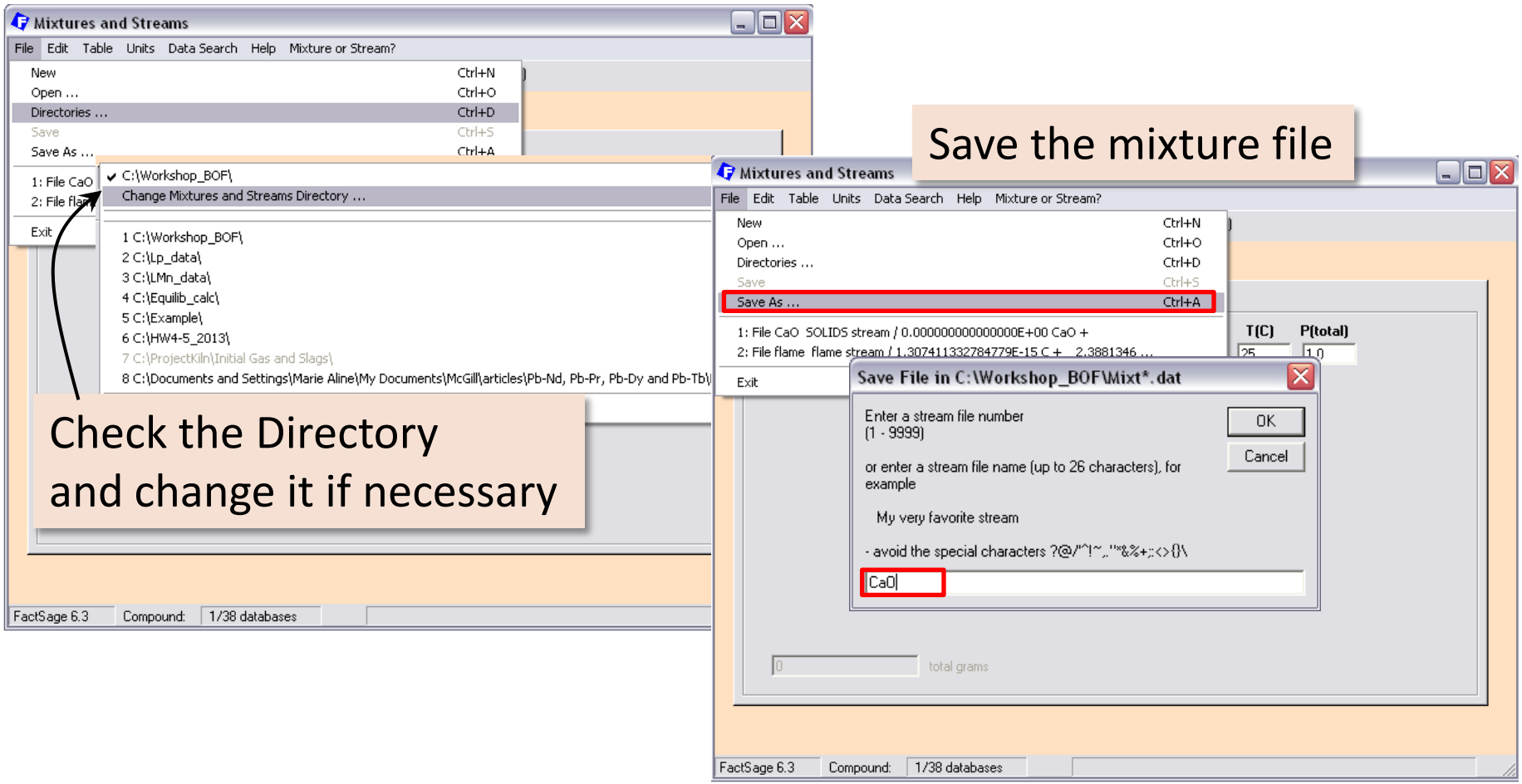
3. Streams initialization – Flux

Equilib calculation cannot be done with reactant amount = 0

⇒ Create the mixture manually



3. Streams initialization – Flux



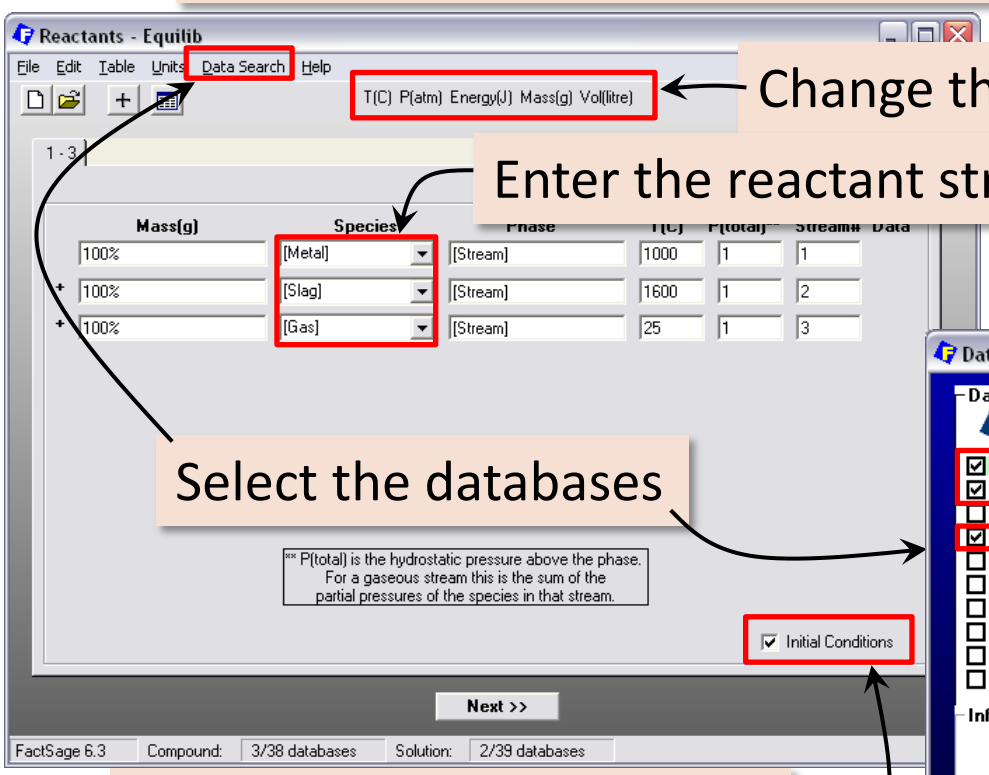
3. Streams initialization – macro

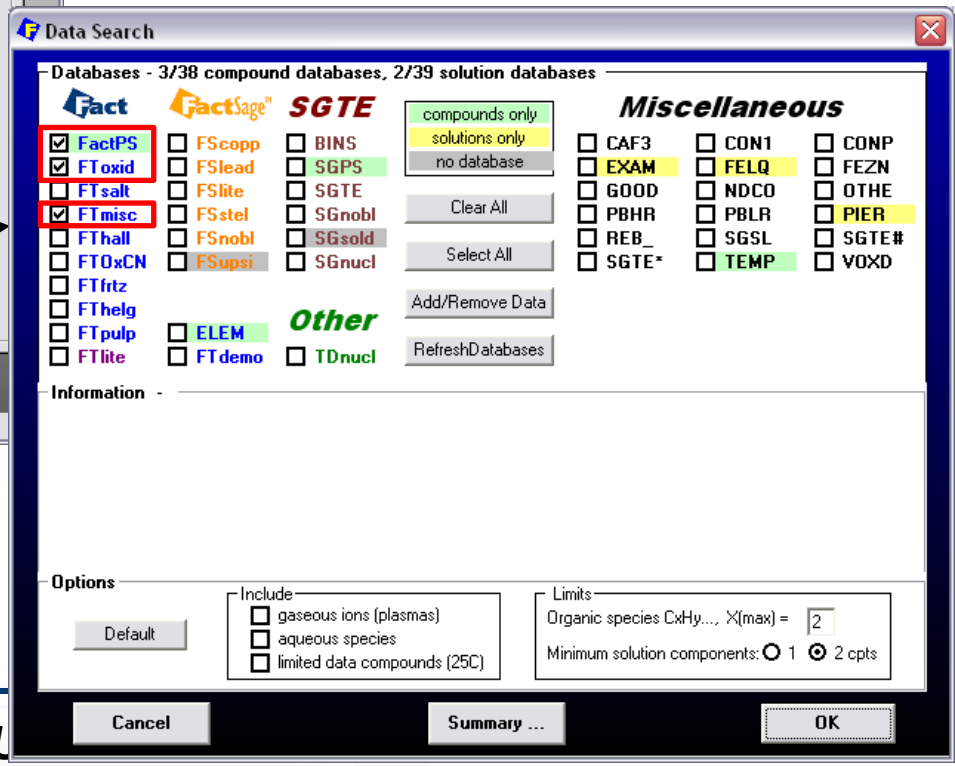
```
1  HIDE                                          // Hide the equilib window
2
3  // Declaration of variables:
4  VARIABLE %MyDir. %temperature
5
6  %Mydir. = C:\Workshop_BOF\                    // path definition
7
8  OLE1 %Mydir.BOF_inoutput.xls Sheet1           // creation of OLE link
9
10 // ****************************** Initialisation ******************************
11
12 OPEN %MyDir.EquiMetal_init.dat                // open the equilib file
13 %3 = 3                                        // position of the column to read
14 %1 = 1 TO 4                                   // loop on the equilib reactants
15     %2 OLE1 READ R3C%3                        // read and store reactant amounts
16     SET REACTANT %1 MASS %2                   // overwrite the reactant amounts
17     %3 STEP                                   // move to the next column
18 %1 LOOP                                       // end of loop
19 %temperature OLE1 READ H2                     // reading and storing Metal temperature
20 SET FINAL T %temperature                      // overwrite the temperature in Equilib
21 CALC                                          // calculate the equilibrium
22 SAVE %MyDir.MixtMetal.dat FTmisc-FeLQ         // save FeLQ as a stream
23
24 OPEN %MyDir.EquiSlag_init.dat                 // open the equilib file
25 %3 = 3
26 %1 = 1 TO 3                                   // loop on the equilib reactants
27     %2 OLE1 READ R6C%3                        // read and store reactant amounts
28     SET REACTANT %1 MASS %2                   // overwrite the reactant amounts
29     %3 STEP                                   // move to the next column
30 %1 LOOP                                       // end of loop
31 %temperature OLE1 READ H5                     // reading and storing slag temperature
32 SET FINAL T %temperature                      // overwrite the temperature in Equilib
33 CALC                                          // calculate the equilibrium
34 SAVE %MyDir.MixtSlag.dat FToxid-SLAGA#1       // save SLAGA#1 as a stream
35
36 OPEN %MyDir.EquiGas_init.dat                  // open the equilib file
37 %1 OLE1 READ C9                               // read and store reactant amounts
38 SET REACTANT 1 MASS %1                        // overwrite the reactant amounts
39 %temperature OLE1 READ H8                     // reading and storing gas temperature
40 SET FINAL T %temperature                      // overwrite the temperature in Equilib
41 CALC                                          // calculate the equilibrium
42 SAVE %MyDir.MixtGas.dat GAS                   // save GAS as a stream
43
44 END                                           // end of macro
```

FactSage™

4. Equilib file for R1

Reaction between hot metal, slag and gas – EquiR1.dat

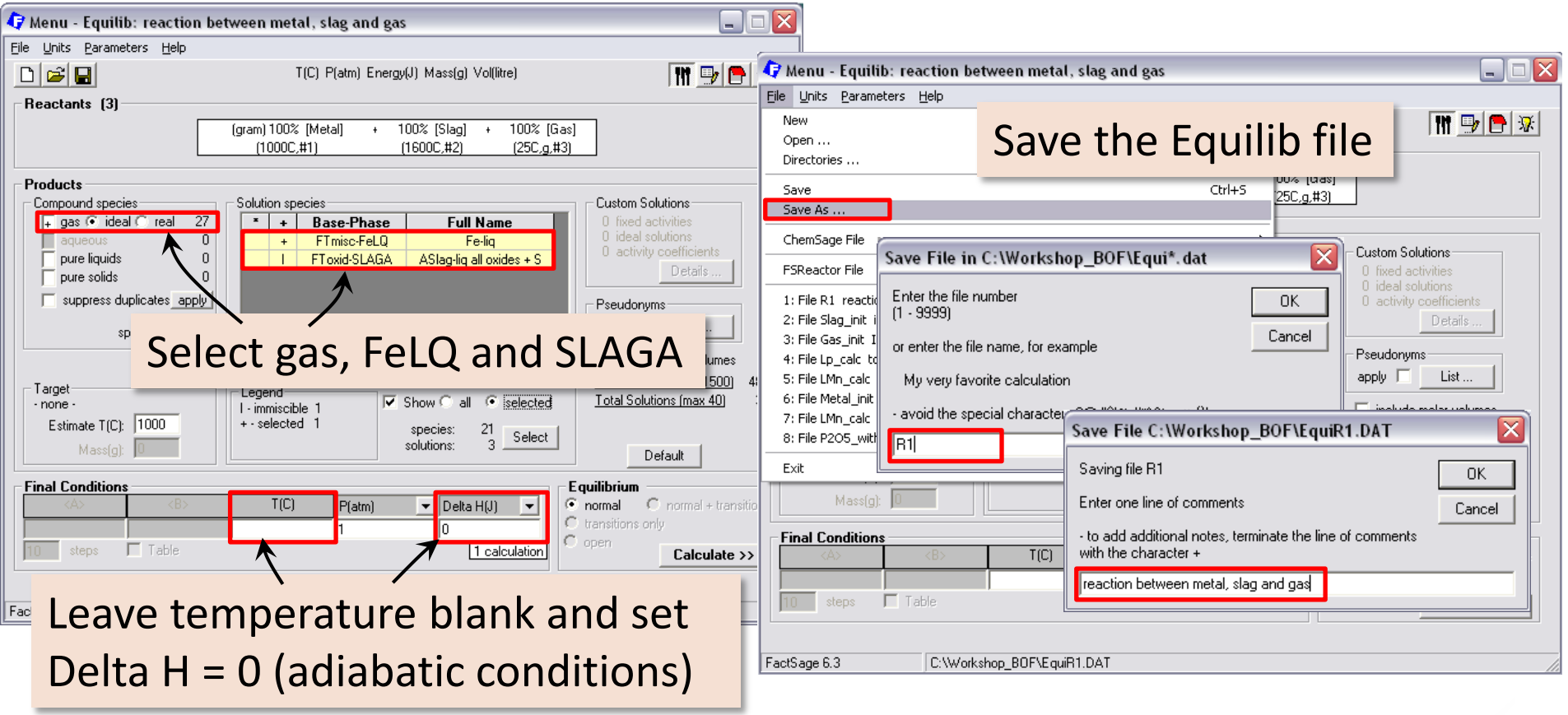




Select initial conditions for adiabatic calculations

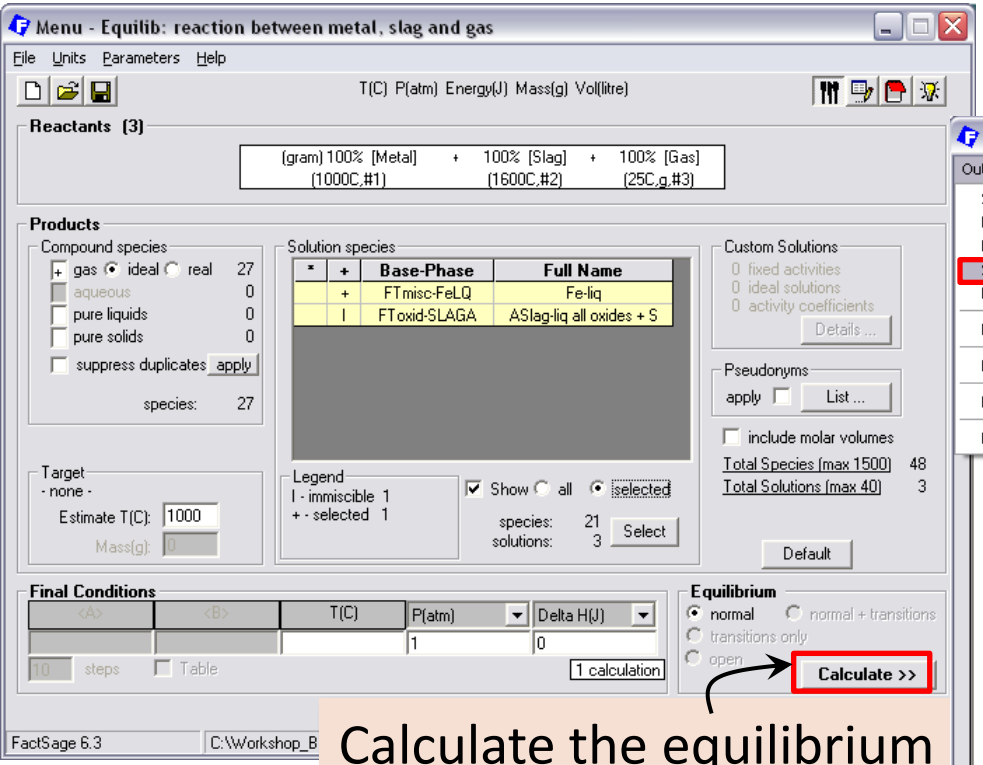
4. Equilib file for R1

Reaction between hot metal, slag and gas – EquiR1.dat



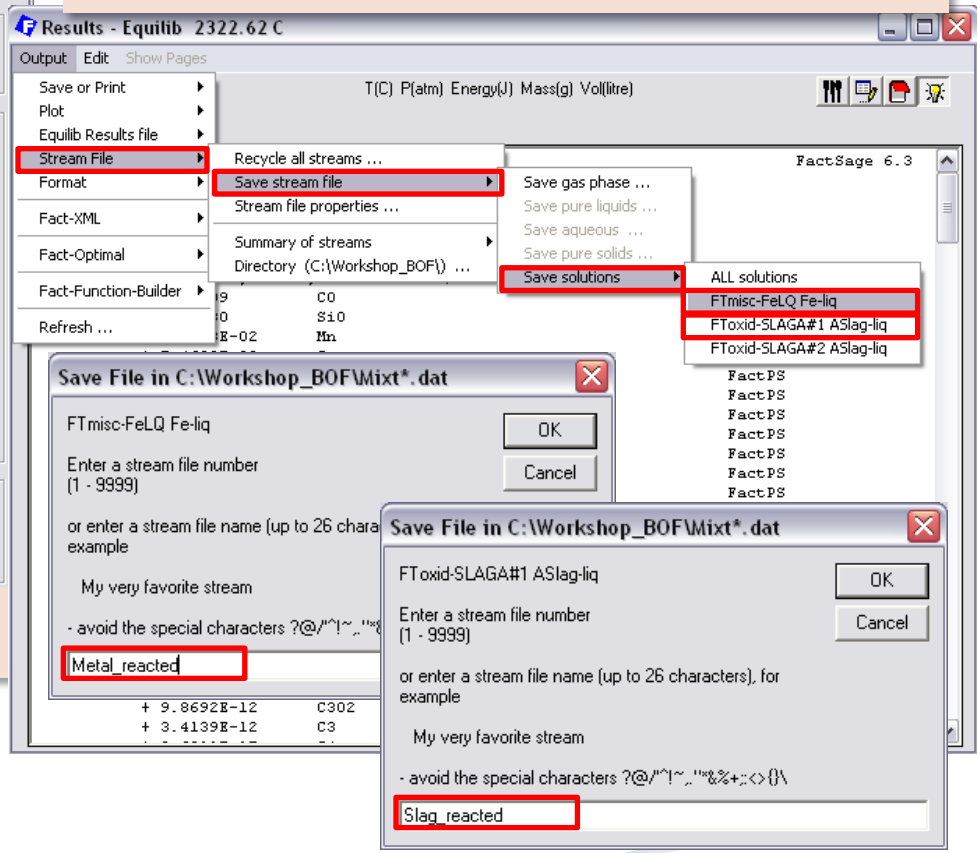
4. Equilib file for R1

Reaction between hot metal, slag and gas – EquiR1.dat



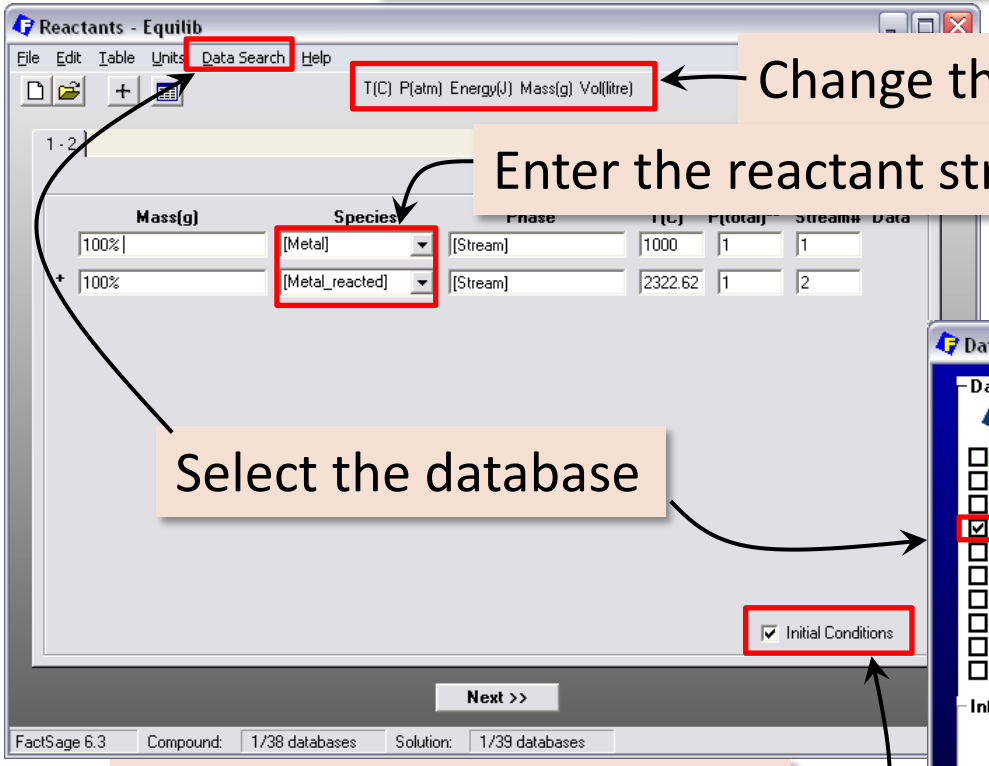
Calculate the equilibrium

Save FeLQ and SLAGA#1 as streams



4. Equilib file for R2

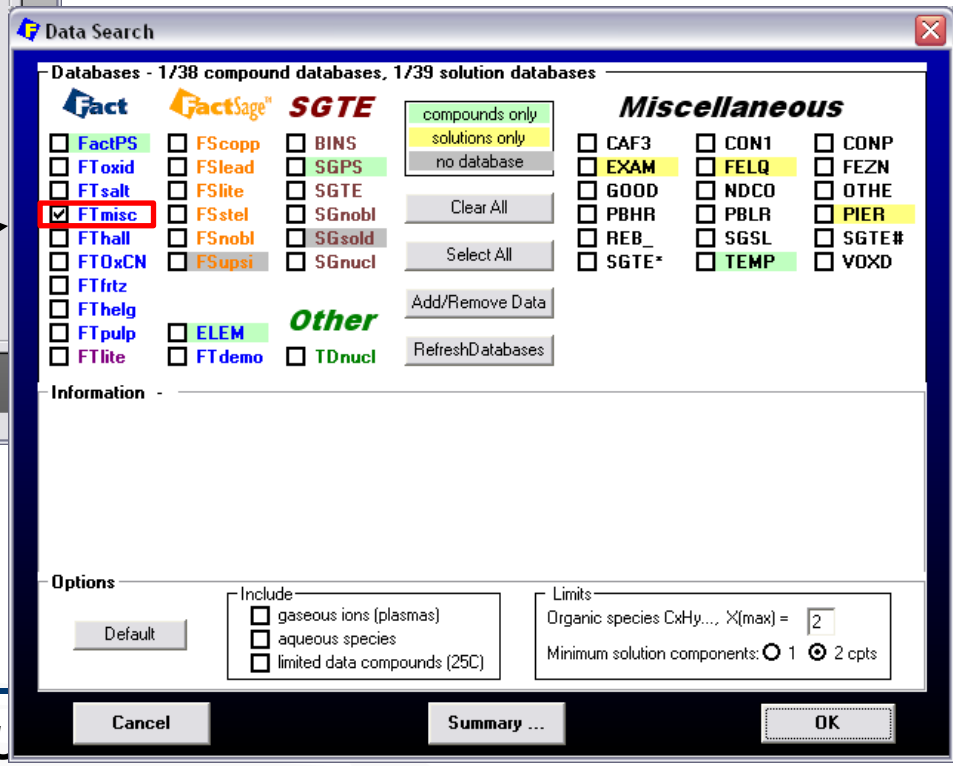
Homogenization in metal – EquiR2.dat



Change the units to °C (T) and g (mass)

Enter the reactant streams for R2

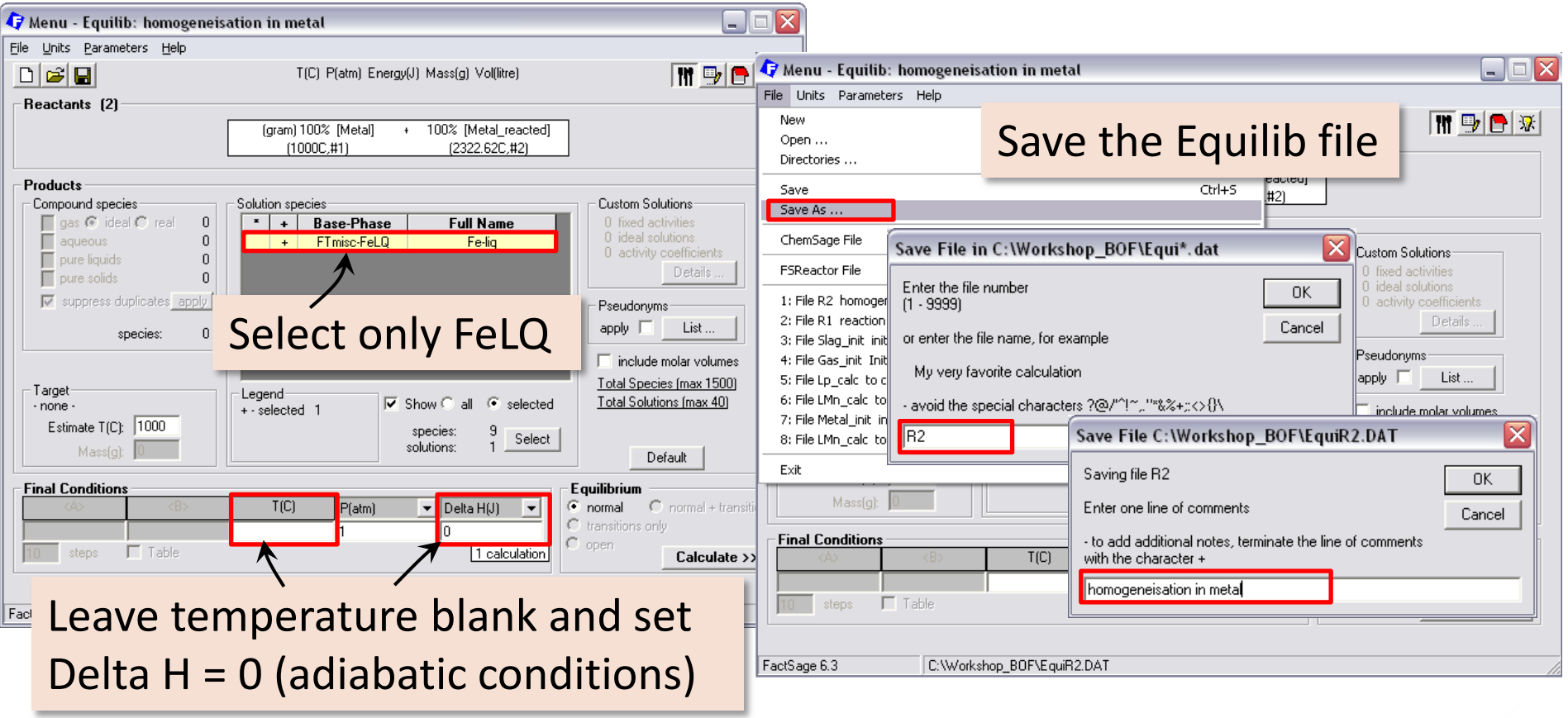
Select the database



Select initial conditions for adiabatic calculations

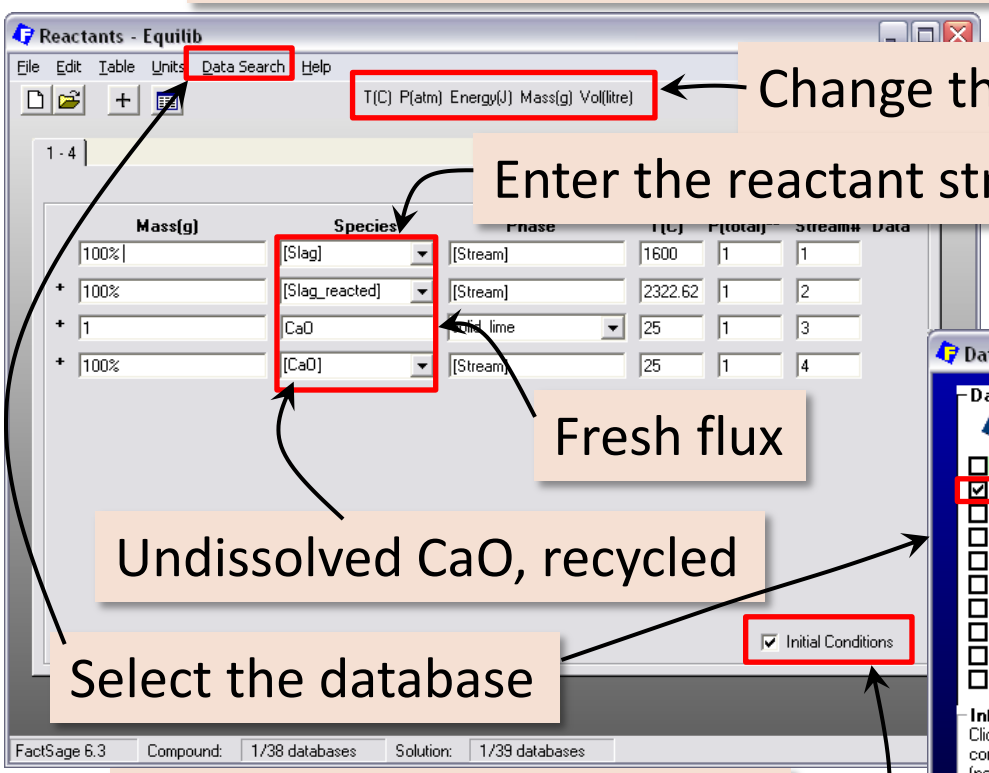
4. Equilib file for R2

Homogenization in metal – EquiR2.dat



4. Equilib file for R3

Homogenization in slag and flux addition – EquiR3.dat



Change the units to °C (T) and g (mass)

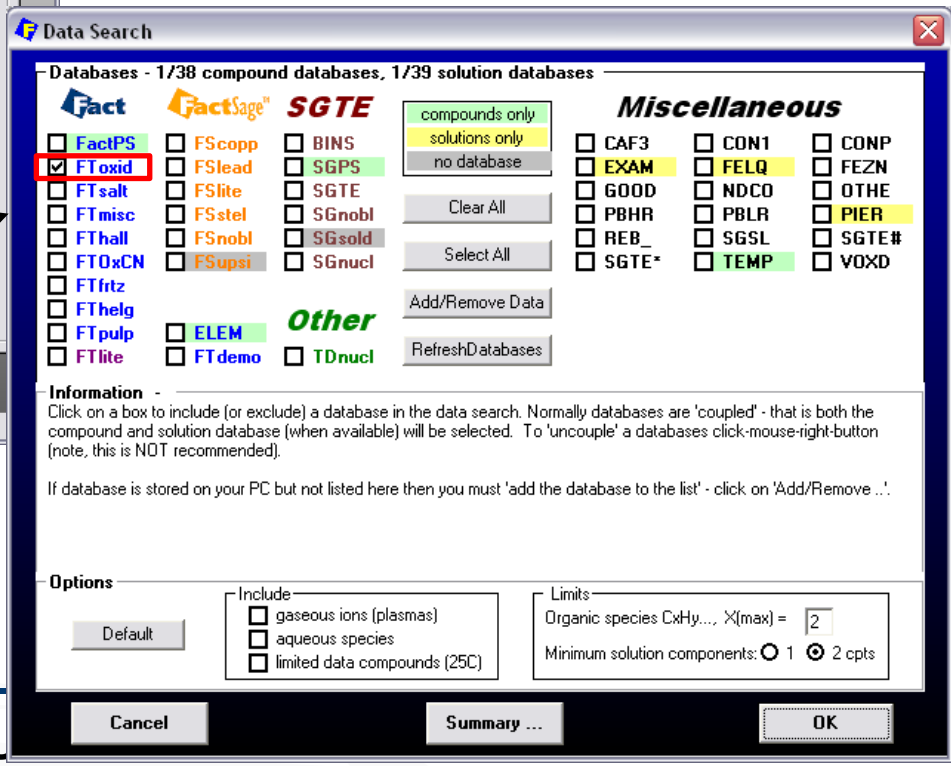
Enter the reactant streams for R3

Fresh flux

Undissolved CaO, recycled

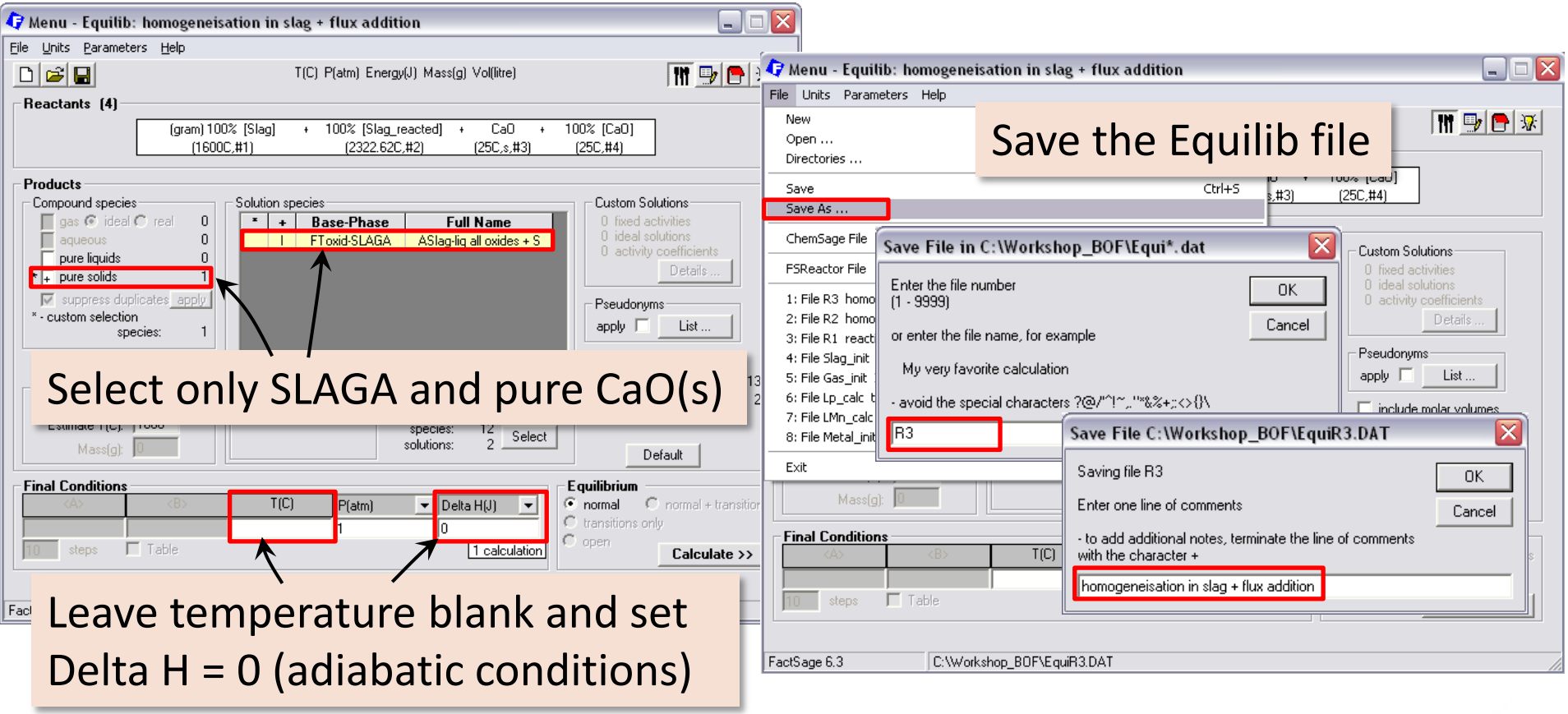
Select the database

Select initial conditions for adiabatic calculations



4. Equilib file for R3

Homogenization in slag and flux addition – EquiR3.dat



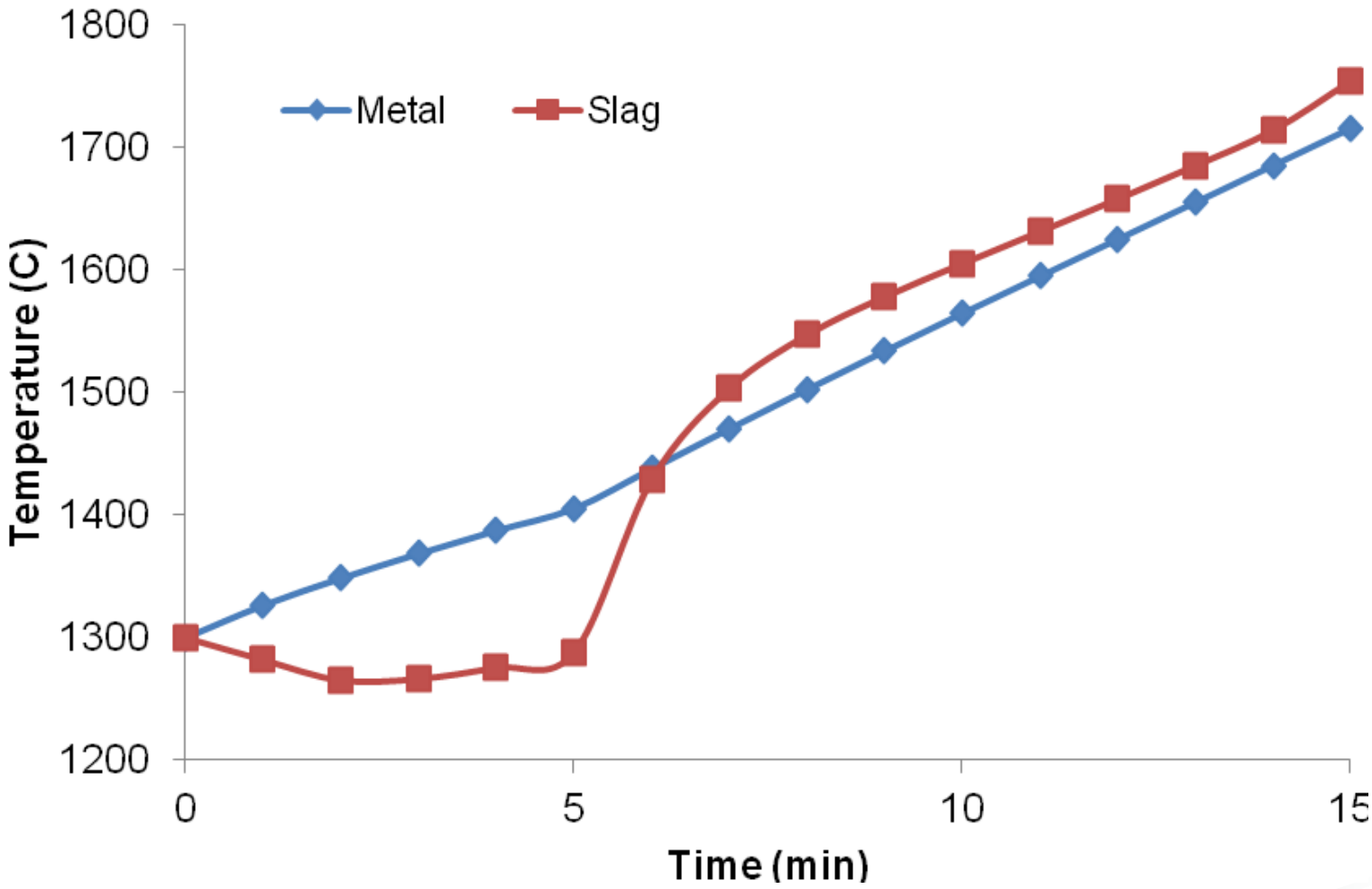
4. Main reactions – macro

```
// ****************************** START OF PROCESS ******************************
VARIABLE %tempflux %time %pos                    // variable declaration for main reactions
%tempflux OLE1 READ H10                          // read and store flux temperature
%pos = 15                                        // first row to read input data

%time = 1 TO 15                                  // loop over the 15 calculations
    OPEN %MyDir.EquiR1.dat                       // open the equilib file
    %1 OLE1 READ R%posC3                         // read the kinetic factor in excel
    SET REACTANT 1 MASS %1                       // overwrite the reactant amounts
    %1 OLE1 READ R%posC7                         // read the kinetic factor in excel
    SET REACTANT 2 MASS %1                       // overwrite the reactant amounts
    %1 OLE1 READ R%posC5                         // read the kinetic factor in excel
    SET REACTANT 3 MASS %1                       // overwrite the reactant amounts
    CALC                                         // calculate the equilibrium
    SAVE %MyDir.MixtMetal_reacted.DAT FTmisc-FeLQ       // save FeLQ as a stream
    SAVE %MyDir.MixtSlag_reacted.DAT FToxid-SLAGA#1     // save SLAGA#1 as a stream

    OPEN %MyDir.EquiR2.dat                       // open the equilib file
    %1 OLE1 READ R%posC4                         // read the kinetic factor in excel
    SET REACTANT 1 MASS %1                       // overwrite the reactant amounts
    CALC                                         // calculate the equilibrium
    SAVE %MyDir.MixtMetal.dat FTmisc-FeLQ        // save FeLQ as a stream

    OPEN %MyDir.EquiR3.dat                       // open the equilib file
    %1 OLE1 READ R%posC8                         // read the kinetic factor in excel
    SET REACTANT 1 MASS %1                       // overwrite the reactant amounts
    %1 OLE1 READ R%posC2                         // read the kinetic factor in excel
    SET REACTANT 3 MASS %1                       // overwrite the reactant amounts
    SET REACTANT 3 T %tempflux                   // overwrite the reactant temperature (flux)
    IF %time = 1 THEN                            // if first calculation,
        SET REACTANT 4 MASS 0                    // force the recycled CaO stream to be 0
    ENDIF                                        // end of if
    CALC                                         // calculate the equilibrium
    SAVE %MyDir.MixtSlag.dat FToxid-SLAGA#1      // save SLAGA#1 as a stream
    SAVE %MyDir.MixtCaO.dat SOLIDS               // save SOLIDS as a stream
    %pos STEP                                    // move to the next row to read inputs
%time LOOP                                       // end of loop

END                                              // end of macro
```

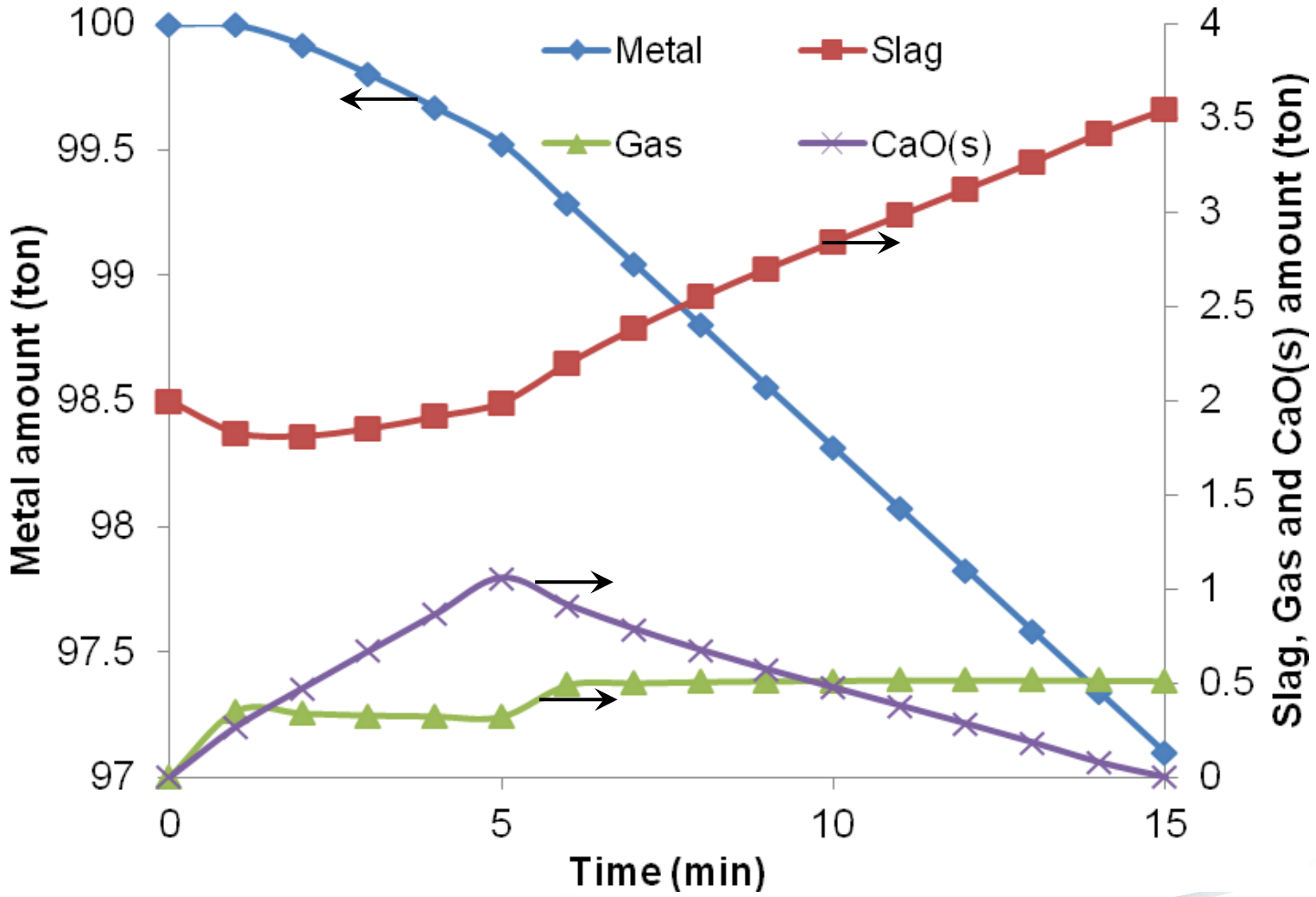
5. Organise the outputs in Excel

- 1 Excel sheet to print out the calculation results for the metal, slag and gas phases after homogenization (R2 and R3)
- Print out for each min (0 to 15 min):
  - Metal temperature, mass of Si, C and Mn in metal, and total mass of metal after homogenization (R2)
  - Amount of gas produced from R1
  - Slag temperature, amount, and mass of each slag species after homogenization (R3)
  - Mass of undissolved CaO(s) after homogenization (R3)

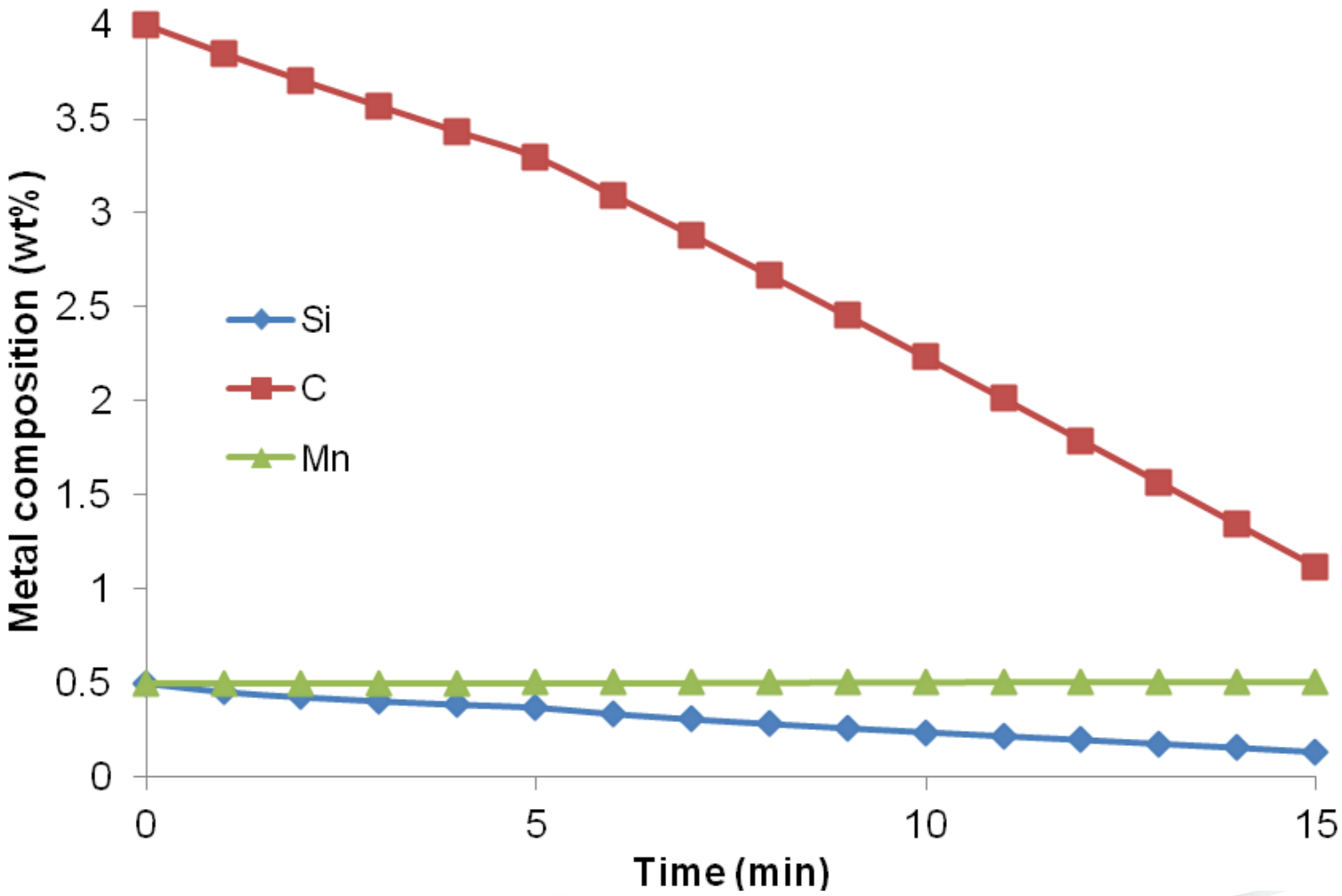
Results – Temperature profile



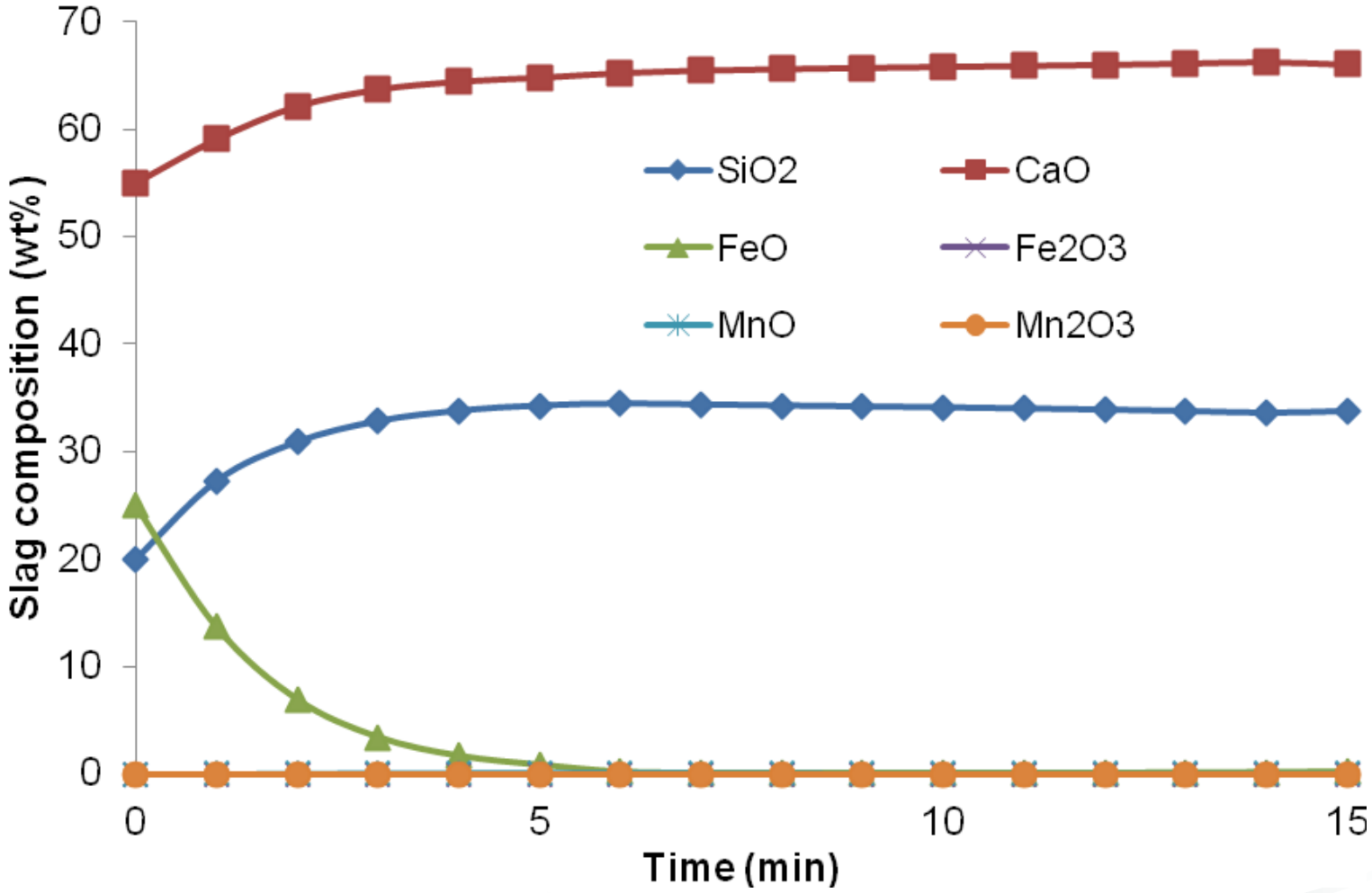
Results – Phases amount



Results – Metal composition



Results – Slag composition

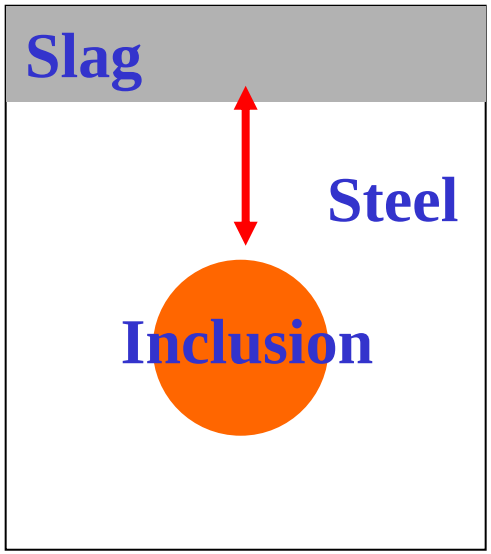


Application III

SLAG/STEEL/INCLUSION INTERACTION

Evolution of inclusion chemistry by indirect interaction with top slag

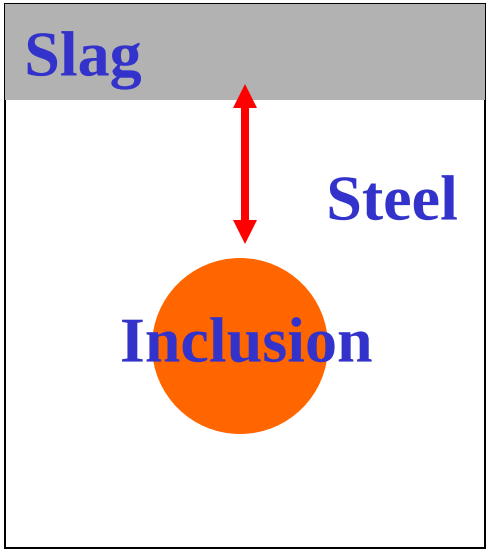
Slag/Steel/Inclusion Reactions

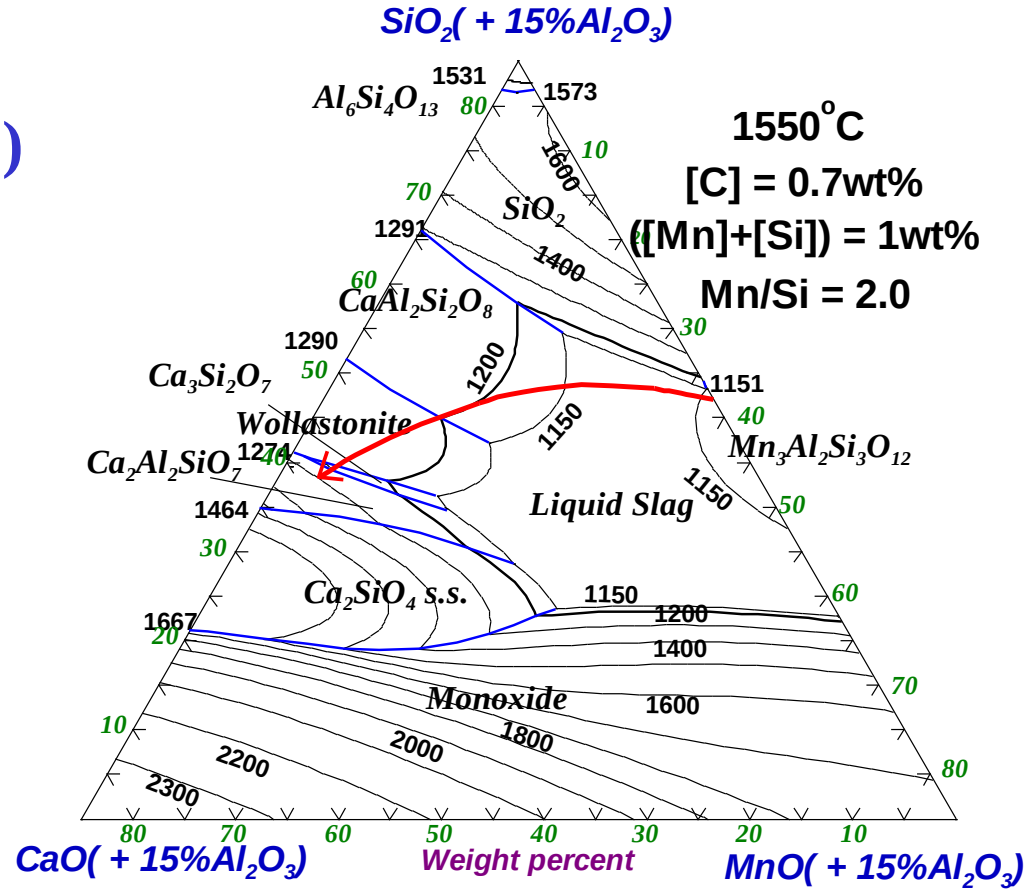


- In FactSage, if we put slag, steel and non-metallic inclusion together and do calculations, it is impossible to distinguish the slag and non-metallic inclusion phase.
- Theoretically, the slag and inclusion compositions should be identical if the entire system is in equilibrium. However, the inclusions typically formed by the deoxidation of molten steel require a time to be completely in equilibrium with molten slag.
- The only option to see the interaction between slag and inclusions is to do two separate calculations, ‘Slag/Steel’ and ‘Steel/Inclusion’, with Steel shared between the calculations. Therefore, the influence of the slag on the inclusion chemistry can be calculated indirectly through the change of the steel chemistry.
- In these calculations, the molten steel after the first equilibration with molten slag should be stored as a mixture (stream) as input for the next equilibration calculation with the inclusions.
- Alternatively, the calculations can be performed using the FactSage macro processing facility.

Modification of inclusion in LF by interaction with top slag

Top-Slag Composition
55CaO-15Al_2O_3–30SiO_2 (wt%)





Slag/Steel/Inclusion Reaction: Macro processing input Excel file

	A	B	C	D	E	F	G	H	I	J
1	Temperature	1600	C							
2	Duration	10	min							
3										
4	Steel amount:	100	kg							
5	Steel composition (wt%)									
6	Fe	Mn	Si	O	Al	Ti	S	Ca	Total	
7	98.9849	0.6	0.4	0.01	0.0001	0	0.005	0	100	
8										
9	Slag amount:	10	kg							
10	Slag composition (wt%)									
11	CaO	MgO	Al2O3	SiO2	FeO	MnO	Total			
12	45	10	15	25	5	0	100			
13										
14										
15										
16										
17										
18	DO NOT ALTER									
19	Fe	Mn	Si	O	Al	Ti	S	Ca	Total	
20	98.9849	0.6	0.4	0.01	0.0001	0	0.005	0	100	
21										
22										
23										
24	CaO	MgO	Al2O3	SiO2	FeO	MnO	Total			
25	4.5	1	1.5	2.5	0.5	0	10			

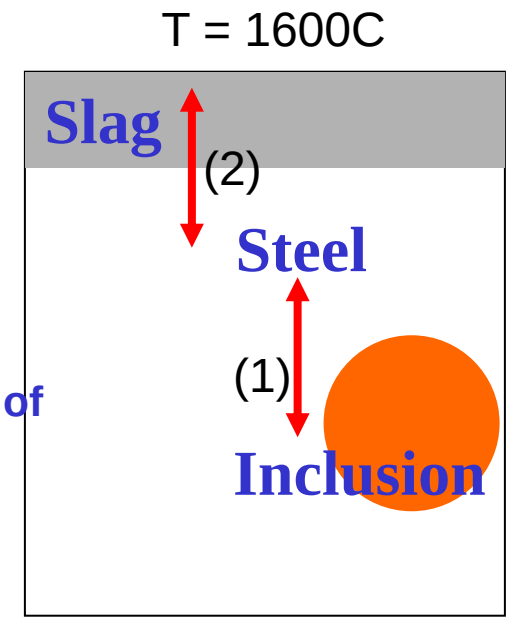
Sheet1 Sheet2 Sheet3

Ready

System temperature

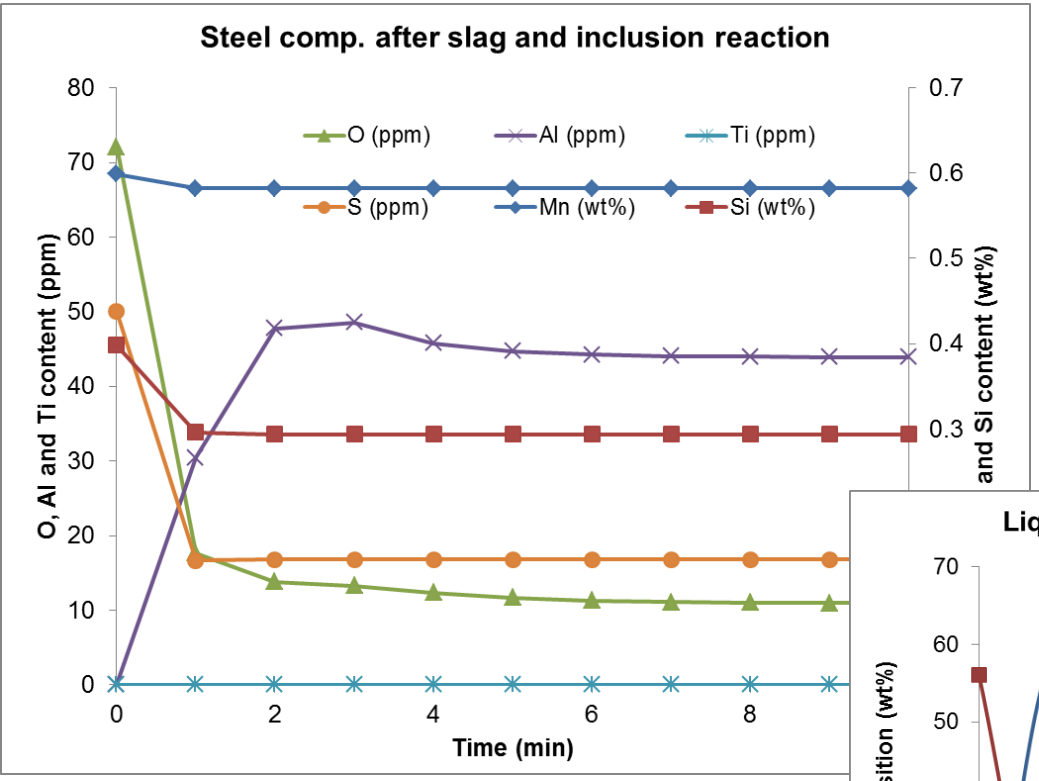
10 times iterations for (1) and (2) rxns.

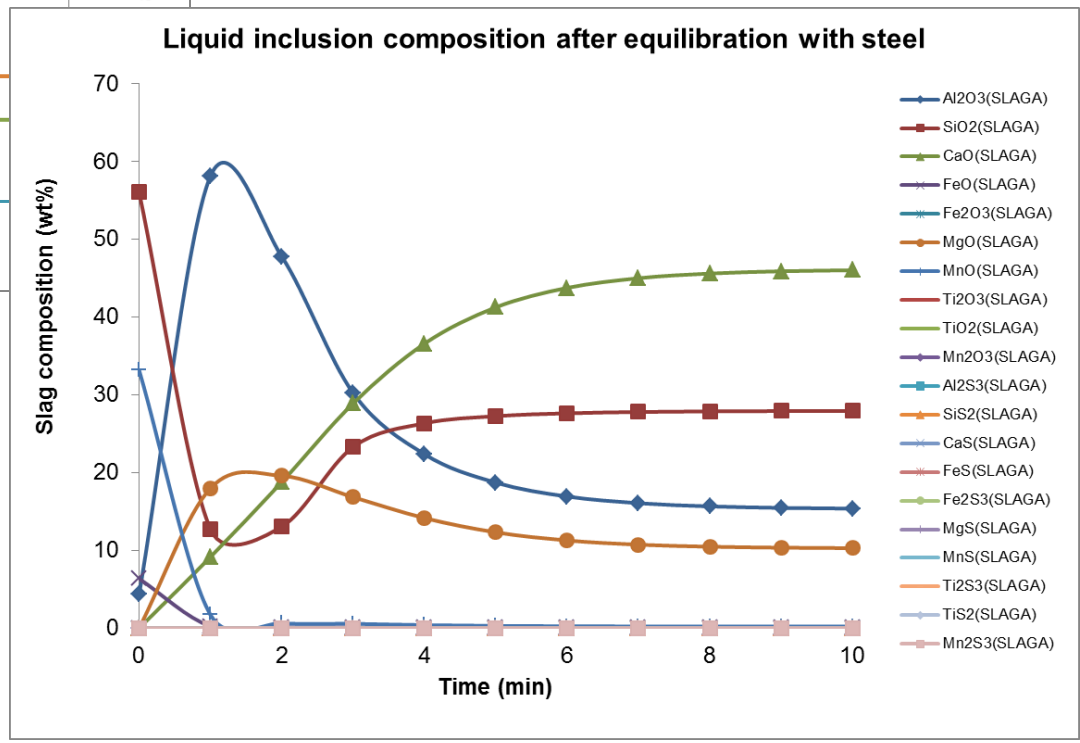
Relative amount is important for the change of inclusion chemistry



Macro process files will be provided separately

Slag/Steel/Inclusion Reaction: Macro processing input Excel file





Reoxidation of Al-killed Ti-bearing steel: macro-processing

Reoxidation by high FeO ladle slag (for example, just after RH process)

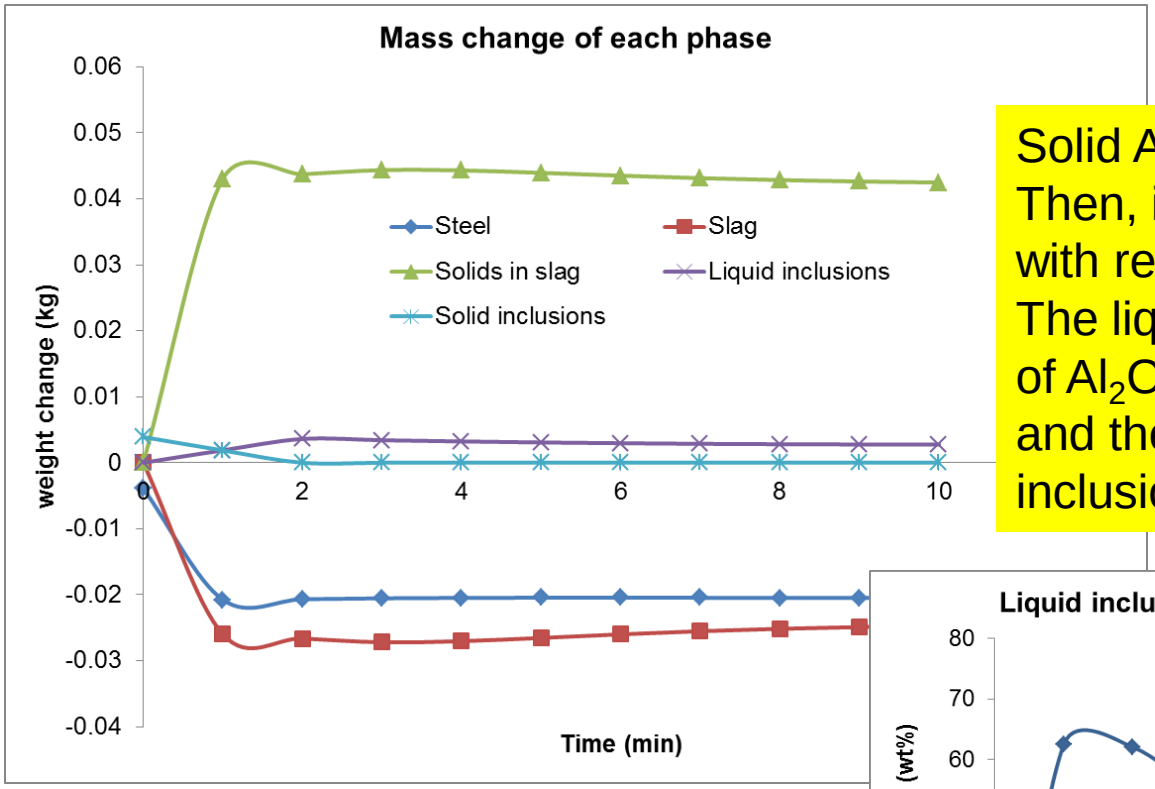
	A	B	C	D	E	F	G	H	I	J
1	Temperature	1600	C							
2	Duration	10	min							
3										
4	Steel amount:	100	kg							
5	Steel composition (wt%)									
6	Fe	Mn	Si	O	Al	Ti	S	Ca	Total	
7	99.8425	0.01	0.01	0.0025	0.03	0.1	0.005	0	100	
8										
9	Slag amount:	0.1	kg							
10	Slag composition (wt%)									
11	CaO	MgO	Al2O3	SiO2	FeO	MnO	Total			
12	40	10	15	30	5	0	100			
13										
14										
15										
16										
17										
18	**DO NOT ALTER**									
19	Fe	Mn	Si	O	Al	Ti	S	Ca	Total	
20	99.8425	0.01	0.01	0.0025	0.03	0.1	0.005	0	100	
21										
22										
23										
24	CaO	MgO	Al2O3	SiO2	FeO	MnO	Total			
25	0.04	0.01	0.015	0.03	0.005	0	0.1			

Sheet1 Sheet2 Sheet3

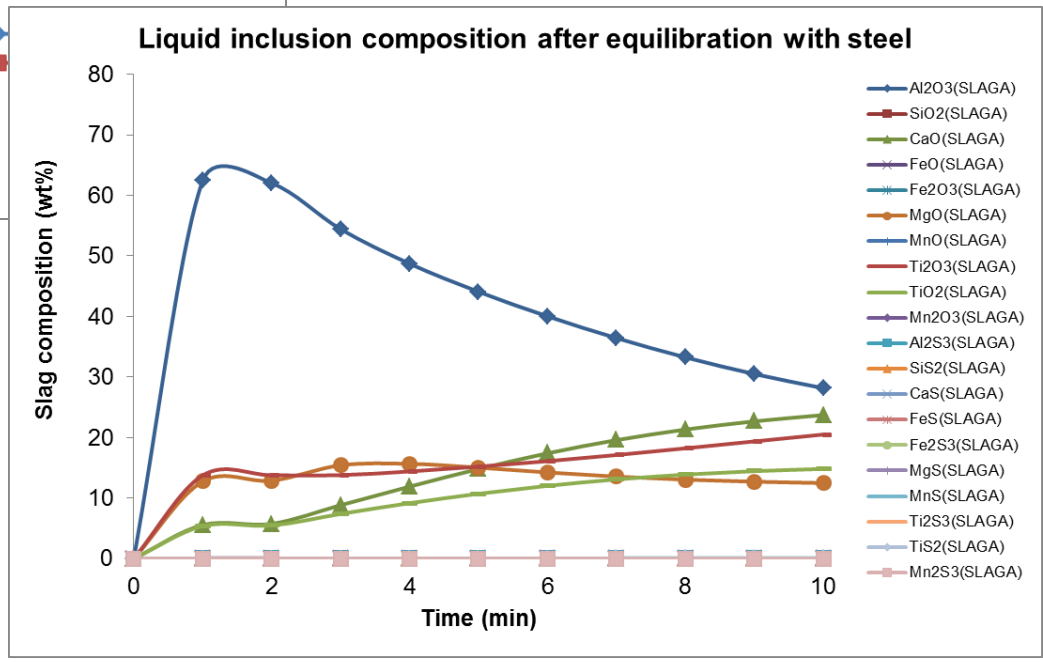
Ready

Ladle slag with 5% FeO

Reoxidation of Al-killed Ti-bearing steel: macro-processing



Solid Al_2O_3 forms after deoxidation. Then, it is converted to liquid inclusions with reoxidation by the slag.
The liquid inclusion is composed mainly of Al_2O_3-TiO_2-Ti_2O_3-MgO in early stages and the CaO content in the liquid inclusion increases with time.



Reoxidation of Al-killed Ti-bearing steel: macro-processing

Reoxidation by high SiO2 tundish slag (in Tundish)

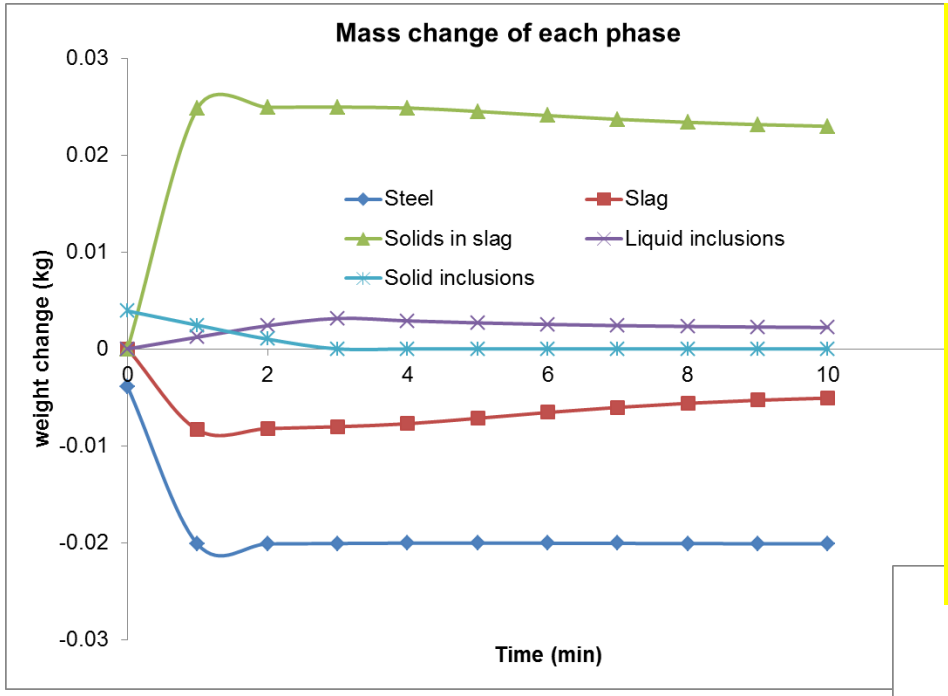
	A	B	C	D	E	F	G	H	I	J
1	Temperature	1600	C							
2	Duration	10	min							
3										
4	Steel amount:	100	kg							
5	Steel composition (wt%)									
6	Fe	Mn	Si	O	Al	Ti	S	Ca	Total	
7	98.8625	0.7	0.3	0.0025	0.03	0.1	0.005	0	100	
8										
9	Slag amount:	0.1	kg							
10	Slag composition (wt%)									
11	CaO	MgO	Al2O3	SiO2	FeO	MnO	Total			
12	35	10	10	40	5	0	100			
13										
14										
15										
16										
17										
18	**DO NOT ALTER**									
19	Fe	Mn	Si	O	Al	Ti	S	Ca	Total	
20	98.8625	0.7	0.3	0.0025	0.03	0.1	0.005	0	100	
21										
22										
23										
24	CaO	MgO	Al2O3	SiO2	FeO	MnO	Total			
25	0.035	0.01	0.01	0.04	0.005	0	0.1			

Sheet1 Sheet2 Sheet3

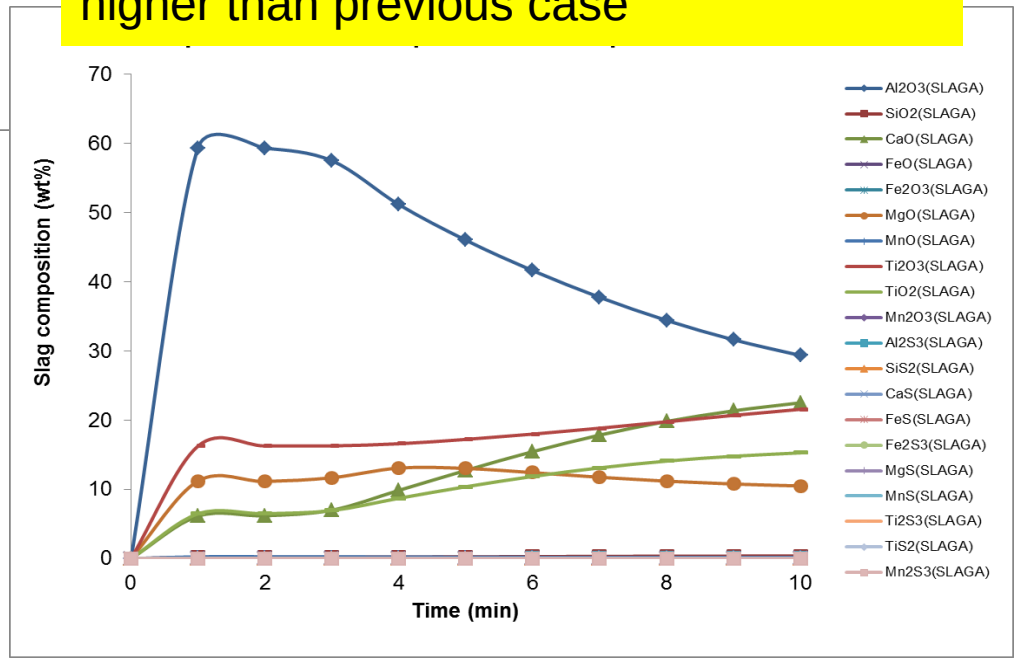
Ready

Tundish slag with 40% SiO2

Reoxidation of Al-killed Ti-bearing steel: macro-processing



Solid Al_2O_3 forms after deoxidation. Then, it is converted to liquid inclusions with reoxidation by the slag (more slowly than in the previous case).
The liquid inlcusion is composed mainly of Al_2O_3-TiO_2-Ti_2O_3-MgO (less MgO than in the previous case) in early stage and the CaO content in the liquid inclusion is increasing with time. Ti_2O_3 level is higher than previous case



Note

Note

Thanks to FactSage Steelmaking Consortium Members

JFE Steel Corporation

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NIPPON STEEL & SUMITOMO METAL

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RHI

Natural Sciences and Engineering Research Council of Canada

Developments of

- **Thermodynamic database**
- **Process simulation model**

Training for FactSage and Process simulation