

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>

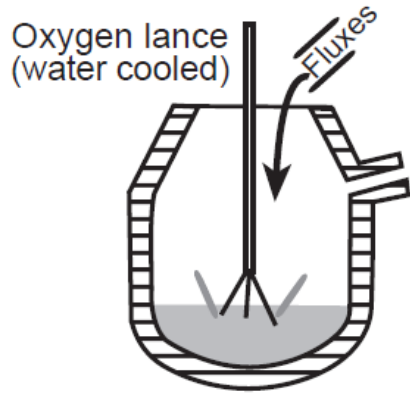
Contents

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

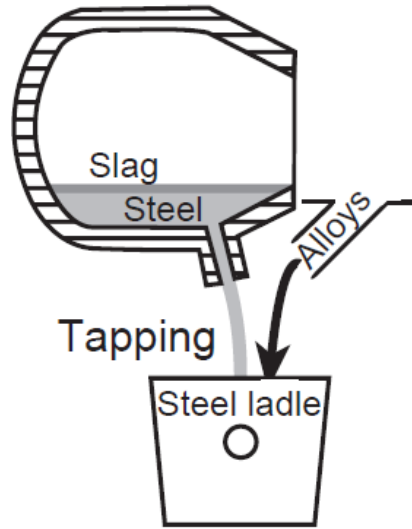
Application I

SECONDARY STEELMAKING

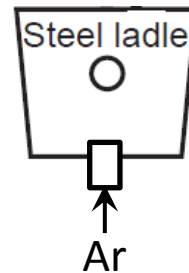
Secondary steelmaking



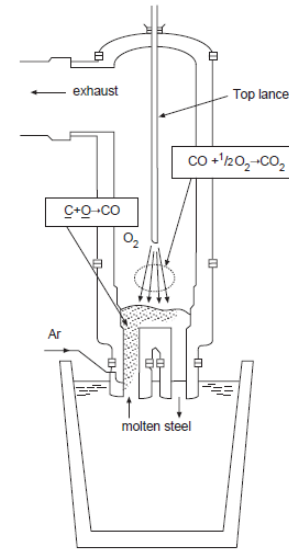
BOF



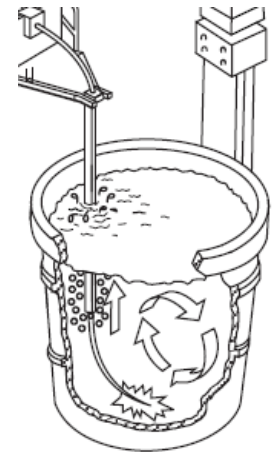
1. Tapping and alloy/flux addition



2. Stirring



3. degassing

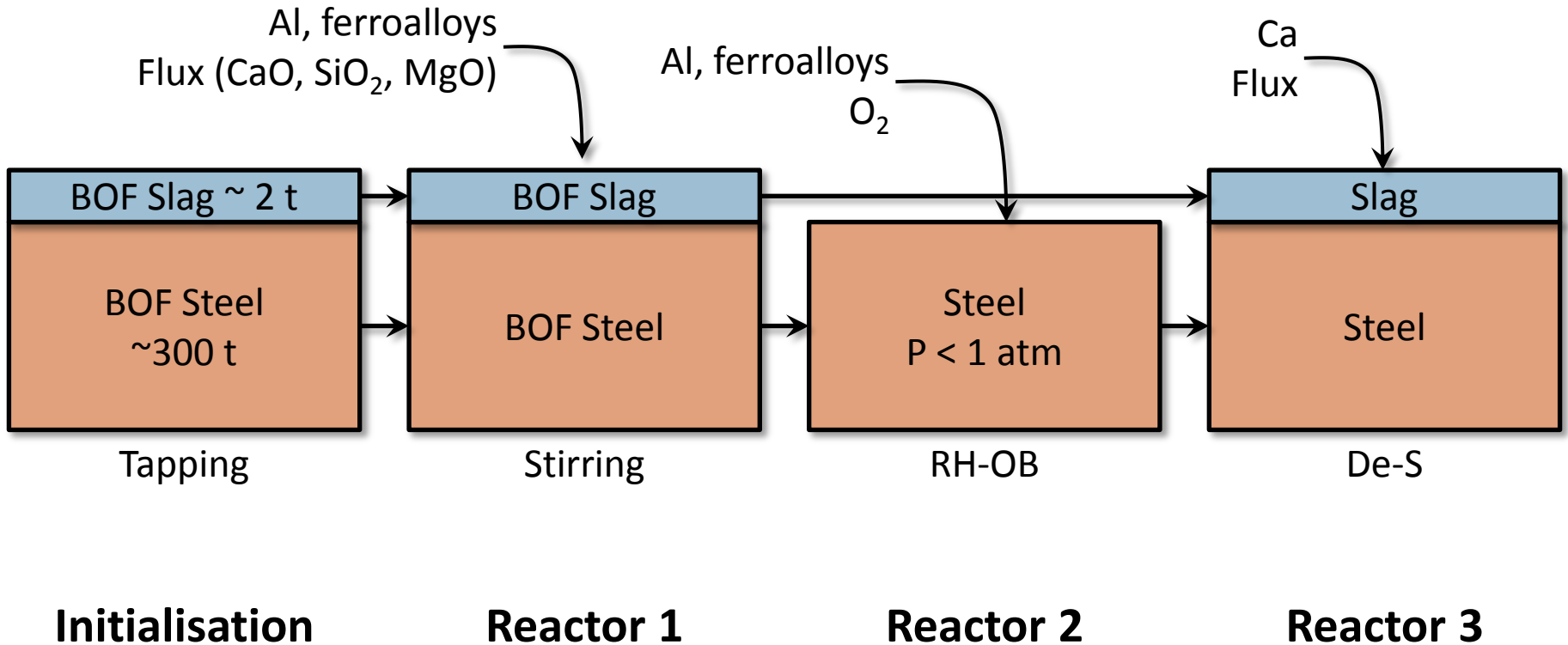


4. Wire feeding powder injection (De-S)

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



Simplifications:

- No kinetic factors
- Isothermal conditions

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

Microsoft Excel window: *inoutput* [Compatibility Mode] - Microsoft Excel

Initial BOF steel and slag composition, amount and temperature

BOF steel								Ferroalloy calculation				element		atom number
comp. (wt%)	Fe	O	C	Si	Mn	S	Total	FeMn	%Fe	%non-ferro	total mass (ton)	Fe	26	
99.74	0.08	0.05	0.02	0.1	0.01	0.01	100	20	80	0.5		Mn	25	
mass (ton)	299.22	0.24	0.15	0.06	0.3	0.03		FeSi	30	70	0.5	Ca	20	
Total amount	300 ton								FeTi	35	65	0.2	S	16
temperature	1600 °C								Fe	Mn	Si	Ti	Si	14
								0.32	0.4	0.35	0.13	Al	13	
												Mg	12	
												O	8	
												C	6	
												Ti	22	

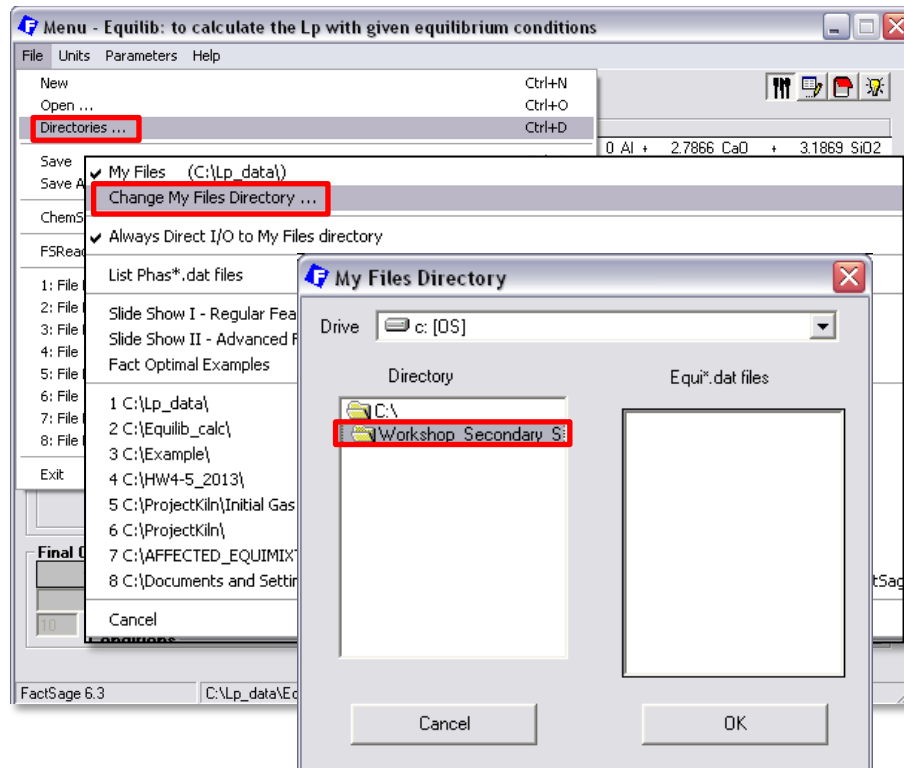
calculation	Stirring station (ton)							RH (atm, ton)					De-S station (ton)				
	Al	Fe	Mn	Si	CaO	SiO2	MgO	Pressure	Al	Fe	Mn	Si	Ti	O2	Ca	CaO	SiO2
1	0.45							0.01							0.06		
2	0.5							0.001								0.06	
3								0.001	0.45						0.06		

Amount of flux, ferroalloys, etc., added in each reactor

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

Reactants - Equilib

File Edit Table Units **Data Search** Help

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

1 - 6

Mass(g)	Species
1	Fe
+ 1	O
+ 1	C
+ 1	Si
+ 1	Mn
+ 1	S

Data Search

Databases - 1/38 compound databases, 1/39 solution databases

<input type="checkbox"/> FactPS	<input type="checkbox"/> FScopp	<input type="checkbox"/> BINS	<input type="checkbox"/> compounds only	<input type="checkbox"/> CAF3	<input type="checkbox"/> CON1	<input type="checkbox"/> COMP
<input type="checkbox"/> FToxid	<input type="checkbox"/> FSlead	<input type="checkbox"/> SGPS	<input type="checkbox"/> solutions only	<input type="checkbox"/> EXAM	<input type="checkbox"/> FELQ	<input type="checkbox"/> FEZN
<input type="checkbox"/> FTsalt	<input type="checkbox"/> FSlite	<input type="checkbox"/> SGTE	<input type="checkbox"/> no database	<input type="checkbox"/> GOOD	<input type="checkbox"/> NDCO	<input type="checkbox"/> OTHE
<input checked="" type="checkbox"/> FTmisc	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGnobl	Clear All	<input type="checkbox"/> PBHR	<input type="checkbox"/> PBLR	<input type="checkbox"/> PIER
<input type="checkbox"/> FTball	<input type="checkbox"/> FSnobl	<input type="checkbox"/> SGsold	Select All	<input type="checkbox"/> REB_	<input type="checkbox"/> SGSL	<input type="checkbox"/> SGTE#
<input type="checkbox"/> FT0xCN	<input type="checkbox"/> FSupsi	<input type="checkbox"/> SGnucl	Add/Remove Data	<input type="checkbox"/> SGTE*	<input type="checkbox"/> TEMP	<input type="checkbox"/> VOXD
<input type="checkbox"/> FTfritz			RefreshDatabases			
<input type="checkbox"/> FThelp	<input type="checkbox"/> ELEM	Other				
<input type="checkbox"/> FTpulp	<input type="checkbox"/> FTdemo	<input type="checkbox"/> TDnucl				
<input type="checkbox"/> FTlite						

Information

Options

Default

Include

- gaseous ions (plasmas)
- aqueous species
- limited data compounds (25C)

Limits

Organic species CxHy... X(max) = 2

Minimum solution components: 1 2 cpts

Cancel Summary ... OK

3. Streams initialization – BOF steel

Initialization of the BOF steel – EquiSteel_init.dat

Menu - Equilib: last system

Reactants (6): (gram) Fe + O + C + Si + Mn + S

Base-Phase	Full Name
FTmisc-FeLQ	Fe-liq
FTmisc-MAT1	Matte
FTmisc-FeS ₂	FeS-liq
FTmisc-MAT2C	CLiq(Matte/Metal)
FTmisc-PYRRC	CPyrrothite
FTmisc-BCCS	bcc

Final Conditions: T(C) 1000, P(atm) 1

Equilibrium: normal

Menu - Equilib: initialisation of the Fe liquid

Save the Equilib file

Save As ...

Save File in C:\Workshop_Secondary_Steelmaking...

Steel_init

Save File C:\Workshop_Secondary_Steelmaking\Eq...

Initialisation of the BOF steel

3. Streams initialization – BOF steel

Initialization of the BOF steel – EquiSteel_init.dat

The screenshot shows the 'Menu - Equilib: last system' window. The reactants are listed as (gram) Fe + O + C + Si + Mn + S. The products section includes a table of solution species:

*	+	Base-Phase	Full Name
		FTmisc-FeLQ	Fe-liq
		FTmisc-MATT	Matte
		FTmisc-FeS_	FeS-liq
		FTmisc-MAT2C	CLiq(Matte/Metal)
		FTmisc-PYRRC	CPyrrhotite
		FTmisc-BCCS	bcc
		FTmisc-FCCS	fcc
		FTmisc-MS-c	MeS_cubic

The 'Final Conditions' section shows T(C) = 1000 and P(atm) = 1. The 'Equilibrium' section has 'normal' selected. A red box highlights the 'Calculate >>' button.

Calculate the equilibrium

Save FeLQ as a stream

The screenshot shows the 'Results - Equilib 1000 C' window. The 'Stream File' menu is open, showing the path: Stream File > Save stream file > Save solutions > FTmisc-FeLQ Fe-liq. A red box highlights the 'Calculate >>' button from the previous window. Below, the 'Save File in C:\Workshop_Secondary_Steelmaking...' dialog is shown with 'BOF_steel' entered in the stream file name field.

3. Streams initialization – BOF slag

Initialization of the BOF slag – EquiSlag_init.dat

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

Enter all the reactant species, in the same order as in the Excel sheet

Select the databases

Mass(g)	Species
1	CaO
+ 1	SiO2
+ 1	FeO
+ 1	MgO
+ 1	MnO

Data Search

Databases - 1/38 compound databases, 1/39 solution databases

Fact	FactSage	SGTE	Miscellaneous		
<input type="checkbox"/> FactPS	<input type="checkbox"/> FScopp	<input type="checkbox"/> BINS	<input type="checkbox"/> CAF3	<input type="checkbox"/> CON1	<input type="checkbox"/> COMP
<input checked="" type="checkbox"/> FToxid	<input type="checkbox"/> FSlead	<input type="checkbox"/> SGPS	<input type="checkbox"/> EXAM	<input type="checkbox"/> FELQ	<input type="checkbox"/> FEZN
<input type="checkbox"/> FTsalt	<input type="checkbox"/> FSlite	<input type="checkbox"/> SGTE	<input type="checkbox"/> GOOD	<input type="checkbox"/> NDCC	<input type="checkbox"/> OTHE
<input type="checkbox"/> FTmisc	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGnobl	<input type="checkbox"/> PBHR	<input type="checkbox"/> PBLR	<input type="checkbox"/> PIER
<input type="checkbox"/> FTball	<input type="checkbox"/> FSnobl	<input type="checkbox"/> SGsold	<input type="checkbox"/> REB_	<input type="checkbox"/> SGSL	<input type="checkbox"/> SGTE#
<input type="checkbox"/> FT0xCN	<input type="checkbox"/> FSupsi	<input type="checkbox"/> SGnucl	<input type="checkbox"/> SGTE*	<input type="checkbox"/> TEMP	<input type="checkbox"/> VOXD
<input type="checkbox"/> FTfritz					
<input type="checkbox"/> FTthelg					
<input type="checkbox"/> FTpulp	<input type="checkbox"/> ELEM	Other			
<input type="checkbox"/> FTlite	<input type="checkbox"/> FTdemo	<input type="checkbox"/> TDnucl			

Options

Include:

- gaseous ions (plasmas)
- aqueous species
- limited data compounds (25C)

Limits:

Organic species CxHy... X(max) = 2

Minimum solution components: 1 2 cpts

Buttons: Cancel, Summary..., OK

3. Streams initialization – BOF slag

Initialization of the BOF slag – EquiSlag_init.dat

Menu - Equilib: last system

Reactants (5): (gram) CaO + SiO2 + FeO + MgO + MnO

		Base-Phase	Full Name
1	FToxid-SLAGA	ASlag-liq all oxides + S	
	FToxid-SPINA	ASpinel	
	FToxid-SPINB	BSpinel	
	FToxid-SPIN?	?Spinel	
	FToxid-MeO_A	AMonoxide	
	FToxid-MeO_B	BMonoxide	

Menu - Equilib: initialisation of the Fe liquid

Save the Equilib file

Save File in C:\Workshop_BOFEqui*.dat

Enter the file number (1 - 9999)

or enter the file name, for example

My very favorite calculation

- avoid the special characters

Slag_init

Save File C:\Workshop_Secondary_Steelmaking\Eq...

Saving file Slag_init

Enter one line of comments

- to add additional notes, terminate the line of comments with the character +

Initialisation of the BOF slag

3. Streams initialization – BOF slag

Initialization of the BOF slag – MixtBOF_slag.dat

Save SLAGA#1 as a stream

Calculate the equilibrium

The screenshot displays the FactSage 6.3 software interface. The main window is titled "Menu - Equilib: last system". The "Reactants (5)" field contains "(gram) CaO + SiO2 + FeO + MgO + MnO". The "Products" section shows a list of "Solution species" with columns for "Base-Phase" and "Full Name". The first entry is "FToxid-SLAGA" with "ASlag-liq all oxides + S" as the full name. The "Equilibrium" section has radio buttons for "normal", "normal + transitions", "transitions only", and "open", with "normal" selected. A "Calculate >>" button is highlighted with a red box and an arrow pointing to it. The "Results - Equilib 1600 C" window is open, showing the "Stream File" menu with "Save stream file" selected. A "Save File" dialog box is open, showing the file name "FToxid-SLAGA#1 ASlag-liq" and a text input field containing "BOF_slag".

3. Streams initialization – macro

```
1 HIDE // Hide the equilib window
2
3 // Declaration of variables:
4 VARIABLE %MyDir. %temperature %Metal_input(6) %Slag_input(5)
5
6 %MyDir. = C:\Workshop_Secondary_Steelmaking\ // path definition
7
8 OLE1 %MyDir.inoutput.xls sheet1 // creation of OLE link
9
10 %Metal_input OLE1 READ B4:G4 // reading and storing initial steel
11 %Slag_input OLE1 READ B11:F11 // reading and storing initial slag
12 %temperature OLE1 READ B6 // reading and storing temperature
13
14 // ***** Initialisation *****
15
16 OPEN %MyDir.EquiSteel_init.dat // open the equilib file
17 %1 = 1 TO 6 // loop on the equilib reactants
18 SET REACTANT %1 MASS %Metal_input(%1) // overwrite the reactant amounts
19 %1 LOOP // end of loop
20 SET FINAL T %temperature // overwrite the temperature in Equilib
21 CALC // calculate the equilibrium
22 SAVE %MyDir.MixtBOF_steel.dat FTmisc-FeLQ // save FeLQ as a stream
23
24 OPEN %MyDir.EquiSlag_init.dat // open the equilib file
25 %1 = 1 TO 5 // loop on the equilib reactants
26 SET REACTANT %1 MASS %Slag_input(%1) // overwrite the reactant amounts
27 %1 LOOP // end of loop
28 SET FINAL T %temperature // overwrite the temperature in Equilib
29 CALC // calculate the equilibrium
30 SAVE %MyDir.MixtBOF_slag.dat FToxid-SLAGA#1 // save SLAGA#1 as a stream
31
32 END // end of macro
```

4. Equilib file for Reactor 1 - stirring

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

Reactants - Equilib

File Edit Table Units **Data Search** Help

T(C) P(atm) Energy(J) Mass(g) Vol(litre) ← Change the units to °C (T) and g (mass)

1 - 9

Mass(g)	Species		
100%	[BOF_steel]		
+ 100%	[BOF_slag]		
+ 0	Al		3
+ 0	Fe		3
+ 0	Mn		3
+ 0	Si		3
+ 0	CaO		3
+ 0	SiO2		3
+ 0	MgO		3

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

Select the databases

Data Search

Databases - 2/38 compound databases, 2/39 solution databases

<input type="checkbox"/> FactPS	<input type="checkbox"/> FScoopp	<input type="checkbox"/> BINS	<input type="checkbox"/> compounds only
<input checked="" type="checkbox"/> FToxid	<input type="checkbox"/> FSlead	<input type="checkbox"/> SGPS	<input type="checkbox"/> solutions only
<input type="checkbox"/> FTsalt	<input type="checkbox"/> FSlite	<input type="checkbox"/> SGTE	<input type="checkbox"/> no database
<input checked="" type="checkbox"/> FTmisc	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGnobl	Clear All
<input type="checkbox"/> FThall	<input type="checkbox"/> FSnobl	<input type="checkbox"/> SGsold	Select All
<input type="checkbox"/> FT0xCN	<input type="checkbox"/> FSupsi	<input type="checkbox"/> SGnucl	Add/Remove Data
<input type="checkbox"/> FTfritz			RefreshDatabases
<input type="checkbox"/> FTfritz			
<input type="checkbox"/> FTfritz			
<input type="checkbox"/> FTpulp	<input type="checkbox"/> ELEM	Other	
<input type="checkbox"/> FTlite	<input type="checkbox"/> FTdemo	<input type="checkbox"/> TDnucl	

Information -
Click on a box to include (or exclude) a database in the data search. Normally databases are 'coupled' - that is both the compound and solution database (when available) will be selected. To 'uncouple' a databases click-mouse-right-button (note, this is NOT recommended).
If database is stored on your PC but not listed here then you must 'add the database to the list' - click on 'Add/Remove ...'

Options

Default

Include

- gaseous ions (plasmas)
- aqueous species
- limited data compounds (25C)

Limits

Organic species CxHy... X(max) = 2

Minimum solution components: 1 2 cpts

Cancel Summary ... OK

4. Equilib file for Reactor 1 - stirring

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

The screenshot shows the FactSage 6.3 Equilib module interface. The main window displays the reaction setup for a reactor. The reactants are listed as 100% BOF steel, 100% BOF slag, and various elements (Al, Fe, Mn, Si, CaO, SiO2, MgO). The products section shows a table of solution species:

Base-Phase	Full Name
FT misc-FeLQ	Fe-liq
FToxid-SLAGA	ASlag-liq all oxides + S

The 'pure solids' option is selected in the products list. A callout box points to this selection with the text: "Select pure solids from FToxid, FeLQ and SLAGA".

Three dialog boxes are overlaid on the interface:

- Save File in C:\Workshop_Secondary_Steelmaking...**: A dialog for entering a file number (1-9999) or a file name. The file name "R1" is entered.
- Save File C:\Workshop_Secondary_Steelmaking\Eq...**: A dialog for saving the file. The file name "R1" is entered. A comment box contains the text: "Reaction between BOF steel, slag, Al, ferroalloys, fluxes".
- Menu - Equilib: reaction between metal, slag and gas**: A menu window with "Save As ..." highlighted.

4. Equilib file for Reactor 1 - stirring

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

The screenshot shows the FactSage 6.3 Equilib interface. The 'Reactants' list includes 100% BOF_steel, 100% BOF_slag, and various elements (Al, Fe, Mn, Si, CaO, SiO2, MgO). The 'Products' list includes 'Fe-liq' (FTmisc-FeLQ) and 'ASlag-liq all oxides + S' (FToxid-SLAGA). The 'Final Conditions' are set to T=1600, P=1, and 1 calculation. The 'Calculate >>' button is highlighted with a red box and an arrow pointing to it.

Calculate the equilibrium

Save Solids, FeLQ and SLAGA#1 as streams

The screenshot shows the 'Stream File' menu open in FactSage 6.3. The 'Save stream file' option is selected, leading to a submenu with 'Save pure solids ...', 'Save solutions', and 'Save gas phase ...'. Three 'Save File in C:\Workshop_Secondary_Steelmaking...' dialog boxes are shown, each with a red box around the filename: 'Steel_reacted', 'Slag_reacted', and 'Solids_reacted'. The 'Calculate >>' button from the previous screenshot is also visible in the background.

4. Equilib file for Reactor 2 - RH

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

Reactants - Equilib

File Edit Table Units Data Search Help

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

1-7

Mass(g)	Species
100%	[Steel_reacted]
+ 0	Al
+ 0	Fe
+ 0	Mn
+ 0	Si
+ 0	Ti
+ 0	O2

Initial Conditions

Next >>

FactSage 6.3 Compound: 2/38 databases Solution: 2/39 databases

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

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

Select the databases

Data Search

Databases - 3/38 compound databases, 2/39 solution databases

<input checked="" type="checkbox"/> FactPS	<input type="checkbox"/> FSscopp	<input type="checkbox"/> BINS	<input type="checkbox"/> compounds only
<input checked="" type="checkbox"/> FToxid	<input type="checkbox"/> FSlead	<input type="checkbox"/> SGPS	<input type="checkbox"/> solutions only
<input type="checkbox"/> FTsalt	<input type="checkbox"/> FSlite	<input type="checkbox"/> SGTE	<input type="checkbox"/> no database
<input checked="" type="checkbox"/> FTmisc	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGnobl	Clear All
<input type="checkbox"/> FTxhall	<input type="checkbox"/> FSnobl	<input type="checkbox"/> SGold	Select All
<input type="checkbox"/> FTxncn	<input type="checkbox"/> FSupsi	<input type="checkbox"/> SGnucl	Add/Remove Data
<input type="checkbox"/> FTfritz	<input type="checkbox"/> ELEM	Other	RefreshDatabases
<input type="checkbox"/> FThelg	<input type="checkbox"/> FTdemo	<input type="checkbox"/> TDnucl	
<input type="checkbox"/> FTpulp			
<input type="checkbox"/> FTlite			

Information -

Click on a box to include (or exclude) a database in the data search. Normally databases are 'coupled' - that is both the compound and solution database (when available) will be selected. To 'uncouple' a databases click-mouse-right-button (note, this is NOT recommended).

If database is stored on your PC but not listed here then you must 'add the database to the list' - click on 'Add/Remove ...'

Options

Default

Include

- gaseous ions (plasmas)
- aqueous species
- limited data compounds (25C)

Limits

Organic species CxHy... X(max) = 2

Minimum solution components: 1 2 cpts

Cancel Summary ... OK

4. Equilib file for Reactor 2 - RH

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

The screenshot shows the FactSage 6.3 Equilib interface. The main window is titled "Menu - Equilib: last system". The "Reactants" field contains "(gram) 100% [Steel_reacted] + 0 Al + 0 Fe + 0 Mn + 0 Si + 0 Ti + 0 O2". The "Products" section shows "gas" selected as the compound species, and "pure solids" selected as the solution species. A table of solution species is visible:

Base-Phase	Full Name
FTmisc-FeLQ	Fe-liq
FToxid-SLAGA	ASlag-liq all oxides + S

Arrows point from the text "Select gas, pure solids from FToxid, FeLQ and SLAGA" to the "gas" and "pure solids" options in the "Products" section, and to the "FToxid-SLAGA" and "FTmisc-FeLQ" entries in the solution species table.

Overlaid on the interface are several dialog boxes and text boxes:

- A text box "Save the Equilib file" is positioned over the "Save As ..." menu option.
- A "Save File in C:\Workshop_Secondary_Steelmaking..." dialog box is open, with "R2" entered in the file name field.
- A "Save File C:\Workshop_Secondary_Steelmaking\Eq..." dialog box is open, with the comment "Reaction in RH between steel, Al, ferroalloys at low P" entered in the text field.

4. Equilib file for Reactor 2 - RH

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

The screenshot shows the FactSage 6.3 Equilib interface. The 'Reactants' field contains: (gram) 100% [Steel_reacted] + 0 Al + 0 Fe + 0 Mn + 0 Si + 0 Ti + 0 O2. The 'Products' section shows a table of solution species:

*	+	Base-Phase	Full Name
	+	FTmisc-FeLQ	Fe-liq
	l	FToxid-SLAGA	ASlag-liq all oxides + S

The 'Calculate >>' button is highlighted with a red box. A callout box points to it with the text 'Calculate the equilibrium'.

Save Solids, FeLQ and SLAGA#1 as streams

The screenshot shows the 'Stream File' menu open in FactSage 6.3. The 'Save stream file' option is selected, leading to a submenu with 'Save pure solids ...' highlighted. Three 'Save File in C:\Workshop_Secondary_Steelmaking...' dialog boxes are shown, each with a red box around the filename:

- FTmisc-FeLQ Fe-liq
- FToxid-SLAGA#1 ASlag-liq
- SOLID

The 'Calculate >>' button from the previous screenshot is also visible in the background.

4. Equilib file for Reactor 3 – De-S

Reaction between steel, slag and flux – EquiR3.dat

Reactants - Equilib

File Edit Table Units **Data Search** Help

T(C) P(atm) Energy(J) Mass(g) Vol(litre) ← Change the units to °C (T) and g (mass)

Mass(g)	Species		
100%	[Steel_RH]		
+ 100%	[Solids_RH]		
+ 100%	[Slag_RH]		3
+ 100%	[Slag_reacted]		4
+ 100%	[Solids_reacted]		5
+ 0	Ca		6
+ 0	CaO		6
+ 0	SiO2		6
+ 0	Ti		
+ 0	Al		

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

To have Al and Ti compounds showing

Select the databases

Data Search

Databases - 2/38 compound databases, 2/39 solution databases

- FactPS
- FToxid
- FTsalt
- FTmisc
- FThall
- FT0xCN
- FTfritz
- FThelp
- FTpulp
- FTlite

- FScoopp
- FSlead
- FSlite
- FSstel
- FSnobl
- FSupsi

- BINS
- SGPS
- SGTE
- SGnobl
- SGnucl

- ELEM
- FTdemo
- TDnucl

Other

Miscellaneous

- CAF3
- EXAM
- GOOD
- PBHR
- REB_
- SGTE*

- CON1
- FELQ
- NDCO
- PBLR
- SGSL
- TEMP

- CONP
- FEZN
- OTHE
- PIER
- SGTE#
- VOXD

Information -

Click on a box to include (or exclude) a database in the data search. Normally databases are 'coupled' - that is both the compound and solution database (when available) will be selected. To 'uncouple' a databases click-mouse-right-button (note, this is NOT recommended).

If database is stored on your PC but not listed here then you must 'add the database to the list' - click on 'Add/Remove ...'

Options

Include

- gaseous ions (plasmas)
- aqueous species
- limited data compounds (25C)

Limits

Organic species CxHy... X(max) = 2

Minimum solution components: 1 2 cpts

Cancel Summary ... OK

4. Equilib file for Reactor 3 – De-S

Reaction between steel, slag and flux – EquiR3.dat

The image shows two screenshots of the FactSage 6.3 software interface. The left screenshot shows the 'Equilib' window for a reaction between RH steel, RH slag, RH solids, reacted slag, and reacted solids. The 'Reactants' list includes 100% Steel RH, 100% Solids RH, 100% Slag RH, 100% Slag reacted, and 100% Solids. The 'Products' list includes pure solids (114). The 'Solution species' table is highlighted with a red box, showing the following entries:

*	+	Base-Phase	Full Name
	+	FT misc-FeLQ	Fe-liq
		FToxid-SLAGA	ASlag-liq all oxides + S

An arrow points from the 'pure solids' entry in the 'Products' list to the 'FToxid-SLAGA' entry in the 'Solution species' table. A text box below this screenshot says: "Select pure solids from FToxid, FeLQ and SLAGA".

The right screenshot shows the 'Save As...' dialog box in the 'Equilib' window. The 'Save As...' option is highlighted in the 'File' menu. A text box above it says: "Save the Equilib file". The 'Save File in C:\Workshop_Secondary_Steelmaking...' dialog box is open, with the file number 'R3' entered in the 'Enter the file number' field. A text box below this dialog says: "Save File C:\Workshop_Secondary_Steelmaking\Eq...". The 'Save File C:\Workshop_Secondary_Steelmaking\Eq...' dialog box is also open, with the file name 'R3' entered in the 'Enter one line of comments' field. A text box below this dialog says: "I, RH slag, RH solids, reacted slag and reacted solids and De-S agents".

4. Main reactions – macro

```
32 // ***** START OF PROCESS *****
33
34 // Declaration of variables:
35 VARIABLE %R1_flux(7) %R2_flux(6) %R3_flux(3) %RH_pressure %pos %num_calc %check %react
36
37 %pos = 17 // position of row to read in excel file
38
39 %num_calc = 1 TO 65536 // loop over the max amount of rows in excel
40 %check OLE1 READ R%posC1 // read the calculation number
41 IF %check = 0 GOTO END // if cell is empty, stop the macro
42 %R1_flux OLE1 READ R%posC2:R%posC8 // reading and storing flux R1
43 %RH_pressure OLE1 READ R%posC9 // reading and storing RH pressure
44 %R2_flux OLE1 READ R%posC10:R%posC15 // reading and storing flux R2
45 %R3_flux OLE1 READ R%posC16:R%posC18 // reading and storing flux R3
46
47 OPEN %MyDir.EquiR1.dat // open the equilib file - reactor 1
48 %react = 3 // position of first reactant to overwrite mass
49 %i = 1 TO 7 // loop over the size of %R1_flux
50 SET REACTANT %react MASS %R1_flux(%i) // overwrite the reactant mass
51 %react STEP // move to the next reactant
52 %i LOOP // end of loop
53 SET FINAL T %temperature // overwrite the temperature in Equilib
54 CALC // calculate the equilibrium
55 SAVE %MyDir.MixtSteel_reacted.dat FTmisc-FelQ // save FelQ as a stream
56 SAVE %MyDir.MixtSlag_reacted.dat FToxid-SLAGA#1 // save SLAGA#1 as a stream
57 SAVE %MyDir.MixtSolids_reacted.dat SOLIDS // save solids as as stream
58
59 OPEN %MyDir.EquiR2.dat // open the equilib file - reactor 2
60 %react = 2 // position of first reactant to overwrite mass
61 %i = 1 TO 6 // loop over the size of %R2_flux
62 SET REACTANT %react MASS %R2_flux(%i) // overwrite the reactant mass
63 %react STEP // move to the next reactant
64 %i LOOP // end of loop
65 SET FINAL T %temperature // overwrite the temperature in Equilib
66 CALC // calculate the equilibrium
67 SAVE %MyDir.MixtSteel_RH.dat FTmisc-FelQ // save FelQ as a stream
68 SAVE %MyDir.MixtSlag_RH.dat FToxid-SLAGA#1 // save SLAGA#1 as a stream
69 SAVE %MyDir.MixtSolids_RH.dat SOLIDS // save solids as as stream
70
71 OPEN %MyDir.EquiR3.dat // open the equilib file - reactor 3
72 %react = 6 // position of first reactant to overwrite mass
73 %i = 1 TO 3 // loop over the size of %R3_flux
74 SET REACTANT %react MASS %R3_flux(%i) // overwrite the reactant mass
75 %react STEP // move to the next reactant
76 %i LOOP // end of loop
77 SET FINAL T %temperature // overwrite the temperature in Equilib
78 CALC // calculate the equilibrium
79
80 %pos STEP // move to the next row in Excel (new process)
81 %num_calc LOOP // end of loop
82 END // end of macro
```


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
```

Macro commands for printing the Equilib results of Reactor 1

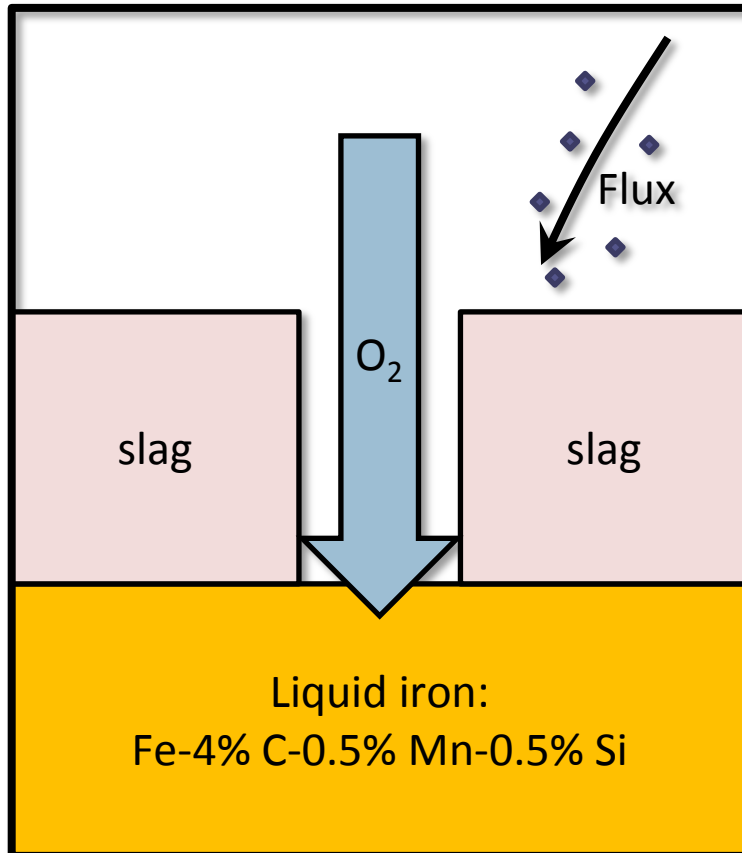
```
// PRINTING:
IF %num_calc = 1 THEN // if first loop, print the names in first row
  %Inc = 1 // start from first column
  %results = calculation // column title
  %results OLE2 WRITE R1C%Inc // write in first row
  %Inc STEP // move to next column
  %1 = 2 TO 4 // loop on the mixture number
  %results = $E_mN%1$ // 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
```

```
%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



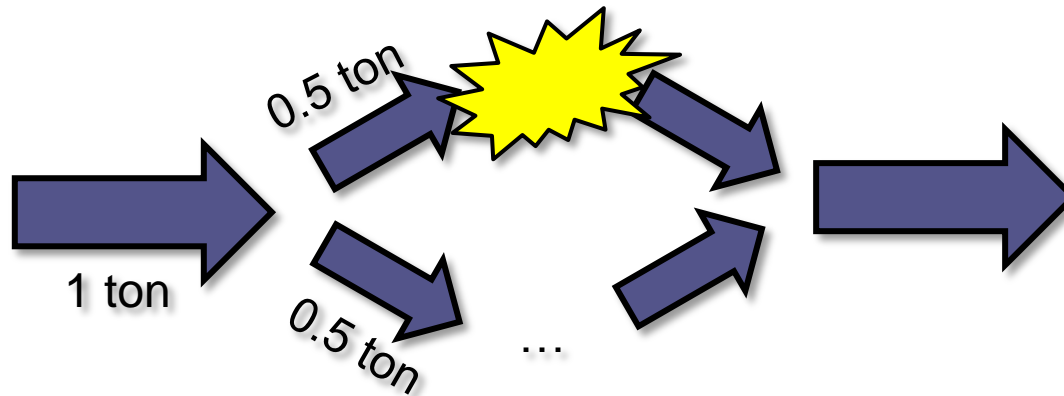
Phase	Amount	Composition	Temperature
Metal	100 ton	95% Fe 4% C 0.5% Mn 0.5% Si	1300 °C
Slag	2 ton	55% CaO 25% FeO 20% SiO ₂	1300 °C
Gas	0.4 ton/min	100% O ₂	25 °C
Flux	0.25 ton/min 1 to 5 min	100% CaO	25 °C

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

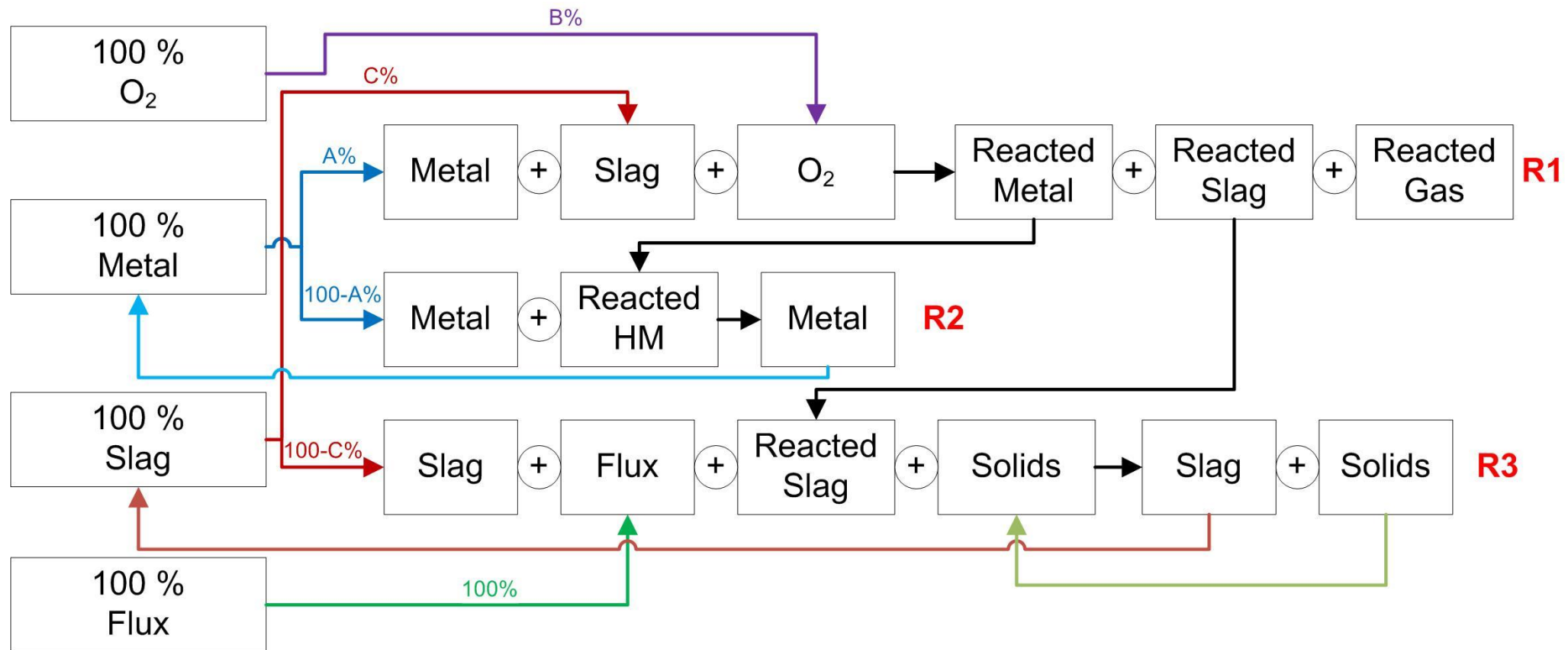


- Finding the suitable proportion of material reacting and non-reacting

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

BOF_inoutput [Compatibility Mode] - Microsoft Excel

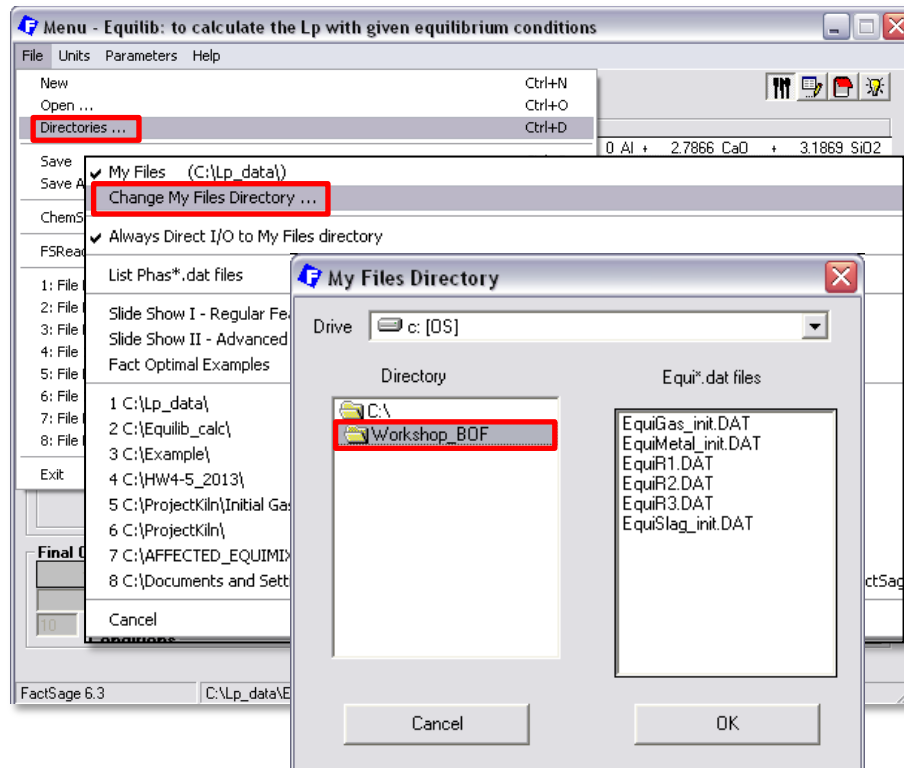
	A	B	C	D	E	F	G	H	I	J	K
1	Metal		Fe	C	Mn	Si	total tons	Temp. (C)			
2		comp. (wt%	95	4	0.5	0.5	100	1300			
3		mass (ton)	95	4	0.5	0.5					
4	Slag		CaO	FeO	SiO2						
5		comp. (wt%	55	25	20		2	1300			
6		mass (ton)	1.1	0.5	0.4						
7	Gas		O2								
8		comp. (wt%	100				0.4	25			
9		mass (ton)	0.4				/min				
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											
31											

Sheet1 Sheet2 Sheet3

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

Menu - Equilib: initialisation of the Fe liquid

Reactants (4) (gram) Fe + C + Mn + Si

+	Base-Phase	Full Name
+	FTmisc-FeLQ	Fe-liq
	FTmisc-BCCS	bcc
	FTmisc-FCCS	fcc

Select only FeLQ solution

Save the Equilib file

Save File in C:\Workshop_BOFEqui*.dat

1: File Metal_init
2: File LMn_calc
3: File LMn_calc
4: File Lp_calc to
5: File P205_wit
6: File P205 - cd
7: File 1 exampl
8: File Estimate

Metal_init

Save File C:\Workshop_BOFEquiMetal_init.DAT

Saving file Metal_init

initialisation of the Fe liquid

3. Streams initialization – Metal

Initialization of the hot metal – EquiMetal_init.dat

Menu - Equilib: initialisation of the Fe liquid

Reactants (4): (gram) Fe + C + Mn + Si

*	+	Base-Phase	Full Name
		FTmisc-FeLQ	Fe-liq
		FTmisc-BCCS	bcc
		FTmisc-FCCS	fcc

Final Conditions: T(C) = 1000, P(atm) = 1

Calculate >>

Save FeLQ as a stream

Results - Equilib 1000 C

Stream File

Save stream file

Save solutions

ALL solutions

FTmisc-FeLQ Fe-liq

Save File in C:\Workshop_BOFWmix*.dat

FTmisc-FeLQ Fe-liq

Enter a stream file number (1 - 9999)

or enter a stream file name (up to 26 characters), for example

My very favorite stream

- avoid the special characters ?@!~",'%%+;<> \

Metal

Calculate the equilibrium

3. Streams initialization – Slag

Initialization of the slag – EquiSlag_init.dat

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

Enter all the reactant species, in the same order as in the Excel sheet

Select the databases

Mass(g)	Species
1	CaO
1	FeO
1	SiO2
0	MnO

Data Search

Databases - 1/38 compound databases, 1/39 solution databases

<input type="checkbox"/> FactPS	<input type="checkbox"/> FScopp	<input type="checkbox"/> BINS	<input type="checkbox"/> compounds only	Miscellaneous		
<input checked="" type="checkbox"/> FToxid	<input type="checkbox"/> FSlead	<input type="checkbox"/> SGPS	<input type="checkbox"/> solutions only	<input type="checkbox"/> CAF3	<input type="checkbox"/> CON1	<input type="checkbox"/> COMP
<input type="checkbox"/> FTsalt	<input type="checkbox"/> FSlite	<input type="checkbox"/> SGTE	<input type="checkbox"/> no database	<input type="checkbox"/> EXAM	<input type="checkbox"/> NDCC	<input type="checkbox"/> FEZN
<input type="checkbox"/> FTmisc	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGnobl	Clear All	<input type="checkbox"/> GOOD	<input type="checkbox"/> PBLR	<input type="checkbox"/> OTHE
<input type="checkbox"/> FTball	<input type="checkbox"/> FSnobl	<input type="checkbox"/> SGsold	Select All	<input type="checkbox"/> PBHR	<input type="checkbox"/> PBLR	<input type="checkbox"/> PIER
<input type="checkbox"/> FT0xCN	<input type="checkbox"/> FSupsi	<input type="checkbox"/> SGnucl	Add/Remove Data	<input type="checkbox"/> REB_	<input type="checkbox"/> SGSL	<input type="checkbox"/> SGTE#
<input type="checkbox"/> FTfritz			RefreshDatabases	<input type="checkbox"/> SGTE*	<input type="checkbox"/> TEMP	<input type="checkbox"/> VOXD
<input type="checkbox"/> FTthelg	<input type="checkbox"/> ELEM	Other				
<input type="checkbox"/> FTpulp	<input type="checkbox"/> FTdemo	<input type="checkbox"/> TDnucl				
<input type="checkbox"/> FTlite						

Options

Include:

- gaseous ions (plasmas)
- aqueous species
- limited data compounds (25C)

Limits:

Organic species CxHy... X(max) = 2

Minimum solution components: 1 2 cpts

Buttons: Cancel, Summary ..., OK

3. Streams initialization – Slag

Initialization of the slag – EquiSlag_init.dat

Menu - Equilib: initialisation of the slag

Reactants (4): (gram) CaO + FeO + SiO2 + 0 MnO

Base-Phase	Full Name
FToxid-SLAGA	ASlag-liq all oxides + S
FToxid-SPINB	BSpinel
FToxid-MeO_A	AMonoxide
FToxid-MeO_B	BMonoxide
FToxid-MeO_?	?Monoxide
FToxid-cPvA	AClinoproxene

Menu - Equilib: initialisation of the Fe liquid

Save the Equilib file

Save File in C:\Workshop_BOFEqui*.dat

1: File Metal_init
2: File LMn_calc
3: File LMn_calc
4: File Lp_calc to
5: File P205_witt
6: File P205 - cc
7: File 1 example
8: File Estimate

Save File C:\Workshop_BOFEquiSlag_init.DAT

initialisation of the slag

Select only SLAGA solution

3. Streams initialization – Slag

Initialization of the slag – EquiSlag_init.dat

Save SLAGA#1 as a stream

Calculate the equilibrium

The screenshot displays the FactSage 6.3 interface. The main window is titled "Menu - Equilib: initialisation of the slag". It shows a list of reactants: (gram) CaO + FeO + SiO2 + 0 MnO. The "Products" section includes a table of solution species:

*	+	Base-Phase	Full Name
1		FToxid-SLAGA	ASlag-liq all oxides + S
		FToxid-SPINB	BSpinel
		FToxid-MeO_A	AMonoxide
		FToxid-MeO_B	BMonoxide
		FToxid-MeO_?	?Monoxide
		FToxid-cPyrA	AClinopyroxene
		FToxid-WOLLA	AWollastonite,
		FToxid-bc2S	aCa2SiO4

The "Final Conditions" section shows T(C) = 1600 and P(atm) = 1. The "Equilibrium" section has "normal" selected. A red box highlights the "Calculate >>" button.

The "Results - Equilib 1600 C" window is open, showing the "Stream File" menu. The "Save stream file" option is selected, leading to a "Save File in C:\Workshop_BOF\Mixt*.dat" dialog box. The dialog box contains the following text:

```
FToxid-SLAGA#1 ASlag-liq
Enter a stream file number
(1 - 9999)
or enter a stream file name (up to 26 characters), for
example
My very favorite stream
- avoid the special characters ?@/!"~.%&+;<>{}
Slag
```

The "Slag" text in the input field is highlighted with a red box.

3. Streams initialization – Gas

Initialization of the gas – EquiGas_init.dat

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

Enter all the reactant species, in the same order as in the Excel sheet

Select the database

The 'Reactants - Equilib' window shows the 'Units' menu and a table with columns for 'Mass(g)' and 'Species'. The 'Species' column contains 'O2'. The 'Data Search' dialog box is open, showing a list of databases with 'FactPS' selected. The 'Miscellaneous' section includes options like 'CAF3', 'EXAM', 'GOOD', 'PBHR', 'REB_', 'SGTE+', 'CON1', 'FELQ', 'NDCO', 'PBLR', 'SGSL', 'TEMP', 'CONP', 'FEZN', 'OTHE', 'PIER', 'SGTE#', and 'VOXD'. The 'Options' section includes 'Include' (gaseous ions, aqueous species, limited data compounds) and 'Limits' (Organic species CxHy... X(max) = 2, Minimum solution components: 1 or 2 cpts).

3. Streams initialization – Gas

Initialization of the gas – EquiGas_init.dat

Menu - Equilib: Initialisation of the gas

Reactants (1): (gram) O2

Products

Compound species	Solution species	Base-Phase	Full Name
<input checked="" type="radio"/> gas	<input checked="" type="radio"/> ideal	<input checked="" type="radio"/> real	3
<input type="radio"/> aqueous	<input type="radio"/>	<input type="radio"/>	
<input type="radio"/> pure liquids	<input type="radio"/>	<input type="radio"/>	
<input type="radio"/> pure solids	<input type="radio"/>	<input type="radio"/>	

Target: Estimate T(K): 1000, Mass(g): 0

Final Conditions: T(C): 25, P(atm): 1, Product H(J):

Equilibrium: normal, normal + transi, transitions only, open

Menu - Equilib: initialisation of the Fe liquid

Save As ...

Save File in C:\Workshop_BOFEqui*.dat

Enter the file number (1 - 9999) or enter the file name, for example: My very favorite calculation - avoid the special characters

Gas_init

Save File C:\Workshop_BOFEquiGas_init.DAT

Saving file Gas_init

Enter one line of comments: - to add additional notes, terminate the line of comments with the character +

Initialisation of the gas

3. Streams initialization – Gas

Initialization of the gas – EquiGas_init.dat

Calculate the equilibrium

Save gas as a stream

Menu - Equilib: Initialisation of the gas

File Units Parameters Help

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

Reactants (1)

(gram) O2

Products

Compound species

- gas ideal real 3
- aqueous 0
- pure liquids 0
- pure solids 0

suppress duplicates apply

species: 3

Target

Estimate T(K): 1000

Mass(g): 0

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
10	steps	25	1	

Equilibrium

- normal
- normal + transitions
- transitions only
- open

Calculate >>

Results - Equilibrium

Output Edit Show

- Save or Print
- Plot
- Equilib Results file
- Stream File
- Format
- Fact-XML
- Fact-Optimal
- Fact-Function-Builder
- Refresh ...

- Recycle all streams ...
- Save stream file
- Stream file properties ...
- Summary of streams
- Directory (C:\Workshop_BOF) ...

- Save gas phase ...
- Save pure liquids ...
- Save aqueous ...
- Save pure solids ...
- Save solutions

The cutoff concentration has been specified to 1.0000E-75

Save File in C:\Workshop_BOF\Mixt*.dat

GAS

Enter a stream file number (1 - 9999)

or enter a stream file name (up to 26 characters), for example

My very favorite stream

- avoid the special characters ?@/!\~`"%%&+:;<>{} \

Gas

OK Cancel

T = 25 C
P = 1 atm
V = 0.76458 dm3

3. Streams initialization – Flux

Equilib calculation cannot be done with reactant amount = 0
⇒ Create the mixture manually

The image shows a composite screenshot of the FactSage 6.3.1 software interface. The main window displays the 'Mixture' module, which is highlighted with a red box and an arrow pointing to it from the text 'Open Mixture module'. The 'Mixture' module is part of the 'Calculate' section. The 'Mixture' module is open, showing a table with columns: Mass(g), Species, Phase, T(C), and P(total). The table contains one entry: 0 g of CaO at 25 °C. A callout box points to this entry with the text 'Enter 0 g CaO at 25 °C'. The 'Data Search' dialog is also open, showing a list of databases. The 'FToxid' database is selected, and a callout box points to it with the text 'Select FToxid database'. The 'Data Search' dialog also shows a list of 'Miscellaneous' databases and 'Options' for the search.

FactSage 6.3.1

Dr. In-Ho Jung

Info: General, Databases, View Data, Compound, Solution

Calculate: Reaction, Predom, **Mixture**, Phase Diagram, OptiSage

Manipulate: Results, Viscosity, Quit

Mixtures and Streams

Mass(g)	Species	Phase	T(C)	P(total)
0	CaO	solid lime	25	1.0

Data Search

Databases - 1/38 compound databases, 0/39 solution databases

FactPS FScopp BINS compounds only EXAM CON1 COMP

Fealt FSlead SGTE solutions only GOOD NDCC OTHE

Fmisc FSlite SGTE no database PBHR PBLR PIER

Fhall FSstel SGnobl Clear All REB_ SGSL SGTE#

FDOxCN FSnobl SGsold Select All SGTE* TEMP VOXD

FTirtz FSupsi SGnucl Add/Remove Data

FTvelg FTpplp FTlite ELEM FTdemo TDnucl RefreshDatabases

Information: Mixture only accesses COMPOUND databases

Options: Include gaseous ions (plasmas) aqueous species limited data compounds (25C) Limits: Organic species CxHy..., X(max) = 0 Minimum solution components: 1 2 cpts

Open Mixture module

Enter 0 g CaO at 25 °C

Select FToxid database

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3. Streams initialization – Flux

Save the mixture file

Check the Directory and change it if necessary

Save File in C:\Workshop_BOFMixt*.dat

Enter a stream file number (1 - 9999)

or enter a stream file name (up to 26 characters), for example

My very favorite stream

- avoid the special characters ?@/!~,"'%&+:;<>{} \

total grams

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
```

4. Equilib file for R1

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

File Edit Table Units **Data Search** Help

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

1-3

Mass(g)	Species	Phase	T(C)	P(total)	Stream#	Data
100%	(Metal)	(Stream)	1000	1	1	
+ 100%	(Slag)	(Stream)	1600	1	2	
+ 100%	(Gas)	(Stream)	25	1	3	

*** P(total) is the hydrostatic pressure above the phase.
For a gaseous stream this is the sum of the partial pressures of the species in that stream.

Initial Conditions

Next >>

FactSage 6.3 Compound: 3/38 databases Solution: 2/39 databases

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

Enter the reactant streams for R1

Select the databases

Select initial conditions for adiabatic calculations

Databases - 3/38 compound databases, 2/39 solution databases

FactPS FSscopp BINS compounds only

FToxid FSlead SGPS solutions only

FTsalt FSlite SGTE no database

FTmisc FSstel SGnobl Clear All

FThall FSnobl SGsold Select All

FT0xCN FSupsi SGnucl Add/Remove Data

FTfritz FTpulp ELEM Other RefreshDatabases

FTlitz FTdemo TDnucl

Information -

Options

Default

Include

gaseous ions (plasmas)

aqueous species

limited data compounds (25C)

Limits

Organic species CxHy... X(max) = 2

Minimum solution components: 1 2 cpts

Cancel Summary ... OK

4. Equilib file for R1

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

The screenshot shows the FactSage 6.3 Equilib window with the following details:

- Reactants (3):** (gram) 100% [Metal] (1000C.#1) + 100% [Slag] (1600C.#2) + 100% [Gas] (25C.g.#3)
- Products:** A table with columns for Base-Phase and Full Name. The selected products are:

Base-Phase	Full Name
+ FT misc-FeLQ	Fe-liq
FT oxid-SLAGA	ASlag-liq all oxides + S
- Final Conditions:** Temperature (T(C)) is blank, and Delta H(J) is set to 0.

Three dialog boxes are overlaid on the window:

- Save File in C:\Workshop_BOFEqui*.dat:** A dialog for entering a file number (1-9999) or a file name. The name **R1** is entered.
- Save File C:\Workshop_BOFEquiR1.DAT:** A dialog for saving file R1 with a comment: **reaction between metal, slag and gas**.
- Save the Equilib file:** A callout box pointing to the 'Save As ...' button in the main window.

Annotations include:

- An arrow pointing to the 'gas' checkbox in the 'Compound species' section with the text: **Select gas, FeLQ and SLAGA**
- An arrow pointing to the 'T(C)' field in the 'Final Conditions' section with the text: **Leave temperature blank and set Delta H = 0 (adiabatic conditions)**

4. Equilib file for R1

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

Menu - Equilib: reaction between metal, slag and gas

Reactants [3]
(gram) 100% [Metal] + 100% [Slag] + 100% [Gas]
(1000C.#1) (1600C.#2) (25C.g.#3)

Products

Compound species	Base-Phase	Full Name
+	FTmisc-FeLQ	Fe-liq
+	FToxid-SLAGA	ASlag-liq all oxides + S

Final Conditions

T(C): 1000
P(atm): 1

Equilibrium

normal + transitions only

Calculate >>

Save FeLQ and SLAGA#1 as streams

Results - Equilib 2322.62 C

Stream File

- Recycle all streams ...
- Save stream file
- Stream file properties ...
- Summary of streams
- Directory (C:\Workshop_BOF) ...

Save solutions

- ALL solutions
- FTmisc-FeLQ Fe-liq
- FToxid-SLAGA#1 ASlag-liq
- FToxid-SLAGA#2 ASlag-liq

Save File in C:\Workshop_BOFMixt*.dat

FTmisc-FeLQ Fe-liq

Enter a stream file number (1 - 9999)

or enter a stream file name (up to 26 characters)

My very favorite stream

Metal_reacted

Save File in C:\Workshop_BOFMixt*.dat

FToxid-SLAGA#1 ASlag-liq

Enter a stream file number (1 - 9999)

or enter a stream file name (up to 26 characters), for example

My very favorite stream

Slag_reacted

Calculate the equilibrium

4. Equilib file for R2

Homogenization in metal – EquiR2.dat

Mass(g)	Species	Phase	T(C)	P(atm)	Energy(J)	Vol(litre)
100%	[Metal]	[Stream]	1000	1		1
+ 100%	[Metal_reacted]	[Stream]	2322.62	1		2

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

Enter the reactant streams for R2

Select the database

Select initial conditions for adiabatic calculations

Databases - 1/38 compound databases, 1/39 solution databases

- FactPS
- FToxid
- FTsalt
- FTmisc
- FTHall
- FT0xCN
- FTfritz
- FTHelg
- FTpulp
- FTlite

Other

- ELEM
- FTdemo
- TDnucl

Options

Include

- gaseous ions (plasmas)
- aqueous species
- limited data compounds (25C)

Limits

Organic species CxHy... X(max) = 2

Minimum solution components: 1 2 cpts

4. Equilib file for R2

Homogenization in metal – EquiR2.dat

Menu - Equilib: homogenisation in metal

File Units Parameters Help

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

Reactants (2)

[gram] 100% [Metal] + 100% [Metal_reacted]
(1000C,#1) (2322.62C,#2)

Products

Compound species

gas ideal real 0
aqueous 0
pure liquids 0
pure solids 0
 suppress duplicates apply

species: 0

Target
- none -
Estimate T(C): 1000
Mass(g): 0

Final Conditions

<A> T(C) P(atm) Delta H(J)
10 steps Table 1 calculation

Equilibrium

normal normal + transi
 transitions only
 open

Calculate >>

Save the Equilib file

Save File in C:\Workshop_BOF\Equi*.dat

Enter the file number
(1 - 9999)

or enter the file name, for example
My very favorite calculation

- avoid the special characters ?@/*~`!%&+:;<>{\

R2

Save File C:\Workshop_BOF\EquiR2.DAT

Saving file R2

Enter one line of comments

- to add additional notes, terminate the line of comments
with the character +

homogenisation in metal

Select only FeLQ

Leave temperature blank and set
Delta H = 0 (adiabatic conditions)

4. Equilib file for R3

Homogenization in slag and flux addition – EquiR3.dat

Mass(g)	Species	Phase	T(C)	P(total)	Stream#
100%	[Slag]	[Stream]	1600	1	1
+ 100%	[Slag_reacted]	[Stream]	2322.62	1	2
+ 1	CaO	fresh flux	25	1	3
+ 100%	[CaO]	[Stream]	25	1	4

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

Databases - 1/38 compound databases, 1/39 solution databases

- FactPS
- FToxid
- FTsalt
- FTmisc
- FToxCN
- FTfritz
- FThelp
- FTpulp
- FTlite
- FSopp
- FSlead
- FSlite
- FSstel
- FSnobl
- FSupsi
- BINS
- SGPS
- SGTE
- SGnobl
- SGnucl
- ELEM
- FTdemo
- TDnucl

Miscellaneous

- CAF3
- EXAM
- GOOD
- PBHR
- REB_
- SGTE*
- CON1
- FELQ
- NDCO
- PBLR
- SGSL
- TEMP
- CONP
- FEZN
- OTHE
- PIER
- SGTE#
- VOXD

Other

Initial Conditions

Information -
Click on a box to include (or exclude) a database in the data search. Normally databases are 'coupled' - that is both the compound and solution database (when available) will be selected. To 'uncouple' a databases click-mouse-right-button (note, this is NOT recommended).

If database is stored on your PC but not listed here then you must 'add the database to the list' - click on 'Add/Remove ...'

Options

Include

- gaseous ions (plasmas)
- aqueous species
- limited data compounds (25C)

Limits

Organic species CxHy... X(max) = 2

Minimum solution components: 1 2 cpts

Cancel Summary ... OK

4. Equilib file for R3

Homogenization in slag and flux addition – EquiR3.dat

Save the Equilib file

Select only SLAGA and pure CaO(s)

Leave temperature blank and set Delta H = 0 (adiabatic conditions)

Save File in C:\Workshop_BOF\Equi*.dat

Save File C:\Workshop_BOF\EquiR3.DAT

homogenisation in slag + flux addition

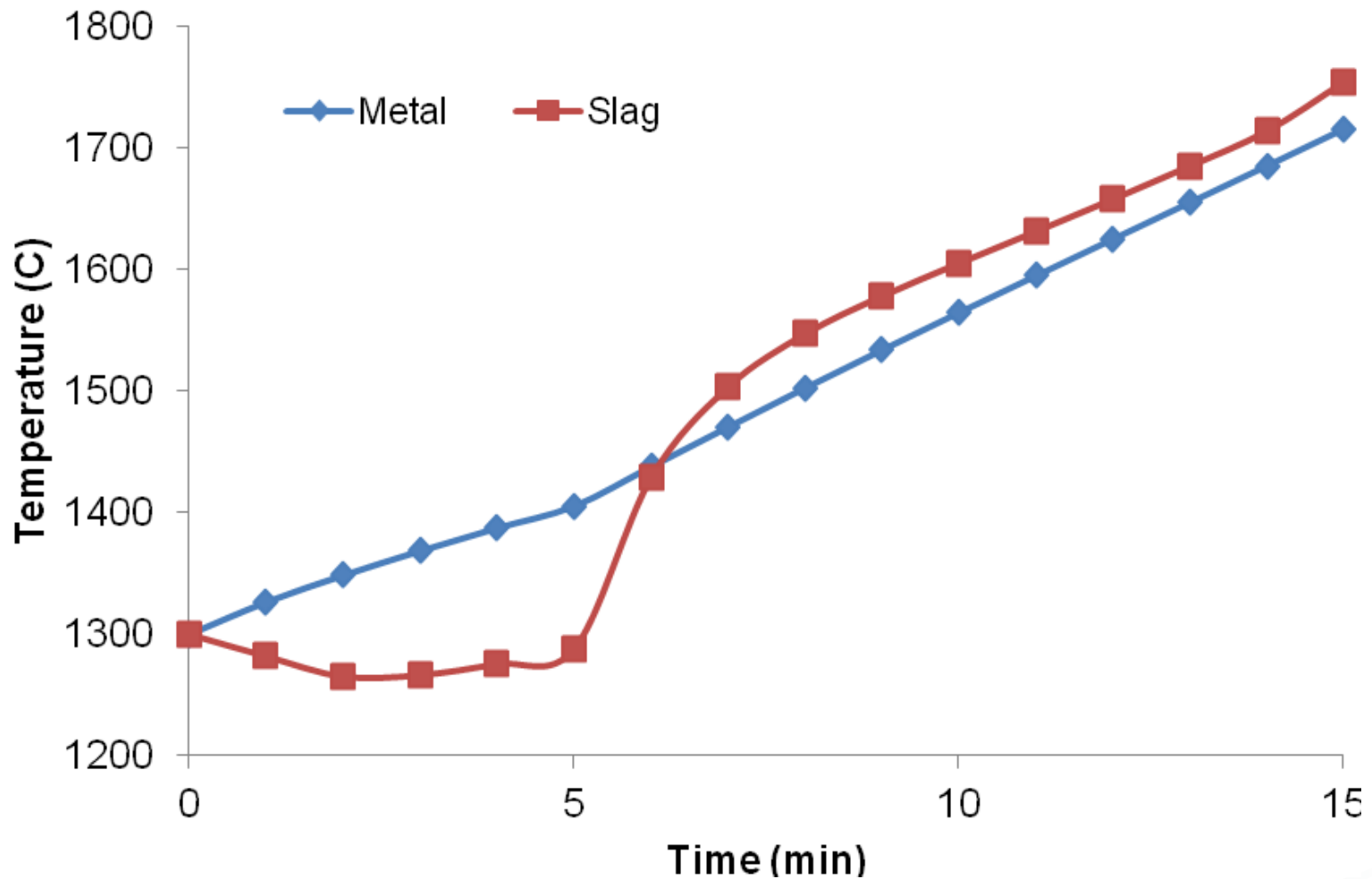
4. Main reactions – macro

```
102 // ***** START OF PROCESS *****
103 VARIABLE %tempflux %time %pos // variable declaration for main reactions
104 %tempflux OLE1 READ H10 // read and store flux temperature
105 %pos = 15 // first row to read input data
106
107 %time = 1 TO 15 // loop over the 15 calculations
108 OPEN %MyDir.EquiR1.dat // open the equilib file
109 %1 OLE1 READ R%posC3 // read the kinetic factor in excel
110 SET REACTANT 1 MASS %1 // overwrite the reactant amounts
111 %1 OLE1 READ R%posC7 // read the kinetic factor in excel
112 SET REACTANT 2 MASS %1 // overwrite the reactant amounts
113 %1 OLE1 READ R%posC5 // read the kinetic factor in excel
114 SET REACTANT 3 MASS %1 // overwrite the reactant amounts
115 CALC // calculate the equilibrium
116 SAVE %MyDir.MixtMetal_reacted.DAT FTmisc-FeLQ // save FeLQ as a stream
117 SAVE %MyDir.MixtSlag_reacted.DAT FToxid-SLAGA#1 // save SLAGA#1 as a stream
118
119 OPEN %MyDir.EquiR2.dat // open the equilib file
120 %1 OLE1 READ R%posC4 // read the kinetic factor in excel
121 SET REACTANT 1 MASS %1 // overwrite the reactant amounts
122 CALC // calculate the equilibrium
123 SAVE %MyDir.MixtMetal.dat FTmisc-FeLQ // save FeLQ as a stream
124
125 OPEN %MyDir.EquiR3.dat // open the equilib file
126 %1 OLE1 READ R%posC8 // read the kinetic factor in excel
127 SET REACTANT 1 MASS %1 // overwrite the reactant amounts
128 %1 OLE1 READ R%posC2 // read the kinetic factor in excel
129 SET REACTANT 3 MASS %1 // overwrite the reactant amounts
130 SET REACTANT 3 T %tempflux // overwrite the reactant temperature (flux)
131 IF %time = 1 THEN // if first calculation,
132 | SET REACTANT 4 MASS 0 // force the recycled CaO stream to be 0
133 | ENDIF // end of if
134 CALC // calculate the equilibrium
135 SAVE %MyDir.MixtSlag.dat FToxid-SLAGA#1 // save SLAGA#1 as a stream
136 SAVE %MyDir.MixtCaO.dat SOLIDS // save SOLIDS as a stream
137 %pos STEP // move to the next row to read inputs
138 %time LOOP // end of loop
139
140 END // end of macro
```

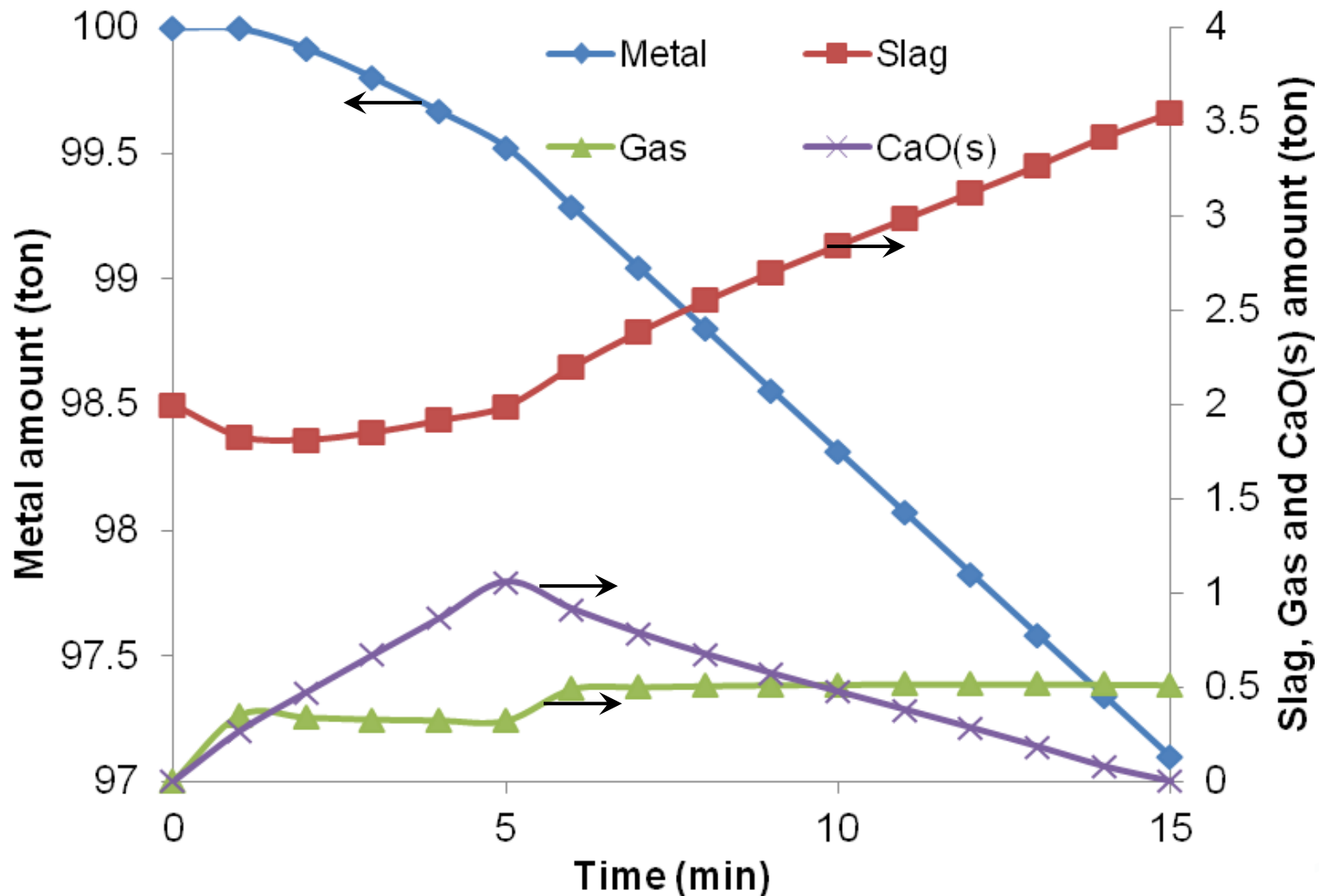
5. Organise the outputs in Excel

- 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)

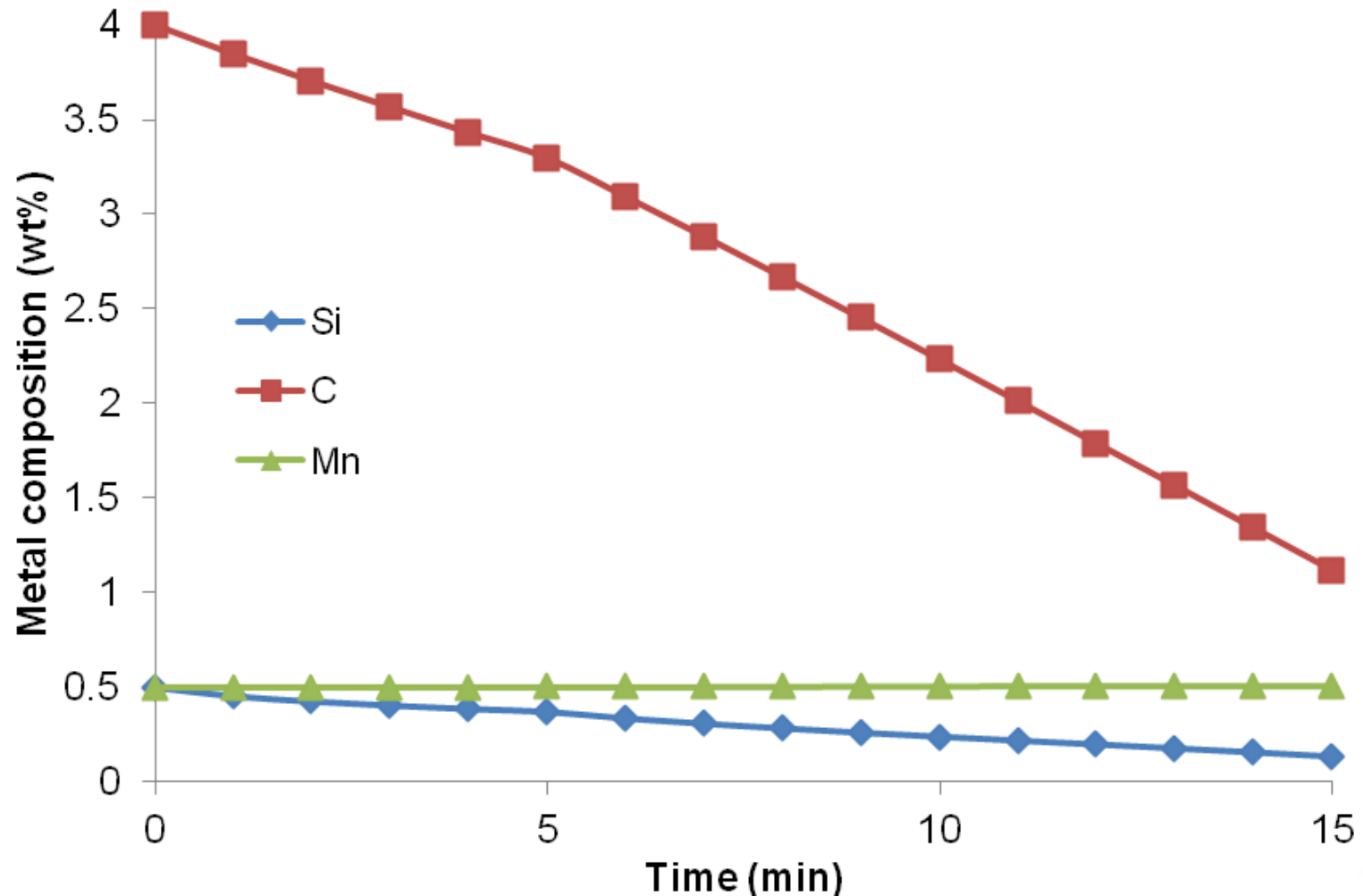
Results – Temperature profile



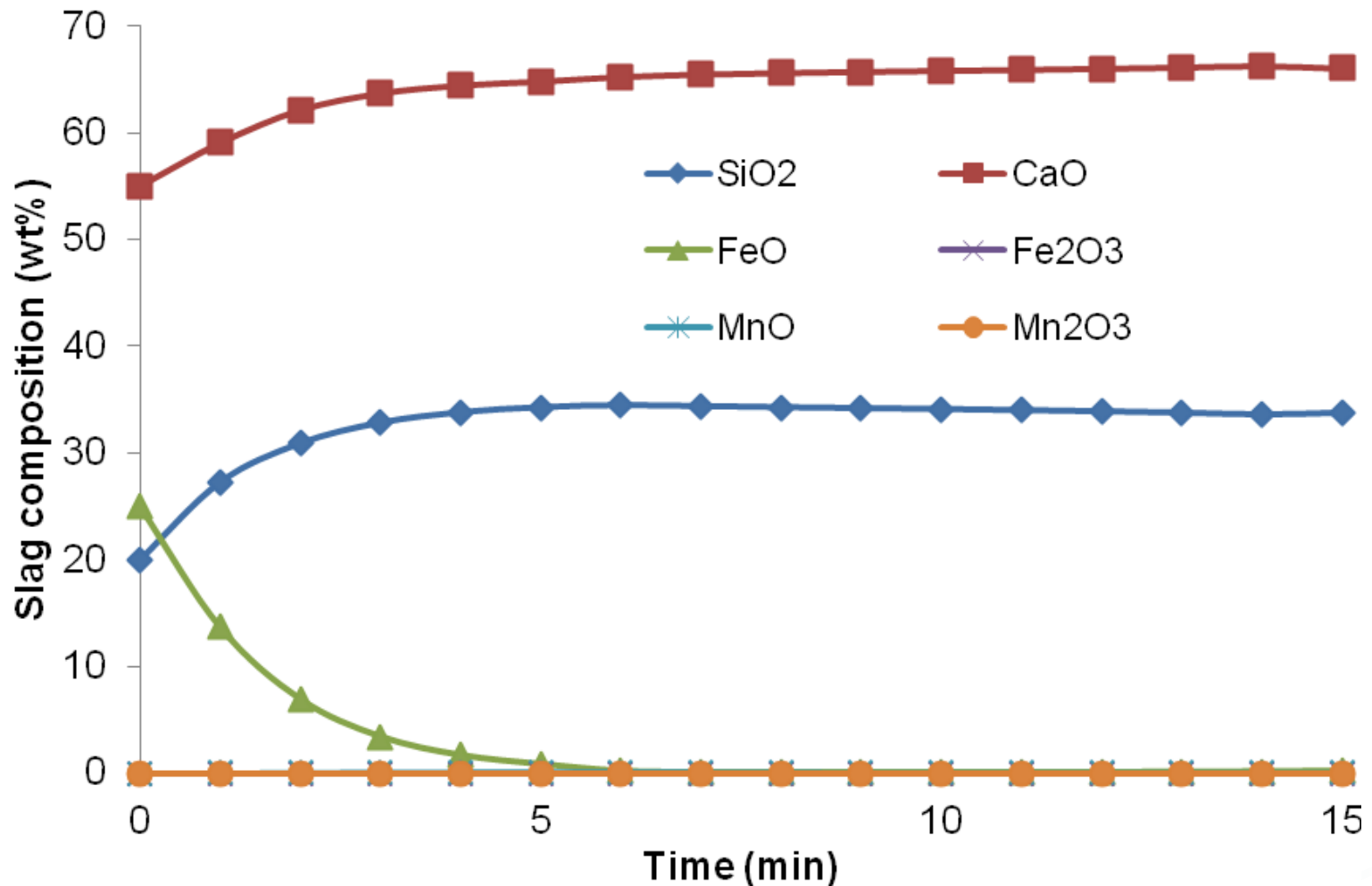
Results – Phases amount



Results – Metal composition



Results – Slag composition

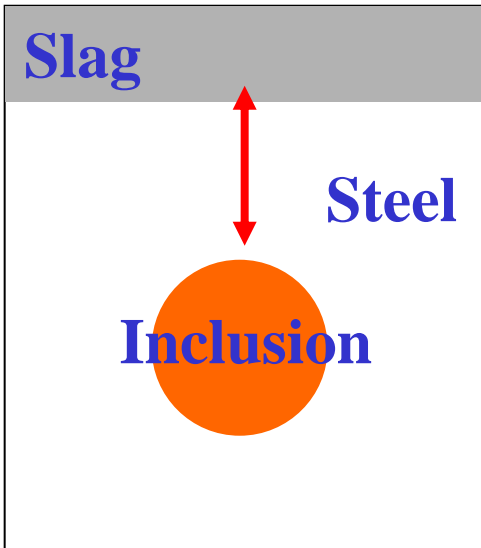


Application III

SLAG/STEEL/INCLUSION INTERACTION

*Evolution of inclusion chemistry by
indirect interaction with top slag*

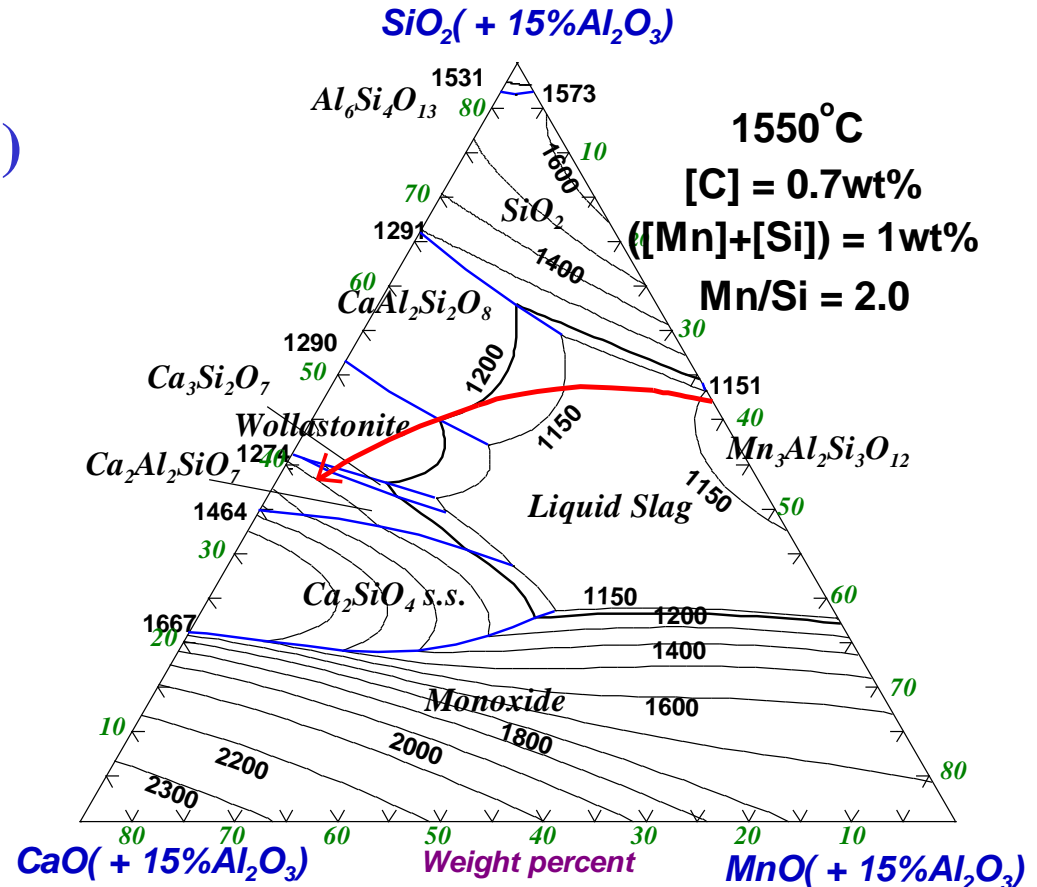
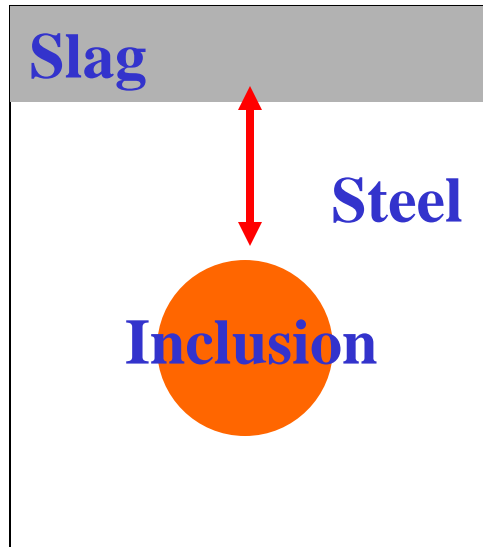
Slag/Steel/Inclusion Reactions



- 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.

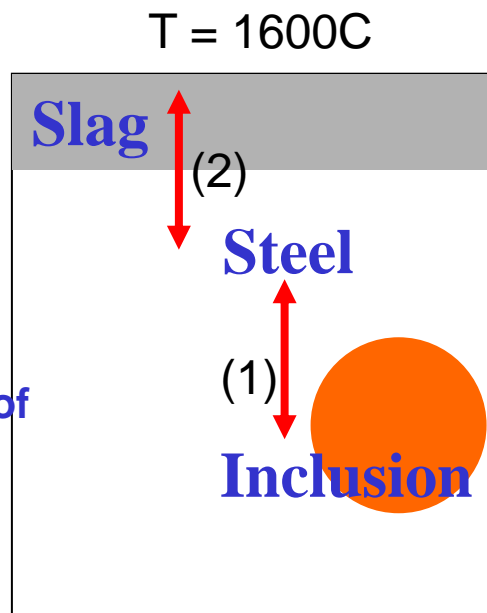
Modification of inclusion in LF by interaction with top slag

Top-Slag Composition
 $55\text{CaO}-15\text{Al}_2\text{O}_3-30\text{SiO}_2$ (wt%)



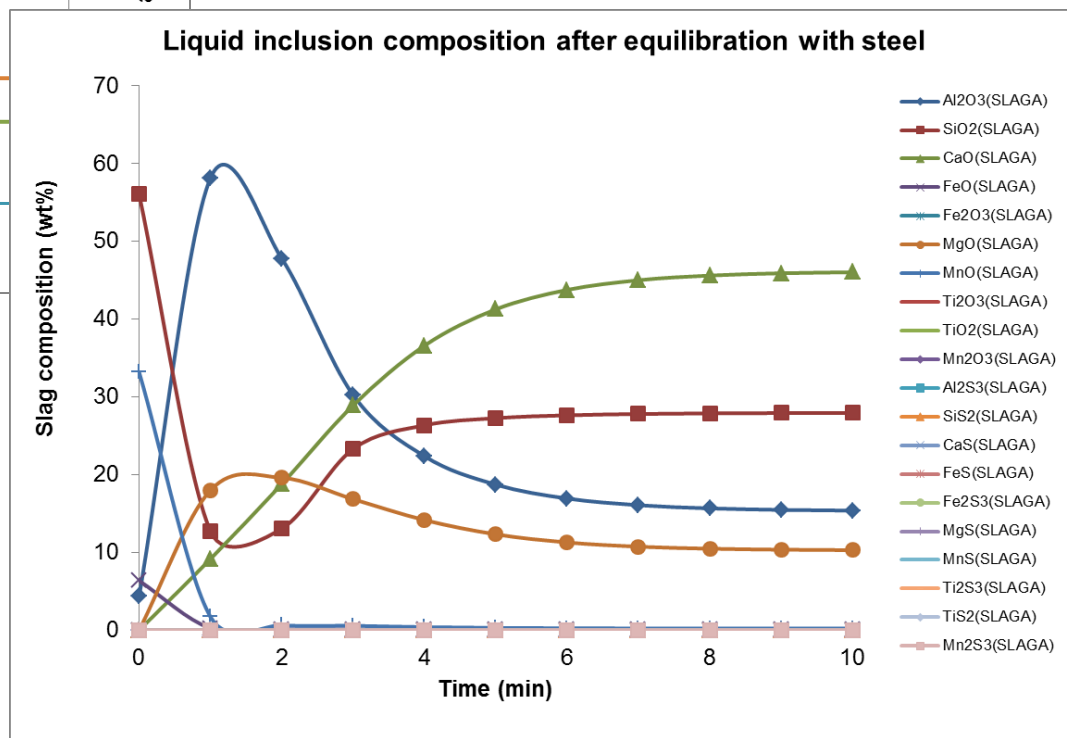
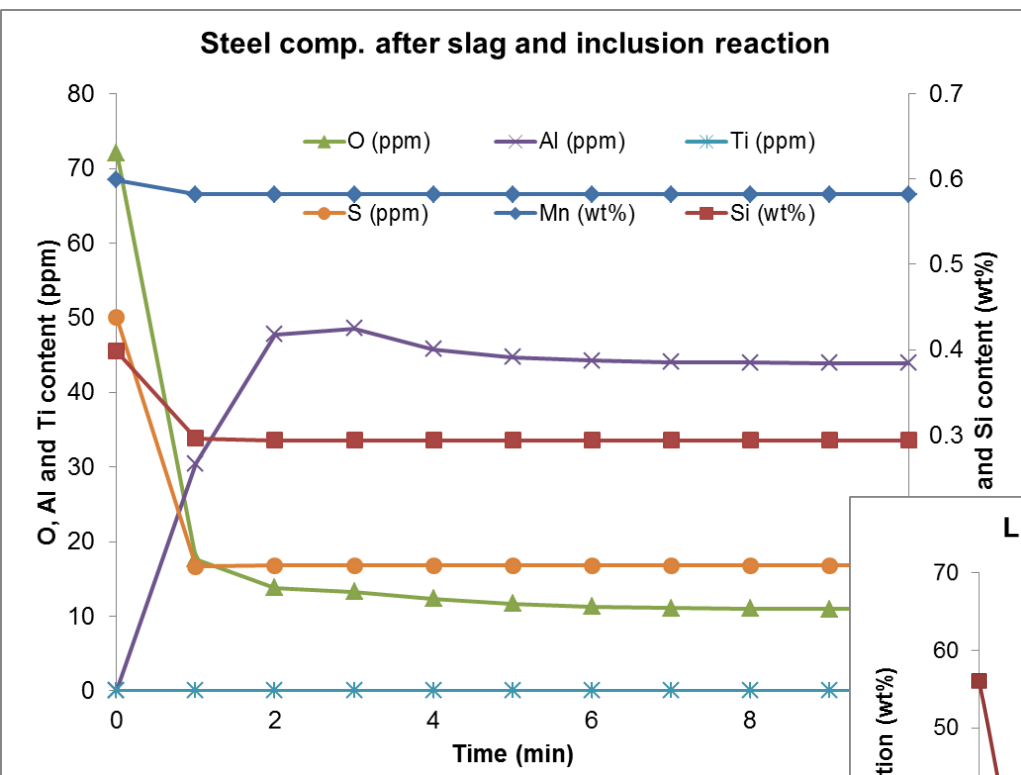
Slag/Steel/Inclusion Reaction: Macro processing input Excel file

	A	B	C	D	E	F	G	H	I	J
1	Temperature	1600 C	System temperature							
2	Duration	10 min	10 times iterations for (1) and (2) rxns.							
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	Relative amount is important for the change of inclusion chemistry							
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			



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

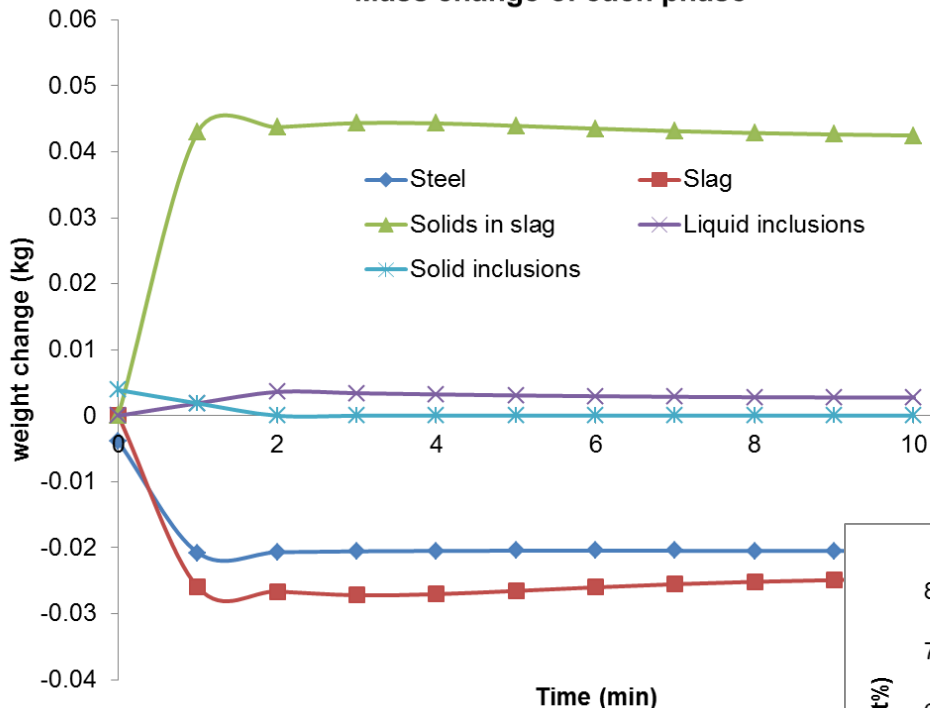
Reoxidation by high FeO ladle slag (for example, just after RH process)

	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			
26										
<div style="display: flex; justify-content: space-between; border: 1px solid gray; padding: 2px;"> Sheet1 Sheet2 Sheet3 </div> <div style="display: flex; justify-content: space-between; border: 1px solid gray; padding: 2px;"> Ready </div>										

Ladle slag with 5% FeO

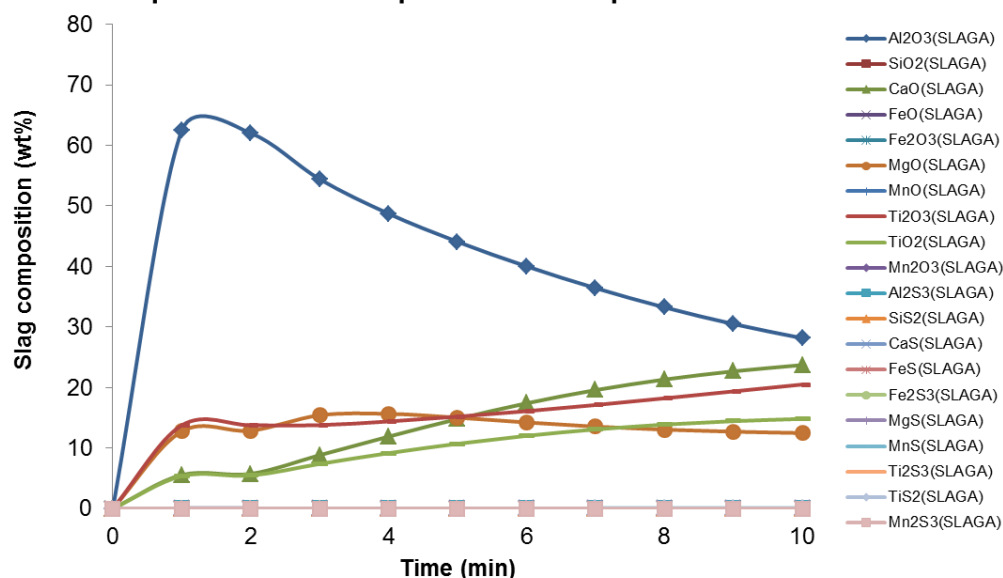
Reoxidation of Al-killed Ti-bearing steel: macro-processing

Mass change of each phase



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.

Liquid inclusion composition after equilibration with steel



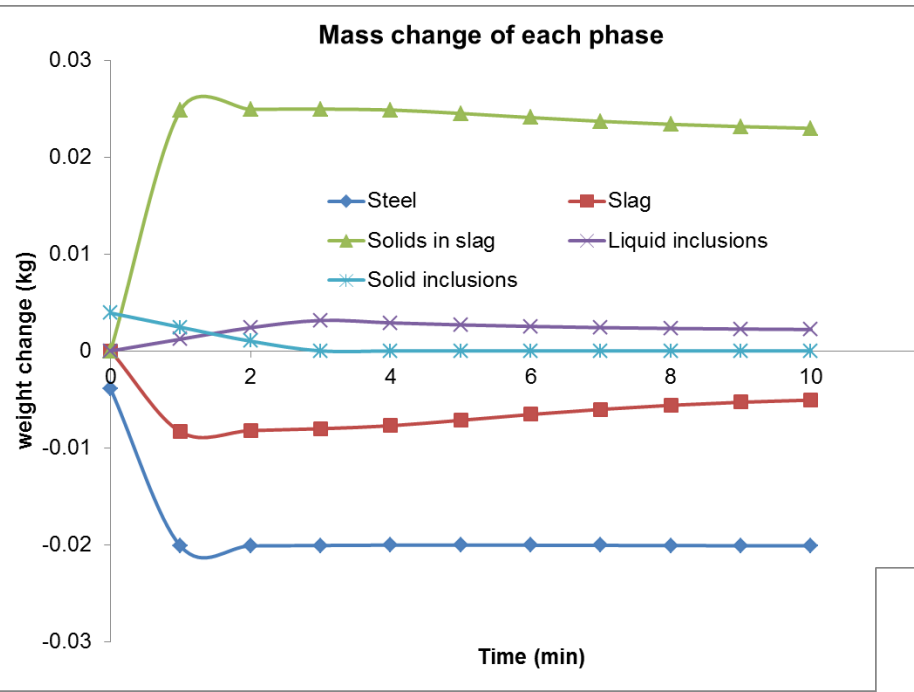
Reoxidation of Al-killed Ti-bearing steel: macro-processing

Reoxidation by high SiO₂ tundish slag (in Tundish)

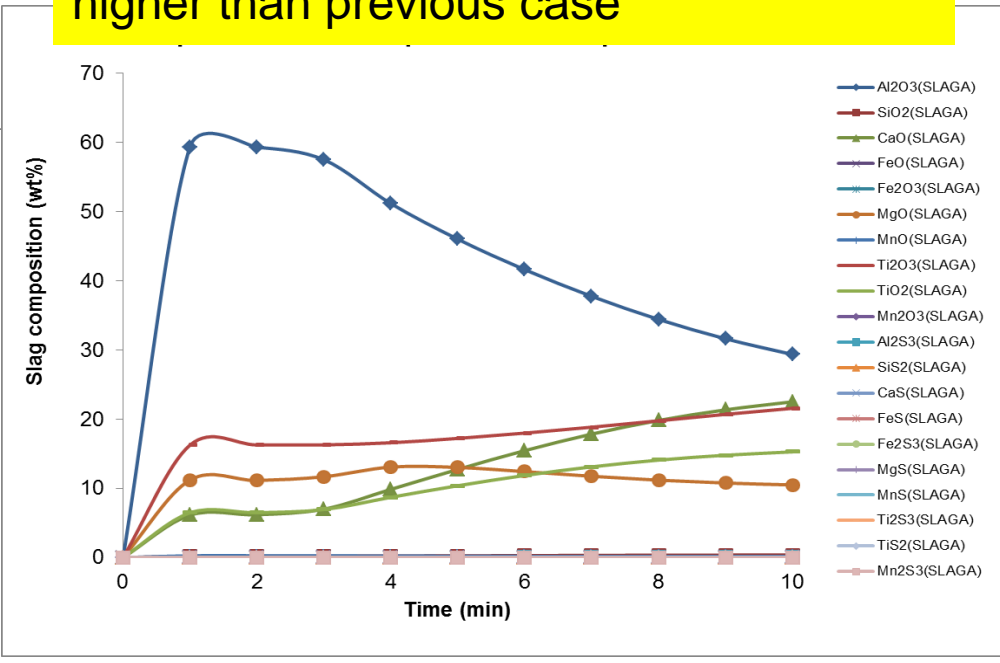
	A	B	C	D	E	F	G	H	I	J
1	Temperature	1600	C							
2	Duration	10	min							
3										
4	Steel amount:	100	kg							
5	Steel composition (wt%)									
6	Fe	Mn	Si	O	Al	Ti	S	Ca	Total	
7	98.8625	0.7	0.3	0.0025	0.03	0.1	0.005	0	100	
8										
9	Slag amount:	0.1	kg							
10	Slag composition (wt%)									
11	CaO	MgO	Al ₂ O ₃	SiO ₂	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	Al ₂ O ₃	SiO ₂	FeO	MnO	Total			
25	0.035	0.01	0.01	0.04	0.005	0	0.1			

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 inclusion 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



Thanks to FactSage Steelmaking Consortium Members

70



Natural Sciences and Engineering
Research Council of Canada

Developments of

- Thermodynamic database
- Process simulation model

Training for FactSage and Process simulation