

# Introduction to Tools in FactSage 8.4 for process modeling – Equilib, FactFlow and FactProSim

**Christopher W. Bale  
and  
Eve Bélisle**

 **CRCT** CENTRE FOR RESEARCH IN  
COMPUTATIONAL THERMOCHEMISTRY

**POLYTECHNIQUE  
MONTREAL** 

This presentation on process simulators is available at  
[www.factsage.com](http://www.factsage.com) <https://factsage.com/process-simulation/>

# Introduction to Tools in FactSage 8.4 for process modeling – Equilib, FactFlow and FactProSim



**Equilib** is a powerful tool for computing complex chemical equilibria but it can be a challenge when used for process modeling.

Users want to perform a series of equilibrium calculations using a user-friendly graphical interface.



**FactFlow** – developed by **Kyota Poëti, Jean-Philippe Harvey, Kentaro Oishi, Khloé Le Boulanger and Patrice Chartrand**

CRCT, Montreal



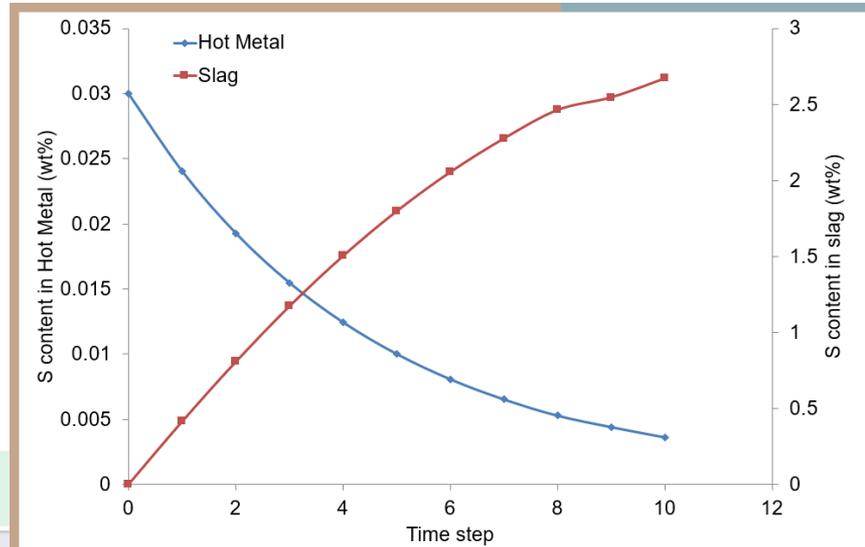
**FactProSim** – developed by **Nishant Kumar, Marie-Aline Van Ende and In-Ho Jung**

Seoul National University, South Korea

# Equilib macro processing

Example of an interactive process simulation of the desulfurisation of hot metal by the top slag.

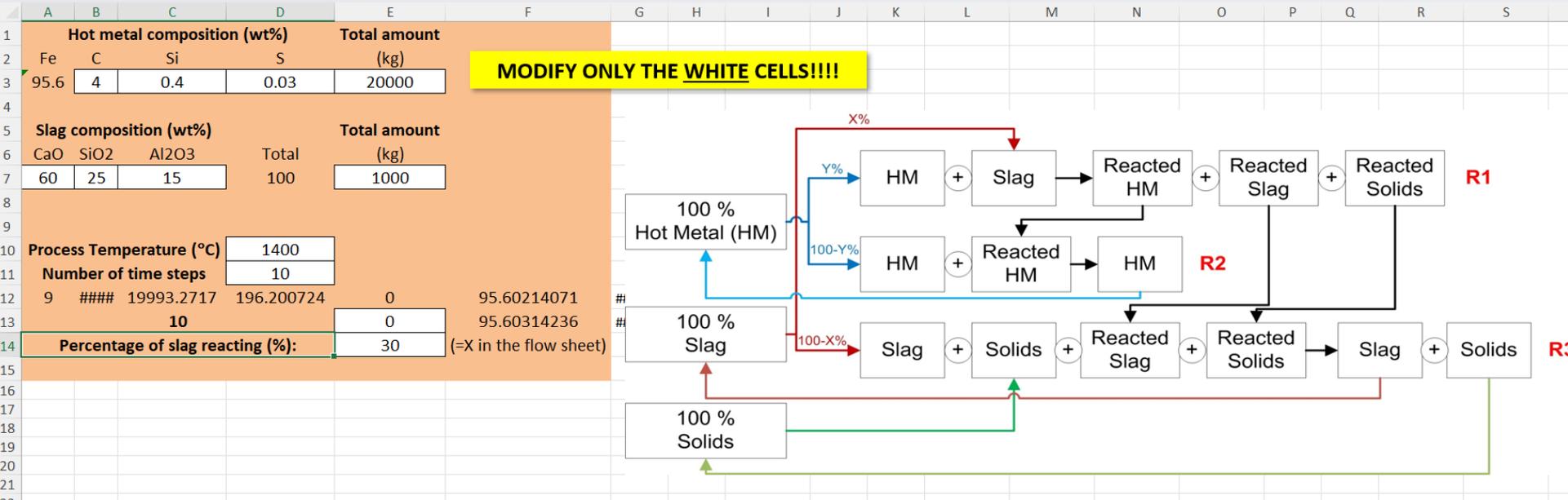
Marie-Aline Van Ende and In-Ho Jung, 2016



File Home Insert Draw Page Layout Formulas Data Review View Automate Help

Comments Share

A14 Percentage of slag reacting (%):

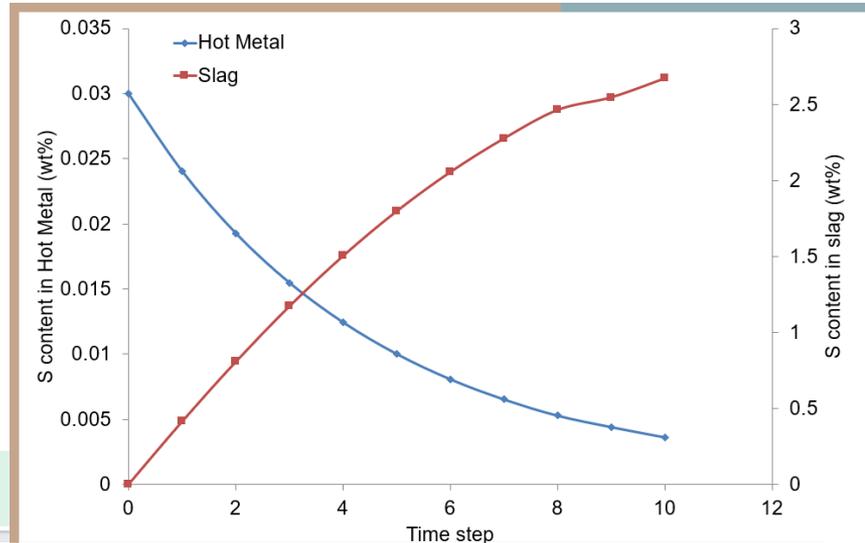


Macro stored in \MACROS\Ex\_Streams\EquiEx\_Streams.mac

# Equilib macro processing

Example of an interactive process simulation of the desulfurisation of hot metal by the top slag.

Marie-Aline Van Ende and In-Ho Jung, 2016



Hot metal composition (wt%)			
Fe	C	Si	S
95.6	4	0.4	0.03

Slag composition (wt%)			
CaO	SiO2	Al2O3	Total
60	25	15	100

Process Temperature (°C)	1400
Number of time steps	10
9	##### 19993.2717 196.200724
10	

Percentage of slag reacting (%):	
----------------------------------	--

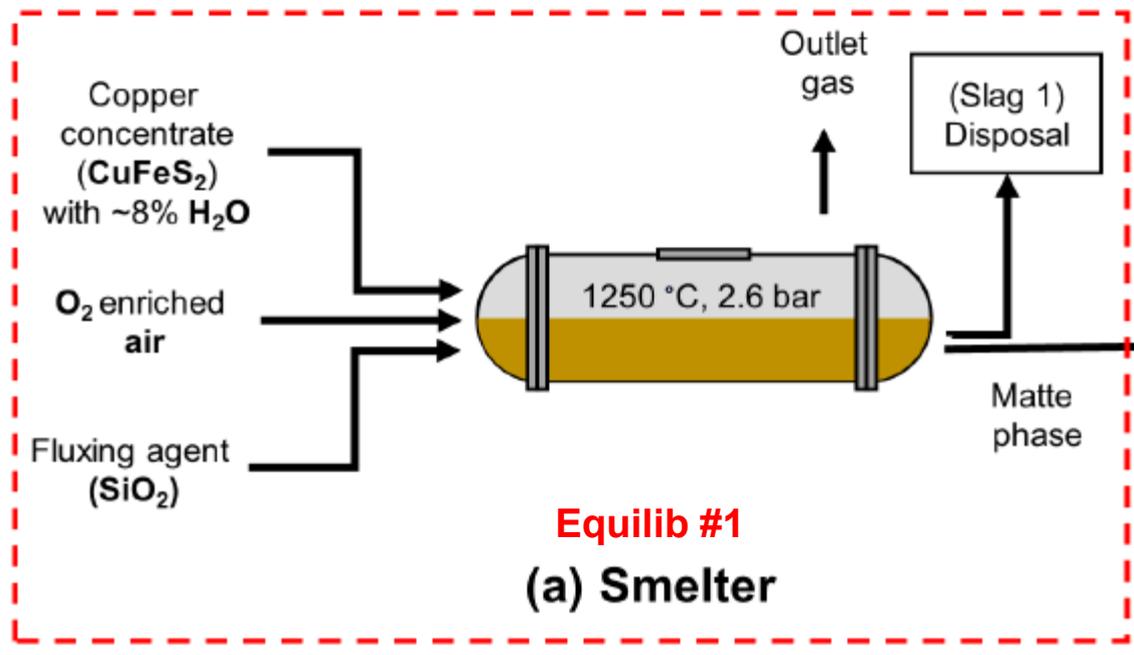
**A Kinetic Ladle Furnace Process Simulation Model: Effective Equilibrium Reaction Zone Model (EERZ model) Using FactSage Macro Processing.** - Metallurgical and Materials Transactions B, 2017.

**EERZ Approach for EAF:** the research extends the EERZ approach to other units like the Electric Arc Furnace (EAF), bridging the gap between melting and refining stages.

Development of the **FactProSim** process simulation package.

Macro stored in \MACROS\Ex\_Streams\EquiEx\_Streams.mac

# **E**quilib process modeling of copper production



**Overall reactions:**



**Databases:** **FactPS** (mainly gas) + **FToxid** (slag) + **FTmisc** (matte)

**Input:** CuFeS<sub>2</sub> (8 wt.% H<sub>2</sub>O) + enriched air (40 vol.% O<sub>2</sub>) + SiO<sub>2</sub> flux

**kgs:** 920 CuFeS<sub>2</sub> + 80 H<sub>2</sub>O + <0.4324 A> O<sub>2</sub> + <0.5676 A> N<sub>2</sub> + <B> SiO<sub>2</sub>



Data Search - Equilib 8.4

Databases - 3/17 compound databases, 2/16 solution databases

**Fact** **FactSage™** **SGTE**

FactPS  FScopp  BINS  compounds only  
 FToxid  FSlead  SGPS  solutions only  
 FTsulf  FSstel  SGTE  no database  
 FTsalt  FSupsi  SGTE  
 FTmisc  
 FTball  
 FTOxCN  ELEM

**Private Databases**  
 Coke  SURF  VIRT

Clear All  
Add/Remove Data

Equilib - Reactants

File Edit Run Macro Table Units Data Search Data Evaluation Help

T(C) P(bar) Energy(J) Quantity(kg) Vol(litre)

1-5

Quantity(kg)	Species	Phase	T(C)	P(total)**	Stream#	Data
920	CuFeS2				1	
+ 80	H2O				1	
+ <0.4324A>	O2				2	
+ <0.5676A>	N2				2	
+ <B>	SiO2				3	

Initial Conditions

Next >>

FactSage 8.4 Compound: 3/17 databases Solution: 2/16 databases

kgs: 920 CuFeS<sub>2</sub> + 80 H<sub>2</sub>O + <0.4324 A> O<sub>2</sub> + <0.5676 A> N<sub>2</sub> + <B> SiO<sub>2</sub>



T(C) P(bar) Energy(J) Quantity(kg) Vol(litre)



## Reactants (5)

(kg) 920 CuFeS2 + 80 H2O + <0.4324A> O2 + <0.5676A> N2 + <B> SiO2

## Products

## Compound species

gas  ideal  real 66  
 aqueous 0  
 pure liquids 25  
 pure solids 98  
 \* - custom selection species: 189

## Target

- none -

Estimate T(K): 1000

Quantity(kg): 0

## Solution phases

*	+	Base-Phase	Full Name
	+	FTmisc-FeLQ	Fe-liq
	+	FTmisc-CuLQ	Cu-liq_or_speiss
	+	FTmisc-FeCu	fcc_Fe-Cu
	+	FTmisc-MATT	Matte
	+	FTmisc-FeS_	FeS-liq
		FToxid-SLAGA	A-Slag-liq all oxides + S
	+	FToxid-SPINC	C-Spinel
	+	FToxid-MeO_A	A-Monoxide

## Legend

| - immiscible 1  
 + - selected 7

 Show  all  selected

species: 51  
solutions: 9

## Custom Solutions

0 fixed activities   
0 ideal solutions

## Pseudonyms

apply

## Volume and physical prop data

assume molar volumes of solids and liquids = 0  
 use only molar volume data  
 use V & phys. property data

 paraequilibrium & Gmin 

Total Species (max 7000) 240

Total Solutions (max 200) 9

Total Phases (max 1500) 133

## Final Conditions

<A>	<B>	T(C)	P(bar)	Product H(J)
0	1000	10	0	1250
2.6				

10 steps  Table

101 calculations

## Equilibrium

normal  normal + transitions  
 transitions only  open

- no time limit -

- recommend you not select both pure liquids and molten solutions -

**Output Quantity Units**

mol  g  lb  kg  tonne  default

**Output**

lower limit :

show only stable phases

show date

**Data Source**

never  
 always  
 >1 cpd or soln database

show bond fractions etc.

show elapsed time (>0.1 sec)

**History**

save previous calculations - see Directory Window

**Time Limit**

elapsed time limit  secs

**Dilute Extrapolation**

Parameter (cal)

species: 189

+	FToxid-SLAG_A	A-Slag-liq all oxides + S
+	FToxid-SPINC	C-Spinel
+	FToxid-MeO_A	A-Monoxide

use only molar volume data  
 use V & phys. property data

paraequilibrium & Gmin

Total Species (max 7000) 240  
 Total Solutions (max 200) 9  
 Total Phases (max 1500) 133

**Target**

- none -  
 Estimate T(K):   
 Quantity(kg):

**Legend**

l - immiscible 1  
 + - selected 7

Show  all  selected

species: 51  
 solutions: 9

**Final Conditions**

<A>	<B>	T(C)	P(bar)	Product H(J)
0	1000	10	0	1250
10	steps	<input type="checkbox"/> Table		

101 calculations

**Equilibrium**

normal  normal + transitions  
 transitions only  open

- no time limit -

- recommend you not select both pure liquids and molten solutions -



T(C) P(bar) Energy(J) Quantity(kg) Vol(litre)



## Reactants (5)

(kg) 920 CuFeS2 + 80 H2O + <0.4324A> O2 + <0.5676A> N2 + <B> SiO2

## Products

## Compound species

gas  ideal  real 66  
 aqueous 0  
 pure liquids 25  
 pure solids 98  
 \* - custom selection species: 189

## Target

- none -

Estimate T(K): 1000

Quant

## Final Condition

&lt;A&gt;

0 1000 10

10 steps

## Solution phases

*	+	Base-Phase	Full Name
	+	FTmisc-FeLQ	Fe-liq
	+	FTmisc-CuLQ	Cu-liq_or_speiss
	+	FTmisc-FeCu	fcc_Fe-Cu
	+	FTmisc-MATT	Matte
	+	FTmisc-FeS_	FeS-liq
I		FToxid-SLAGA	A-Slag-liq all oxides + S
	+	FToxid-SPINC	C-Spinel
	+	FToxid-MeO_A	A-Monoxide

## Legend

I - immiscible 1  
 + - selected 7

 Show  all  selected

species: 51

## Custom Solutions

0 fixed activities  
0 ideal solutions

Details ...

## Pseudonyms

apply 

Edit ...

## Volume and physical prop data

assume molar volumes of  
 solids and liquids = 0  
 use only molar volume data  
 use V & phys. property data

 paraequilibrium & Gmin edit

Total Species (max 7000) 240

Total Solutions (max 200) 9

Species (max 1500) 133

 normal + transitions

 only  open

Calculate &gt;&gt;

This **Equilib** example is stored in your computer in the file **Cu-without-E-waste.equi**.

- recommend you not select both pure liquids and molten solutions -

# 1000 kg feed + <A> kg enr-air + 0 kg SiO<sub>2</sub> , 1250 C

Equilib - Results A=680 (page 69/101) page 69/101

Output Edit Show Pages Final Conditions

680 kg enr-air T(C) P(bar) Energy(J) Quantity(kg) Vol(litre)

A=500 | A=510 | A=520 | A=530 | A=540 | A=550 | A=560 | A=570 | A=580 | A=590 | A=600 | A=610 | A=620 | A=630 | A=640 | A=650 | A=660 | A=670 | **- A=680 -** | A=690 | A=700 | A=710 | A=720 | A=730 | A=740

FactSage 8.4

(kg) 920 CuFeS<sub>2</sub> + 80 H<sub>2</sub>O + <0.4324A> O<sub>2</sub> + <0.5676A> N<sub>2</sub> +

(kg) <(0)> SiO<sub>2</sub> =

24743. mol gas\_ideal  
 (8.8285E+05 gram, 24743. mol, 1.2052E+06 litre, 7.3254E-04 gram.cm-3)  
 (1250 C, 2.6000 bar, a=1.0000)

( 0.55685	N <sub>2</sub>
+ 0.26054	SO <sub>2</sub>
+ 0.17588	H <sub>2</sub> O
+ 2.8879E-03	H <sub>2</sub>
+ 1.9588E-03	S <sub>2</sub>
+ 8.4696E-04	SO
+ 6.7954E-04	H <sub>2</sub> S
+ 3.0515E-04	SSO

**gas**

+ 476.21 kg Matte  
 (4.7621E+05 gram, 9296.0 mol)  
 (1250 C, 2.6000 bar, a=1.0000)  
 ( 23.085 wt.% S  
 + 10.024 wt.% Fe  
 + 66.891 wt.% Cu)

**476 kg matte**

System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Cu	5012.7	3.1854E+05	0.53924	0.66891
Fe	854.78	47735.	9.1952E-02	0.10024
S	3428.4	1.0993E+05	0.36881	0.23085

+ 320.94 kg Spinel  
 (3.2094E+05 gram, 1386.2 mol)  
 (1250 C, 2.6000 bar, a=1.0000)

( 20.526	wt.% Fe <sub>3</sub> O <sub>4</sub>
+ 23.606	wt.% Fe <sub>3</sub> O <sub>4</sub> [1-]
+ 45.108	wt.% Fe <sub>3</sub> O <sub>4</sub> [1+]

**spinel**

# 1000 kg feed + <A> kg enr-air + 0 kg SiO<sub>2</sub> , 1250 C

Equilib - Results A=680 (page 69/101) EQUIINTE Intel 2025-06-01 page 69/101

Output Edit Show Pages Final Conditions

680 kg enr-air

A=500 | A=510 | A=520 | A=530 | A=540 | A=550 | A=560 | A=570 | A=580 | A=590 | A=600 | A=610 | A=620 | A=630 | A=640 | A=650 | A=660 | A=670 | **A=680** | A=690 | A=700 | A=710 | A=720 | A=730 | A=740

PHASE:	EQUIL AMOUNT	MOLE FRACTION	FUGACITY	DATABASE
gas_ideal	mol		bar	
N2	1.3778E+04	5.5685E-01	1.4478E+00	FactPS
SO2	6.4466E+03	2.6054E-01	6.7741E-01	FactPS
H2O	4.3517E+03	1.7588E-01	4.5728E-01	FactPS
H2	7.1456E+01	2.8879E-03	7.5086E-03	FactPS
S2	4.8466E+01	1.9588E-03	5.0929E-03	FactPS
SO	2.0956E+01	8.4696E-04	2.2021E-03	FactPS
H2S	1.6814E+01	6.7954E-04	1.7668E-03	FactPS
SSO	7.5502E+00	3.0515E-04	7.9338E-04	FactPS
TOTAL:	2.4743E+04	1.0000E+00	1.0000E+00	
System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Cu	3.0944E-02	1.9664	5.1310E-07	2.2273E-06
Fe	8.1491E-02	4.5508	1.3512E-06	5.1547E-06
S	6597.7	2.1155E+05	0.10940	0.23963
O	17274.	2.7637E+05	0.28642	0.31304
N	27556.	3.8597E+05	0.45691	0.43718
H	8881.3	8951.9	0.14726	1.0140E-02
PHASE: Matte_FTmisc	kg	MASS FRACTION	ACTIVITY	DATABASE
S	1.0993E+02	2.3085E-01	4.2210E-03	FTmisc
Fe	4.7735E+02	1.0024E-01	5.5998E-03	FTmisc
Cu	3.1854E+02	6.6891E-01	7.2814E-02	FTmisc
TOTAL:	4.7621E+02	1.0000E+00	1.0000E+00	
System component	Amount/mol	Amount/gram	Mole fraction	Mass fraction
Cu	5012.7	3.1854E+05	0.53924	0.66891
Fe	854.78	47735.	9.1952E-02	0.10024
S	3428.4	1.0993E+05	0.36881	0.23085
PHASE: Spinel_FToxid	kg	MASS FRACTION	ACTIVITY	DATABASE
Fe3O4	6.5876E+01	2.0526E-01	1.8088E-01	FToxid
Fe3O4[1-]	7.5761E+01	2.3606E-01	1.0152E-01	FToxid
Fe3O4[1+]	1.4477E+02	4.5108E-01	2.6259E-01	FToxid
Fe3O4[2-]	3.4474E+01	1.0741E-01	1.9933E-02	FToxid

476 kg matte

Output

Edit Show Pages Final Conditions

Save or Print As ...

Repeat Save

Plot

Plot Results ...

Equilib Results file

Repeat Plot - gram vs Alpha ...

Stream File

Format

Fact-XML

Fact-Optim

Fact-Functi

Refresh ...

Swap loops

+ 856.86  
(8.5686E

fraction

where "A"

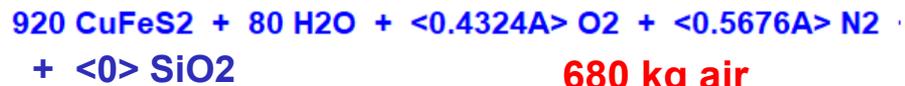
Show only  
Cut-off list

T(C) P(bar) Energy(J) Quantity(kg) Vol(litre)

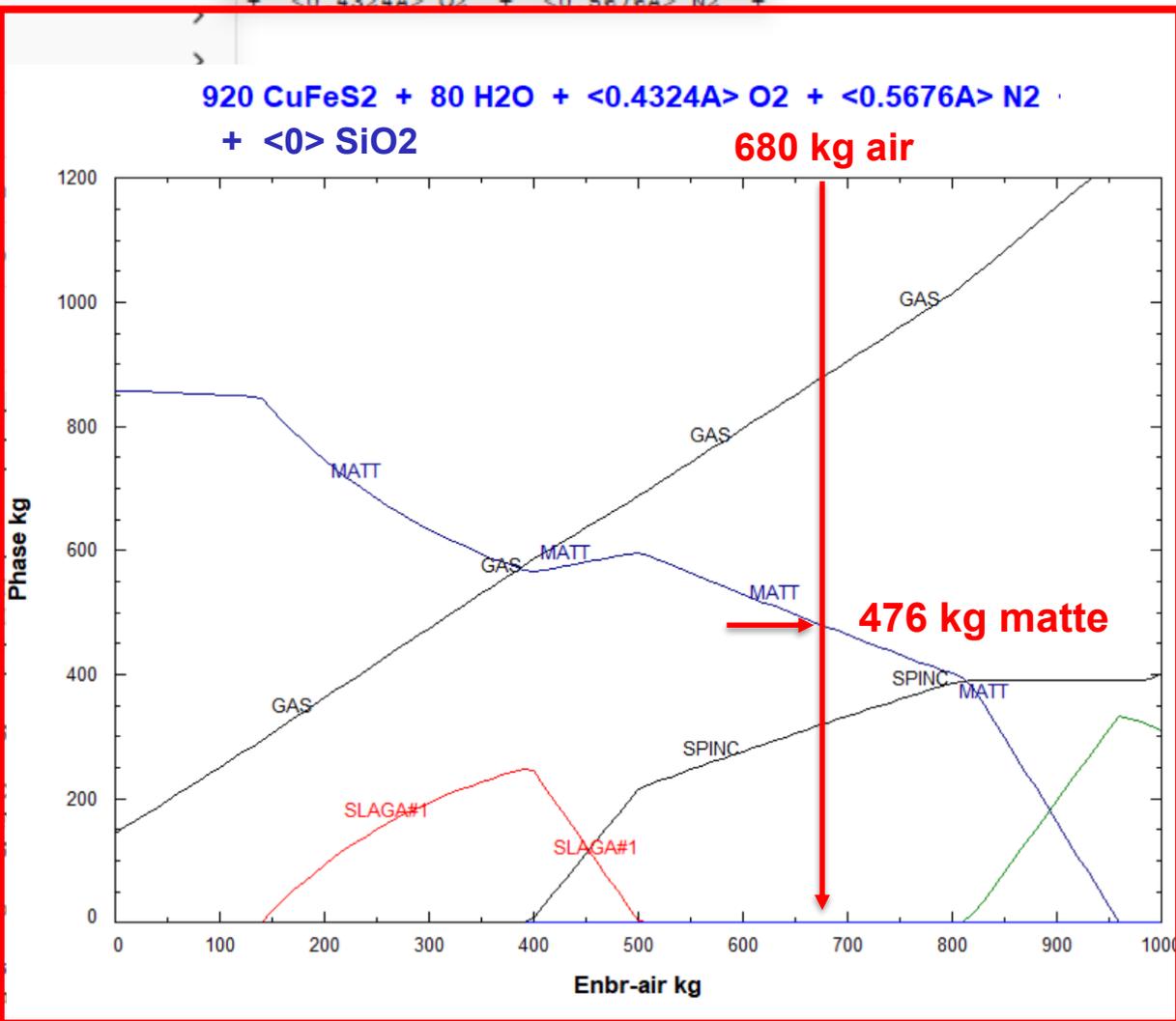
=170 | A=180 | A=190 | A=200 | A=210 | A=220 | A=230 | A=240

110 | A=120 |

FactSage 8.4



680 kg air



**Fact-XML**

Output Edit Show Pages Final Conditions



T(C) P(bar) Energy(J) Quantity(kg) Vol(litre)



A=130 A=140

XML Viewer - [C:\FACTSAGE84\_ALCOA\Xml\_out.xml]

A=0 A=10 A=

File Units Tools **Graph** Help

(kg) 920 Cu

(kg) < (0)>

5370.9

(1.4314E

+ 856.86

(8.5686E

fraction

where "A"

Show only

Cut-off l

Fact Format **AtomSage** Format

```
<?xml version="1.0" encoding="utf-8"?>
<!-- Reference :
T = temperature
P = pressure
V = volume
n = moles
g = grams
a = activity
X = mol fraction
w = weight %
mw = molecular weight
Z = G (Gibbs energy), H (enthalpy), S (entropy)
Zint = integral G, H, S or Cp
Zpar = partial G, H, S or Cp
Zintxs = integral excess G, H or S
Zparxs = partial excess G, H or S
-->
<file id="001" version="5.60" user="01" ...
#EData: Contents Equi0.dat
<FILE>
FILE 0 10:14 22Dec25 Alcoa Tec
last system
'O' '13'
'TC' 'BAR' 'J' 'NOVPT' 'NOPHYS' 'CUT' '1e-
'O' '10'
'CXHY' '2' 'NOGIONTK' '2000' 'NODEMO'
'O' '7'
'LIM' '250' '10000' '1.000E-35' '1.000E+0
'O' '6'
'NOTRNS' 'TRNIM' '0' 'NOPARA' '7 1
```

**Graph - Setup**

Saved graphs... f Function Builder

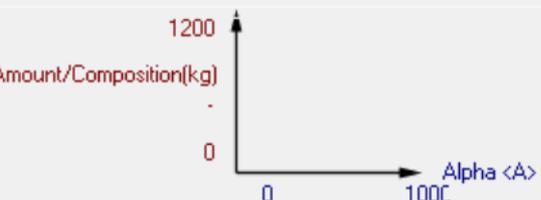


Figure Settings

Font size : 14

# labels per line : 4

line colors... Title

Full Screen

**Y-Axis**

Amount/Composition Y + variable

f1=

MIN	MAX	STEP	Label every
0	1200	Default	100

**X-Axis**

Alpha <A> X + variable

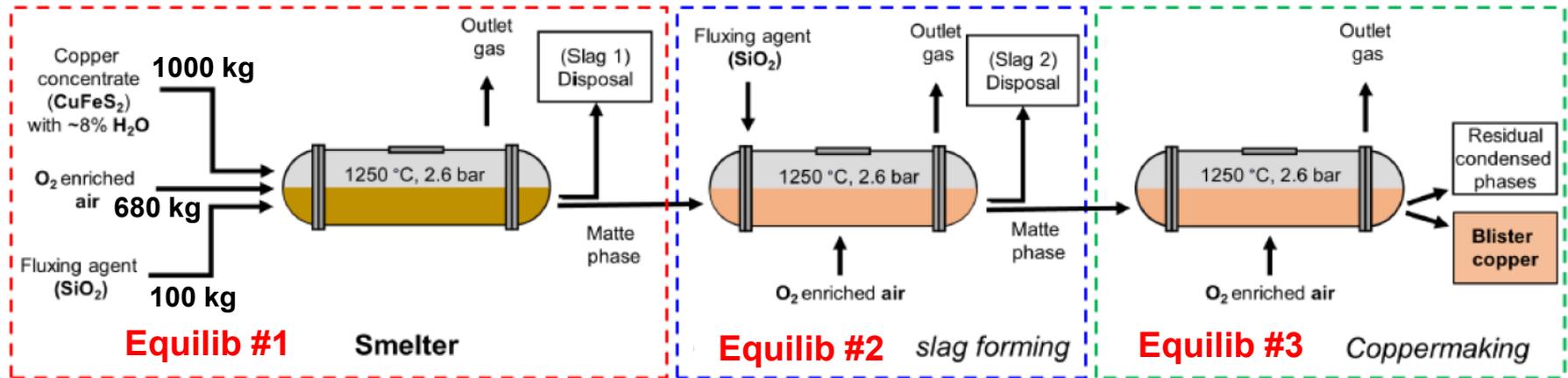
f =

MIN	MAX	STEP	Label every
0	1000	Default	1

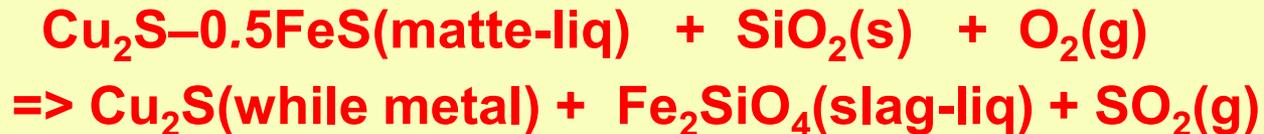
Species/phases:

	Species	Phase	Data	Amount/Co...	MIN	MAX	Pseudonym
<input type="checkbox"/>	CuO_Tenorite	s	FToxid	0.000E+00	0.000E+00	0.000E+00	
<input type="checkbox"/>	Cu2O_solid	s	FToxid	0.000E+00	0.000E+00	0.000E+00	
<input type="checkbox"/>	CuFeO2_solid	s	FToxid	0.000E+00	0.000E+00	0.000E+00	
<input type="checkbox"/>	CuFe2O4_tetrag...	s	FToxid	0.000E+00	0.000E+00	0.000E+00	
<input checked="" type="checkbox"/>	Gas	-		1.431E+02	1.289E+03	1.431E+02	
<input type="checkbox"/>	Fe-liq	-	FTmisc	0.000E+00	0.000E+00	0.000E+00	
<input type="checkbox"/>	Cu-liq_or_speiss	-	FTmisc	0.000E+00	0.000E+00	1.291E+01	
<input type="checkbox"/>	fcc_Fe-Cu	-	FTmisc	0.000E+00	0.000E+00	0.000E+00	
<input checked="" type="checkbox"/>	Matte	-	FTmisc	8.569E+02	0.000E+00	8.569E+02	
<input type="checkbox"/>	FeS-liq	-	FTmisc	0.000E+00	0.000E+00	0.000E+00	
<input checked="" type="checkbox"/>	Slag-liq#1	-	FToxid	0.000E+00	0.000E+00	9.621E-01	
<input type="checkbox"/>	Slag-liq#2	-	FToxid	0.000E+00	0.000E+00	0.000E+00	
<input type="checkbox"/>	Spinel	-	FToxid	0.000E+00	0.000E+00	6.817E+00	
<input type="checkbox"/>	Monoxide	-	FToxid	0.000E+00	0.000E+00	0.000E+00	

Clear  mol  mol fract.  gram  Wt. fract.  Wt. %  kg  lb

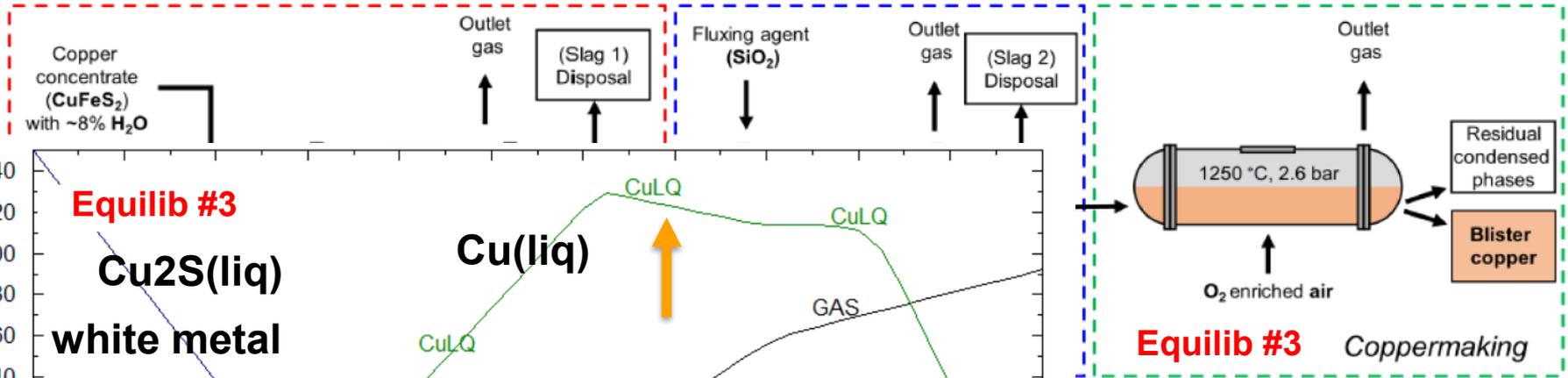


Matte **Equilib #1** (smelter) is input for **Equilib #2** (slag forming)

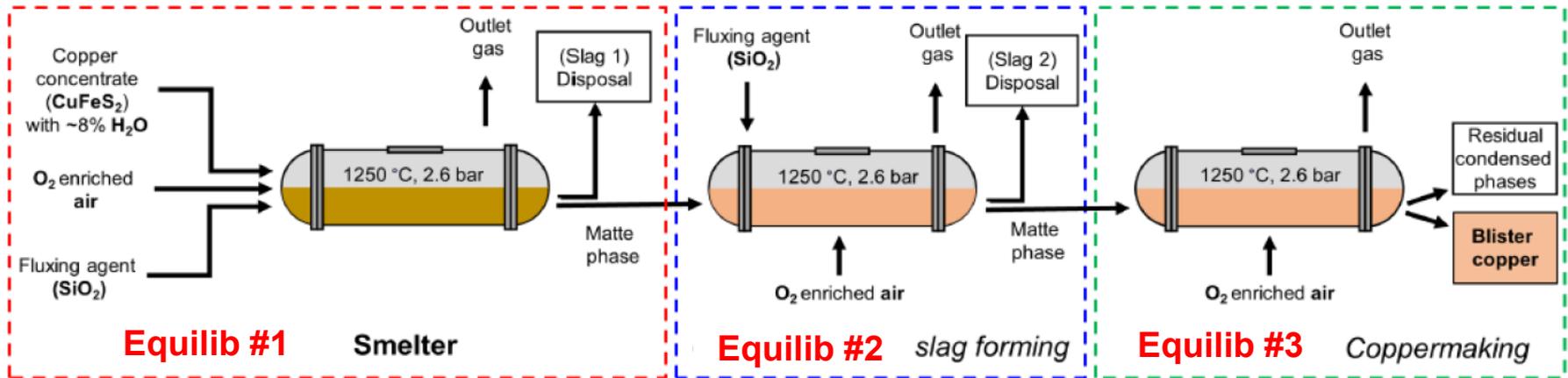


Matte (white metal) from **Equilib #2** (slag forming) is input for **Equilib #3** (copper making)

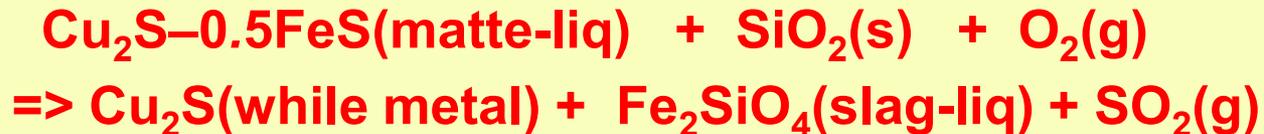




slag forming)  
 +  $\text{O}_2(\text{g})$   
 liq) +  $\text{SO}_2(\text{g})$   
 input for **Equilib #3**  
 ter copper) +  $\text{SO}_2(\text{g})$



Matte **Equilib #1** (smelter) is input for **Equilib #2** (slag forming)



Matte (white metal) from **Equilib #2** (slag forming) is input for **Equilib #3** (copper making)



Sequentially executing stream-related tasks in **Equilib** can be done by **macro processing**. But this is time-consuming and difficult to automate.

Let us employ the process simulation packages **FactFlow** and **FactProSim**.

# Equilib precursor for FactFlow and FactProSim

The screenshot shows the 'Equilib - Reactants' application window. The 'File' menu is open, and the 'FactFlow files' sub-menu is selected. The 'FactFlow' label is highlighted in a yellow box. The 'FactFlow files' sub-menu is also highlighted with a red box, and the 'Summary of .equi files' option is highlighted with a red box.

File	Shortcut
New	Ctrl+N
Open ...	Ctrl+O
Directories ...	Ctrl+D
FactFlow files	>
FactProSim files	>
ChemSage files	>
TDB files	>
Macro processing	>

FactFlow files
Information ...
FactFlow directory
Summary of .equi files
Summary of .equi files - long
Summary of .cst files
Summary of .cst files - long

The screenshot shows the 'Equilib - Reactants' application window. The 'File' menu is open, and the 'FactProSim files' sub-menu is selected. The 'FactProSim' label is highlighted in a yellow box. The 'FactProSim files' sub-menu is also highlighted with a red box, and the 'Summary of .equi files' option is highlighted with a red box.

File	Shortcut
New	Ctrl+N
Open ...	Ctrl+O
Directories ...	Ctrl+D
FactFlow files	>
FactProSim files	>
ChemSage files	>
TDB files	>
Macro processing	>
Exit	

FactProSim files
Information ...
FactProSim folder
Summary of .equi files
Summary of .equi files - long
Summary of .cst files
Summary of .cst files - long
Summary of .ppf files

# Summary of Equilib .equi files in FactProSim

```
Equilib Files *.equi in C:\FACTSAGE84\FactProSim\Projects\
File Edit
This summary is stored in C:\FACTSAGE84\FactProSim\Projects\Summary_EQUI.txt
Summary of Equilib .equi files in FactProSim \FactProSim\Projects\*.equi
=====
1.1 **** Equi-file BOF_database.equi: (BOF_database.cst)
Path: C:\FactSage84\FactProSim\Projects\BOF_simulation\BOF_database.equi:
Reactants: Fe + C + Mn + Si + CaO + FeO + SiO2 =
Compound databases: FactPS FTmisc FToxid
Solution databases: FTmisc FToxid

2.1 **** Equi-file BOF_database.equi (BOF_database.cst):
Path: C:\FactSage84\FactProSim\Projects\BOF_simulation2\BOF_database.equi:
Reactants: Fe + C + Mn + Si + CaO + FeO + SiO2 =
Compound databases: FactPS FTmisc FToxid
Solution databases: FTmisc FToxid

3.1 **** Equi-file DeOx_database.equi:
Path: C:\FactSage84\FactProSim\Projects\DeOx_simulation\DeOx_database.equi:
Reactants: Fe + Al + C + Mn + Si + O + Ca + Mg + CaO + Al2O3 + SiO2
+ FeO + MnO + MgO =
Compound databases: FactPS FTmisc FToxid
Solution databases: FTmisc FToxid

4.1 **** Equi-file DeS_database.equi:
Path: C:\FactSage84\FactProSim\Projects\DeS_simulation\DeS_database.equi:
Reactants: Fe + C + Si + S + CaO + SiO2 + Al2O3 =
Compound databases: FactPS FTmisc FToxid
Solution databases: FTmisc FToxid
```

# Summary of Equilib .equi files in FactProSim

```
Equilib Files *.equi in C:\FACTSAGE84\FactProSim\Projects\
File Edit
This summary is stored in C:\FACTSAGE84\FactProSim\Projects\Summary_EQUI.txt
Summary of Equilib .equi files in FactProSim \FactProSim\Projects\*.equi
=====
1.1 **** Equi-file BOF_database.equi: (BOF_database.cst)
Path: C:\FactSage84\FactProSim\Projects\BOF_simulation\BOF_database.equi:
Reactants: Fe + C + Mn + Si + CaO + FeO + SiO2 =
Compound databases: FactPS FTmisc FToxid
Solution databases: FTmisc FToxid
2.1 **** Equi-file BOF_database.equi (BOF_database.cst):
Path: C:\FactSage84\FactProSim\Projects\BOF_simulation2\BOF_database.equi:
Reactants: Fe + C + Mn + Si + CaO + FeO + SiO2 =
Compound databases: FactPS FTmisc FToxid
Solution databases: FTmisc FToxid
3.
Pa
Re
+
Co
Sc
BOF_database.equi and BOF_database.cst files are coupled.
The cst file is a mini database that contains the data on all the
species and phases selected in the equi file.
4.1 **** Equi-file DeS_database.equi:
Path: C:\FactSage84\FactProSim\Projects\DeS_simulation\DeS_database.equi:
Reactants: Fe + C + Si + S + CaO + SiO2 + Al2O3 =
Compound databases
Solution databases
The cst file will be used by ChemApp
when running FactFlow and FactProSim .
```

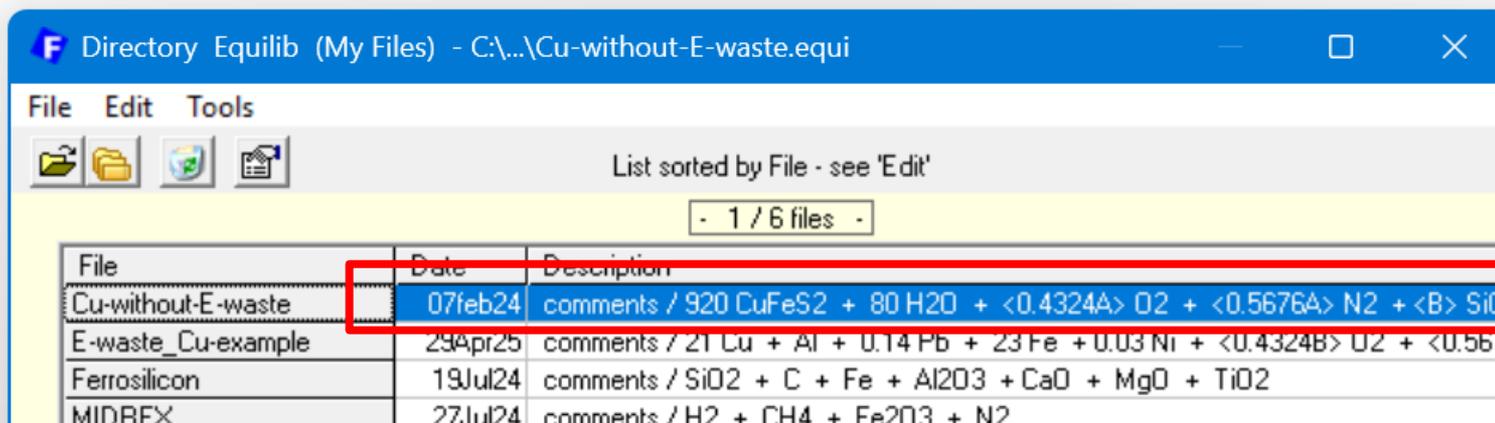
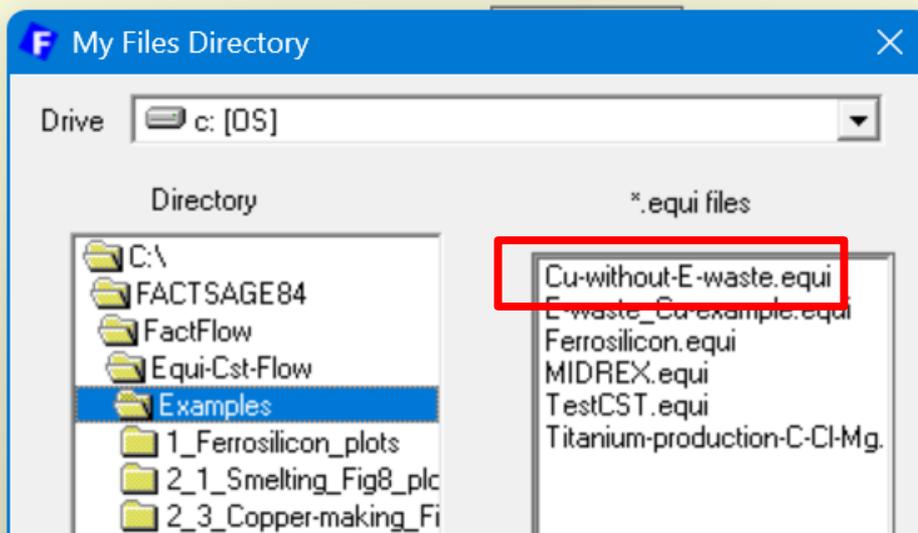
# Summary of Equilib .equi files in

# FactFlow

```
Equilib Files *.equi in C:\FACTSAGE84\FactFlow\Equi-Cst-Flow\
File Edit
This summary is stored in C:\FACTSAGE84\FactFlow\Equi-Cst-Flow\Summary_EQUI.txt
Summary of Equilib .equi files in FactFlow                               \FactFlow\Equi-Cst-Flow\*.equi
=====
1.1 **** Equi-file Cu-without-E-waste.equi:      (Cu-without-E-waste.cst)
Path: C:\FactSage84\FactFlow\Equi-Cst-Flow\Examples\Cu-without-E-waste.equi:
Reactants: 920 CuFeS2 + 80 H2O + <0.4324A> O2 + <0.5676A> N2 + <B> SiO2 =
Compound databases: FactPS FTmisc FToxid
Solution databases: FTmisc FToxid
.....
1.3 **** Equi-file Ferrosilicon.equi:            (Ferrosilicon.cst)
Path: C:\FactSage84\FactFlow\Equi-Cst-Flow\Examples\Ferrosilicon.equi:
Reactants: SiO2 + C + Fe + Al2O3 + CaO + MgO + TiO2 =
Compound databases: FactPS FTlite FToxid
Solution databases: FTlite FToxid
1.4 **** Equi-file MIDREX.equi:
Path: C:\FactSage84\FactFlow\Equi-Cst-Flow\Examples\MIDREX.equi:Reactants: H2 + CH4 + Fe2O3 + N2
Compound databases: FactPS FSstel FToxid
Solution databases: FSstel FToxid.
.....
1.6 **** Equi-file Titanium-production-C-Cl-Mg.equi:
Path: C:\FactSage84\FactFlow\Equi-Cst-Flow\Examples\Titanium-production-C-Cl-Mg.equi:Reactants: TiCl4
+ <A> Mg + O + C =
Compound databases: FactPS FToxid FTlite
Solution databases: FToxid FTlite
-----
1. Summary of Equilib .equi files in C:\FactSage84\FactFlow\Equi-Cst-Flow\Examples\
6 files found
14:36:59 2025-12-23
```



Open **Cu-without-E-waste.equi** stored in  
 \FactFlow\Equi-Cst-Flow\Examples\



This system is identical to the **Equilib** example on process modeling of copper production that we created earlier.

File Units Parameters Help



Reactants (5)

(kg) 920 CuFeS2 + 80 H2O + <0.4324A> O2 + <0.5676A> N2 + <B> SiO2

Products

Compound species

- gas  ideal  real 66
- aqueous 0
- \* pure liquids 25
- \* pure solids 98
- \* - custom selection species: 189

Solution phases

*	+	Base-Phase	Full Name
	+	FTmisc-FeLQ	Fe-liq
	+	FTmisc-CuLQ	Cu-liq_or_speiss
	+	FTmisc-FeCu	fcc_Fe-Cu
	+	FTmisc-MATT	Matte
	+	FTmisc-FeS_	FeS-liq
		FToxid-SLAGA	A-Slag-liq all oxides + S
	+	FToxid-SPINC	C-Spinel
	+	FToxid-MeO_A	A-Monoxide

Custom Solutions

- 0 fixed activities
- 0 ideal solutions

Pseudonyms

apply  Edit ...

Volume and physical prop data

- assume molar volumes of solids and liquids = 0
- use only molar volume data
- use V & phys. property data

paraequilibrium & Gmin edit

Total Species (max 7000) 240

Total Solutions (max 200) 9

Target

- none -

Estimate T(K): 1000

Quantity(kg)

Legend

- | - immiscible 1
- + - selected 7

Show  all  selected

species: 51

Select

We will create a new folder **Equi-Cst-Flow\Montreal-Workshop\** and save this example as **Cu-smelting.equi**

Final Conditions

<A>

0 1000 10

10 steps  Table

101 calculations

Calculate >>

- recommend you not select both pure liquids and molten solutions -

File Units Parameters Help

New Ctrl+N  
Open ... Ctrl+O  
Directories ... Ctrl+D

Save  
Save As ...  
Save Equilib Results

ChemApp File >

ChemSage File >

FactFlow Files

FactProSim File

- 1: File Cu-without-E-waste
- 2: File MIDREX
- 3: File Ferrosilic
- 4: File Ex\_Fe-de
- 5: File Cu-smelt

Exit

Create a new folder **Equi-Cst-Flow\Montreal-Workshop** and save both **Cu-smelting.equi** and **Cu-smelting.cst** in it.

Chemsage .cst file

Chemsage file saved in  
C:\FactSage84\FactFlow\Equi-Cst-Flow\Montreal-Workshop\Cu-smelting.cst

OK

Save FactFlow files (.equi, .cst)

Save FactFlow files and Run

Help ...

paraequilibrium & Gmin

Total Species (max 7000)	258
Total Solutions (max 200)	10
Total Phases (max 1500)	134

Equilibrium  
 normal  normal + transitions

transitions only  open

- no time limit -

- recommend you not select both pure liquids and molten solutions -

0	1000	10	0	1250	2.6	
10	steps	<input type="checkbox"/> Table			101 calculations	

File Units Parameters Help

New Ctrl+N  
Open ... Ctrl+O  
Directories ... Ctrl+D

Save  
Save As ...  
Save Equilib Result

ChemApp File &gt;

ChemSage File &gt;

FactFlow Files

FactProSim File

1: File Cu-witho

2: File MIDREX

3: File Ferrosilic

4: File Ex\_Fe-de

5: File Cu-smelt

Exit

0 1000 10

10 steps

Create a new folder **Equi-Cst-Flow\Montreal-Workshop** and save both **Cu-smelting.equi** and **Cu-smelting.cst** in it.

Chemsage .cst file



Chemsage file saved in

C:\FactSage84\FactFlow\Equi-Cst-Flow\Montreal-Workshop\Cu-smelting.cst

OK

Save FactFlow files (.equi, .cst)

Save FactFlow files and Run

Help ...

paraequilibrium &amp; Gmin edit

Total Species (max 7000) 258

Total Solutions (max 200) 10

Total Phases (max 1500) 134

Equilibrium

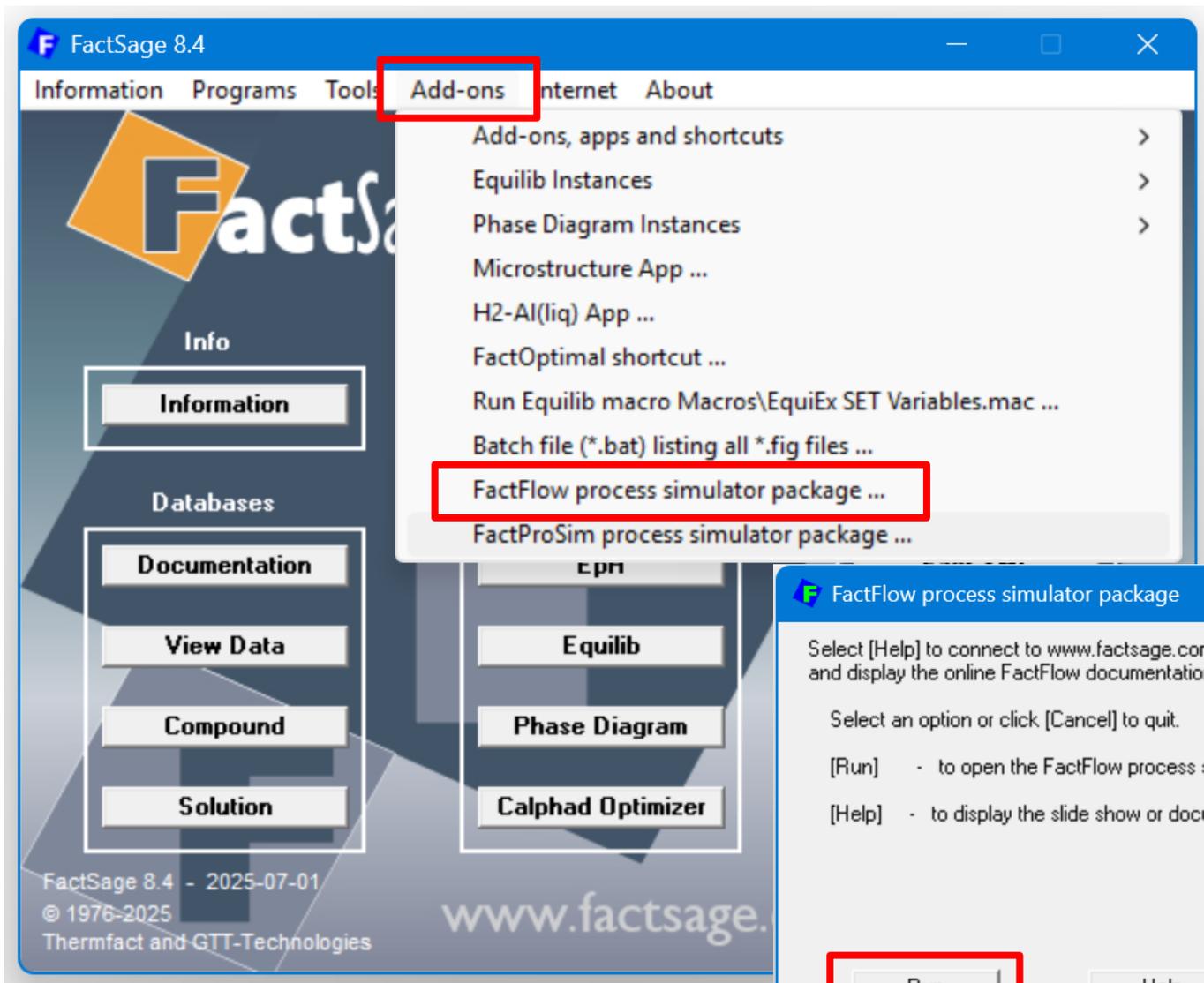
 normal + transitions

only

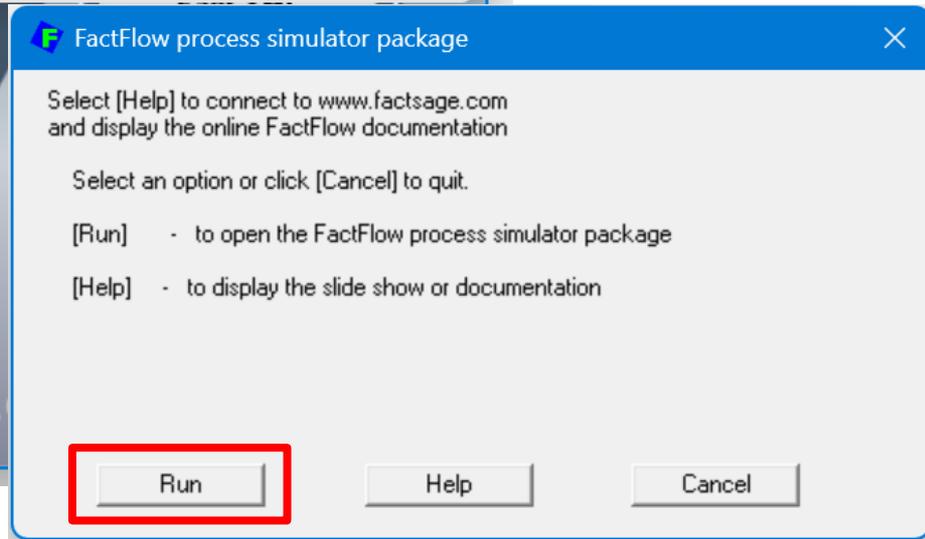
 open

Calculate &gt;&gt;

- recommend you not select both pure liquids and molten solutions -



The screenshot shows the FactSage 8.4 application window. The 'Add-ons' menu is open, and the 'FactFlow process simulator package ...' option is highlighted with a red box. The main interface features several buttons for navigation and simulation, including 'Information', 'View Data', 'Compound', 'Solution', 'Equilib', 'Phase Diagram', and 'Calphad Optimizer'. The bottom of the window displays the version 'FactSage 8.4 - 2025-07-01' and the copyright '© 1976-2025 Thermfact and GTT-Technologies'.



The dialog box titled 'FactFlow process simulator package' contains the following text:

Select [Help] to connect to [www.factsage.com](http://www.factsage.com) and display the online FactFlow documentation

Select an option or click [Cancel] to quit.

[Run] - to open the FactFlow process simulator package

[Help] - to display the slide show or documentation

At the bottom, the 'Run' button is highlighted with a red box.

FactFlow

File Settings About Help

**Run** T K P atm Energy J Quantity mol Plot Default Settings Run Settings  Show stream text >>

Input Exit

Splitter Mixer

Equilib Reactor Recycle node

Heat Exchanger

▼ New project  
Summary  
CST: None

Demonstration of FactFlow



Run

T K ▾

P atm ▾

Energy J ▾

Quantity mol ▾

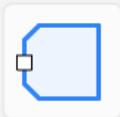
Plot Default Settings

Run Settings

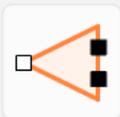
Show stream text  >>



Input



Exit



Splitter



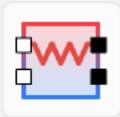
Mixer



Equilib Reactor



Recycle node



Heat Exchanger

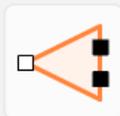
▼ New project  
Summary  
CST: None



Input



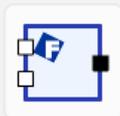
Exit



Splitter



Mixer



Equilib Reactor



Recycle node

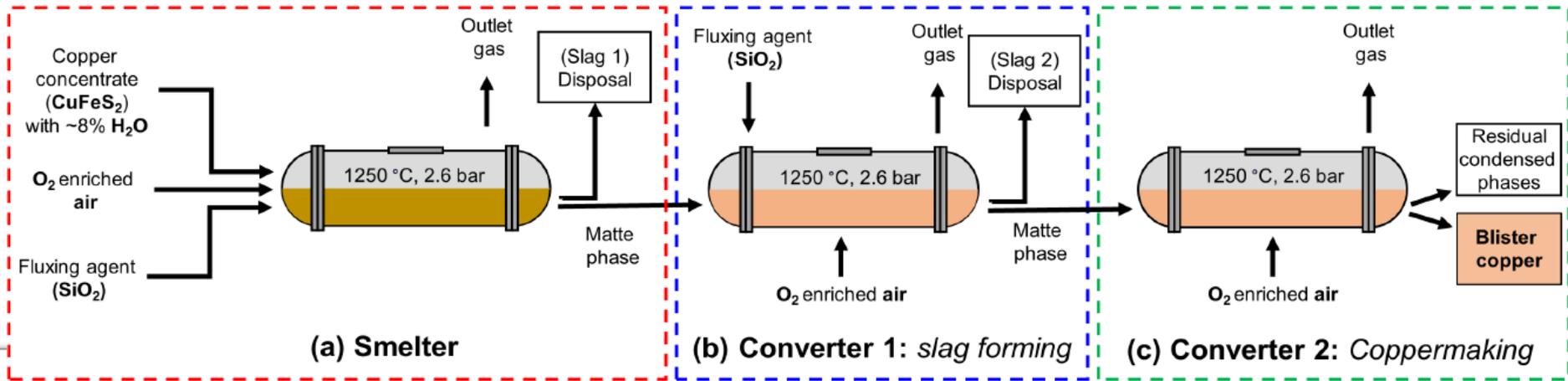


Heat Exchanger

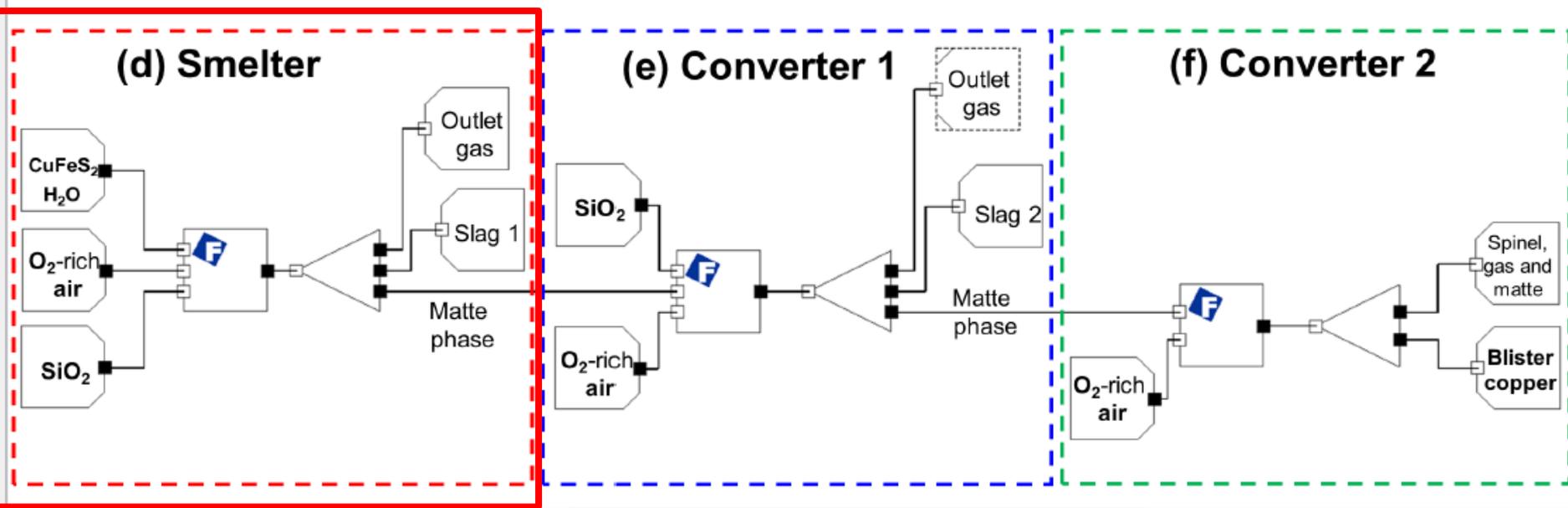
▼ New project  
Summary  
CST: None

Click **Help** to display the **User Manual** as shown below.

The screenshot shows the FactFlow software interface with the Help menu open. The menu bar includes File, Settings, About, and Help. The Help menu is highlighted, and a yellow box in the main window points to it. The interface includes a Run button, Unit selection, Run Settings button, Stream text overlay control, and Max runs and recycling iterations. The Flowsheet canvas displays a process flow diagram with various nodes and streams. The Project tree on the left shows a hierarchy of nodes including Gas input, Copper input, SiO2 input, Smelter, Slag output, Converter, and Phase splitter. A mouse icon indicates navigation: Right-click + drag.



Alpha (?) 0

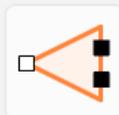




Input



Exit



Splitter



Mixer



Equilib Reactor

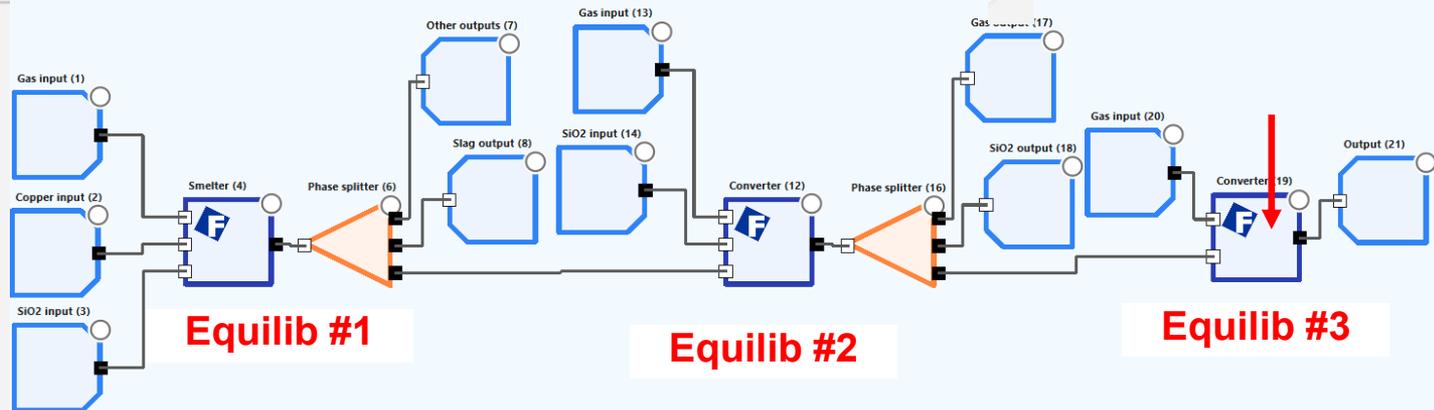


Recycle node



Heat Exchanger

- ▼ New project
  - Summary
  - CST: None



**Equilib #1**

**Equilib #2**

**Equilib #3**

**Results (Converter 19)**

**Equilib #3**

Inputs			Outputs					
Name	Phase	Quantity (kg)	Name	Phase	Quant	Activity	Qty Min (kg)	Qty Max (kg)
> Matte	Liquid	389.796	> Matte	Liquid	349.968		21.7721	349.968
> gas_ideal	Gas	20	> Cu-liq_or_speiss	Liquid	31.123		31.123	328.175
			> gas_ideal	Gas	28.05		28.05	291.802
			> Spinel	Solid	0.655154		0.655154	0.850173
			> Slag-liq#1	Liquid	0			

Run 1 ▾

Recycling iteration 1 ▾

Plot

Elemental Analysis

Show log

Export to Excel

### Equilib #3

Inputs

Search name

Name	Phase	Quantity (kg)
> Matte	Liquid	389.796
> gas_ideal	Gas	20

Outputs

Search name

Name	Phase	Quant	Activity	Qty Min (kg)	Qty Max (kg)
> Matte	Liquid	349.968		21.7721	349.968
> Cu-liq_or_speiss	Liquid	31.123		31.123	328.175
> gas_ideal	Gas	28.05		28.05	291.802
> Spinel	Solid	0.655154		0.655154	0.850173
> Slag-liq#1	Liquid	0			

Plot Options

X axis

Run

Run Cancel

Run variables > Air\_kg

Run 1

Recycling iteration 1

Plot

Elemental Analysis

Show log

Export to Excel

**Run** T K

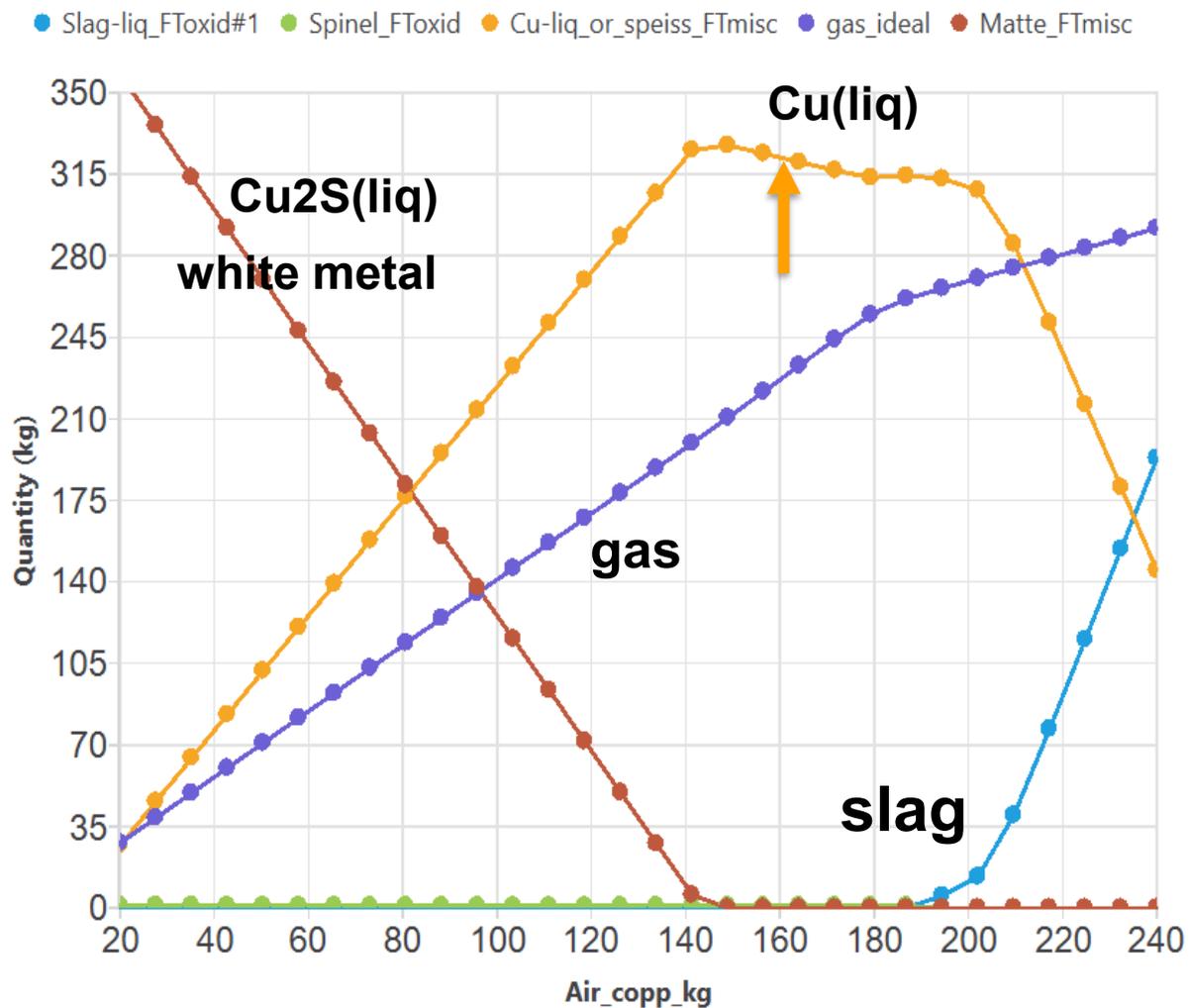
Results (Converter 19)

Inputs

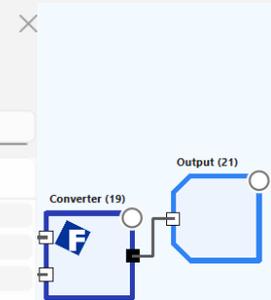
Search name

Name	Phase
> Matte	Liquid
> gas_ideal	Gas

**Equilib #3**



stream text



Run 1

Recycling iteration 1

Elemental Analysis

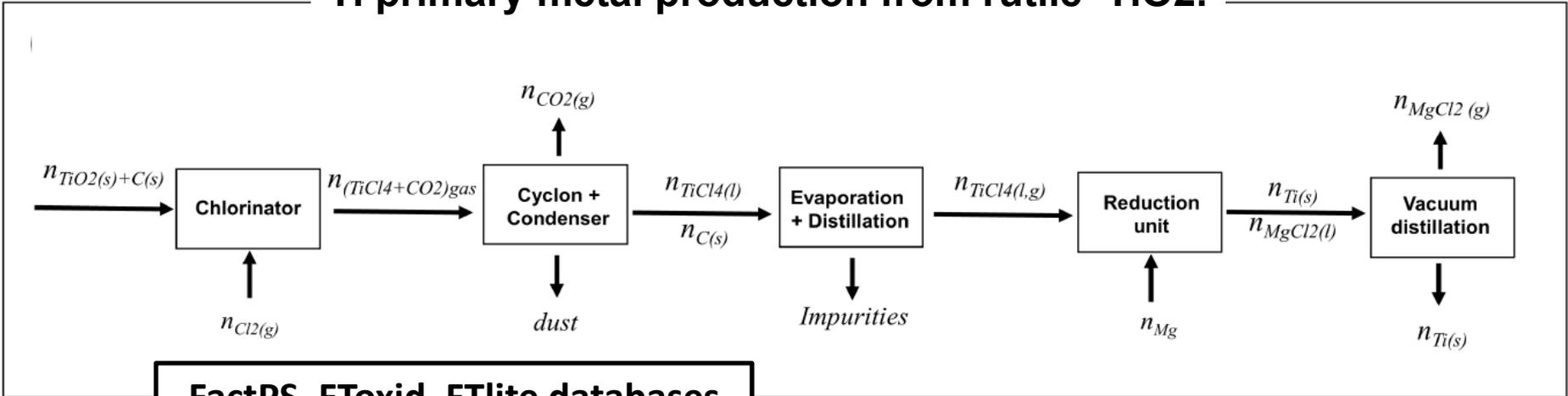


Show log

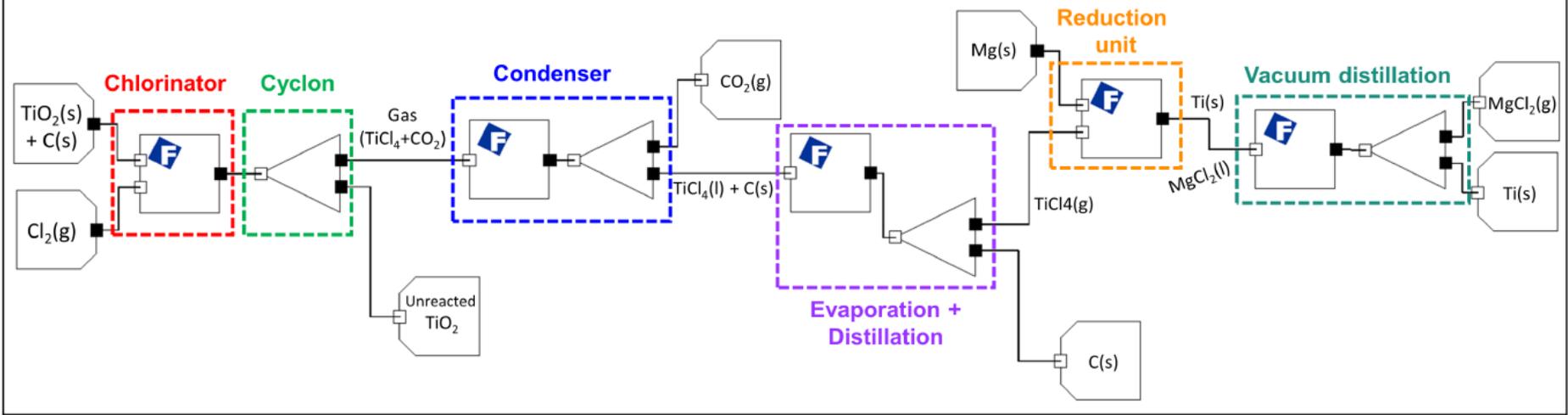


Export to Excel

## Ti primary metal production from rutile TiO<sub>2</sub>.



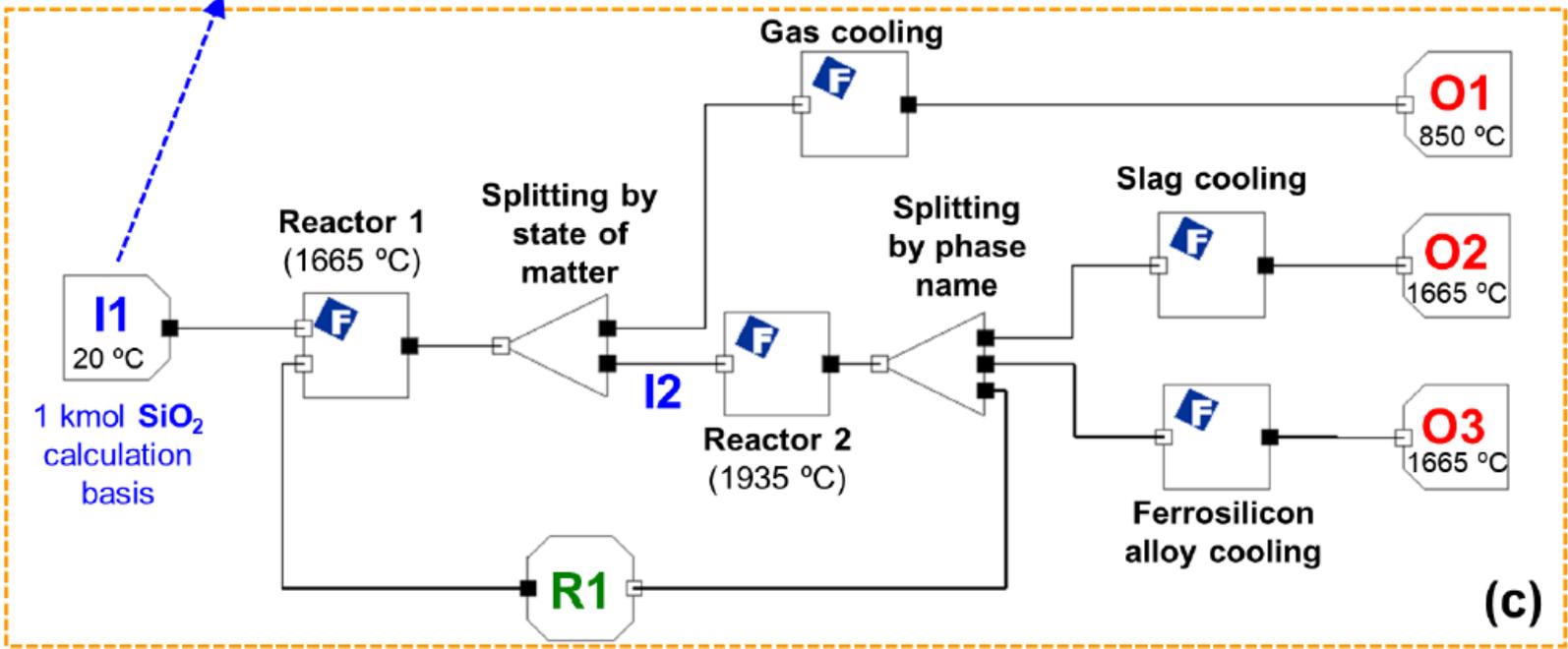
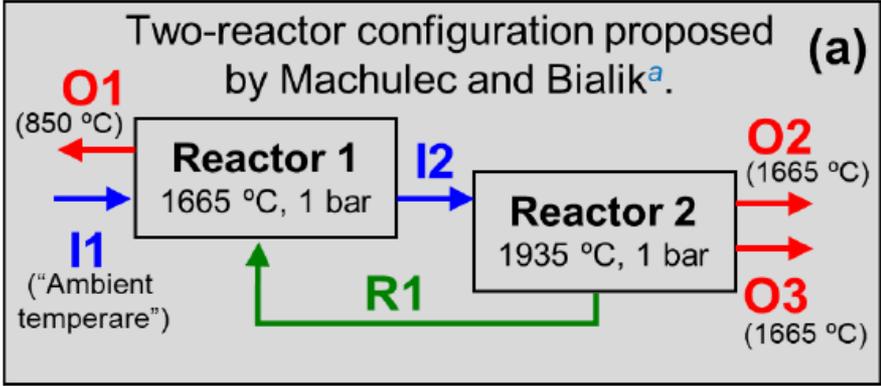
**FactPS, FToxid, FTlite databases**



# Modeling of an electric arc furnace to produce ferrosilicon using recycling loops

**92.716 kg of input stream (I1):**  
 64.80 wt% SiO<sub>2</sub> (i.e. 1 kmol SiO<sub>2</sub>)  
 24.50 wt% C  
 8.440 wt% Fe  
 1.650 wt% Al<sub>2</sub>O<sub>3</sub>  
 0.484 wt% CaO  
 0.131 wt% MgO  
 0.009 wt% TiO<sub>2</sub>

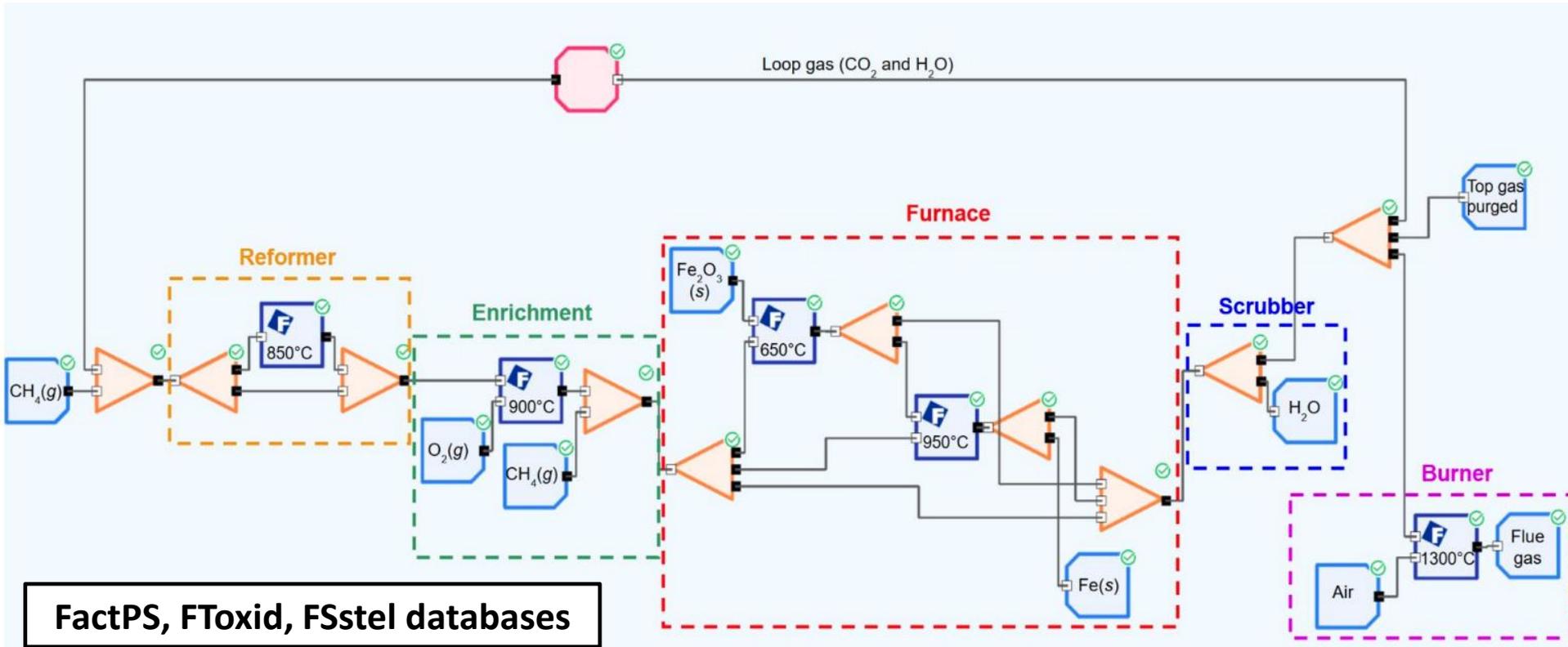
**FactPS  
 FToxid  
 FSstel  
 databases**



**I1:** Input raw materials  
**I2:** Input condensed phases in reactor 2  
**O1:** Output gas from reactor 1

**O2:** Output slag from reactor 2  
**O3:** Output metal from reactor 2  
**R1:** Recycling of gas from reactor 2

# MIDREX direct iron reduction process





## In addition **FactFlow**

- has a dedicated **Analysis Module** for viewing, plotting and comparing results across runs or recycling iterations from within the interface.
- has a graphical interface for defining **custom variables** that vary across parametric runs and recycling iterations to easily perform parameter studies.
- has a powerful **Function Builder** enabling the use of mathematical expressions, conditional logic, and looping structures to control node behavior and variable values.
- can define **runs** and **recycling iterations** and **maximum iterations**; define **new run variables** and **recycle iteration variables** by importing them from an **Excel** file; define variables names for **temperature** or **pressure** fields of **Equilib Reactors**, for **quantities** in Input nodes, for **percentage splits** in splitter nodes



Click **Add-ons** to open the **FactProSim** process simulation package

The image shows the FactSage 8.4 software interface. The 'Add-ons' menu is open, and the 'FactProSim process simulator package ...' option is highlighted with a red box. Below the main window, a dialog box titled 'FactProSim process simulator package' is displayed. The dialog box contains the following text:

Select an option or click [Cancel] to quit.

[Run] - to open the FactProSim process simulator package

[Help] - to display the slide show or documentation

The 'Run' button at the bottom of the dialog box is highlighted with a red box.



# FactProSim process simulation package

FactProSim

New Save Load CST Units Steps 1 Run Stop Help About

Modules

- Input Stream
- Stream
- Splitter
- Equilib
- Heat Ex

Arrange

- Align Vertical
- Align Horizontal

Tools

- Excel Files
- Initializer
- Rearrange Process IDs

Unsaved\*

100 %

Version: 2.1.9316



Click **Help** to display the **Installation Guide** and **Program description**

The screenshot shows the FactProSim software interface with several panels and toolbars. The main window displays a flowchart workspace with a toolbar at the top containing buttons for New, Save, Load, Steps (with a value of 1), Run, Units, CST, About, and Help. The Help button is highlighted with a red box. A smaller inset window shows a zoomed-in view of the same interface, with a red box around the Help and About buttons. The interface is divided into several panels: Modules (Input Stream, Stream, Splitter, Equilib, Heat Ex), Arrange (Align Vertical, Align Horizontal), and Tools (Excel Files, Initializer, Rearrange Process IDs). The status bar at the bottom left shows the version number 2.1.9316.

**Toolbar**

**Modules Panel**

**Arrange Panel**

**Extra Tools**

**Diagram (flowsheet) Workspace**

**Zoom and view controls**

**Run the simulation**

**Enter the number of steps (= number of Times the flowsheet is repeated during run)**

**Load an existing diagram (ppf, encrypted)**

**Save the current diagram (ppf, encrypted)**

**Create a new blank diagram**  
⚠ The current diagram will be lost if unsaved

**Load a database file (\*.cst)**

**Abort the simulation (activated during run)**

**Display developers names And contact information**

**Open the user manual for FactProSim**



# FactProSim process simulation

The screenshot shows the FactProSim software interface. The top menu bar includes 'New', 'Save', 'Load', 'CST', and 'Units'. The 'CST' menu is highlighted with a red box. A red arrow points from the 'CST' menu to a yellow text box containing the first step of the process. Below this, a 'Load CST Database' dialog box is open, showing the file path 'C:\FactSage84\FactProSim\Projects\Montreal-Workshop\Cu-smelting.cst'. A second yellow text box points to the 'LOAD' button in this dialog. In the bottom right, a file explorer window is open, showing the file 'Cu-smelting.cst' in the 'Montreal-Workshop' folder. A third yellow text box points to the 'File name' field in the file explorer, which contains 'Cu-smelting.cst'. The software interface also shows a 'Module' palette with icons for 'Input Stream', 'Stream', 'Splitter', 'Equilib', and 'Heat Ex', and an 'Arrange' section with 'Align Vertical' and 'Align Horizontal' options. The version number '2.1.9316' is visible in the bottom left corner.

1. First copy **\Cu-smelting.cst** file from **FactFlow\Equi-Cst-Flow\Montreal-Workshop\** to **FactProSim\Projects\Montreal-Workshop\**

2. Then load **Cu-smelting.cst**

3. Then save **FactProSim** flowsheet **Cu-smelting.ppf**



# FactProSim process simulation

FactProSim

New Save Load CST Units Steps 1 Run Stop Help About

Modules

- Input Stream
- Stream
- Splitter
- Equilib
- Heat Ex

Arrange

- Align Vertical
- Align Horizontal

Tools

- Excel Files
- Initializer
- Rearrange Process IDs

Unsaved\*

100 %

Version: 2.1.9316



# FactProSim process simulation

FactProSim

New Save Load CST Units Steps 1 Run Stop Help About

Modules

- Input Stream
- Stream
- Splitter
- Equilib
- Heat Ex

Arrange

- Align Vertical
- Align Horizontal

Tools

- Excel Files
- Initializer
- Rearrange Process IDs

Unsaved\*

100 %

1. Feed

2. Enr-air

3. Flux

1

4. Gas

5. Slag

6. Matte

Version: 2.1.9316



# FactProSim process simulation

FactProSim

New Save Load CST Units Steps 1 Run Stop Help About

Modules

- Input Stream
- Stream
- Splitter
- Equilib
- Heat Ex

Arrange

- Align Vertical
- Align Horizontal

Tools

- Excel Files
- Initializer
- Rearrange Process IDs

Unsaved\*

100 %

1\_ Feed

2. Enr-air

3.. Flux

1

4. Gas

5. Slag

6. Matte

Input Stream

Local Units

Description: Enriched-air 40% O2 for smelter

Name: 2. Enr-air

Temperature (C): 25

Amount (kg): 680

Pressure (bar): 1

Excel Link:

Equation:

Gas Phase Species

- N
- N2
- N3
- O
- O2
- O3
- NO
- N2O
- NO2
- NO3
- N2O3
- N2O4
- N2O5

Solution Phases

- Fe-liq\_FTmisc
- Cu-liq\_or\_speiss\_F

Components

ADD

Mass Percent

Mass Percent	Species
43.24	O2
56.76	N2

Total%: 100

Total Selection: 2

Total Selection: 0

OK Schedule

Version: 2.1.9316



# FactProSim process simulation

FactProSim

New Save Load CST Units Steps 1 Run Stop Help About

Modules

- Input Stream
- Stream
- Splitter
- Equilib
- Heat Ex

Arrange

- Align Vertical
- Align Horizontal

Tools

- Excel Files
- Initializer
- Rearrange Process IDs

Unsaved\*

100 %

1\_Feed

2. Enr-air

3.. Flux

1

4. Gas

5. Slag

6. Matte

Equilib

Local Units

Description: Smelter - Equilib #1

Excel Link Equation Gas Phase Species All Solution

Temperature (C) Check Schedu

Enthalpy (J) Check Schedu

Pressure (bar) Check Schedu

Process ID 1

Incoming Streams	Outgoing Streams
2. Enr-air	4. Gas
1_Feed	5. Slag
3.. Flux	6. Matte

Gas Phase Species	Solution
<input checked="" type="checkbox"/> H	<input checked="" type="checkbox"/> Fe-l
<input checked="" type="checkbox"/> H2	<input checked="" type="checkbox"/> Cu-
<input checked="" type="checkbox"/> N	<input checked="" type="checkbox"/> fcc-
<input checked="" type="checkbox"/> N2	<input checked="" type="checkbox"/> Mat
<input checked="" type="checkbox"/> N3	<input checked="" type="checkbox"/> FeS
<input checked="" type="checkbox"/> NH	<input checked="" type="checkbox"/> Pitz
<input checked="" type="checkbox"/> NH2	<input checked="" type="checkbox"/> Slag
<input checked="" type="checkbox"/> NH3	<input checked="" type="checkbox"/> Slag
<input checked="" type="checkbox"/> HNNH	<input checked="" type="checkbox"/> Spi
<input checked="" type="checkbox"/> N2H4	<input checked="" type="checkbox"/> Mor
<input checked="" type="checkbox"/> O	
<input checked="" type="checkbox"/> O2	

Skip if No Reactants

Total Selection: 66

OK

Sc

Version: 2.1.9316



# FactProSim process simulation

FactProSim

New Save Load CST Units Steps 1 Run Stop Help About

Modules

- Input Stream
- Stream
- Splitter
- Equilib
- Heat Ex

Arrange

- Align Vertical
- Align Horizontal

Tools

- Excel Files
- Initializer
- Rearrange Process IDs

Unsaved\*

```
graph LR; I1[1_Feed] --> E1[1]; I2[2.Enr-air] --> E1; I3[3..Flux] --> E1; E1 --> S4[4.Gas]; E1 --> S5[5.Slag]; E1 --> S6[6.Matte]; S6 --> E2[2]; S7[7.Flux] --> E2; S8[8.Enr-air] --> E2; E2 --> S9[9.Off gas]; E2 --> S10[10.Matte]; E2 --> S11[11.Slag]; S10 --> E3[3]; S12[12.Enr-air] --> E3; E3 --> S13[13.Gas]; E3 --> S14[14.Other]; E3 --> S15[15.Cu];
```

Version: 2.1.9316



# FactProSim process simulation

FactProSim [ ] X

New Save Load CST Units Steps 1 Run Stop Help About

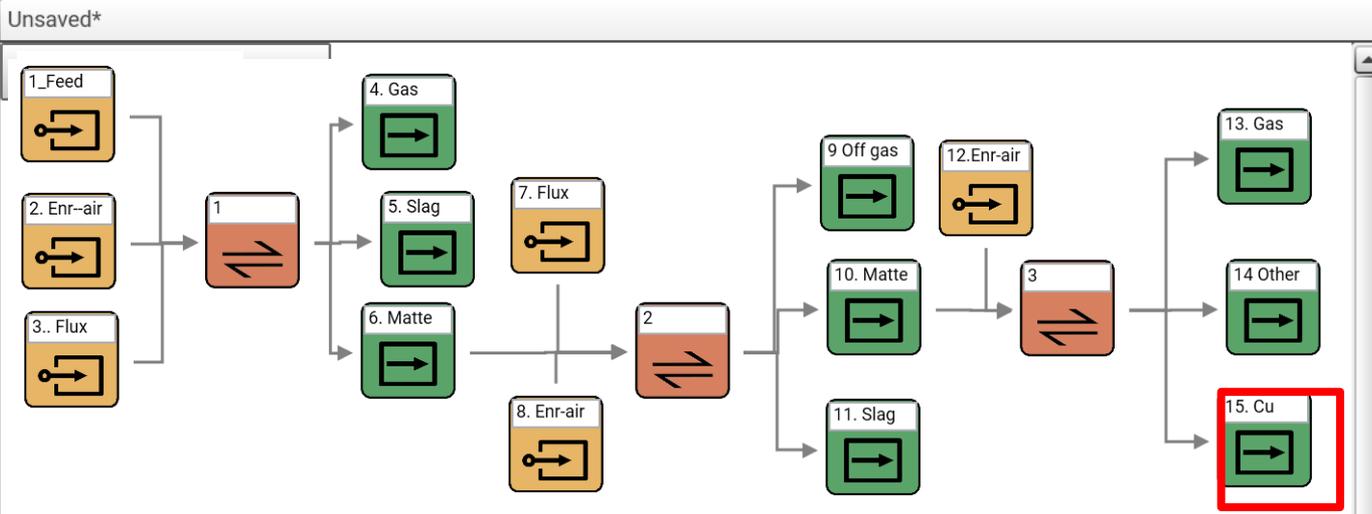
Modules

Input Stream Stream Splitter

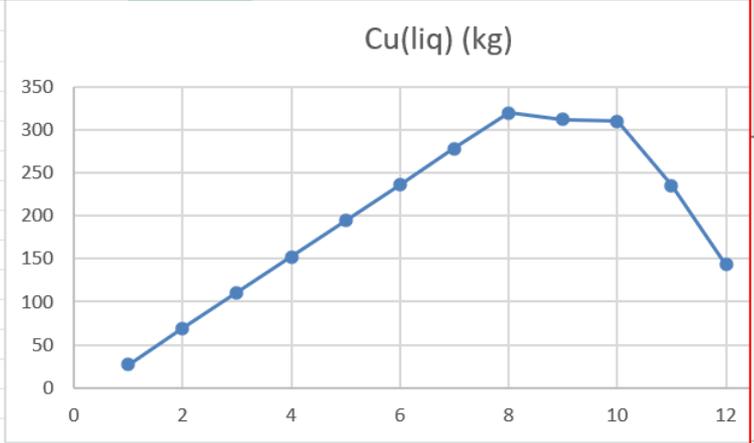
Equilib Heat Ex

Arrange

Align Vertical Align Horizontal



	Cu(liq)		Ftmisc			
	Amt. kg	Cu	Fe	S	O	
1	27.04221	0.969325	4.39E-05	0.028763	0.001868	
2	68.90019	0.969283	4.38E-05	0.0288	0.001873	
3	110.761	0.969269	4.38E-05	0.028813	0.001874	
4	152.6226	0.969262	4.38E-05	0.028819	0.001875	
5	194.4845	0.969258	4.38E-05	0.028823	0.001876	
6	236.3464	0.969255	4.38E-05	0.028825	0.001876	
7	278.2085	0.969253	4.38E-05	0.028827	0.001876	
8	320.0705	0.969251	4.38E-05	0.028829	0.001876	
9	312.6345	0.995337	1.08E-05	0.00266	0.001992	
10	310.5967	0.976031	2.26E-07	0.00014	0.023829	
11	235.5166	0.971535	2.12E-08	0.000107	0.028359	
12	143.4671	0.971462	1.03E-08	9.9E-05	0.028439	





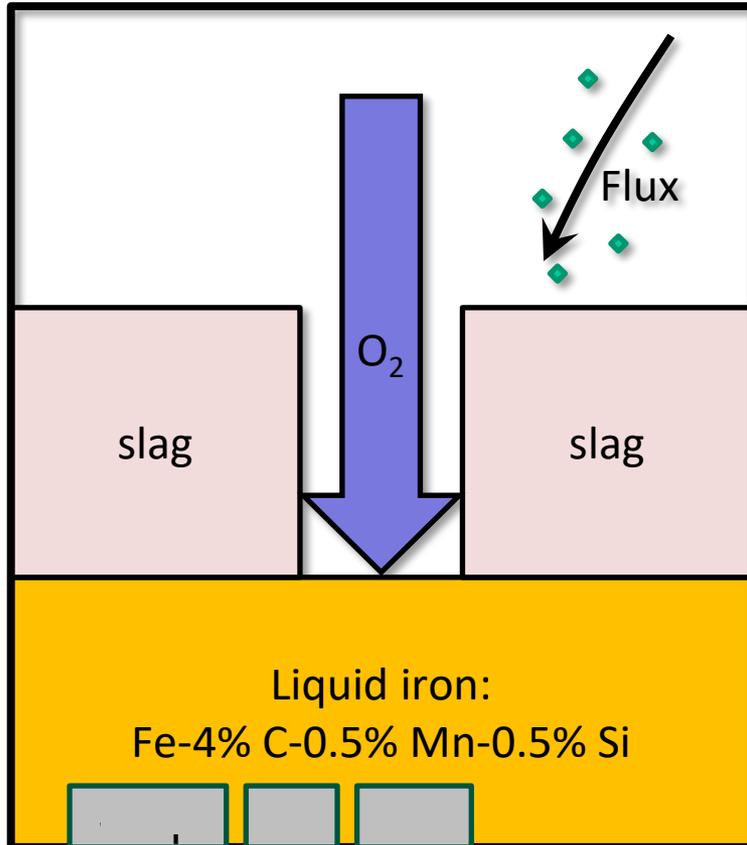
## FactProSim examples

- **Simulation of Al addition in the ladle.**
- **Desulfurization of Hot Metal.**
- **Process simulation of the BOF process.**
- **Process simulation of the BOF process with post-combustion and heat recovery.**

All examples are associated with development of complex industrial process simulations, some using the **Effective Equilibrium Reaction Zone (EERZ)** model approach.

**FactPS, FToxid, FTmisc databases**

## FactProSim process simulation of the BOF process

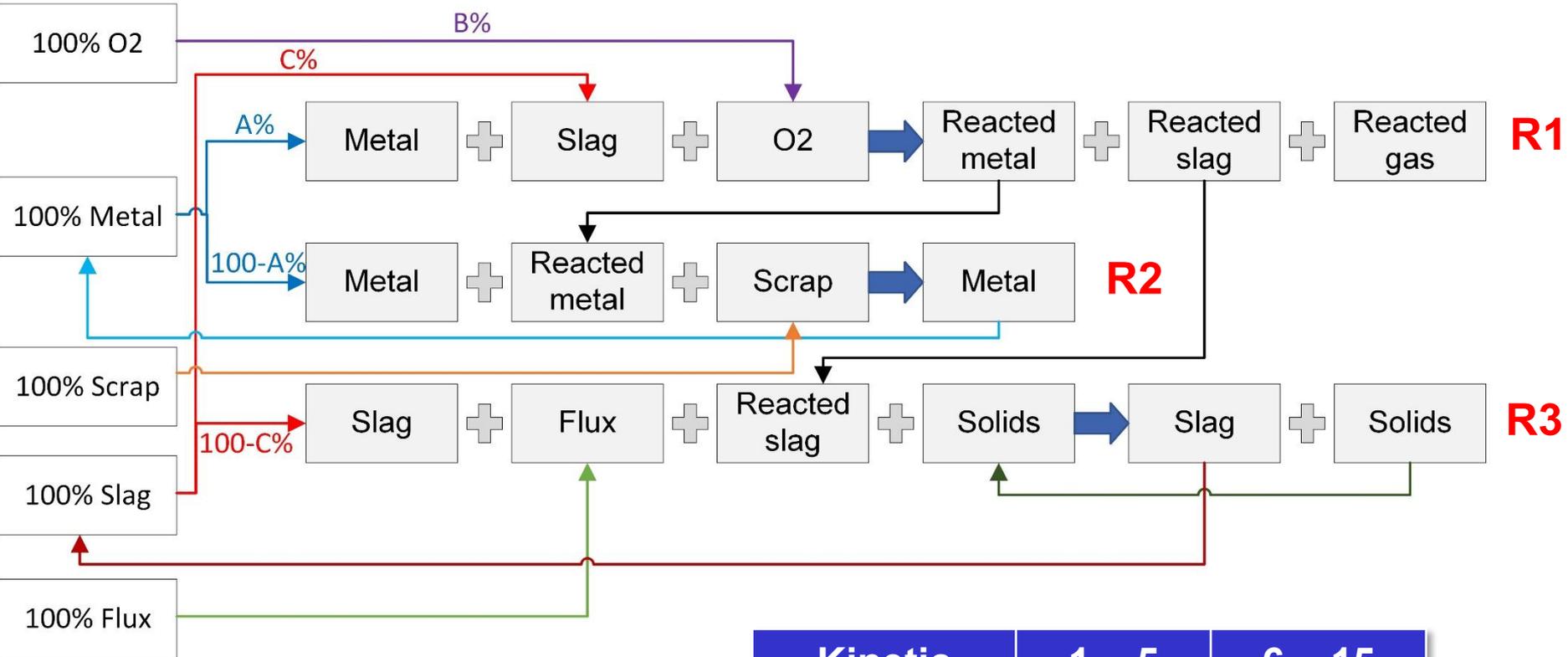


Phase	Amount	Composition	Temperature
Metal	100 ton	95% Fe 4% C 0.5% Mn 0.5% Si	1300 °C
Slag	2 ton	55% CaO 25% FeO 20% SiO <sub>2</sub>	1300 °C
Gas	0.57 ton/min	100% O <sub>2</sub>	25 °C
Flux	0.25 ton/min 1 to 10 min	100% CaO	25 °C
Scrap	2 ton/min 1 to 9 min	100% Fe	25 °C

Process duration : 15 min

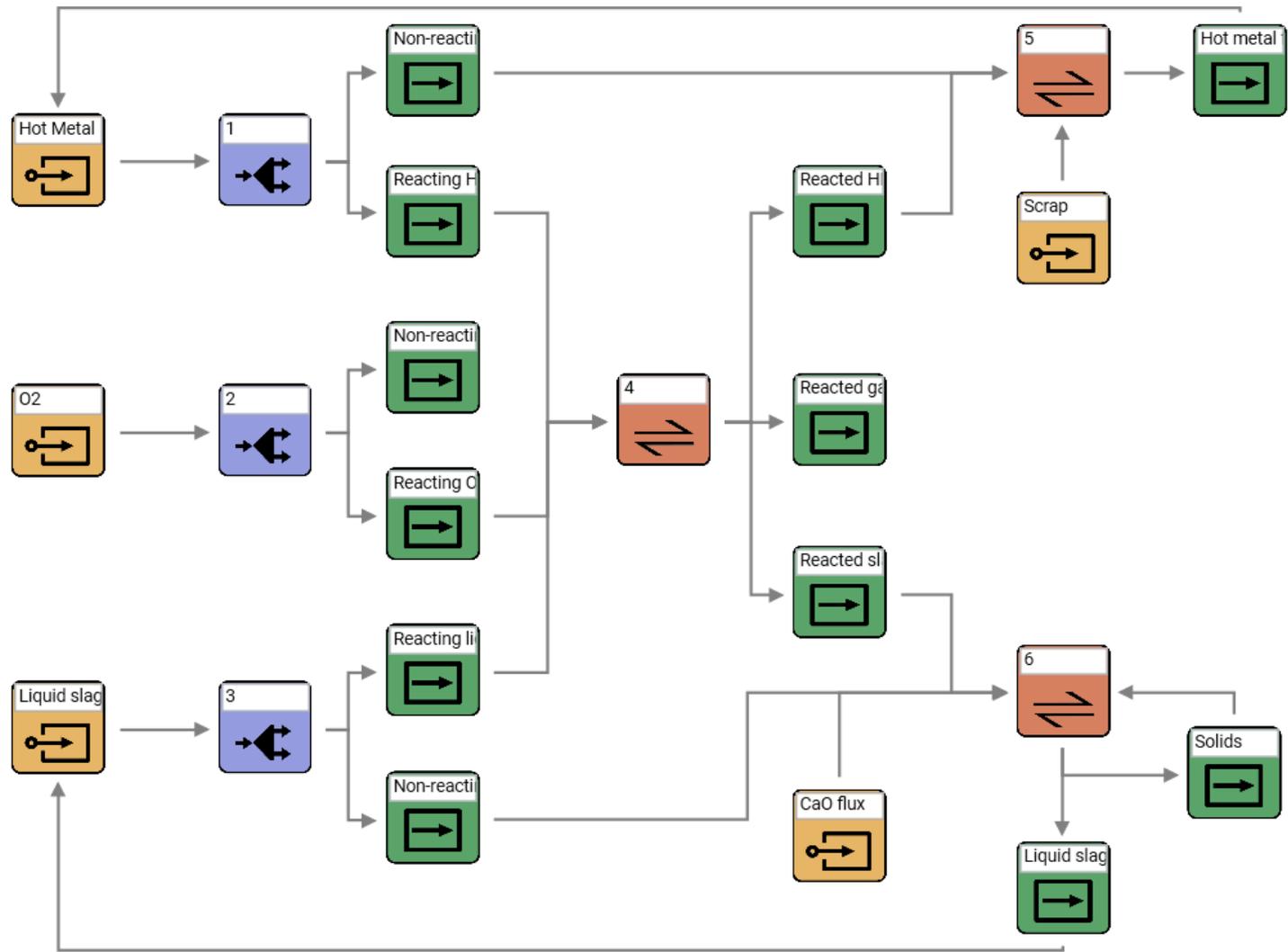
All reactions under adiabatic conditions

# FactProSim process simulation of the BOF process

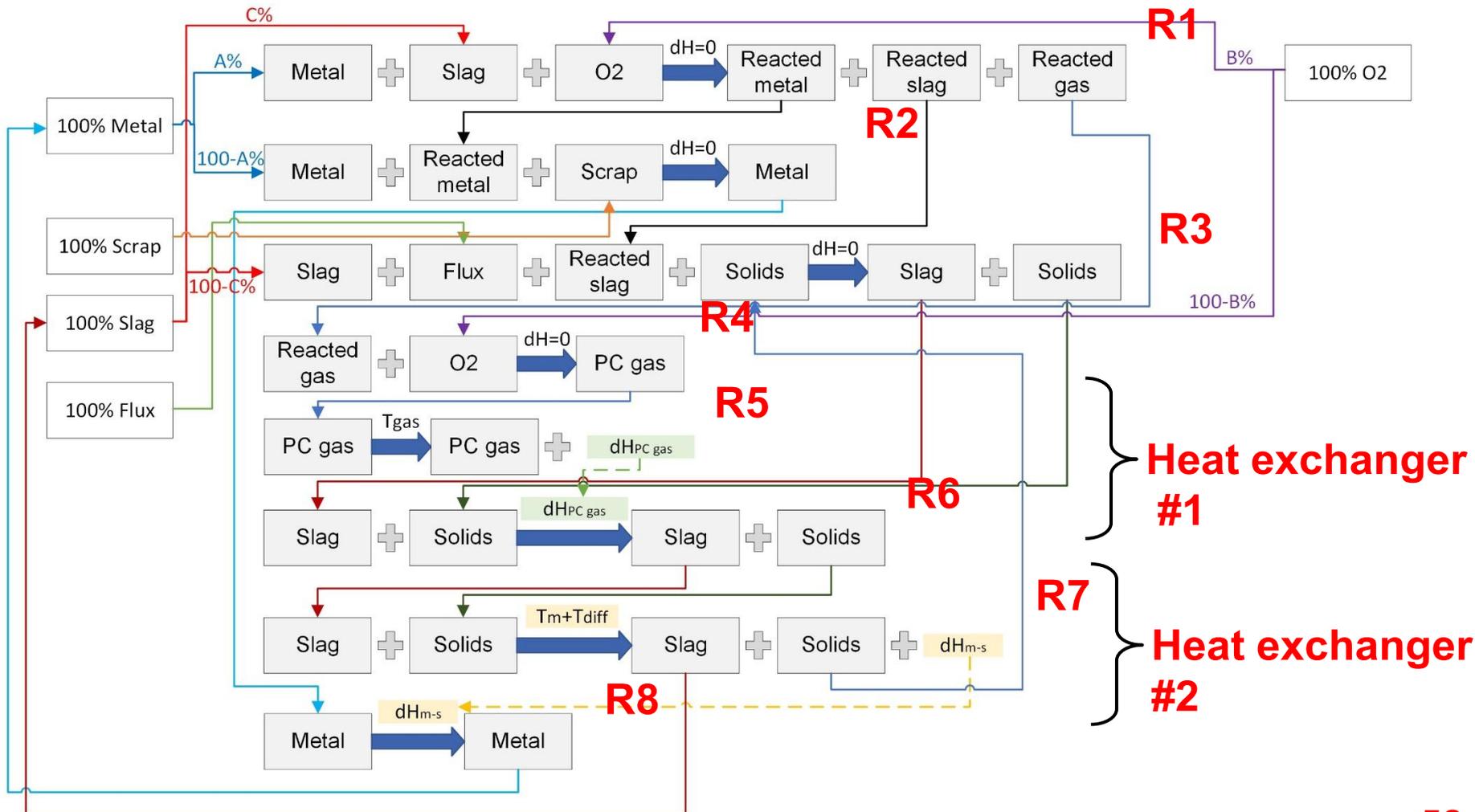


Kinetic factor	1 ~ 5 min	6 ~ 15 min
A	10%	30%
B	50%	80%
C	50%	80%

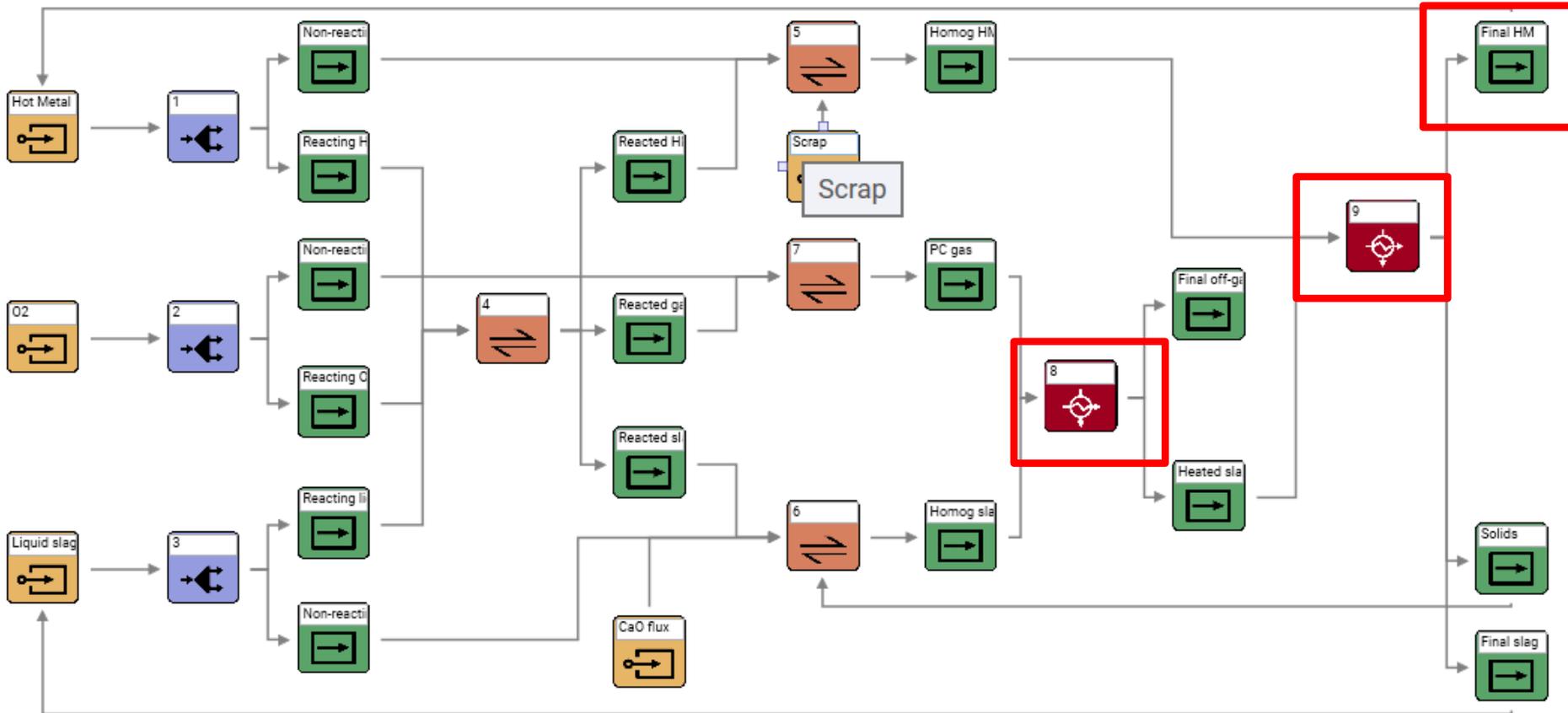
# FactProSim process simulation of the BOF process



# FactProSim process simulation of the BOF process - with post-combustion and heat recovery



# FactProSim process simulation of the BOF process - with heat exchangers



## FactProSim process inputs in Excel file

Metal	Comp. (wt%)				Amount (ton)	Temp. (C)
	Fe	C	Mn	Si		
	95	4	0.5	0.5	100	1300
Slag	CaO	FeO	SiO2		Amount (ton)	Temp. (C)
	55	25	20			
Gas	O2				Amount (ton)	Temp. (C)
	100					
Flux	CaO				Amount (ton)	Temp. (C)
	100					
Scrap	Fe				Amount (ton)	Temp. (C)
	100					

Input data and process conditions saved in Excel file BOF data.xlsx

dH (kJ)      0

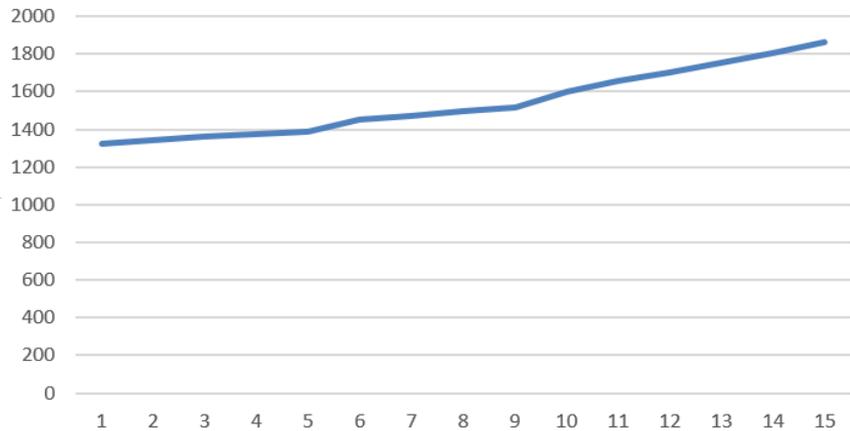
Time (min)	O2 (ton)	CaO (ton)	Kinetic factors			Scrap (ton)	off-gas temp. (C)	Temp difference between slag and HM
			Metal (A,%)	Gas (B,%)	Slag (C,%)			
1	0.57	0.25	10	50	50	2	2500	100
2	0.57	0.25	10	50	50	2	2500	100
3	0.57	0.25	10	50	50	2	2500	100
4	0.57	0.25	10	50	50	2	2500	100
5	0.57	0.5	10	50	50	2	2500	100
6	0.57	0.35	30	80	80	2	2500	100
7	0.57	0.25	30	80	80	2	2500	100
8	0.57	0.25	30	80	80	2	2500	100
9	0.57	0.25	30	80	80	2	2500	100
10	0.57	0.25	30	80	80	0	2500	100
11	0.57	0	30	80	80	0	2500	100
12	0.57	0	30	80	80	0	2500	100
13	0.57	0	30	80	80	0	2500	100
14	0.57	0	30	80	80	0	2500	100
15	0.57	0	30	80	80	0	2500	100



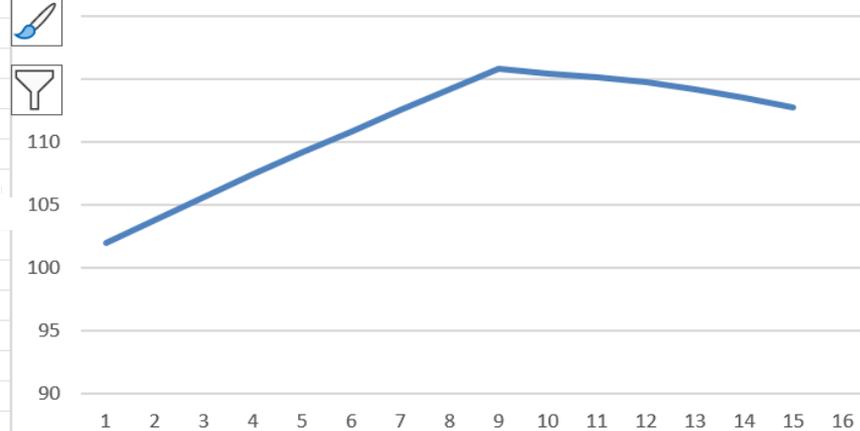
# Results of the process simulation – composition of the hot metal saved in the Excel file BOF data.xlsx

Step	Temperature	Fe-liq Amount	all Fe	amounts C	kg Ca	Mn	O	Si	CaO	SiO	MnO	Fe	Mn
1	1323.38212	101.9315	0.953522	0.037117	5.78E-10	0.004901	5.85E-07	0.004459	6.92E-07	6.58E-08	3.33E-08	0.953522	0.004901
2	1344.00426	103.789	0.956661	0.034444	4.82E-10	0.004808	1.18E-06	0.004085	1.12E-06	1.1E-07	6.87E-08	0.956661	0.004808
3	1360.90463	105.6092	0.959568	0.031927	4.55E-10	0.00472	1.83E-06	0.003782	1.62E-06	1.42E-07	1.08E-07	0.959568	0.00472
4	1376.53413	107.4107	0.962317	0.029533	4.62E-10	0.004636	2.57E-06	0.003508	2.31E-06	1.68E-07	1.54E-07	0.962317	0.004636
5	1385.15886	109.2026	0.964949	0.027247	4.6E-10	0.004556	3.45E-06	0.003241	3.34E-06	1.91E-07	2.1E-07	0.964949	0.004556
6	1450.55668	110.8593	0.968658	0.024175	5.43E-10	0.004481	4.16E-06	0.002679	2.83E-06	1.63E-07	2.5E-07	0.968658	0.004481
7	1474.34466	112.5106	0.97223	0.0212	7.58E-10	0.004416	5.23E-06	0.002143	4.81E-06	1.44E-07	3.21E-07	0.97223	0.004416
8	1496.8733	114.1603	0.975695	0.018313	1.07E-09	0.004349	6.78E-06	0.001627	8.63E-06	1.26E-07	4.22E-07	0.975695	0.004349
9	1516.99294	115.81	0.979047	0.015479	1.53E-09	0.004282	9.19E-06	0.001165	1.69E-05	1.09E-07	5.81E-07	0.979047	0.004282
10	1602.06973	115.4589	0.981967	0.012874	3.91E-09	0.004286	1.37E-05	0.000826	3.23E-05	1.01E-07	8.52E-07	0.981967	0.004286
11	1659.168	115.1076	0.984816	0.010191	9.82E-09	0.004284	2.37E-05	0.000586	9.86E-05	1.11E-07	1.48E-06	0.984816	0.004284
12	1703.80631	114.733	0.987527	0.007547	9.44E-09	0.004247	6.25E-05	0.000413	0.000199	1.86E-07	3.88E-06	0.987527	0.004247
13	1753.35709	114.2286	0.989745	0.005394	4.52E-09	0.004009	0.000255	0.000291	0.000291	4.89E-07	1.49E-05	0.989745	0.004009
14	1808.32677	113.561	0.991319	0.00384	3.67E-09	0.00358	0.000622	0.000205	0.000402	7.92E-07	3.2E-05	0.991319	0.00367
15	1864.15615	112.7554	0.992297	0.002736	4.17E-09	0.003118	0.001103	0.000145	0.000553	9.51E-07	4.86E-05	0.992297	0.003118

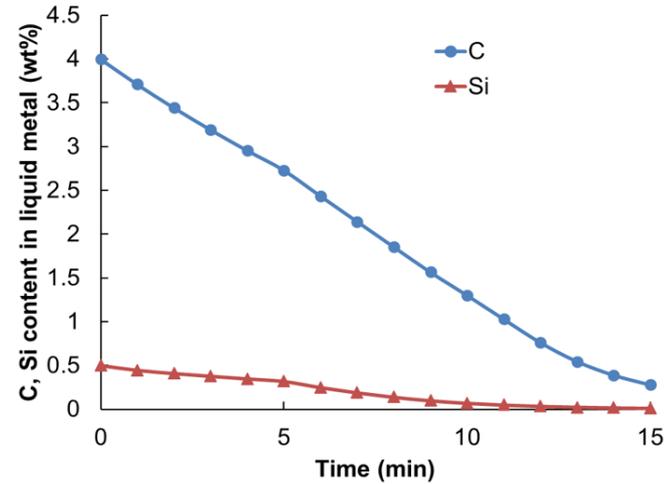
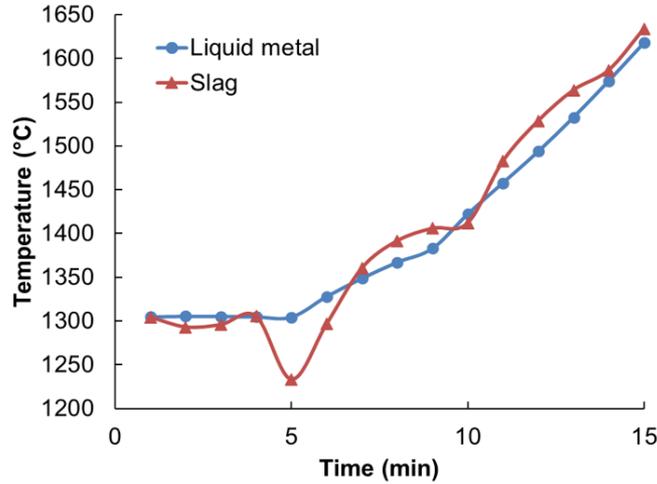
Temperature (C)



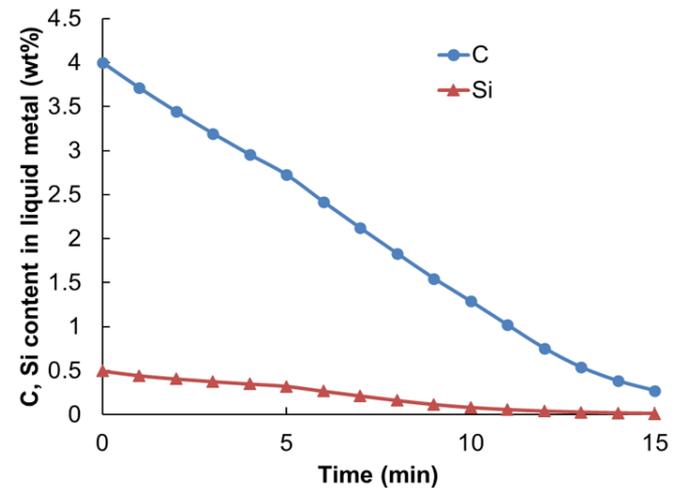
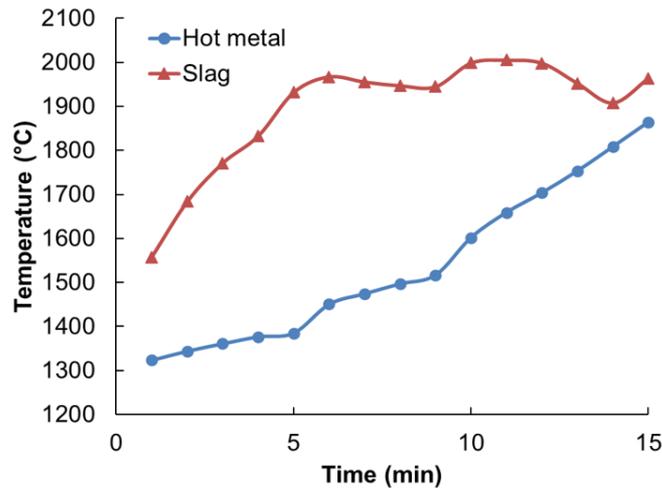
Amount

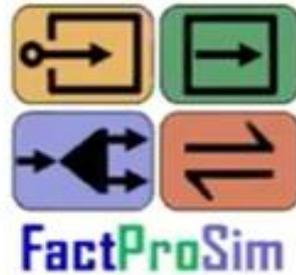


## Plots for BOF\_Simulation



## Plots for BOF\_Simulation2 (with heat exchangers)

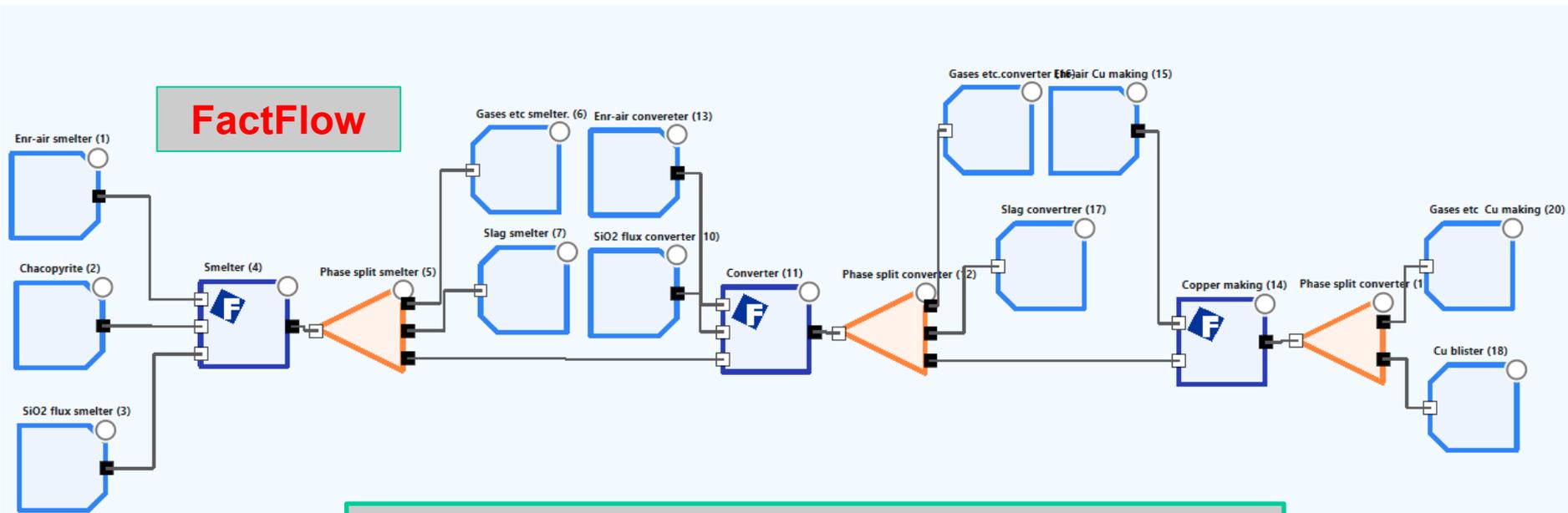




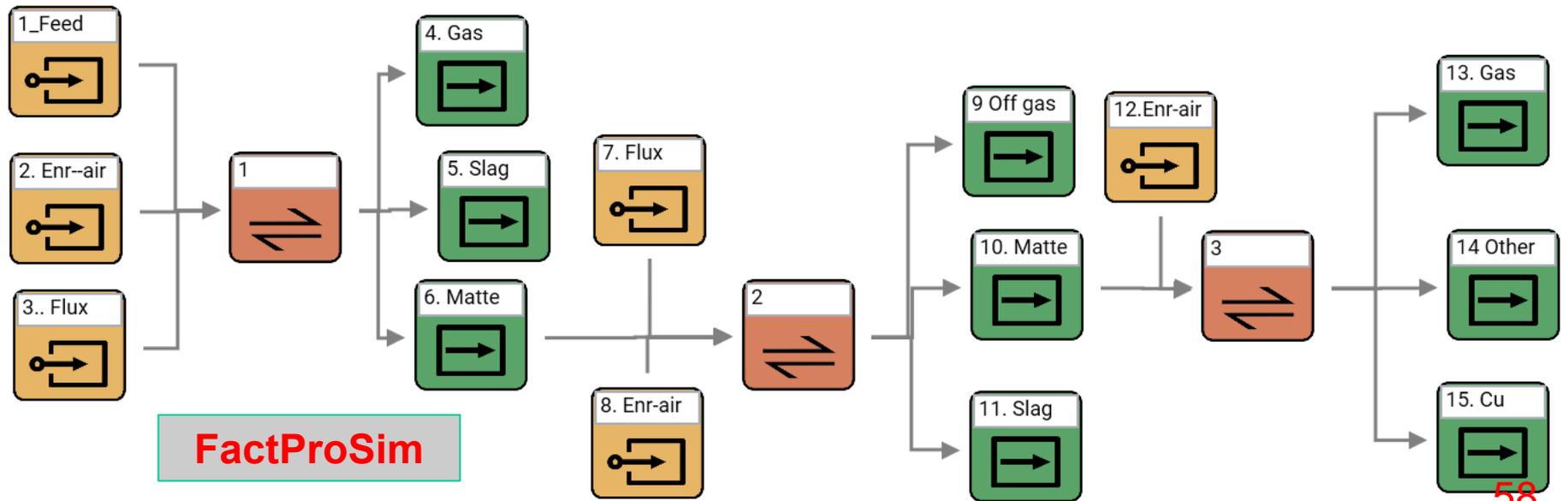
In particular, **FactProSim**:

- enables the **simulation of batch processes**, incorporating time-dependent conditions and parameters.
- allows for the **creation of custom equations** where elements from the flowsheet can be incorporated.
- is designed for the **development of complex industrial process simulations using the Effective Equilibrium Reaction Zone (EERZ) model approach**.

**FactProSim** was initially developed for the **Steelmaking Consortium** at Seoul National University, which comprises **14 industrial partners** around the world. It has been employed by consortium members to develop their own process simulations. Continuous enhancements and new functionalities, including more user-friendly graphic outputs, will be introduced to enhance its versatility and flexibility, and to meet users' needs.



**Flowsheets - similar look and feel**



# Conclusions

## FactFlow and FactProsim simulation packages

- have been developed in parallel and offer user-friendly graphical interfaces
- access the same databases **FactPS**, **FToxid**, **Ftlite** ... **SGPS**, **SGTE2024** ... **etc.**
- employ the same Gibbs energy minimization algorithms (**ChemApp**)
- calculate the same chemical equilibria
- but they have different applications.



**FactFlow** is designed for users to execute a series of stream-related **Equilib** tasks without having to save equilibrated streams (\*.mixt files) and recycle them. **FactFlow** is particularly useful for simulating high temperature pyrometallurgical processing operations under equilibrium conditions.



**FactProSim** is primarily designed for the steelmaking industry, for example the simulation of additions in the ladle, desulfurization of hot metal and the BOF process with post-combustion and heat recovery. It is associated with the development of complex industrial process simulations involving kinetics and some using the **Effective Equilibrium Reaction Zone (EERZ)** model approach. 59

**Thank you!**

**Chris Bale and Eve Bélice**

For more info on the process simulators visit

**[www.factsage.com](http://www.factsage.com)**

**<https://factsage.com/process-simulation>**