

# Development of a Melter Gasifier Model in gPROMS with ChemApp Multicomponent/Multiphase Calculation Routines



**Orestis Almpanis-Lekkas<sup>1</sup>, Bernd Weiss<sup>2</sup>, Walter Wukovits<sup>1</sup>**

**1 Vienna University of Technology, Institute of Chemical Engineering, 1060 Vienna, Austria**

**2 Siemens VAI Metals Technologies GmbH, Ironmaking Technology–Smelting/Direct Reduction, Linz, Austria**





Motivation

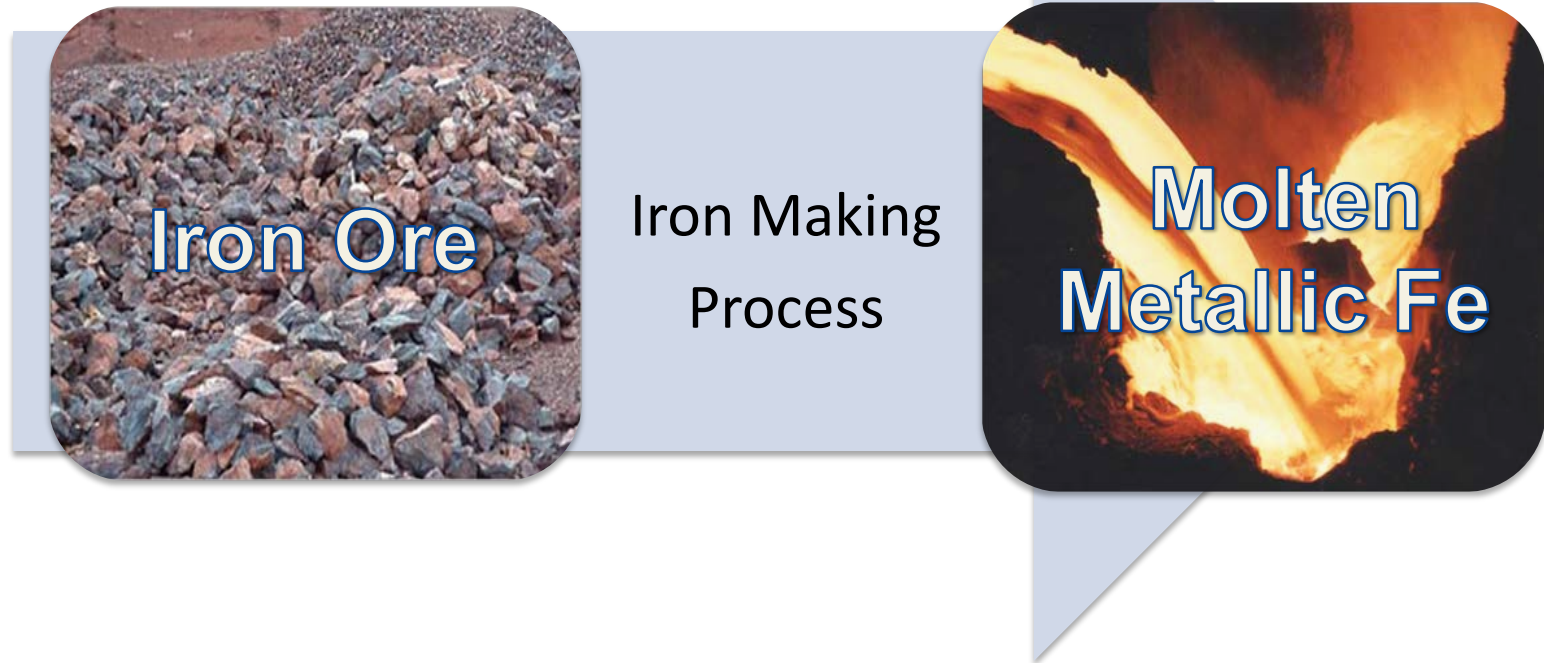
Method

Testing /Evaluation

Melter Gasifier Model

Simulation Results

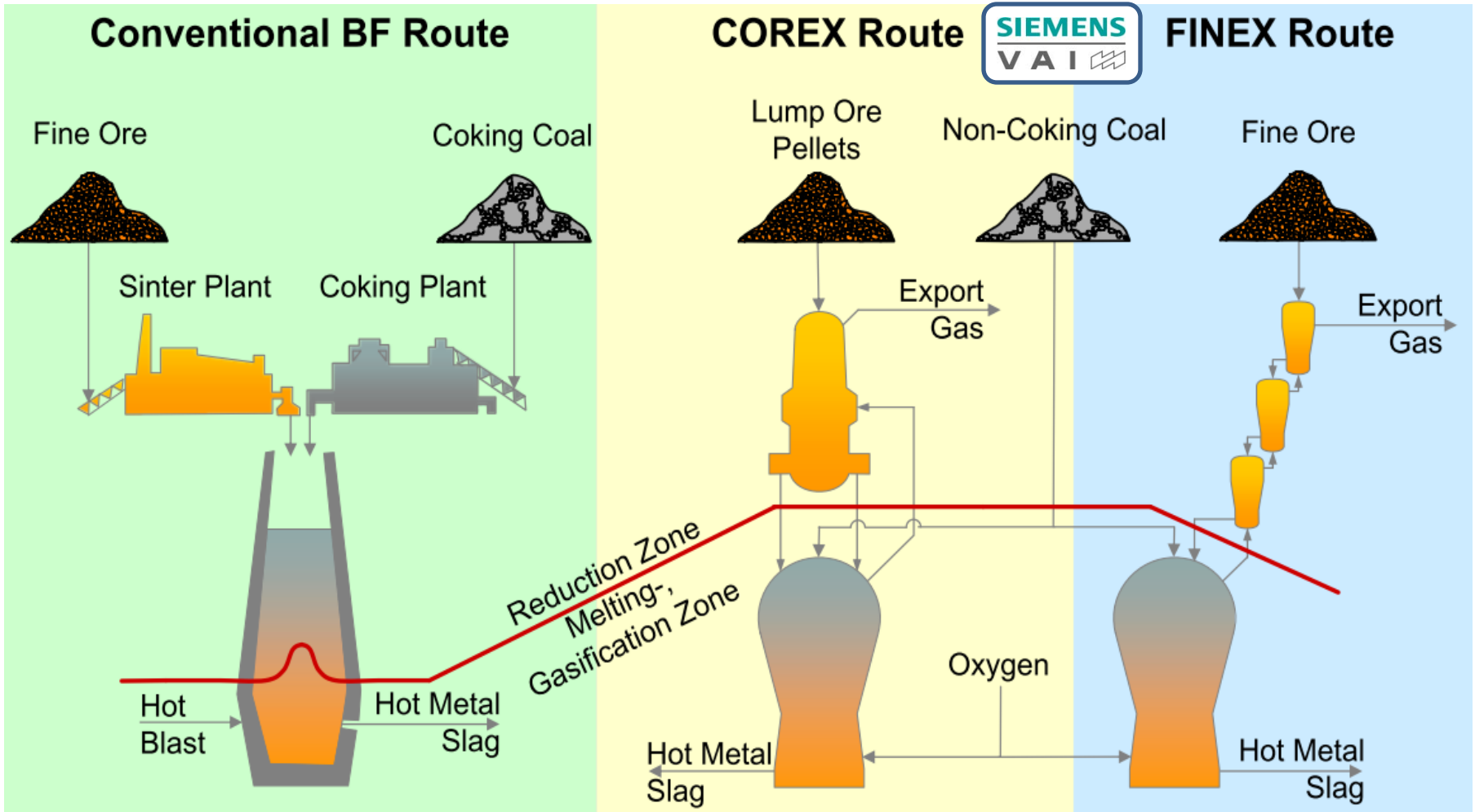
Summary



basic mechanism : **iron oxide reduction at high temperatures**

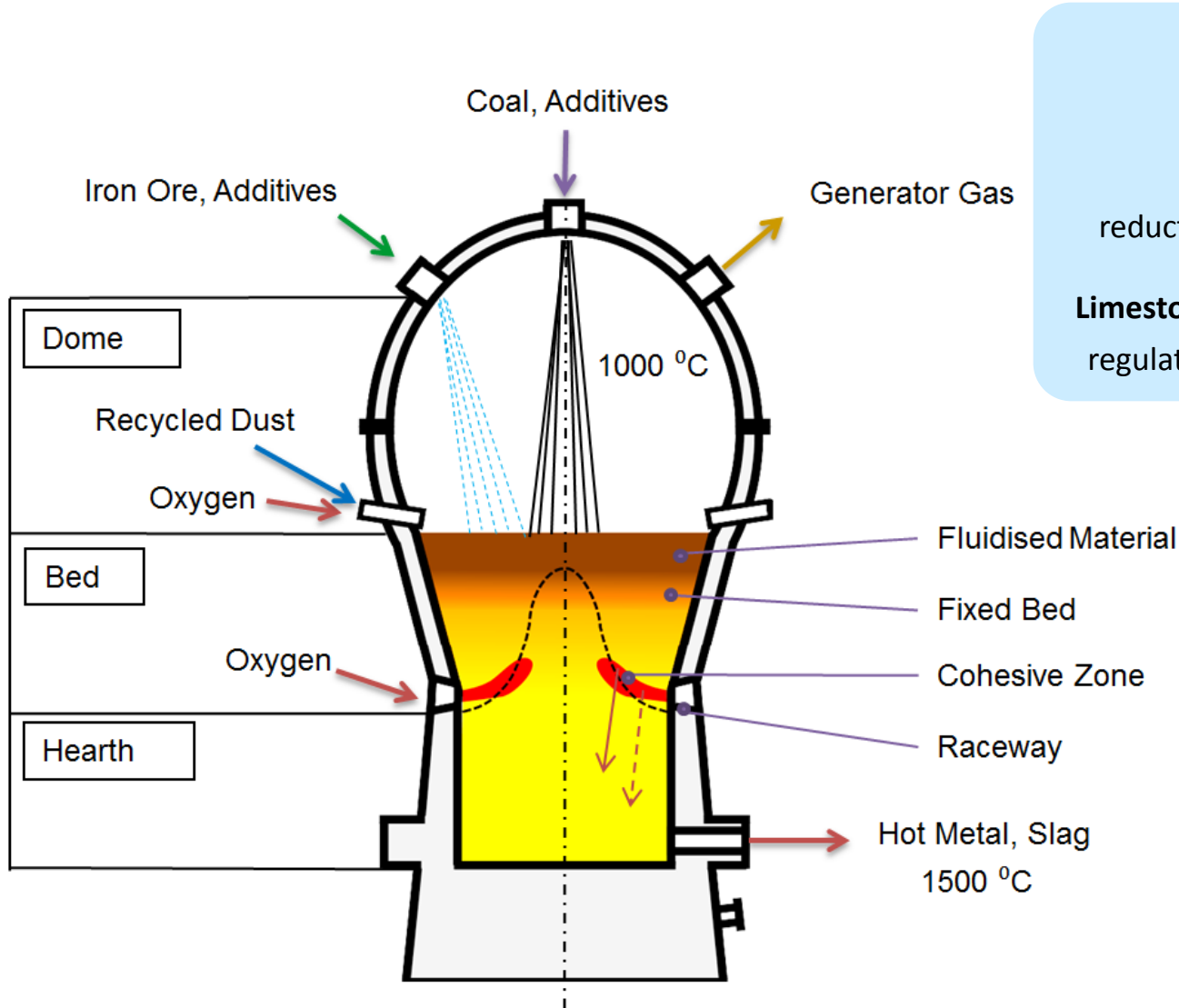


# Ironmaking Processes



**Corex and Finex advantages** → lower capital investment and operating cost (15-20%)  
→ lower SO<sub>x</sub>, NO<sub>x</sub> and dust emission

# Melter Gasifier



**HCl, DRI (Iron Ore)**  
iron and iron oxide supply

**Coal, Coke, PCI (Fuels)**  
reduction gas generation, heat supply

**Limestone, Dolomite, Quartz (Additives)**  
regulation of hot metal and slag quality

**Freeboard**  
dust reactions  
gas reactions

**Bed**  
drying  
final reduction  
final calcination  
fuel gasification

**Hearth**  
hot metal & slag removal



## gPROMS

- developed by Process System Enterprise (PSE)
- equation-oriented modeling & simulation software
- flow-sheeting interface
- sophisticated implementation of Newton solver
- gPROMS capabilities
  - steady-state simulation
  - dynamic simulation
  - parameter estimation
  - model-based experiment design
  - steady-state and dynamic optimisation

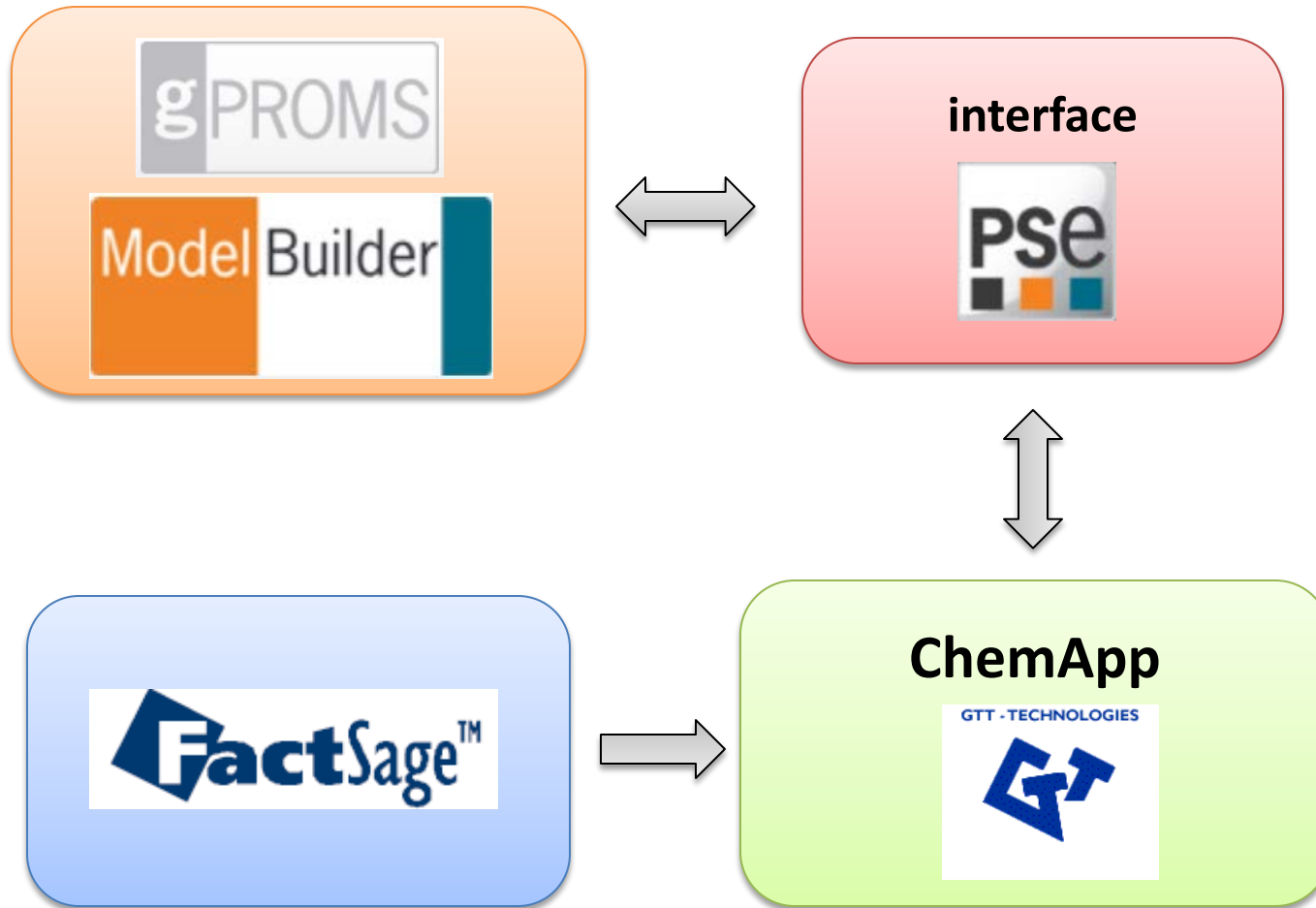
GTT - TECHNOLOGIES



## ChemApp

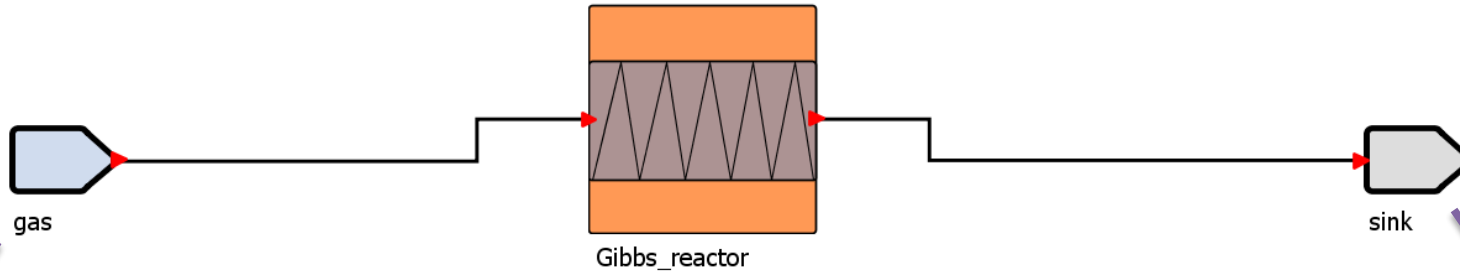
- a library of subroutines for the thermodynamic calculations
- uses thermodynamic data files (.cst or .dat) exported from FactSage
- calculation of complex multicomponent, multiphase chemical equilibria and their associated energy balances
- not a standalone program
- in combination with FactSage it provides rich component list in the field of metallurgy

# Software Tool Combination





# Using ChemApp in gPROMS



```

non_equilibrium_CS_mass_percent("Fe2O3_hematite(s)#Fe2O3_hematite(s)") = normalised_inlet_mass_percent("Fe2O3");
non_equilibrium_CS_mass_percent("Fe3O4_magnetite(s)#Fe3O4_magnetite(s)") = normalised_inlet_mass_percent("Fe3O4");
non_equilibrium_CS_mass_percent("K2O_solid(s)#K2O_solid(s)") = normalised_inlet_mass_percent("K2O");
    
```

gas (source\_gas)

Temperature units: degrees Celsius  
 Pressure units: barg  
 Composition specification: mol %  
 Flowrate specification: mol/h

Specify

Temperature: 25 degrees Celsius  
 Pressure: 5.3 barg  
 Uniform for entire array  Per element

gas	mol %
H2	19.1139365
H2O_gas	6.3771926
H2S	0
O2	0
CO	46.2605203
CO2	28.2483506
CH4	0
C6H6	0
N2	0

Flow rate: 614.58742 mol/h

VARIABLE RESULTS

Flowsheet.gas.outlet.mass\_percent

Time ... 0.0 Actual ...

components	mass_percent
"FeCO3"	0.0
"Fe2O3_H2O"	0.0
"H2O_liq"	0.0
"H2"	1.431225
"H2O_gas"	4.267083
"H2S"	0.0
"CO"	48.12723
"CO2"	46.17446
"CH4"	0.0
"C6H6"	0.0
"N2"	0.0
"C_vol_coal"	0.0
"C_vol_coke"	0.0
"H_vol"	0.0
"N_vol"	0.0
"O_vol"	0.0
"S_vol"	0.0

VARIABLE RESULTS non\_equilibrium\_CS\_mass...

Flowsheet.Gibbs\_reactor.non\_equilibrium\_CS\_mass\_percent

Time [0.0 .. 0.0] Fixed at 0.0 Actual = 0.0

phase\_constit... Rows

phase constituents	value
"CaO_liquid(liq)#CaO_liquid(liq)"	0.0
"Mn_liquid(liq)#Mn_liquid(liq)"	0.0
"Fe_liquid(liq)#Fe_liquid(liq)"	0.0
"Na2O_liquid(liq)#Na2O_liquid(liq)"	0.0
"Al2O3_liquid(liq)#Al2O3_liquid(liq)"	0.0
"K2O_liquid(liq)#K2O_liquid(liq)"	0.0
"TiO2_liquid(liq)#TiO2_liquid(liq)"	0.0
"MnO_liquid(liq)#MnO_liquid(liq)"	0.0
"P_liquid(liq)#P_liquid(liq)"	0.0
"S_liquid(liq)#S_liquid(liq)"	0.0

VARIABLE RESULTS

Flowsheet.gas.outlet.mass\_percent

Time ... 0.0 Actual ...

components	mass_percent
"FeCO3"	0.0
"Fe2O3_H2O"	0.0
"H2O_liq"	0.0
"H2"	1.431225
"H2O_gas"	4.267083
"H2S"	0.0
"O2"	0.0
"CO"	48.12723
"CO2"	46.17446
"CH4"	0.0
"C6H6"	0.0
"N2"	0.0
"C_vol_coal"	0.0
"C_vol_coke"	0.0
"H_vol"	0.0
"N_vol"	0.0
"O_vol"	0.0
"S_vol"	0.0

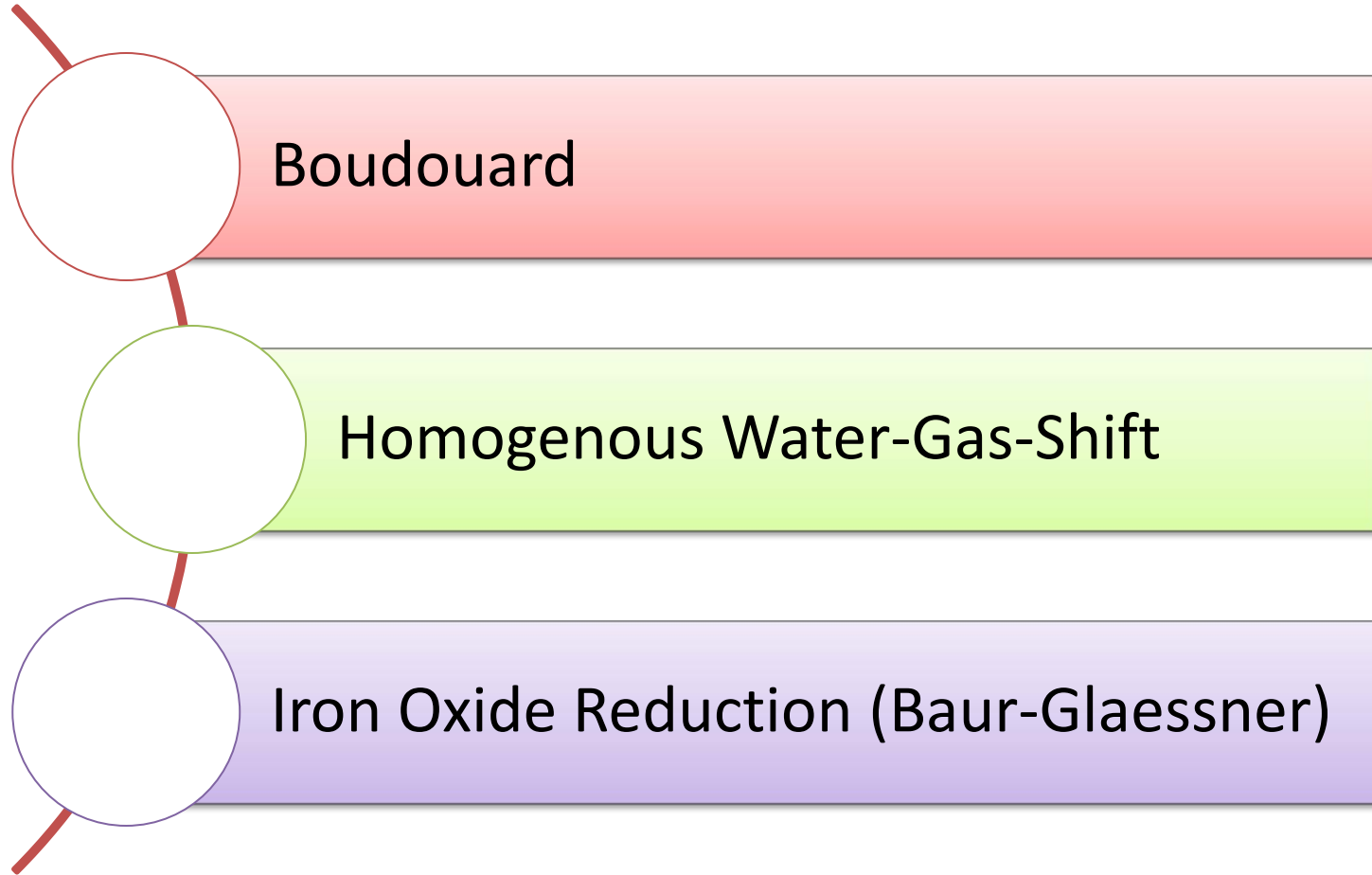
```

# Equilibria calculation
equilibrium_CS_mass_percent = phys_prop_CS.EquilibriumAmount(temperature , pressure , non_equilibrium_CS_mass_percent() ) ;
    
```

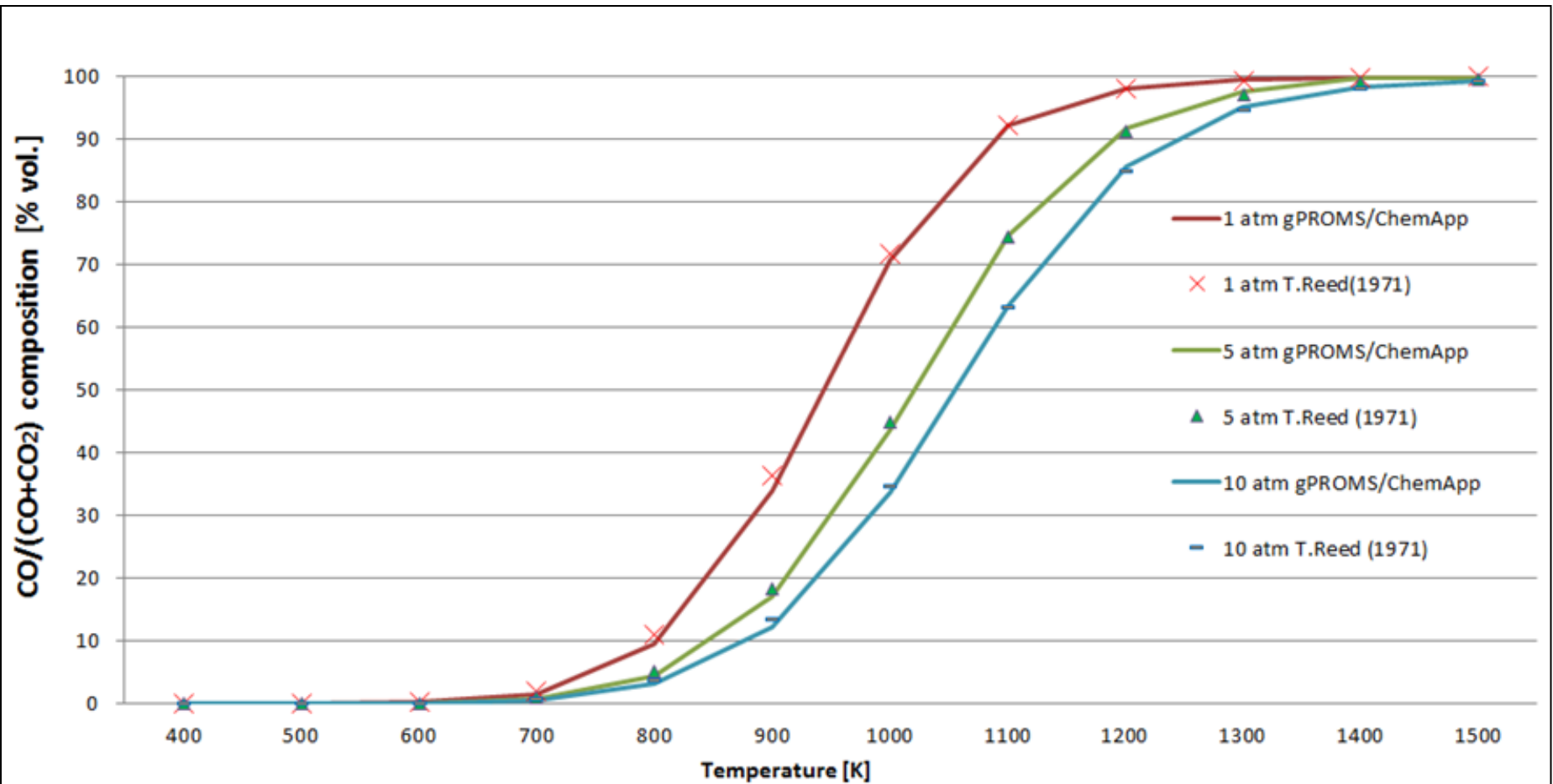
```

outlet.mass_percent("FeO") = equilibrium_CS_mass_percent("FeO_wustite(s)#FeO_wustite(s)");
outlet.mass_percent("Fe2O3_H2O") = equilibrium_CS_mass_percent("Fe2O3(H2O)_solid(s)#Fe2O3(H2O)_solid(s)");
outlet.mass_percent("FeCO3") = equilibrium_CS_mass_percent("FeCO3_siderite(s)#FeCO3_siderite(s)");
    
```

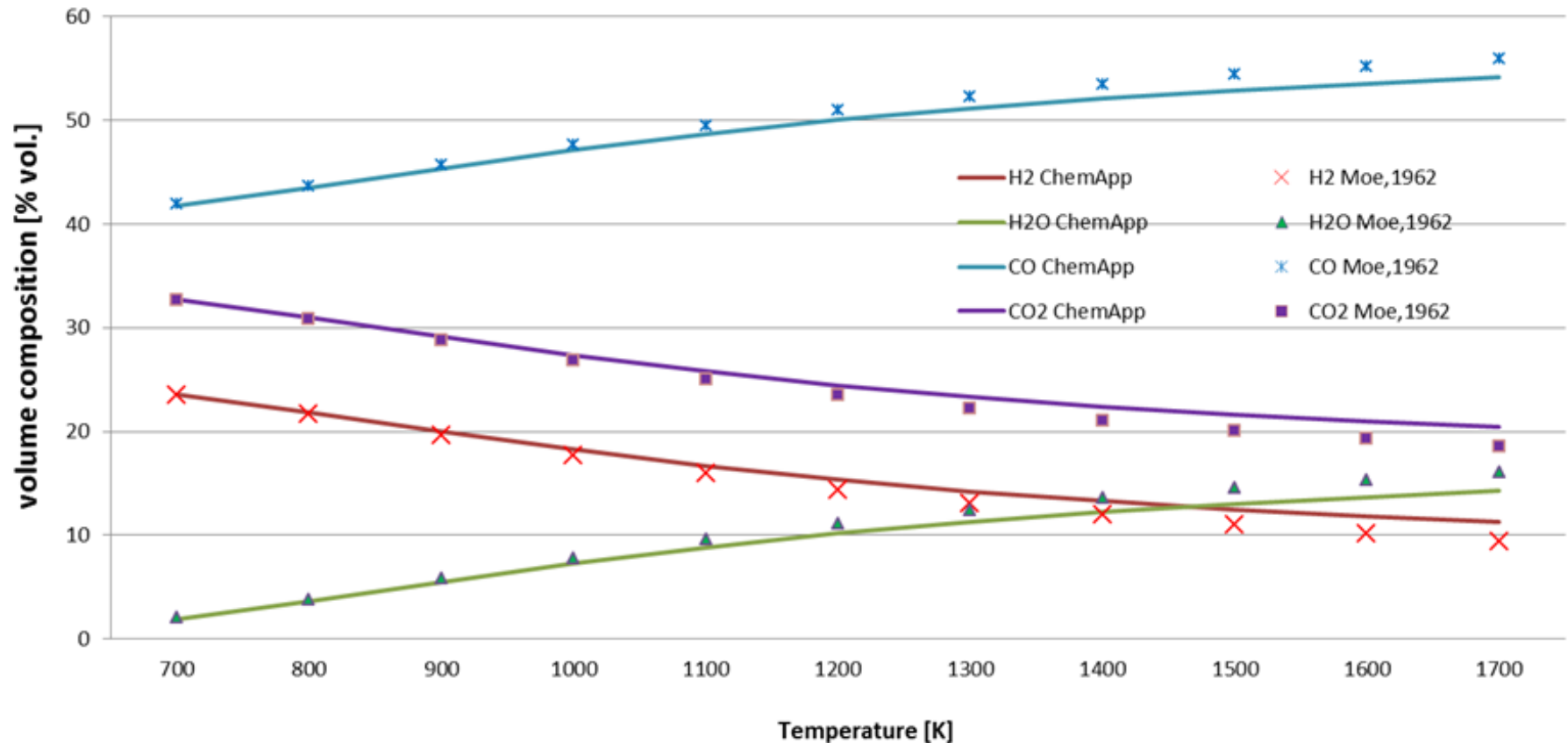




# Boudouard Equilibrium

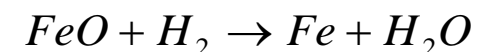
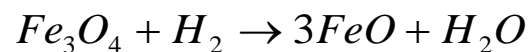
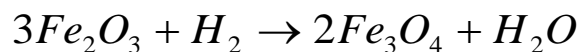
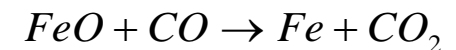
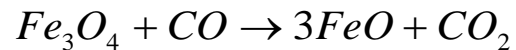
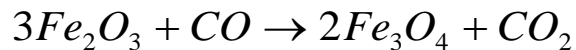
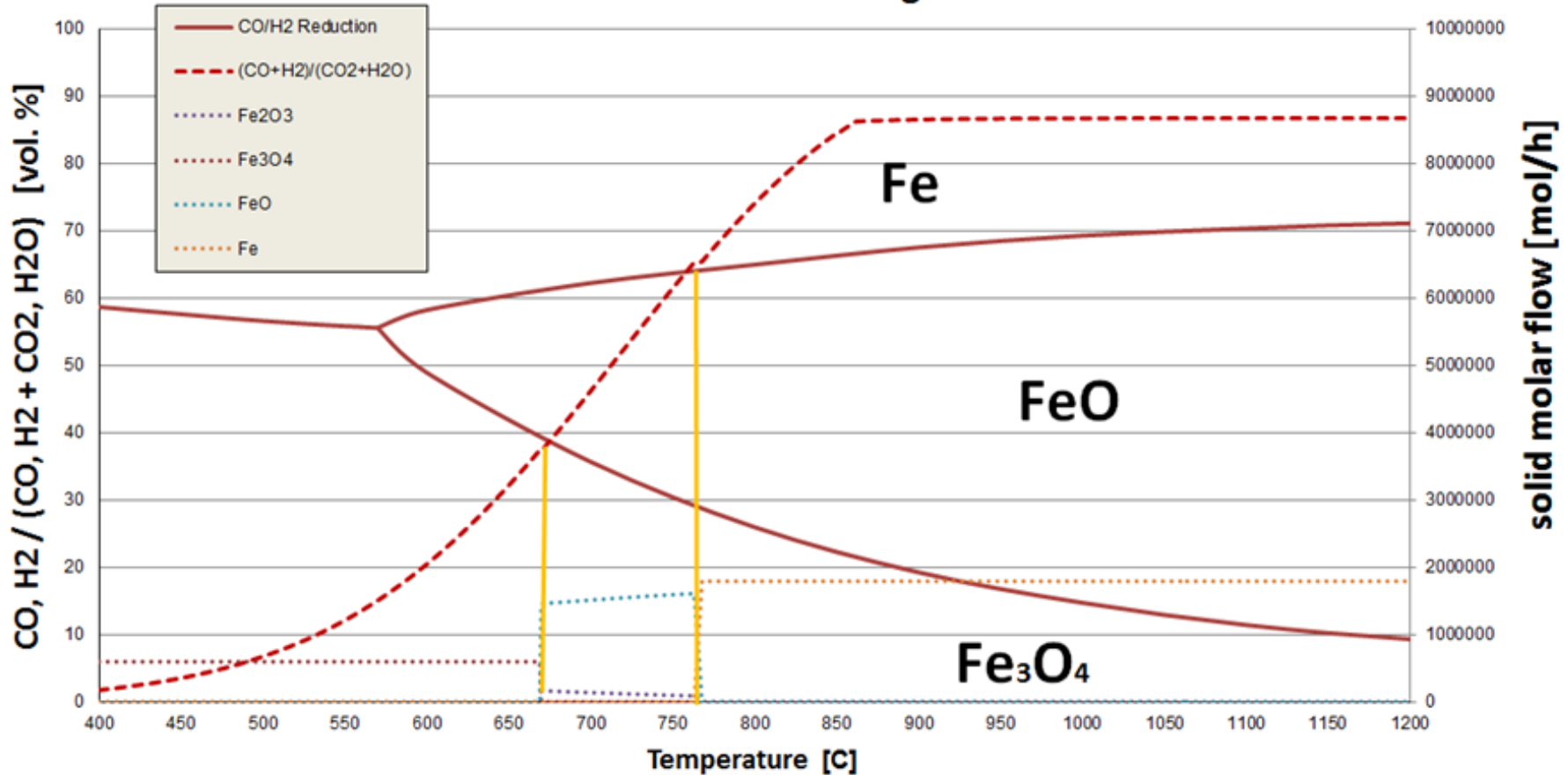


# Homogenous Water-Gas-Shift Equilibrium



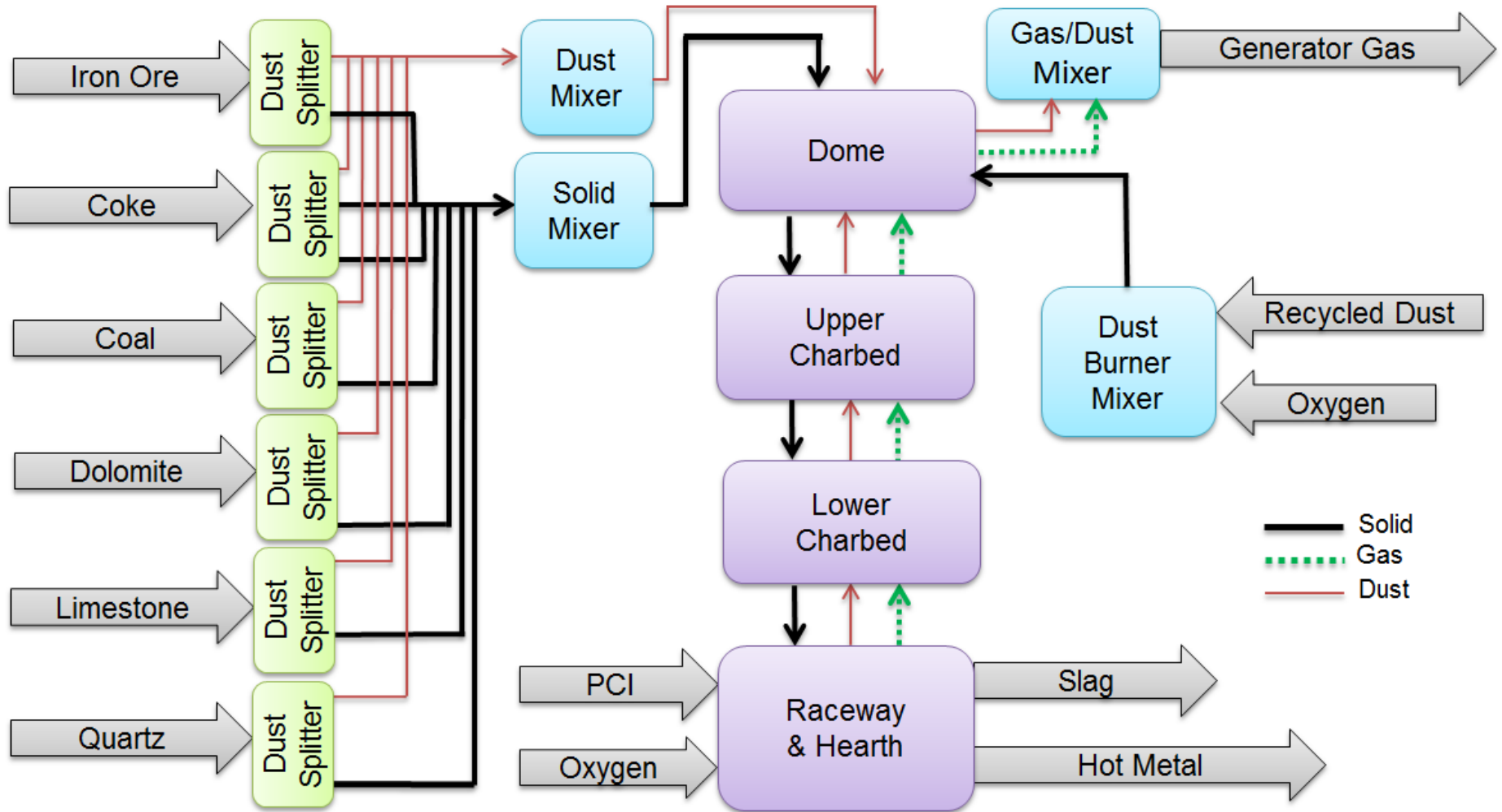
# Iron Oxide Reduction in Equilibrium

Baur-Glössner Diagram

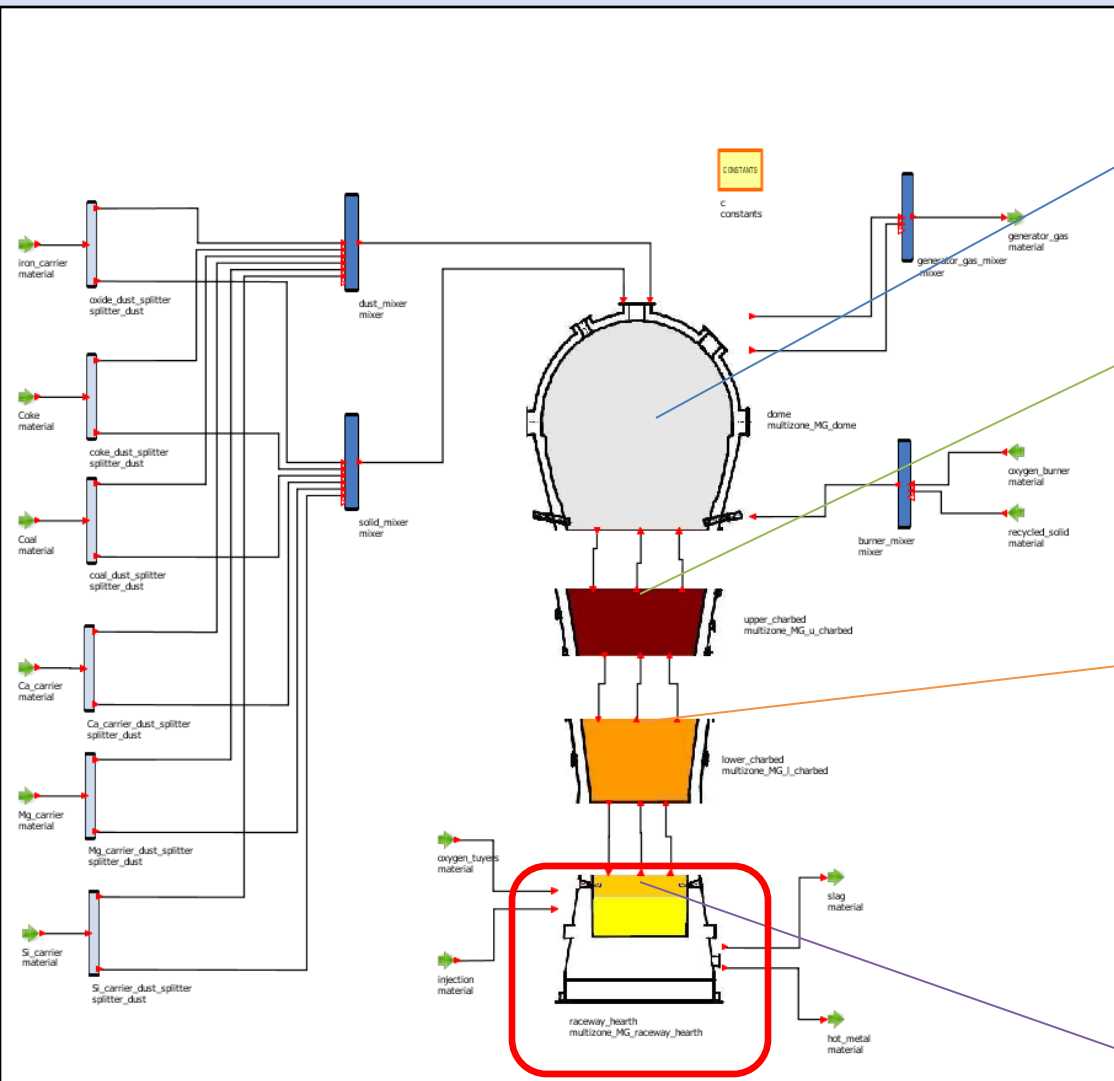




# Melter Gasifier Model Structure



# Reactions Considered in Model Zones



zone calculated with ChemApp

dust reaction	oxide reduction / calcination
recirculated dust combustion	$C + O_2 \rightarrow CO_2$
WGS equilibrium	$CO_2 + H_2 \leftrightarrow CO + H_2O$

drying	$H_2O_{liquid} \rightarrow H_2O_{gas}$
pyrolysis	$volatile\ matter \rightarrow CO_2, CO, H_2O, CH_4, C_6H_6, H_2, H_2S, N_2$
Mg calcination	$MgCO_3 \rightarrow MgO + CO_2$
Boudouard Equilibrium	$CO_2 + C \leftrightarrow 2CO$
WGS equilibrium	$CO_2 + H_2 \leftrightarrow CO + H_2O$

oxide reduction	$3Fe_2O_3 + CO \rightarrow 2Fe_3O_4 + CO_2$
	$3Fe_2O_3 + H_2 \rightarrow 2Fe_3O_4 + H_2O$
	$Fe_3O_4 + CO \rightarrow 3FeO + CO_2$
	$Fe_3O_4 + H_2 \rightarrow 3FeO + H_2O$
	$FeO + CO \rightarrow Fe + CO_2$
	$FeO + H_2 \rightarrow Fe + H_2O$
Ca calcination	$CaCO_3 \rightarrow CaO + CO_2$
WGS equilibrium	$CO_2 + H_2 \leftrightarrow CO + H_2O$

C in hot metal	direct definition
S distribution	$S_{distr} = \frac{[W_{S,Slag}]}{[W_{S,HM}]}$
P distribution	$Mn_{port} = \frac{[m_{Mn, HM}]}{[m_{Mn, HM}] + (m_{Mn, Slag})}$
Mn distribution	$P_{port} = \frac{[m_{P, HM}]}{[m_{P, HM}] + (m_{P, Slag})}$

# Defining Hot Metal / Slag Components

**Reactants - Equilib**

File Edit Table Units Data Search Help

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

1 - 10 | 11 - 17

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
99856.24	Fe				1	
+ 4770	C				1	
+ 530	Si				1	
+ 605.26	Mn				1	
+ 134.62	P				1	
+ 43.46	S				1	
+ 204.5665	FeO				1	
+ 14897.3508	CaO				1	
+ 4673.117126	MgO				1	
+ 12415	SiO2				1	

Initial Conditions

Next >>

FactSage 6.3 Compound: 3/15 databases Solution: 2/14 databases



**Menu - Equilib: Hot Liquids**

File Units Parameters Help

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

Reactants (17)

(gram) 99856.24 Fe + 4770 C + 530 Si + 605.26 Mn + 134.62 P + 43.46 S + 204.5665 FeO + 14897.3508 CaO + 4673.117126 MgO + 12415 SiO2

Products

Compound species

- gas  ideal  real 0
- aqueous 0
- pure liquids 14
- pure solids 1
- suppress duplicates
- \* custom selection species: 15

Target

- none -

Estimate T(K): 1000

Mass(g): 0

Solution species

*	+	Base-Phase	Full Name
		FSstel-M7C3	M7C3
		FSstel-CBCC	CBCC_A12
		FSstel-CUB	CUB_A13
		FSstel-MNS	(Mn,Fe)S_Q
		FSstel-FES	(Fe,Mn)S_P
		FSstel-M3SI	M3SI
		FSstel-FE1S	Fe1Si1
		FSstel-FE5S	FE5Si3

Legend

- immiscible 1

+ selected 2

Show all  selected

species: 50

solutions: 4

Custom Solutions

- fixed activities
- ideal solutions
- activity coefficients

Pseudonyms

apply

include molar volumes

Total Species (max 1500) 65

Total Solutions (max 40) 4

Equilibrium

- normal
- normal + transitions
- transitions only
- open

Final Conditions

<A>	<B>	T(C)	P(bar)	Product H(J)
10	steps	1500	3.6	1 calculation

FactSage 6.3 C:\FactSage\Equil8.DAT

**Fstel-LIQU (Hot Metal):** Al, Al<sub>2</sub>O, AlO, C, Ca, CaO, CaS, Fe, FeS, Mg, MgO, MgS, Mn, MnO, MnS, O, P, S, Si, SiO, Ti, Ti<sub>2</sub>O, TiS

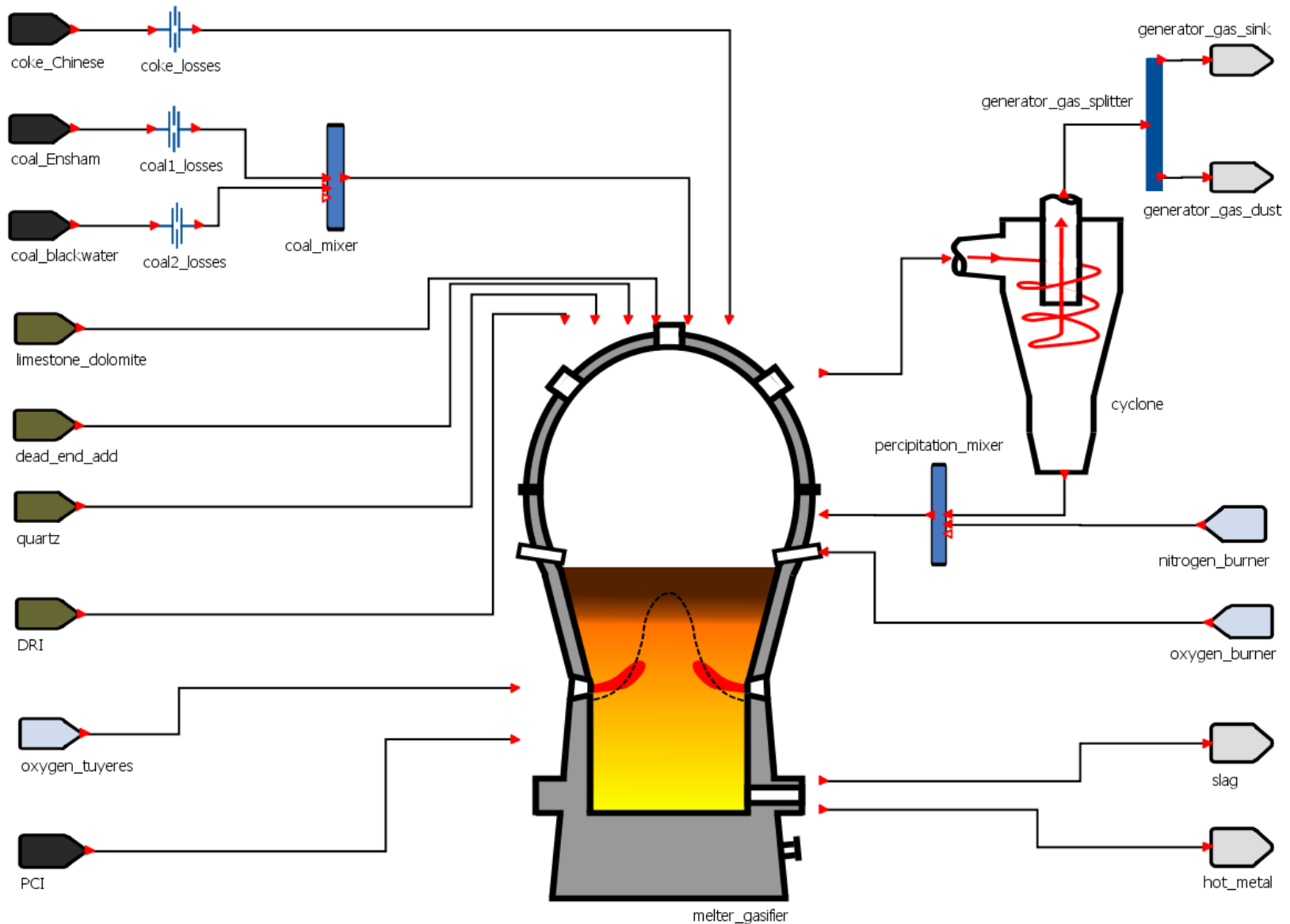
**Fmisc-FeLQ (Hot Metal):** Al, Al<sub>2</sub>O, AlO, C, Ca, CaO, Fe, Mg, MgO, Mn, MnO, O, P, S, Si, SiO, Ti, Ti<sub>2</sub>O, TiO

**FToxid\_SLAGA (Slag):** Al<sub>2</sub>O<sub>3</sub>, Al<sub>2</sub>S<sub>3</sub>, CaO, CaS, Fe<sub>2</sub>O<sub>3</sub>, Fe<sub>2</sub>S<sub>3</sub>, FeO, FeS, MgO, MgS, Mn<sub>2</sub>O<sub>3</sub>, Mn<sub>2</sub>S<sub>3</sub>, MnO, MnS, SiO<sub>2</sub>, Si<sub>2</sub>, Ti<sub>2</sub>O<sub>3</sub>, Ti<sub>3</sub>, TiO<sub>3</sub>, TiS<sub>2</sub>

**FToxid\_SLAGC (Slag):** Al<sub>2</sub>O<sub>3</sub>, Ca<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>, CaO, Fe<sub>2</sub>O<sub>3</sub>, Fe<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>, FeO, FePO<sub>4</sub>, K<sub>2</sub>O, K<sub>3</sub>PO<sub>4</sub>, Mg<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>, MgO, Na<sub>2</sub>O, Na<sub>3</sub>(PO<sub>4</sub>), SiO<sub>2</sub>, Ti<sub>2</sub>O<sub>3</sub>, TiO<sub>2</sub>

**FToxid\_SLAG? (Slag):** Al<sub>2</sub>O<sub>3</sub>, Ca<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>, CaC, CaCO<sub>3</sub>, CaO, CaS, CaSO<sub>4</sub>, Fe<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>, Fe<sub>2</sub>O<sub>3</sub>, Fe<sub>3</sub>(PO<sub>4</sub>), FeO, FePO<sub>4</sub>, FeS, K<sub>2</sub>CO<sub>3</sub>, K<sub>2</sub>O, K<sub>2</sub>S, K<sub>2</sub>SO<sub>4</sub>, K<sub>3</sub>PO<sub>4</sub>, Mg<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>, MgCO<sub>3</sub>, MgO, MgS, MgSO<sub>4</sub>, Mn<sub>2</sub>O<sub>3</sub>, MnO, MnS, MnSO<sub>4</sub>, Na<sub>2</sub>CO<sub>3</sub>, Na<sub>2</sub>O, Na<sub>2</sub>S, Na<sub>2</sub>SO<sub>4</sub>, Na<sub>3</sub>(PO<sub>4</sub>), SiC, SiO<sub>2</sub>, Ti<sub>2</sub>O<sub>3</sub>, TiC, TiO<sub>2</sub>

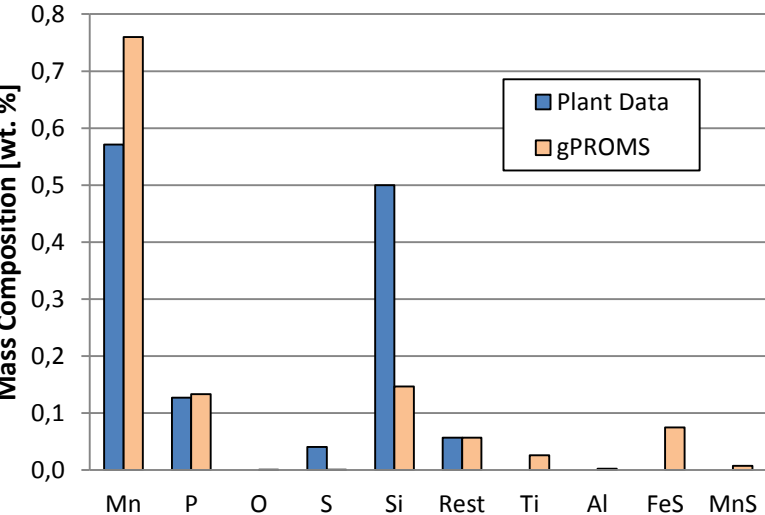
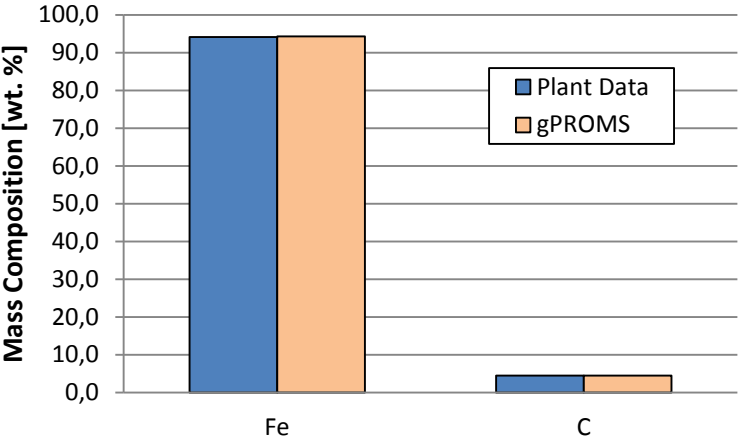
# Multizone Melter Gasifier Flowsheet



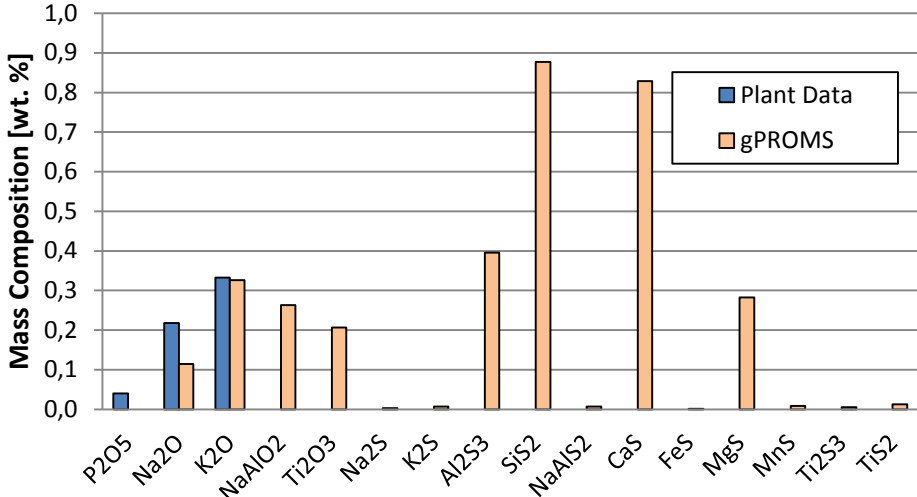
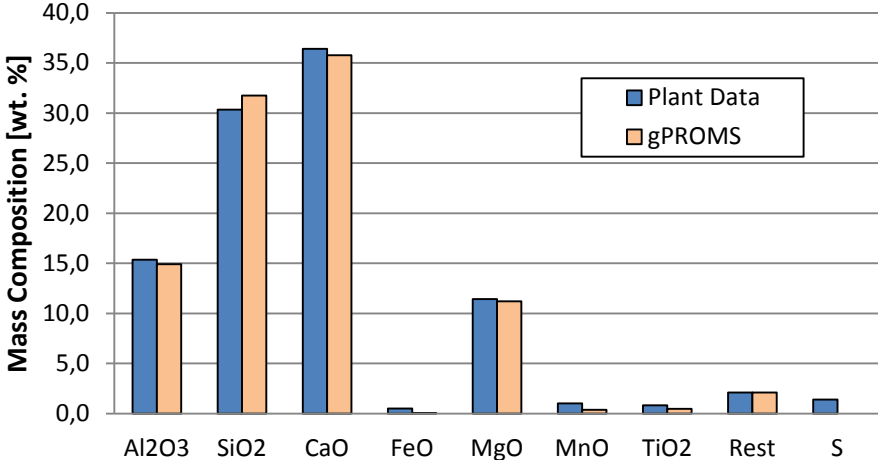


# Simulation Results

## Hot Metal

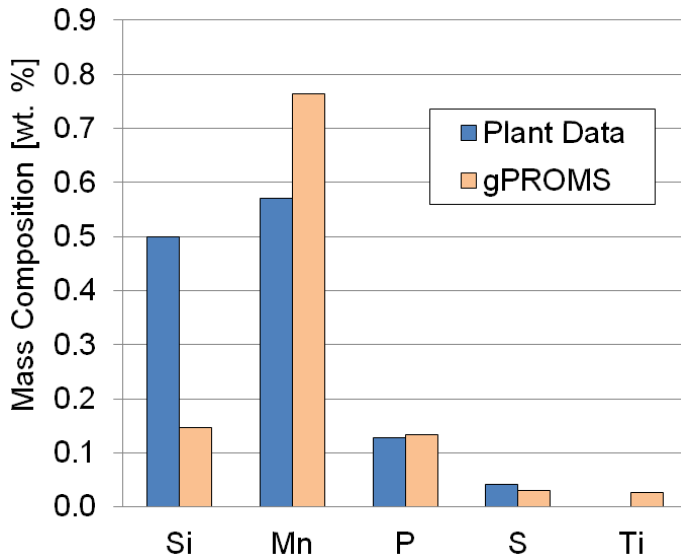
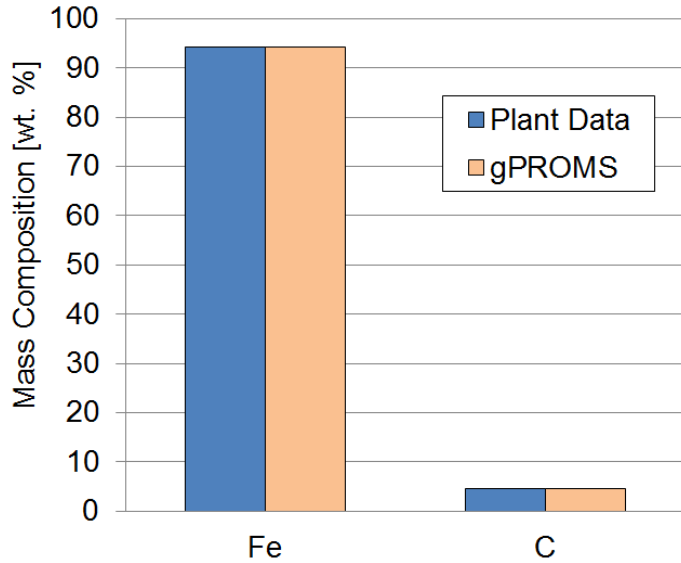


## Slag

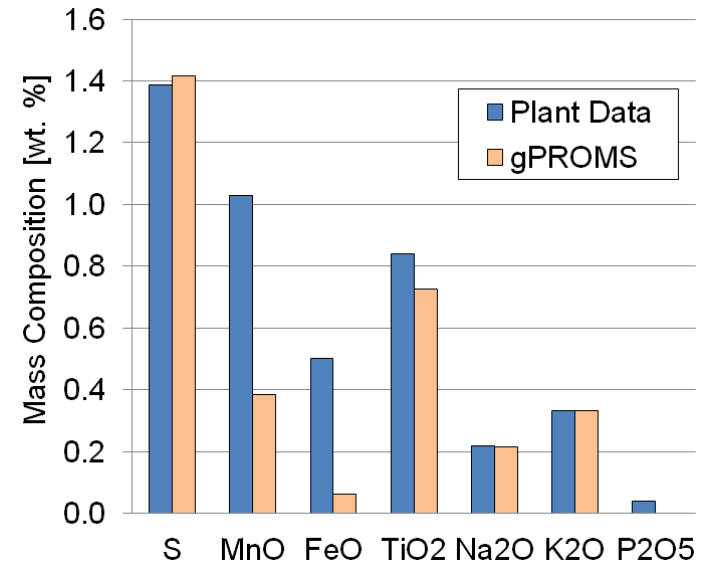
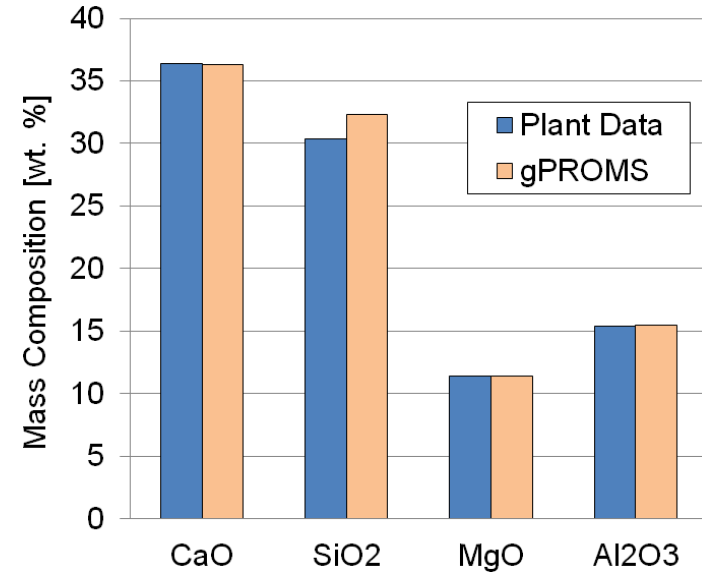


# Transformed Simulation Results

## Hot Metal



## Slag



- a communication structure between gPROMS and ChemApp was established
- several equilibrium reactions were tested successfully for the evaluation of the software tool communication
- a multizone model of a melter gasifier was developed with ChemApp calculation routines implemented in the “Raceway & Hearth” zone
- the simulation results were in good accordance with the real plant data for the major components
- deviation was observed in the Si, Mn components that are crucial for the product quality
- further investigation should be made for the determination of the cause of deviation

# Thank you for your Attention!



We would like to thank SIEMENS VAI Metals Technologies for the collaboration and the financial support