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

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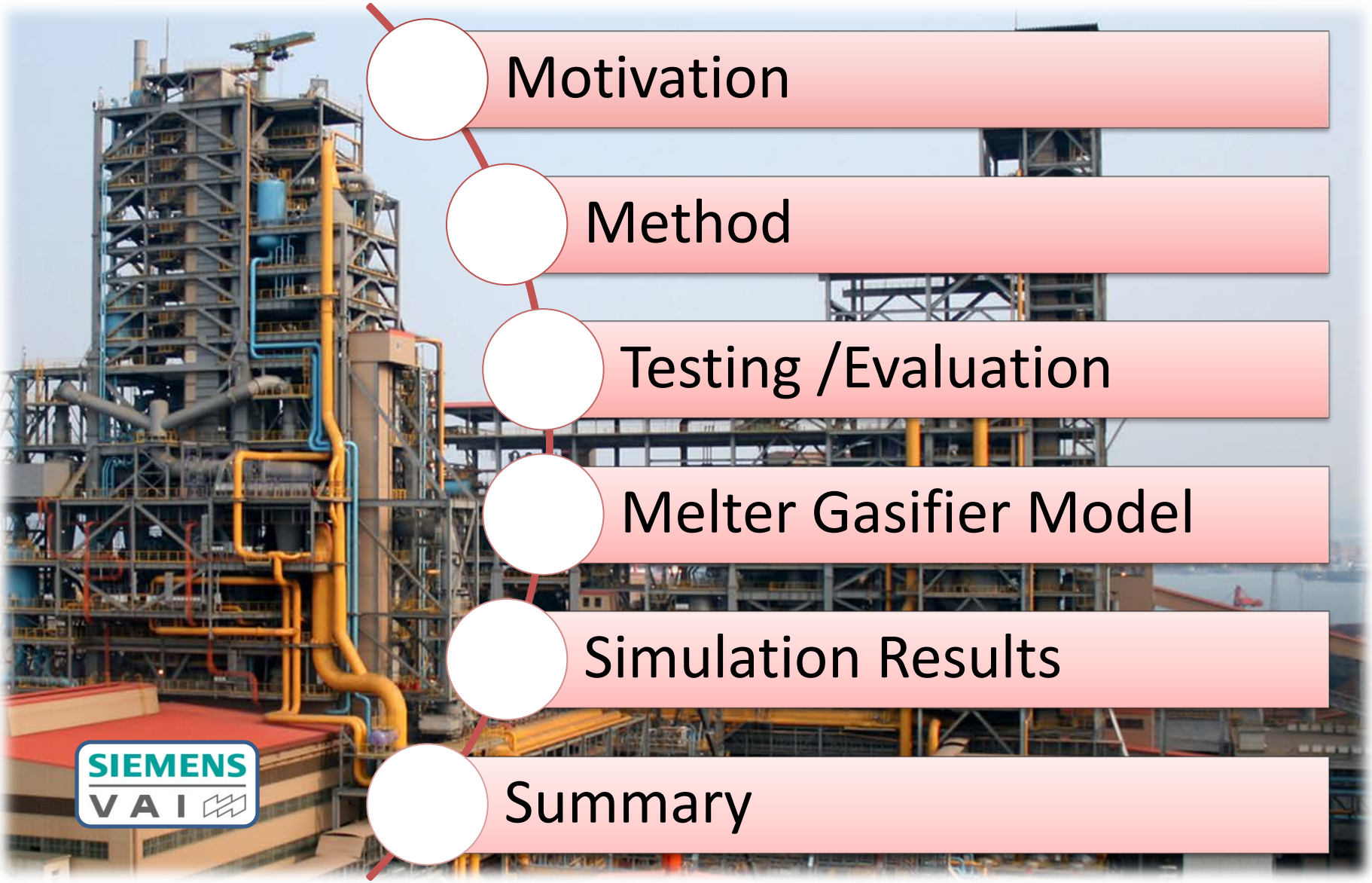
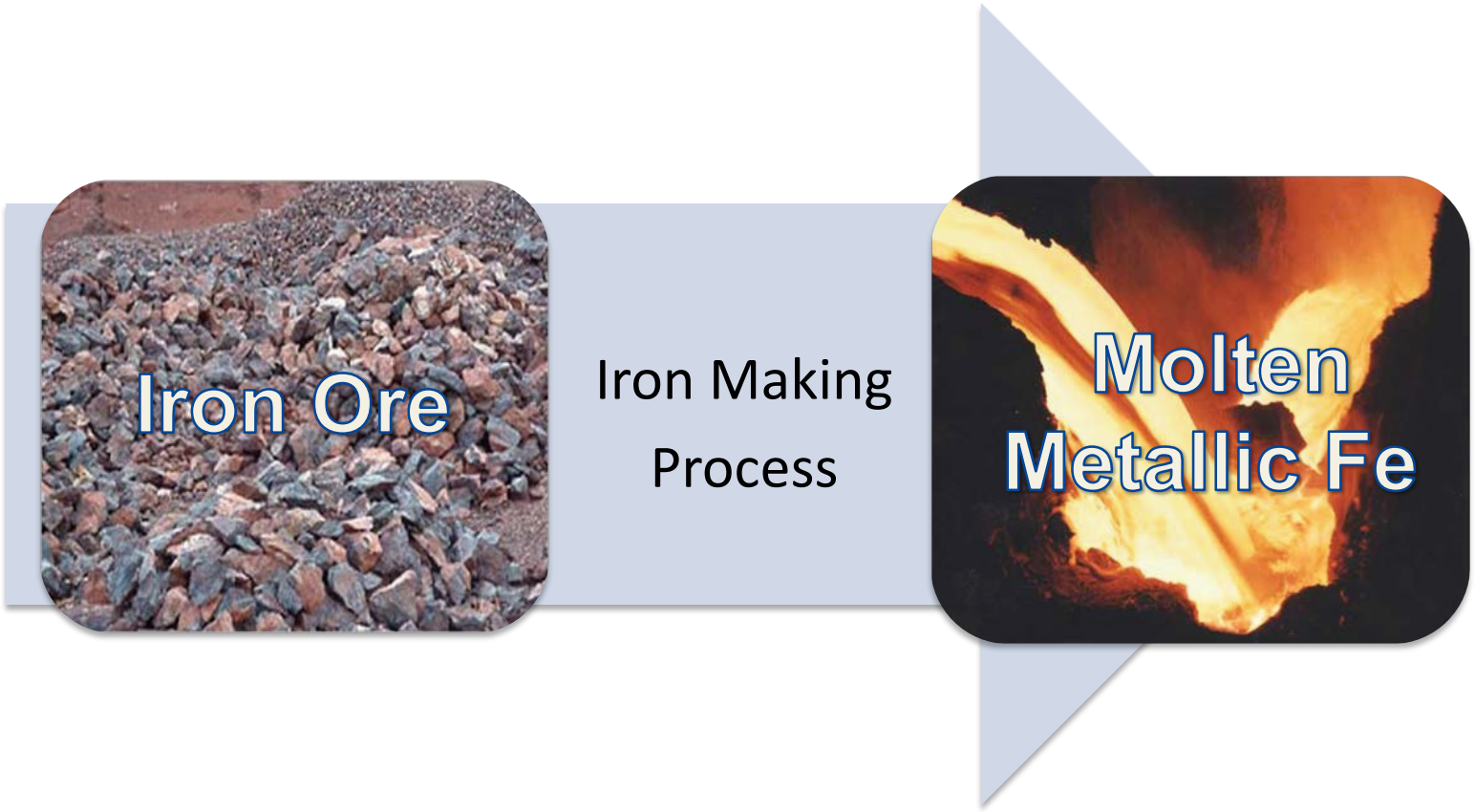
Outline


Motivation
Method
Testing /Evaluation
Melter Gasifier Model
Simulation Results
Summary
SIEMENS
VAI

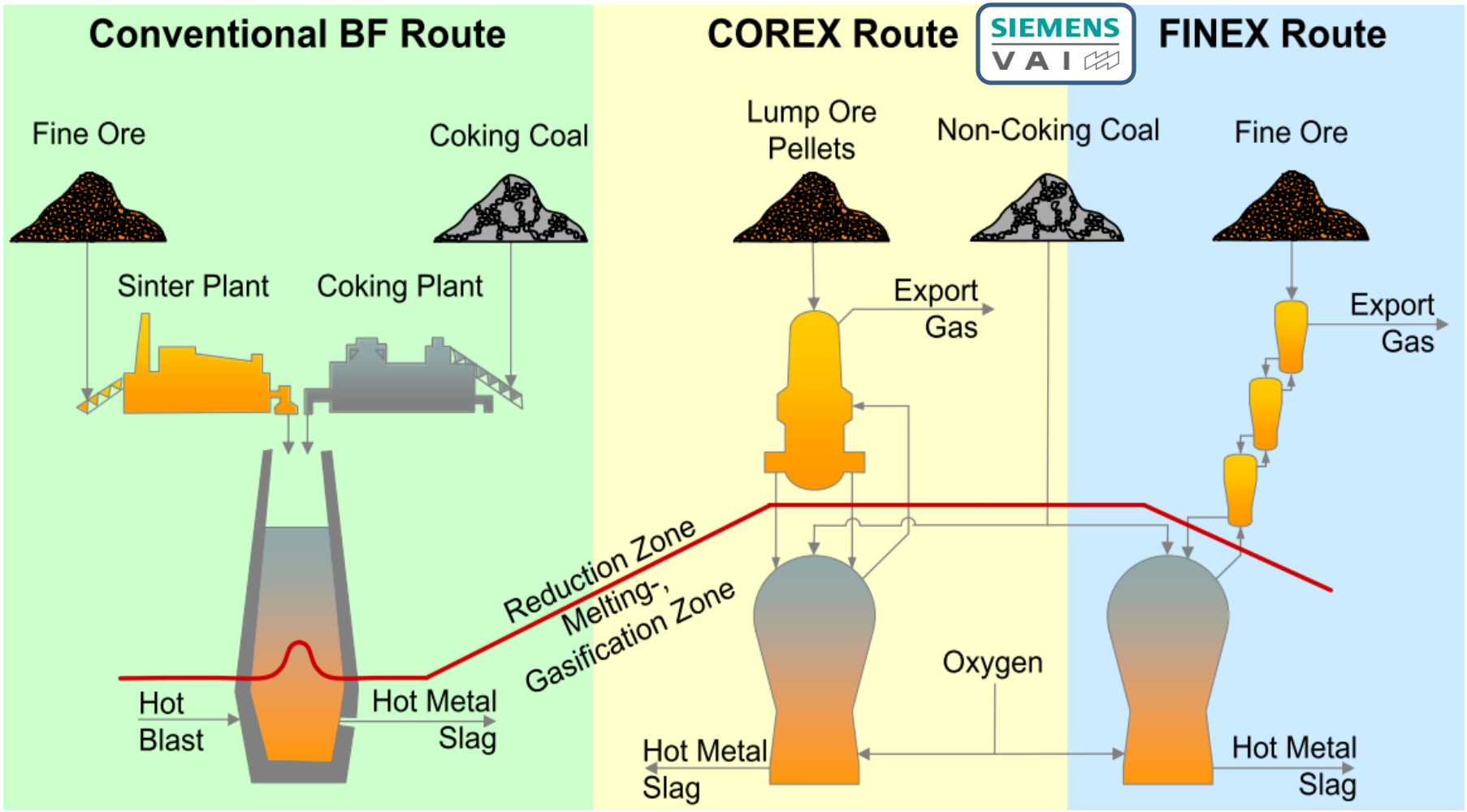
Ironmaking



basic mechanism : iron oxide reduction at high temperatures

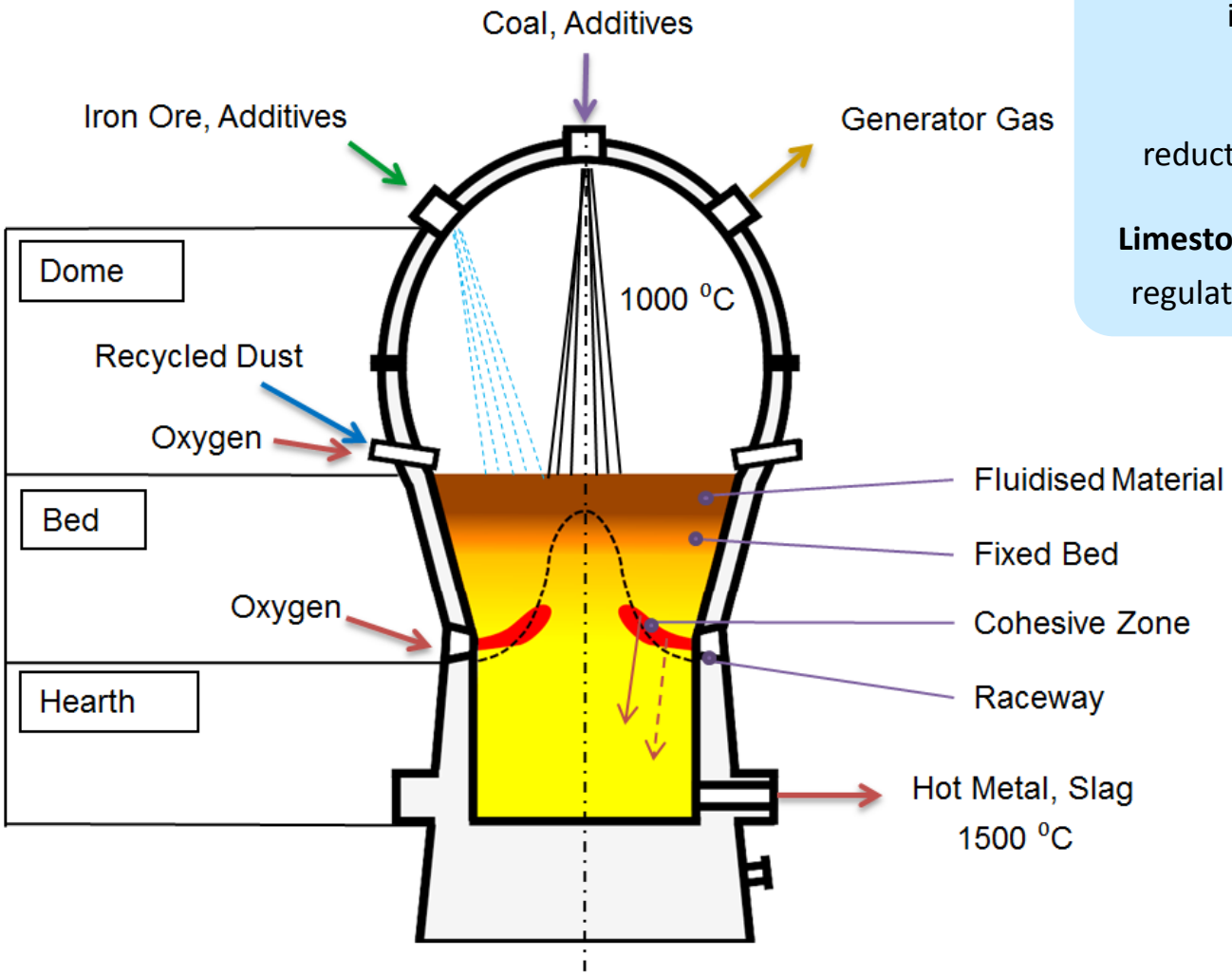
(e.g. $Fe_2O_3 + 3CO \rightarrow 2\mathbf{Fe} + 3CO_2$)

Ironmaking Processes



Corex and **Finex** advantages → lower capital investment and operating cost (15-20%)
→ lower SOx, NOx and dust emission

Melter Gasifier



HCI, 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

Software Tools

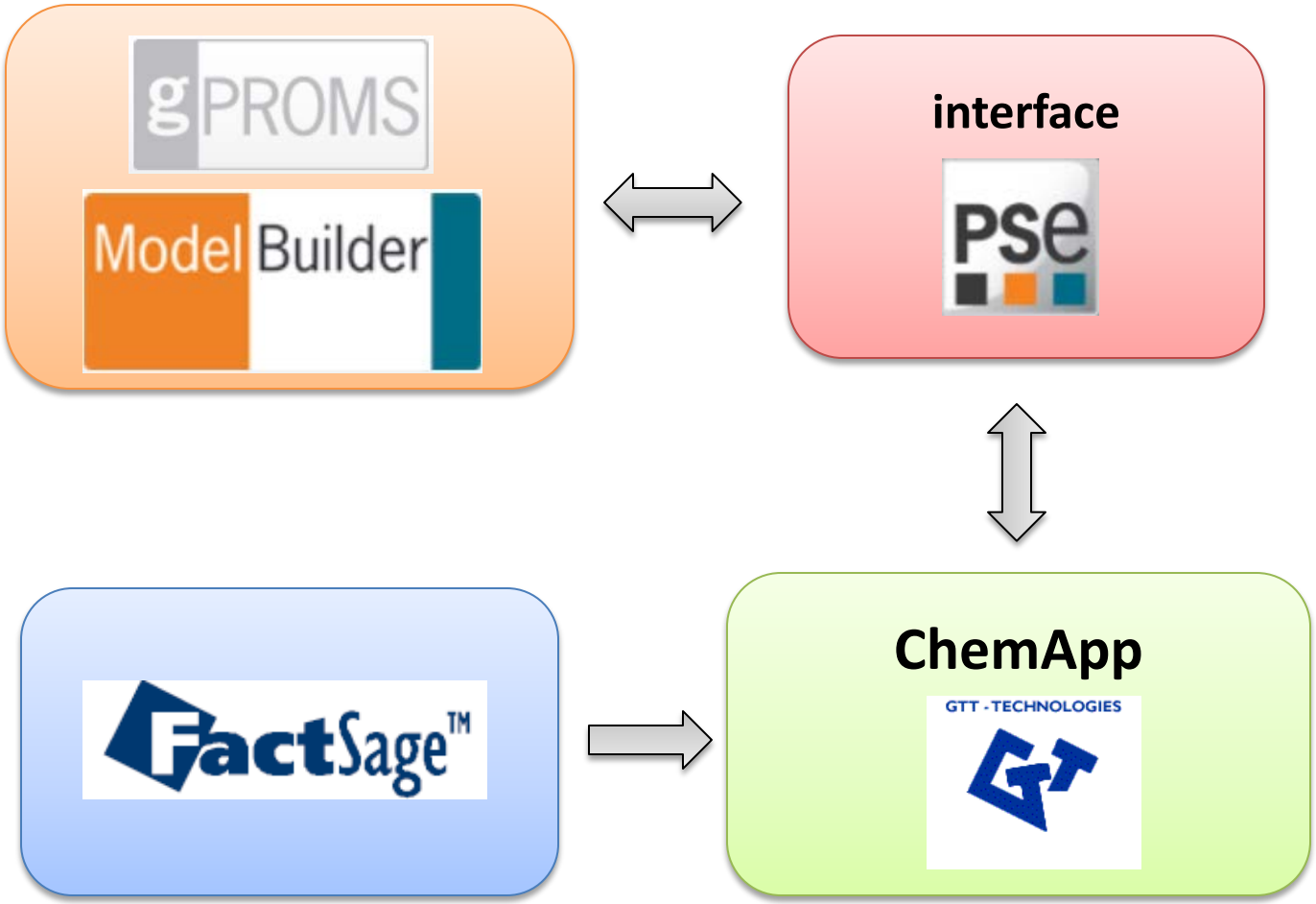
gPROMS

- 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

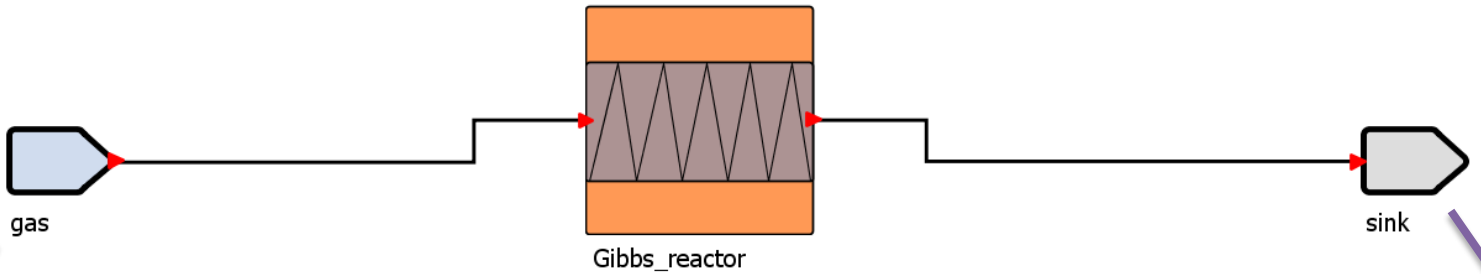
ChemApp

- 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

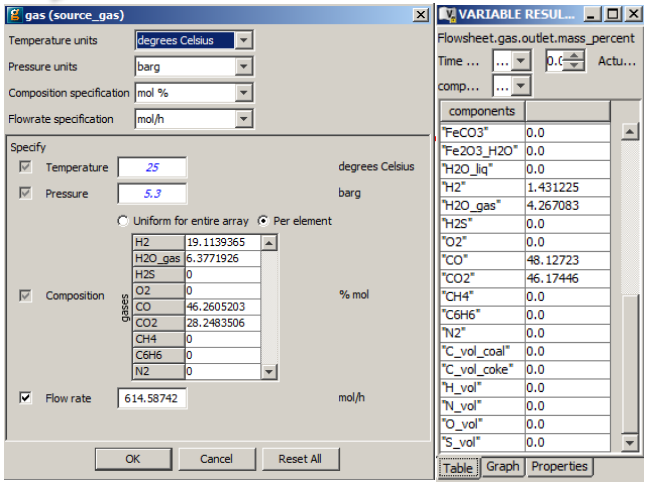
Software Tool Combination

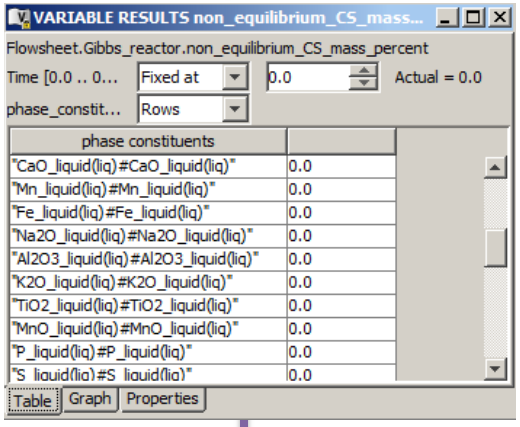


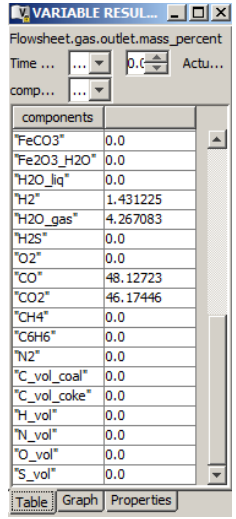
Using ChemApp in gPROMS




```
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");
```



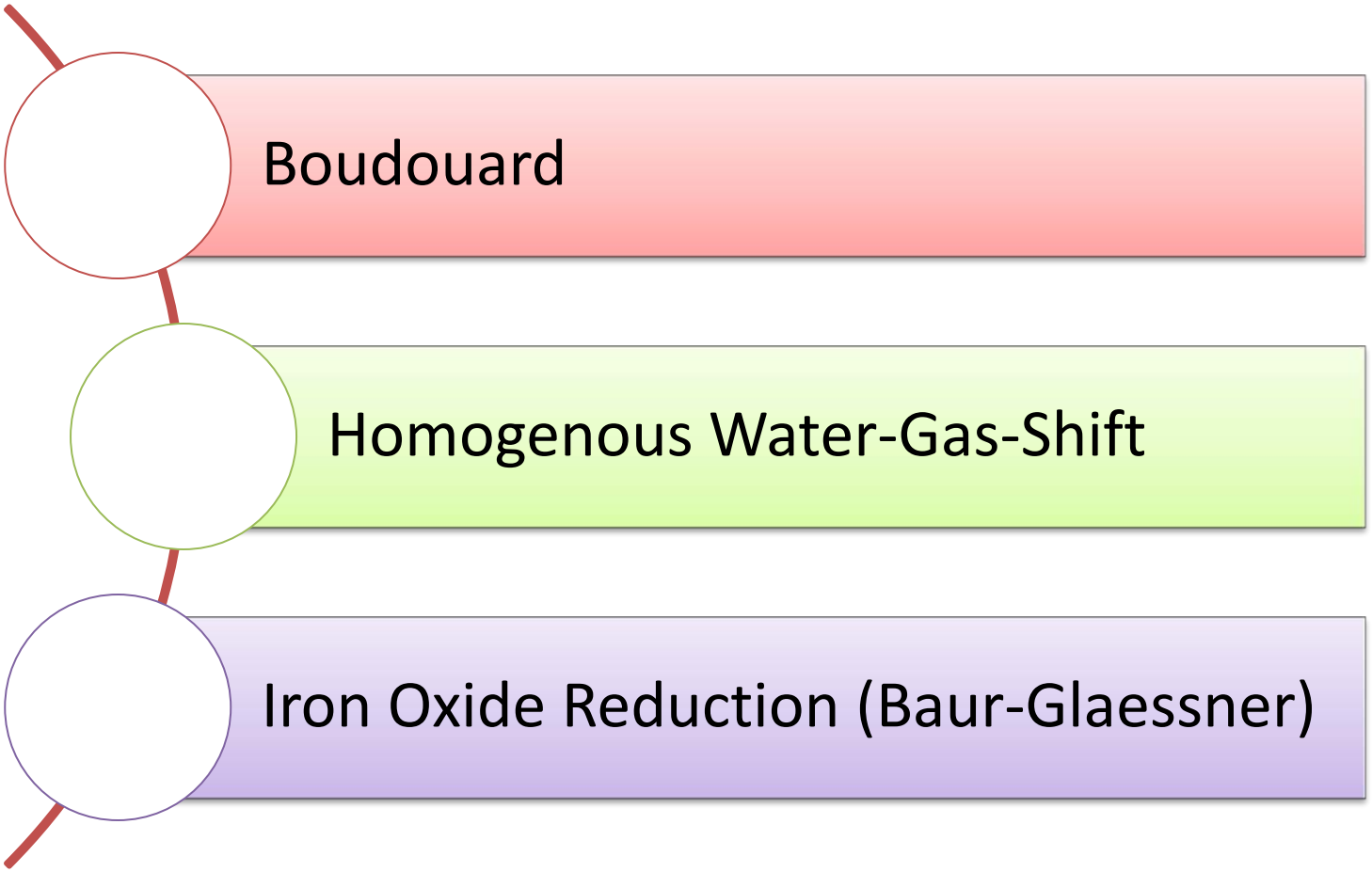




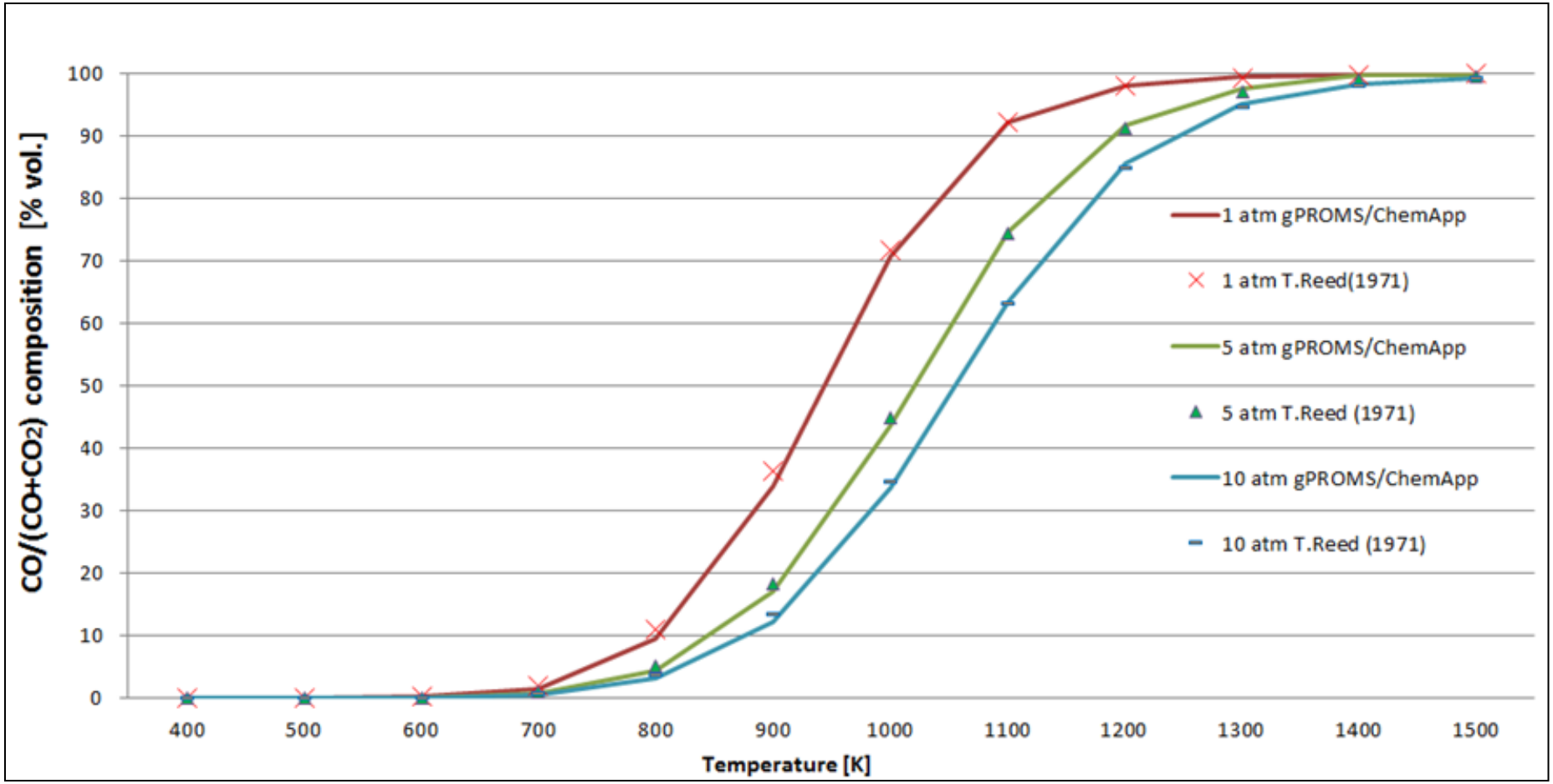

```
# Equilibria calculation
equilibrium_CS_mass_percent = phys_prop_CS.EquilibriumAmount(temperature , pressure , non_equilibrium_CS_mass_percent() ) ;
```

```
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)");
```

Testing the Software Combination



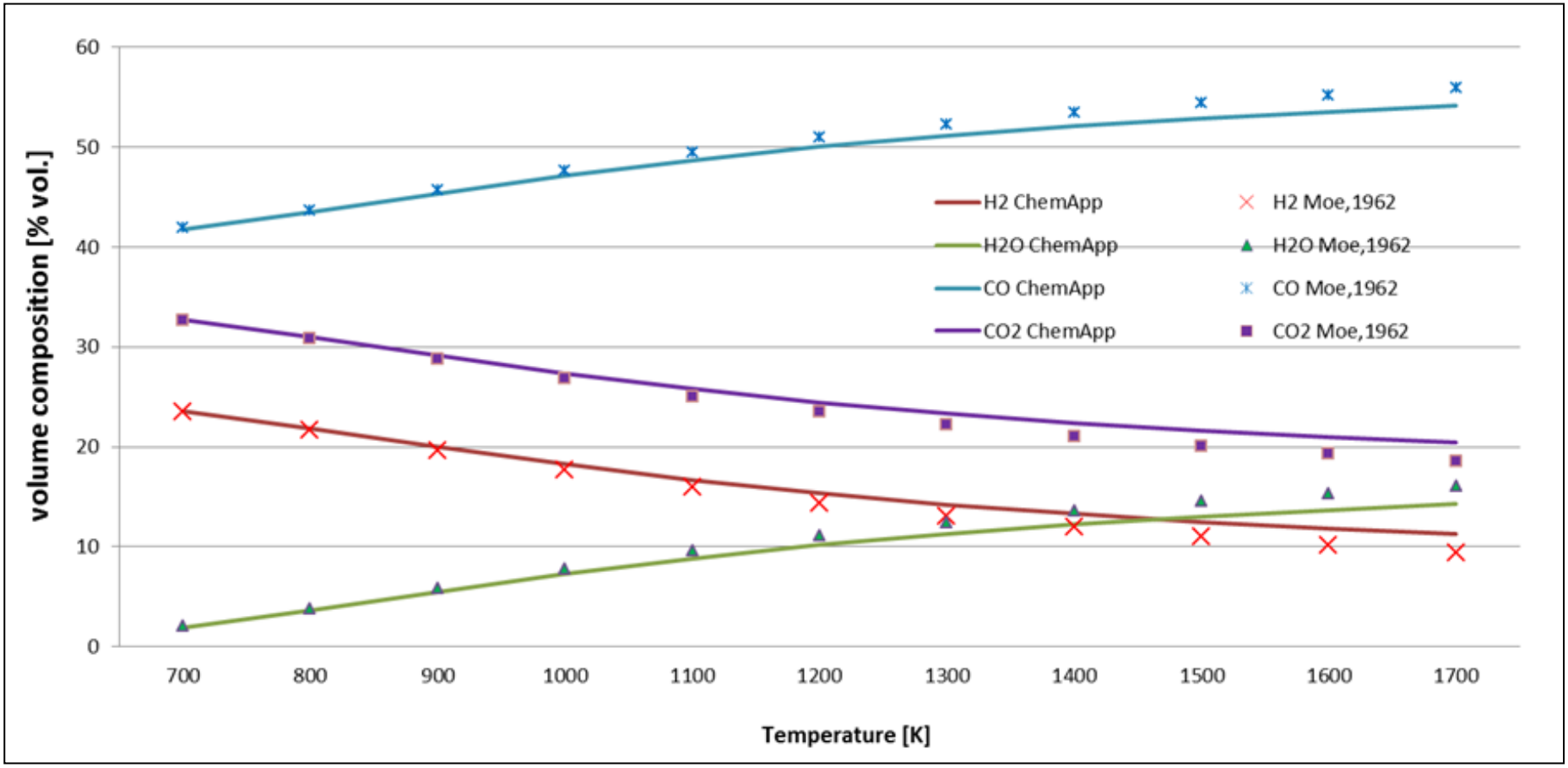
Boudouard Equilibrium



$$CO_2 + C \leftrightarrow 2CO$$

T. Reed, *Free Energy of Formation of Binary Compounds, MIT Press, Cambridge, MA, 1972*

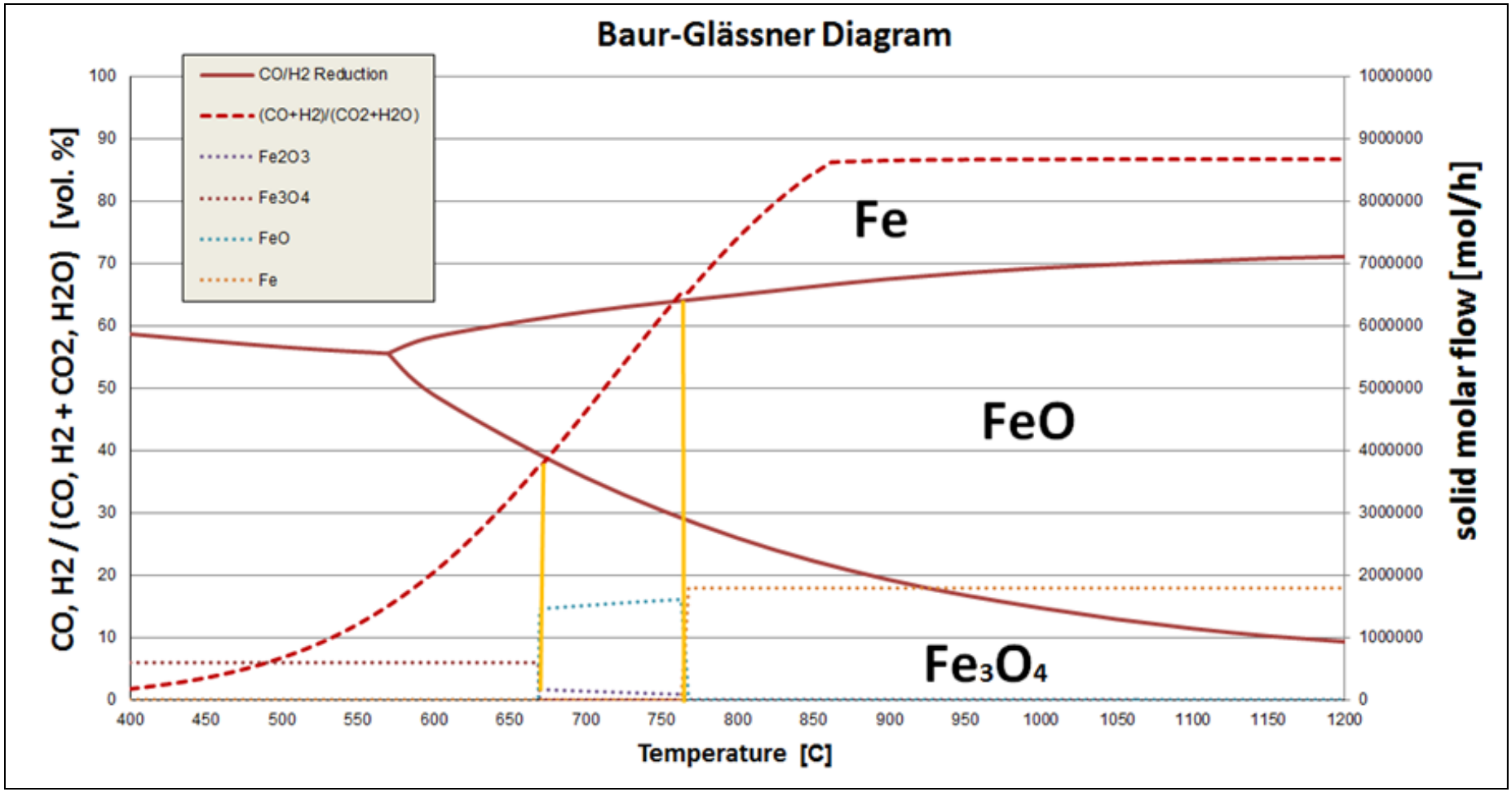
Homogenous Water-Gas-Shift Equilibrium



$$CO_2 + H_2 \leftrightarrow CO + H_2O$$

J.M. Moe, *Design of Water-Gas Shift reactors, Chemical Engineering Progress, 58 (3), 33, 1962*

Iron Oxide Reduction in Equilibrium

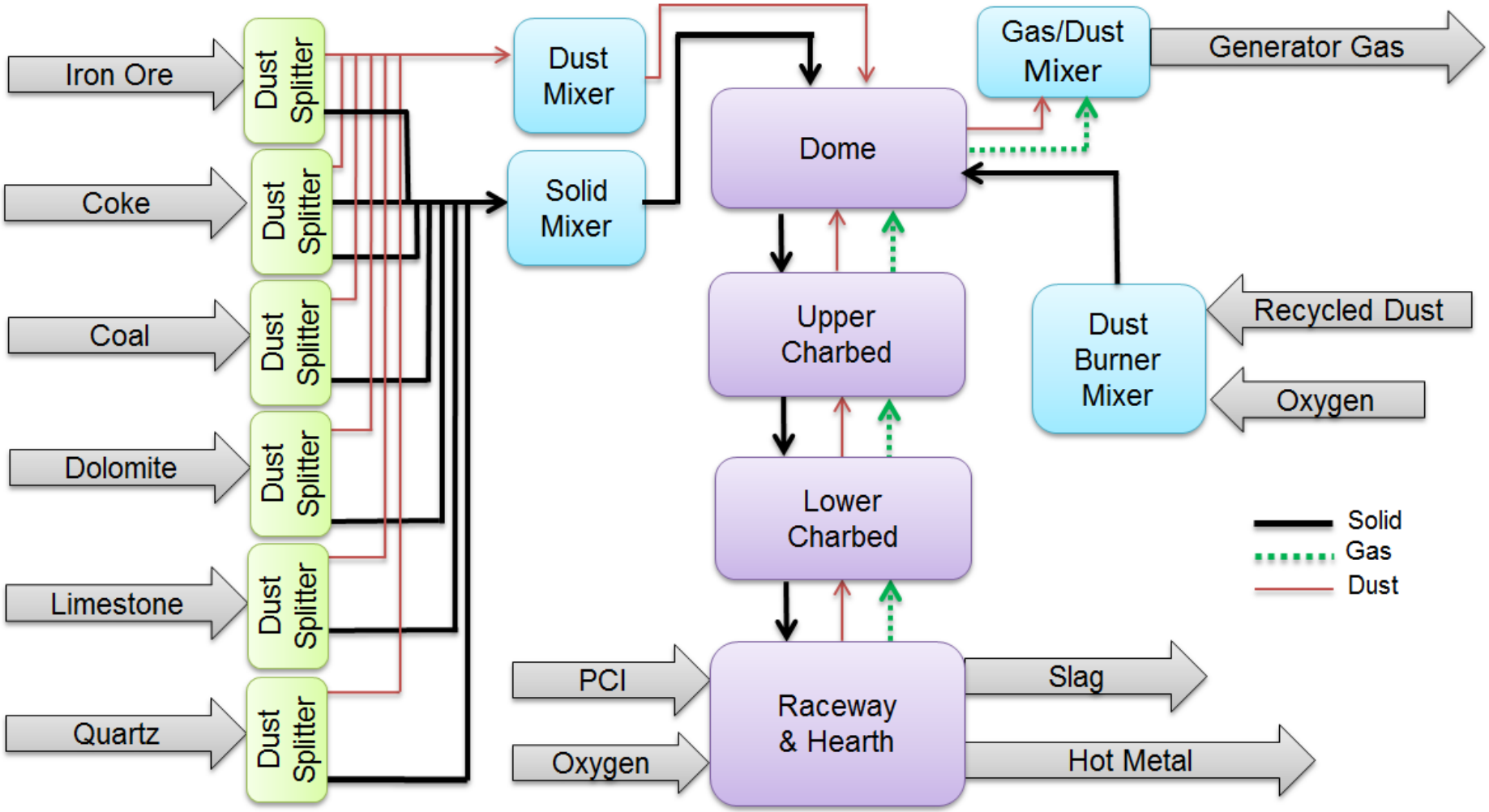


$$3Fe_2O_3 + CO \rightarrow 2Fe_3O_4 + CO_2 \qquad Fe_3O_4 + CO \rightarrow 3FeO + CO_2 \qquad FeO + CO \rightarrow Fe + CO_2$$

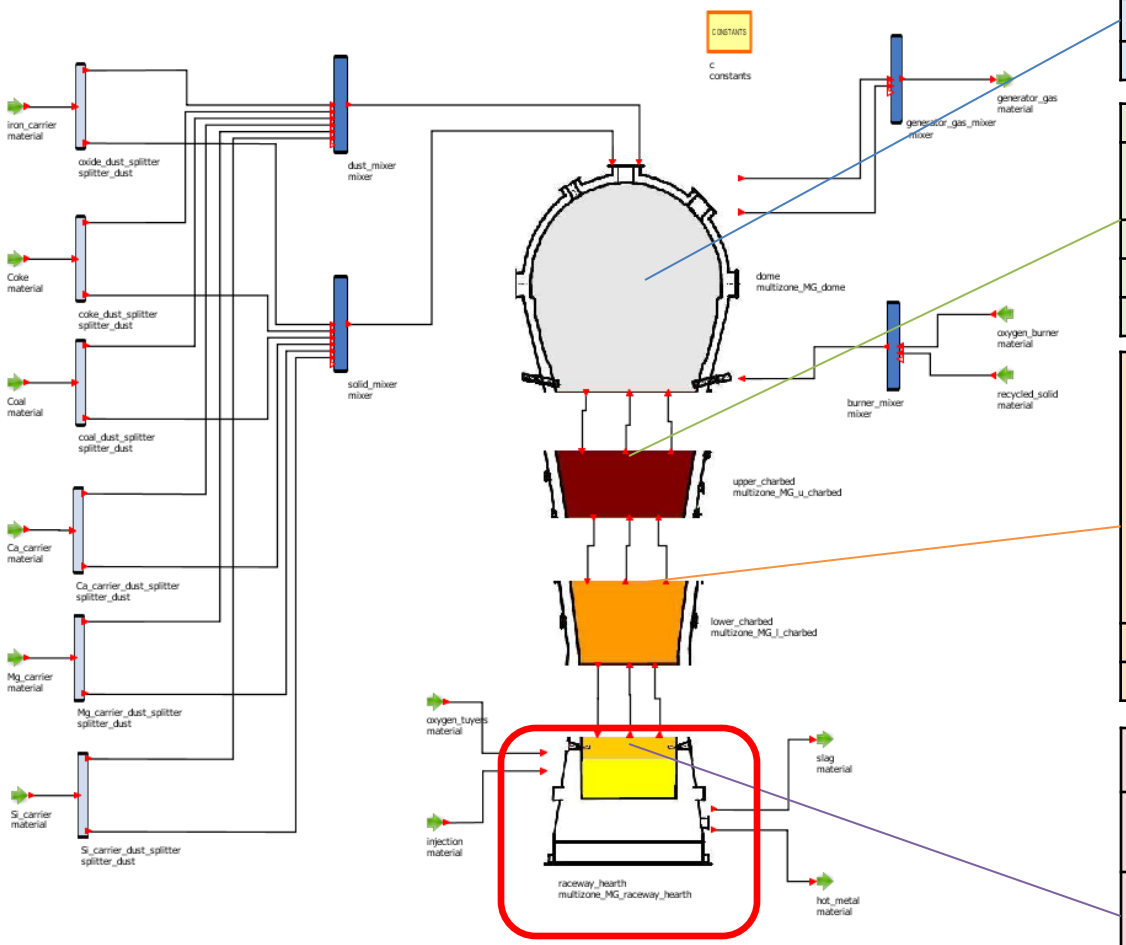
$$3Fe_2O_3 + H_2 \rightarrow 2Fe_3O_4 + H_2O \qquad Fe_3O_4 + H_2 \rightarrow 3FeO + H_2O \qquad FeO + H_2 \rightarrow Fe + H_2O$$

T. Tappeiner, *Ganzheiliche Betrachtung des Einsatzes von LRI im Hochofen zur CO2-Minimierung, MIT Press, Leoben, 2011*

Melter Gasifier Model Structure



Reactions Considered in Model Zones



zone calculated with ChemApp

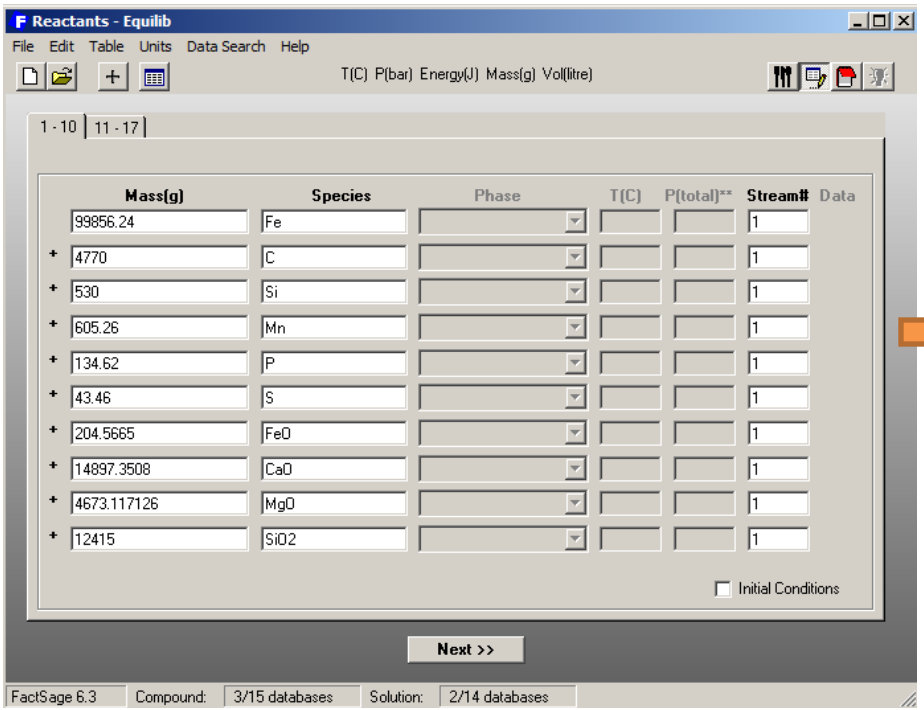
dust reaction	oxide reduction / calcination
recirculated dust combustion	$C + O_2 \rightarrow CO_2$
WGS equilibrium	$CO_2 + H_2 \leftrightarrow CO + H_2O$

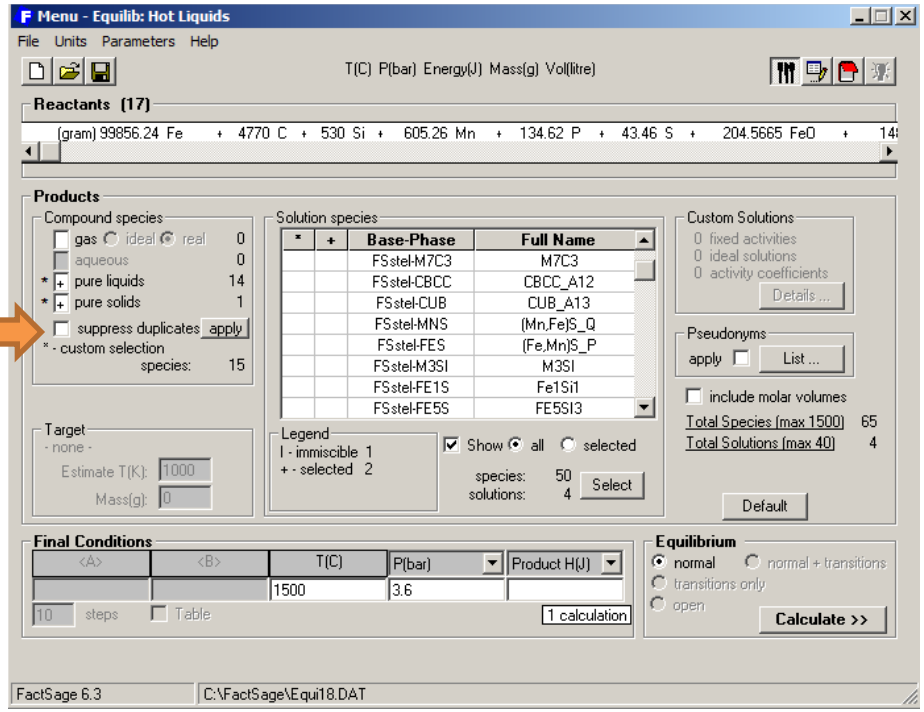
drying	$H_2O_{liquid} \rightarrow H_2O_{gas}$
pyrolysis	$volatile\ matter \rightarrow CO_2, CO, H_2O, CH_4, C_6H_6, H_2, H_2S, N_2$
Mg calcination	$MgCO_3 \rightarrow MgO + CO_2$
Boudouard Equilibrium	$CO_2 + C \leftrightarrow 2CO$
WGS equilibrium	$CO_2 + H_2 \leftrightarrow CO + H_2O$

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	$Mn_{port} = \frac{\dot{[m}_{Mn,HM}]}{\dot{[m}_{Mn,HM}] + \dot{(m}_{Mn,Slag})}$
Mn distribution	$P_{port} = \frac{\dot{[m}_{P,HM}]}{\dot{[m}_{P,HM}] + \dot{(m}_{P,Slag})}$

Defining Hot Metal / Slag Components





Fstel-LIQU (Hot Metal): Al, Al2O, AlO, C, Ca, CaO, CaS, Fe, FeS, Mg, MgO, MgS, Mn, MnO, MnS, O, P, S, Si, SiO, Ti, Ti2O, TiS

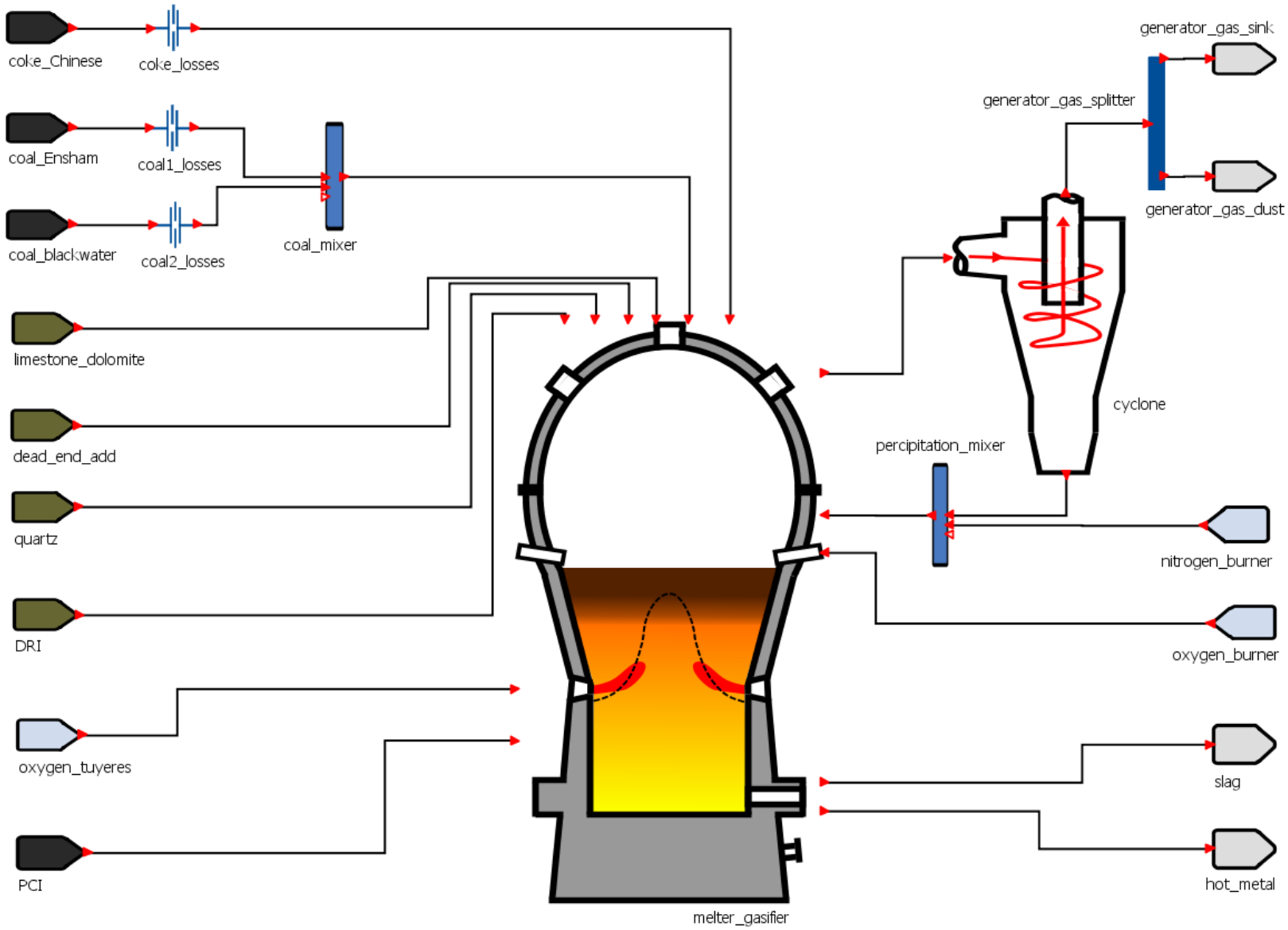
Fmisc-FeLQ (Hot Metal): Al, Al2O, AlO, C, Ca, CaO, Fe, Mg, MgO, Mn, MnO, O, P, S, Si, SiO, Ti, Ti2O, TiO

FToxid_SLAGA (Slag): Al2O3, Al2S3, CaO, CaS, Fe2O3, Fe2S3, FeO, FeS, MgO, MgS, Mn2O3, Mn2S3, MnO, MnS, SiO2, SiS2, Ti2O3, TiS3, TiO3, TiS2

FToxid_SLAGC (Slag): Al2O3, Ca3(PO4)2, CaO, Fe2O3, Fe3(PO4)2, FeO, FePO4, K2O, K3PO4, Mg3(PO4)2, MgO, Na2O, Na3(PO4), SiO2, Ti2O3, TiO2

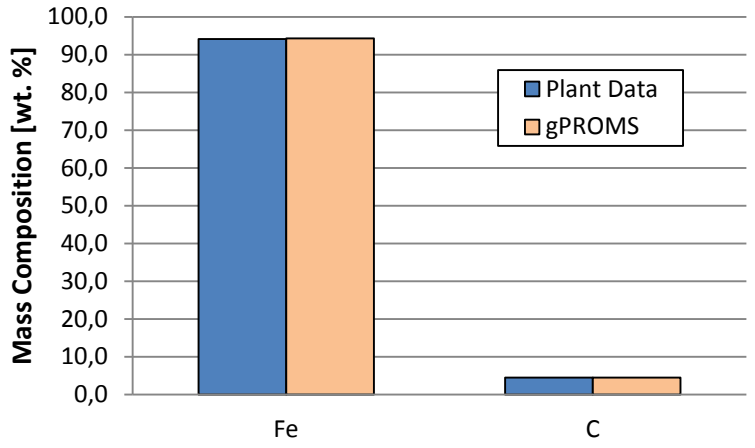
FToxid_SLAG? (Slag): Al2O3, Ca3(PO4)2, CaC, CaCO3, CaO, CaS, CaSO4,Fe2(SO4)3, Fe2O3, Fe3(PO4), FeO, FePO4, FeS, K2CO3, K2O, K2S, K2SO4, K3PO4, Mg3(PO4)2, MgCO3, MgO, MgS, MgSO4, Mn2O3, MnO, MnS, MnSO4, Na2CO3, Na2O, Na2S, Na2SO4, Na3(PO4), SiC, SiO2, Ti2O3, TiC, TiO2

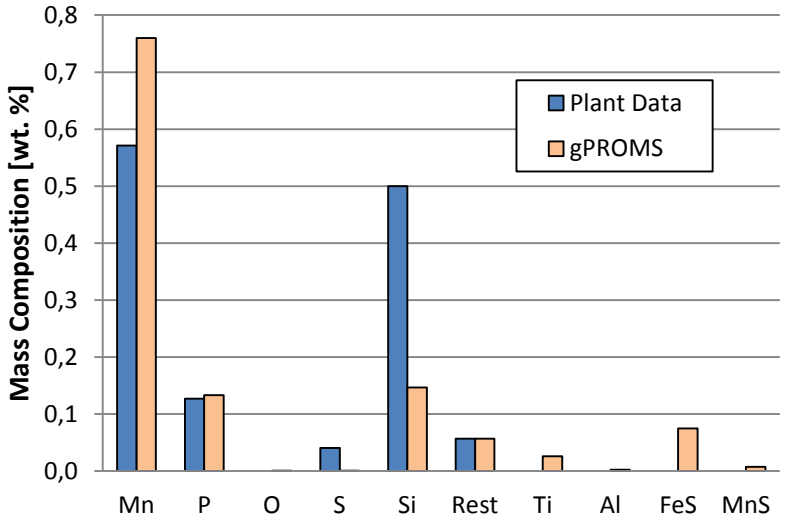
Multizone Melter Gasifier Flowsheet



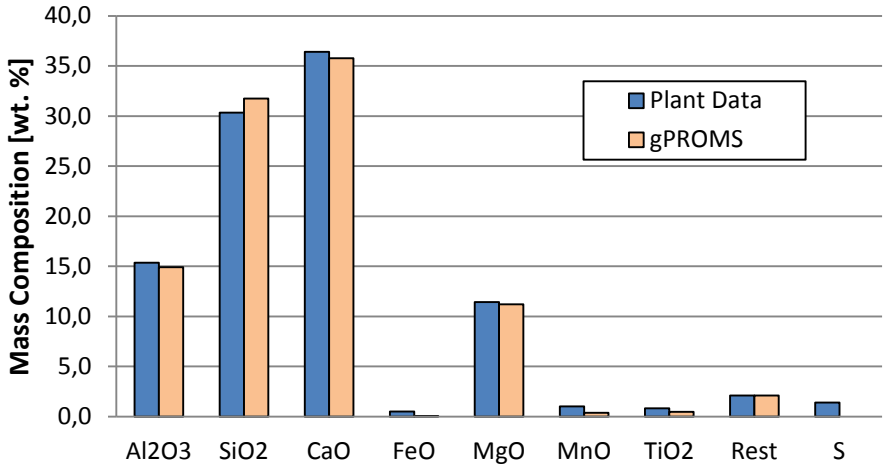
Simulation Results

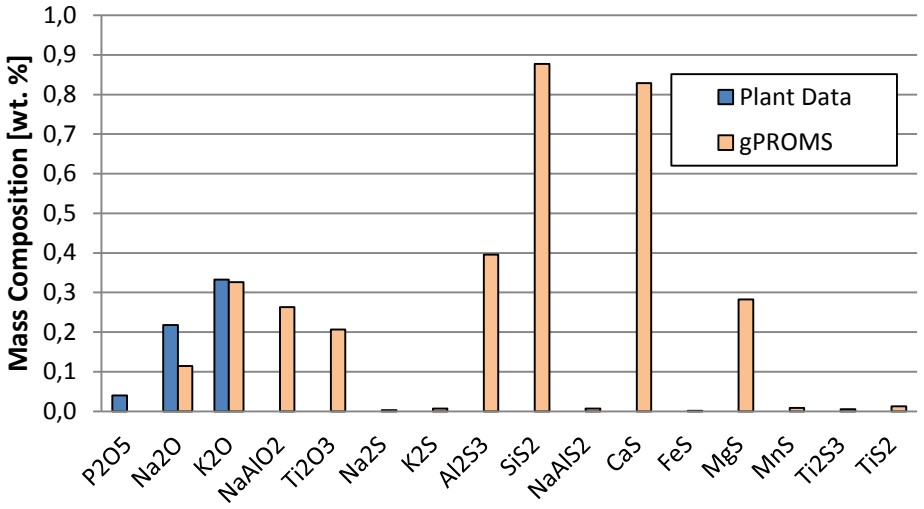
Hot Metal





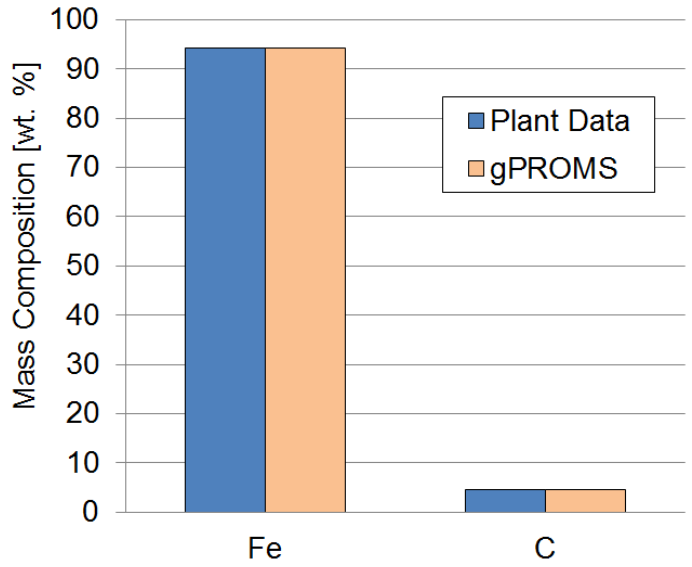
Slag

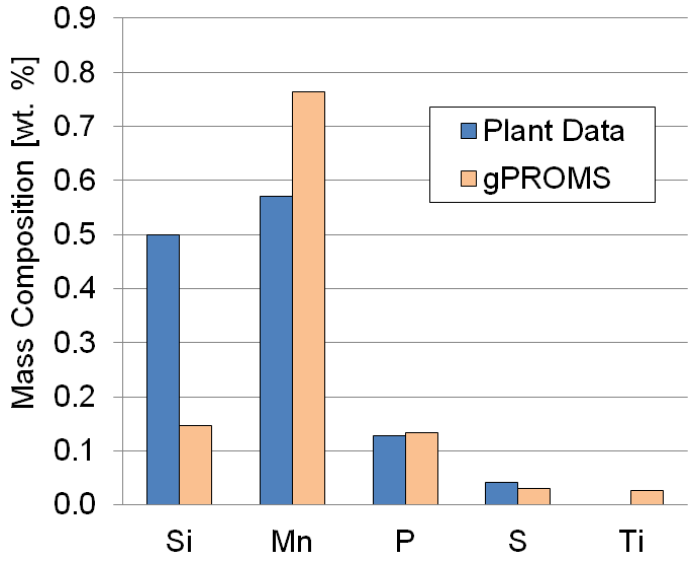




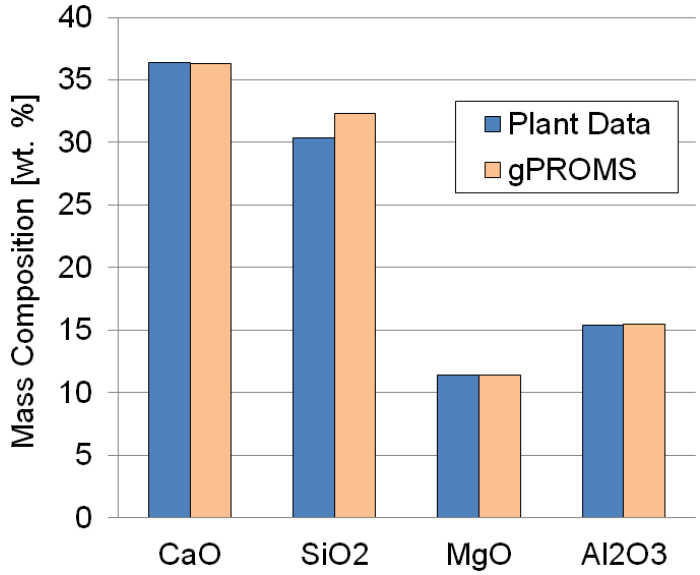
Transformed Simulation Results

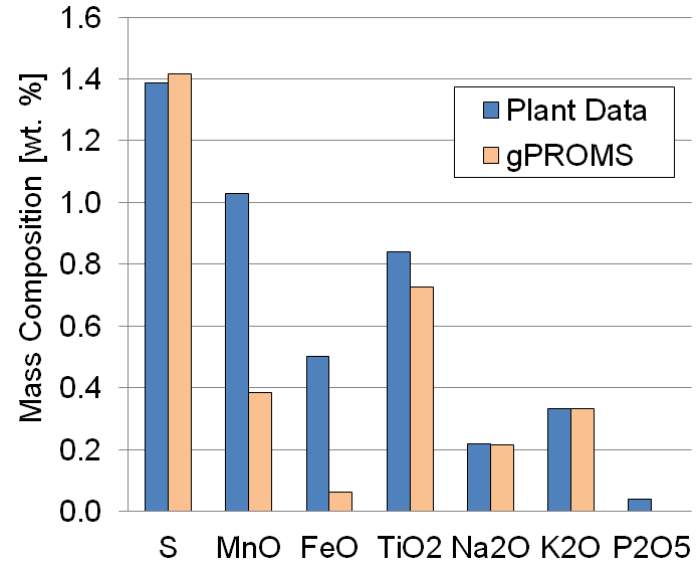
Hot Metal





Slag





Summary

- 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