Multizone model of a melter-gasifier reactor in gPROMS and its extension with complex phase equilibrium calculations in ChemApp

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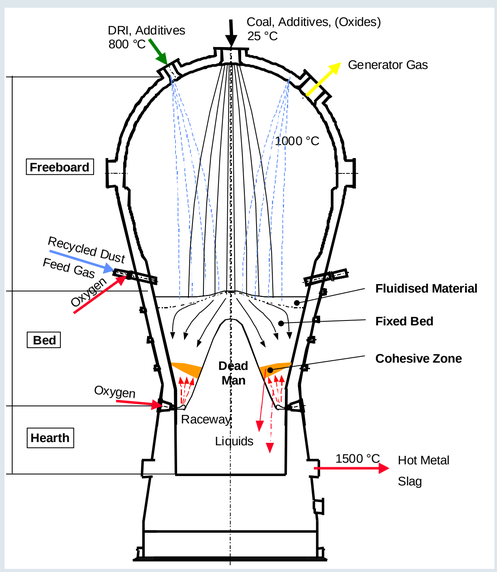
Introduction

The Corex® and Finex® processes are the industrially realized alternatives to the blast furnace route for hot metal production. Due to their more economical and ecological characteristics, their use has been gaining ground over the last two decades. The heart of these processes is the melter-gasifier (MG) reactor. The target of this work is to present the developed multizone MG model in gPROMS and its future extension for complex equilibrium calculations in ChemApp. For this purpose the following software tools have been used:

- gPROMS ModelBuilder version 3.6.0
- FactSage version 6.3.1
- ChemApp version 6.1.6

Melter-Gasifier Process

In the MG unit, the iron ore reduction is completed by the reduction gas (CO, H_2) and further smelted in order to leave the system in hot liquid form. The generator gas exits the melter-gasifier through its top and is further processed in order to pre-reduce the iron ores either in a shaft (Corex®) or in a fluidised bed reactor cascade (Finex®).



inputs
iron ore, additives, fuel

outputs
hot metal , slag, generator gas

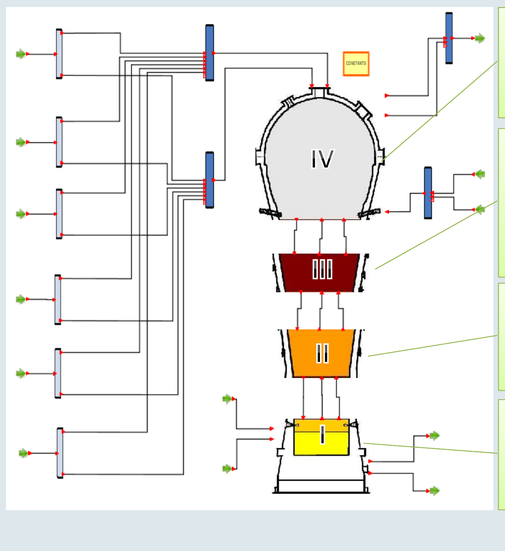
reactor type
continuous reactor

flow principle
counter-current gas-solid flow

processes/ reactions
additive calcination
oxide reduction
coal pyrolysis
coal gasification
smelting

gPROMS Model

The steady state MG multizone model is based on empirical and equilibrium correlations. The model is divided into four reaction zones with more than fourty components considered in gaseous, liquid/molten and solid phase.



dome
dust reactions
re-circulated C burning
water-gas-shift equilibrium

upper charbed
drying
pyrolisis
Mg calcination
Bourdouard equilibrium
water-gas-shift equilibrium

lower charbed
oxide reduction
Ca calcination
water-gas-shift equilibrium

raceway & hearth
coal gasification
melting
water-gas-shift equilibrium

Basic Model Equations

mass balance

$$\sum_{in}\left(m_{in}\cdot c_{in,k}\cdot si_{k,i}\cdot\frac{MW_i}{MW_k}\right)=\sum_{out}\left(m_{out}\cdot c_{out,k}\cdot si_{k,i}\cdot\frac{MW_i}{MW_k}\right)$$

enthalpy balance

$$\sum_{in}\left(m_{in}\cdot c_{in,k}\cdot h_k(T)\right)=\sum_{out}\left(m_{out}\cdot c_{out,k}\cdot h_k(T)\right)+H_{losses}$$

reaction stoichiometry

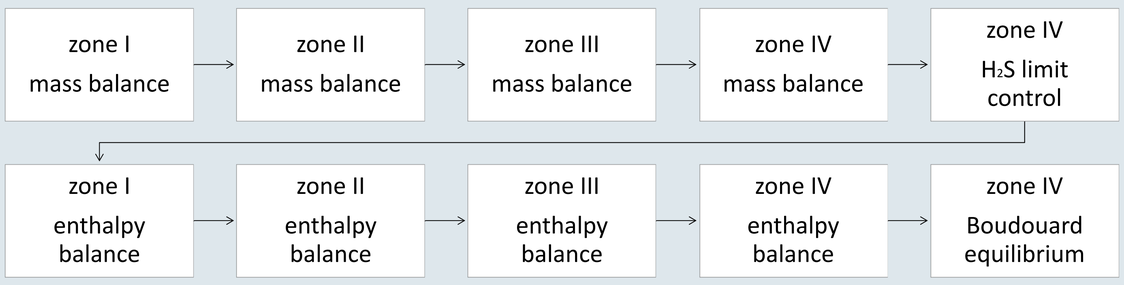
$$\sum_{in}\left(m_{in}\cdot\frac{c_{in,k}}{MW_k}\cdot RD\right)=\sum_{out}\left(m_{out}\cdot\frac{c_{out,j}}{MW_j}\right)$$

equilibrium conditions

$$K_{react}=f(T,p)$$

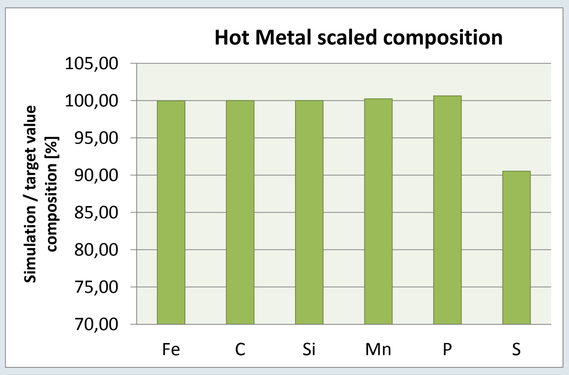
Simulation Initialisation

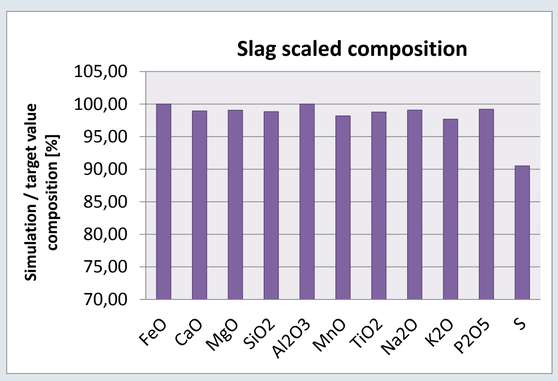
The initialisation of the non-linear system in the case of the melter-gasifier is complex, as all the equations in each zone are coupled with each other due to the counter-current nature of the flow. The following initialisation procedure sequence proved to be robust for a variety of simulation cases.

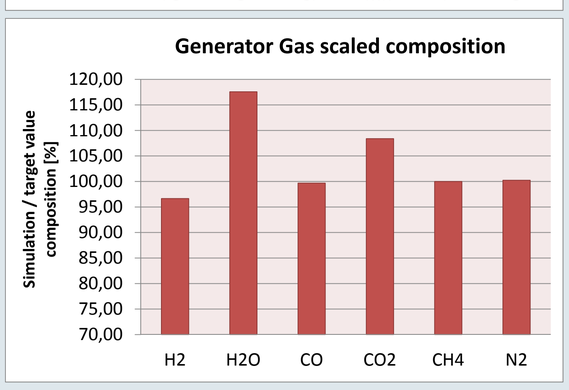


Model Validation

The model was validated based on plant data provided by Siemens VAI. The results are given scaled in percent of the target values. The main interest is focused on the hot metal, the slag, the generator gas and their most important components.



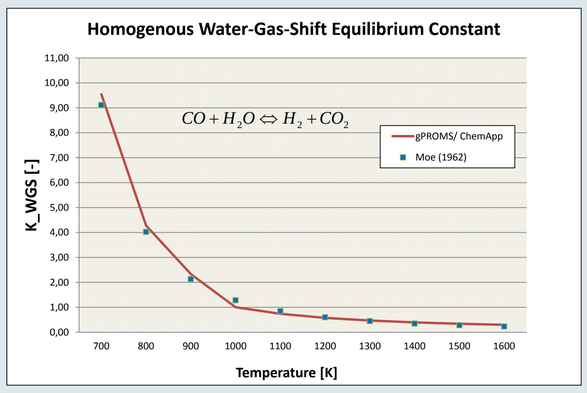


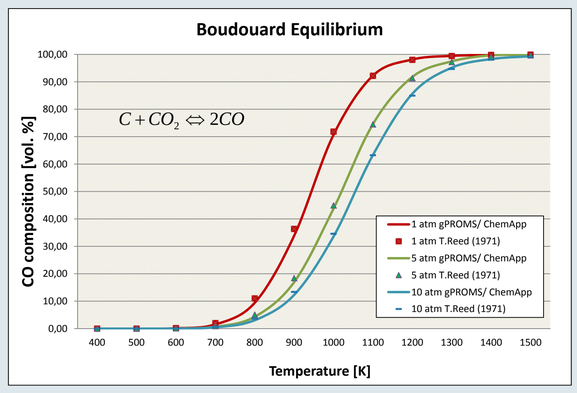


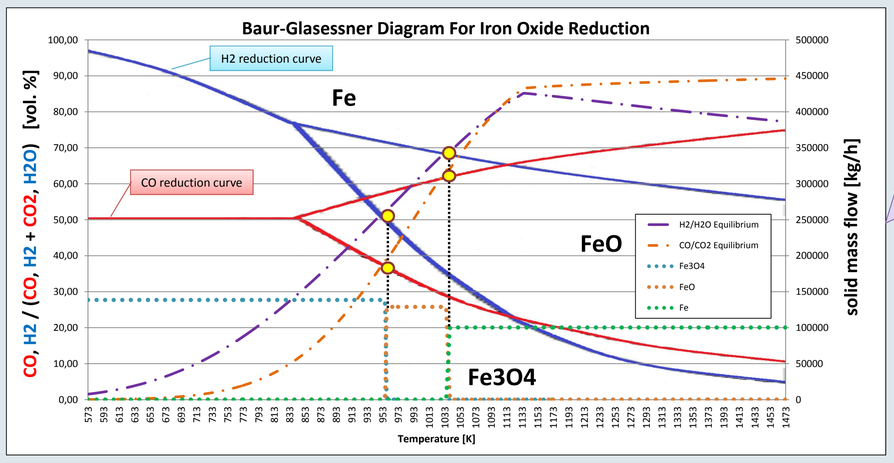
Model equilibrium extension with ChemApp

- library of subroutines for Gibbs minimisation equilibrium calculations
- multicomponent/multiphase systems support
- extensive databank in the field of metallurgy
- ChemApp requires compound properties exported by FactSage
- the interface between gPROMS-ChemApp has been developed by PSE

As a first step for increasing the model fidelity with equilibrium calculations, it was chosen to investigate the basic “isolated” reactions in gPROMS/ChemApp and to compare the simulation results with literature data.







iron oxide reduction @ 4,5 bar

reduction gas
175000 Nm³/h
66 vol. % CO
21 vol. % H2

iron ore
200000 kg/h
68 wt. % Fe3O4

Conclusions

- the multizone MG model simulation results presented minor deviation within tolerance
- a robust initialisation procedure was developed for a variety of simulation cases
- the preliminary investigation showed that ChemApp in combination with gPROMS can handle well multicomponent /multiphase systems in equilibrium

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Acknowledgements

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