Modelling of a steelmaking BOF unit operation and its extension with the multicomponent/multiphase equilibrium approach of ChemApp

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Introduction

The Linz-Donawitz (LD) is a basic oxygen steelmaking (BOF) process that is accounted for the major world wide production of steel. The development of this technology in 1953 lead to reduced plant capital costs and increased productivity. The target of this work is the development of a mathematical model within the environment of the gPROMS ModelBuilder for the simulation of the LD process. Additionally, the extension of the existing Primetals library from ironmaking to steelmaking is envisaged.

LD Converter Process

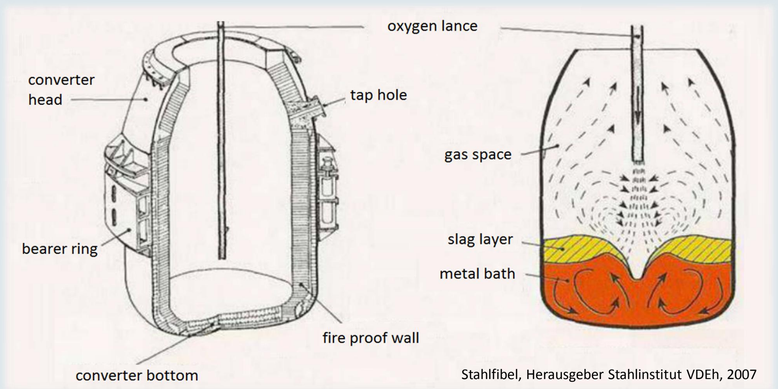
In the LD process hot metal is transformed into steel by blowing pure oxygen through a lance in a converter. The main target of this unit operation is the oxidation of the species that affect the steel quality negatively and their removal through the slag and gas phase. The process is autothermal since heat is generated by the oxidation reactions.

The iron carriers of the process are mainly hot metal and scrap. The choice of an optimal charging ratio between these inputs is crucial for the thermal and chemical stability of the operation. Additionally, additives (dolomite, limestone or burnt lime) are fed into the device for controlling the slag basicity to the required levels. Finally, nitrogen and argon are used as purge gases.

unit operation type
batch reactor

process inputs
hot metal
slag
scrap
dolomite
limestone
burnt lime
oxygen
nitrogen
argon

process outputs
BOF gas
slag
steel



Stahlfibel, Herausgeber Stahlinstitut VDEh, 2007

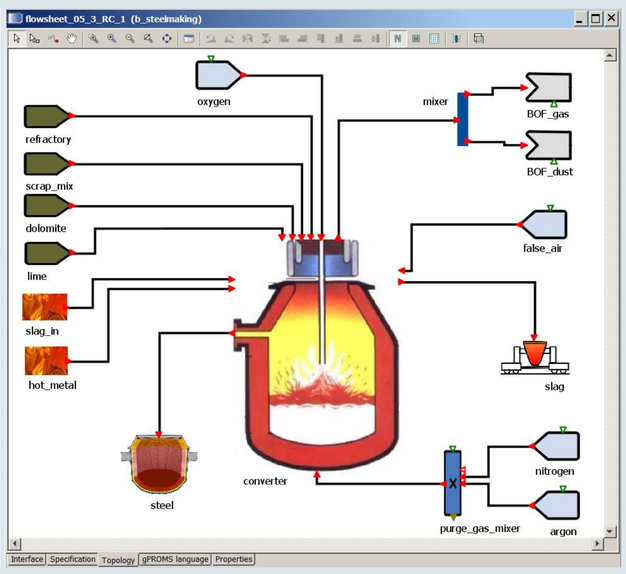
BOF converter basic reactions			
iron oxidation	$Fe + 0{,}5\ O_2 \rightarrow FeO$ $FeO + Fe_2O_3 \rightarrow Fe_3O_4$ $2\ FeO + 0{,}5\ O_2 \rightarrow Fe_2O_3$ $3\ FeO + 0{,}5\ O_2 \rightarrow Fe_3O_4$	phosphate formation	$3\ CaO + P_2O_5 \rightarrow Ca_3(PO_4)_2$ $4\ CaO + P_2O_5 \rightarrow Ca_4P_2O_9$ $3\ FeO + P_2O_5 \rightarrow Fe_3(PO_4)_2$ $Fe_2O_3 + P_2O_5 \rightarrow 2\ FePO_4$ $3\ MnO + P_2O_5 \rightarrow Mn_3(PO_4)_2$
non iron metal oxidation	$2\ Al + 1{,}5\ O_2 \rightarrow Al_2O_3$ $Ca + 0{,}5\ O_2 \rightarrow CaO$ $2\ Cr + 1{,}5\ O_2 \rightarrow Cr_2O_3$ $Mg + 0{,}5\ O_2 \rightarrow MgO$ $Mn + 0{,}5\ O_2 \rightarrow MnO$ $2\ Na + 0{,}5\ O_2 \rightarrow Na2O$ $Ni + 0{,}5\ O_2 \rightarrow Ni$ $Si + O_2 \rightarrow SiO_2$ $Ti + O_2 \rightarrow TiO_2$	silicate formation	$Al_2O_3 + SiO_2 \rightarrow Al_2SiO_5$ $CaO + SiO_2 \rightarrow CaSiO_3$ $2\ CaO + SiO_2 \rightarrow Ca_2SiO_4$ $3\ CaO + SiO_2 \rightarrow Ca_3SiO_5$ $FeO + SiO_2 \rightarrow FeSiO_3$ $2\ FeO + SiO_2 \rightarrow Fe_2SiO_4$ $MnO + SiO_2 \rightarrow MnSiO_3$ $2\ MnO + SiO_2 \rightarrow Mn_2SiO_4$
oxidation & combustion	$C + 0{,}5\ O_2 \rightarrow CO$ $C + O_2 \rightarrow CO_2$ $H_2 + 0{,}5\ O_2 \rightarrow H_2O$	sulfide formation	$Fe + S \rightarrow FeS$ $Ca + S \rightarrow CaS$ $Mn + S \rightarrow MnS$ $2\ Na + S \rightarrow Na_2S$

Model

The model is based on mass and enthalpy balances. The nature of the physical and chemical processes that take place in the converter is complex, since heat and mass transfer occur in multicomponent/multiphase systems. Therefore, the distribution of the components between the steel and slag phase will be handled with empirical distribution coefficients. The simulation of the LD process follows the design specification principle. This means that the system inputs are calculated, so that user defined specifications at the outlet are fulfilled.

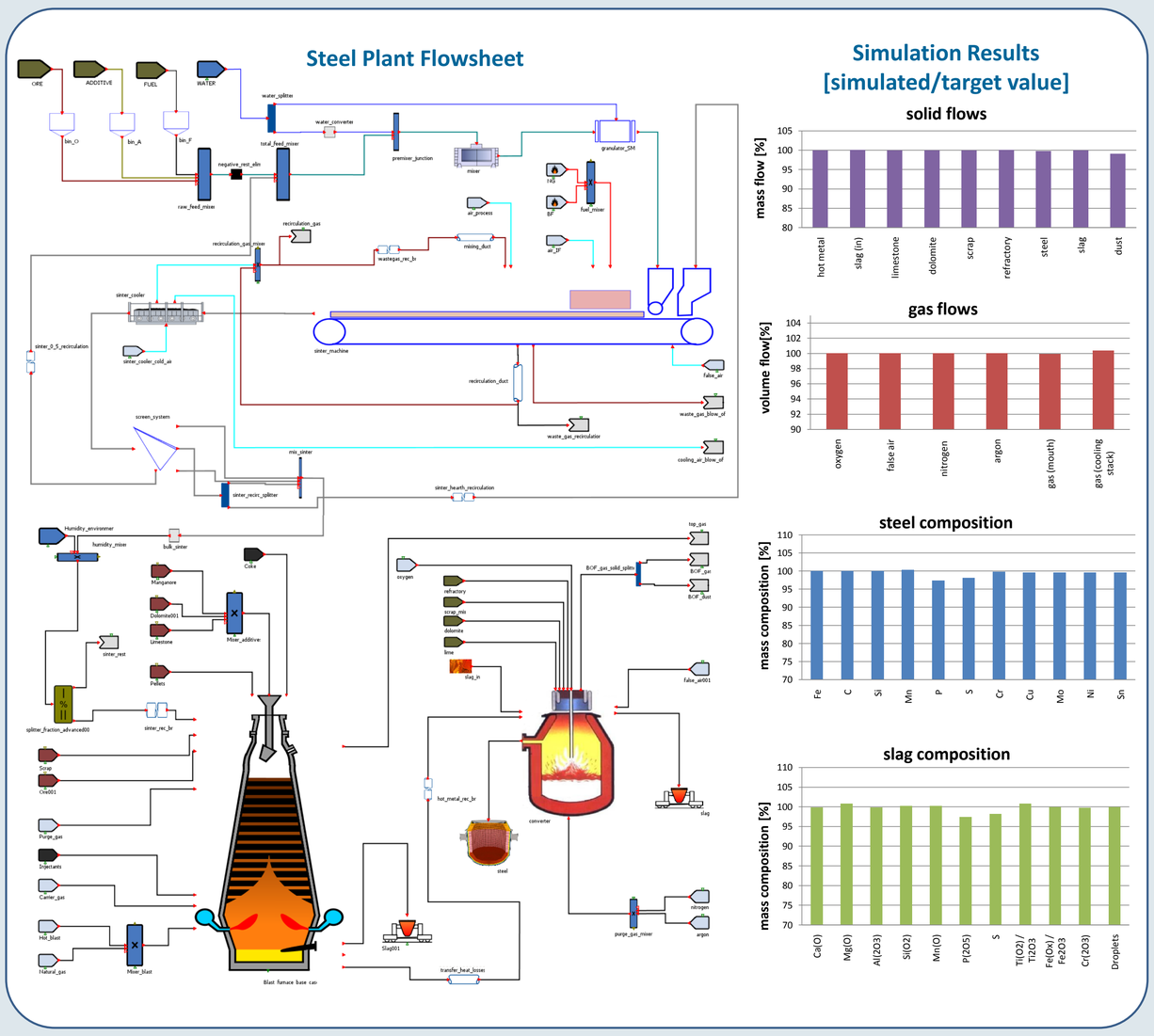
basic model equations	
mass balance	$\sum_{in}\left(m_{in}\cdot c_{in,k}\cdot si_{k,i}\cdot\frac{MW_i}{MW_k}\right)=\sum_{out}\left(m_{out}\cdot c_{out,k}\cdot si_{k,i}\cdot\frac{MW_i}{MW_k}\right)$
enthalpy balance	$\sum_{in}\left(m_{in}\cdot c_{in,k}\cdot h_k(T)\right)=\sum_{out}\left(m_{out}\cdot c_{out,k}\cdot h_k(T)\right)+H_{losses}$

main inlet flows	calculation criterion
lime / limestone	basicity
dolomite	MgO content of Slag
scrap	energy balance (work in progress)
hot metal	steel productivity
slag in	manually defined
oxygen	gas post combustion degree at mouth
dilution air	gas post combustion degree



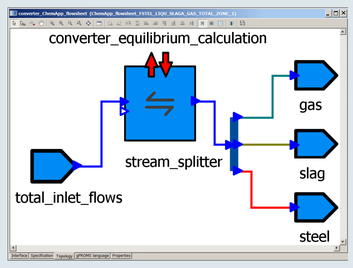
Simulation Results

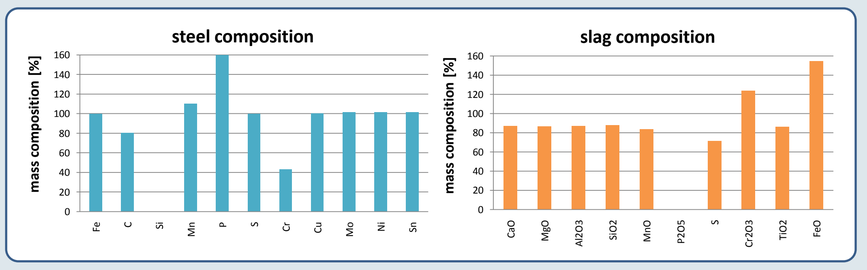
The converter model was used in the flowsheet of a steel plant. For this simulation the sintering plant and blast furnace models of the Primetals library were used. The converter results are given as a ratio between the simulation and the target values provided by Primetals Technologies.



Equilibrium approach

The metallurgical reactions of the converter process evolve in the model described above based on empirical distributions between the steel and the slag phases. These coefficients are defined by the user. In order to increase the model fidelity, an attempt to calculate this multicomponent/ multiphase mixture with the ChemApp thermodynamic equilibrium routines took place. This could assist in the creation of a predictive model based on first principles. As a first step, a single equilibrium zone was set up in a flowsheet, using the total feed of the converter as an input. The scaled composition (against target values) of steel and slag are of main interest in order to gain insight to the deviations resulting from this first simple equilibrium model attempt.





Conclusions & Outlook

- A mass and enthalpy balance model of a converter was created within the environment of the gPROMS ModelBuilder.
- The simulation results are in good accordance with the target values provided by Primetals Technologies.
- An investigation with the equilibrium routines of ChemApp for a simple single zone converter model showed significant deviations for Si, P and Cr.
- In the future a multizonal implementation of the model should be attempted for increasing the model fidelity and describing the process in a better way.

References

A. Babich, D. Senk, H.W. Gudenau, K.T. Mavromatis, Ironmaking Textbook, RWTH Aachen University, Aachen (2008)

R.J. Fruehan, The Making, Shaping and Treating of Steel, Vol. 2: Steelmaking and Refining Volume, 11th edition, The AISE Steel Foundation, United States of America (1998)

K. Hack, The SGTE casebook – Thermodynamics at Work, Bourne Press, Bournemouth, United Kingdom (1996)

J. Schenk, Eisen- und Stahlmetallurgie I, lecture notes, Montan University Leoben, Leoben (2013)

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PRIMETALS TECHNOLOGIES

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