Development of an Industrial Iron-Making Melter Gasifier Model with Multiphase Equilibrium Calculations

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The Corex® and Finex® processes are the only industrially proven alternative options for hot metal production compared to the traditional blast furnace iron-making route. Due to their more economical and ecological characteristics, their use has been gaining ground over the last two decades. The main unit operation of these processes is the melter gasifier device. The target of this work is to create a prototype multizone model of the melter gasifier and implement it in the platform of gPROMS ModelBuilder. For the calculation of the elemental distribution between the hot metal and the slag phases, the thermodynamic equilibrium routines of ChemApp are used. The simulation results showed a good fitting with plant data for most of the important components (Fe, C, CaO, MgO, CaO, Al_2O_3, S). Deviations were observed in the Mn and Si components. Through this work, predictive simulations of Corex® and Finex® iron-making processes can take place and a better understanding is gained in regard to the thermodynamic equilibrium. This knowledge can contribute in the direction of both process and design optimisation.

1. Introduction

The target of the iron making processes is to produce hot metal with high iron content through the use of iron ore (mainly consisting of iron oxides) as raw material. The blast furnace is the traditional industrial iron making process. In this technology, iron ore, fuel and additives (limestone, dolomite, quartz) are driven in the furnace, while hot blast is blown in the bottom of the reactor, so that the reduction of iron oxides and the melting of the product take place (Babich, 2008). Corex® and Finex® are innovative iron making processes developed by Siemens VAI for the production of hot metal (see Figure 1).

The basic differentiation point of Corex® and Finex® processes is the iron ore pre-reduction stage and the use of oxygen instead of hot blast (air). The pre-reduction takes place either in a reduction shaft (Corex®) or in a series of fluidised bed reactors (Finex®). Due to these technologies, the sinter and coking plants are not needed for the pre-treatment of the iron ore and the coal. This fact gives the ability to use low cost raw materials, while both capital investment and production costs are lower. Additionally, SO_x, NO_x, and dust emissions are significantly lower, due to the treatment and recirculation of the generator gas (Hasanbeigi, 2014).

The melter gasifier (see Figure 2) is the basic unit operation of the Corex® and Finex® processes. In this device, the final reduction of iron ore takes place through the reduction gas that mainly consists of CO and H_2. This gas is produced by the gasification of fuels (coal, coke and pulverised coke injection) with oxygen. The ore is smelted in order to leave the unit as hot metal and slag. The regulation of additive inputs is applied in order to control the quality of the produced hot metal and slag, by moving impurities into the slag. The target of this work is to create a mathematical model of the melter gasifier for the calculation of the process mass and energy balances within the environment of gPROMS ModelBuilder® that is developed by Process Systems Enterprise (PSE, 2013). This software is an equation oriented modelling and simulation tool that was selected due to its flexibility in defining various components and phases, as well as its flowsheeting capability.
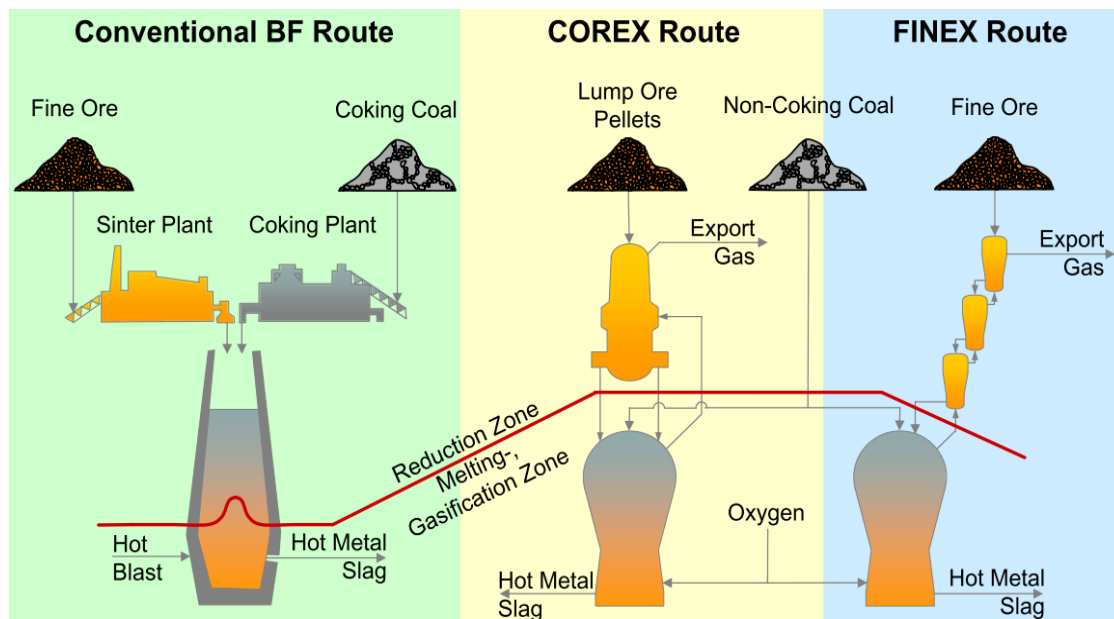
Figure 1: Corex®, Finex® and Blast Furnace processes (Grill 2009)

In the bottom of the melter gasifier, the nature of the metallurgical, physical and chemical processes that take place is complex, since heat and mass transfer occur in multicomponent and multiphase systems. The implementation of a mathematical model describing the whole device with the kinetic approach is a difficult task. Even with the most detailed models, it is impossible to receive reasonable results, mainly due to the big amount of unknown information required. This issue is usually handled with empirical coefficients. The problem with the empirical parameters is that by applying different operation conditions (e.g. different feed mixtures and temperatures), the model results tend to present a significant deviation from reality. Therefore, empirical models cannot be used for predictive simulation in a wide range of process operation.

In this direction, thermodynamics can provide an answer. Due to the significant residence time of the hot liquid phases (up to 3 hours) and the high temperatures (1,500 °C), it is expected that the process should reach equilibrium. In this work, an attempt has been made to simulate the elemental distribution between the hot metal and slag phases with the Gibbs minimisation approach. For this reason, the combination of FactSage and ChemApp thermodynamic software packages is used (Erikson, 2008). Such an approach has not been used in the literature for a melter gasifier process before.

ChemApp is developed by GTT Technologies and consists of sub-routines which provide all the necessary tools for the calculation of complex multicomponent and multiphase chemical equilibria based on Gibbs minimisation. FactSage is a software providing the thermodynamic properties required for this task. The main advantage of the FactSage-ChemApp solution is the ability to calculate the state of equilibrium of extensive component systems that cover the field of metallurgy.

2. Model

The melter gasifier follows the counter-current gas/solid/liquid flow scheme. The device is divided into four zones: the dome, the upper charbed, the lower charbed and the raceway & hearth zones according to the allocated chemical reactions.

The dome is the top spherical part. The homogeneous water-gas-shift reaction, the Boudouard equilibrium and the decomposition of volatile compounds produced by pyrolysis evolve here. The produced gas (generator gas) leaves the device through a duct. Additional heat is provided through the combustion of recycled dust, through burners found on the sides of the globe. The solids are charged through the upper part without undergoing any changes, since their residence time is very limited. A part of the solid input is mixed with the gas phase and exits the system in the form of dust. The dust undergoes the drying, pyrolysis, calcination and reduction reactions.

The bed (charbed) part of the melter gasifier is positioned between the dome and the hearth. In the upper fluidised part of the bed, drying, pyrolysis and calcination take place along with additional dust generation from solid materials. In the lower fixed bed, the final calcination and reduction of iron ore are fulfilled.
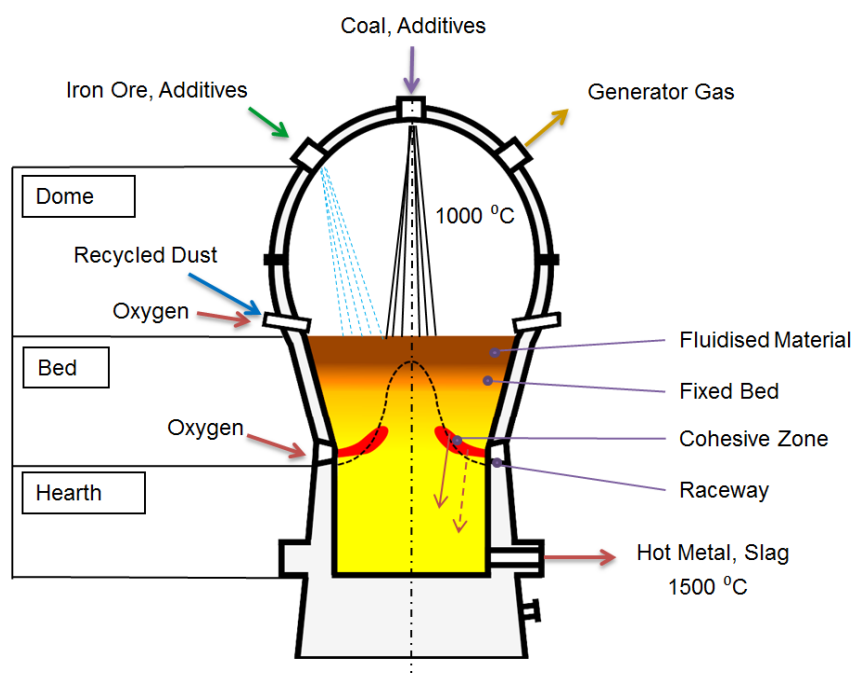
Figure 2: Melter gasifier device

The hearth zone starts at the level of the raceway. Oxygen is injected through tuyeres for the gasification of the solid carbon. This step produces the reduction gas as well as the required heat for melting the solids. A part of the carbon is dissolved in the liquid iron through carburisation. The produced molten liquid consists of the hot metal and slag phase. There is interaction between the elements of the hot metal solution and the oxides of the slag solution. Both phases flow through the hearth and are finally removed through tap holes from the bottom of the device.

The overview of the basic reactions taking place in the melter gasifier is presented in Table 1 (Oeters, 2013).

The topology of the developed steady state multizone model is presented in Figure 3. The boxes shown represent sub-models in the topology of the main model. The thick lines represent the solid flows, the thin lines represent the dust flows and the discontinuous lines represent the gas flows.

Each solid input is separated into dust and solid flows in splitters. All these streams are mixed accordingly in dust and solid mixers that are connected to the upper part of the dome. The recycled dust is mixed with oxygen and combusted in the dome. Additionally, generator gas and dust exit the system through this zone. All the zones are connected with each other through down-streaming solid and up-streaming dust/gas flows. At the raceway & hearth zone an additional mixture of pulverised coke injection with oxygen provides the required heat for the reactions.

Table 1: Basic melter gasifier process reactions

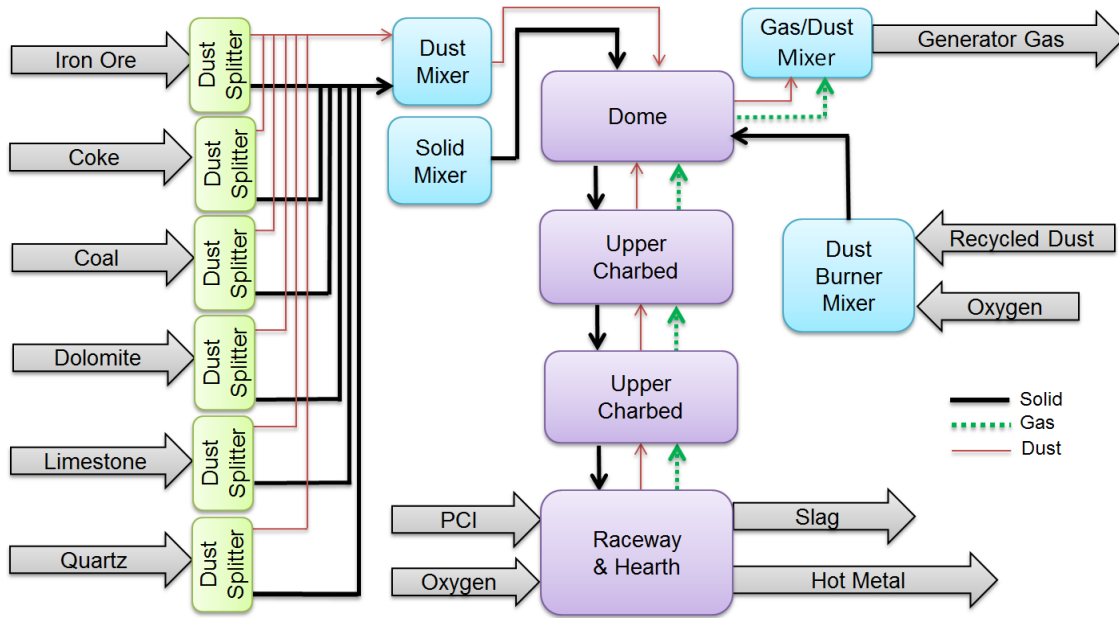| carbon combustion	$C + O_2 \rightarrow CO_2$		$3Fe_2O_3 + CO \rightarrow 2Fe_3O_4 + CO_2$
carbon partial oxidation	$C + \frac{1}{2}O_2 \rightarrow CO$	oxide reduction	$3Fe_2O_3 + H_2 \rightarrow 2Fe_3O_4 + H_2O$
Boudouard equilibrium	$CO_2 + C \leftrightarrow 2CO$		$Fe_3O_4 + CO \rightarrow 3FeO + CO_2$
WGS equilibrium	$CO_2 + H_2 \leftrightarrow CO + H_2O$		$Fe_3O_4 + H_2 \rightarrow 3FeO + H_2O$
Mg calcination	$MgCO_3 \rightarrow MgO + CO_2$		$FeO + CO \rightarrow Fe + CO_2$
Ca calcination	$CaCO_3 \rightarrow CaO + CO_2$		$FeO + H_2 \rightarrow Fe + H_2O$
		carburisation	$3Fe + C \leftrightarrow Fe_3C$

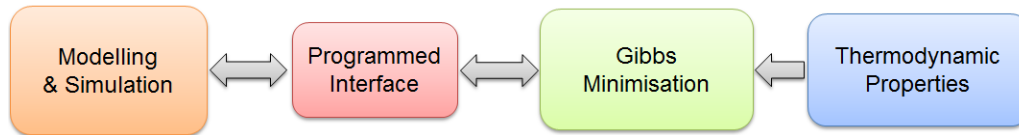*Figure 3: Melter Gasifier multizone model topology*

Figure 4: Software communication structure.

In each zone, the mass and energy balance are considered. The reactions presented in Table 1 are assigned in the mathematical model of each zone accordingly. The reactions that take place between the hot meal and the slag in the hearth are handled with the equilibrium approach.

For calculating the thermodynamic equilibrium, a software communication scheme between ChemApp and gPROMS was created (Figure 4). In principle FactSage is the software providing the databases in order to generate the thermodynamic properties of a selected component system. These properties are used in the Gibbs-minimisation routines of ChemApp. During the numerical iterations, information is exchanged between gPROMS (modelling & simulation software) and ChemApp (Gibbs minimisation software) in both directions through an interface developped by Process System Enterprises.

The components involved in the equilibrium calculations were selected from the solution databases of FactSage. The solutions are optimised sets of components according to experimental results for a better representation of reality. The differentiation point in comparison to pure substances is, that the solutions take into account the excess free energy in the Gibbs minimisation. The excess free energy expresses the phase interaction among the constituents of a solution. The hot metal and slag solution phases used (Table 2) cover the component requirements of the melter gasifier metallurgical process. The only incompatibility appears in the absence of phosporous compounds in the slag phase.

Table 2: Selected solution phases

Solution Phase	Components
Hot Metal	Fe, C, M, P, O, S, Si, Ti, Al, Mg, AlO, Al_2O, MnO, SiO, TiO, Ti_2O, MgO, FeS, MnS, Ca, CaO, TiS, CaS, MgS
Slag	Na_2O, K_2O, Al_2O_3, SiO_2, CaO, FeO, MgO, MnO, TiO_2, $NaAlO_2$, Ti_2O_3, Fe_2O_3, Mn_2O_3, Na_2S, K_2S, Al_2S_3, SiS_2, $NaAlS_2$, CaS, FeS, Fe_2S_3, MgS, MnS, Ti_2S_3, TiS_2, Mn_2S_3

Table 3: Simulation operation conditions

Melting Rate [t/h]	Operation Pressure [bar]	Hot Metal Temperature [˚C]
106	4,5	1500

3. Simulation Results

The simulation was performed for a melter gasifier used in a Corex® process. The reference data were supplied by Siemens VAI. The basic operation conditions are given in Table 3.

In Figures 5-8 the simulation results of the major (high percentage) and minor (low percentage) components are presented. The point of interest is to check if the elemental distribution between the hot metal and slag phases is matching the target values. The component system presented in Table 4 is not identical to the one provided by the plant data analyses (e.g. no CaS in the slag). Therefore, a transformation of the simulated composition components to the Siemens VAI data components took place in order to offer a more representative comparison.

It is observed that the major components in both hot metal (Fe,C) and slag (CaO, MgO, Al_2O_3) are fitting well with the plant data. The largest deviation appears in the Si and Mn distribution. The amount of Si in the hot metal appears to be lower since a part of it is found in the slag as SiO_2. The opposite is observed in the case of Mn, since more of it is found in the hot metal, leaving less MnO in the slag. These differences might appear either due to the thermodynamic data used (e.g. absence of P in the slag) or as a result of the process not reaching equilibrium. The S that is important for the hot metal product quality seems to fit well with the target values. In the data provided by Siemens VAI there were no Ti components available in the analysis of the hot metal, since it is not important for the process at this step. Therefore, in the data all the Ti is found as TiO_2 in the slag. In reality Ti is expected to be found in the hot metal phase (Adema, 2014). The simulation results presented only a small amount of Ti dissolved in the liquid iron. The absence
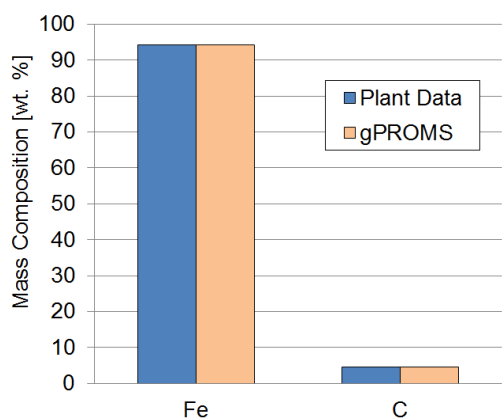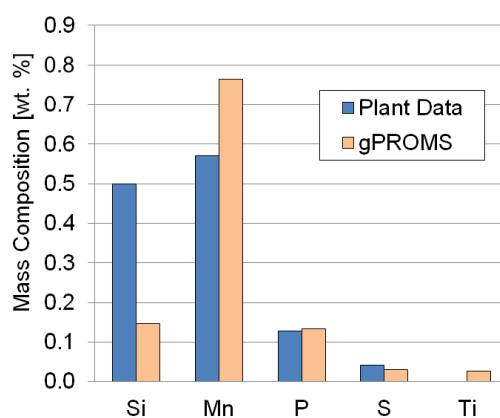

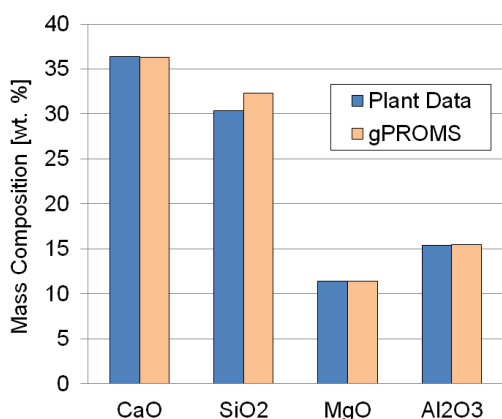*Figure 5: Hot metal major composition*

Figure 6: Hot metal minor composition
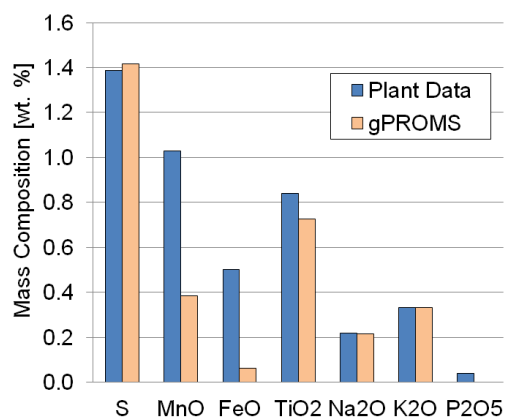

Figure 7: Slag major composition

Figure 8: Slag minor composition

of phosphorous components in the slag causes all the elemental phosphor to be found in the hot metal phase due to the mass balance. Finally, the deviation in the FeO is expected, since the simulation assumes infinite residence time in the state of equilibrium, whereas in reality, rate based steps hinder the complete reduction (Wei 2013).

4. Conclusions and Outlook

A prototype multizone mathematical model of an industrial iron-making melter gasifier was developed within the environment of gPROMS. The most challenging part was to find an approach that would accurately calculate the hot metal and slag composition. In this direction, the thermodynamic routines of ChemApp were used. Such an approach has not been used previously in the literature. The simulation results were in good accordance with plant data for all important major and minor components besides Si/SiO_2 and Mn/MnO. This deviation appears either due to the thermodynamic properties used, or due to the fact that the process does not reach equilibrium in reality.

The developed melter gasifier model can be used for predictive simulation of Corex® and Finex® processes. The main advantage is the deterministic background of the model that can lead through investigations to sensible sensitivity analyses as well as process changes. This can lead to better understanding of the phenomena taking place and can contribute in the direction of the process optimisation.

In the future more emphasis should be given in investigations connected with the thermodynamic background of the calculation routines. More specifically, different solutions from newer versions of the Gibbs minimization routines should be used. Additionally, user defined phase constituents containing P, Si and Mn could be programmed based on literature data.

Acknowledgements

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