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Modelling of an ironmaking melter gasifier unit operation with multicomponent/multiphase equilibrium calculations

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ABSTRACT

The blast furnace is the traditional ironmaking process for the production of hot metal with high iron content. The Corex® and Finex® processes are the main alternative technological solutions in this field of industrial activity. Their main advantages are focused in better economic and environmental characteristics. The melter gasifier is the most important unit operation of both processes. The aim of this paper is to describe the development and implementation of a predictive mathematical model of a multizone melter gasifier. The process modelling and simulation software used for this task is the gPROMS ModelBuilder. For the calculation of the hot metal/slag mixture chemistry, the Gibbs minimisation routines for multicomponent/multiphase systems were implemented through FactSage and ChemApp. A communication scheme between gPROMS and FactSage/ChemApp was established. The validation of this methodology took place by comparing the basic iron making reactions against literature. Special attention was given in the numerical stability by designing a dedicated initialisation strategy. The agreement between simulation results and plant data proved to be successful for the main components (iron, carbon, calcium oxide, magnesium oxide, aluminium oxide, sulphur). Deviation appeared for the silicon and manganese components. This work contributes in making accurate predictions for the hot metal and slag chemistry based on thermodynamic first principles. The reliable calculation presents the opportunity to apply rigorous optimisations that can lead to higher process efficiency. This reflects the potential of reducing fuel consumption, thus leading to lower environmental emissions.

1. Introduction

The aim of the ironmaking processes is the production of hot metal with high iron content. The basic raw material used is iron ore (mainly consisting of iron oxides). The blast furnace is the main ironmaking route (Strezov et al., 2013). In this technology, iron ore, fuel and additives (limestone, dolomite, quartz) are charged in the furnace, while hot blast is injected in the bottom of the reactor, so that the reduction of iron oxides and the melting of the product takes place (Babich et al., 2008).

Corex® and Finex® are among others the main alternative commercial ironmaking processes (Nill, 2008), developed by Siemens VAI for the production of hot metal (Fig. 1). The basic differentiation point between these processes is the iron ore pre-reduction stages 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®) (Moya and Pardo, 2013). Due to these technologies, the sinter and coking plants are not required for the pre-treatment of iron ore and coal. This fact enables the use of low cost raw materials, while both capital investment and production costs are lower. Additionally, depending on the operation the emissions can be approximately lowered up to 90% for sulphur oxides (SO_x), nitric oxides (NO_x) and dust compared to the conventional blast furnace route, due to the treatment and recirculation of the generator gas (Grill, 2009). These emissions have a severe impact in humans, since they are causing problems in the respiratory system. The environment is also largely affected due to their connection with acid rain. Finally, the lower fuel consumption results in lower carbon dioxide (CO_2) production that accounts largely for the global warming that is connected to the greenhouse effect.

The melter gasifier is the core unit operation of the Corex® and Finex® processes. In this device, the final reduction of iron ore takes place through the reduction gas (generator gas) that mainly

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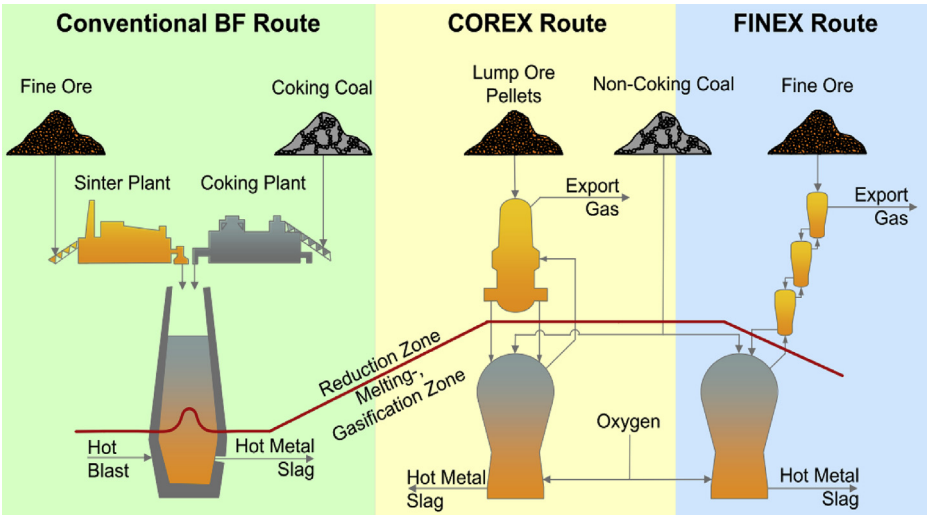

Fig. 1. Corex®, Finex® and blast furnace processes (Grill, 2009).

consists of carbon dioxide (CO) and hydrogen (H_2) (Hasanbeigi et al., 2014). 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 (Dash and Das, 2009). Additive inputs are 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 predictive mathematical model of the melter gasifier for the calculation of the process mass and energy balances.

The amount of literature publications related to the melter gasifier device is limited. This can be explained by the fact that the know-how of this technology is patented by Siemens VAI that is the constructor of Corex and Finex plants. Despite this fact there are some published models regarding the mathematical modelling of the process. Pal and Lahiri have created a three zone melter gasifier model consisting of the free board, the fluidized bed and the moving bed zones (Pal and Lahiri, 2003). In the moving bed zone, the tuyere region is two-dimensional and the rest is one-dimensional. The model is based on multiphase conservation of mass, momentum, and heat but it does not give an insight on the hot metal and slag phases. The team of Gang, Xun-Liang and Zhi has developed a two dimensional model describing the gas flow in a Corex melter gasifier (Gang et al., 2011). This work focuses mainly on the gas velocity and the pressure drop in the device. In the dissertation of Holzleithner a detailed three dimensional model of the moving coal bed inside a melter gasifier is described (Holzleithner, 2013). The developed CFD model takes into account the population balances of the carbon, along with their particle size distributions. The mass energy and momentum balances are the basic principles considered.

In this current thesis the main focus of the model is to calculate the hot metal and slag chemistry in order to accurately predict the end product. The Gibbs minimization multicomponent/multiphase equilibrium approach is used in this direction. Such an approach has not been investigated in the past. By creating a reliable validated model it should be possible to further optimise the process towards a lower fuel consumption that would lead to lower emissions.

2. Method

In order to implement the model of the melter gasifier, the combination of the appropriate software tools was investigated. In this direction, the conclusion was that the combination of gPROMS and ChemApp seemed to be the most suitable solution.

The gPROMS ModelBuilder® 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. Additionally it enables the user to control the initialisation of the blocks of mathematical equations through *initialisation procedures*. This may help the user to develop numerically robust models.

FactSage and ChemApp are developed by GTT Technologies (Eriksson and Königsberger, 2008). FactSage is a standalone program that contains component and solution property databases and among several features can perform equilibrium calculations as well as plot equilibrium diagrams. ChemApp consists of subroutines, which provide all the necessary tools for the calculation of complex multicomponent and multiphase chemical equilibria based on Gibbs minimisation. ChemApp is not a standalone tool, but instead can be connected with programmed interfaces to different process simulation tools. 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.

In the approach implemented in ChemApp and FactSage (Hack, 1996), the total Gibbs free energy of a phase φ with i, j, k phase constituents is given by Equations (1)–(4). The x_i represents the molar fraction of the mixture for each constituent, while the L parameters represent the excess Gibbs free energy interaction coefficients. This equation consists of the ideal, the reference and the excess Gibbs energy part. The reference term represents the free energy of formation. The ideal part represents the free energy of the pure substances at the defined conditions. The excess term considers the phase interaction among the constituents and is usually defined through experimental data or literature sources.

$$G_m^{\varphi} = G_m^{ref} + G_m^{id} + G_m^{ex,\varphi} \quad (1)$$

$$G_m^{ref} = \sum x_i^0 \cdot G_i^{\varphi} + RT \quad (2)$$

$$G_m^{id} = \sum x_i \cdot \ln x_i \quad (3)$$