

Modelling of Trace Material Flow Distribution in a Melter Gasifier based on Thermodynamic Multiphase Equilibrium Calculations

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In combination with a complex global market environment, the iron and steel industry is dealing with increasing demands for reduction of environmental and greenhouse emissions. Alternative iron making technologies such as Corex® and Finex® can offer solutions for these challenges. The melter gasifier is the central unit operation of these well-established alternative iron making processes. Both offer considerable advantages with respect to economic characteristics and environmental emissions.

Similar to the conventional iron making process of the blast furnace route, a variety of different input materials is required for these processes including coal, coke, lump or fine ore, iron ore pellets as well as limestone and dolomite. Most of these raw materials also carry minor amounts of unwanted compounds such as alkali or zinc-based species. The presence of these materials inside a melter gasifier can lead to instability, problematic process conditions and refractory damages. A better understanding of the distribution of these problematic species is therefore of great importance to plant manufacturers and operators. A variety of different multiphase reactions are responsible for the distribution of trace materials within the melter gasifier. In order to get a better understanding of the complex nature of these reactions, a thermodynamic investigation was carried out using calculation routines of HSC Chemistry and FactSage.

Based on the findings of this investigation, a multi-zone model was developed using the simulation platform of the gPROMS ModelBuilder®. The model is separated into distinct reaction zones across the height of the melter gasifier to depict the main iron ore reduction process as well as the governing reactions of trace material components. Validation of the model was carried out using reference data of existing plants. The model described in this work is used to analyse the behaviour of trace materials within a melter gasifier. Due to the highly integrated material flows of the Corex® and Finex® iron making processes, the impact on their operational characteristics can be investigated as well. Through this it is possible to optimise the raw material input of these processes, potentially leading to reduced fuel demand and environmental emissions.

1. Introduction

Iron making can be classified into two different process routes for production of metallic iron. The first category of processes is known as direct reduction processes such as Midrex®, HYL® or Finmet®. In these processes the oxygen content of iron oxide contained in the raw material is removed leading to the solid product called direct reduced iron or DRI (Babich et al., 2008). The second category includes production technologies used to produce metallic iron in liquid form, so-called pig iron or hot metal. Of these processes, only a limited number was established on an industrial scale. The traditional blast furnace process is by far the most important process route while Corex® and Finex® (see Figure 1) represent the only two technological alternatives which are commercially available (Hasanbeigi et al., 2014).

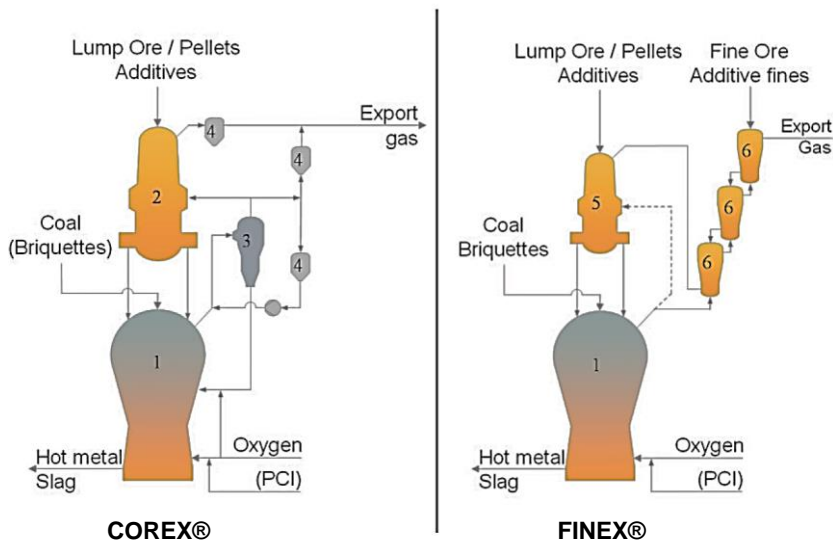


Figure 1: Corex® and Finex® process flow sheets; 1) melter-gasifier, 2) reduction shaft, 3) hot gas cyclone, 4) process gas scrubber, 5) hot compacted iron bin, 6) fluidized bed reactor (Wieder, et al., 2009)

Corex® and Finex® are so-called smelting reduction processes which can produce pig iron directly with non-coking coal. In addition to this they are more flexible with respect to raw material quality and operation conditions while having a lower environmental impact than the conventional blast furnace route. Iron ore reduction and smelting are separated as reduction of iron ore is moved to a pre-reduction stage represented by a reduction shaft or fluidised bed reactors. Gasification of coal to produce reducing gas and heat for smelting as well as direct reduction of the pre-reduced iron ore to metallic iron are located in the so-called melter-gasifier (Flickenschild, et al., 2012). This melter-gasifier (see Figure 2) therefore acts as the final reduction stage of both the Corex® and Finex® processes (Almpanis-Lekkas et al, 2014)

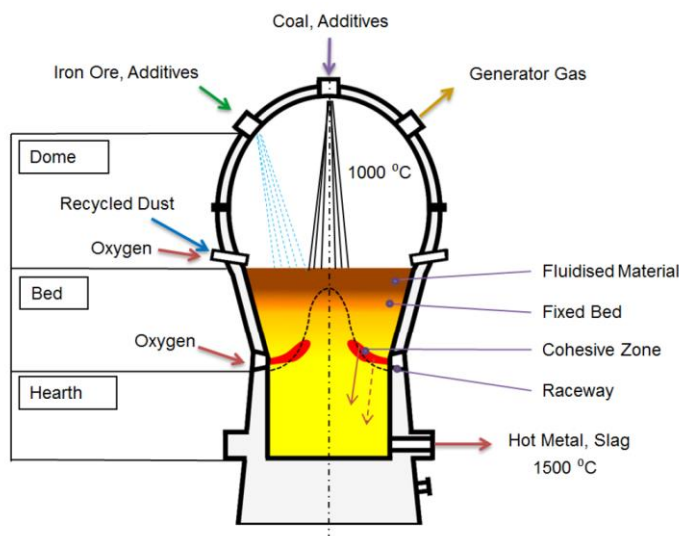


Figure 2: Melter-gasifier device (Almpanis-Lekkas et al, 2014)

In general iron ores used for iron making contain several trace elements such as potassium, sodium or zinc. If such elements transfer to gaseous form in high temperature parts of the blast furnace, ascend to low temperature zones and condense, a circle is formed which may lead to accumulation inside the blast furnace. The accumulation of trace elements in a blast furnace may lead to decreasing productivity, increasing reducing agent demand and refractory wear or even to unstable process conditions (Babich et al., 2008). Due to their similarity, a comparable situation applies for the melter-gasifier device (Pichler, 2017).

2. Thermodynamic investigation

To get a better understanding of the complex nature of trace element reactions and circulating flows inside of iron making reactors, Pichler (2017) carried out a thermodynamic investigation of the stability of specific alkali components under typical conditions in a blast furnace and a melter-gasifier. The results of this work were specific multi-stage models describing the distribution of alkali-components in each reaction zone. Figure 3 gives an overview of the structure of the corresponding blast furnace model. The underlying thermochemical equilibrium calculations were carried out using the thermochemical program FactSage (Bale et al., 2016).

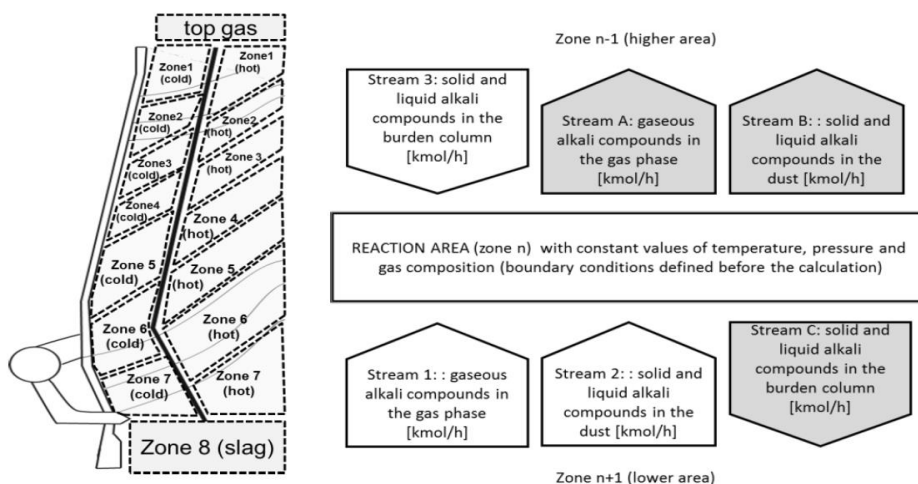


Figure 3: Reaction zones of alkali model and general overview of input and output streams (Pichler, 2017)

The prevalent process conditions like gas composition, temperature and pressure which are required for these equilibrium calculations were based on industry and literature data. Both models include alkali components of potassium and sodium as well as halogenic components based on chlorine and fluorine. This allows for the prediction of alkali enrichment in specific zones and visualization of corresponding material flows inside the iron making devices (Pichler et al. 2016).

As an alternative software program for thermochemical calculations, HSC Chemistry has been used to describe iron ore reduction by Zhang et al. (2013) as well as circulating alkali components by Ilijana et al. (2013). It was also used to provide enthalpy data for the development of a black box melter-gasifier model (Almpanis-Lekkas, 2012) and other metallurgical unit operations (Almpanis-Lekkas, 2015). To corroborate the results the thermochemical modelling approach described by Pichler (2017), the calculated equilibrium compositions of different reaction zones of the multi-stage blast furnace model have been compared to results derived from the equilibrium module of HSC Chemistry.

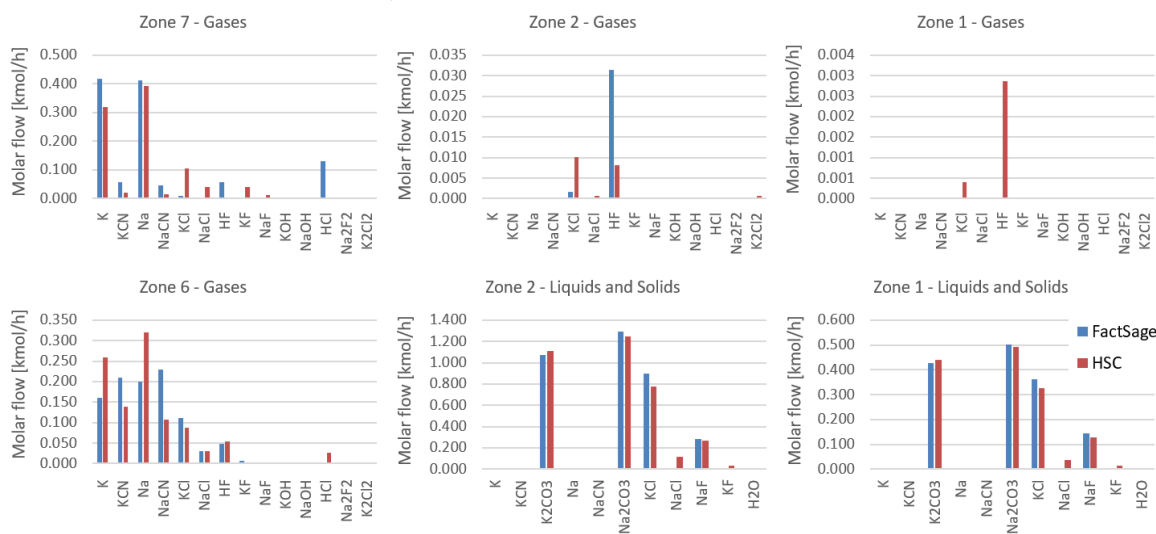


Figure 4: Comparison of equilibrium molar flows calculated by FactSage and HSC Chemistry

Results of this comparison are given in Figure 4 for selected zones. For zones representing lower parts of the blast furnace (zone 7), HSC Chemistry delivers results comparable to the reference values of FactSage. Equilibrium zones representing higher parts of the blast furnace (zones 1 and 2) also show similar results for liquid and solid components. However, in the case of gaseous components significant differences are visible. The deviations observed for gaseous components are related to differences of the underlying enthalpy and entropy databases of FactSage and HSC Chemistry.

3. Modelling

The melter-gasifier model described in this work is based on a multi-zone model which was developed for the simulation platform of the gPROMS ModelBuilder® (Almpanis-Lekkas, 2015). This model was furthermore used as a basis to investigate the applicability of FactSage based hot metal / slag equilibrium calculations (Almpanis-Lekkas et al., 2016). In general, the model is divided into four main reaction zones which are distributed along the height of the melter-gasifier. A specific set of chemical reactions is allocated to each of these zones corresponding with the actual chemical and metallurgical reactions taking place. The material streams between the zones follow a counter-current gas/solid flow scheme. Reactions like drying, pyrolysis, carbon gasification and iron ore reduction are included by means of reaction degrees. Equilibrium formulations for gas and solid/gas reactions like the homogeneous water-gas-shift reaction and the Boudouard reaction are implemented through chemical equilibrium formulations. Empiric element conversion and distribution factors are used for the depiction of three-phase metallurgical reactions.

Based on the results of the thermodynamic investigations described in Chapter 2, the melter-gasifier multi-zone model has been extended by several reactions to depict the behaviour of trace elements such as potassium, sodium, chlorine and zinc. For each zone it is assumed that the gaseous trace components fully ascend to higher zones with the general gas and dust stream while the solid and liquid trace components are descending to lower reaction zones with the general solid stream. Figure 5 gives an overview of the additional reactions which have been added to each zone of the model. Starting at the bottom zone of raceway and hearth, silicon decomposition and direct reduction of alkali components are located leading to liquid alkali oxide and elemental alkali gas. Part of the elemental alkali gas reacts with carbon and nitrogen to form gaseous alkali cyanides. Volatile chlorine entering the melter-gasifier through the tuyères due to injection of substitute reducing agents like pulverised coal (PCI) is forming gaseous hydrogen chloride. In the lower charbed zone solid alkali halides are transformed to their gaseous form. Several reactions are added to the upper charbed zone where gaseous alkali gas and alkali cyanides form solid alkali carbonates with the carbon dioxide of this zone. The produced alkali carbonates are however immediately decomposed forming solid alkali oxides. Parts of these alkali oxides react with gaseous hydrogen chloride and hydrogen fluoride to form solid alkali halides. Additionally, solid zinc oxide is reduced with carbon monoxide leading to elemental zinc gas. In the current version of the model there are no additional reactions allocated to the dome zone.

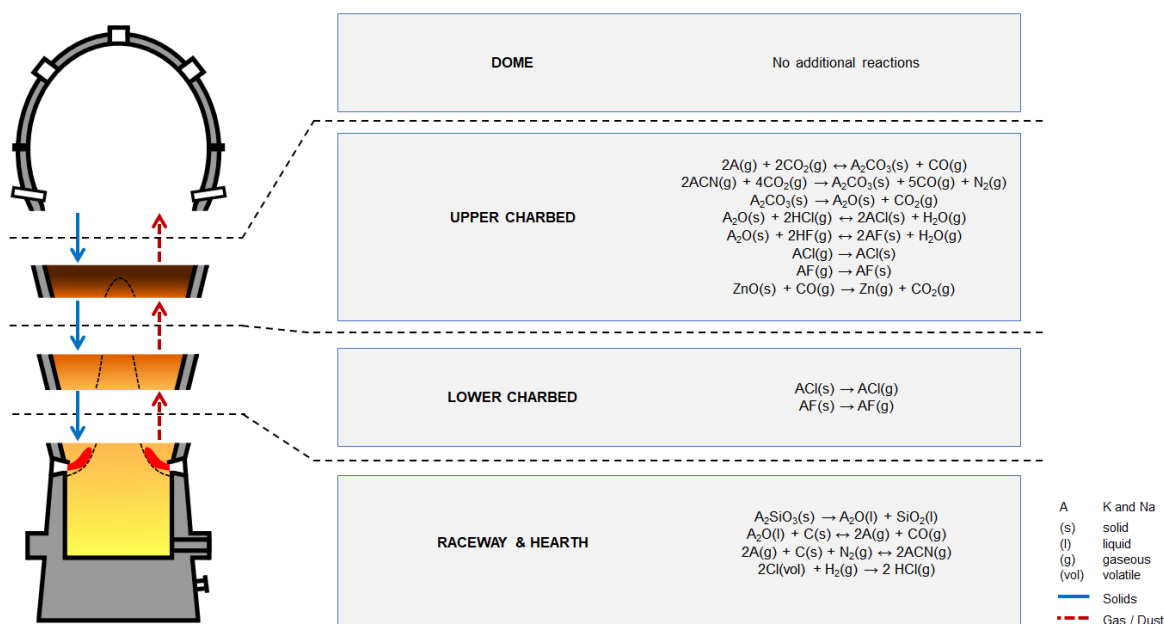


Figure 5: Trace element reactions of the extended melter-gasifier multi-zone model

4. Simulation results

The preceding model has been validated using data for melter-gasifier operation under different process conditions (Almpanis-Lekkas, 2015). The reference values were provided by Primetals Technologies for two Corex® processes with different production capacities (C2000, C3000) and for a Finex® process (F2_0M). Based on this data, the extended melter-gasifier model was used in this work to calculate the flow distribution of the newly added trace components.

Figure 6 illustrates the calculated mass specific distribution of potassium components across the zones of the melter-gasifier model for the F2_0M scenario. Solid raw materials appear to be responsible for the main input of potassium related species. On the other hand, the main amount of potassium is discharged as part of the slag produced in the process. The highest amount of potassium components can be found at the interface between lower and upper charbed due to the counter current flow of gaseous and solid matter. Figure 7 shows a comparison of elemental potassium and chlorine flow distribution for the F2_0M, C3000 and C2000 scenarios. All three processes lead to a similar distribution pattern in the case of chlorine. For F2_0M however, a minor input is visible at the raceway and hearth zone due to injection of pulverised coal which contains small amounts of chlorine.

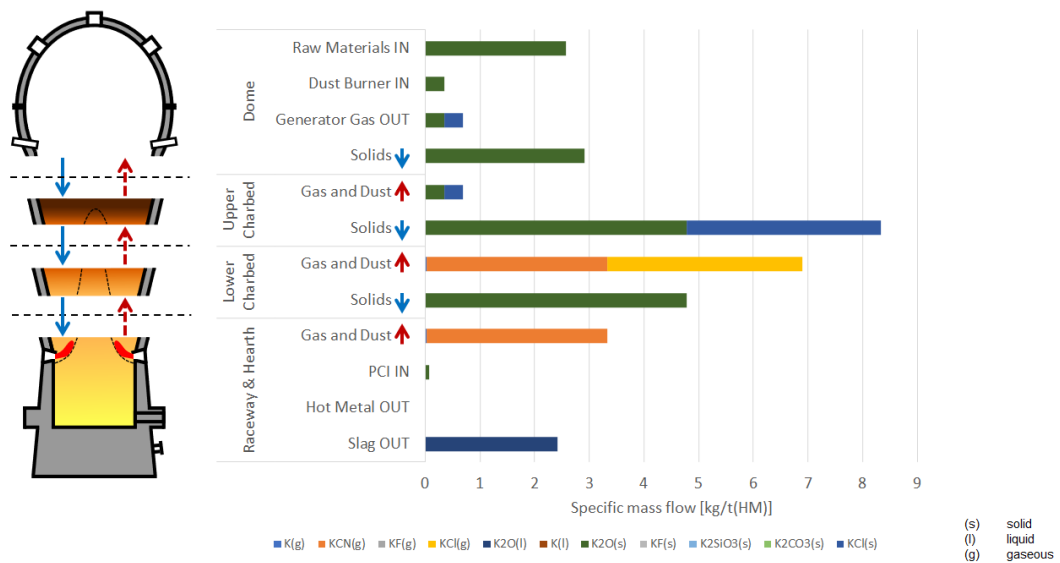


Figure 6: Potassium flow distribution for F2_0M process scenario

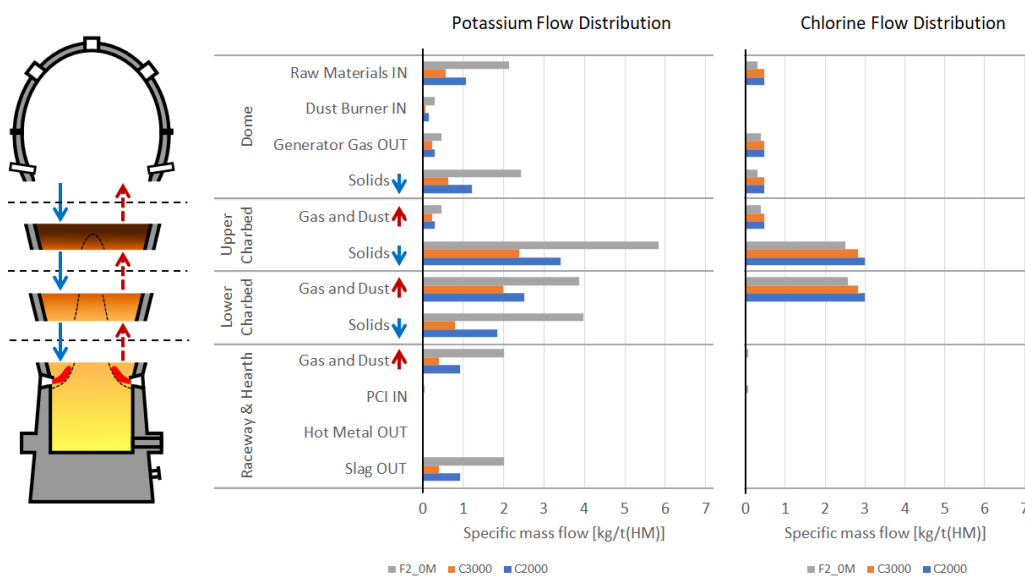


Figure 7: Comparison of elemental potassium and chlorine flow distribution for different process scenarios

In contrast to chlorine, the differences between the three process scenarios are much larger for the flow distribution of potassium. It can be observed, that the input stream of F2_0M exceeds those for C2000 and C3000 significantly. This leads to a larger specific output of potassium through slag. The amount of circulating matter is increased as well. However, all flow distributions qualitatively appear to follow a similar pattern.

5. Conclusions and outlook

The visualization of the flow distribution of specific trace components presented in this work allows for a deeper understanding of their behavior in metallurgical processes. With the current version of the model it is possible to simulate the flow path of several trace components inside the melter-gasifier. This enables a better assessment of their potential influence on operation in different areas of the reactor.

The extended melter-gasifier model represents the first step of an ongoing effort to simulate the behaviour of trace elements in metallurgical processes within gPROMS ModelBuilder®. In the future, further developments are envisaged to be made regarding the implementation of trace elements such as lead, mercury, nickel, cobalt and copper. In addition to this, other metallurgical devices like a blast furnace, reduction shaft, electric arc furnace and basic oxygen converter should be extended in a similar manner. This would lay the ground for a comprehensive analysis of trace element flow distributions along all major iron and steel production routes.

Acknowledgments

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