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Mathematical modeling of the shaft furnace process for producing DRI based on the multiphase theory

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Abstract

A numerical model based on transport equations for momentum, energy and chemical species for the gas and solid phases is proposed to simulate the inner phenomena in the direct reduction of the shaft furnace process for producing directly reduced iron (DRI). The model is verified using industrial data for productivity, raw materials and final composition of the DRI product. The model is used to evaluate operational practices using new raw materials and the composition of the reducing gas in the process. Three cases were considered, which correspond to available raw materials commercialized by different suppliers. The effects on the gas and solid inner temperatures, pressure and phase composition distributions are quantified. The simulation results indicated that good agreement for overall parameters of the process could be achieved and afterwards, detailed features of the inner conditions of the process are predicted.

Keywords: DRI, multiphase theory, mathematical modeling, shaft furnace.

1. Introduction

The shaft furnace reactors are used in several industries for processing granular materials due to their flexibility, scale and economic aspects. The processes based on shaft reactors can be used for several operation units with flexibilities for the scale of the production and raw materials used. In general, the iron direct reduction processes use a large amount of energy and raw materials, which depend particularly on the ores and pellet qualities and the shaft furnace operating conditions. Besides, depending on the reactor capacity, the charging system and the granulometric distribution of the granular materials play an important role

on the productivity and efficiency of the process. Process modeling using advanced computers techniques have been useful for successfully analyzing the actual status and new technologies in several metallurgical reactors. Based on fundamental phenomena, the models can be used to propose new technologies able to increase the efficiency of the process and quantify their environmental impact. Direct reduction processes based on shaft furnace are widely used in the actual metallurgy industry especially for mini mill facilities. In the shaft furnace DRI process, the raw material quality is of special importance due to the guaranty of efficient heat and mass transfer in the reduction and cooling zones, in addition to the softening properties due to the steaking phenomenon. Comprehensive mathematical models could play an important role for direct reduction plant operations by demonstrating the effects of process alternatives and expediting the decision-making process, as well helping the adequate selection of raw material. The field of non-catalytic gas reaction modeling is a very active research area in chemical engineering and metallurgy process fields (Austin *et al,* 1997, Yagi, 1993, Castro *et al* 2001, 2011, 2013, Dong *et al,* 2014, Kuang *et al,* 2014). Some attempts have been made in order to develop mathematical models of the direct reduction shaft furnace (Dong *et al,* 2014). One of the most important applications in the industrial scale is the reduction of iron oxides. In this work, a comprehensive mathematical model for the direct reduction of iron oxides in the shaft furnace has been developed and used to simulate the steady state condition of a commercial shaft furnace for pellets and lump ore reductions. The model is used to predict the productivity and efficiency of the gas shaft furnace. The effects of all external parameters, such as the reducing gases flow rate and temperature, ore types and their characteristics, on the process behavior can be examined in order to determine the optimum operating conditions of the shaft furnace for direct reduction of pellets and lump ores in commercial plants. The model is used to study self-catalytic reforming in the transition zone. This study newly presents the simulation of the inner conditions of the shaft furnace DRI process using self-catalytic reforming in order to decrease the specific reducing gas in the process and hence decreasing the specific gas and energy consumption.

2. Methodology

The methodology used in this investigation is based on the construction of a multiphase multicomponent tridimensional mathematical model for steady state conditions able to simulate the inner variables of the shaft furnace used to produce directly reduced iron (DRI) in a commercial scale reactor.

2.1 Model principles

The shaft reduction process involves complex phenomena of momentum, energy and mass transfer. Usually, the direct reduction of shaft furnace is divided into 3 zones: the reduction, transition and cooling zones. In the reduction zone, the major reactions of solid gas are mainly controlled by the heat supply and local gas composition. In the transition zone, the reducing gas is fed at temperatures around 1100 °C and the final reduction step usually takes place. A first step to construct the mathematical model is to define the computational domain and the boundary conditions representing the real reactor features. Figure 1 shows a schematic view of the shaft furnace and the constructed computational mesh used throughout the simulation carried out in this paper. The computational mesh was selected after continuous refinement of the computational grid using 1% of maximum error for velocity, pressure and temperature fields. To successfully model the direct reduction process, detailed rate equations for the reduction steps and heat transfer mechanism are needed. In the transition zone, new opportunities for improvement on heat efficiency can be generated by using some amount of oxygen injection with partial combustion of the hydrogen releasing energy for burden heat and endothermic reactions in the reduction zone.

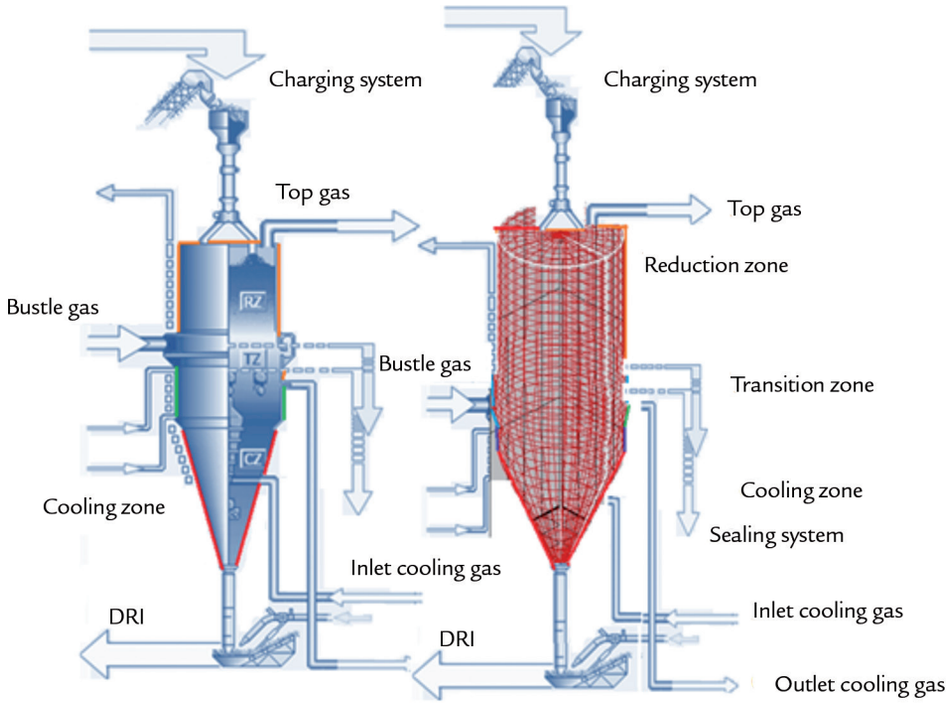

Figure 1
Schematic view of the shaft furnace process and the constructed computational mesh for simulating the reactor using the multiphase theory.

For each of these phases, velocity, temperature and concentration fields are calculated while the gas phase is assumed as a continuum with a pressure field. Figure 2 shows the modeling principles for the multiphase multicomponent formulation used in this study for treating the packed bed composed of pellets of different diameters and lump ore with the gas flow through the arrangement of particles. The phase interactions are considered using momentum interaction for individual gas-solid packed beds and the heat transfer is computed for each individual granular material. The chemical reactions take into account the individual characteristics of the granular materials. The rate equations considered in this model can be found elsewhere (Yagi, 1993, Austin *et al*, 1997, Castro *et al*, 2011).

2.2 Model equations

The mathematical model is based on transport equations of momentum, energy and mass conservations. The model is formulated assuming the size and composition distributions for several classes of pellets with their own reduction kinetics laws. The heat transfer is considered convective and conduction simultaneously taking place within the bed structure. The general equations are presented for the solid phases classes and gas separately.

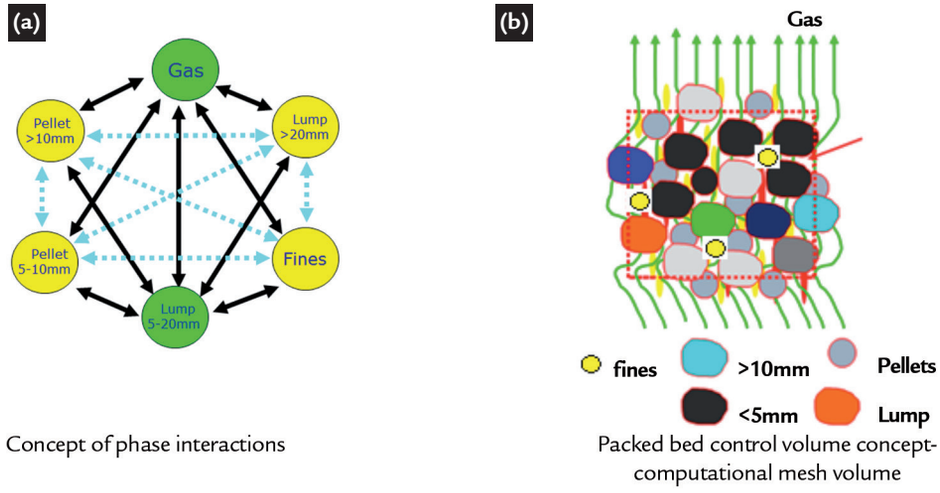

Figure 2
Multiphase and multicomponent modeling concept applied for the packed bed composed of different classes of pellets and lump ore.

Granular classes momentum conservation:

$$\frac{\partial\left(\rho_i \varepsilon_i u_{i,k} u_{i,j}\right)}{\partial x_k} = \frac{\partial}{\partial x_k}\left(\mu_s \frac{\partial u_{i,j}}{\partial x_k}\right) + F_j^{i-l} + F_i^{l} \qquad (1)$$

Mass conservation of solid fractions:

$$\frac{\partial\left(\rho_i \varepsilon_i u_{i,k}\right)}{\partial x_k} = \sum_{m=1}^{Nreacts} M_n r_m \qquad (2)$$

Enthalpy balance for solid fractions:

$$\frac{\partial\left(\rho_i \varepsilon_i u_{i,k} H_i\right)}{\partial x_k} = \frac{\partial}{\partial x_k}\left(\frac{k_i}{C_{p_i}} \frac{\partial H_i}{\partial x_k}\right) + E^{i-l} + \sum_{m=1}^{Nreacts} \Delta H_m r_m \qquad (3)$$

Chemical species of solid phases

$$\frac{\partial\left(\rho_i \varepsilon_i u_{i,k} \phi_n\right)}{\partial x_k} = \frac{\partial}{\partial x_k}\left(D_n^{eff} \frac{\partial \phi_n}{\partial x_k}\right) - \sum_{m=1}^{Nreacts} M_n r_m \qquad (4)$$

Gas momentum transfer:

$$\frac{\partial\left(\rho_g \varepsilon_g u_{g,k} u_{g,j}\right)}{\partial x_k} = \frac{\partial}{\partial x_k}\left(\mu_g \frac{\partial u_{g,j}}{\partial x_k}\right) - \frac{\partial P}{\partial x_j} - F_j^{i-l} \qquad (5)$$

Mass conservation of the gas phase:

$$\frac{\partial\left(\rho_g \varepsilon_g u_{g,k}\right)}{\partial x_k} = -\sum_{m=1}^{Nreacts} M_n r_m \tag{6}$$

Enthalpy conservation of gas phase:

$$\frac{\partial\left(\rho_g \varepsilon_g u_{g,k} H_g\right)}{\partial x_k} = \frac{\partial}{\partial x_k}\left(\frac{k_g}{C_{p_g}}\frac{\partial H_g}{\partial x_k}\right) - E^{g-p} - \sum_{m=1}^{Nreacts}\Delta H_m r_m \tag{7}$$

Chemical species

$$\frac{\partial\left(\rho_g \varepsilon_g u_{g,k} \phi_n\right)}{\partial x_k} = \frac{\partial}{\partial x_k}\left(D_n^{eff}\frac{\partial \phi_n}{\partial x_k}\right) + \sum_{m=1}^{Nreacts} M_n r_m \tag{8}$$

Semi empirical relations for the gas solid momentum transfer:

$$F_j^{g-i} = \left[1.75\rho_g + \frac{150\mu_g}{\left|U_g - U_i\right|}\left(\frac{\varepsilon_i}{d_i\varphi_i}\right)\right]\left(\frac{\varepsilon_i}{\left(1-\varepsilon_i\right)^3 d_i\varphi_i}\right)\left|U_g - U_i\right|\left(u_{g,j} - u_{i,j}\right) \tag{9}$$

Effective energy transfer among solid phases and gas:

$$E^{g-i} = \frac{6\varepsilon_i}{d_i\varphi_i}\frac{k_g}{\left(d_i\varphi_i\right)}\left[2 + 0.39\left(\frac{\rho\left|U_g\right|}{\mu_g}\left(d_i\varphi_i\right)\right)^{1/2}\left(\frac{\mu_g C_{p,g}}{k_g}\right)^{1/3}\right]\left(T_g - T_i\right) \tag{10}$$

$$\varepsilon_g = 1 - \sum \varepsilon_i \tag{11}$$

Where ε_i stands for the individual solid volume fractions of the pellets classes and ε_g is the gas volume fraction, k is the thermal conductivity di is the average particle diameter of the pellet class. The index i represents the classes of the pellets considered in the solid charged. The indexes j and k are for coordinates component direction n is chemical species and m the indicator of the reactions, M is the molecular weight of the species, P is gas pressure, F is the component of momentum interactions among the phases and *r* is the rate of chemical reactions. ρ,ε,Cp, k and ΔH are phase density, volume fractions, heat capacity, heat conductivity and heat due to chemical reactions, respectively. T and U are the phase temperature and velocity fields, respectively. The quantity E^{i-l} is the heat transfer among the phases and accounts for convective and radiation heat transfer. The gas-solids momentum interactions are represented by F^{i-l} for each coordinate direction, given in Eq. (10). The above equations coupled with the rate of chemical reactions of reduction based on the 3-interface model for H_2 and CO (Castro *et al,* 2001, 2011) and the rate equations for self-reforming reactions are solved simultaneously. In the cooling zone, the carburization of the DRI is considered as a first order reaction controlled by the carbon deposition from the methane.

2.3 Numerical method

The set of differential equations, Eqs. (1)-(9) are discretized using the finite volume method. The gas velocity and pressure field coupling are solved using the SIMPLE algorithm (Mealaen, 1992). For all equations, the discretized algebraic equations are determined using the power law scheme (Mealaen, 1992). The system of algebraic equations were solved using the line-by-line iterative procedure based on the tri-diagonal algorithm. The convergence criterion assumed a maximum error of 10^{-5} for the momentum and energy equations, in addition to a mass balance of the individual species of less than 1%. The numerical grid was selected by continuous refinement until the average error reached less than 1%. The solution algorithm uses the iterative sequence of updating all properties and interphase interactions of momentum, mass and energy by calculating all the source terms based on the actual variables, thus solving the momentum, chemical species and energy for all phases and updating all variables. Repeat this procedure until convergence of all variables is achieved.

3. Results and discussions

The numerical results are presented comparing the use of 3 pellets with similar geometalurgical characteristics and distinguished size distributions. Figure 3 shows the size distributions for pellets A, B and C. Pellet A is a typical raw material used in the shaft furnace. Pellets B and C are obtained by controlling the green pellet formation and sieving after firing. Figure 4 shows the gas flow and temperature distributions for the reference operation with pellet A. The inner temperature condition and the average gas composition at the outlet agreed with the industrial data within a 2% of average error. The productivity and mass flow rates of solid materials are in agreement with the industrial data within 1%. Figures 4, 5 and 6 comparatively show the gas flow rates and temperature distributions for the size distributions presented in Figures 3 (a), (b) and (c), respectively. As can be observed, the inner temperature of the central region of the reactor decreased for the distributions shown in Figures 3 (b) and (c). The reason for such behavior is mainly due to the changes in the gas flow rates. It is worthy to mention that the metallization was aimed constant and the solid inflow was adjusted, which promotes inner temperature and gas flow changes, as evidenced in Figures. 4, 5 and 6.

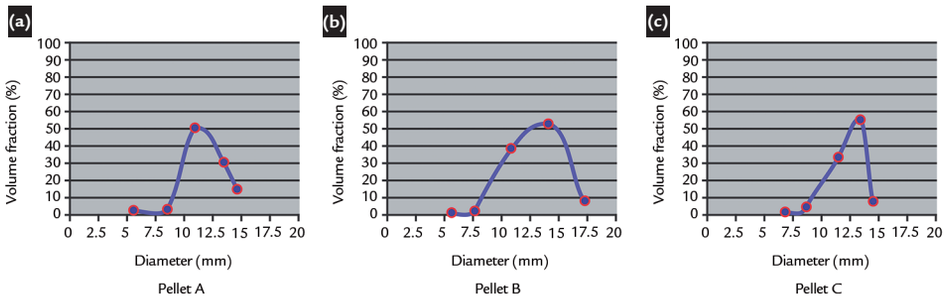

Figure 3
Granulometric fractions distributions for the comparison of 3 pellets with similar geometallurgy characteristics.

The gas flow rates at the inlet are imposed as boundary conditions and the outlet mass flow rate was compared with the measured one with agreement discrepancy of less than 5%. This discrepancy is explained due to the complex reactions and rate equations taking into account the local variables, which are measured under conditions that simulate the process parameters.

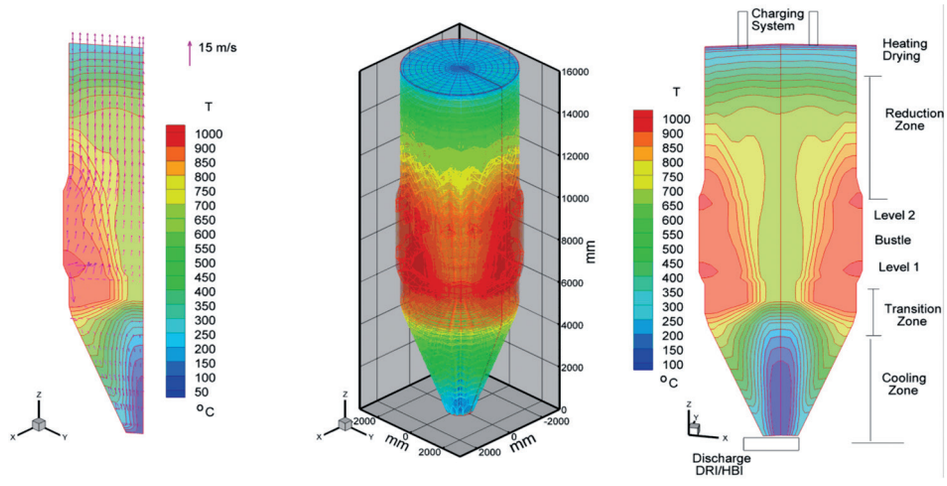

Figure 4
Gas flow characteristics and temperature distributions for the operation with 90% pellet A and 10% lump ore. Actual shaft furnace operational conditions – Reference case for the simulations.

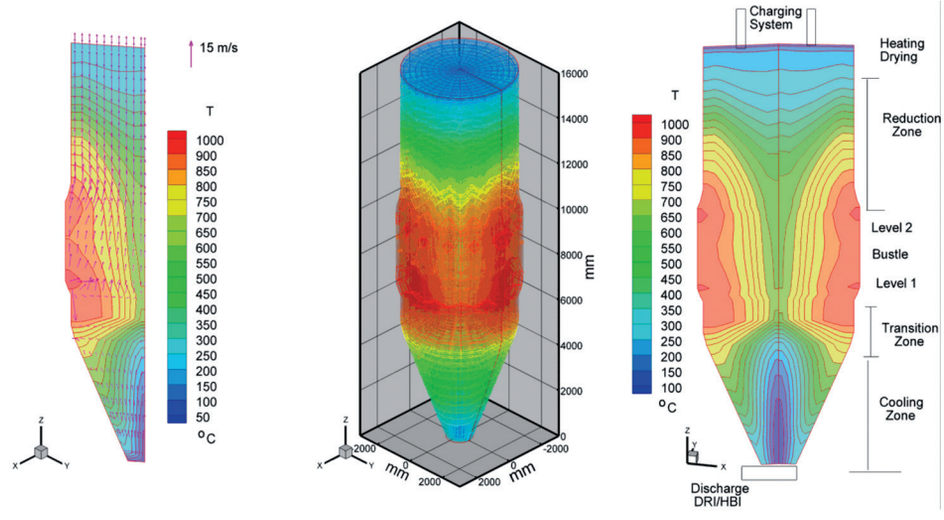

Figure 5
Gas flow characteristics and temperature distributions for the operation with 90% pellet B and 10% lump ore- Same operational conditions for the reference case.

Figures 5 and 6 show the inner variables for pellets B and C, respectively. As can be observed, when the granulometric distribution is narrowed, the temperature profile moves upward. The reason for this behavior is attributed to the enhanced heat and mass transfer due to more uniformity of the gas flow.

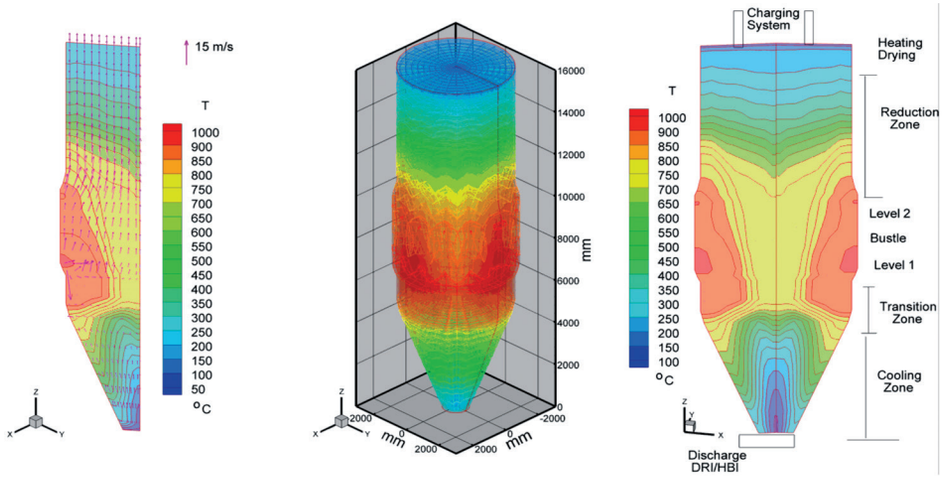

Figure 6
Gas flow characteristics and temperature distributions for the operation with 90% pellet C and 10% of lump ore - Same operational conditions for the reference case.

Figure 7 shows the self-catalytic effect by adding CH_4 and O_2 in the bustle zone which promotes reactions of gas reforming and post combustion of H_2, CO which supply heat for enhancing the reduction zone temperature.

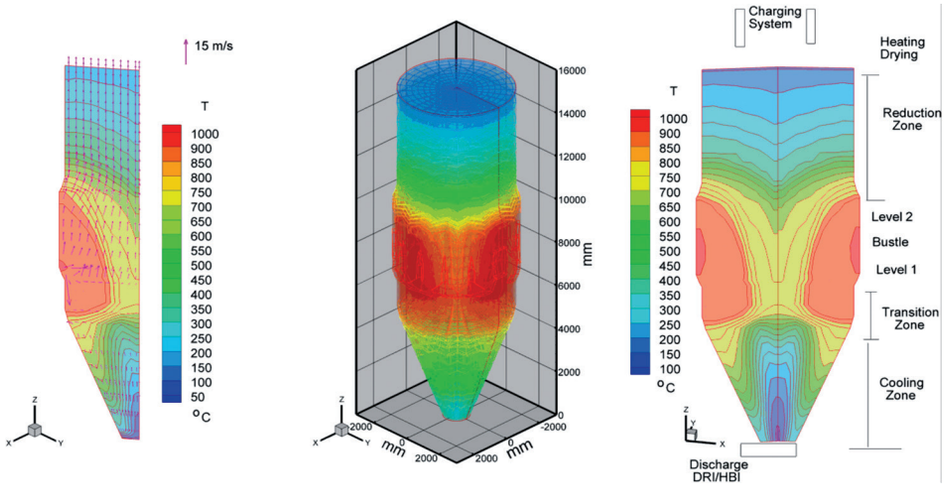

Figure 7
Effect of the self-catalytic reactions (1.8% CH_4 and 1.5 % O_2 added to flow rate).

This technology can be used with restriction due to the possibility of excessively increasing the temperature and hence allowing the clustering phenomena. However, as can be observed in Fig. 7, the temperature distribution in the reduction zone is restored and well distributed allowing better reduction conditions within the reactor with operation stability. In this study, Fig. 7 shows that under these operational conditions, the performance of the reactor can be improved. The self-catalytic effect is mainly obtained with the reduced iron in the transition zone of the reactor acting as an activated surface for the CH_4 reforming reactions and the partial combustion furnishes additional energy for the reforming reactions.

4. Conclusions

This paper analyzed the shaft furnace for direct reduction as a multiphase multicomponent momentum, energy and mass transfer reactor by applying a comprehensive mathematical model. The effect of process variables and raw materials were investigated. The model indicated that further improvements on the energy efficiency and environmental benefits could be obtained by using self-catalytic reactions and compensation of the heat supply using partial combustion of natural gas with oxygen up to 1.5% on the reducing gas inlet for the same metallization of the DRI product.

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