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Modeling of iron ore reactions in blast furnace

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ABSTRACT

Iron ore (pellet, sinter and lump ore) is gradually reduced to iron in blast furnace. The reductions are a serial of heterogeneous gas solid reactions that take place from the top of the furnace and throughout the shaft region of the furnace. Two major categories of iron ore reaction model had been developed and applied for modeling the iron ore reduction: Un-Reacted shrinking Core (URC) model and grain model. The URC model had been widely adopted in blast furnace numerical model due to its simplicity for numerical implementation. However, the URC model assumes the reaction taking place in a sharp interface inside the iron ore. The sharp interface assumption may not be valid in the entire reaction stage due to the porous natural of the iron ore. The grain model was proposed to overcome such limitation. But the complexity of the grain model restricts its application to single ore granule reaction process and it has not been applied full blast furnace modeling. In this paper, a novel methodology is proposed to implement the grain model to predict iron ore reduction in blast furnace. The model considers the gas diffusion in porous iron ore, the dynamic composition changes of iron ore along the radius of the iron ore, the iron ore transport in blast furnace. The gas flow and interphase heat transfer are also considered. The result reveals the detailed heat and mass transfer process for the iron ore reduction in blast furnace shaft.

1. Introduction

Iron ore (pellet, sinter and lump) is gradually reduced to iron in blast furnace. The reductions are a serial of heterogeneous gas solid reactions that take place from the top of the furnace and throughout the shaft region of the furnace. For full blast furnace numerical modeling, the accurate prediction of the reaction kinetics is essential as the reaction rates will be used as the source term for the conservation equations in the blast furnace computational fluid dynamics (CFD) model. The overall reaction rate of a single ore will be determined by the total resistance generated by following general steps [1]. (i) gas film resistance: mass transfer of gaseous reactant from the bulk flow to the ore surface; (ii) production layer resistance: diffusion of the gaseous reactant through the porous reduced solid layer; (iii) intrinsic chemical resistance: chemical reaction resistance between the metal-oxide and the gaseous reactant.

Depending on the iron ore porosity, two major categories of models have been developed and applied for modeling the iron ore reduction: Un-Reacted shrinking Core (URC) model [1,2] and grain model [3,4]. The basic assumption of the URC model is that the chemical reaction only takes places in a sharp interface between the reacted and unreacted zone. The one interface [5] and three interfaces [6] URC models are the most frequently used ore reduction model in the blast furnace modeling. However, the assumptions of the URC model are valid in the two following situations. The first situation is that the URC model can be used to predict the reduction process of dense pellet, i.e., the gaseous reactant is restricted in the reaction interface. Second situation is that the URC model is also applicable when the intrinsic chemical resistance is negligibly small, i.e., the chemical reaction is much faster than the gas diffusion in the production layer.

The grain model is proposed to overcome the limitation of the URC model. The grain model allows the chemical reaction and gaseous diffusion proceeds simultaneously in iron ore composed of small grains. The reaction takes place in the volumetric region rather than being constrained to a sharp interface. Therefore, the reaction rate varies locally along the radius of the ore. The additional resistance may also be considered due to the diffusion of the solid product layer for each individual grain [3]. Unlike the URC model, the analytical solution for the grain model is usually

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Nomenclature

A_i	chemical reaction resistance
B_i	diffusion resistance
C_A	reactant gas concentration, mol/m^3
C_{CO}	concentrate of CO inside the pellet, mol/m^3
C_{CO_2}	concentrate of CO_2 inside the pellet, mol/m^3
C_p	heat capacity, J/(kg K)
D_0	throat diameter, m
D_{CO}^e	effective diffusivity of CO inside pellet, m^2/s
$D_{CO_2}^e$	effective diffusivity of CO_2 inside pellet, m^2/s
$D_{e,i}$	effective diffusivity of the product layer, m^2/s
D_e'	Effective diffusive coefficient of CO through the surface layer, cm^2/s
F	gas film resistance
k_i	reaction constant, cm/s
$K_{e,i}$	equilibrium constant
L	vertical distance of the burden profile, m
r	radial direction, m
r_0	radius of the iron pellet, m
r_g	radius of the grain, m
R	gas constant, J/(K mol)
R_i	reaction rate, mol/(m^3 s)
S_0	specific surface area, cm^2/cm^3
T	temperature, K
$\vec{\boldsymbol{u}}_{\boldsymbol{b}}$	burden velocity, m/s
v_0	reduction rate of the concentrates, mol/(cm^3 s)
X_0	local un-reacted degree
α	shape factor of the concentrate
β	micro-structure of the fine pellets
γ	fracture factor
ε	porosity
τ	tortuosity
ρ	density, m^3/kg
ψ_{mg}	volumetric fraction of the iron concentrate

unavailable, thus the discretization along the ore radius is required to apply the grain model to blast furnace numerical method in a moving bed fashion. Therefore, the grain model has been limited to apply to single ore reduction in batch furnace or fixed beds reduction [3,4]. Recently, blast furnace numerical models in one-dimension [7,8], two-dimensions [9–11] and three-dimensions [12,13] have been developed extensively. However, all the aforementioned blast furnace models implement the URC model for iron ore reduction. The difficulty to implement grain model in blast furnace is mainly because that discretization along the ore radius in a moving bed fashion is required. In this paper, a novel method is developed to incorporate the grain model into the blast furnace model. This novel method not only applies to the iron ore reduction in blast furnace but also suits for the general moving bed reduction system such as shaft furnace. In addition, the URC model and grain model in blast furnace modeling are compared.

2. Numerical model

2.1. Iron ore reaction in blast furnace shaft

The reduction of iron ore proceeds via the successive steps $Fe_2O_3 \rightarrow Fe_3O_4 \rightarrow FeO \rightarrow Fe$ in blast furnace. This paper is based on the framework of the blast furnace numerical model developed previously [11,14]. The focus of the present study is to implement the grain model into the blast furnace model and compare with the URC model. As listed in Table 1, the two different models, i.e., URC and grain, have been applied to the indirect reduction of the iron ore by CO and H_2 as listed in Table 1 R1–R6. Other reactions such as the coke reactions (Boudouard reaction, water gas reaction), flux decomposing, water gas shift reaction, direct reduction of FeO are also considered. Blast furnace coke undergoes three main reactions in the shaft. These are the Boudouard reaction (7), the water–gas reaction (8) and the direct reduction reaction ($C + FeO = Fe + CO$) which is, kinetically, a combination of reaction (3) and reaction (7) or a combination of reaction (6) and reaction (8). The detail description of the models for other reactions is published elsewhere [14,21].

2.2. One interface unreacted shrinking core model

As shown in Fig. 1, the URC model [1,2,15] assumes that the reduction of an iron oxide sphere occurs at the surface with the formation of an outer shell of metallic iron. The shell grows into the core in the radial direction until the entire oxide is completely reduced to iron.

The complex process of iron ore reduction is simplified to three rate control processes, namely, gas film resistance, diffusion resistance through the product layer (reduced oxide shell), and chemical reaction resistance at the metal-oxide interface. The expression for the reaction rate for a single pellet is expressed as

$$R_i = \frac{4\pi r_0^2\left(C_R - \frac{C_P}{K_{e,i}}\right)\cdot\frac{K_{e,i}}{(1+K_{e,i})}}{F + B_i + A_i} \tag{1}$$

Table 1
Chemical reactions considered in the CFD model.

Reaction	No.	Chemical equation	Rate
Indirect reduction by CO	R-1	$3Fe_2O_3(s) + CO(g) \rightarrow 2Fe_3O_4(s) + CO_2\ (g)$	R_1
	R-2	$Fe_3O_4(s) + CO(g) \rightarrow 3FeO(s) + CO_2\ (g)$	R_2
	R-3	$FeO(s) + CO(g) \rightarrow Fe(s) + CO_2\ (g)$	R_3
Indirect reduction by H_2	R-4	$3Fe_2O_3(s) + H_2(g) \rightarrow 2Fe_3O_4(s) + H_2O\ (g)$	R_4
	R-5	$Fe_3O_4(s) + H_2(g) \rightarrow 3FeO(s) + H_2O\ (g)$	R_5
	R-6	$FeO(s) + H_2\ (g) \rightarrow Fe(s) + H_2O\ (g)$	R_6
Boudouard reaction	R-7	$C(s) + CO_2\ (g) \rightarrow 2CO\ (g)$	R_7 [14,21]
Water gas reaction	R-8	$C(s) + H_2O(g) \rightarrow CO + H_2\ (g)$	R_8 [14,21]
Flux decomposition	R-9	$MeCO_3(s) \rightarrow MeO(s) + CO_2(g)$, Me = Ca, Mg	R_9 [14,21]
Water gas shift reaction	R-10	$H_2\ (g) + CO_2\ (g) \rightarrow H_2O(g) + CO(g)$	R_{10} [14,21]
Direct reduction of liquid FeO	R-11	$C(s) + FeO\ (l) \rightarrow Fe\ (l) + CO\ (g)$	R_{11} [14,21]