

3D MULTIPHASE MULTICOMPONENT MATHEMATICAL MODEL OF THE SHAFT FURNACE FOR SELF-REDUCING PROCESS¹

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Abstract

DRI demand continues increasing due to shortage of high quality scrap for the steel production using electric arc furnace. In this context, the shaft furnace based on self-reducing process becomes alternative to supply the demand of metallics. This technology has the advantage of possible recycling solid waste materials from iron and steelmaking industries since the self-reducing agglomerate are mixtures of fine ore/ residues and reducing agent. The principal characteristic is the "internal environment of the agglomerate", this results in high rates of reduction (extraction of the oxygen from the ore) due to the kinetic conditions. The present paper aims to develop a mathematical model capable of simulating the operating conditions of the shaft furnace with self-reducing agglomerate, lump coal and secondary gas injection. The model used the technique of finite volume to solve the transport equations of momentum, energy and chemical species of both, solid and gas phases considered in this model. The main finds of this paper are: a) the self-reducing furnace can operates with a mixture of self-reducing briquettes and anthracite, b) the productivity of the process can achieve 35.5 t/m³/day, c) the process produces outlet gas with high calorific value.

Key words: Self-reducing agglomerates; Mathematical modeling; Shaft furnace

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1 INTRODUCTION

DRI demand continues increasing due to shortage of high quality scrap iron for the steel production through electric arc furnace. In this context, the shaft furnace based on self-reducing process becomes an alternative to supply the demand of metallic. It is possible to recycle the remainders of iron and steelmaking industries since the self-reducing agglomerate are mixtures of fine ore/ residues and reducing agent. The principal characteristic is the "internal environment of the agglomerate", this results in high rates of reduction (extraction of the oxygen from the ore) due to the kinetic conditions.

Another differential is regard with the environment because it does not need lump ore and coke. Without the units most polluting of the ironmaking process – Sinter and Coke Plants- the system guarantees a friendly environment operation.

The self-reducing agglomerates are cold bonded, since they cannot be fired (the carbon will burn), usually produced from a mixture of fines of iron ore or residues and a carbonaceous material. It could be coal of different qualities and ash levels, charcoal, coke breeze, petroleum coke and others⁽¹⁾. One of the principal characteristic is related to the reaction rate: due to the contact of the reactants and their small size and nitrogen free environment, high rates of reduction (extraction of the oxygen of the ore) can be achieved.

In order to have better understandings of the phenomena in the self-reducing process, some researches have been carried out. D'Abreu and collaborators had carried out some research aiming to analyze the behavior of the self-reducing pellets.⁽¹⁻⁴⁾ They had presented an analysis of the impact of the temperature, type of atmosphere and composition of the ferrous and carbonaceous materials, on the kinetic of self-reducing technology, in two types of carbon-bearing agglomerates for temperatures between 1000 and 1300°C.⁽²⁾ On the other hand, It was studied the morphological aspects of the metallic iron phases from self-reducing briquettes in the range of temperature of 1000 to 1350°C.⁽³⁾ Efforts have been made in order to quantify the metallic phase of iron using digital techniques of microscopy in reduced briquettes of magnetite-coal under atmosphere of N₂ at 1200°C using time intervals of 5 min until 45 minutes.

Moreover, researches have been developed mathematical modeling of fundamental phenomena of heat and mass transfer, as well as the kinetic of the self-reduction process. In this context, Castro et al. have developed a total mathematical model using finite volumes technique to simulate the superior region of the self-reducing reactor.⁽¹⁾ The proposed model considers two phases (solid and gas) and conservation equations for mass, momentum and energy are solved simultaneously for the two phases in the reactor. The solid phase consists of self-reducing briquettes, granular coals and other iron bearing materials.

The present paper aims to develop a mathematical model capable of simulating the operating conditions of the shaft furnace with self-reducing agglomerate, lump coal and secondary gas injection. The energy produced by the carbon monoxide combustion of secondary gas injection is used for preheating and reducing the agglomerates. Inside of the reactor occur the self-reduction and the heat exchange and momentum phenomena between ascendant gas and solid descendent (briquette and coal). The kinetic rates of all self-reduction reactions and coal combustion-gasification in the interior of the briquette have been modeled according to models obtained from literature.⁽¹⁻¹⁶⁾

2 MATHEMATICAL MODELING

The model of the shaft furnace of the self-reducing process, presented here, consists in the formulation of the phenomena that occur in the interior of the reactor as a two-phase system. The phase interactions are coupled by the source terms appearing on the momentum, energy and chemical species transport equations. The transport equations are discretized and solved based on the finite volume method. In general, the heat, momentum and mass transfer equations in the interior of the shaft furnace are represented by the general conservation equation (eq.1). In this equation the sources terms represent the interactions with the other phases. Γ_ϕ is the effective transfer coefficient which depends on the state variable to be solved. The source term (S_ϕ) include all terms not enclosed in the left side of the equation. Equation 1 is a typical equation computed by finite volume method. The momentum and energy transfer models had been collected from the literature and adapted for the conditions of the furnace in previous works^(1, 5, 10). The mechanisms and kinetics models of the main self-reducing reactions⁽¹²⁻¹⁶⁾, volatile and coal combustion had been presented in previous works, being only adapted for the conditions of the self-reduction reactor.^(1,5-16)

$$\frac{\partial(\rho_i \varepsilon_i \phi_{i,k})}{\partial t} + \text{div}(\rho_i \varepsilon_i \vec{V}_i \phi_{i,k}) = \text{div}(\Gamma_{\phi_{i,k}} \text{grad}(\phi_{i,k})) + S_{\phi_{i,k}} \quad (1)$$

The phases considered in this model are, solids, (self-reducing briquettes lump coal), that are loaded for the top and gases. The gaseous phase corresponds to injection and gases generated by chemical reactions.

In Table 1 the chemical species are presented for each phase. Each chemical specie correspond to partial differential equation as presented in eq. 1

Table 1 Two-phase model considered to describe the shaft furnace of the self-reduction process (40 partial differential equations, eq.1)

Phases	Chemical Species	
Gas (u_1, u_2, u_3, p, T)	CO, CO ₂ , O ₂ , H ₂ , H ₂ O, N ₂ , SiO	
Solid (u_1, u_2, u_3, p, T)	Self-reducing briquettes	C, volatile, SiC, Fe ₂ O ₃ , Fe ₃ O ₄ , FeO, Fe, CaO, Al ₂ O ₃ , MgO, SiO ₂ , H ₂ O, gangue
	Lump coal	C, volatile, S, SiC, H ₂ O, CaO, Al ₂ O ₃ , MgO, SiO ₂ , gangue

The reactor dimension was adopted from industrial data with internal volume of 3,36 m³. The Figure 1 shows the grid constitution for the numerical simulation.

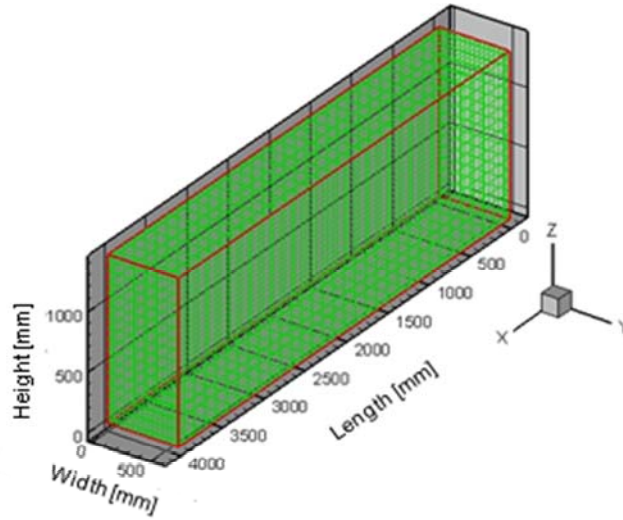


Figure 1: Grid constitution for the numerical simulation

The lump coal charged provides to the process peculiar characteristic of heat and mass transfer due to liberation of volatile material in the interior of the granular bed. Devolatilization models of coals for PCI are widely divulged in literature.^(6,7,9,11) In this work a model was adapted to represent the volatilization in granular coal as follows:

Volatiles combustion

1	Volatile (coal, fines) + $\alpha_1 O_2 \rightarrow \alpha_2 CO_2(g) + \alpha_3 H_2O(g) + \alpha_4 N_2(g)$
$R_1 = 23,6 \cdot k_{\text{eff}} \left(\frac{\mu_g \varepsilon_t}{\rho_g k_t} \right)^{1/4} \left(\frac{\varepsilon_t}{k_t} \right) \min \left(\varepsilon_c \rho_c \omega_{VM_{pc}}, \varepsilon_g \rho_g \omega_{O_2} \frac{M_{VM}}{\alpha_1 M_{O_2}} \right)$	
2	volatile(coal, fines) + $\alpha_5 CO_2(g) \rightarrow \alpha_6 CO(g) + \alpha_7 H_2(g) + \alpha_8 N_2(g)$
$R_2 = 23,6 \cdot k_{\text{eff}} \left(\frac{\mu_g \varepsilon_t}{\rho_g k_t} \right)^{1/4} \left(\frac{\varepsilon_t}{k_t} \right) \min \left(\varepsilon_c \rho_c \omega_{VM_c}, \varepsilon_g \rho_g \omega_{CO_2} \frac{M_{VM}}{\alpha_5 M_{CO_2}} \right)$	
$k_t = (0,03 \vec{U}_g)^2; \varepsilon_t = \frac{k_t^{0,5}}{0,01}$	
$k_{\text{eff}} = 1,5 \times 10^{-4} (T_{\text{film}})^{1,25} \text{EXP} \left(\frac{-25300}{8314 T_{\text{film}}} \right)$	

The stoichiometric coefficients of the volatile combustion equations are determined as follows

$$\delta = \frac{\omega_{C_{VM}}}{M_C} + \frac{\omega_{H_{VM}}}{M_H} + \frac{\omega_{O_{VM}}}{M_O} + \frac{\omega_{N_{VM}}}{M_N}; \quad \alpha_1 = \frac{\omega_{C_{VM}}}{\delta M_C} + \frac{\omega_{H_{VM}}}{4\delta M_H} - \frac{\omega_{O_{VM}}}{2\delta M_O}; \quad \alpha_2 = \frac{\omega_{C_{VM}}}{\delta M_C};$$

$$\alpha_3 = \frac{\omega_{H_{VM}}}{4\delta M_H}; \quad \alpha_4 = \frac{\omega_{O_{VM}}}{2\delta M_O}; \quad \alpha_5 = \frac{\omega_{C_{VM}}}{\delta M_C} - \frac{\omega_{O_{VM}}}{2\delta M_O}; \quad \alpha_6 = \frac{\omega_{C_{VM}}}{\delta M_C} + \alpha_5; \quad \alpha_7 = \frac{\omega_{H_{VM}}}{\delta M_H};$$

$$\alpha_8 = \frac{\omega_{N_{VM}}}{2\delta M_N}$$

3 RESULTS/DISCUSSION

In this section it will be presented and discussed the main internal aspects of the shaft furnace and the main forecasts of operational parameters. Table 2 shows the chemical characteristics of raw materials used in this simulation. The metallic charge is a typical self-reducing briquette and the coal is anthracite with low volatile.

Table 2: Self-reducing agglomerate and lump coal composition [%]

Self-reducing agglomerate components											
C	volatile	Fe2O3	Fe3O4	FeO	Fe	H2O	gangue	SiO2	Al2O3	MgO	CaO
14,8	0,5	66,2	-	1,1	-	4,4	-	2,8	2,7	4,0	4,0
Lump coal components (anthracite)											
C	volatile	H2O	gangue	S	SiC	SiO2	Al2O3	MgO	CaO		
70,8	15,11	-	7,05	0,5	-	3,02	-	2,0	2,03		

In the Figure 2, the temperature profile for the gas and solid phases foreseen by the model are presented. It was observed considerable increased of the temperatures of gas and solid in the region of the secondary tuyeres due to oxygen injection that reacts with the CO that comes from the inferior zone of the furnace, liberating heat that immediately is transferred to the descending solid charge.

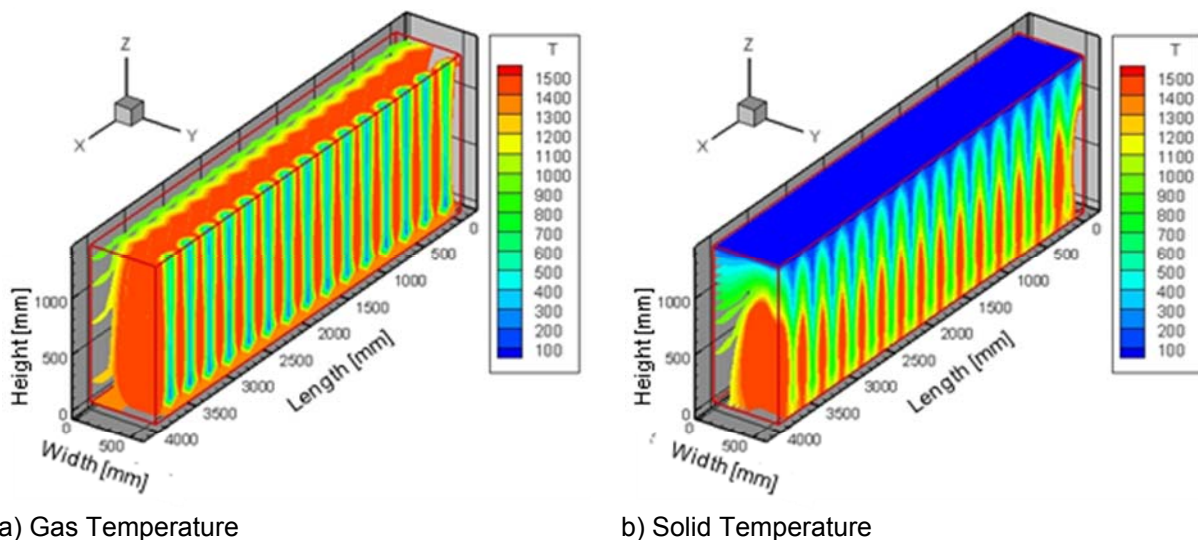


Figure 2: Temperature profiles in self-reducing shaft furnace

In Figure 3 is presented distribution of pre-reduced oxides of iron in the interior of the self-reduction reactor. It is observed that hematite is quickly reduced to

magnetite and magnetite remains until approximately the middle of the height of the shaft, where it is finally reduced to wustite and iron. The predominant region where wustite located is the periphery of the shaft while the reduced iron is located in the central region due to gaseous stream, temperature profile of solid and gas and CO concentration due to secondary combustion that impose favorable reducing conditions in the central region. It can be observed that DRI composition varies strongly from the center to the periphery.

In Figure 4 are presented the three-dimensional fields of reduced fraction, charge descent velocity and the reduction conditions in the gaseous atmosphere. The reduced fraction is located in the central region as a result of a rich atmosphere in CO (c). On the other hand, CO₂ produced by reduction of iron oxides is consumed through the “solution loss” reaction and the remaining gas is liberated for the top (d). The profile of charge descent velocity presents a standard behavior of lower velocity next to the furnace walls (b). It is due to attrition between charge and wall.

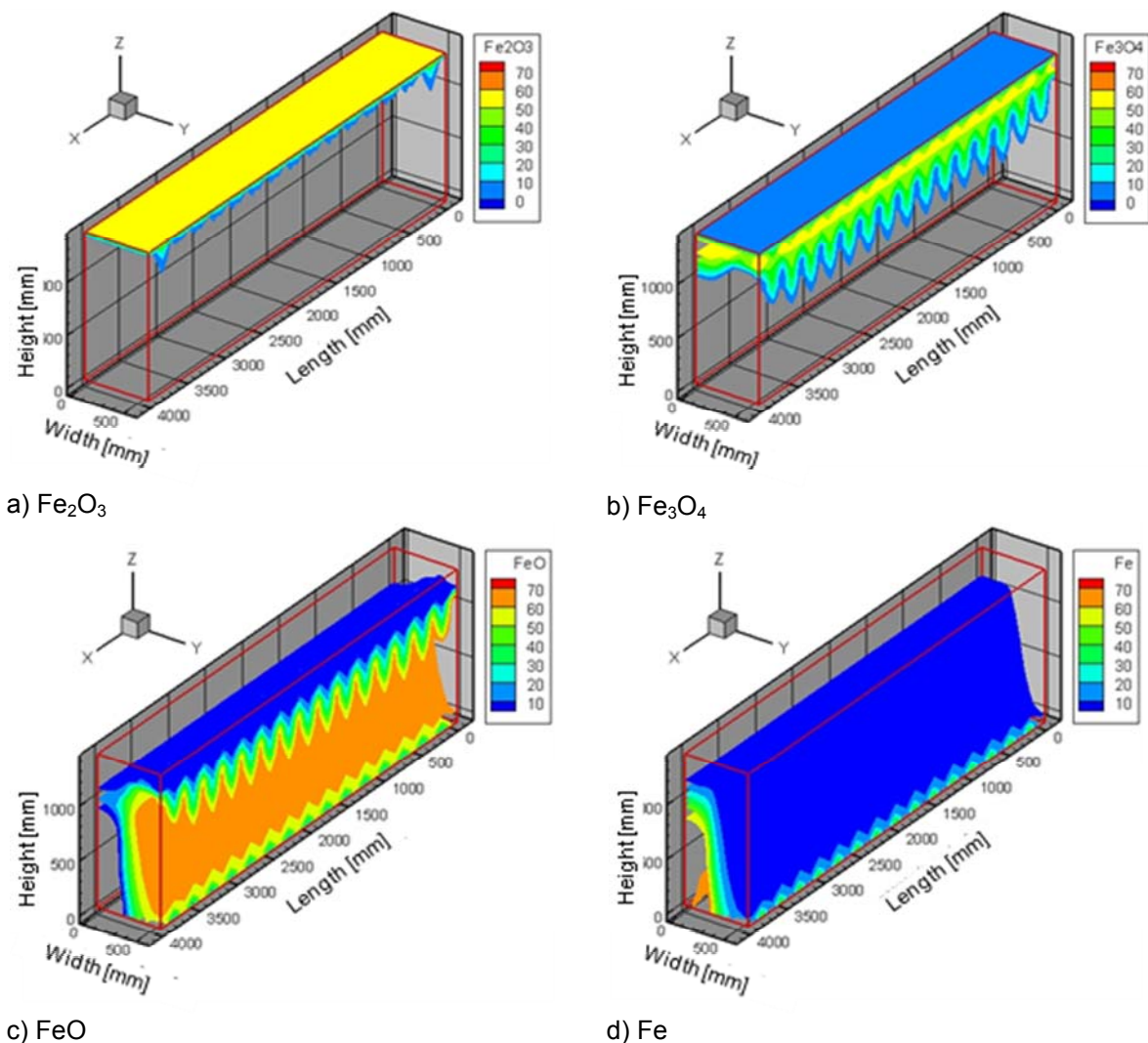
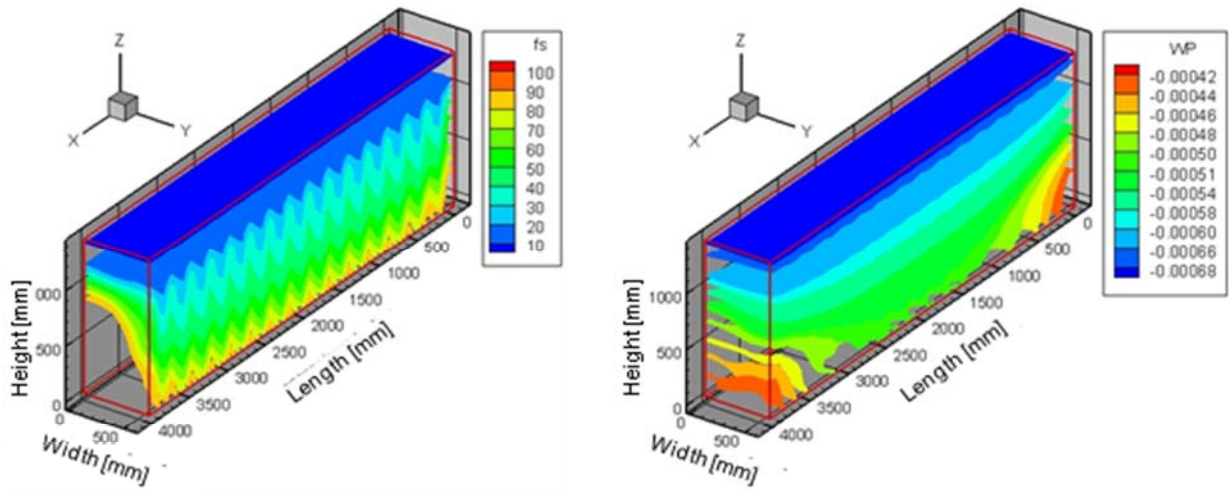


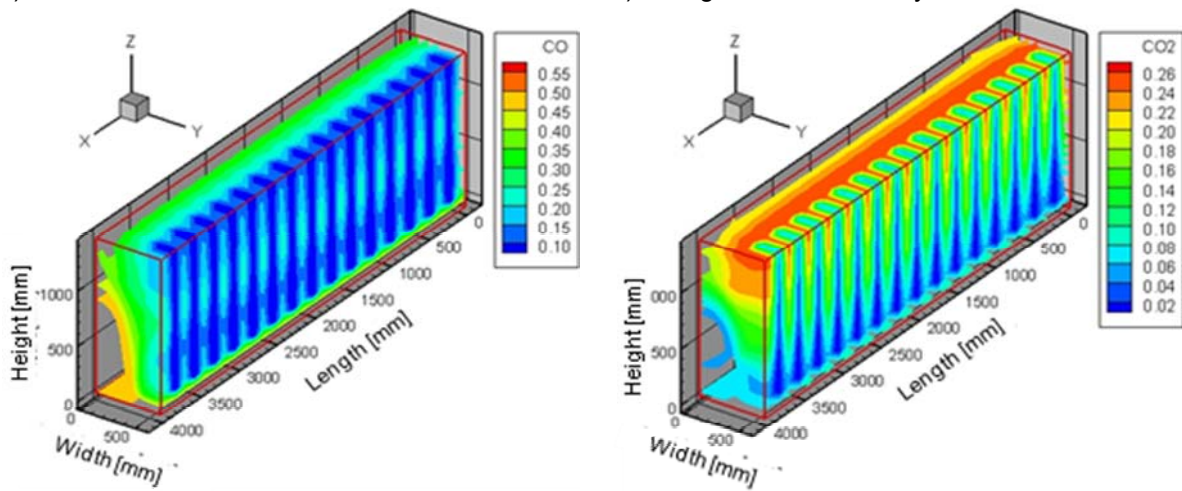
Figure 3: Distribution of pre-reduced oxides and reduced iron ore

Operational global parameters of the reactor calculated by the model are presented in Tables 3, 4 and 5. High productivities can be obtained through this process. Although the production scale is small when compared with the blast furnace production, it is high when compared with typical processes of DRI production.



a) Fractional conversion

b) Charge descent velocity



c) CO

d) CO₂

Figure 4: Internal conditions of the shaft furnace operating with self-reducing agglomerates

Table 3: Principal operational parameters.

Charge [kg/t DRI]	1555	Top gas temperature [°C]	590
Productivity [t/m ³ /day]	34.5	Gas production [Nm ³ /t DRI]	4000
Production [t/day]	118	Secondary injection [Nm ³ /t DRI]	1650
Average residence time [min]	35	Char production [kg/t DRI]	56
Metallization [%]	80	CO/CO ₂	1.9

Table 4: Top gas composition

N ₂ [% vol]	O ₂ [% vol]	CO [% vol]	CO ₂ [% vol]	H ₂ [% vol]	H ₂ O [% vol]
53.4	4.5	24.5	12.8	1.69	3.10

Table 5: Chemical composition of self-reducing agglomerate and granulated char produced [%].

Briquettes produced											
C	Volatile	Fe ₂ O ₃	Fe ₃ O ₄	FeO	Fe	H ₂ O	gangue	SiO ₂	Al ₂ O ₃	MgO	CaO
4,87	-	0,47	1,01	2,42	70,3	-	-	4,32	4,22	6,18	6,18
Granulated char											
C	Volatile	H ₂ O	gangue	S	SiC	SiO ₂	Al ₂ O ₃	MgO	CaO		
84,2	-	-	7,29	-	-	3,65	-	-	4,86		

4 CONCLUSIONS

A model capable to predict of satisfactory form the internal behavior of the self-reduction reactor was developed. The prediction of the evolution of the pressure, temperature and chemical composition of the two phases can be calculated by the model. The model predicts rapid initial reduction of hematite to magnetite, but slow reduction from magnetite to iron. It was observed considerable increased of the temperatures of gas and solid in the region of the secondary injection.

Also, the simulation gives the principals aspects of the distribution of gas through the charge, as well as the charge movement in the interior of the reactor and residence time of solids in the shaft furnace. The residence time calculated was 35 min and the CO/CO₂ relation was 1.9.

Operational parameters such as productivity, temperature of the top gas and chemical composition of products had been calculated successfully. Results of simulation had indicated that approximately 80% of metallization degree can be attained in this process. The productivity of the process was of 35 t/m³/d with a top gas volume of approximately 4000 Nm³/tDRI.

5 NOMENCLATURE

D- Effective Diffusivity for specie <i>i</i> (m ² /s)	ε _{<i>i</i>} - Shape factor for phase <i>i</i>
d- Particle diameter for phase <i>i</i> (m)	ω _{<i>j</i>} - molar fraction for phase <i>j</i>
M _{<i>j</i>} - Molecular weight of specie (Kg/mol)	S _φ - Source Terms
P- Pressure (Pa)	Sh- Sherwood number(-)
R _{<i>i</i>} - Rate of reaction <i>n</i> (mol/m ³ /s)	φ _{<i>i</i>} - fractional conversion of iron ore
T- temperature (K)	ρ- Density
α- stoichiometric coefficient	Γ- Transfer coefficient

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