Computational Analysis of The Performance of Shaft Furnaces with Partial Replacement of The Burden with Self-Reducing Pellets Containing Biomass

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The shaft furnace knowed Midrex™ is used for the production of direct reduced iron with the use of reformed gas. Another process based on shaft reactors is the Tecoreo process, which exhibits the great advantage of using self-reducing agglomerates. Therefore, it was proposed a combination of the shaft furnace for direct reduction with self-reducing pellet burden. In addition, with the aim of improving the furnace efficiency and reducing the need for reformed gas, the injection of natural gas and oxygen into the bustle region is proposed. Thus, it is possible exploit the advantages of direct reduction involving high amounts of hydrogen and faster reactions of the self-reducing process to decrease the CO₂ emission, compared to that of blast furnace. The energy profile, productivity, and carbon emission of the traditional shaft furnace were compared with the simulated results after partial replacement of the burden with self-reducing pellets containing fines of elephant grass charcoal. The simulation results for a combination of 15% of self-reducing pellets in the burden with 2.5% oxygen and natural gas injection were the best among the scenarios simulated, with the productivity being 2.7 ton/m³/day and the decrease in the amount of reformed gas being 10%.

Keywords: numerical simulation, shaft furnace, self-reducing pellets, biomass.

1. Introduction

The shaft furnace used in direct reduction processes has some advantages, such as lower energy demand due the absence of metal melting, the use of different sources of reducing agents, the use of reformed gas as a reducing agent in the fuel option, and the produced sponge iron exhibiting a lower carbon concentration when compared with that of pig iron, which can demand less refining operations. These technologies are especially attractive on a particular economic and market situation where the demand for steel can be attended by compact reactors providing high energy efficiency.

The shaft furnace is a continuous flow reactor that is charged with iron ore pellets and lump iron ores that descend by gravity while they are reduced to iron by the reducing gas in counter-current flow. The phenomena that take place within the reactor are complex and involve multiple phases and chemical species. In order to understand the inner phenomena, it is convenient to distinguish four different zones in the furnace: heating, reducing, transition, and cooling zones. In the reduction zone, the transformation of the iron oxides to iron occurs at temperatures above 900 °C, concluding in the cooling zone, where the product is cooled and carburized.

A large number of mathematical models have been proposed to predict the direct reduction occurring in the shaft furnace by using transport phenomenon 1-3. The models have been successfully used to forecast the energy balance, productivity, and overall mass balance of the furnace. These models have been useful in analyzing new operating conditions and proposals for new developments 4-9.

However, owing to the difficulty in describing the complex phenomena, the computational models proposed in the literature have been simplified 5-9. The assumptions for the transport equations concerning spatial analysis, which can be one-dimensional 1,2 or two-dimensional, are commonly applied 5-5; yet, the analysis is carried out in the steady state regime 6-7.

A combination of the shaft furnace for the production of DRI (direct reduced iron) with partial replacement of the burden with self-reducing pellets has not yet been investigated, but, there are proposals of the variations in the burden of the shaft furnaces investigated by means of computational resources, however, those proposals are in terms of changing the burden distribution 10-11. Zhou et al. have proposed that the burden of the blast furnace was charged alternating coke and ore layers of different permeability. It was observed the energy profile of the blast furnace and, when the burden is mixed, the gas and burden along the radial direction are of the same temperature, and the gas temperature and pressure at the furnace wall are in good agreement with the measured data in the operating blast furnace. This also may be noted in Austin et al. 12-15 and Castro et al.’s research 16.

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Previous investigations of the behavior of the shaft furnace charged with pellets and using reformed reducing gas were performed by using computational simulations, and the results suggested the possibility of reaching around 93% of the metallization degree 8-10. However, a large amount of reducing gas is required, and hydrogen reduction is efficient only at high temperatures. Matos et al. 17 investigated the use of self-reducing briquettes in a mini blast furnace and concluded that both the thermal reserve zone and the fuel rate decreased. A combination of these techniques was proposed by Castro et al. 11 and the results showed promising features. However, further investigations are required to confirm and suggest a better combination of the operational parameters.

This study has important advantages with regard to the inner phenomena, in that it is expected to improve the efficiency of the process owing to the high reactivity resulting from the bigger contact area among the reactants and the presence of a larger inner porous area, compared to that of DRI pellets. Furthermore, the shaft furnace reactor can be made more compact (shorter), and some studies have suggested that the specific CO₂ emissions could be decreased 10,11. However, a balance of the inner porosity with a suitable mechanical resistance is required. Therefore, to investigate the feasibility of these concepts, it was developed a multiphase and multicomponent mathematical model based on mass, momentum, and energy conservation equations for predicting the inner temperature distribution of a shaft furnace on an industrial scale. It was proposed rate equations that represent the new raw material used in the model, based on previous experimental studies 18 and for DRI pellets with composition considered in previous works 10,11, 19. It was developed simulation scenarios based on a reference case involving actual operation and those based on partial substitution of the charge with SRP (self reduced pellet).

### 2. Materials and Methods

The methodological approach considered in this study comprised formulation of a detailed model based on multiphase and multicomponent phenomenon and the complementary rate equations determined experimentally to account for the overall rate of the new self-reducing raw material using CEG (charcoal from elephant grass). In this model, the shaft furnace is described as a multiphase multiphase reactor, where the pellets are treated as phases of different sizes and compositions; these phases interact among themselves as lumps and gaseous phases to exchange energy, mass, and momentum. The energy, mass, and momentum interactions among the granular particles were computed by considering the characteristics of the granular material.

The kinetic rate equations for the SRP and the composition parameters for the implementation of the model were obtained experimentally by the slow sample heating (heat rate of 5°C/min) until to reach three different temperatures and so, each temperature was maintained in isothermal runs until the chemical transformations are completed, totally. The experiments were performed in a TGA/DSC Q600 furnace using inert atmosphere. The kinetic parameters used in this study were previously published by the authors 18.

The shaft furnace burden in the model of this paper was composed by iron ore, SRP and DRI pellets, coke and others. So, in the Table 1 the final compositions of the SRP, DRI pellets, CEG, and materials for producing the SRP with biomass, are listed. For mixture of SRP, 20% of its composition is CEG.

An example of the reaction rates measured in this study is shown in Figure 1. The time evolution of the mass conversion fraction exhibited the typical behavior for isothermal conditions, which were used to determine the kinetic rate constant based on Arrhenius plot 18. A low heating rate was used until the temperatures 900 °C, 1000 °C, and 1100 °C were reached, therefore, the samples were kept in a constant temperature range for one hour. Details of the experimental runs and rate formulations can be found elsewhere 18.

The time evolution of the converted samples can be characterized as follows. Above 300 °C, the change in mass is explained by the release of combined associated water molecules through vaporization, since H₂O molecules can be associated to molecules of iron oxides, like FeO(OH) and Fe³⁺O(OH), and calcium oxide (Ca(OH)₂), apart from being present in the hydrocarbons that compose the carbon source used 20-23. With continuous heating up to 600 °C for around 120 min, a chemical transformation occurs due to the breaking of the molecules of the volatile materials, followed by CaCO₃ decomposition and the solution loss reaction; this is because this type of carbon source is more reactive than coke owing to its porosity and activation energy 21.

From this moment onwards, the change in mass is abrupt, because, as the appropriate temperature is reached, it favors the indirect reduction of the oxides by the gaseous product CO: Fe₃O₄ → FeO and FeO → Fe, which is represented by the two high peaks observed beyond 180 min at 1100 °C (Figure 1).

Table 1. Chemical compositions of the feed charge of the shaft furnace simulation.

| % Compounds | Fe₂O₃ | FeO | SiO₂ | Al₂O₃ | CaO | MgO | ZnO | P | S | MnO | PbO | Cₑ | Vol. | Ash. |
|-------------|-------|-----|------|-------|-----|-----|-----|---|---|-----|-----|----|------|------|
| SRP         | 53.5  | 0.41| 1.12 | 0.29  | 8.07| 1.32| 3.43| 0.02| 0.32| 0.71 | 0.05| 11.24| 6.52 | 2.2  |
| DRI*        | 96.71 | 0.39| 1.5  | 0.42  | 0.84| 0.11| 0   | 0  | 0  | 0   | 0   | 0   | 0    |
| Charcoal    | 0     | 0   | 0    | 0     | 0   | 0   | 0   | 0  | 0  | 0   | 0   | 0   | 0    |
| Ashes       | 0.24  | 9.21| 0.51 | 0.47  | 0.47| 0.19| 0   | 0  | 0  | 0   | 0   | 0   | 0    |

* Composition of DRI was obtained from author 10,11, 19.
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2.1 Calculation

The computational model was implemented with the reaction kinetic constants obtained experimentally. The system of differential equations was solved through the finite volume technique by using suitable initial and boundary conditions. The solid burden inlet was interactively adjusted until the final metallization reached 95% in order to compare the calculations on the same basis. The main output parameters were obtained, namely, the productivity, bustle gas pressure, and residence time of the charge in the furnace, as schematically shown in Figure 2.

The governing equations were solved through the finite volume technique that was applied to a non-orthogonal mesh by using Fortran software. Equation 1 is the governing equation that describes the phenomena of mass, momentum, and energy transfers for each species i in phase k, where the sources terms \( S_{\phi_k} \) represent the interactions among other phases in terms of the momentum, energy, and mass transfers involved in the chemical reactions. The transfer coefficient \( \Gamma_{\phi_k} \) assumes different meanings depending on the equation solved. The details pertaining to these model principles have been previously published by Castro et al. [8-11, 16].

\[
\frac{\partial (\rho \cdot \varepsilon \cdot \chi_{\phi_k})}{\partial t} + \nabla \cdot (\rho \cdot \varepsilon \cdot \boldsymbol{U} \cdot \chi_{\phi_k}) = \nabla \cdot (\Gamma_{\phi_k} \cdot \nabla (\chi_{\phi_k} \cdot \phi_k)) + S_{\phi_k} \tag{1}
\]

The subscripts i, j, and k represent the classes of pellets considered in the feed charge and the components of the directions of the coordinates, respectively. The subscripts g and s represent gaseous and solid species, respectively, \( n \) represents a chemical species, and \( m \) is the number of reactions. The parameters that appear in the set of equations listed above are defined in the nomenclature list below.

These equations are coupled with the chemical reaction rates of the self-reformation and self-reduction of CO and \( \text{H}_2 \) and solved simultaneously.

The governing equations are described for the solid and gaseous phases of each phenomenon, as presented in Table 2.

The chemical species considered in this model are summarized in Table 3.

The rates of the reactions occurring among the chemical species directly affect the governing equations and can be found in the literature.

According to the assumptions mentioned, seven operating cases of the furnace were proposed: the first case is the reference for the other cases, and, for the other six cases, new operational conditions are proposed for analyzing the partial substitution of the charge with SRP.

The base case furnace was simulated by using 100% of DRI pellets, and the atmosphere displayed the characteristic composition of Midrex furnaces (55.2% \( \text{H}_2 \), 30% CO, 10% CO\(_2\), and 4.8% \( \text{CH}_4 \)).

Table 4 shows the cases defined and the operating parameters modified, where the self-reducing charge was...
Table 2. Governing equations for all the species considered in this work.

\[ \frac{\partial (\rho, \varepsilon_i, u_{ij})}{\partial x_k} = \frac{\partial}{\partial x_k} \left( \mu_i \frac{\partial u_{ij}}{\partial x_k} \right) + F_{j}^{i} + F_{i}^{j} \]  

(2) 

Mass conservation of solid fractions

\[ \frac{\partial (\rho, \varepsilon_i, u_{ij})}{\partial x_k} = \sum_{n} M_n r_n \]  

(3) 

Enthalpy balance of solid fractions

\[ \frac{\partial (\rho, \varepsilon_i, u_{ij}, H_i)}{\partial x_k} = \frac{\partial}{\partial x_k} \left( D_{ij}^{\text{eff}} \frac{\partial \Theta_i}{\partial x_k} \right) + E_{j}^{i} - \sum_{n} M_n r_n \]  

(4) 

Chemical species of solid phases

\[ \frac{\partial (\rho, \varepsilon_i, u_{ij}, \Theta_i)}{\partial x_k} = \frac{\partial}{\partial x_k} \left( D_{ij}^{\text{eff}} \frac{\partial \Theta_i}{\partial x_k} \right) - \sum_{n} M_n r_n \]  

(5) 

Gas momentum transfer

\[ \frac{\partial (\rho, \varepsilon_i, u_{ij})}{\partial x_k} = \frac{\partial}{\partial x_k} \left( \mu_i \frac{\partial u_{ij}}{\partial x_k} \right) - \frac{\partial P}{\partial x_k} F_{j}^{i} \]  

(6) 

Mass conservation of the gas phase

\[ \frac{\partial (\rho, \varepsilon_i, u_{ij})}{\partial x_k} = \sum_{n} M_n r_n \]  

(7) 

Enthalpy conservation in the gas phase

\[ \frac{\partial (\rho, \varepsilon_i, u_{ij}, H_i)}{\partial x_k} = \frac{\partial}{\partial x_k} \left( D_{ij}^{\text{eff}} \frac{\partial \Theta_i}{\partial x_k} \right) - \sum_{n} M_n r_n \]  

(8) 

Chemical species

\[ \frac{\partial (\rho, \varepsilon_i, u_{ij}, \Theta_i)}{\partial x_k} = \frac{\partial}{\partial x_k} \left( D_{ij}^{\text{eff}} \frac{\partial \Theta_i}{\partial x_k} \right) - \sum_{n} M_n r_n \]  

(9) 

Semi empirical relations for the gas-solid momentum transfer

\[ \frac{\partial (\rho, \varepsilon_i, u_{ij}, \Theta_i)}{\partial x_k} = \frac{\partial}{\partial x_k} \left( D_{ij}^{\text{eff}} \frac{\partial \Theta_i}{\partial x_k} \right) - \sum_{n} M_n r_n \]  

(10) 

Effective energy transferred between the solid and gaseous phases

\[ E_{j}^{i} = \begin{cases} 1.75 \rho_i + \frac{150 \mu_i}{U_{ij} - U_i} \left( \frac{\varepsilon_i}{d}, \Phi_i \right) \\ \left( 1 - \varepsilon_i \right) \left( d, \Phi_i \right) \end{cases} \]  

(11) 

Table 3. The chemical species considered in this model.

| Phase          | Chemical Species                                      |
|----------------|-------------------------------------------------------|
| Gas            | CO, CO₂, O₂, H₂, H₂O, N₂                              |
| Solid          | Fe₂O₃, Fe₃O₅, FeO, Fe, CaO, Al₂O₃, MgO, SiO₂, H₂O, gang |
| DRI Pellet     | Fe₂O₃, Fe₃O₅, FeO, Fe, CaO, Al₂O₃, MgO, SiO₂, H₂O, gang |
| SRP            | C, Volatiles, Fe₂O₃, Fe₃O₅, FeO, Fe, CaO, Al₂O₃, MgO, SiO₂, H₂O, gang |
| Coke           | C, Volatiles, SiC, SiO₂, Al₂O₃, CaO, MgO, H₂O, gang    |
| CEG            | C, Volatiles, SiC, SiO₂, Al₂O₃, CaO, MgO, H₂O, gang    |
| Slag           | FeO, SiO₂, Al₂O₃, CaO, MgO, gang                       |
### Table 4. Cases examined according to the operating parameters modified.

| Parameters                                | Base       | Case A   | Case B   | Case C     | Case D   | Case E   | Case F   |
|-------------------------------------------|------------|----------|----------|------------|----------|----------|----------|
| Self-reducing charge                      | 100% DRI   | 5%       | 15%      | 20%        |          |          |          |
| Decrease in height in the reduction zone  | x          | x        | x        | 15%        | 30%      | 40%      | 40%      |
| Composition in the cooled zone            | x          | x        | x        | 50% CH₄ reduction | x        | x        | x        |
| Composition of bustle gas                 | x          | x        |          | 2.5% O₂ addition | ΔP recuperation | ΔP recuperation | No recuperation of ΔP |

### Table 5. Parameters modified for the computational simulation.

| Parameters                                | Operational range                      |
|-------------------------------------------|----------------------------------------|
| Height and volume of the reduction zone   | 5.0 – 7.5 m and 100 – 140 m³           |
| Flow rate of the reducing gas             | 40 – 60 NL/min                         |
| Fraction of self-reducing charge          | 0 – 20%                                |
| Size of the pellets                       | 4 – 18 mm                              |

### Figure 3. Temperature distributions for the base case of the shaft furnace operation.

### Figure 4. Temperature distribution of case A, containing 5% of self-reducing pellets.
Figure 5. Temperature distribution of case B, in which 15% of the charge was replaced with self-reducing pellets, 2.5% of oxygen was added to the bustle gas, and the CH$_4$ in the cooling gas was reduced by 50%.

In addition, the fines of carbon in the agglomerates reduce the consumption of the cooling gas by 50%, which is replaced by the treated gas (top outlet), since a part of the carburizing process involves the carbon present in the self-reducing pellets in the transition zone and the injected gas. This replacement saves natural gas from being consumed and helps maintain the pressure in the reduction zone.

For the cases represented in Fig. 5 and 6, additional oxygen was injected in the bustle zone. This allowed the increase of the self-reducing charge due to the energy gain from the oxygen reactions. An increase of the higher temperature region is observed in the central region of the reduction zone, compared to case A. However, the productivity of case C, compared to case B, is increased by 5% for the same degree of metallization and volume of injected gas. Case C presents a great advantage compared to the previous cases, since the reactor can be resized based on the necessary requirements in order to avoid degradation of the load, since self-reducing pellets display lower mechanical resistances compared to that of DRI. In addition, it is expected that reducing the height of the furnace will also reduce the “sticking” phenomenon, which occurs when necks are formed between the pellets.

To increase the proportion of self-reducing pellets in the charge to 20%, it is necessary to further reduce the height of the reduction zone to avoid charge degradation and attempt...
to recover the pressure loss in the charge by injecting more gas into the bustle. The results of cases D, E, and F can be seen in Fig. 7 and 8.

Fig. 7 shows that, upon replacement of the feed load with 20% of SRP, the temperature distribution throughout the reactor volume decreases; however, it is possible to resize the reactor up to a height 40% less than the initial height without any interference in the energy distribution of the equipment, compared to the previous case in which 30% of the height was reduced.

Case F is compared with case E in Fig. 8, and it is observed that when the amount of gas injected into the bustle increases, the temperature distribution remains unchanged in the reduction and transition zones, compared to that of case E; however, there is an energy gain in the cooling zone, and the productivity of case E is almost 2% higher than that of case F.

The residence time of the charge inside the reactor under usual operating conditions is about 6 h, with the average productivity being approximately 12 ton/m$^3$/day. When comparing the cases D, E, and F with the base case, it is observed that the residence time of the charge inside the furnace decreases drastically to almost 50% of that inside a commercial reactor, as observed in Table 6.
Table 6. Operating parameters obtained for the cases simulated in this study.

| Parameters                  | Base   | Case D | Case E | Case F |
|-----------------------------|--------|--------|--------|--------|
| Productivity (ton/m³/dia)   | 11.85  | 13.41  | 14.53  | 13.09  |
| Metallization (%)           | 93.66% | 95.34% | 94.80% | 94.76% |
| Average residence time (h)  | 5 h 57 min | 3 h 46 min | 3 h 09 min | 3 h 29 min |
| Carbon Emission (kgC/tonDRI)| 34.55  | 37.39  | 37.36  | 37.39  |

Composition of gas (kg/tonDRI)

| Component | Base       | Case D       | Case E       | Case F       |
|-----------|------------|--------------|--------------|--------------|
| CH₄       | 19.92      | 21.92        | 22.11        | 22.02        |
| H₂         | 54.07      | 57.32        | 57.8         | 57.55        |
| N₂         | 7.23       | 7.97         | 8.03         | 7.99         |
| CO₂       | 51.89      | 57.14        | 57.61        | 57.37        |
| H₂O       | 9.6×10⁻⁴  | 5.42×10⁻⁴   | 1.04×10⁻³   | 6.18×10⁻⁴   |

Composition of top gas (Nm³/tonDRI)

| Component | Base       | Case D       | Case E       | Case F       |
|-----------|------------|--------------|--------------|--------------|
| N₂        | 0.51       | 0.49         | 0.49         | 0.49         |
| CO₂       | 24.34      | 27.37        | 27.36        | 27.39        |
| CO₂       | 10.21      | 10.02        | 10.00        | 10.00        |
| H₂O       | 43.79      | 33.29        | 32.96        | 33.16        |

Specifically, case E was the best case obtained, since its productivity reached 2.7 tons/m³/day, which is higher than that of the base case; this case is also superior in terms of carbon emissions, compared with those of cases D and F.

Despite considerable increases in the CO₂ and CO emissions through the outlet gas in all the cases in which the self-reducing load was considered, increasing concentration of the other gases characteristic of the synthesis gas in the outlet stream is also observed. This implies that the bustle flow can be further reduced or recovered after condensation of the water and reuse of the energy, thus improving the reduction potential. In addition, the carbonaceous source considered in the self-reducing pellets is not obtained from a fossil source, but from biomass, which is a renewable source.

4. Conclusion

This study investigated the energy gain and productivity improvement of shaft furnaces through computational simulations, when it is proposed the burden partial replacing by self-reducing agglomerates, containing CEG. For this purpose, the numerical model based on the governing equations transport within the reactor was implemented by using the kinetic parameters obtained experimentally. From the simulation results, it has been proven that the combination between self-reduction and self-reformation phenomena in the direct reduction on shaft furnaces increase the productivity and decrease the residence time of the load inside the furnace in an abrupt manner.

Owing to the addition of these processes, it was possible to analyze the resizing of the reactor, the energy demand on reduction, and the increase in the productivity, and reasonably avoid degradation of the pellets and the so-called sticking phenomenon. In addition, the carbonaceous source is obtained from a renewable raw material, biomass of elephant grass, which replaces coke, a fossil source.

The consumption of natural gas in the cooling zone was reduced because a part of the carburizing of the load was carried out by the self-reducing pellets and a part of the cooling gas was replaced by the treated gas; the consumption also decreased owing to the re-dimensioning of the reactor, which lowered the demand for reformed gas.

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