Numerical Simulation Model of the Iron Ore Sintering Process Directly Describing the Agglomeration Phenomenon of Granules in the Packed Bed

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Comprehensive numerical simulation model was developed to describe the structural changes in the iron ore sintering bed by using the discrete element method (DEM). The heat wave propagation through the sintering bed was incorporated by combining the solutions of the various reaction rates and gas–granule heat transfer with the calculation of the granule movement by DEM. Simulations were conducted under different conditions, i.e., different carbon content and melting temperature of the granules. Results show that both carbon content and melting temperature of the granule influence the final structure of the sintering bed. The obtained structural change of the sintering bed show that the proposed model is a potential tool to analyse the agglomeration phenomena occurring in the iron ore sintering process under various conditions.

KEY WORDS: iron ore sintering; DEM; simulation; agglomeration; granules; heat transfer; structural change; packed bed.

1. Introduction

Most iron ores are agglomerated through sintering to have appropriate size range and metallurgical properties as a burden of blast furnace for ironmaking. During sintering, structural changes occur in the packed bed of mixed and granulated raw materials to form a porous solid cake permeated by voids. The resulting structure is an important factor that directly affects product yield and properties of sinter, e.g., strength and reducibility, which are required in the blast furnace operation. Such importance have led to many studies to find out experimentally the factors that determine the structural characteristics of the sinter cake. These include the use of X-ray CT scan, which is capable of non-destructive and/or real-time in-situ observations of the structure of sintering bed and sinter cake. This technique provides us significant information on the structural change in the sintering bed such as “snapshots” in time. However, the mechanism and way of control of the structural change are not yet sufficiently understood due to its complex nature.

On the other hand, many numerical simulation studies of iron ore sintering process which consider major reactions and heat transfer have been tried. However, they have not been able to directly take into account the structural changes occurring in the sintering bed. Recently, the authors have proposed a numerical simulation model to study the agglomeration phenomena in the iron ore sintering. The model can directly describe the structural change of the packed bed of granules by using the discrete element method (DEM). However, in this model the heat wave propagation through sintering bed was only simply represented in the simulation by introducing a virtual high temperature zone that uniformly moves downward.

In the actual iron ore sintering, the heat wave propagation is influenced by the various physicochemical and thermal phenomena involved in the process. These include in particular, (i) gas flow across the bed, (ii) gas–granule heat exchange, (iii) drying of the moist granules and the condensation of water at the lower bed, (iv) chemical reactions, e.g., dehydration of combined water, limestone decomposition, carbon combustion, (v) melting and solidification of materials and (vi) the changes in the structure, particularly the variation of void fraction/porosity, which strongly affects the permeability of the bed.

In this study, an improved DEM model for the iron ore sintering has been developed by combining the solution of the mathematical equations to describe the above physicochemical and thermal mechanisms involved in the sintering process. The present paper gives the outline of the model and its results of calculation under different conditions.

2. Outline of the Model

The model is essentially based on the works of Higuchi and Muchi to describe the physicochemical and the thermal mechanisms involved in the sintering process. It utilizes the Ranz equation for heat transfer in packed beds and includes a two stage drying process and rate equations for carbon combustion and limestone decomposition. The used symbols are listed in Table 1 together with the initial values of process parameters and constants.
The change in gas temperature, $T_g$, with respect to bed depth is described by Eq. (1) as a function of the heat exchange between the gas and granules.

$$-\frac{G}{d} \frac{\delta T_g}{\delta z} = A_h h_{fg} (T_g - T_w) + C_{fg} T_g \left( \Delta M_T \rho \nu'_{fg} + \Delta M_T \nu'_{fg} \right)$$

The change in the temperature of the granule, $T_s$, is determined in several stages. First, a two-step drying process was introduced in the early stage of sintering. When the moisture content of the granule is greater than a critical value, $W_c$, all the heat from the gases are used in water vaporization. In this case, $T_s$ will not change:

$$\frac{\delta T_s}{\delta t} = 0 \quad \text{when } W_s > W_c$$

Once the moisture level is lower than the critical value, some of the heat from the gases is transferred to the granule. Then, the change in $T_s$ is given by the equation:

$$\frac{\delta T_s}{\delta t} = -A_{rg} \nu_r \left( \frac{W_w}{W_c} \right)$$

When no moisture remains in the layer of material, the rate of change of $T_s$ is a function of the heat transferred.
from the gases, the heat gained form carbon combustion and the heat loss by limestone decomposition. However, other contributing factors, i.e., fusion and solidification of materials, are present at elevated temperatures. To account for this, the specific heat of the granule is modified by a melting/solidifying function, $f_m$, to allow for the latent heat of fusion and solidification. The equation is given by:

$$\rho_c (C_v-f_m) \frac{dT_d}{dt} = A_i h_p (T_g - T_d) + \Delta H_m n_c r'_c - \Delta H_p f'_p$$

(when $W_s=0$) ........................(4)

The change in oxygen concentration in the gas phase with bed depth is given by:

$$-G\delta C_{O_2}/\delta z = n_{r'_c} \rho_g + c_{O_2} (\Delta M_n n_{r'_c} + \Delta M_p n_{r'_p})$$ .............................(5)

Where the rate of the oxygen concentration change is determined by the reaction rates and the dilution effect of the gases by using an equation of continuity. The change in carbon dioxide concentration in the gas phase is described in a similar manner to Eq. (5) by:

$$-G\delta C_{CO_2}/\delta z = \rho_g (n_{r'_c} + n_{r'_p}) + c_{CO_2} (\Delta M_n n_{r'_c} + \Delta M_p n_{r'_p})$$ .............................(6)

The change in the moisture concentration of the granules is given as a function of the drying rate by the equation:

$$-\delta W'_g/\delta t = 6 r'_s/(\rho_d \bar{d})$$ ..............................(7)

The change in the un-reacted carbon particle size is obtained by:

$$\delta r'_c/\delta t = \Delta M_f (4 \pi r'_c^2)$$ ..............................(8)

Similarly, the un-reacted limestone particle size is given by:

$$\delta r'_c/\delta t = \Delta M_f (4 \pi r'_p^2)$$ ..............................(9)

Other equations used in the calculation are given in the Appendix.

3. Simulation Procedure

The calculation field is a cylindrical configuration similar to a sinter pot (see Fig. 1). The sinter pot was initially filled randomly with both granules and carbon particles assuming coke particles having no ash component. The number of carbon particles depends on the specified carbon contents in the mixture. Carbon content was set at 3.0, 3.5 or 4.0 mass%. The calculation field was divided into equal thin layers along the height direction with a depth, $\Delta z$, equal to the diameter of the granule. A particular granule is regarded to belong to a certain thin bed if the center of its mass is located in that bed. In this manner, the number of granules or number of carbon particles in each bed can be determined. The position of the granules/particles was used in determining various bed parameters such as void fraction and specific surface area (SSA).

The same granule assumed in the previous DEM model for iron ore sintering process was used in the simulation, and volume fraction of fine adhering layer was set at 0.5 (see Fig. 2). Part or the entire adhering layer will melt depending on the temperature profile of the bed. The volume fraction of melt, $M_f$, is given by:

$$M_f = (T_s - T_{m_1})/(T_{m_2} - T_{m_1})$$ ..............................(10)

Where, $T_s$, $T_{m_1}$ and $T_{m_2}$ are the average granule temperature, and initiation and completion temperatures for melting of adhering materials, respectively. $T_{m_1}$ is set at 1 373 K considering inhomogeneity of bed temperature. $T_{m_2}$ is derived from the CaO–Fe₂O₃ phase diagram as shown in Fig. 3. It is corresponding to the liquidus temperature of adhering materials of granule and is varied as indicated by lines a–a’, b–b’ and c–c’ in the figure. These lines are for the composition of 15, 15.5 and 20 mass% CaO and the values of $T_{m_2}$ are 1 478, 1 550 and 1 600 K, respectively. Using the value of $M_f$ calculated by this manner, the diameter of un-melted granule is estimated assuming the melt-formation occurs from the outside of the granule.

Based on the melting state of the granules, the
granule/particle movement is calculated using the DEM model proposed in previous paper. The forces acting on the granules consist of the inter-granular contact forces and the force due to gravity. The component of the inter-granular contact forces will depend on the value of $M_f$ and temperature of granules. When the temperature of granules is below $T_{m1}$, the inter-granular contact forces have only the elastic and damping components. Above $T_{m1}$, bonding force, $H_p$, is considered in the calculation of the inter-granular contact forces. When the temperature of the granules has again cooled down below $T_{m1}$, the position of the granules relative to each other is maintained by applying the average force acting on the granules to each granule.

A flow chart of the simulation procedure is shown in Fig. 4. At the start, the initial values and constants were inputted. Then the bed and gas parameters for each position were evaluated under these conditions. The heat and mass transfer equations were simultaneously integrated by using the Adams–Moulton’s predictor-corrector method. The DEM model was then used to determine movement and change in the position of each granule/particle. The data were saved and the iteration was repeated until the set sintering time elapsed.

4. Results and Discussion
4.1. Effect of Carbon Content on the Temperature Profile of Bed

Figure 5 shows the example of the calculated temperature profile of the sintering bed at different position in the height direction. In this case, gas flow rate was set at 1.3 Nl/s (0.45 Nm/s) during ignition and 2.7 Nl/s (0.95 Nm/s) after ignition. Ignition temperature of the gas was 1 600 K and was reduced to 305 K after ignition. Total ignition time was 90 s. A horizontal dotted line at 1 373 K indicates $T_{m1}$. $T_{m2}$ was 1 550 K, i.e., CaO concentration of adhering materials of the granules was 17.5 mass% (see Fig. 3).

The comparison of the temperature profiles using different carbon content is shown in Fig. 6. The temperatures shown in the figure are calculated at 2.5 cm and 5.5 cm from the bed top. Higher carbon content in the mixture results in higher maximum bed temperature. Also, the duration time above the $T_{m1}$ is longer for higher carbon content. Both the higher maximum bed temperature and longer duration time above the melting temperature leads to a larger melt fraction of granules.

Figure 7 shows the “snapshots” of the structural change of the sinter obtained from the simulation using carbon par-
Particle size of 5 mm and carbon content of 3.5 mass%. The temperature profile across the bed calculated at 340 s is also shown in the figure. It indicates the approximate location and size of the sinter/melt zone. The "snapshots" show a reduction of bed height with progress in sintering time. Less agglomeration of granules occurs at the upper bed compared to the lower bed. Figures 5 and 6 show that the maximum temperature in the lower bed is higher than in the upper bed. This means that under the condition of the present calculation, granules in the lower bed have a higher melt fraction resulting in more extensive agglomeration.

The "snapshots" showing the comparison of the structure of the sintering bed for different levels of carbon content is shown in Fig. 8. These are taken at 340 s. The temperature profiles across the bed and the approximate location of the melt zone are also shown in the figure. Increasing the amount of carbon in the mixture leads to higher maximum bed temperature and thicker melt zone. This combination results in more agglomeration of granules.

4.2. Effect of Completion Temperature of Melting, $T_{m2}$

The comparison of the structural changes of the sintering bed for different $T_{m2}$ of the adhering materials of granules is shown in Fig. 9. The lowering of $T_{m2}$ results in a relatively extensive agglomeration of the granules. Agglomeration of granules in the upper bed is more noticeable at lower $T_{m2}$. An increase in the reduction of the bed height is also observed.
4.3. An Attempt to Characterize the Agglomeration State of Granules

The effect of carbon content and $T_{m2}$ on the change in the structure of the bed is further analyzed by comparing the distribution of the “co-ordination number” of the granules in the bed after sintering simulation. “Co-ordination number” can be calculated with a definition that it gives the average number of granules directly touched to one granule. Therefore, the larger number implies that the denser and probably firmly bound clusters are formed. Figure 10 shows the comparison of the co-ordination number distribution obtained by the calculations with different carbon contents. Increasing carbon content result in the distribution with higher co-ordination number. Higher bed temperature with longer holding time leads to a larger amount of melt formed and more extensive agglomeration of granules. The comparison of the co-ordination number distribution is shown in Fig. 11 which is obtained with different completion temperatures of melting, $T_{m2}$, for the adhering materials of granules. Ratio of granules with higher co-ordination number increases with lowering $T_{m2}$.

It may be worth to relate such structural data obtained from the final structure of sintering bed to the physical properties of actual sinter cake such as product yield and strength. This is an important future subject together with the development of an efficient algorithm to reduce calculation time.

5. Conclusions

A comprehensive simulation model which can directly describes the structural change of the iron ore sintering bed was developed by combining solutions of the gas–granule heat transfer equations with the DEM calculations of granule movement. A sinter pot configuration is used as a calcu-
lation field in the DEM simulation. It was first randomly filled with both granules and carbon particles. Carbon content and completion temperature of melting, $T_m$ (liquidus temperature), for the adhering materials of the granules were varied assuming its chemical components are represented by CaO–Fe$_2$O$_3$ system.

The “snapshots” show a reduction of bed height with progress in sintering time. Less agglomeration of granules occurs at the upper bed compared to the lower bed. Higher carbon content in the mixture and lower completion temperature of melting result in higher maximum bed temperature and longer holding time at high temperature. These lead to a larger melt fraction of the granules and hence extensive agglomeration.

An analysis of the final bed structure was attempted by introducing the co-ordination number of the granules which expresses the average number of granules directly touched to one granule. Increasing carbon content and lowering completion temperature of melting lead to the distribution with higher co-ordination number.

REFERENCES

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Appendix. Supplementary Formulae used in the Calculation

\[ n_c = \frac{V}{(1 - e)/(4 \pi r_c^3/3)} \] ...........................(A-1)
\[ n_m = \frac{V}{(1 - e)/(4 \pi r_m^3/3)} \] ...........................(A-2)
\[ f_m = H_m/(T_m - T_m) \quad \text{(when, } T_m < T_m < T_m) \] ...........................(A-3)
\[ f_m = 0 \quad \text{(when, } T_m > T_m \text{ or } T_m > T_m) \] ...........................(A-4)
\[ \text{Re} = \frac{Gd}{(\mu e)} \] ...........................(A-5)
\[ \text{Sc} = \frac{\mu (p D_{CO_2})}{(p)} \] ...........................(A-6)
\[ \text{Sh} = 2 + 0.7 \text{Re}^{0.5} \text{Sc}^{0.3} \] ...........................(A-7)
\[ \text{Pr} = \frac{C_p \mu}{k_g} \] ...........................(A-8)
\[ \text{Nu} = 2 + 0.7 \text{Re}^{0.5} \text{Pr}^{0.3} \] ...........................(A-9)
\[ h_p = \text{Nu} \frac{k_g}{d_p} \] ...........................(A-10)
\[ k_c = 0.0653 \times 10^7 T_c^{0.5} \exp[-44000/(RT)]^{14} \] ...........................(A-11)
\[ k_c' = (d_p/(Sh D_{CO_2}) + 1/k_c)^{-1} \] ...........................(A-12)
\[ r_c' = 4 \pi r_c^3 k_c' C_{O_2} \] ...........................(A-13)
\[ R_c' = n_c r_c' \] ...........................(A-14)
\[ K_i = \exp(-5211/T + 7.35) \] ...........................(A-15)
\[ k_i = 0.152 \times 10^7 \exp[-40000/(RT)]^{15} \] ...........................(A-16)
\[ k_i' = 1/[(d_p/(Sh D_{CO_2}) + d_p/(d_p - 2r_c)/(2r_c D_p)) + (d_p/2r_c)2K_i/(k_i R_t)] \] ...........................(A-17)
\[ C_{O_2} = K_i/(R_t) \] ...........................(A-18)
\[ r_i' = 4 \pi r_i^3 (C_{O_2} - C_{CO_2}) k_i' \] ...........................(A-19)
\[ R_i' = n_i r_i' \] ...........................(A-20)
\[ r_w' = h_g(T_g - T_s)/H_w \quad \text{(when, } W_s > W_c) \] ...........................(A-21)
\[ r_w' = h_g(T_g - T_s)/(W_s/W_c)/H_w \quad \text{(when, } 0 < W_s < W_c) \] ...........................(A-22)