Simulation of sintering of iron ore bed with variable porosity

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Phoenics User Conference
Melbourne, 2004

Introduction (I)

In steelmaking industry, blast furnace continues to be the major reactor owing its extremely high energy efficiency and productivity. Stable blast furnace operation requires the property control of raw materials charged into the furnace. The major iron-bearing raw materials called burden are composed of sintered iron ores.

Figure 1 presents schematically an iron ore sintering process. In the process, crushed coke and limestone are mixed and granulated with fine blend ore, whereupon the raw mixture is charged as a packed bed on a continuous traveling grate called the sinter strand. A burner hood at the beginning of the sinter strand ignites the coke in the mixture at the surface of the bed. Then, the combustion is self-supporting and provides sufficient heat to cause partial melting/solidifying leading to the agglomeration of the raw materials. To maintain the coke combustion, air is sucked down through the bed by using a series of windboxes mounted underneath the sinter strand. The agglomerated bed called sinter cake is discharged at the end of the sinter strand where it is crushed and screened.

In the sintering process, the particle size of the mixture has been long recognized to have the major influence on the operation stability. Too small granules result in poor bed-permeability and possible destabilizing of flame propagation. Nevertheless, constantly increasing trend towards using lower grade iron ores with very fine particle size has caused the need for improvement in the sintering process performance. Commonly used methods are the use of granulation binder, prolongation of granulation time and so forth. These methods, however, lead to an increase in the production cost, a decrease in the operational efficiency/productivity and often deterioration of sinter quality.
Introduction (II)

The alternative method being developed is based on subdividing the iron ores into two parts, coarser and finer particles. The finer part is preliminary pelletized and then it is calmly mixed with the coarse part to be distributed over the bed as it is shown in Fig. 2. Packed bed prepared in such a way is expected to have a higher permeability and therefore provides more stable operation and good controllability of the sintering process.

The aim of the present study was to develop Phoenics Q1 and Ground codes for the simulation of this new sintering process using pre-granulated pellets, in order to predict the influence of such parameters as pellet size and fraction, void fraction of the packed bed and coke content on the heat propagation process during the sintering process. The developed codes allow transient two-dimensional simulation of the gas flow, heat and mass transfers through the sintering bed of variable void fraction under one-phase mode.
Principle of big pellet aging

Induction bed for combustion/sintering

Control of heat transfer/distribution by permeation and convectional gas flow

Longer time aging by heat transfer from the induction bed

Pregranulation
Charging of raw materials
Design of size and agglomeration
(Parameters should be considered)
† coke/ore properties and ratios
limestone
(Science)
† Flow mechanics, material science
transport phenomena
(Others) Ignition, suction, crushing of sintered cake, screening method
way to use return ore

Computational domain and its physical prototype

Air inlet
Preheated air
External shell:
- ε = 0.4
- d_p = 2 mm
- Fe_2O_3, C
CaCO_3

Spherical pellet:
- ε_0 = 0.25
- R = 2.5 cm
- d_p = 0.5 mm
- Fe_2O_3

Packed bed

O A
Axis
Z

B C
Exhaust gas outlet
The sintering process chemistry

- CaCO\textsubscript{3} = CaO + CO\textsubscript{2}  \quad Q_2 = -1.61 \times 10^6 \text{ J/kg} \\
- C + O\textsubscript{2} = CO\textsubscript{2}  \quad Q_1 = 3.28 \times 10^7 \text{ J/kg} \\
- CaO + Fe\textsubscript{2}O\textsubscript{3} = (CaO \cdot Fe\textsubscript{2}O\textsubscript{3})  \quad Q_3 = -1.37 \times 10^6 \text{ J/kg} \\
- (CaO \cdot Fe\textsubscript{2}O\textsubscript{3}) = CaFe\textsubscript{2}O\textsubscript{4}  \quad Q_4 = 5.07 \times 10^5 \text{ J/kg}

Hematite (Fe\textsubscript{2}O\textsubscript{3}) – 0.82 \\
Carbon (C) – 0.03 \\
Limestone (CaCO\textsubscript{3}) – 0.15

The process related physical phenomena

1. Momentum transfer
2. Two phase heat transfer
   - convection (gas) 
   - diffusion (gas, solid) 
   - radiation (interparticle space) 
   - heat exchange (gas-solid interface) 
   - heat generation (C combustion) 
   - heat absorption (CaCO\textsubscript{3} decomposition, CaO \cdot Fe\textsubscript{2}O\textsubscript{3} melting) 
3. Mass transfer (only gas phase)
   - convection (O\textsubscript{2}, N\textsubscript{2}, CO\textsubscript{2}) 
   - diffusion (O\textsubscript{2}, N\textsubscript{2}, CO\textsubscript{2}) 
   - gas sourcing (CO\textsubscript{2}) and sinking (O\textsubscript{2})
The model variables and parameters

**Solved variables**
- Pressure, $P_1$
- Velocity, $V_1, W_1$
- Gas temperature, $T_{EM1}$
- $O_2$ mass fraction in gas, $Y_{O2}$
- $CO_2$ mass fraction in gas, $Y_{CO2}$
- $N_2$ mass fraction in gas, $Y_{N2}$
- Solid enthalpy, $SOLH$

**Parameters**
- Solid temperature, $SOLT$
- Carbon mass fraction, $MFC$
- Hematite mass fraction, $MFH$
- Limestone mass fraction, $MFL$
- Calcia mass fraction, $MFA$
- Melted phase mass fraction, $MFM$
- Solidified phase mass fraction, $MFS$
- Reaction heat effects

**Mass fraction and temperature dependent properties**
- Gas
  - density
  - viscosity
  - heat capacity
  - thermal conductivity
  - $O_2$ diffusivity
- Solid
  - density
  - heat capacity
  - thermal conductivity
  - porosity

**Setting method**
- Inform
- Group 19. Finish of iz slab
- Group 19. Finish of time step
- Group 9

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Kinetics of graphite combustion

\[
C + O_2 = CO_2
\]

\[
r_c = \rho_g Y_{O2} A_{p,c} k_{ov}
\]

Combustion rate

\[
A_{p,c} = \frac{6(1-\varepsilon)}{d_c} Y_c
\]

Specific area

\[
k_{ov} = \frac{1}{\frac{1}{k_r} + \frac{1}{k_m}}
\]

Overall rate coefficient

\[
k_r = k_0 T_s^{0.5} \exp \left( -\frac{E_a}{RT_s} \right)
\]

Chemical reaction rate coefficient

\[
k_m = Sh \frac{D_{O2}}{d_c}
\]

Mass transfer rate coefficient
Sherwood and Nusselt numbers for sphere

\[ Sh = \frac{k \cdot d}{D_{02}} = 2.0 + 0.6 \left( \frac{U_e \cdot d_e}{v_g} \right)^{1/2} \left( \frac{v_g}{D_{02}} \right)^{1/2} \]

\[ Nu = \frac{h \cdot d_e}{\lambda} = 2.0 + 0.6 \left( \frac{U_e \cdot d_e}{v_g} \right)^{1/2} \left( \frac{v_g}{\lambda} \right)^{1/2} \]

\[ U_\infty = \left( V C_1^2 + W C_1^2 \right)^{0.5} \]

Kinetics of the other reactions

**Assumptions**
- The reaction rates are controlled by heat supply (1,2) or removal (3)
- The reactions proceed within a temperature interval \( \Delta T \) around the corresponding thermodynamic temperature \( T_d \)

\[ \Delta T = 10 \]  
\[ T_d = 1123 \text{ K} \]

**Example for reaction (1)**

\[ f_1(T) = 1 - \frac{1}{1 + e^{\frac{T - T_d}{\Delta T}}} \]

\[ r_l = f_1(T) \left( \frac{dH}{dt} + \rho c_p (1 - e) Y_{CaCO_3} + Q_c r_c \right) \]

\( f_l \) – function of kinetic factor
\( r_l \) – reaction rate
\( Q_l \) – reaction heat
\( Q_c \) – graphite combustion heat
\( r_c \) – graphite combustion rate
Initial porosity

Wall effect

Mathematical formulation

Zone $B: \varepsilon = \varepsilon_{0,B} = 0.25$
Zone $A: \varepsilon = \varepsilon_{0,A} = 0.4$

Transition zone:

$$\varepsilon = \frac{(0.9 - \varepsilon_{0,A}) R_B + \delta - r_B + \varepsilon_{0,A}}{\delta}$$

Equation of motion

$$\frac{\partial}{\partial t} \left( \rho_g \phi_g \right) + \frac{\partial}{\partial x_k} \left( \rho_g U \phi_g - \Gamma_{\phi,g} \frac{\partial \phi_g}{\partial x_k} \right) = S_{\phi,g}$$

where $\phi_g = U; \Gamma_{\phi,g} = \rho_g v_g; U = VC1, WC1$

$$S_{\phi,g} = \frac{150 \mu_g U (1 - \varepsilon)^2}{d_p^2} + \frac{1.75 \rho_g U^2 (1 - \varepsilon)}{\varepsilon}$$

Ergun equation

$d_p$ - particle diameter
$\varepsilon$ - void fraction (porosity)
$\mu_g$ - gas viscosity
$\rho_g$ - gas density

Group 13. Boundary & Special Sources

PATCH (ERGUN , PHASEM, 0.0, 0.0, 0.0, 0.0, 1.0, 200)
COVAL (ERGUN , WC1 , GRND1 , 0.0)
COVAL (ERGUN , VC1 , GRND1 , 0.0)
Equations of continuity and mass conservation

\[
\frac{\partial (\rho_g \overline{U})}{\partial x} = S_{1,g}; \quad \frac{\partial (\rho_g Y_i)}{\partial t} + \frac{\partial (\rho_g \overline{U} Y_i - \Gamma_{0,g} \frac{\partial Y_i}{\partial x_k})}{\partial x_k} = S_{Y_i,g} \\
\]

(i = CO₂, O₂, N₂)

\[
S_{Y_{CO₂,g}} = \frac{r_c}{\varepsilon} \frac{M_{CO₂}}{M_c} + \frac{r_l}{\varepsilon} \frac{M_{CO₂}}{M_{CaCO₃}} \\
S_{Y_{O₂,g}} = -\frac{r_c}{\varepsilon} \frac{M_{O₂}}{M_c}; \quad S_{Y_{N₂,g}} = 0 \\
S_{1,g} = S_{Y_{CO₂,g}} - S_{Y_{O₂,g}}
\]

Equation of energy conservation (gas phase)

\[
\frac{\partial}{\partial t} (\rho_g C_{p,g} T_g) + \frac{\partial}{\partial x_k} \left( \rho_g \overline{U} C_{p,g} T_g - \Gamma_{T,g} \frac{\partial (C_{p,g} T_g)}{\partial x_k} \right) = S_{ex} + (1 - \gamma) S_c
\]

Concept of C combustion

\[
C + O₂ = CO₂ \quad \text{CaCO₃} = CaO + CO₂
\]

\[
q1 \quad \text{PATCH (REACA ,FREEVL,.3,.0,.0,.0,.0,.0,.1,.2)} \quad \text{COVAL (REACA ,P1 , FIXFLU , GRND3 )} \quad \text{COVAL (REACA ,YCO₂ , 0.0, GRND3 )} \quad \text{COVAL (REACA ,YO₂ , 0.0, GRND3 )}
\]

Gas-particle heat exchange rate

\[
S_{ex} = \frac{Nu \lambda_g}{d_h} A_p (T_s - T_g) \\
\Gamma_{T,g} = \frac{\lambda_g (T_s)}{C_{p,g}(T_g)} A_p = \frac{6(1 - \varepsilon)}{d_h}
\]

\[Nu - \text{Nusselt number, } \lambda_g - \text{gas thermal conductivity, } d_h - \text{hematite particle diameter, } T_s - \text{solid temperature, } T_g - \text{gas temperature, } A_p - \text{specific gas-particle area, } C_{p,g} - \text{gas heat capacity, } Q_c - \text{graphite combustion heat, } r_c - \text{rate of graphite combustion}\]
Equation of energy conservation (solid phase)

\[
\frac{\partial}{\partial t}(\rho H_s) - \frac{\partial}{\partial x_k} \left( \Gamma_{H,s} \frac{\partial H_s}{\partial x_k} \right) = \ldots = - \frac{\partial}{\partial x_k} \left( \Gamma_{H,s} \frac{\partial H_s}{\partial x_k} \right) = S_{ex} + S_{t,s} + \gamma S_b + S_o
\]

\[S_{t,s} = \frac{(1-\varepsilon)\rho_s}{\Delta t} (H_{x,old} - H_s)\]

\[\Gamma_{H,s} = \frac{\lambda_{eff}(T_s, Y_s)}{C_{p,s}(T_s, Y_s)}\]

\[\lambda_{eff} = \lambda_C Y_C + \lambda_{CaCO_3} Y_{CaCO_3} + \lambda_{CaO} Y_{CaO} + \lambda_{Fe_2O_3} Y_{Fe_2O_3} + \lambda_{Rad}\]

\[\lambda_{Rad} \text{ - radiative conductivity according to Rosseland diffusion model}\]

\[\lambda_{Rad} = \frac{16}{3} \sigma T_s^3 / \sigma_s; \quad \sigma_s = \frac{3}{2} \frac{(1-\varepsilon)}{d_h} \eta; \quad T_s = \frac{H_s}{C_{p,s}}\]

\[\sigma \text{- Stephan-Boltzmann constant (=5.67x10}^{-8}\text{), } \sigma_s \text{- scattering coefficient}\]

\[\eta \text{- the reflectivity coefficient (=0.5), } T_s \text{ - solid temperature}\]

Equation of energy conservation (solid phase)

\[-\frac{\partial}{\partial x_k} \left( \Gamma_{H,s} \frac{\partial H_s}{\partial x_k} \right) = S_{ex} + S_{t,s} + \gamma S_b + S_o\]

\[S_{H,ex} = \frac{Nu\lambda_s A_p (T_g - T_s)}{d_h}\]

\[S_o = -Q_i r_i - Q_m r_m + Q_f r_s\]

\[Q_i \text{ and } r_i \text{ are heat effect and rate of appropriate reactions}\]

\[l \text{ - } CaCO_3=CaO+CO_2\]

\[m \text{ - } CaO+Fe_2O_3=(CaO·Fe_2O_3)\]

\[f,s \text{ - } (CaO·Fe_2O_3)=CaFe_2O_4\]
Boundary and initial conditions

**Initial chemical composition and porosity**

<table>
<thead>
<tr>
<th>Zone</th>
<th>Fe$_2$O$_3$</th>
<th>C</th>
<th>CaCO$_3$</th>
<th>Porosity</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.82</td>
<td>0.03</td>
<td>0.15</td>
<td>0.40</td>
</tr>
<tr>
<td>B</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.25</td>
</tr>
</tbody>
</table>

**Air velocity at inlet**

$W_1$ is defined from condition $\rho_g \times W_1 = \text{const} (1.2)$

$V_1 = 0$

**Initial temperature**

$T_g = T_i = 25^\circ C$

**Air temperature at inlet**

Setting of solver options

- **Grid type**: BFC 20x48
- **Time dependence**: unsteady 1s $\times$ 600 step = 600 s
- **Flow**: laminar
- **One-phase mode (ONEPHS=T)**
- **Total number of iteration**: 100
- **Global convergence criteria**: 0.5%
- **Equation formulation**: Elliptic GCV
- **Differencing schemes**: Hybrid
Example of calculated results. Velocity vector

\begin{align*}
  t &= 90 \text{ s} \\
  180 \text{ s} \\
  330 \text{ s}
\end{align*}

Example of calculated results. Solid phase temperature

\begin{align*}
  t &= 90 \text{ s} \\
  180 \text{ s} \\
  330 \text{ s}
\end{align*}
Example of calculated results. Graphite concentration

t = 90 s    180 s    330 s

Example of calculated results. Heat generation

t = 90 s    180 s    330 s
Example of calculated results. Lime concentration

\[ t = 90 \text{ s} \quad 180 \text{ s} \quad 330 \text{ s} \]

Example of calculated results. Melted phase concentration

\[ t = 90 \text{ s} \quad 180 \text{ s} \quad 330 \text{ s} \]
Example of calculated results. Solid phase concentration

\[ t = 90 \text{ s} \quad 180 \text{ s} \quad 330 \text{ s} \]

Example of calculated results. Porosity

\[ t = 90 \text{ s} \quad 180 \text{ s} \quad 330 \text{ s} \]
Conclusions

- Phoenics code has been applied to the problem of iron ore sintering process which includes coke ignition and flame front propagation through the sintering bed.

- It is shown that Phoenics can be used to simulate transient two-phase problems under one-phase setting option.

- Ground coding allows to simulate gas flow, heat and mass transfer through bed of variable porosity.

- The predicted results seem to be realistic but the model needs to be validated against experimental data.