The efficiency of a blast furnace ironmaking operation is largely dependent on the physical and chemical properties of the iron ore and coke. The reducibility of iron ore and the reactivity of coke are key parameters that affect the blast furnace coke rate. To reduce the coke rate via pulverized coal injection (PCI) and natural gas injection additions, it is important to understand the behavior of the burden materials inside the furnace in order to further reduce the coke rate while maintaining process stability — particularly as the rates of the injected fuels reach very high levels.\textsuperscript{1,2} It is well understood that a significant portion of the coke rate is attributed to the coke solution loss reactions that occur in the shaft region of a blast furnace where the iron ore and coke undergo gas-solid reactions. The solution loss is characterized as the degree of direct reduction from the coupling reaction of FeO reduction and coke gasification, while the reaction kinetics are dependent on the iron ore and coke interaction that affects the gas flow, thermal condition and overall efficiency of the blast furnace operation. Burden distribution and tuyere practices also affect coke reactivity, but are not considered here.

Increasing the reducibility of iron ore will decrease the overall coke rate due to the iron ore having a higher degree of reduction in the upper shaft and before reaching the higher temperature region below, where coke gasification from direct reduction is favored.\textsuperscript{3} As the iron ore is transformed in a stepwise fashion from Fe\textsubscript{2}O\textsubscript{3} to Fe\textsubscript{3}O\textsubscript{4} to FeO and then to Fe in the blast furnace, the effects of each stepwise reaction rate have not been sufficiently investigated.

There are two schools of thought regarding the optimization of coke reactivity for a blast furnace operation. Low-reactivity coke is normally preferred for the blast furnace, as coke with less reactivity will possess higher strength after reaction, thus resulting in better bed permeability and less solution loss in the shaft. However, a number of researchers suggest that high-reactivity coke could lower the thermal reserve zone temperature.\textsuperscript{4,5} With a lower thermal reserve zone temperature, the equilibrium point of FeO to Fe reduction will shift lower down in the shaft region and allow for more indirect reaction to take place. It is also reported that there are benefits from having a combination of coke with high reactivity and sinter ore with high reducibility.\textsuperscript{5}

**CFD Model**

**Blast Furnace Shaft CFD Model**

The blast furnace shaft simulator that was developed in this paper, a computational fluid dynamics (CFD) model is employed to investigate changes in ore and coke reaction rates in the shaft region of a blast furnace. The CFD analysis shows that a specified combination of the reaction rates of ore and coke significantly affects the solution loss reaction of the coke in the shaft region. The effects of each individual reaction rate, as well as the combination of reaction rates, are studied.
previously is used in this study to conduct the simulation. The chemical reactions listed in Table 1 are considered in the model. R1–R8 are gas-solid reactions. R9 is the decomposition of the carbonate fluxes that generate CO2 gas. R10 and R11 are the homogeneous gas reaction and the direct reduction of liquid FeO below the CZ lower boundary, respectively.

Iron Ore Reduction Model — The one-interface, unreacted, shrinking-core (URC) model is used to model the reduction of the iron ore. The complex process of iron ore reduction has been simplified to three rate control processes — gas film resistance, diffusion resistance through the reduced iron shell and intrinsic chemical reaction resistance at the metal-oxide interface. The expression for the reaction rate for one ore particle is shown in Equation 1.

\[
R_i = \frac{4\pi r_0^2}{s} \left( \frac{C_A}{K_{s,i}} + \frac{C_B}{K_{s,i}} \right) \frac{K_{s,i}}{1 + K_{s,i}} \left( \frac{mol \, CO}{s} \right), \quad i = 1 - 6
\]

(Eq. 1)

The gas film resistance is \( F = \frac{1}{\beta_A} \left( \frac{s}{m} \right) \).

The diffusion resistance is \( B_i = \frac{r_0}{D_s} \left[ (1 - f_i) \frac{r_0}{D_s} - 1 \right] \left( \frac{s}{m} \right) \).

The intrinsic chemical reaction resistance is \( A_i = \frac{1}{K_{s,i}} \left( \frac{1}{1 + K_{s,i}} \right) \left( \frac{s}{m} \right) \).

The fraction of reduction is defined as \( f_i = \frac{weight \, of \, oxygen \, removed \, from \, iron \, oxide}{weight \, of \, removable \, oxygen} \).

\( r_0 \) is the radius of the iron ore.

The effective diffusivity is expressed as \( D_{ei} = D_e \frac{\varepsilon_{ei}}{\tau} \).

The porosity for different layers is \( \varepsilon_{HM} = 0.008 + 0.992 \varepsilon_0, \varepsilon_{MW} = 0.122 + 0.878 \varepsilon_0 \) and \( \varepsilon_{WF} = 0.435 + 0.565 \varepsilon_0 \).

\( \varepsilon_0 \) is the original ore porosity before reaction.

\( \tau \) is the tortuosity which is estimated as 2.8.

\( K_{s,i} \) are the equilibrium constants.

The kinetic constant of each individual reduction step is \( k_i = k_s \exp \left( -\frac{E_i}{RT_i} \right) \).

The values of the frequency factors and activation energies for the six reductions are adopted from the literature.

Coke Reaction Model — Blast furnace coke undergoes two main reactions (R7 and R8) in the shaft. The gas diffuses through the porous coke, while the reaction takes place in the coke void zone instead of at a sharp interface. It is assumed that the reaction is first-order and irreversible. The kinetic diffusion model adopted from literature is used to determine the extent of the chemical reaction at the internal surface of the lump coke. The gas film resistance is determined using the modified effectiveness factor. The expression for the reaction rate for a single coke particle is shown in Equation 2.

### Table 1

<table>
<thead>
<tr>
<th>Reaction</th>
<th>No.</th>
<th>Chemical equation</th>
<th>Rate</th>
<th>Activation energy, kcal/mol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Indirect reduction of iron oxide by carbon monoxide</td>
<td>R1</td>
<td>(3Fe_2O_3(s) + CO(g) \rightarrow 2Fe_3O_4(s) + CO_2(g))</td>
<td>(R_{1})</td>
<td>27.2</td>
</tr>
<tr>
<td></td>
<td>R2</td>
<td>(Fe_3O_4(s) + CO(g) \rightarrow 3FeO(s) + CO_2(g))</td>
<td>(R_{2})</td>
<td>17.6</td>
</tr>
<tr>
<td></td>
<td>R3</td>
<td>(FeO(s) + CO(g) \rightarrow Fe(s) + CO_2(g))</td>
<td>(R_{3})</td>
<td>16.6</td>
</tr>
<tr>
<td>Indirect reduction of iron oxide by hydrogen</td>
<td>R4</td>
<td>(3Fe_2O_3(s) + H_2(g) \rightarrow 2Fe_3O_4(s) + H_2O(g))</td>
<td>(R_{4})</td>
<td>22.0</td>
</tr>
<tr>
<td></td>
<td>R5</td>
<td>(Fe_3O_4(s) + H_2(g) \rightarrow 3FeO(s) + H_2O(g))</td>
<td>(R_{5})</td>
<td>17.0</td>
</tr>
<tr>
<td></td>
<td>R6</td>
<td>(FeO(s) + H_2(g) \rightarrow Fe(s) + H_2O(g))</td>
<td>(R_{6})</td>
<td>15.2</td>
</tr>
<tr>
<td>Boudouard reaction</td>
<td>R7</td>
<td>(C(s) + CO_2(g) \rightarrow 2CO(g))</td>
<td>(R_{7})</td>
<td>56.9</td>
</tr>
<tr>
<td>Water gas reaction</td>
<td>R8</td>
<td>(C(s) + H_2O(g) \rightarrow CO + H_2(g))</td>
<td>(R_{8})</td>
<td>52.4</td>
</tr>
<tr>
<td>Flux decomposition</td>
<td>R9</td>
<td>(MeCO_3(s) \rightarrow MeO(s) + CO_2(g)), Me = Ca, Mg</td>
<td>(R_{9})</td>
<td>33.6</td>
</tr>
<tr>
<td>Water gas shift reaction</td>
<td>R10</td>
<td>(H_2(g) + CO_2(g) \rightarrow H_2O(g) + CO(g))</td>
<td>(R_{10})</td>
<td>—</td>
</tr>
<tr>
<td>Direct reduction of liquid FeO</td>
<td>R11</td>
<td>(C(s) + FeO(l) \rightarrow Fe(l) + CO(g))</td>
<td>(R_{11})</td>
<td>—</td>
</tr>
</tbody>
</table>
The intrinsic chemical reaction rate is defined as

\[ R_i = \frac{4}{3} \pi r_p^3 \rho_p \eta_i A \left( \frac{kg\ C}{s} \right), \quad i = 7, 8 \]  
(Eq. 2)

The intrinsic chemical reaction rate is defined as

\[ A = \rho_p A_k \frac{RT}{M_r} \]

\( \rho_p \) is the apparent density of the coke.

\( A_g \) defines the specific internal surface area of a coke particle that is assumed constant during reaction.

\( M_r \) is the molecular weight of the reactant gases (carbon dioxide for R7 and water vapor for R8).

The diffusion rate is expressed as \( B = \frac{D_e}{r_p} \cdot r_p \).

\( r_p \) is the radius of the coke particle.

\( D_e \) is the effective diffusion coefficient in the coke pores.

The Thiele modulus is defined as

\[ \Phi = \frac{A_{\text{reaction rate}}}{A_{\text{internal diffusion rate}}} = \sqrt{\frac{A}{B}}. \]

The effectiveness factor without the gas film mass transfer is defined as

\[ \eta = \frac{1}{\sqrt{\tanh(\Phi) - 1}} \]

The modified effectiveness factor, taking the gas film resistance into consideration, is expressed as

\[ \eta = \frac{1}{\sqrt{\frac{1}{\tanh(\Phi)} - 1}} \cdot \frac{1}{Bi} \]  
when \( \Phi \leq 100 \), \( \eta = \frac{1}{\Phi} \) when \( \Phi > 100 \).  

\( Bi \) is the mass transfer Biot number.

The effects of CO on intrinsic chemical reaction constants are considered as \( k_i = \frac{k_{CO}}{1 + k_{CO} P_{CO}} \) for R7. \(^{11}\)

The effect of \( H_2 \) on \( k_8 \) is neglected \(^{12}\) and \( k_8 = k_{H_2O} \) for R8. The reaction rate of coke is set to zero when the temperature of the coke is less than 700°C.

Other Reactions — The flux decomposition reaction R9 is greatly dependent on the decomposition pressure. The unreacted core model is also applied to the flux decomposition reaction. The water gas shift reaction R10 is assumed to reach equilibrium above 1,273 K.\(^{13}\) Above the CZ lower boundary, the direct reduction of solid FeO, \( \text{C(s)} + \text{FeO(s)} \rightarrow \text{Fe(s)} + \text{CO} \) takes place in two steps,\(^{14}\) via R3 and then R7 or R6, and then R8. Therefore, the direct reduction of solid FeO is not modeled but implicitly included through the gas solid reactions R3, R7, R6 and R8. Below the CZ lower boundary, where the reactivity of the hot coke increases dramatically, no CO\(_2\) or H\(_2\)O exists,\(^{15}\) and R11 is assumed to take place.

Baseline case results: gas streamline (a), CO\(_2\)/\((\text{CO}+\text{CO}_2)\) (b) and ore reduction degree (c).
The blast furnace has a working volume of 2,081 m³. The ore layers inside the CZ possess much lower voids W/(m²·K) to match the total heat loss from the furnace shell. The bosh gas temperature is assumed at 2,300 K for all cases. The gas streamlines in Figure 1a illustrate the zigzag flow pattern that is caused from the difference in the voids of the coke and ore layers. The ore layers inside the CZ possess much lower voids due to the fusion of the iron ore burden, making it virtually impermeable, thus forcing the ascending gas to pass through the coke slits between the ore layers. Figure 1b shows the CO gas utilization (ηCO) superimposed with the isothermal line of ore temperature. The ηCO starts to increase from zero in the CZ ore layer as the coke solution loss takes place in the coke layer in CZ, thus reducing ηCO to a low level again. The degree of reduction is superimposed with the ore isothermal lines, as shown in Figure 1c. Coke-only burden is assumed in the center chimney of the furnace, so there is no degree of reduction at this location. The simulation results match the measured top gas composition within 5% and top gas temperature within 10%. Upon validation, parametric cases focusing on the effects of ore reducibility and coke reactivity were considered.

**Results and Discussion**

**Baseline Case** — Actual operating blast furnace conditions were selected to conduct the CFD simulation. The blast furnace has a working volume of 2,081 m³, productivity of 4,989 MTHM, 1 atm top pressure, 65 kg/MTHM pulverized coal injection rate and a natural gas injection rate of 52.1 Nm³/MTHM. The heat transfer coefficient for wall heat loss is set to 150 W/(m²·K) to match the total heat loss from the furnace shell. The bosh gas temperature is assumed at 2,300 K for all cases. The gas streamlines in Figure 1a illustrate the zigzag flow pattern that is caused from the difference in the voids of the coke and ore layers. The ore layers inside the CZ possess much lower voids due to the fusion of the iron ore burden, making it virtually impermeable, thus forcing the ascending gas to pass through the coke slits between the ore layers. Figure 1b shows the CO gas utilization (ηCO) superimposed with the isothermal line of ore temperature. The ηCO starts to increase from zero in the CZ ore layer as the coke solution loss takes place in the coke layer in CZ, thus reducing ηCO to a low level again. The degree of reduction is superimposed with the ore isothermal lines, as shown in Figure 1c. Coke-only burden is assumed in the center chimney of the furnace, so there is no degree of reduction at this location. The simulation results match the measured top gas composition within 5% and top gas temperature within 10%. Upon validation, parametric cases focusing on the effects of ore reducibility and coke reactivity were considered.

**Effects of Ore Reaction Rates** — To simplify the complicated factors that impact the reducibility of iron ore and reactivity of coke, a constant scaling value known as the reaction rate factor $\alpha$ is applied to modify the overall reaction rate ($R_i' = \alpha R_i$). In reality, ore with varying reducibility and coke with varying reactivity may vary the parameters of the Arrhenius equation, porosity, effective diffusivity, etc. Those variations should be taken into consideration for a more accurate description of the behavior of ore and coke with varying reactivity. In this paper, the simplification has been made to apply the reaction rate factor to represent a relative change of the reactivity of ore and coke. For the baseline case, $\alpha = 1$ is assumed for all the reactions.

In Figure 2, the scaling of the rate is transformed to the equivalent temperature from the Arrhenius equation using the activation energy provided in Table 1. The relative rate is obtained by normalizing to the rate at 1,223 K (950°C), which is the ISO standard industry experiment temperature for testing ore reducibility. Figure 2 provides assessments to map the magnitude of the effects of the reaction rate factor on coke reaction with CO do not affect overall coke rate significantly. The effects of the reactivity of each stepwise reaction are studied from case groups A4–A6. The
reaction rate of Fe$_2$O$_3$ to Fe$_3$O$_4$ has minor effects on the coke consumption. However, the reaction rates of Fe$_3$O$_4$ to FeO, as well as FeO to Fe (indirect reaction), noticeably affect the coke rate. The early generation and rapid indirect reduction of FeO are key for lowering the amount of direct reduction of FeO. All the iron ore reactions are scaled in case group A7, which reflect the overall ore reducibility. The top gas CO utilization $\eta_{\text{CO}}$ reduces as the reducibility of the ore decreases. The top gas temperature and H$_2$ utilization $\eta_{\text{H}_2}$ remain almost constant in those cases.

The effect of overall ore reducibility on the coke rate is shown in Figure 4a. As the ore reducibility increases, the coke rate decreases slightly. Decreasing the reducibility leads to very high coke rate due to the increase in direct reduction. Figure 4b shows that the top gas CO utilization changes correspondingly with the ore reducibility. However, the H$_2$ utilization increases from the low reducibility case to about 50% at the baseline case level. The H$_2$ utilization does not improve with further increases in ore reducibility.

Figure 5a shows the iso-reduction degree lines of two cases in case group A7. In the higher ore reducibility case ($\alpha = 2$), the reduction degree is higher in the middle section of the shaft, indicating that the generation of FeO from Fe$_3$O$_4$ is accelerated. The acceleration improves the final reduction stage of FeO to Fe and reduces the direct reduction. The corresponding solution loss of case group A7 is given in Figure 5b. The total coke consumed in the shaft region is defined by reactions R7, R8 and R11. The solution loss has been divided into two parts according to the regions where the reactions are taking place, i.e., above CZ lower boundary (R7 and R8) and below CZ lower boundary (R11). The solution loss above the CZ lower boundary decreases slightly as the ore becomes less reactive due to the driving force of the product gases CO$_2$ and H$_2$O from the ore reduction weakening in the high-temperature region. Consequently, a large amount of FeO is reduced by R11 below the CZ lower boundary, and the net solution loss increases.

Effects of Coke Reaction Rates — Coke reactivity plays an important role in blast furnace efficiency. The coke is consumed from three reactions (R7, R8 and R11) in the blast furnace shaft. All of the unreduced FeO below the CZ lower boundary will react with coke. Therefore, the solution loss below the CZ lower boundary is determined from the amount of unreduced FeO instead of the reactivity of coke. However, the reactivity of coke largely affects the coke consumed above the CZ lower boundary. The same reaction rate factor was applied to reflect the
coke with varying reactivity. Similarly, the equivalent temperature of the relative reaction rate is plotted in Figure 6. The reference temperature for the coke reactivity index (CRI) is carried out at 1,373 K (1,100°C) as per ASTM procedure.\textsuperscript{18}

Figure 7a shows the effects of individual coke reaction with CO\textsubscript{2} and H\textsubscript{2}O. The coke rate is more sensitive to the reactivity with H\textsubscript{2}O. Due to the high-temperature region, FeO is more reactive with H\textsubscript{2} than CO. Increasing the coke reactivity enhances the direct reduction of solid FeO via the path of R6 and then R8. The effects of the overall coke reactivity on the top gas utilization are shown in Figure 7b. A larger drop in H\textsubscript{2} utilization is observed compared to the CO utilization when the coke reactivity is high.

From Figure 7a, it is noted that when coke reactivity decreases, the coke rate remains nearly constant. Figure 8 shows each portion of the solution loss for varying coke reactivity. The solution loss above CZ is significantly reduced as the coke becomes less reactive. However, the amount of coke consumed below the CZ increases due to the unreacted FeO, resulting in no significant change in the total amount of solution loss. When the coke reactivity is high, the solution loss below CZ approaches a minimal point. The solution loss above CZ, however, increases steadily, which will lead to an increase in the net solution loss.

For case group B3, the effects of coke reactivity on CZ location and shape are shown in Figure 9a. The position of the CZ is lower and the CZ becomes thinner as the coke reactivity increases. The CFD model does not take coke strength into consideration. As a result, a lower overall pressure drop is observed in the high-reactivity-coke case, which could allow for more wind flow in the blast furnace, thereby increasing productivity. The reason for CZ is explained as follows. Coke reactions R7, R8 and R11 are highly endothermic. In the low-reactivity-coke case, the heat of the gas is absorbed by R11 below the CZ lower boundary. The bosh gas has already lost energy due to the endothermic reaction R11 before it makes contact with the solid burden, leading to a lower melting rate of the solid burden. However, the hot gas retains most of its energy when it is in contact with the solid burden for the high-reactivity-coke case. The resultant CZ is much thinner than in the low-reactivity-coke case. Figure 9b shows the ore iso-temperature line for three cases with varying coke reactivity. Figure 9c shows the
average iron ore temperature along the height of the blast furnace shaft. The average ore temperature in the lump zone (dry zone) is decreased when the reactivity of coke is high. However, the coke rate does not decrease for this specific operating condition. The reason is that as the temperature of the lump zone is lower, the reaction is kinetically slow, even though the reaction R3 is thermodynamically favorable. The distribution of the degree of reduction is shown in Figure 9d. The reduction of iron ore slows down when the lump zone temperature decreases. In order to achieve a low coke rate from highly reactive coke, it may be necessary to increase the reducibility of the iron ore at low temperature. A low coke rate operation from using low-reactivity coke has also been reported in the literature.19,20

Combined Effects of Ore and Coke Reaction Rates — As mentioned earlier, solution loss is determined from the combined effects of coke reactivity and ore reducibility. Case groups C1–C3 examine the combined effects. As shown in Figure 10, the coke rate is more sensitive to coke reactivity when the ore reducibility is poor. As the ore reducibility increases, the coke rate is kept at a near-constant value. Therefore, it is essential to maintain the coke less reactive when the ore reducibility is low.

Summary

The effects of iron ore reducibility and coke reactivity on the blast furnace operation have been numerically investigated using a CFD model. The effects of each individual reaction rate, as well as the combination of reaction rates, have been studied. The reaction rate of ore and coke is scaled by a constant factor to vary the reducibility and reactivity. The findings for the specified blast furnace operation are summarized as follows:

- The early generation and rapid indirect reduction of FeO are the key for lowering the amount of direct reduction of FeO.
- The position of the CZ is lower in the shaft region, and the thickness of CZ becomes thinner as the coke reactivity increases.
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