

# Promotion of CO Oxidization and Inhibition of NO Formation by Gaseous Iron Species during High-Temperature Off-Gas Combustion

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**ABSTRACT:** The promotion of CO oxidization and inhibition of NO formation by gaseous iron species were analyzed using the Sandia SENKIN program. It is shown that the relative ratio of CO oxidization dramatically varies with combustion time at early burning stage in the presence of iron species, and all peak values are greater than 2.4. The relative ratio of CO oxidization decreases with the increase of air stoichiometric ratio and CO concentration in off-gas. The circulation reactions of Fe–FeO/FeO<sub>2</sub>–Fe achieve the catalytic effect on CO oxidization. Gaseous iron species can greatly inhibit NO formation, NO reduction ratio can reach above 70% at  $T = 2073$  and  $2273$  K, and gaseous iron species can effectively inhibit NO formation when combustion temperature is not higher than  $2273$  K during the off-gas combustion. There are O<sub>2</sub> competitive reactions between thermal NO formation and Fe oxidization, and high chemical activity of iron species inhibits thermal-NO formation.

## 1. INTRODUCTION

A large amount of high-temperature off-gas is produced during oxygen converter steelmaking, the major compositions of off-gas are CO and CO<sub>2</sub>, CO concentration varies from 15 to 70%, and off-gas temperature can reach 1900 K.<sup>1</sup> In the meantime, off-gas entrains a large amount of fine dusts (Fe, FeO, Fe<sub>2</sub>O<sub>3</sub>, etc.) and the amount of the dusts entrained by off-gas is about 80–150 g/m<sup>3</sup>.<sup>2</sup>

The high-temperature off-gas is a precious valuable fuel. It is often discharged into the cooling stack to be combusted, and the peak temperature of flame can reach above 2000 °C where CO<sub>2</sub> may decompose and NO<sub>x</sub> is significantly formed.<sup>3</sup> CO emission concentration can reach above 2000 mg/m<sup>3</sup> which is always over emission standards (300 mg/m<sup>3</sup> in China).<sup>4,5</sup> CO is a toxic gas which is dangerous to human health. High CO emission results in not only atmospheric pollutant but also fuel loss. NO<sub>x</sub> is a known precursor to the formation of ozone and acid rain, and it can react with volatile organic compounds to form photochemical smog.<sup>6</sup>

Iron oxide catalyst is widely used either as single metal oxide or as a mixed oxide in industrial processes, and iron oxide exhibits intermediate activity in the complete oxidation of methane and carbon monoxide.<sup>7–9</sup> NO reduction by iron species has been studied in fluidized bed, and the results indicate that iron or its oxides cause a chemical reduction of NO in the presence of CO.<sup>10</sup> It has been discovered that injection of iron-containing compounds into the combustion and reburning zones of conventional gas- and coal-fired combustors can increase the efficiency of NO<sub>x</sub> reduction by up to 20% in comparison with that which can be achieved by basic reburning.<sup>11</sup>

During the combustion of high-temperature off-gas entraining a large amount of dust containing iron and iron oxides, gaseous iron species is present at  $T > 2073$  K, and it has effects on CO oxidization and NO formation. A detailed chemical kinetic mechanism for gaseous iron-species inhibition of flames, iron pentacarbonyl (Fe(CO)<sub>5</sub>) mechanism, has been introduced,<sup>12</sup> and modeling with the mechanism supports the premise that the inhibition is primarily a gas-phase phenomena. Many researchers

used the Fe(CO)<sub>5</sub> mechanism to investigate the influence of Fe(CO)<sub>5</sub> on combustion flames, and the mechanism was validated by experimental results.<sup>12–16</sup> Understanding the behaviors of promotion of CO oxidization and inhibition of NO formation by gaseous iron and iron oxides at high-temperature off-gas combustion is important for the control of CO and NO emissions. There are no reports in the literature of NO by iron-containing compounds in steelmaking off-gas combustion conditions. The goal of this work is to gain better understanding of the mechanisms of the promotion of CO oxidization and inhibition of NO formation by gaseous iron species. In the paper, the combustion of off-gas in the presence of gaseous iron species was simulated using the Sandia SENKIN program, and the promotion of CO oxidization and inhibition of NO formation by gaseous iron species were analyzed.

## 2. KINETIC MODEL

The chemical kinetic behavior of reactants was modeled with the Sandia SENKIN program of CHEMKIN subroutines.<sup>17,18</sup> The program solves the conservation equations for mass and energy. It can calculate the temporal evolution of mole fractions of species for a homogeneous mixture in a closed reactor and it can account for finite-rate elementary chemical reactions and perform kinetic sensitivity analysis. Therefore, the SENKIN model is appropriate to investigate the mechanisms of CO oxidization and NO reduction by gaseous iron species in the process of high-temperature off-gas combustion in a closed chamber. The reaction pathway flux analysis is performed using MixMaster (a Python program that is part of the Cantera suite), which is based on a conserved scalar approach to reaction fluxes.<sup>19</sup>

The chemical kinetic model of off-gas combustion is from Linteris et al.<sup>20</sup> In the mechanism, the CO/H<sub>2</sub>/O<sub>2</sub> system is from

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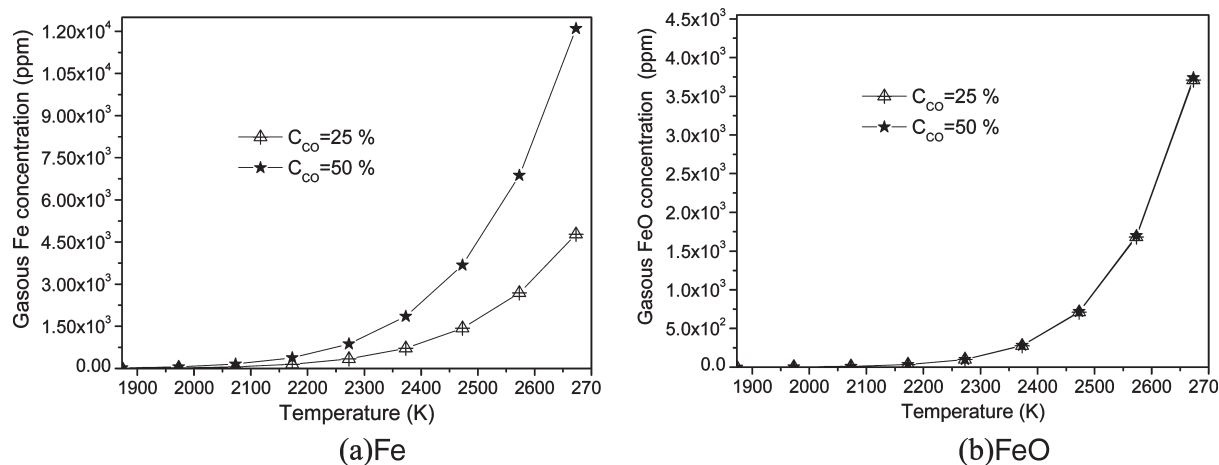


Figure 1. Initial concentration of gaseous iron species in high-temperature off-gas.

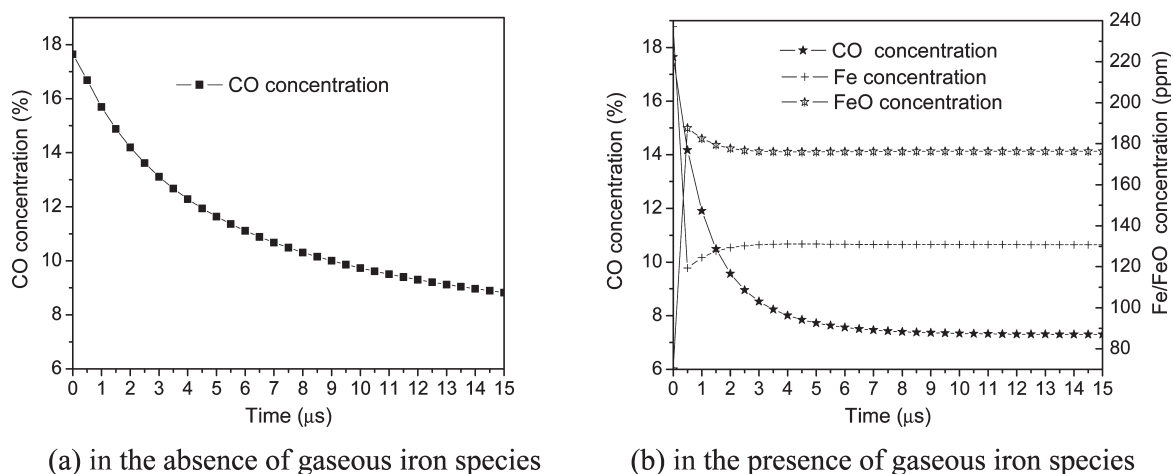


Figure 2. Concentrations of CO, gaseous Fe, and FeO during off-gas combustion at the initial  $C_{CO} = 25\%$ ,  $SR = 0.7$ , and  $T = 2273$  K.

Allen and Yetter,<sup>21</sup> based upon that from Kim et al.,<sup>22</sup> while the gaseous iron species mechanism is from Rumminger et al.<sup>23</sup> The CO/H<sub>2</sub>/O<sub>2</sub> submechanism has been extensively validated by experimental data in ref 22, and the iron submechanism has been validated using flame speed data and diffusion flame extinction data.<sup>16,23–25</sup>

### 3. SIMULATION CONDITIONS

In the combustion simulation of high-temperature off-gas containing gaseous iron species by Sandia SENKIN model with the mechanism from Linteris, it is a case for an adiabatic constant pressure system ( $P = 1.01$  bar). The initial compositions of off-gas are CO and CO<sub>2</sub>, and the oxidizer is air. In the paper,  $C_{CO}$  is the initial CO concentration in off-gas, and  $C_{CO,0}$  is the initial CO concentration in the gas mixture of off-gas and air during combustion. The promotion of CO oxidation and inhibition of NO formation by gaseous iron species are investigated at  $C_{CO} = 25\%$  and  $50\%$ .

According to the analysis data of dust sampled at the cooling stack outlet (72.0% Fe<sub>2</sub>O<sub>3</sub>, 0.80% SiO<sub>2</sub>, and 9.04% CaO, 120 g/m<sup>3</sup>),<sup>2</sup> using chemical equilibrium calculation by HSC chemistry 7.0,<sup>26</sup> the initial concentrations of gaseous iron species in high-temperature off-gas were calculated, as shown in Figure 1. Because the high-temperature off-gas originates from the high-temperature

steel-smelting bath during converter steelmaking process, it can be considered that the gaseous Fe species is in an equilibrium saturated state in the high-temperature off-gas, thus the initial concentration of gaseous iron species calculated by chemical equilibrium is reasonable. The results of chemical equilibrium calculation indicate that the gaseous compositions of iron-containing species are Fe and FeO; the concentrations of gaseous Fe and FeO increase with the increase of temperature; with the increase of CO concentration, the concentration of gaseous Fe increases, but FeO concentration is not effected.

Moisture content of air supplied for combustion is 0.6 wt %. Air stoichiometric ratio (SR) represents the fuel–air mixture composition:

$$SR = (\text{actual air supplied}) / (\text{stoichiometric air demand of fuel}) \quad (1)$$

In the paper, the influences of SR on CO oxidation and NO formation are investigated, and SR ranges from 0.3 to 1.2.

### 4. RESULTS AND DISCUSSION

**4.1. Catalytic Effect of Gaseous Iron Species on CO Oxidation.** Figure 2 compares the variations of CO concentrations during off-gas combustion in the presence and absence of gaseous

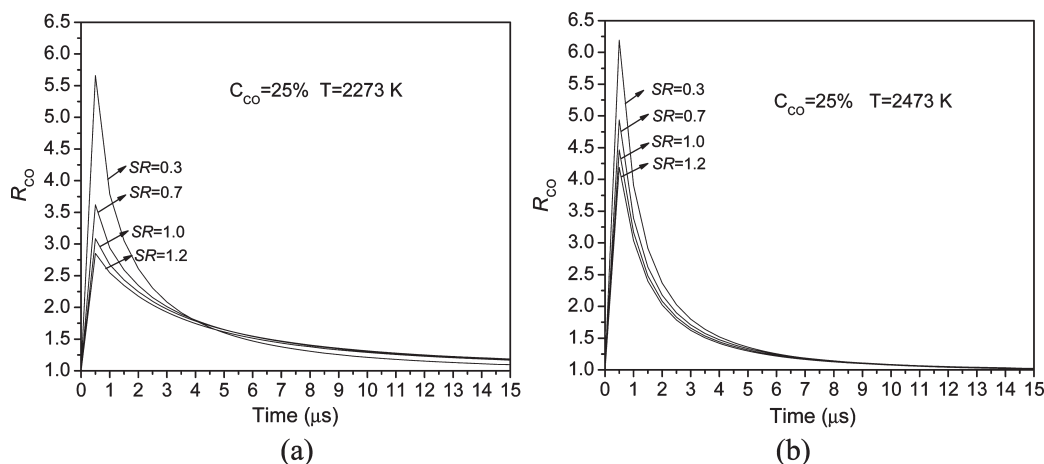


Figure 3. Influence of SR on the relative ratio of CO oxidation at  $C_{CO} = 25\%$ .

iron species at  $C_{CO} = 25\%$ ,  $SR = 0.7$  and  $T = 2273$  K, and the concentrations of gaseous iron species are also provided in the presence of gaseous iron species during off-gas combustion. CO concentration in the presence of gaseous iron species decreases faster than that in the absence of gaseous iron species, indicating that gaseous iron species during off-gas can greatly promote CO oxidation.

To estimate the contribution of gaseous iron species to CO oxidation, the relative ratio of CO oxidation is defined as ( $R_{CO}$ )

$$R_{CO} = \frac{C_{CO,0} - C_{CO,2}}{C_{CO,0} - C_{CO,1}} \quad (2)$$

where  $C_{CO,0}$  is the initial CO concentration in the gas mixture of off-gas and air during off-gas combustion;  $C_{CO,1}$  is the CO concentration in the absence of gaseous iron species during off-gas combustion;  $C_{CO,2}$  is the CO concentration in the presence of gaseous iron species during off-gas combustion.  $R_{CO} > 1$  means that the presence of gaseous iron species during off-gas combustion is conducive to CO oxidation, and the higher  $R_{CO}$ , the more significant the catalytic effect of gaseous iron species on CO oxidation.

In Figure 3, the relative ratio of CO oxidation is shown as a function of time at  $C_{CO} = 25\%$  and  $SR = 0.3-1.2$ . The simulation results indicate the following: at early burning stage ( $t < 3 \mu s$ ),  $R_{CO}$  dramatically varies with combustion time, it has a peak value when combustion time is  $0.5 \mu s$  or so, all of the peak values of  $R_{CO}$  are greater than 2.7, and increasing SR makes  $R_{CO}$  decrease; at  $t > 5 \mu s$ ,  $R_{CO}$  moderately decreases with combustion time and tends to 1, and SR has little effect on  $R_{CO}$ ;  $R_{CO}$  at  $T = 2473$  K is higher than that at  $T = 2273$  K.

In Figure 4, the relative ratio of CO oxidation is shown at initial  $C_{CO} = 50\%$  and  $SR = 0.3-1.2$ . When comparing  $R_{CO}$  at  $C_{CO,0} = 25\%$  and  $50\%$  (see Figures 3 and 4), increasing  $C_{CO}$  makes  $R_{CO}$  decrease.

To understand the influence mechanism of gaseous iron species on CO oxidation, the normalized sensitivity of CO concentration toward reactions is calculated. The sensitivity analysis coefficients are obtained through perturbation of the pre-exponential factor  $A$  in the Arrhenius equation of reactions, and the normalized sensitivity coefficient ( $S_i$ ) is defined as

$$S_i = \frac{\partial \ln c}{\partial \ln k_i} \quad (3)$$

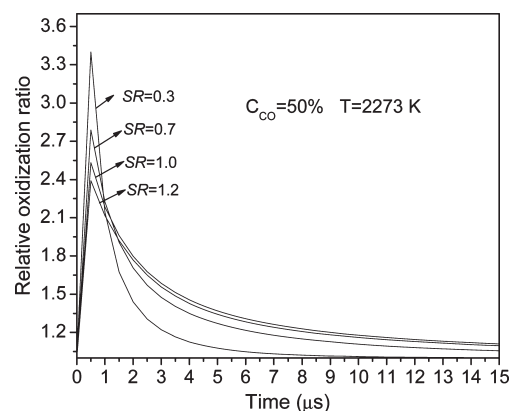
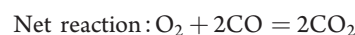
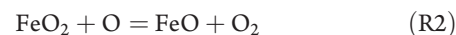


Figure 4. Influence of SR on relative CO oxidation ratio at  $C_{CO} = 50\%$ .

where  $c$  is CO concentration, and  $k_i$  is the pre-exponential factor  $A$  in the Arrhenius equation of the reaction  $i$ . The value of the sensitivity coefficient indicates a positive or negative influence on  $c$  by  $k_i$ , a positive value means that the value of  $c$  increases as  $k_i$  increases and a negative value means that the value of  $c$  decreases as  $k_i$  increases. The reason for the high value of this coefficient is that the reaction is the key chain branching step and strongly promotes CO oxidation.

As known from Figure 5, the normalized sensitivity coefficients of reactions R1R1–R4R4 are the top 4, meaning the four reactions are most important for CO oxidation. All of the reactions R1R1–R4R4 involve gaseous iron species, and these reactions comprise the catalytic CO oxidation.



Therefore, during the combustion of high-temperature off-gas, gaseous iron species have great catalytic effect on CO oxidation.

The peak values of the sensitivity coefficient of reactions R1R1–R4R4 coincide in time at the early stage of off-gas combustion. These reactions are responsible for the rapid increase of the relative ratio of CO oxidation at early burning stage in Figures 3 and 4, indicating that gaseous containing-iron species during off-gas can greatly promote CO oxidation.

The primary reaction pathways for CO and iron species are shown in Figure 6. Figure 6a indicates that the most important reaction of CO oxidation in the absence of iron species is

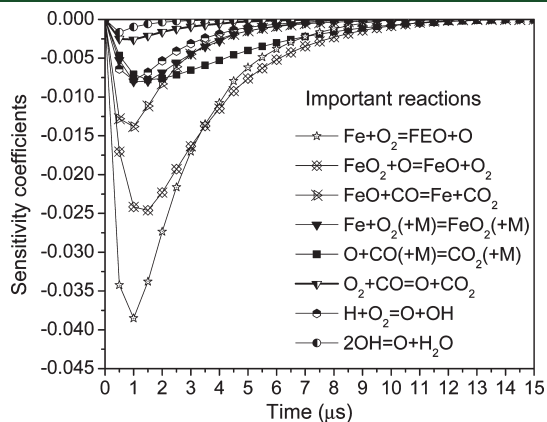
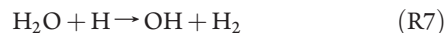


Figure 5. Sensitivity of CO concentrations toward the most important reactions at  $C_{\text{CO}} = 25\%$ ,  $T = 2273 \text{ K}$ , and  $\text{SR} = 0.7$ .

OH is crucial to CO oxidation. OH radical is formed to accelerate CO oxidation in the presence of even a small quantity of hydrogen-containing material.<sup>27</sup> For off-gas combustion, off-gas contains virtually no hydrogen-containing material, OH only originates from  $\text{H}_2\text{O}$  vapor supplied by combustion air stream, and OH is principally obtained by the following mechanisms:



Therefore, during off-gas combustion,  $\text{H}_2\text{O}$  vapor supplied by combustion air stream is very important, and the absence of  $\text{H}_2\text{O}$  may make the oxidation of CO extremely slow.

Figure 6b illustrates the reaction pathways for CO oxidation in the presence of gaseous iron species. It indicates that there are three reaction pathways of CO oxidation: (1)  $\text{FeO} + \text{CO} = \text{Fe} + \text{CO}_2$ ; (2)  $\text{OH} + \text{CO} = \text{H} + \text{CO}_2$ ; (3)  $\text{O} + \text{CO} = \text{CO}_2$ . The first reaction pathway is the most important pathway and accounts for 72% contribution for CO oxidation. Here, a portion of Fe is converted first to  $\text{FeO}_2$  and then to  $\text{FeO}$ , the remainder of the Fe is directly converted to  $\text{FeO}$ , and  $\text{FeO}$  participates in CO oxidation to be reduced into Fe. In the series of reactions, and the circulation reactions of  $\text{Fe}-\text{FeO}/\text{FeO}_2-\text{Fe}$  achieve the catalytic effect on CO oxidation, which predominates CO oxidation. The secondary pathway of CO oxidation is the same as that in the absence of iron species mentioned in Figure 6a; it accounts for 26% contribution for CO oxidation in the presence of iron species which accounts for 84% in the absence of iron species, and the pathway originates from the reaction of CO and  $\text{H}_2\text{O}$  vapor supplied by combustion air

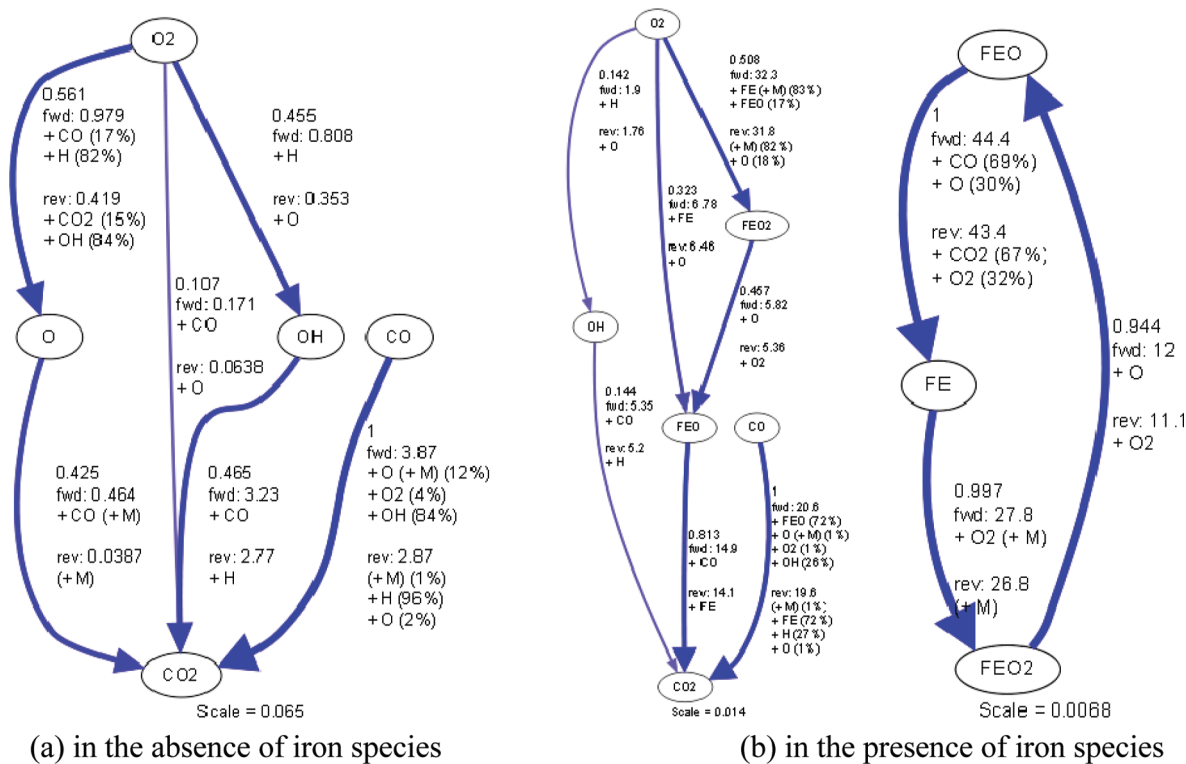
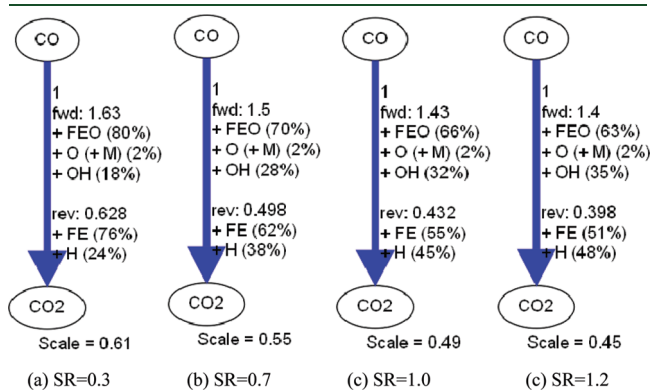


Figure 6. Schematic diagram of reaction pathways for CO and iron species at  $C_{\text{CO}} = 25\%$  in off-gas,  $T = 2273 \text{ K}$ ,  $\text{SR} = 0.7$ , and  $t = 1 \mu\text{s}$ . The percentages presented in some paths represent the contribution of that path to the consequent species. Large arrows represent the important paths for both consumed and produced species.

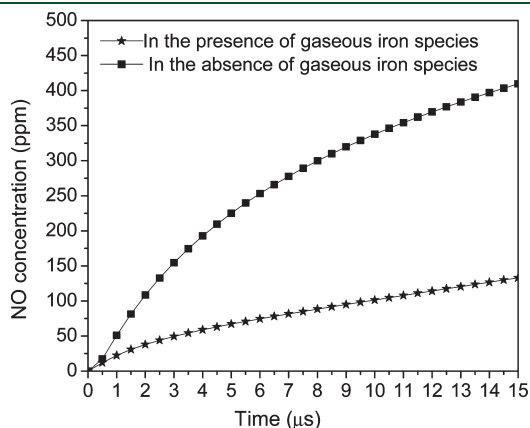


stream. The third reaction pathway CO oxidation accounts for only 1% contribution for CO oxidation, and it is negligible.

Based on the above analysis of sensitivity and reaction pathways, the influences of SR, temperature, and  $C_{CO}$  on the relative ratio of CO oxidation are discussed. Figures 3 and 4 indicate that increasing SR makes the relative ratio of CO oxidation decrease at the early combustion stage. To investigate the reason, the schematic diagrams of reaction pathways for CO oxidation



**Figure 7.** Schematic diagrams of reaction pathways for CO oxidation at  $C_{CO} = 25\%$  in off-gas,  $T = 2273\text{ K}$ , and  $t = 1\ \mu\text{s}$ .



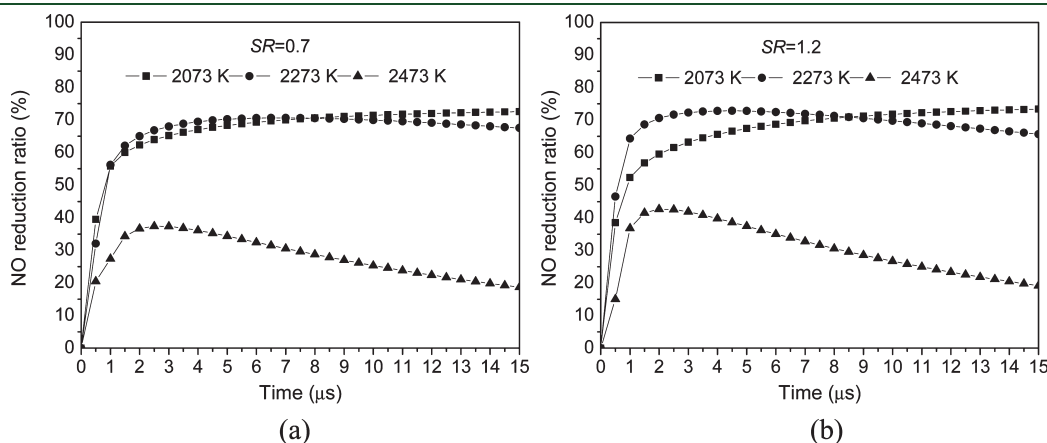
**Figure 8.** NO concentration during off-gas combustion in the presence and absence of gaseous containing-iron species at initial  $C_{CO} = 25\%$  in off-gas,  $SR = 0.7$ , and  $T = 2273\text{ K}$ .

at different SR are presented in Figures 7. The results indicate that, with the increase of SR, the contribution rate of R3 ( $\text{FeO} + \text{CO} = \text{Fe} + \text{CO}_2$ ) for CO oxidation decreases, but the contribution rate of R5 ( $\text{OH} + \text{CO} = \text{H} + \text{CO}_2$ ) for CO oxidation increases. When SR increases from 0.3 to 1.2, the increasing air supplied dilutes the concentration of gaseous iron species in the gas mixture of off-gas and air, the initial concentration Fe species decreases from 285 to 196 ppm, but the initial concentration  $\text{H}_2\text{O}$  vapor supplied by air stream increases from 48 to 133 ppm. Since the reaction rate of R3 is larger than that of R5, the decrease of the initial concentration Fe species with SR is not conducive to CO oxidation. The catalytic effect of gaseous iron species on CO oxidation reduces, thus the relative ratio of CO oxidation decreases with the increase of SR at early stage of off-gas combustion (see Figures 3 and 4). In Figure 3, the reason for the increase of the relative ratio of CO oxidation with the increase of temperature is as follows: the reaction rate coefficients have exponential relationship with combustion temperature, increasing temperature strengthens catalytic effect of gaseous iron species on CO oxidation, and then the relative ratio of CO oxidation at  $T = 2473\text{ K}$  is higher than that at  $T = 2273\text{ K}$  (see Figure 3). In Figures 3 and 4, the reason for the decrease of the relative ratio of CO oxidation with the increase of  $C_{CO}$  is as follows: the off-gas combustion with high-concentration CO needs more air provided, and a large amount of combustion air results in the decrease of the concentration of gaseous iron species, the catalytic effect of gaseous iron species on CO oxidation is weakened, and then the relative CO ratio of oxidation decreases at early stage of off-gas combustion with the decrease of  $C_{CO}$  as compared between Figure 3 and Figure 4.

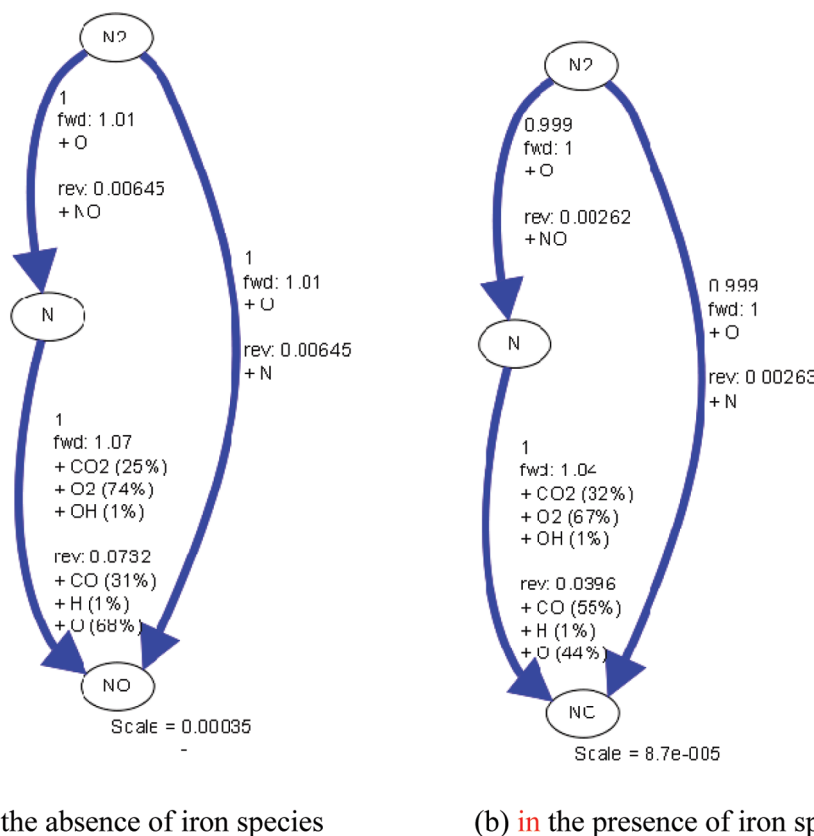
**4.2. Catalytic Effect of Gaseous Iron Species on NO Formation.** Figure 8 compares the variations of NO concentration during off-gas combustion in the presence and absence of gaseous iron species at  $C_{CO} = 25\%$ ,  $SR = 0.7$  and  $T = 2273\text{ K}$ . NO concentration in the presence of gaseous iron species is much lower than that in the absence of gaseous iron species, indicating that gaseous iron species can greatly inhibit NO formation.

To estimate the effect of gaseous iron species on NO formation, NO reduction ratio is defined as  $R_{NO}$

$$R_{NO} = \frac{C_{NO,2} - C_{NO,1}}{C_{NO,2}} \times 100\% \quad (4)$$



**Figure 9.** Influence of temperature and SR on relative CO oxidation ratio at  $C_{CO} = 25\%$ .



**Figure 10.** Schematic diagram of reaction pathways for NO formation at  $C_{CO} = 25\%$ ,  $T = 2273$  K,  $SR = 1.2$ , and  $t = 1 \mu s$ . The percentages presented in some paths represent the contribution of that path to the consequent species. Large arrows represent the important paths for both consumed and produced species.

where  $C_{NO,1}$  is the NO concentration in the presence of gaseous iron species, and  $C_{NO,2}$  is the NO concentration in the absence of gaseous iron species.

Figure 9 shows NO reduction ratio of off-gas in the presence of gaseous iron species at  $SR = 0.7$  and  $1.2$ . NO reduction ratio can reach above 70% at  $T = 2073$  and  $2273$  K, but it is less than 50% at  $T = 2473$  K. NO reduction ratio slightly increases with the increase of SR. The results indicate that gaseous iron species can effectively inhibit NO formation when combustion temperature is not higher than  $2273$  K during the off-gas combustion.

Figure 10 shows NO formation pathways during the off-gas combustion in the absence and presence of gaseous iron species, and the results indicate that major reaction pathways of NO formation in the absence and presence of gaseous iron are similar, where  $N_2/N$  mainly reacts with  $O_2$  and  $O$  to form NO.

To understand NO formation mechanism, by using the rate of production (ROP) analyses, NO production rates of reactions were calculated (see Figure 11). The top three reactions during high-temperature off-gas combustion in the absence and presence of gaseous iron are the same, and they are following reactions:



Reactions R8R8 and R9R9 are thermal-NO or Zeldovich-NO; thermal-NO is produced from the reaction of nitrogen

and oxygen gases in the air during combustion, especially at high temperatures. Reaction R8R8 has a very high activation energy due to the strong trip bond in the  $N_2$ -molecule, and is thus sufficient at high-temperature. The formation of thermal-NO is determined by a set of highly temperature-dependent chemical reactions known as the extended Zeldovich mechanism.

The presence of  $CO_2$  has a significant effect on NO formation by reaction R10R10, the high concentration of  $CO_2$  makes more NO formation. At initial stage of off-gas combustion, NO production rates of the reactions R8R8 and R9R9 rapidly increase because of high  $O_2$  concentration, and then the production rates decreases with combustion time because of the decrease of  $O_2$  concentration (see Figure 11).

As compared with the NO production rates during off-gas in the absence of gaseous iron, the NO production rates are noticeably low in the presence of gaseous iron, indicating that gaseous iron species plays a key role in the NO reduction. To investigate the reasons for the inhibition mechanism of NO formation by gaseous iron species, the normalized sensitivity of NO concentration toward reactions involving gaseous iron species reactions is calculated, and the top three sensitivities of NO concentration toward reactions involving gaseous iron reactions are shown in Figure 12.

The sensitivity analysis reflects the relative importance of different reactions with respect to the NO mole fraction. Figure 11 indicates that the reactions of iron species greatly influence NO formation, and the top three reactions are the

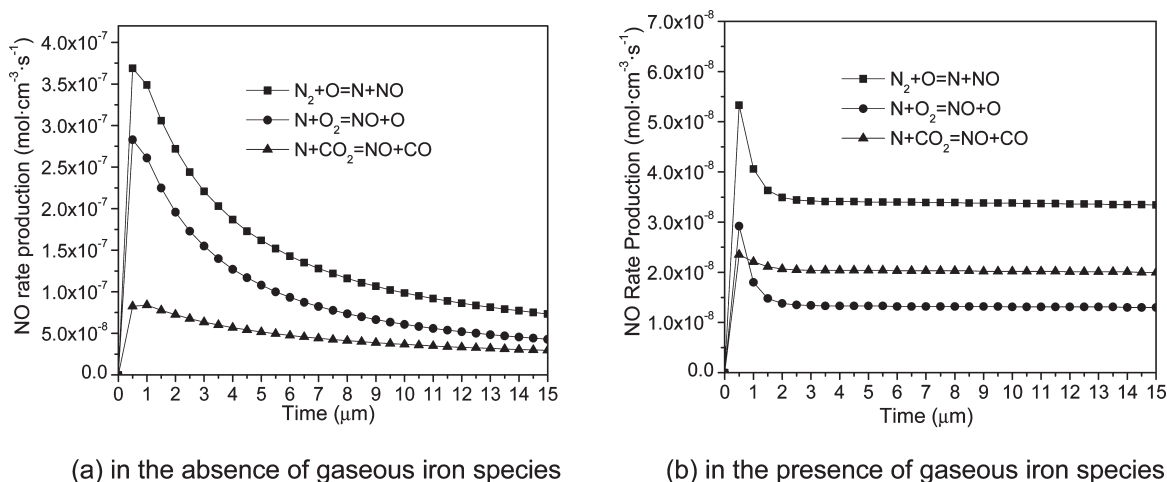


Figure 11. Rate of production (ROP) analyses of NO formation at  $C_{CO} = 25\%$ ,  $T = 2273$  K, and  $SR = 1.2$ .

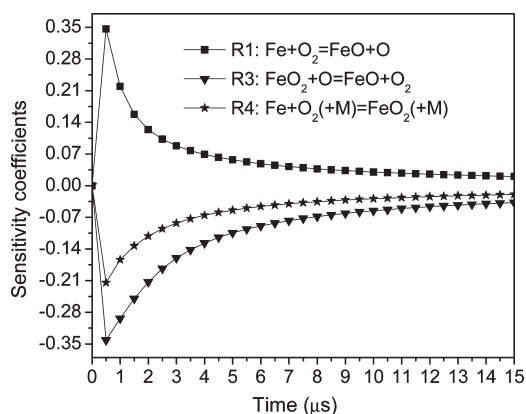
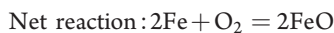


Figure 12. Sensitivity of NO concentrations toward the most important reactions at  $T = 2273$  K,  $SR = 1.2$ , and  $C_{CO} = 25\%$ .

following:



Reactions R1R1, R3R3, and R4R4 play a key role not only in CO oxidation but also in NO formation.  $\text{O}_2$  is very important for thermal-NO formation. As mentioned above, reactions R1R1–R4R4 have the catalytic effect of CO oxidation, and they play a role of  $\text{O}_2$  transfer for CO oxidation. The circulation reactions of  $\text{Fe}-\text{FeO}/\text{FeO}_2-\text{Fe}$  predominate CO oxidation, but thermal NO greatly depends on  $\text{O}_2$ . Thus, there are  $\text{O}_2$  competitive reactions between thermal NO formation and Fe oxidation. High chemical activity of iron species easily reacts with  $\text{O}_2/\text{O}$  (see Figure 6b), thus thermal-NO formation is inhibited. In short, the gaseous iron species promotes CO oxidation and inhibits NO formation in the combustion of off-gas.

## 5. CONCLUSION

In the paper, a numerical simulation of the promotion of CO oxidation and inhibition of NO formation by gaseous iron

species during the combustion of converter steelmaking off-gas was performed using the Sandia SENKIN program of CHEMKIN subroutines. In the presence of iron species, at early burning stage ( $t < 3 \mu\text{s}$ ),  $R_{CO}$  dramatically varies with combustion time, all of the peak values of  $R_{CO}$  are greater than 2.4, and increasing SR makes  $R_{CO}$  decrease. These reactions comprise the catalytic CO oxidation:  $\text{Fe} + \text{O}_2 = \text{FeO} + \text{O}$ ,  $\text{FeO}_2 + \text{O} = \text{FeO} + \text{O}_2$ ,  $\text{Fe} + \text{O}_2 = \text{FeO}_2$ ,  $\text{FeO} + \text{CO} = \text{Fe} + \text{CO}_2$ . The circulation reactions of  $\text{Fe}-\text{FeO}/\text{FeO}_2-\text{Fe}$  achieve the catalytic effect on CO oxidation. Gaseous iron species can greatly inhibit NO formation, and NO reduction ratio can reach above 70% at  $T = 2073$  and  $2273$  K. Gaseous iron species can effectively inhibit NO formation when combustion temperature is not higher than  $2273$  K during the off-gas combustion. There are  $\text{O}_2$  competitive reactions between thermal NO formation and Fe oxidation, and high chemical activity of iron species inhibits thermal-NO formation.

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## NOMENCLATURE

- $C_{CO}$  = initial CO concentration in off-gas (%)
- $C_{CO,0}$  = initial CO concentration in the gas mixture of off-gas and air during combustion (%)
- $C_{CO,1}$  = CO concentration in the absence of gaseous iron species during off-gas combustion (%)
- $C_{CO,2}$  = CO concentration in the presence of gaseous iron species during off-gas combustion
- $T$  = combustion temperature (K)
- $SR$  = air stoichiometric ratio
- $R_{CO}$  = the relative ratio of CO oxidation
- $R_{NO}$  = NO reduction ratio (%)
- $S_j$  = the normalized sensitivity coefficient

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