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ABSTRACT

In this study, a computational fluid dynamics (CFD) model was developed to study the flow and heat transfer characteristics of a 320 MW oxy-fired boiler with dry and wet flue gas recirculation (FGR). The results show that there exist significant differences in the composition and physical properties of flue gas between the air- and oxy-combustion modes and these differences may lead to remarkable differences in the flow, temperature and heat transfer distributions of boiler. Specifically, since the specific heat of CO₂ and H₂O are higher than that of N₂, the flue gas heat capacity of the oxy-combustion case with wet FGR is significantly higher than the air-combustion case leading to lower furnace temperature and heat absorption of furnace wall. Moreover, since the density of CO₂ is higher than N₂, the overall flow velocity in oxy-fired boiler is lower than that of air-fired boiler, which subsequently affects the boiler flow and temperature distributions in the furnace. The differences in the flow and heat transfer distributions between oxy-fired and air-fired boilers should be taken into consideration when designing new oxy-fuel combustion systems or retrofitting existing air combustion systems to minimize costly modifications to the boiler’s heating surfaces.

Keywords: oxy-fuel combustion; radiation heat transfer; flue gas recirculation; coal combustion; numerical simulation

1. INTRODUCTION

Oxy-fuel combustion is recognized as one of the most promising technologies of CO₂ capture [1, 2]. It has been widely studied in small scale problems [3-6]. However, to date the experience on the design and operation of full scale oxy-fired boilers are still rather limited. Experiments on large scale boilers are extremely costly and technically impractical. Then CFD becomes a viable option to study the large scale oxy-fired boilers. In this study we conducted a numerical study on the combustion and heat transfer characteristics of a full scale 320 MW oxy-fired boiler. In oxy-fuel combustion, N₂ is removed by air separation unit (ASU) and coal is burning with the high-purity O₂. The flue gas is then mainly composed of CO₂ and H₂O rather than N₂ in air combustion. Moreover, in order to control combustion temperature, FGR is usually applied to oxy-fuel combustion systems. Depending on if the water vapor is removed from the recirculated flue gas, H₂O concentration in flue gas may also vary over a broad range. Because there exist remarkable differences in the gas properties among N₂, CO₂ and H₂O, the properties of the flue gas mixture (density, heat capacity and radiation properties) of oxy-fuel combustion may significantly differ from those of air combustion. This may dramatically affect the flow, temperature and heat transfer characteristics of oxy-fuel boilers. Particularly, in coal-fired boiler radiation is the dominant heat transfer mechanism in the furnace contributing more than 90% of total heat transfer to the furnace water wall [7]. Because of the significantly higher concentration of the absorbing gases, CO₂ and H₂O, the radiation properties of the gas mixture change dramatically. This may strongly affect the furnace heat transfer distribution of the oxy-fired boilers.

Thus, in this study a full scale 320 MW oxy-fired boiler with FGR is numerically studied with particular attention focused on the different furnace wall heat transfer characteristics resulted from different flue gas composition between the air- and oxy-combustion modes. The results from the present study are going to provide guidance to the design of new oxy-combustion systems or retrofit of existing air combustion systems.
2. MATHEMATICAL MODELS

ANSYS Fluent is used as the computational platform to implement the CFD models presented in this study. Realizable $k$-$\varepsilon$ model is used for turbulence closure [8]. Coal particles are tracked in Lagrangian framework using stochastic tracking method [9]. Coal devolatilization is modeled using a first-order single reaction rate model [10] with the rate parameters obtained from a separate FLASHCHAIN model [11]. The volatile matter is represented by a single virtual substance $C_6H_{12}O_{8}S_2N_2$ [12-14]. Assuming that char is composed of pure carbon and ash, the values of $a$, $b$, $c$, $d$ and $e$ can be determined by the mass balance of each volatile element.

The heterogeneous reactions of char include:

\begin{align}
C_{\text{char}} + 0.5O_2 & \rightarrow CO \quad (1) \\
C_{\text{char}} + CO_2 & \rightarrow 2CO \quad (2) \\
C_{\text{char}} + H_2O & \rightarrow H_2+CO \quad (3)
\end{align}

where $C_{\text{char}}$ is the carbon in the char. The char surface reaction rate is calculated by the kinetic/diffusion-limited rate model [15] with the rate parameters given in the table below.

<table>
<thead>
<tr>
<th>Diffusion rate constant</th>
<th>Pre-exponential factor</th>
<th>Activation energy (kJ/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C + O_2$</td>
<td>$4.374 \times 10^{-12}$</td>
<td>79</td>
</tr>
<tr>
<td>$C + CO_2$</td>
<td>$2.811 \times 10^{-12}$</td>
<td>147</td>
</tr>
<tr>
<td>$C + H_2O$</td>
<td>$2.811 \times 10^{-12}$</td>
<td>162</td>
</tr>
</tbody>
</table>

The CO and H$_2$ generated at the char surface are transported to the bulk gas and further oxidized to CO$_2$ and H$_2$O. The combustion reaction of the volatile matter $C_6H_{12}O_{8}S_2N_2$ is modeled with a two-step reaction scheme. Then the homogeneous reactions include

\begin{align}
C_6H_{12}O_{8}S_2N_2 & + \left( \frac{a}{4} + \frac{b}{2} - \frac{c}{2} + \frac{d}{2} \right)O_2 \rightarrow \\
& \alpha CO + \frac{b}{2}H_2O + dSO_2 + eN_2 \\
& CO + 0.5O_2 \rightarrow CO_2 \\
& H_2 + 0.5O_2 \rightarrow H_2O
\end{align}

For most of engineering applications, combustion is extremely intense such that the reaction rate is overall limited by the mixing between the fuel and oxidizer. Thus, Eddy-Dissipation Model (EDM) is used to calculate the homogeneous chemical reaction rates [16, 17]. The Discrete Ordinate Method (DOM) is used to simulate the radiation heat transfer. The emissivity of the gas mixture is calculated using weighted-sum-of-gray-gas model (WSGGM). In WSGGM the emissivity of gas mixture is approximated by the weighted sum of emissivities of several fictitious gray gases,
are particularly suitable for the radiation calculation of oxy-combustion problems.

3. BOILER GEOMETRY AND OPERATING DATA

Figure 2 shows the schematic of the furnace geometry of the 320 MW boiler with burner and heating surfaces arrangement. The height, width and depth of the boiler are 56.2 m, 14.0 m and 14.0 m, respectively. The mesh is constructed with 4.06 million hexahedral structured cells. This boiler is firing bituminous coal. The coal property data is summarized in Table 2.

Three cases are studied in the present study, including air combustion, oxy-fuel combustion with dry FGR and oxy-fuel combustion with wet FGR, hereafter referred to as Air, Oxy-Dry and Oxy-Wet cases respectively. The model parameters of the Air case are determined based on the design and operating data of the boiler. All three cases use the same total coal flow rate (123.5 t/h). Different FGR modes (wet or dry FGR) and FGR flow rates affect the furnace inlet O\(_2\) and gas flow rates, and subsequently affect the flow, temperature and heat transfer distributions in the furnace. For the ease of comparison, this study maintain the same burner inlet O\(_2\) and gas mass flow rates for all three cases based on which the needed excess air ratio and FGR ratio for the Oxy-Dry and Oxy-Wet cases can be determined, as shown in Table 3. Here the FGR ratio denotes ratio of recycled flue gas volume flow rate to that of total gas flow and we have assumed that the air used in the oxy-combustion cases is composed of 95% O\(_2\) and 5% N\(_2\) by volume. Note that because the recirculated
flue gas contains excess oxygen, the excess air ratios of oxy-fuel combustion cases can be significantly lower than that of air-combustion case to maintain the same inlet \(O_2\) flow rate.

<table>
<thead>
<tr>
<th>Cases</th>
<th>Air</th>
<th>Oxy-Dry</th>
<th>Oxy-Wet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Excess air ratio</td>
<td>1.235</td>
<td>1.056</td>
<td>1.063</td>
</tr>
<tr>
<td>FGR ratio</td>
<td>74.30%</td>
<td>77.48%</td>
<td>78.63%</td>
</tr>
</tbody>
</table>

Table 3. Excess air ratio, FGR ratio and furnace inlet gas composition

Since \(t_f\) of \(N_2\), \(CO_2\) and \(H_2O\) (at 2000 K) are 1285 J/(kg·K), 1373 J/(kg·K) and 2839 J/(kg·K), respectively, and that the \(H_2O\) concentration of Oxy-Wet case is much higher than the other two cases. Thus the \(c_p\) of the gas mixture of Oxy-Wet case is considerably higher than the other two cases, resulting in lower furnace temperature. Since the \(c_p\) of \(CO_2\) is only slightly higher than \(N_2\), the large difference in \(CO_2\) concentration between the Oxy-Dry and Air cases only results in slightly higher \(c_p\) of the Oxy-Dry case. However, the furnace temperature of the Oxy-Dry case shown in Fig. 4 appears slightly higher than the Air case, opposite to what is expected from the comparison of \(c_p\) between the two cases. This can be explained by the differences in flow and furnace temperature distributions between the two cases. As seen in Fig. 3, because the inlet gas velocity of Oxy-Dry case is significantly lower than the Air case, its rotational flow in the furnace is relatively weaker so that the high temperature flame locates near the center of furnace and away from the furnace wall. As seen in Eq. (7), the overall emissivity of flue gas drops exponentially with the path length \(L\). As a result, the overall radiation heat absorption by the furnace wall is reduced (as seen in Table 5) and this effect dominates over that of higher \(c_p\).

Figure 4 shows the furnace cross-corner sectional temperature distributions for different cases. It is seen that the furnace temperature of the Oxy-Wet case is lower than that of the Air case, while the Oxy-Dry case is slightly higher. The difference in furnace temperature among the three cases is firstly caused by the difference in the specific heat \(c_p\) of the gas mixture. Table 5 gives the mass fraction of major flue gas composition, specific heat of flue gas (at 2000 K), and total heat absorption of furnace wall of different cases. Note that the \(c_p\) of \(N_2\), \(CO_2\) and \(H_2O\) (at 2000 K) are 1285 J/(kg·K), 1373 J/(kg·K) and 2839 J/(kg·K), respectively, and that the \(H_2O\) concentration of Oxy-Wet case is much higher than the other two cases. Thus the \(c_p\) of the gas mixture of Oxy-Wet case is considerably higher than the other two cases, resulting in lower furnace temperature. Since the \(c_p\) of \(CO_2\) is only slightly higher than \(N_2\), the large difference in \(CO_2\) concentration between the Oxy-Dry and Air cases only results in slightly higher \(c_p\) of the Oxy-Dry case. However, the furnace temperature of the Oxy-Dry case shown in Fig. 4 appears slightly higher than the Air case, opposite to what is expected from the comparison of \(c_p\) between the two cases. This can be explained by the differences in flow and furnace temperature distributions between the two cases. As seen in Fig. 3, because the inlet gas velocity of Oxy-Dry case is significantly lower than the Air case, its rotational flow in the furnace is relatively weaker so that the high temperature flame locates near the center of furnace and away from the furnace wall. As seen in Eq. (7), the overall emissivity of flue gas drops exponentially with the path length \(L\). As a result, the overall radiation heat absorption by the furnace wall is reduced (as seen in Table 5) and this effect dominates over that of higher \(c_p\).
As a result, the temperature of Oxy-Dry case appears slightly higher than that of Air case. Oxy-Dry case is distributed over a smaller area of furnace wall although its peak heat flux is higher. This is the reason why the overall furnace wall heat absorption of the Oxy-Dry case (297.6 MW) is lower than that of the Air case (314.5 MW).

| Table 5. Mass fraction of major flue gas components, specific heat of flue gas, and heat absorption of furnace wall under different combustion modes |
|---------------------------------|--------|--------|--------|
| Air | Oxy-Dry | Oxy-Wet |
| N₂  | 0.708  | 0.038  | 0.034  |
| CO₂ | 0.207  | 0.876  | 0.773  |
| H₂O | 0.043  | 0.039  | 0.147  |
| c_p (J/kg·K) | 1373 | 1430 | 1595 |
| Heat absorption (MW) | 314.5 | 297.6 | 276.2 |

Figure 5 shows furnace wall heat flux distributions for different cases. Comparing the three cases, it is seen that the peak heat flux of Oxy-Dry case is higher than that of Air case while the Oxy-Wet case is significantly lower, which is consistent with temperature distributions shown in Fig. 4. This is because radiation is proportional to the fourth power of temperature, and hence, becomes extremely sensitive to temperature variations at higher temperatures. As such, the level of peak heat flux is largely determined by the peak flame temperature in the furnace. The heat flux distribution pattern over the entire furnace wall, however, is dependent on the overall furnace temperature distribution. Because the flame of the Oxy-Dry case locates near the center of the furnace, the heat flux in majority of furnace wall area is lower than that of the Air case except for the area corresponding to the location of the highest flame temperature. As a result, the high heat flux region of the Oxy-Dry case is distributed over a smaller area of furnace wall although its peak heat flux is higher. This is the reason why the overall furnace wall heat absorption of the Oxy-Dry case (297.6 MW) is lower than that of the Air case (314.5 MW).

5. CONCLUSION

A numerical study was conducted on the flow and heat transfer characteristics of a full scale 320 MW oxy-fired boiler. In order to properly account for the impact of different gas composition of oxy-combustion on radiation heat transfer, Johansson’s WSGGM was firstly implemented into the CFD model framework to make the CFD model suitable for the radiation calculation of oxy-combustion. Then, numerical studies were conducted for the oxy-fired boiler with both dry and wet FGR. The following conclusions were drawn based on the simulation results:

1. The differences in the composition and physical properties of flue gas between different combustion modes may result in considerable differences in the flow, temperature and heat transfer distributions of boiler.
2. The specific heat of flue gas of oxy-combustion with wet FGR is significantly higher than that of the air-combustion case, leading to lower furnace temperature and reduced furnace wall heat absorption.
3. Because the density of CO₂ is higher than that of N₂, the gas volume flow rate of oxy-combustion with dry FGR is significantly lower than that of air-combustion case which consequently leads to remarkable differences in the furnace flow and temperature distributions.
4. The differences in the flow, temperature and heat transfer distributions resulted from the differences in the composition and properties of flue gas of oxy-combustion need to be systematically considered when designing new oxy-combustion or retrofitting existing air-combustion systems.

REFERENCE