CFD Analysis of a Water Vaporization Process in a Three-Dimensional Spouted Bed for Flue Gas Desulfurization

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ABSTRACT: In this work, the gas—solid flow and water vaporization process are simulated by the method of Euler—Eulerian two-fluid model in a three-dimensional spouted bed, which have a significant influence on the desulfurization efficiency. The results of simulation indicate that the change trends of the particle volume fraction are similar under superficial gas velocities of 0.7 and 0.8 m/s. The degree of particle pulsation is the highest at the bottom of the spout area, and the degree of gas pulsation is the highest at the junction of the annulus area and spout area. The temperatures of gas, liquid, and particles are also analyzed. The results demonstrate that in the spout area, the gas temperature is much higher than that of the liquid and particles, but the three phases are uniformly mixed and have similar temperatures in other areas. Moreover, water vaporization mainly occurs at the junction of the annulus area and the spout area, a small amount of liquid is vaporized at the center of the spout area, and basically no vaporization reaction occurs in the outer radius of the annulus area. With the increase in gas velocity, gas temperature, and liquid temperature and the decrease in gas humidity, water vaporization reaction is promoted.

1. INTRODUCTION

In recent years, a large number of coal-fired emissions such as sulfur dioxide (SO2) have caused serious pollution to the environment, and the scope of pollution continues to increase, leading to serious global environmental problems.1−11 In the increasingly stringent environmental protection policy, removing sulfur dioxide from flue gas has become a challenging and urgent task. Therefore, it is necessary to control the content of sulfur dioxide to reduce the harm to the environment.6−11 Nowadays, the process of semi-dry flue gas desulfurization (FGD) has become a new type of desulfurization technology with great application prospects.12−15 Ma et al.16−18 explored the impact of influencing parameters such as the adiabatic saturation temperature and absorbent diameter on the efficiency of semi-dry FGD in a powder-particle spouted bed (PPSB). Also, the effects of CO2 and O2 on the removal of SO2 in flue gas were also studied through experiments. The results show that the O2 concentration will not affect the removal of SO2 within the experimental range. Lu et al.19 investigated the outlet concentration, desulfurization efficiency, and sulfur fixation of calcium-based desulfurization agents under varying levels of relative humidity (0−45%) to improve relative humidity. The experimental results show that a significant improvement of the FGD efficiency can be achieved by an increase in relative humidity. The dynamics of the spouted bed filled with particles were researched by Freitas and Freire20 through experimentation. They determined the velocity of particle and the rate of recirculation in the bed, and analyzed the influence of different operating parameters on spouted bed dynamics. Ren et al.21 studied the flow pattern and flow pattern conversion of the spouted bed. The influence of some important parameters (such as minimum spout velocity and pressure drop) on flow characteristics is discussed. The results show that the flow pattern mainly depends on the height of the stationary bed.

Even though the experiment can accurately observe the flow and evolution processes in the bed, they are not sufficient to determine the hydrodynamics and the details of spouting. In order to overcome these difficulties, the simulation method can quickly be used to obtain the physical parameters and the details of spouting. Therefore, through the simulation method, it is possible to experimentally study and simulate the gas—solid two-phase flow to improve the design and operation of the reactor.22−26 Wang et al.27 used the multi-fluid model and the kinetic theory of granular flows (KTGF) to experimentally study and simulate the gas—solid two-phase flow in the bed. Comparing the experiment with the simulation, it shows that the results of the drag coefficient model used in the simulation are consistent with the experiment. This research laid the foundation for further research on the numerical simulation of the spouted bed. The two-fluid model is used to study the influence of the wall boundary conditions of...
the solid phase in the fluid on the flow characteristics of the spouted bed by Lan et al.\textsuperscript{28} Using the method of comparing numerical prediction with experimental results, the simulation shows that the wall boundary conditions of the solid phase in the fluid play an essential role in the numerical modeling. Wu et al.\textsuperscript{29,30} used the CFD method to simulate the semi-dry FGD process in the two-dimensional spouted bed and analyzed the influence of different operating parameters on the desulfurization efficiency (such as temperature and superficial gas velocity). They carried out numerical simulation and optimization analysis of the two-dimensional integral multi-jet spouted bed. The desulfurization process in the spouted bed involves a multi-phase reaction system in which the liquid phase provides a place for the desulfurization process, and it has a great influence on the desulfurization efficiency. All in all, studying the evaporation process of water is of great significance for improving the desulfurization efficiency. All in all, studying the reaction characteristics and powder retention process in the system.

According to the above summary, this article uses the two-fluid model (TFM) and KTG method to simulate the gas–solid two-fluid and the process of water vaporization in the three-dimensional PPSB.

2. MATHEMATICAL MODEL

2.1. Gas–Solid Two-Fluid Flow Model. The two-fluid method was applied for gas and solid phases in three-dimensional PPSB. The interaction between the continuums is described by the Navier–Stokes equation. The main equations are summarized below.

The mass conservation equations are expressed as follows:

For the particle phase:
\[
\frac{\partial}{\partial t}(\alpha \rho_P u) + \nabla \cdot (\alpha \rho_P u) = 0
\]  
(1)

For the gas phase:
\[
\frac{\partial}{\partial t}(\alpha \rho_G v) + \nabla \cdot (\alpha \rho_G v) = 0
\]
(2)

The momentum conservation equations are expressed as follows:

For the particle phase:
\[
\frac{\partial}{\partial t}(\alpha \rho_P u) + \nabla \cdot (\alpha \rho_P u) = -\rho_P \nabla P + \alpha \rho_P K_p (u_P - u) + \nabla \cdot \tau_P
\]
(3)

For the gas phase:
\[
\frac{\partial}{\partial t}(\alpha \rho_G v) + \nabla \cdot (\alpha \rho_G v) = -\rho_P \nabla P + \alpha \rho_P K_g (u_P - u) + \nabla \cdot \tau_g
\]
(4)

where \( K_p \) denotes the drag coefficient between the gas phase and the particle phase and \( \tau_r \) represents the gas stress tensor.

The granular temperature equation is shown as follows:
\[
\frac{3}{2} \frac{\partial}{\partial t}(e_{pG} \theta) + \nabla \cdot (e_{pG} \theta) u_P = \nabla P I + \nabla \cdot (k \nabla \theta) - r_i + q_i
\]
(5)

The expression of momentum transfer coefficient between interfaces is as follows:\textsuperscript{31}
\[
\beta_{gs} = \begin{cases}
\frac{3}{4} C_d \frac{\alpha \rho_P u_P - u}{d} \alpha_g^{-2.65}, & \alpha_g \geq 0.8 \\
\frac{150 \alpha^2 u}{\alpha d_i^2} + 1.75 \frac{\alpha \rho_P u_P - u}{d_i}, & \alpha_g < 0.8
\end{cases}
\]
(6)

where
\[
C_d = \begin{cases}
\frac{24}{\alpha_g Re} [1 + 0.15(\alpha_g Re)^{0.687}] & \text{Re} \leq 1000 \\
0.44 & \text{Re} > 1000
\end{cases}
\]
(7)

2.2. Water Evaporation Model. The rate of water vapor per unit area of the slurry is as follows:\textsuperscript{32}
\[
m_w = \frac{D_h}{2R_d} Sh B_M \rho_{total}
\]
(8)

where \( Sh \) denotes the Sherwood dimensionless number,\textsuperscript{33} formulated as
\[
Sh = (2.0 + 0.552 Re^{1/2} Sc^{1/3})(1 + B_M)^{2/3}
\]
(9)

where
\[
B_M = \frac{Y_{sat}(1 - \phi)}{1 - Y_{sat}}
\]
(10)

\( \phi \) denotes the gas relative humidity. The equation can be written as follows:
\[
\phi = \frac{\rho_{hi,0}}{P_{sat}(MIN(T_{hi, sat}, T))}
\]
(11)

The mass transfer area of water vaporization is written as follows:
\[
A_T = \alpha_s \alpha_w \frac{6e_w}{d_{pc}}
\]
(12)

The area covered by water on the particle surface is represented by \( \alpha_s \) and \( \alpha_w \) denotes the influence of the volume fraction of the liquid phase on the area of mass transfer. They can be calculated by the following equations, respectively.
\[
\alpha_s = MIN\left( \frac{e_w d_{pc}}{12 e_{w} d_{pc}}, 1 \right)
\]
(13)

\[
\alpha_w = \begin{cases}
1.0 & e_w \leq 0.0001 \\
\frac{1}{100000(e_w - 0.0001) + 1} & e_w > 0.0001
\end{cases}
\]
(14)

The source term of mass transfer \( m_\bullet \) in the water vaporization process is expressed as follows:
\[
m_\bullet = m_w A_T
\]
(15)

In the course of water vaporization, gas transfers heat to water, while water transfers heat to gas in the form of latent heat evaporation. The energy source terms of the gas and liquid phases are shown below:
diagram and computational grid of the spouted bed. According to the experimental settings, the filling height of the particles is 107 mm, the diameter of the cylindrical and the nozzle of the spouted bed are 53.5 and 14.3 mm, respectively. The cone angle is 60°, and the total height of the bed is 260 mm. The relevant settings for the boundary conditions are the following: the gas inlet and the water inlet are defined as the velocity inlet, the gas outlet is defined as the pressure outlet, and the remaining faces are set as the wall boundary condition. The inlet gas temperature is 520 K, and the temperature of the water is set to 300 K. The grid independence test of the three-dimensional computational model of the bed is shown in Figure 2. The grid numbers were set to 153,455, 213,745, 312,910, and 431,150. It was found that the number of grids of 312,910 was sufficient to ensure a grid-independent solution. Thence, the total number of grid cells was set to 312,910.

The physical properties of the relevant phase composition are listed in Table 1. The mass and heat transfer process in the water vaporization process adopted the method of user-defined function (UDF). Pressure–velocity coupling adopted the SIMPLE algorithm. The turbulent kinetic energy, momentum, and turbulent dissipation rate equations adopted a second-order upwind discretization scheme. The phase volume fraction adopted a first-order upwind discretization scheme.

3. RESULTS AND DISCUSSION

This chapter mainly includes two parts: the gas–solid two-phase flow process and water vaporization process. The distribution of particle volume fraction, radial and axial velocity of the particle, radial and axial velocity of the gas, particle granular temperature, and gas turbulent kinetic energy in the process of gas–solid two-phase flow are discussed and analyzed by a numerical simulation method. The distribution of water, gas–liquid–solid three-phase temperature, the rate of water vaporization, and the factors affecting the rate are discussed in the process of water vaporization.

3.1. Flow of Gas–Solid Two-Phase

Figure 3 illustrates the contours of the particle volume fraction under super gas velocities of 0.7 and 0.8 m/s. From Figure 3a, we can observe that contours of volume fraction at 7.04 and 7.20 s are similar. As time progresses, the flow of gas–solid two-phase in the three-dimensional spouted bed circulated every 0.16 s, indicating that the flow of gas–solid two-phase is periodic and the spouted bed has reached a stable state. While the super gas velocity is 0.8 m/s, the cycle time is 0.16 s.

In general, the flow of fluid in a traditional spouted bed can be divided into three areas: fountain, spout, and annulus area. However, the spouting state in the bed does not form a three-zone structure. Instead, as the gas enters, it first forms a large bubble-like shape in the bed, and then the bubbles keep getting bigger and moving up slowly against the particles, accounting for the size of the spouted bed. In this case, the ratio of bed diameter to gas inlet diameter is 3.74, while the ratio of the traditional spouted bed is generally greater than 8. Consequently, the ratio of the cross section of the continuous gas column to the cross section of the annulus area is larger than that in the ordinary spouted bed throughout the three-dimensional spouted bed.
are similar. The difference is that the higher the gas velocity, the higher the fountain height.

Figure 4 presents the volume fraction distribution of the particle as a function of radial distance under different superficial gas velocities and different bed heights. When the heights are 0.04 and 0.08 m and the superficial gas velocity is 0.8 m/s, the changing trend of volume fraction of particle along the radial distance is similar. However, when the superficial gas velocity is 0.7 m/s, the volume fraction of particle at the center of the bed is higher at 0.04 m due to the presence of particles between adjacent bubbles. At the height of 0.12 m, the higher volume fraction of particle in the middle of the bed is because the particle group sprays upward to form a fountain under the action of the gas. Overall, the distribution trends of particle volume fraction are similar under different superficial gas velocities. The following section analyzes the data when the velocity is 0.7 m/s.

Figure 5a exhibits the contours of the radial velocity of particles in the three-dimensional spouted bed. The particles radial velocity is symmetrical along the center with opposite directions. The particles move with the opposite direction in the cone because they first move toward the center and then move upward under the action of the gas. However, the particles in the cylindrical part move in opposite directions on both sides owing to effect of the airflow. From Figure 5b, the axial velocity of the particles in the center of the bed is the largest, and the downward movement velocity of the particles on both sides of the bed is small. The reason that the axial velocity at the junction of the cone and the cylinder is higher is due to the fact that the particles move downward under the action of pressure and their gravity and then are driven upward by the incoming gas.

Figure 6 presents the contours of the radial and axial velocities of the gas phase in the three-dimensional spouted bed. It can be observed that the gas radial velocity is symmetrical along the central axis of the bed, and the direction is opposite. This proves that the movement of the gas at the cone, the middle of the spout.
area, and the fountain area is a circular movement in opposite directions. As the particles are affected by gravity, pressure and bed structure, the particles tend to gather toward the center, causing the gas to move in the opposite direction. The contours of the axial velocity of gas phase are illustrated in Figure 6b. Since the upper layer of gas is less affected by the force of top particles, the axial velocity of the gas is larger at the top of the spout area.

The degree of particle fluctuation can be evaluated by the granular temperature of the particles. As observed in Figure 7, the granular temperature of the particles is the highest at the bottom of the spout area, higher in the fountain area, and near to zero in the annulus area. It means that under the action of gas, the pulsation fluctuation of particles in the bottom inlet area is greater than that in other areas.

Figure 8 shows the granular temperature of particle along the radial distance at the heights of 0.03, 0.06, 0.09, and 0.12 m. When the height is 0.03 m in the center of the bed, it is observed that the granular temperature of the particles is higher, corresponding to the contours diagram in Figure 7. When the heights are 0.06, 0.09, and 0.12 m respectively, the granular temperature of the particles does not change significantly, which is almost zero. This is because the gas velocity decreases as the bed height increases, resulting in a decrease in particle fluctuation intensity.

Figure 9 exhibits the contours of gas turbulent kinetic energy. Specifically, the gas turbulent kinetic energy is the largest at the junction of the annulus area and spout area, and it gradually decreases to zero when the gas enters the annulus area. The gas in the spouted bed drives the particles to move upward, resulting in a smaller particle volume fraction in the area of the spout. Therefore, the intensity of gas turbulence in this area gradually increases. The distribution of the gas turbulent kinetic energy along the radial distance at the heights of 0.03, 0.06, 0.09, and 0.12 m is shown in Figure 10. Gas turbulent kinetic energy is an essential parameter for evaluating the degree of gas fluctuation. In addition, when the heights are selected as 0.06 and 0.09 m, the turbulent kinetic energy of the gas in the spout area is the largest, corresponding to the cloud diagram in Figure 9.

3.2. Water Vaporization Process. Figure 11 demonstrates the contours of the volume fraction of water at different times in

Figure 6. Contours of radial and axial velocities of gas (unit: m/s).

Figure 7. Contours of particle granular temperature (unit: m²/s²).

Figure 8. Particle granular temperature as a function of the radial distance.

Figure 9. Contours of gas turbulent kinetic energy (unit: m²/s²).

Figure 10. Gas turbulent kinetic energy as a function of the radial distance.

Figure 11. Contours of the volume fraction of water at different times.
the three-dimensional spouted bed. In this case, the superficial gas velocity is 0.7 m/s. It can be observed from the figure that the water mainly gathers at the top of the annulus area of the bed 1 s after the addition of water. As the flow time progresses, the water is dispersed by the particles and airflow in the fountain area, then flows downward along the wall under the action of its gravity and the downward circulating particles in the annulus area, and finally adheres to the surface of the particles. At the sixth second after the addition of water in the annulus area of the spouted bed, the volume fraction of water reaches 0.0003, and it becomes relatively stable in the subsequent time.

The temperatures of gas, particles, and liquid are illustrated in Figure 12. From Figure 12a, because the content of liquid and water in the spout area is low and the heat loss is lower, the gas temperature in this area is high. Meanwhile, in in the annulus area, the gas transfers heat to a large amount of liquid, resulting in a lower temperature in this area. As demonstrated in Figure 12b, contours of the temperature of particles. The particles at the bottom of the spout area are heated by the high-temperature gas. Since the evaporation of water is an endothermic reaction, it absorbs a large amount of heat in other areas, resulting in similar particle temperatures in these areas. Figure 12c is the contours of the liquid temperature; the liquid mainly gathers in the area outside the spout area, and at the junction of the annulus area and the fountain area, the liquid receives the heat transferred by the high-temperature gas, and thus the liquid temperature is higher. The three-phase of gas, liquid, and particles are completely mixed in the fountain area; the liquid transfers heat to the particles, causing a slight drop in temperature.

Figure 13 displays the contours of the water vaporization rate at different times. It is found from the figure that as time progresses, there is no obvious change in the contours of water vaporization rate, indicating that water vaporization has reached a stable state at 17.4 s. Water is added from the top of the bed and contacts the high-temperature gas for vaporization reaction. Due to the high-temperature gas is mainly concentrated in the spout area, the liquid reacts with the gas at the junction of the annulus area and the spout area, where the water vaporization rate is the highest. Moreover, in the center of the spout area, the water vaporization rate is low, and only a small amount of water is vaporized in the annulus area.

Figure 14 describes the distribution of water vaporization rate along the radial distance at different heights. It can be observed that when the heights are 0.03 and 0.06 m, the rate of water vaporization first increases and then decreases as a function of the radial distance and finally tends to a constant value. The maximum is at the junction of the annulus area and the spout area; this is because the liquid phase temperature in this area is higher, which promotes the vaporization of water. As the heights increase to 0.09 and 0.12 m, the gas temperature is lower within this range of height, resulting in a lower rate of water vaporization.

As far as we know, gas velocity, gas temperature, liquid temperature, and gas humidity play a significant role in the water vaporization rate. Figure 15 lists the impacts of gas velocity, gas temperature, liquid temperature, and gas humidity on the water vaporization rate when the bed height is 0.06 m. Figure 15a,b exhibits the influence of gas velocity and gas temperature on the water vaporization rate. Along the radial distance, the changing trends of Figure 15a,b are similar. The gas velocity and gas temperature both drop sharply and then maintain a relatively stable value in the area of annulus. Meanwhile, the evaporation rate of water in the spout area rises sharply, then drops sharply at the junction with the annulus area, and finally reaches a steady state. The reason for the decrease in gas velocity and temperature is the axial movement of the particles; this leads to an increase in the driving force for heat and mass transfer between the gas phase and liquid phase. Therefore, the evaporation rate of water is high in this area. Due to the low gas temperature and velocity in the annulus area, the mass and heat transfers between phases are reduced, resulting in a low water vaporization rate. According to the change curves of the liquid temperature and water vaporization rate, as illustrated in Figure 15c, the liquid temperature and water vaporization rate both increase first, then decrease, and finally stabilize. However, as a function of the radial distance, the water content is increasing, causing the liquid temperature to lag behind the water vaporization rate. In addition, the gas temperature and the water content are higher at the junction of the annulus area and the fountain area, and the promotion of water vaporization is stronger. Figure 15d presents the change curves of the gas humidity and water vaporization rate as a function of the radial distance.
distance. It can be seen from the figure that the change trend of gas humidity is to increase first and then gradually remain stable in the annulus area. Meanwhile, the change trend of water evaporation rate is to first rise sharply, then drop sharply, and finally remain stable. This is because the low gas humidity promotes the mass transfer, thereby promoting the degree of evaporation.

4. CONCLUSIONS
In this paper, the flow behaviors of the gas—solid two-phase flow and water vaporization process in a three-dimensional PPSB are investigated using the CFD method. Additionally, the influence of different factors on the water vaporization rate is also discussed. The conclusions are drawn as follows:

i In the three-dimensional PPSB, the three-phase heat transfer is mainly concentrated outside the spout area; the process of water vaporization mainly occurs at the junction between the annulus area and the spout area.

ii Increasing gas velocity, gas temperature, and liquid temperature and decreasing gas humidity can promote the evaporation of water.

iii The ultimate goal of the water vaporization process is to achieve wet desulfurization and dry treatment of desulfurized products. In the follow-up research, this goal and the impact of parameters on the desulfurization rate need to be further explored.

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Notes

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NOMENCLATURE

| Symbol | Unit          | Description                                      |
|--------|---------------|--------------------------------------------------|
| $v$    | [m/s]         | velocity vector                                  |
| $d_p$  | [mm]          | particle diameter                                |
| $g_0$  | [–]           | radial distribution coefficient                  |
| $h$    | [J/kg]        | enthalpy                                         |
| $\mathbf{I}$ | [–]     | unit tensor                                      |
| $Y_{sat}$ | [–]     | vapor mass fraction at gas–liquid interface     |
| $U$    | [m/s]         | superficial gas velocity                         |
| $T$    | [K]           | thermodynamic temperature                        |
| $\tau$ | [n/m]         | stress tensor                                    |
| $S_c$  | [–]           | Schmidt dimensionless number                     |

Greek symbols

| Symbol | Description |
|--------|-------------|
| $K_g$  | gas-particle drag coefficient |
mixture of biomass and coal with various oxygen carriers.

Simulation of Chemical Looping Combustion using ASPEN Plus for a screen desulfurization system.

on removal of SO2 from flue gas in the semidry FGD process with a

Chem. Eng. Res. Des.

sulfur dioxide abatement with hydrogen peroxide solutions in a packed

3

[kg/m³] density

s

[i] phase type (particle or gas)

s

solid

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