Analysis of Desulfurization Characteristics in Coal-Fired Power Plant by Numerical Simulation and Computer Simulation

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Abstract. In this paper, the spray tower of a wet flue gas desulphurization system in a coal-fired power plant is studied. The flue gas and slurry droplet are two-way coupled with Euler-Lagrange method. The heat and mass transfer and the ion reaction in SO2 removal are also considered. The results show that the error between simulation removal efficiency and practical value is within 5% under the above models. Adjusting liquid-gas ratio and opening spray layer are beneficial to the SO2 removal, and the optimal liquid-gas ratio is 16 L/m3. Balance gas velocity is needed, because an overlarge velocity will significantly reduce removal efficiency.

Keywords: Spray tower, Computational fluid dynamics, Coupling model, Spray layer, Liquid-gas ratio.

1. Introduction

The wet flue gas desulphurization (WFGD) system is the main technology in large coal-fired power plants to remove sulphur currently. In recent years, with the continuous improvement of environmental protection requirements, which reduces the emission standard of SO2 from 200 mg/m3 to 35 mg/m3, the coal-fired power units have been upgraded to achieve this ultra-low criterion [1]. As the key equipment of the WFGD system, the design and operation condition affect the SO2 removal efficiency directly. Moreover, due to the severe environment in the spray tower, there are often failures such as the blockage of spray pipe, the deterioration of slurry and the blockage of mist eliminator. These faults affect the operating stability of the WFGD system.

With the development of the computational fluid dynamics (CFD) technology, many researchers have established flow and absorption models of desulfurization systems by means of numerical simulation. Barwick Company of the United States first introduced CFD technology into the design and improvement of desulfurization system [2], and increased the mass transfer between gas and liquid by adding an open-hole tray in the absorption tower to improve the desulfurization efficiency. Lin et al. [3] numerically simulated the resistance characteristics in the spray tower of a 300MW WFGD system by using Fluent software, and emphatically investigated the resistance characteristics in the spray tower under different tower diameters. The design parameters like spray layer spacing, spray layer number and operating conditions such as different load and liquid-gas ratio are studied.
Some researchers investigated the mass transfer and reaction characteristics of single droplets absorbing SO$_2$, and established a calculation model of liquid mass transfer coefficient based on Higbie's osmotic theory [4]. Marocco et al. [5] explored the interaction between the heat and mass transfer in the absorber and the chemical reaction in the liquid phase, predicted the pressure drop and absorption performance of the desulfurization spray device, and verified the applicability of the calculation model. Qu et al. [6] established a desulfurization system model with coupled flow model, chemical reaction model and mass transfer model. The flow characteristics, SO$_2$ absorption characteristics and pH distribution characteristics of liquid droplets in the desulfurization tower are predicted based on the above models.

In this paper, a coupled flow model of flue gas and liquid droplets is established based on the Euler-Lagrange method, and the operation in the desulfurization tower is numerically simulated considering the heat and mass transfer as well as chemical reactions in the desulfurization process, and the flow, heat and mass transfer characteristics of the desulfurization system are analyzed to provide guidance for the actual operation.

2. Methodology

2.1. Structure description

The WFGD spray absorption tower of a 330MW coal-fired generating unit is the study object, and its cross-sectional structure and main components are shown in Fig. 1. The slurry is extracted from the slurry tank at the bottom of the tower by the circulation pump and then enters the spraying layer along the pipeline and is sprayed out by the nozzles of the spray layer. The raw flue gas enters from the inlet near the bottom of the tower, flows counter-currently with the sprayed slurry and reacts fully, and then removes the possible entrained liquid droplets through the mist eliminator arranged above and flows out from the flue gas outlet at the top, thus removing SO$_2$ from the flue gas [7].

Fig. 1. Schematic diagram of the spray power.

Because the position of the slurry tank has a weak influence on the flue gas flow and droplet spraying process in the tower, only the gas space above the slurry tank is considered in the modeling process [8]. The overall calculated height of the absorber tower is 25.1 m. Four spray layers are arranged in a stepped manner in the tower, with heights of 9.75, 11.45, 13.15, and 14.85 m. The actual structure of the spray layers and mist eliminator is more complex, and it is simplified to a porous media model. Each spray layer is arranged with 48 nozzles, and the nozzles use one-way hollow cone atomization nozzles.

2.2. Model simplifications and assumptions

Considering that the desulfurization process for practical applications involves complex engineering equipment and reaction processes, the two-phase flow of flue gas and liquid droplets in the absorption
tower is somewhat simplified to save computational resources under the condition of ensuring computational accuracy [6].

1. The flue gas is an incompressible fluid and the physical parameters are kept constant.
2. The duct structure in the tower, including the spray tower and mist eliminator, is simplified to the effect of the porous media region on the flow field.
3. Droplets are considered as rigid particles with diameters obeying the Rosin-Rammler (R-R) distribution. The variation of droplet traction coefficient due to evaporation, mass transfer, etc. is not considered.
4. The absorption of SO2 in the slurry tank is neglected, and the calculation area is the part above the slurry tank.
5. The spray slurry touches the wall surface and is assumed to flow down the wall surface. The calculation of the droplet trajectory and the resulting source term is stopped when the droplet hits the wall during the calculation.
6. Only the chemical reactions related to the absorption of SO2 are considered.

2.3. Numerical model

2.3.1. Control equation for gas phase. Considering the flue gas as an ideal gas mixed with SO2 and air, the mass transfer process of SO2 with the evaporation of water is considered, involving the mass and momentum changes caused by the evaporation of water from liquid droplets. The control equations are as follows.

$$\frac{\partial p}{\partial t} + \frac{\partial}{\partial x_i}(p u_i) = S_{\text{mass}}$$ (1)

$$\frac{\partial}{\partial t}(p u_i) + \frac{\partial}{\partial x_j}(p u_i u_j) = \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} (\rho g_i + \rho g_i) + S_{\text{mom,j}}$$ (2)

$$\frac{\partial}{\partial t} (\rho e) + \frac{\partial}{\partial x_j} (\rho eu_j) = -p \frac{\partial u_j}{\partial x_j} + \left[ \lambda_{\text{eff}} \frac{\partial T}{\partial x_j} + u_j \frac{\partial T}{\partial x_j} \right] + S_{\text{en}}$$ (3)

$$\frac{\partial}{\partial t} (\rho \omega_k) + \frac{\partial}{\partial x_j} (\rho \omega_k u_j) = \frac{\partial}{\partial x_j} \left( \rho \frac{\partial \omega_k}{\partial x_j} \right) + S_{\text{en, mass}}$$ (4)

where $\rho$ is density; $u$ is velocity; $S$ is source term, $p$ is pressure; $g$ is gravity acceleration; $\tau$ is stress tensor; $\rho e$ is internal energy per unit mass; $\lambda$ is thermal conductivity; $\omega$ is mass fraction; subscriptions $i$ and $j$ are direction components; subscription $k$ is component $k$; subscriptions mass, mom and en are mass, momentum and energy, respectively; subscript eff is effective value.

2.3.2. Control equation for droplet. The limestone slurry is treated as an inert particle, and the particle mass variation is defined by a user-defined function. The mass conservation equation for droplet particles is as follows.

$$\frac{\partial m_i}{\partial t} = S_{\text{mass}}$$ (5)

Where $m$ is mass and subscript $d$ represents droplet.
Due to the volume fraction of slurry droplets is less than 12% [9], the discrete phase model (DPM) model is suitable to describe the droplet motion. The control equation is

$$\frac{du_i}{dt} = g\left(\frac{\rho_d - \rho_g}{\rho_d}\right) - \frac{3}{4} \left[\frac{\rho_d(u_d - u_g)^2}{\rho_d d} C_D \right]$$

(6)

Where $C_D$ is traction factor and subscript $g$ represent gas.

The discrete-phase orbital random wander model was used to simulate the droplet turbulent diffusion phenomenon due to random pulsations in the continuous phase. The gas-phase pulsation values are considered as each homogeneous and remain constant over the characteristic time of the vortex cluster [10].

The heat exchange between droplets and flue gas mainly includes convective heat exchange between particles and flue gas and latent heat of vaporization from water evaporation. Neglecting the reaction heat released from limestone dissolution and SO$_2$ absorption reaction, the energy conservation equation of droplet particles is as follows.

$$m_d c_d \frac{dT_d}{dt} = h(T - T_d) A_d + L S_{H_2O}$$

(7)

Where $T$ is temperature, $A$ is the surface of the droplets, $L$ is the latent heat of droplet, $c$ is the specific heat and $h$ is the heat transfer coefficient and can be determined by

$$\text{Nu} = \frac{h d}{\lambda} = 2 + 0.6 \text{Re}_{d}^{1/2} \text{Pr}^{1/3}$$

(8)

Where $\text{Re}_{d}$ is the Reynolds number of the droplet and can be calculated as

$$\text{Re}_{d} = \frac{\rho_d |u - u_d|}{\mu}$$

(9)

And $\mu$ is dynamic viscosity.

2.3.3. Control equation for particle evaporation. For the evaporation process of droplet particles, the mass transfer driving force is the difference between the partial pressure of water vapor in the mainstream flue gas and the saturated water pressure under the temperature corresponding to the droplet surface. Using the user-defined function in Fluent to couple the mass transfer rate term of water evaporation as the source term into the calculation of the continuous phase, the mass transfer rate is calculated as follows.

$$S_{H_2O} = k_{H_2O} \left(p_{H_2O} - p_{H_2O,s}\right) A_d M_{H_2O}$$

(10)

Where $k$ is the mass transfer coefficient, subscript $s$ represents the saturated state under the local temperature, and $M$ is the mole mass. The following formula can be used to determine $k$ as [11]

$$\text{Sh} = \frac{k_{H_2O} dRT}{D_{H_2O}} = 2 + 0.6 \text{Re}_{d}^{1/2} \text{Pr}^{1/3}$$

(11)
2.3.4. Control equation for SO2 absorption. The desulfurization process is a chemical absorption process. Since the absorption of SO2 is a fast reaction process, it can be determined that the reaction rate should be determined by the mass transfer rate [12]. Based on the simplification and assumptions of Section 2.2, only the mass transfer process of SO2 in the absorption process is needed to consider. The mass transfer model of SO2 is established using the double film theory, and its relevant control equations are as follows.

\[ S_{SO_2} = k_o p_{SO_2} A_j M_{SO_2} \]  

(12)

Where \( k_o \) is the total mass transfer coefficient.

2.3.5. Boundary conditions. The ambient pressure is set to atmospheric pressure. The flue gas, consisting of air and SO2, enters the tower from the inlet at the bottom with a flow rate of 1246212 m³/h, where the SO2 concentration is 5000 mg/m³ and the inlet temperature is 150 °C. The wall is set up as a non-slip adiabatic wall. The outlet pressure is 1 atmosphere.

The liquid droplets are sprayed from the nozzle to the conical space below, and the action with the flue gas is two-way coupled. The slurry volume of each spray layer is 6000 m³/h. The droplets will be captured when they move to the surrounding wall or to the position of the demister.

3. Result and discussion

3.1. Gas flow characteristics

The flow diagram of the gas phase in the tower for different numbers of spray layers is shown in Fig. 2. As can be seen, after the flue gas enters the spray tower, it rapidly deflects and has the maximum velocity and deflection angle at the upper end of the inlet section. It bears the strongest impact and corrosion effect, which requires attention to protection in practice. When only the first spray layer is open, the bottom space and the middle of the tower has large vortexes, where gas velocity distribution is turbulent. With the increase in the number of spraying layers, the tower vortex size gradually reduced; especially while opening three or four layers of spraying. The gas phase velocity distribution is more uniform, large-scale vortex below the flue gas inlet is generally eliminated, reducing the loss of energy.
3.2. SO$_2$ concentration distribution
When one spray layer is opened, the SO$_2$ concentration distribution in the vertical section is shown in Fig. 3. At the flue gas inlet, the SO$_2$ concentration is higher. When the flue gas comes in contact with the sprayed slurry, the SO$_2$ is gradually absorbed. In the vertical direction, the vast majority of the reaction occurs near the flue gas inlet, and the SO$_2$ concentration gradually plateaus on the way to the gas flow outlet. The difference in radical concentration distribution is mainly determined by local flow direction. The concentration in the middle of the tower is smaller than other places because there is a clear flue gas vortex [see Fig. 2(a)], which makes the flue gas residence time longer and SO$_2$ absorption more adequate.

3.3. Operation characters
The liquid to gas ratio is an important factor affecting the desulfurization efficiency and is also the main parameter for operational regulation. The simulation results and actual values are compared in Fig. 4 in the range of 8-20 L/m$^3$ of liquid to gas ratio. It can be seen that the good agreement is achieved between them, indicating that the model used in this paper has sufficient accuracy.
It can be seen that in the low liquid-gas ratio region (8~16 L/m$^3$), the desulfurization efficiency rises rapidly with the increase of liquid-gas ratio, and the increase of efficiency is about 30%. When the liquid-gas ratio reaches 18 L/m$^3$, the desulfurization efficiency rises slowly, and the increase of desulfurization efficiency is about 2%. Considering the operating economy of desulfurization system, the best liquid-gas ratio should be selected at about 16 L/m$^3$.

As can be seen from Fig. 5, the desulfurization efficiency increases gradually with the increase of the number of spraying layers. When only the first spray layer is open, the desulfurization efficiency is only 73%, while when the second spraying layer is opened, the desulfurization efficiency can reach 90%. This is due to the fact that the location of the first two spray layers is located in the flue gas inlet area where the heat and mass exchange is most intense, and a large amount of SO$_2$ is absorbed in this area. When the third and fourth spray layer is opened to absorb the remaining SO$_2$, the amount of SO$_2$ absorbed at this time gradually tends to saturate because the concentration of SO$_2$ in the flue gas is already relatively low, and the mass transfer rate is also low. In order to meet the environmental requirements, the fourth layer of spraying can be closed to improve the operating economy.

The relationship between inlet flue gas flow rate and desulfurization efficiency is shown in Fig. 6. When the flue gas velocity increases from 3 m/s to 12 m/s, the desulfurization efficiency decreases by about 1.5%. This is due to the fact that as the flue gas flow rate increases, the residence time of liquid droplets in the tower becomes shorter and the reaction time with the flue gas becomes shorter, which
makes some of the SO\textsubscript{2} in the flue gas not fully react with the droplets and results in a decrease in the desulfurization efficiency.

4. Conclusions
In this paper, a coupled CFD model of flue gas flow, droplet evaporation and SO\textsubscript{2} absorption was developed for a spray tower of a 330 MW coal-fired power plant desulfurization system. The flue gas flow and SO\textsubscript{2} concentration distribution in the tower are investigated, and the factors that significantly affect the desulfurization efficiency, such as liquid to gas ratio, number of spray layers and flue gas inlet flow rate, are studied separately, and the main conclusions are as follows.

(1) When flue gas enters the tower, it has the maximum flow velocity and SO\textsubscript{2} concentration at the entrance, and it is easy to form a vortex at the bottom and middle of the tower. Increasing the number of spray layers can effectively weaken the vortex and play a rectifying role. The vortex makes the flue gas residence time increase, which is conducive to SO\textsubscript{2} removal.

(2) Desulfurization efficiency increases with the increase of liquid to gas ratio, the best liquid to gas ratio is 16 L/m\textsuperscript{3}; the more spray layers open, also conducive to increasing the desulfurization efficiency, the fourth layer may be closed; flue gas flow rate increases is not conducive to SO\textsubscript{2} removal, because the time is too short to make the reaction is not sufficient.

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