Simulation Study on the Desulfurization Efficiency Based on Swirl Atomizing

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ABSTRACT

Based on the kinetics of chemical reaction, the theory of turbulent diffusion and the theory of mass transfer, the turbulent flow of flue gas in the desulfurization tower was described by standard $k-\varepsilon$ model, and Lagrangian discrete phase model was employed to solve the particle momentum. The SO$_2$ absorption model of wet flue gas desulfurization (WFGD) tower was established, and swirl atomizing layer (SAL) was installed on the tower. The concentration distribution of SO$_2$ was simulated using CFD method. The results showed that SAL could improve the desulfurization efficiency.

INTRODUCTION

The SO$_2$ absorption was the core part of WFGD. According to the mechanism of chemical reaction, the absorption was essentially a gas-liquid reaction. In order to achieve high desulfurization efficiency, the absorption equilibrium, oxidative equilibrium and crystallization equilibrium were needed happen at the same time. In 1995, Gerbec etc. [1] established the unsteady model of WFGD. And chemical equilibrium and precipitation and dissolution of salt ware built into the model, which laid a foundation of quantitative description of chemical reaction in desulfurization tower.

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CFD could guide the engineering design and optimization, because it could reduce physical model test, shorten the development cycle, save the cost of study and get a lot of local and transient data. It had been introduced to study flow field in tower and concentration distribution. Xiao etc.[3]studied the effect on flow field under several different inlet boundary conditions. Geng Ping [4] by numerical simulation, it illustrated that conventional spray layer was easy to form dead zone and gas corridor. Liu J.Y.[5]by numerical simulation, found the flow field, the droplet trajectories, the escape rate and the residence time in WFGD tower. 

From the research situation at home and abroad, the numerical simulation study of WFGD tower were mainly concentrated in flow field and rarely quantitative description of desulfurization. Based on the kinetics of chemical reaction, the theory of turbulent diffusion and the theory of mass transfer, The SO2 absorption model of WFGD 460000Nm3/h handling capacity was established. The SO2 concentration distribution and the desulfurization efficiency of tower could be calculated.

PHYSICAL AND MATHEMATICAL MODEL

Physical Model

The physical model was limestone/gypsum WFGD tower of 460000Nm3/h handling capacity of a coal-fired power plant[6]. Absorption region of the desulfurization tower was selected as area calculation, leaving out the demister and spray beam. To facilitate the numerical simulation, the physical model were simplified reasonably.

Two-Film Theory

According to the theory of chemical absorption, Calculation of Hatta [7] showed that the reaction was rapid, who was controlled by mass transfer of SO2. 

In 1923, the two-film theory, a classic dynamics theory of mass transfer between interface, was proposed by W.G. Whitman and L.K. Lewis. Some researchers [8-12] both at home and abroad applied the theory to study the SO2 absorption and obtained some achievements.

$$N_A = k_c (P_A - P_{Ac})$$  \hspace{1cm} (1)

$$k_c = \frac{DP}{RT\delta_c P_H}$$  \hspace{1cm} (2)
The process of FGD was conducted in gas, liquid and solid phase.
Considering limestone fully dissolving in the slurry, the resistance of gas film controlled the process, which were described by equation (1).

NA was the mass transfer rate of SO2, mol/(m2⋅s); kG was defined by equation(2), the mass transfer rate of gas film, mol/(m2⋅s⋅Pa); PA, PAi was partial pressure of SO2 in the main body and interface phase, Pa; D was molecular diffusion coefficient, m2/s; P was the total pressure, Pa; R was gas constant, J/(mol⋅K); T was thermodynamic temperature, K; PM was logarithmic mean partial pressure of inert constituent in the main body and interface phase, Pa; δG was gas film thickness and Related to the Reynolds number.

Combining test data of the WFGD tower in operation conditions, a semi-rational derivate formula was showed by equation (3).

\[
N_A = \alpha_1 \cdot \frac{\sqrt{u d}}{T}(P_A - \frac{\alpha_2}{c_{Bi}})
\]  

(3)

Where \(\alpha_1, \alpha_2\) was empirical constant; \(u\) was the relative velocity of gas and slurry particles, m/s; \(d\) was the average diameter of particles, m. Using user-defined functions (UDF) described the absorption rate equation of SO2, being got on the basis of equation (3). So the absorption process of SO2 could be simulated by CFD.

**User-Defined Functions**

In simulation, source item had the relationship with the mass transfer rate of SO2described by equation(4):

\[
M_s = -m_L \cdot N_A \cdot S_V
\]

(4)

Where, \(M_s\) was absorption mass source; \(m_L\) was molar mass of slurry; \(S_V\) was the surface density of discrete phase described by equation(5)

\[
S_V = \frac{m}{(1/6)\pi d^3 \cdot \rho \cdot \pi d^2 \cdot 1/V}
\]

(5)

Where, \(\rho\) was the mass flow rate of slurry, kg/m3; \(V\) was the volume flow rate of gas, m3.
The relationship between MS and other parameters was loaded into the source term of SO2 in UDF, together with other control equations for iterative calculation. Its derivative of related transport equation variables was added to UDF, in order to improve the stability and convergence of iterative calculation.

A three-dimensional mathematical model was developed to simulate flow field of desulfurizing tower. The grid number was more than 1.5 million. Gas flow was 460000 Nm3/h, the density of flue gas was 1.12kg/m3, the inlet velocity of flue gas was 7.8m/s, the inlet concentration of SO2 was 1168mg/m3.

**RESULTS AND DISCUSSIONS**

**Velocity Flow Field Analysis**

Figure 1 showed that, when closing the SAL, the streamline was inhomogeneous and a large number of flue gas, soaring as soon as it entered, didn’t fully mix with slurry soared, which against the absorption of SO2. Figure 2 showed that opening the SAL could solve the problems of inhomogeneous streamline and short contact time in conventional absorption of SO2.

**Concentration Distribution of SO2**

![Figure 1. The gas streamline when closing the SAL.](image1)

![Figure 2. The gas streamline when opening the SAL.](image2)

The SO2 concentration distribution in X-Z section at Y=0, closing and opening SAL, was respectively shown in Figure 3 and Figure 4. The SAL was installed at elevation z = 6.66m in the tower.

The concentration distribution of SO2 in X-Y section at Z=6, Z=8, Z=10 and Z=15m and the outlet average mass fraction of SO2, closing and opening SAL, was respectively shown in Figure 5 and Figure 6.
Figure 5 and Figure 6 showed that, when opening SAL, the concentration gradient of SO2 was less with the increasing of the depth of section. The concentration gradient of SO2 tended to zero in section at Z=15m. The outlet average mass fraction of SO2 increased to 0.00754% from 0.00613%, when closing SAL. That is to say, the desulfurization efficiency increased to 94.17% from 92.82%.

Those figures showed that the increase of the gas local velocity was bad for the absorption of SO2. Although the increase of the gas local velocity might strengthen the turbulent intensity of droplets, indirectly enhancing the mass transfer by increasing the mass transfer coefficient, meanwhile it reduced the local liquid gas ratio. Because of SO2 being soluble in water, the influence of liquid gas ratio on the absorption of SO2 was higher than that of turbulent intensity, consequently the increase of the gas local velocity reduced the absorption rate of SO2. SAL could optimize the gas velocity and improve the absorption rate of SO2.

CONCLUSIONS

Combining two-film theory, based on the kinetics of chemical reaction, the theory of turbulent diffusion and the theory of mass transfer, the concentration distribution of SO2 and velocity flow field analysis were simulated, conclusions as follows:
1. When opening SAL, the distribution of flow field became inhomogeneous, and the absorption efficiency of SO2 improved obviously.
2. While opening SAL, desulphurization efficiency was increased by 1.72%.
3. The simulation results agreed with the experimental approximately. The model could be used to estimate the desulfurization efficiency in engineering.

REFERENCES