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Numerical Simulation on Flue Gas Desulfurization by Activated Carbon Absorption in Circulation Fluidized Bed

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Abstract: Using standard *k-e* model, Euler model, mass transport and finite rate chemical reaction model to simulate the flow and chemical reaction in the CFD reactor. Theoretical knowledge was applied to analyze the simulation results, verified the feasibility of the numerical simulation. Researched the reaction temperature, O_2 content in the flue gas and the molar ratio of carbon -sulfur of affection on the desulfurization, obtained preferably operating parameters, expects to provide valuable reference for industrial production of later.
Key words: CFD; Powdered activated carbon; Flue gas desulphurization; Numerical simulation

1 Introduction

The current environmental pollution situation in China remains severe, with air pollution and acid rain being prominent environmental challenges. A significant part of this issue is attributed to the substantial emissions of SO_2 from industrial coal combustion. With the implementation of the government's 14th Five-Year Plan for energy conservation and emissions reduction, the coordination between economic development and environmental sustainability is receiving increasing attention. Coal is still the most important fossil fuel in China, and this traditional energy structure is unlikely to change in the short term, meaning that flue gas desulfurization will continue to be the mainstream method for controlling SO_2 pollutionI (Figure 1) [1].

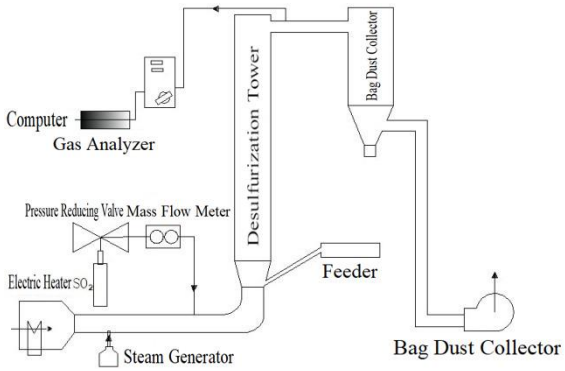

Figure 1 Process Flow of Activated Carbon Circulating Fluidized Bed

The active carbon circulating fluidized bed flue gas desulfurization technology, based on the principle of circulating fluidized beds, has excellent heat and mass transfer performance within the tower during desulfurization, allowing for thorough mixing of activated carbon and flue gas, as well as handling large volumes of flue gas. The wear on the powder adsorbent is reduced, and the manufacturing process for the adsorbent is relatively simple. This technology is an advanced flue gas purification method that has been widely applied, but it still possesses broad prospects for development[2]. This research utilizes numerical simulation methods to investigate the effects of reaction temperature, the O_2 content in flue gas, and carbon-sulfur molar ratio on the desulfurization effectiveness, obtaining useful fundamental parameters.

2 Model Establishment

2.1 Physical Model

The simulation in this paper is based on a complex three-dimensional model of a circulating fluidized bed reactor, as shown in Figure 2. The main structure of the reactor is a vertical cylinder with a height of 2.0 meters and a diameter of 0.3 meters. The flue gas inlet section of the reactor is funnel-shaped, with an inlet diameter of 0.18 meters and a vertical height of 0.2 meters. The powdered activated carbon inlets have a diameter of 0.02 meters and are located on either side of the bottom end, inclined at a 45-degree angle to the vertical. The outlet diameter after the flue gas treatment is 0.05 meters, situated at the top end, 0.05 meters from the uppermost point. A non-structured tetrahedral meshing method with a step size of 0.02 was used to discretize

the reactor structure, dividing the reactor into a combination of 270,000 computational cells, as shown in Figure 2. To analyze the practical issues of this model, a segregated computation approach was adopted with single-precision accuracy for calculations, using an unsteady state method for iterations[3].

Figure 2. Physical Model and Mesh Partitioning

To facilitate quicker and more convenient calculations without significantly affecting the overall results, the model can be simplified with the following assumptions: only the chemical reaction of activated carbon adsorbing SO_2 is considered; the reaction heat is ignored; the activated carbon particles are assumed to have uniform size and isotropic properties; the effect of the inherent reactivity of activated carbon on the reaction is disregarded; for simulation purposes, the volumetric fraction of SO_2 set in the model is assumed to be slightly higher than that in actual conditions.

2.2 Mathematical Model

(1) Establishing the standard k-e model

The turbulence kinetic energy equation:

$$\frac{\partial(\rho k)}{\partial t}+\nabla\cdot(\rho U\kappa)-\left[\left(\mu+\frac{\mu_r}{\delta_k}\right)\nabla\kappa\right]=P+G-\rho \mathrm{e} \tag{1}$$

The turbulence dissipation equation:

$$\frac{\partial(\rho \mathrm{e})}{\partial t}+\nabla\cdot(\rho U\mathrm{e})-\nabla\left[\left(\mu+\frac{\mu_r}{\delta_k}\right)\nabla\kappa\right]=C_t\frac{\mathrm{e}}{\kappa}\left[P+C_3\max\left(G,0\right)\right]-C_2\rho\frac{\mathrm{e}^2}{\kappa} \tag{2}$$

Where P is the shear production term, and G is the volumetric production term[4].

(2) Establishing the Euler model for multiphase flows

The Euler model is selected, ignoring the effects of lift, added mass force, and wall slip boundaries.

Mass conservation equation:

$$\frac{\partial}{\partial \mathrm{t}}\left(\alpha_{\mathrm{q}}\rho_{\mathrm{q}}\right)+\nabla\bullet\left(\alpha_{\mathrm{q}}\rho_{\mathrm{q}}\mathrm{u}_{\mathrm{q}}\right)=\sum_{\mathrm{q}=1}^{\mathrm{n}}\mathrm{m}_{\mathrm{pq}} \tag{3}$$

Where u is the velocity, m is the transported quantity, a is the volume fraction, and ρ is the density.

Momentum conservation equation:

$$\frac{\partial}{\partial \mathrm{t}}\left(\alpha_{\mathrm{v}}\rho_{\mathrm{v}}\mathrm{u}_{\mathrm{v}}\right)+\nabla\bullet\left(\alpha_{\mathrm{v}}\rho_{\mathrm{v}}\mathrm{u}_{\mathrm{v}}\mathrm{u}_{\mathrm{v}}\right)=-\alpha_{\mathrm{v}}\nabla\mathrm{p}+\nabla\tau+\alpha_{\mathrm{v}}\rho_{\mathrm{v}}\mathrm{g}+R_{\mathrm{vs}}+\mathrm{m}_{\mathrm{sv}}\mathrm{u}_{\mathrm{sv}} \tag{4}$$

$$\frac{\partial}{\partial \mathrm{t}}\left(\alpha_{\mathrm{s}}\rho_{\mathrm{s}}\mathrm{u}_{\mathrm{s}}\right)+\nabla\bullet\left(\alpha_{\mathrm{s}}\rho_{\mathrm{s}}\mathrm{u}_{\mathrm{s}}\mathrm{u}_{\mathrm{s}}\right)=-\alpha_{\mathrm{s}}\nabla\mathrm{p}+\nabla\tau+\alpha_{\mathrm{s}}\rho_{\mathrm{s}}\mathrm{g}+R_{\mathrm{sv}}+\mathrm{m}_{\mathrm{vs}}\mathrm{u}_{\mathrm{vs}} \tag{5}$$

Where u is the velocity, m is the transported quantity, a is the volume fraction, ρ is the density, p is the pressure of the two phases, ∇τ is the stress variable, R is the drag force, and g is the acceleration due to gravity [5].

(3) Material transport and finite-rate chemical reaction model

The conservation equation adopts the following general form:

$$\frac{\partial}{\partial \mathrm{t}}\left(\rho Y_{\mathrm{i}}\right)+\nabla\bullet\left(\rho\vec{\mathrm{v}}Y_{\mathrm{i}}\right)=-\nabla\overrightarrow{J_{\mathrm{i}}}+R_{\mathrm{i}}+S_{\mathrm{i}} \tag{6}$$

Where R_i is the net production rate of the chemical reaction, and S_i is the additional production rate due to the discrete phase and user-defined source terms.

3 Analysis of Simulation Results

3.1 Influence of Temperature

Temperature is a crucial process parameter in the desulfurization process using powdered activated carbon. In this simulation, while keeping other processing conditions constant, the temperature within the reactor was varied to study the effect of reaction temperature on the desulfurization performance of powdered activated carbon in the circulating fluidized bed. Figure 3 illustrates the correlation between desulfurization performance of powdered activated carbon and temperature, with a carbon to sulfur molar ratio of approximately 60 and reactor temperatures ranging from 313.15 K to 343.15 K. The results indicate that as the temperature increases, the effect of temperature on the desulfurization performance of powdered activated carbon initially promotes the reaction up to an optimal temperature, after which it begins to inhibit performance. Below 333.15 K, the changes in desulfurization efficiency with increasing temperature are not significant; however, in the temperature range above 333.15 K, the desulfurization efficiency actually decreases with rising temperature. In the initial stage of SO_2 removal using powdered activated carbon, the process is primarily governed by physical adsorption. As the surrounding temperature increases, the rate of physical adsorption slows down. Subsequently, activated SO_2 can be oxidized to SO_3, which then combines with water vapor to form sulfuric acid. Although an increase in temperature facilitates the oxidation reaction, the higher reaction temperature, while promoting the chemical reaction, is detrimental to the physical adsorption of SO_2 by powdered activated carbon. Additionally, the increase in reactor temperature significantly reduces the amount of water vapor that can be adsorbed, resulting in the generated sulfuric acid not being effectively removed from the active centers on the surface of the powdered activated carbon, further contributing to a decline in desulfurization efficiency.

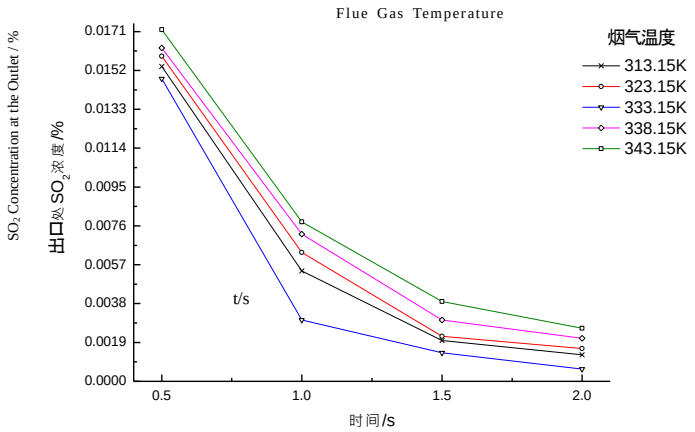

Figure 3 Curve of Temperature's Influence on Desulfurization Effect

3.2 Influence of O_2 Concentration

Research analysis indicates that when there is no oxygen in the flue gas, SO_2 cannot be oxidized; this means it can only undergo weak physical adsorption and cannot engage in chemical adsorption. As the concentration of oxygen increases, chemical adsorption begins to take place. The higher the concentration, the stronger the adsorption effect, leading to better desulfurization performance. Figure 4 presents the curve illustrating the impact of the volumetric fraction of O_2 in flue gas on desulfurization efficiency. At very low levels of O_2 concentration, the simulation results show that the desulfurization efficiency of powdered activated carbon is quite low, remaining below 20%. As the volumetric fraction of O_2 is increased, the desulfurization efficiency gradually improves. When the O_2 volumetric fraction rises from 2% to 6%, the rate of increase in desulfurization efficiency is rapid. However, when the volumetric fraction of O_2 increases from 6% to 8%, the rate of increase in desulfurization efficiency begins to slow down. Considering economic factors and other comprehensive issues, it is concluded that a volumetric fraction of O_2 in the flue gas at 6% represents an optimal condition for desulfurization.

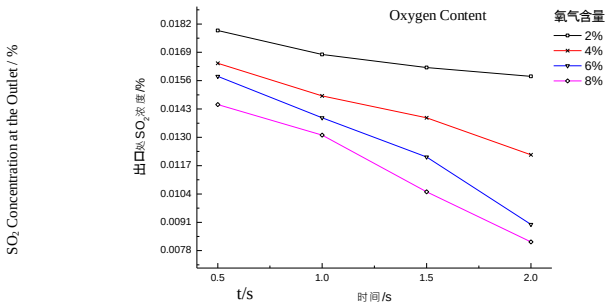

Figure 4 Curve of O_2 Concentration's Influence on Desulfurization Effect

3.3 Influence of Carbon to Sulfur Molar Ratio

An increase in the carbon to sulfur molar ratio leads to an enlarged surface area of the adsorption micropores, which in turn increases the active surface area available for oxidation. This favors the adsorption of SO_2 by the activated carbon. However, as the mass concentration of powdered activated carbon in the reactor continues to increase, the very small particle size and high specific surface area of the activated carbon can lead to agglomeration. This agglomeration can result in the blockage of some voids, thereby increasing mass transfer resistance and decreasing the availability of active sites, ultimately slowing the increase in desulfurization efficiency. The impact of changes in the carbon to sulfur molar ratio on the desulfurization efficiency of powdered activated carbon is illustrated in Figure 5. When the carbon to sulfur molar ratio is 20, the desulfurization efficiency of powdered activated carbon is relatively low. As the carbon to sulfur molar ratio increases, the desulfurization efficiency also rises, although the trend of this increase exhibits stage-wise changes. When the ratio increases from 20 to 60, the change in desulfurization efficiency is significant; however, when the ratio rises from 60 to 100, the change in desulfurization efficiency becomes less pronounced. Considering the mixing of gas and solid phases within the reactor and various economic factors, it is concluded that a carbon to sulfur molar ratio of 60 achieves a relatively optimal desulfurization state.

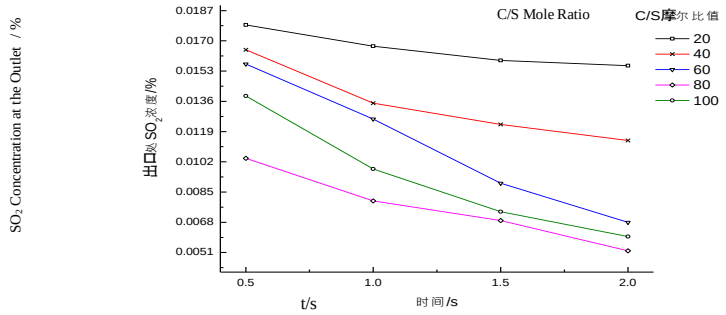

Figure 5 Curve of Carbon to Sulfur Ratio's Influence on Desulfurization Effect

4 Conclusion

The numerical simulation results obtained were analyzed in conjunction with theoretical insights, validating the feasibility of the simulation method. It is concluded that during the desulfurization operation of activated carbon circulating fluidized bed, controlling the temperature at 333.15 K, increasing the O_2 concentration in the flue gas to 6%, and adjusting the carbon to sulfur molar ratio to 60 are optimal operating parameters that can achieve good desulfurization effects.

Declaration of Conflicting Interests

The author(s) declared no potential conflicts of interest with respect to the research, author-ship, and/or publication of this article.

Data Sharing Agreement

The datasets used and/or analyzed during the current study are available from the corresponding author on reasonable request.

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