Simulation research of SCR optimal operation

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Abstract: Selective catalytic reduction technology (SCR) has high denitrification efficiency. It is the main techniques adopted in our country of flue gas denitrification. Due to lack of effective NH₃ spraying methods and means, stock of low efficiency, high rate of ammonia escape problems, secondary pollution is serious in the actual operation of the existing SCR system. In this paper, using computational fluid dynamics (CFD) method, establishing of three dimensional numerical model of SCR system. Flue gas flow and the NH₃/NOx distribution characteristics were analyzed by numerical simulation in SCR system. Studying on the effect of different parameters on the ammonia injection of the reactor entrance speed of the first layer of the catalyst entrance section and the distribution of the NH₃/NOx molar ratio, then providing optimizational parameters of the ammonia injection.

1. Introduction
The emission of nitrogen oxides from coal combustion is one of the major sources of atmospheric pollutants. NOx can directly harm human health. It can also lead to the formation of acid rain and photochemical smog and cause atmospheric greenhouse effect. One of the key technologies in the design and operation of SCR ammonia injection systems is how to ensure that the mixed flue gas flow rate and NH₃/NOx concentration distribution at the inlet of the catalyst layer can be more uniform, thus ensuring higher denitrification efficiency and avoiding ammonia slip. Therefore, reasonable control of the NH₃/NOx molar ratio and its uniformity of distribution are essential for improving the operational performance of the SCR system[1-3].

In this paper, a 660 MW supercritical unit is used as the object, and a three-dimensional numerical model of the SCR system is established using the CFD method. The flue gas flow and the NH₃/NOx distribution characteristics are simulated. The flow of SCR reactor in different ammonia injection parameters is investigated. Study of the effects of NH₃/NOx molar ratio distribution uniformity and deviation. The research results can provide guidance for the optimization of SCR system operation for similar units.

2. Simulation Research and Methods

2.1 Mathematical model
The section size of the flue gas at the inlet of the SCR is 3.2m×10m, the section size of the flue gas in the injection section is 3.2m×13.95m, and the distance between the two layers of the sprayed ammonia grid is 1.762m, and there are 8 ammonia injection pipes on each floor. Figure 1 shows the layout of ammonia injection pipes. The size of the upper ammonia injection pipe is φ76mm×2.5mm, and the size of the lower ammonia injection pipe is φ76mm×1.5mm. The monolayer catalyst size is 11.2m×13.95m×0.875m. Three-dimensional modeling of SCR system using pre-processing software GAMBIT. Figure 2 shows the geometric model of the flue gas denitrification SCR system.

2.2 Calculating the Mathematical Model
This paper uses FLUENT software to select the reasonable mathematical model based on the theory of computational fluid dynamics to carry out the optimization research of SCR reactor.

Because of the limited conditions, the smoke condition in the SCR system is assumed and simplified as follows[4]: (1) Uniform distribution of inlet gas velocity, temperature, component concentration, etc.; (2) Temperature difference between the actual system inlet and outlet is small, assuming that the system adiabatic and isothermal; (3) The actual system has a small air leakage, so the air leakage of the system is not considered; (4) The ash in the flue gas has little influence on the content of this study, so the impact of ash is not considered; (5) The flow assumption is steady flow; (6) Flue gas components and reducing agent gas are assumed to be ideal gases; (7) Catalyst layer pressure drop is simulated with porous media and a pressure loss equivalent to the actual operating value is generated.

The models used for the numerical simulation of SCR process are: (1) The k-ε model with swirl correction is used to simulate the turbulent flow; (2) The model of the porous catalyst is used for the simulation of the catalyst structure; (3) The multi-component transport model is selected for the mixing simulation of various substances. In the solution process, the turbulent kinetic energy, the turbulent flow energy dissipation rate, and the momentum equation all adopt the first-order upwind style. The pressure and velocity coupling is based on the SIMPLICE C algorithm.

2.3 Standard Deviation Criteria
One of the goals of the flow field optimization of the SCR system is to realize the uniformity of airflow distribution within the system[5]. At present, the most commonly used is the RMS standard of the United States, which is the relative rms method. Its formula is as follows:

\[ Cv = \left( \frac{1}{n} \sum_{i=1}^{n} \left( \frac{v_i - \phi}{\phi} \right)^2 \right)^{1/2} \times 100\% \]

Cv—the velocity distribution homogeneity deviation coefficient; n—the number of measurement points of the velocity measurement section; vi—the airflow velocity of the measurement point, m/s; \( \phi \)—the average cross-sectional airflow velocity measured, m/s. Its formula is \( \phi = \frac{1}{n} \sum_{i=1}^{n} v_i \).

Uniform distribution of NH3/NOx molar ratio is another objective of the flow field optimization of the SCR system. The unevenness of the ammonia injection concentration is indicated by the symbol \( C_{\rho} \).
\[ C_\rho = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (\rho_i - \xi)^2} \times 100\% \]

\[ \xi = \frac{1}{n} \sum_{i=1}^{n} \rho_i \]

The uniformity of the mixing of NH\textsubscript{3} and NO\textsubscript{x} is considered to be better if the coefficient of deviation of the distribution of the flue gas velocity distribution \( C_\text{v} < 15\% \) and the coefficient of variation of the distribution ratio NH\textsubscript{3}/NO\textsubscript{x} molar ratio \( C_\rho < 5\% \).

### 3. Simulation Results and Analysis

The internal structure of the deflector, rectifier grille, etc. of the SCR system in this article is well-designed and fixed, and will not be adjusted. The ammonia injection rate parameter of the ammonia injection pipe also has a great influence on the uniformity of the NH\textsubscript{3}/NO\textsubscript{x} molar ratio of the first catalyst inlet section in the SCR reactor. Therefore, this article mainly optimizes the ammonia injection operating parameters of the SCR system. Three programs of ammonia injection parameters were studied.

The NH\textsubscript{3}-air mixture of the upper and lower ammonia nozzles of program 1 has the same injection rate; the mixture gas rate of the upper ammonia tube of program 2 is slightly less than the speed of the lower layer, and the speed of each layer of the nozzle remains the same; program 3 is based on program 2, adjust and optimize the speed of different ammonia spouts for each layer. The velocity parameters of the flue gas inlets and the ammonia injection inlets of the three programs are shown as Table 1. In the BMCR condition, the temperature of the inlet of the flue gas is consistent with that of the former at 657 K, the velocity of the flue gas is set at 20 m/s, and the temperature of the ammonia injection inlet is consistent with that of the former at 293 K.

| Injecting Number | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  |
|-------------------|----|----|----|----|----|----|----|----|----|
| **Program 1**     |    |    |    |    |    |    |    |    |    |
| Upper and lower levels | 15.5 | 15.5 | 15.5 | 15.5 | 15.5 | 15.5 | 15.5 | 15.5 | 15.5 |
| **Program 2**     |    |    |    |    |    |    |    |    |    |
| Upper level       | 14.5 | 14.5 | 14.5 | 14.5 | 14.5 | 14.5 | 14.5 | 14.5 | 14.5 |
| Lower level       | 16.5 | 16.5 | 16.5 | 16.5 | 16.5 | 16.5 | 16.5 | 16.5 | 16.5 |
| **Program 3**     |    |    |    |    |    |    |    |    |    |
| Upper level       | 15.5 | 13.0 | 17.0 | 17.5 | 16.5 | 15.0 | 14.0 | 13.5 | 12.0 |
| Lower level       | 16.0 | 14.0 | 15.0 | 13.0 | 15.5 | 16.5 | 17.0 | 16.5 | 19.0 |

#### 3.1 Flow uniformitys

Figure 3 shows the velocity profile of the central section of the SCR denitration system. It can be seen that the baffles have a great influence on the velocity field of the flue gas, especially the six disk-guiding grids at the corners, which promote the mixing of flue gas and NH\textsubscript{3} by increasing the disturbance of the flue gas. The presence of the 10 curved baffles above the SCR reactor and the rectifier changes the flow direction of the mixed flue gas, so that the velocity of the flue gas entering the first catalyst layer remains as uniform as possible in the Z direction.
3.2 Analysis of simulation results of mixed smoke concentration field

Figure 5 and Figure 6 show the NOx molar concentration and the NH3/NOx molar ratio of the first catalyst inlet section in the SCR reactor, respectively. According to the comparison between scenario 1 and scenario 2, under the condition that the ammonia injection rate of the next layer is slightly higher than the ammonia injection rate of the upper layer, the uniformity of the NH3/NOx molar ratio of the first catalyst inlet cross section in the SCR reactor will be significant. The improvement in the uniformity of the velocity of the first-stage catalyst inlet cross section in the SCR reactor is not significant. This is mainly due to the fact that the relative share of ammonia gas is relatively small, and the rate of ammonia injection is changed while the total amount of ammonia injection is unchanged. The velocity of the cross section of the first layer catalyst in the SCR reactor does not change much. However, because the amount of ammonia in the lower layer increases, the amount of ammonia in the previous time decreases, and the time for mixing the lower layer of ammonia and flue gas is long, and NH3 and NOx are more mixed. Uniformly, the uniformity of the NH3/NOx molar ratio of the first catalyst inlet cross section in the SCR reactor will be significantly improved.
The plan 3 is the optimization made on the basis of plan 1 and plan 2. That is, on the basis that the ammonia injection rate of the next layer is slightly greater than the ammonia injection rate of the upper layer, the ammonia injection rate parameter of each nozzle at each layer is adjusted. By calculation, the uniform coefficient \( C_{\rho 1} = 5.42\% \) of the \( \text{NH}_3/\text{NO}_x \) molar ratio of the plan 1, the uniform coefficient \( C_{\rho 2} = 3.95\% \) of the \( \text{NH}_3/\text{NO}_x \) molar ratio of the plan 2, the uniform coefficient \( C_{\rho 3} = 1.75\% \) of the \( \text{NH}_3/\text{NO}_x \) molar ratio of the plan 3. The results show that the uniformity of the \( \text{NH}_3/\text{NO}_x \) molar ratio distribution at the entrance of the first layer of catalyst in the SCR reactor has been greatly improved by reasonably adjusting the parameters of the ammonia gas vents.

In summary, this paper provides three kinds of ammonia injection programs. The numerical simulation method is used to analyze and compare the flow field and mixed smoke concentration field of the three programs. The results show that the speed parameters of the ammonia injection pipe can be rationally optimized. Targeted control of the amount of ammonia injected in different regions can achieve uniform mixing of \( \text{NH}_3 \)-air and flue gas, ultimately ensuring that the SCR system has a high denitration efficiency and low \( \text{NH}_3 \) escape rate.

4. Conclusion

This paper uses computational fluid dynamics (CFD) method to establish a three-dimensional numerical model of the SCR system. The numerical simulation of the flue gas flow and \( \text{NH}_3/\text{NO}_x \) distribution characteristics in the SCR system is conducted. The SCR reactor in different ammonia injection parameters is studied. The effect of the uniformity of the inlet velocity field and \( \text{NH}_3/\text{NO}_x \) molar ratio distribution of the layer of catalyst entrance. By reasonably optimizing the speed parameters of the ammonia injection pipe, the corresponding amount of ammonia injection in different regions can be controlled in a targeted manner, uniform mixing of \( \text{NH}_3 \)-air and flue gas can be achieved, and ultimately ensuring that the SCR system has a high efficiency of denitration and low \( \text{NH}_3 \) escape rate.

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