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Energy Procedia 17 (2012) 801 – 812

Energy
Procedia

2012 International Conference on Future Electrical Power and Energy Systems

Optimization and Numerical Simulation of the Flow Characteristics in SCR System

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Abstract

Selective Catalytic Reduction (SCR) DeNO_x is the main flue gas denitrification technology, and the efficiency of SCR DeNO_x system depends on whether the flue gas and ammonia distributions of the velocity and concentration fields are uniform in the reactor. Combined with the porous medium model and component transport equations, the numerical simulations were carried on for the SCR system of the 1000MW coal-fired station, and the velocity fields and concentration fields in different cases were obtained. The results showed that: the corner vane cascades and rectifier grills installed, the non-uniformity of flue gas velocity is less than 15% at the catalyst inlet within the reactor. Under the premise of the best flow field, the vortex mixers can ensure the full blending of the ammonia and flue gas in the reactor. The reliability of numerical simulation is verified through the cold model test, and then the design of the SCR system is guided effectively by the numerical simulations.

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Keywords-SCR denitrification; numerical simulation; porous medium; flow field

1. Introduction

The Selective Catalytic Reduction (SCR) of NO_x is a mature flue gas post-processing technique [1]. SCR DeNO_x systems with large equipment size and limits of stack layout make considerable demands on velocity of flue gas, ammonia nitrogen ratio, temperature fields and ash distributions. It should be studied deeply how to obtain a uniform flow field of flue gas and an adequate mixing of flue gas and ammonia, which will provide guidance for the independent design of SCR units, and it also possesses a great significance on energy saving and emission reduction of coal-fired power plants.

At present, the internal flow mechanism in SCR systems is a hot issue. Methods of experimental testing and numerical simulation are two main ways on studying SCR. Whether the results of numerical simulation are correct, it should be tested by experiments, on the other hand, flow phenomenon can be recognized comprehensively and profoundly through the numerical results, and the project amount of experiments can be reduced, the period of study can be shortened and level of research can be improved. Numerical simulation and experimental test are interdependent and complementary.

The reference [2] conducted the laboratory-scale and pilot-scale on SCR DeNO_x, and the experimental and numerical research on flow and mixing of gas in reactor were finished. Based on the SCR mathematical model and the probability distribution of SCR system, a simulation method was proposed to analyze the influence of uncertainty factor on SCR reactor. In reference [3], the research was based on guide plates in SCR reactor of 600MW power plant. The appropriate shapes of guide plates and reasonable flow in SCR reactor were obtained by using Fluent. In reference [4], the investigation concentrates on the ammonia's flow field in AIG, and the results of the research could offer reference to the design and improvement of the SCR system. The reference [5] simulated SCR system. The result showed that the position of guide plate influenced greatly the velocity distribution before the entrance section of catalyst, which is believed to be beneficial to performance improvement of SCR reactors.

In this paper, the numerical simulations were carried on for the SCR system of the 1000MW coal-fired station and some specified scheme were optimized, such as SCR reactor, ammonia injection system, vortex mixer and so on. The flow filed and concentration filed was obtained in BMCR operating conditions and the reliability of numerical simulation results was verified by the cold test.

2. The Scheme of Research

The simulated schemes were shown in table 1. This physical dimension is based on actual dimension of SCR system. SCR is with two-reactor structure. The geometry model was shown in figure 1. The calculations included the following sections:

Case 1: To determine the SCR system structure without vane cascades, rectifier grilles and vortex mixer. The flow characteristic, velocity filed and pressure distribution in the SCR system, especially in every corner, was investigated, which will provide the reference for designing the vane cascades, rectifier grilles and vortex mixer in following cases.

TABLE I The scheme of numerical simulation

Cases	SCR	Vane cascades	Rectifier grilles	Vortex mixer	Simulation characteristics
1	yes	no	no	no	Flow field
2	yes	yes	no	no	
3	yes	yes	yes	no	
4	yes	yes	yes	yes	Concentration field

Case 2: To determine the vane cascades including its shape, number and position.

Case 3: To determine the rectifier grilles including its structure and scale.

Case4: To determine the vortex mixer including its shape, installed angle, and nozzle location, so that ammonia and nitrogen oxides mix completely.

2.1 Vortex mixer

The ammonia injection system adopts the vortex mixer in the SCR units shown in figure 2, which is with the characteristics of strong adaptability for flu gas, better mixture effects and small numbers of ammonia nozzle, and the vortex mixer does not require maintenance. When diluted ammonia injects onto the disc through pipes, ammonia blends into flu gas completely to meet the concentration requirement. In this paper five vortex mixers were adopted, the angles between the disk of vortex mixer and horizontal direction is 60 degree. The center of five vortex mixer is stretched out horizontally in a straight line.

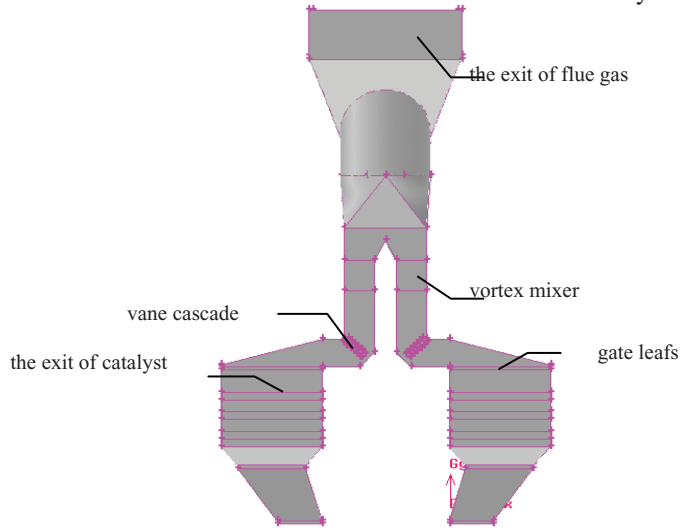


Figure 1. The physical model of SCR system

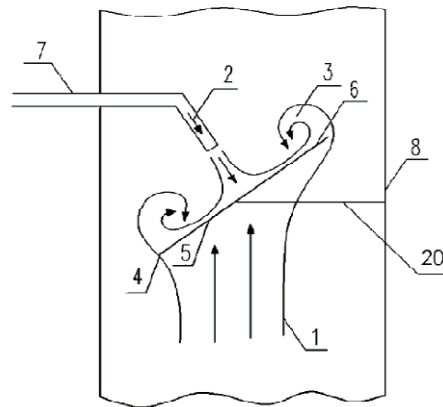


Figure 2. The schematic diagram of vortex mixer

- 1-flue gas 2- ammonia 3-vortex 4-disk
- 5-upwind side 6-downwind side 7- ammonia nozzle
- 8-gas duct 20-bearing beam

3. Mathematical Model and Numerical Method

In the boilers of large power station, the process of SCR DeNOx is very complicated. It involves the design of reactor structure, turbulent flow and mix of flue gas and ammonia in the SCR system, heat and mass transfer, multi-component transport and chemical reaction and so on. Because of limited conditions, the assumptions need to be specified on actual process before building model:

Owing to small temperature difference between the inlet and outlet of SCR system, the system is considered to be adiabatic. No consider the effect of ash, because the influence of ash on research content is small. In the upstream flue gas of reactor, the flue gas component don't occur chemical reaction. Flow is steady and the physical parameter of fluid is constant.

3.1 General governing equation

The general governing equation in three-dimensional Cartesian coordinate is shown equation (1), which each variable expression is as follows [6]:

$$\frac{\partial(\rho\phi)}{\partial t} + \text{div}(\rho u\phi) = \text{div}(\Gamma \text{grad}\phi) + S \quad (1)$$

3.2 Turbulence model

Standard $k - \varepsilon$ two equation model can be expressed as

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho k u_i)}{\partial x_i} = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k - \rho \varepsilon \quad (2)$$

$$\frac{\partial(\rho \varepsilon)}{\partial t} + \frac{\partial(\rho \varepsilon u_i)}{\partial x_i} = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + \frac{C_{1\varepsilon} \varepsilon}{k} G_k - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} \quad (3)$$

3.3 The porous medium model

Catalyst is the core of SCR. In the paper, the honeycomb type SCR catalyst is adopted. If catalyst bed is constructed physically using numerical simulation, the grid of model will reach thousands upon thousands, which is restrained by computer. Consequently the porous medium model was adopted to simulate the flow in the catalyst bed and rectifier grilles.

The resistant formula of porous medium model can be expressed as

$$\Delta p = - \left(\frac{\mu v}{\alpha} + \frac{C_2 \rho v^2}{2} \right) \Delta m \quad (4)$$

Where $\rho = 1.293 \text{ kg/m}^3$, α is porous medium permeability, μ is viscosity coefficient, C_2 is pressure jump coefficient, Δm is the thickness of air distribution plate.

3.4 Component transport equations

Because SCR system involves mixture of a variety of gas composition, so transport model is used to simulation. The general equation is adopted as follow:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \bar{v} Y_i) = -\nabla \bar{J}_i + R_i + S_i \quad (5)$$

In the equation, R_i is the net production rate of chemical reaction, S_i is the extra production rate by discrete-phase.

3.5 Numerical method

The control volume method is used to discretize the governing equations, while the pressure-velocity coupling item is based on SIMPLE algorithm and the finite difference scheme of convection-diffusion equation is the second-order upwind scheme. Unstructured tetrahedron grid in GAMBIT is used to discretize the computational zone, where the grid is more densely in the area with high turbulence level.

The inlet velocity of flue gas is defined 12m/s according to the entrance size of SCR system in the BMCR condition. The boundary conditions include velocity inlet, pressure outlet and no slip wall. Turbulence parameters are defined according to turbulence intensity and hydraulic diameter. The enhanced wall function is adopted to near wall regions. The porous medium model is used for rectifier grilles and catalyst layer. The five ammonia nozzles of vortex mixer are set to velocity boundary.

4. The Analysis of Computational Results

4.1 The result of case 1

Figure 3 shows that pressure and velocity results of SCR reactor on symmetry plane ($Z=0$) of case 1. Figure 4 reveals that internal pressure result of SCR reactor on the left side. From the distribution of velocity and pressure we can see that velocity and pressure field becomes non-uniformity before flue gas enter catalyst through corner. Flue gas deflects laterally of the SCR reactor under the action of inertial force and centrifugal force. After the corner, the velocity of flue gas changes largely before catalyst entrance in the SCR reactor and a recirculation zone forms. Correspondingly, pressure gradient of catalyst entrance section is large, which will affect mixing effect of ammonia. Consequently, to improve velocity field of whole SCR system, the turning corner need to be designed reasonably, and guide device need to be installed in the corner. From the results we can see that flow field inside the vertical flue duct is uniformity, while the velocity and pressure field is non-uniformity before the catalyst through corner. The velocity distribution of flue gas is non-uniformity in the catalyst entrance section of SCR reactor and recirculation zone still exists in the section, so the guide devices are designed according to the results.

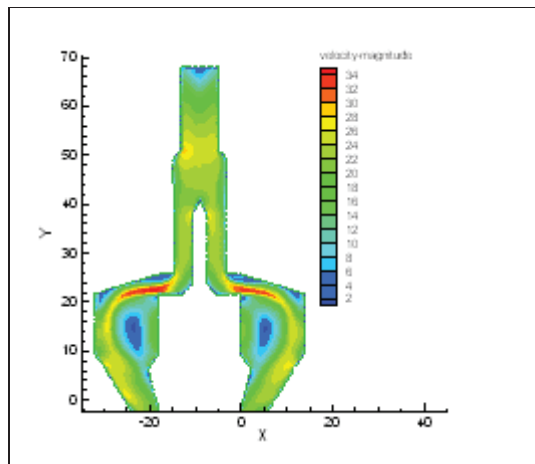


Figure 3. the velocity distribution on Z=0 section (case 1)

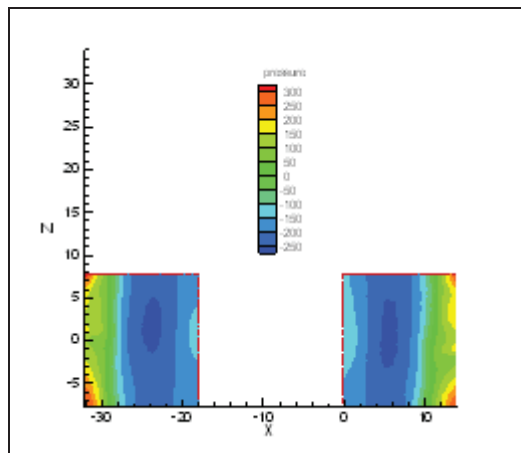


Figure 4. the pressure distribution on catalyst entrance section(case 1)

4.2 The result of case 2

Guide cascades are further designed and installed based on the case 1. The calculation results are shown in figure 5-6. From the figures, guide cascades improve the flow effectively in the first corner of the SCR system, where the distribution of velocity and pressure is uniformity, while the flow before catalyst entrance is still non-uniformity, so SCR system should be designed further.

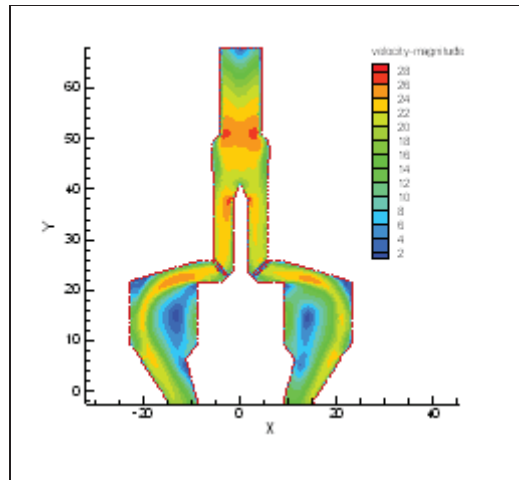


Figure 5. the velocity distribution on Z=0 section(case 2)

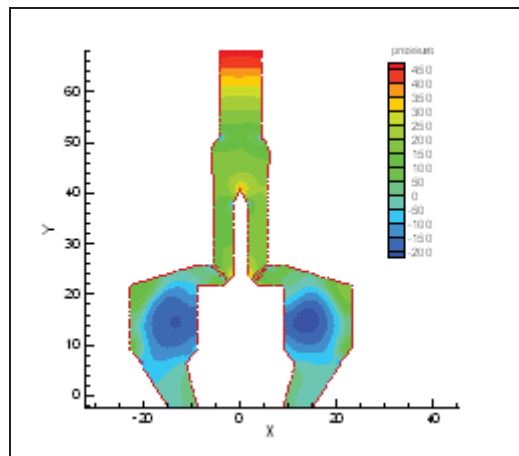


Figure 6. the pressure distribution on catalyst entrance section(case 2)

4.3 The result of case 3

Rectifier grilles are further designed and installed based on the case 2. The calculation results are shown in figure 7-8. From the figures we can see that velocity field of flue gas can be improved by rectifier grilles. When gas flowing through the corner, the separation phenomenon disappears, secondary flow disappears, and the velocity distribution on catalyst entrance section is also uniform. As shown in figure 9, the velocity values on catalyst entrance is between 4m/s and 6m/s, which the ratio of value between 4m/s and 5m/s is 96.1%. The non-uniformity of flue gas is less than 15% on the first catalyst layer of the reactor, so the flow field of this SCR system has achieved satisfactory result.

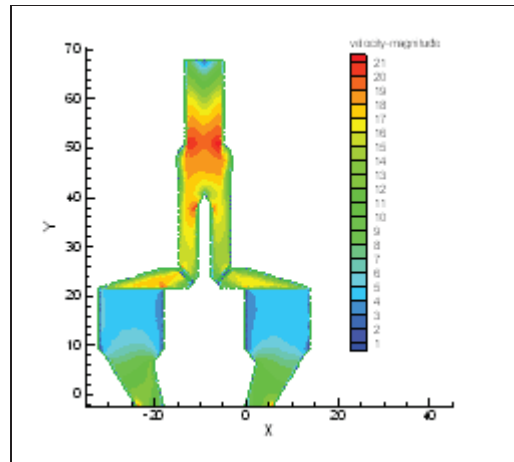


Figure 7. the velocity distribution on Z=0 section(case 3)

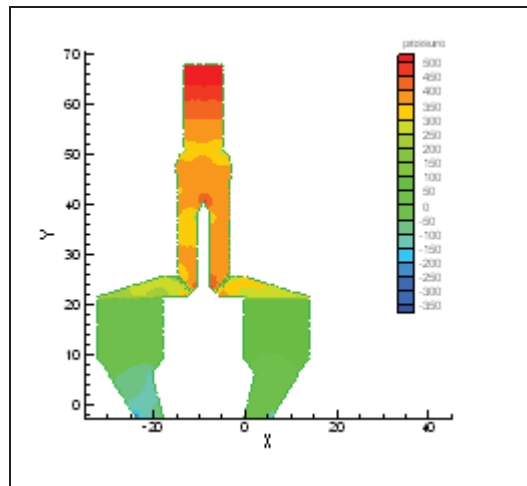


Figure 8. the pressure distribution on catalyst entrance section(case 3)

4.4 The result of case 4

In order to achieve the goal of mixing uniformity between ammonia and flue gas, the disk diameter, layout position and angle of vortex mixer need to be optimized and five nozzles need to be adjusted in the best field of SCR system. Figure 10 shows the velocity and pressure distribution on symmetric plate of the SCR system with vortex mixers, while figure 11 shows the concentration distribution on that plane, and figure 12 reveals ammonia concentration distribution at the catalyst inlet.

It can be seen from the calculation results that ammonia injected from pipes mix fully with flue gas in the reactor. The mixing gas goes through vane cascades and rectifier grills, and then the flow field becomes uniform before gas entering into the first catalyst. Ammonia and flue gas mix completely in the upstream vertical flue duct, the two kinds of gas mix further under the action of vane cascades and

rectifier grills. The concentration distribution of ammonia becomes uniformity at the catalyst inlet, achieving mixed uniformity between ammonia and nitrogen oxides, improving the efficiency of DeNOx.

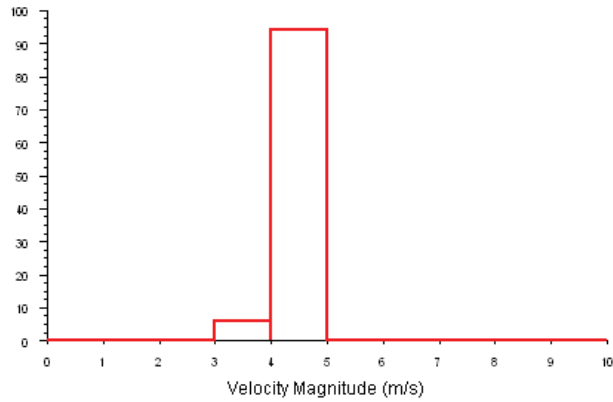


Figure 9. the velocity statistic distribution on catalyst entrance section(case 3)

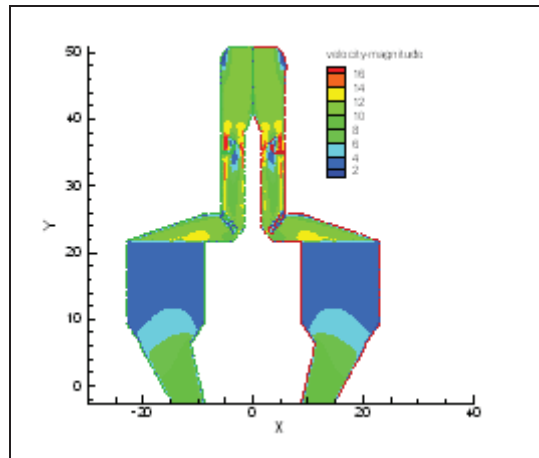


Figure 10(a). the velocity result on Z=0 section(case 4)

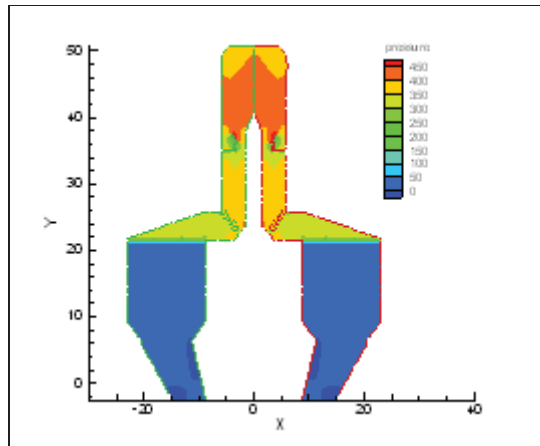


Figure 10(b). the pressure result on $Z=0$ section(case 4)

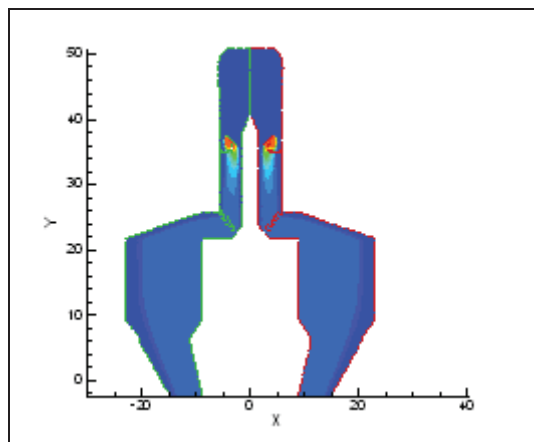


Figure 11. the ammonia concentration result on $Z=0$ section(case 4)

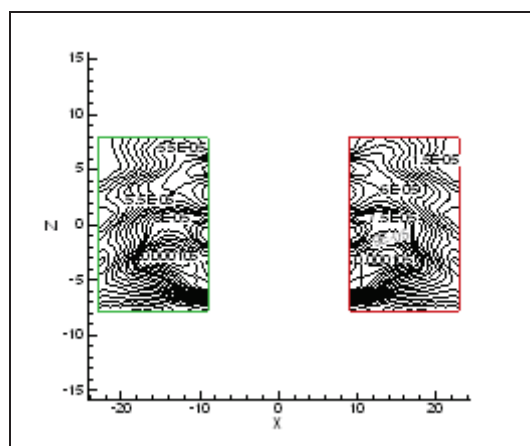


Figure 12. the ammonia concentration result on catalyst entrance section(case 4)

5. Comparison Between Cfd And Test Results

In order to test reliability and accuracy of the results of numerical simulation, physical flow model was set up to get flow and concentration distributions, which the geometry size of SCR model is 1:15. The laboratory designing principles meet the geometric similarity, motion similarity and dynamic similarity. In the process of test, Reynolds number of inlet section is 353000 and so the experiment is completed in self-modeling area. The test model and vortex mixers are shown in figure 13.

The velocity at catalyst inlet is measured by using special five-hole anemometer probe. Five-hole probe gathers gas pressure signals, and then pressure converts into electrical signal by pressure sensor-transmitter. Electrical signal is magnified by signal conditioning module, which the signal is converted digital signal by data collection module and enters into a computer. The velocity values of the experiments and calculations are compared in the figure 14, which the result shows that the values of calculation agree well with that of experiment, consequently the numerical simulation method of this paper has good reliability.



Figure 13. SCR test system

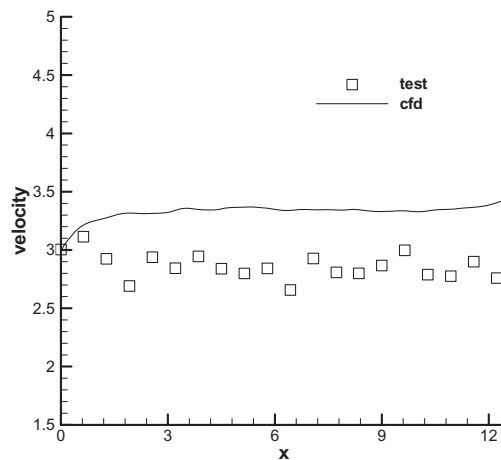


Figure 14. Comparison of CFD and test at catalyst inlet, $Z=0$

6. Conclusions

The reasonable structure and size of SCR system is obtained by numerical simulation on above-mentioned four designed schemes and the numerical calculation guides the design of SCR DeNO_x system effectively.

- The value of calculation agrees well with that of experiment, and the numerical simulation method has good reliability.
- The non-uniformity of flue gas at catalyst inlet is less than 15% by designing the vane cascades and rectifier grills.
- In the best field of SCR system, the disk diameter, layout position, angle of vortex mixer is optimized and ammonia and flue gas mixes fully in the reactor.

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