# Research and Application of Multi-dimension Numerical Simulation Optimization for SCR DeNOx Flow Field

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**Abstract.** CFD has been the main method of optimization for SCR DeNOx flow field. In order to optimize the SCR DeNOx flow field efficiently, we propose multi-dimension numerical simulation method. With 2D and 3D numerical simulation successively, the time of flow field optimization for a single SCR DeNOx project can be reduced greatly. Therefore, multi-dimension numerical simulation method can provide effective guidelines for SCR DeNOx flow field optimization. Via physical model test verification, it reveals that multi-dimension numerical simulation results are accurate and reliable.

## 1. Introduction

SCR (Selective Catalytic Reduction) DeNOx technology has the advantages of small ground occupation, high denitrification efficiency, technology maturity, ect, which is the most widely used technology of flue gas denitrification at present. Its basic principle is that the diluted reducing agent-ammonia is sprayed into the flue gas with temperature of 290~430℃, and after the flue gas and the ammonia are evenly mixed, the ammonia and nitrogen oxides have a redox reaction under the action of the catalyst that causes the nitrogen oxides to be reduced to harmless nitrogen and water.

Denitrification efficiency, ammonia slip rate and catalyst life are the main basis for evaluating SCR DeNOx performance. In addition to the catalyst itself, the flow field is a key factor affecting SCR DeNOx performance in engineering application. The ideal flow field can not only improve the SCR DeNOx efficiency and reduce the ammonia escape rate, but also can reduce catalyst blockage due to dust deposits with low gas velocity or catalyst abrasion due to high gas velocity, thereby prolonging the service life of the catalyst. Therefore, it is essential to optimize the flow field in a SCR DeNOx system.

In recent years, CFD (Computational Fluid Dynamic) has been widely used to optimize the SCR DeNOx system in engineering application. Through CFD, gas flow and ammonia concentration distribution device, including the guide vanes, rectifier grille, mixer, ect., is set in a SCR DeNOx facility. And then, with cold flow model test verification, the specific structure of SCR DeNOx device is ultimately detemined. The objective of optimization is to adjust the location, number and size of gas flow and ammonia concentration distribution device to obtain the following index:

- Uniform velocity distribution upstream the first layer catalyst is obtained: relative standard deviation of velocity in cross section is less than 15%;
- Uniform ammonia concentration upstream the first layer catalyst is obtained: relative standard deviation of ammonia concentration in cross section is less than 5%.

The relative standard deviation is referred to quantitatively evaluate the data uniformity in test cross section a. The smaller the value is, the more uniform the data is. Cv is represented:

$$C_v = \frac{1}{\overline{x}} \left( \frac{\sum\limits_{i=1}^{n} (x_i - \overline{x})}{n-1} \right)^{1/2} \tag{1}$$

In the formula, Cv－Relative standard deviation; $x_i$－measured data, such as velocity, concentration; $\overline{x}$ －Average value of measured data; n－Number of measured data in cross section.

## 2. Method of Multi-dimension Numerical Simulation Optimization for SCR DeNOx Flow Field

The difficulty in optimizing the SCR DeNOx flow field is to distribute the flue gas velocity and ammonia concentration uniformly d above the cross section of the 1st layer catalyst as Cv is less than 15% and 5% respectively. At present, CFD simulations method of optimizing the flow field in gas SCR DeNOx device is mainly based on experience of arranging guide vanes in the size-varied duct and the turning duct, providing rectifiers above the catalyst, ect (as shown in Figure 1). Then, 3D flow field simulation is carried out, and the structure, number, location and size of the flow guide vanes are adjusted until the flow field satisfies SCR DeNOx optimization design requirements. Due to large number of numerical simulation grids of SCR DeNOx flow field (possibly up to 10 million), each case (each adjustment corresponds to one case) takes a long time to calculate. In addition, lack of effective guidance, the method is provided with certain blindness, resulting in the whole optimization work time-consuming.
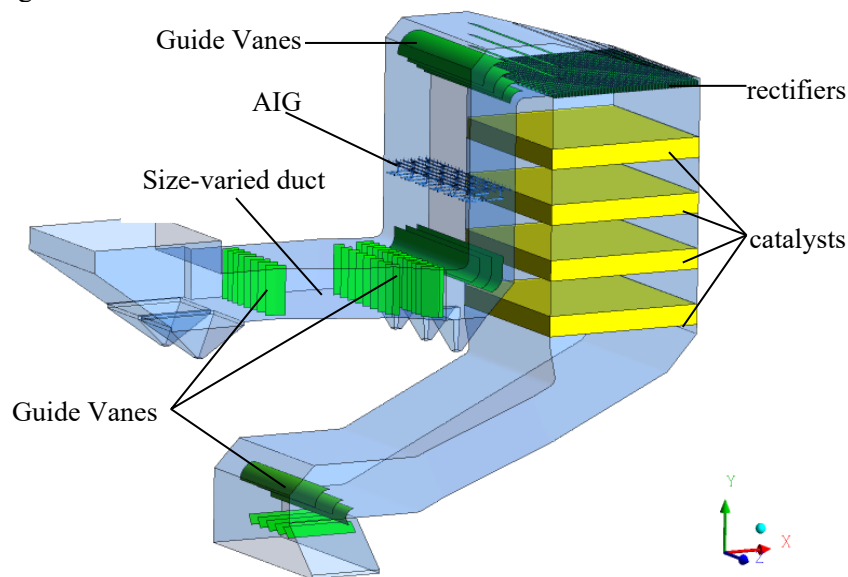


**Figure 1.** Layout of flow distributed devices for a 350MW SCR DeNOx facility in a power plant.

In order to improve the SCR DeNOx flow field optimization efficiency, "method of multi-dimension numerical simulation optimization for SCR DeNOx flow field" is put forward to greatly shorten the optimization time of SCR DeNOx flow field. The method refers to optimize 2D and 3D flow field of SCR DeNOx reactor step by step with 2D and 3D geometry, and takes an idea of adopting least number of flow field adjustments and shortest calculation time for each case to reach the flow optimization index.

The specific implementation process of the multi-dimensional numerical simulation optimization method of SCR DeNOx flow field is given below.

### 2.1. 2D flow field numerical simulation optimization

2D CFD simulation optimization are carried out according to the main view  (the main view reflects the flow characteristics of the flue gas along the main flow direction) of SCR DeNOx reactor structure. In this process, only flow distribution is investigated without ammonia injection. The flow conditioning devices are installed on the main flow direction, including designing the guide vanes in the turning duct, setting the small baffle in the slope flue, setting the rectifier above the catalyst and then, the main flow direction guide vanes are adjusted. When the cross-section velocity Cv above the AIG and the 1st layer catalyst is less than 10%, it indicates that velocity is well distributed, and the structure of the flow guide device on the main flow direction can be determined in the meantime. In addition, the relative standard deviation of the velocity upstream the first layer catalyst is required to be less than 10% instead of 15%, so that the velocity distribution in the 3D flow field is more uniform.

In the process of 2D flow field CFD optimization, it consumes very little time to calculate each case, and several cases can be carried out in a short time, owing to less 2D modeling grid. Therefore, the flow guide vanes structure in the primary flow direction can be determined quickly. Determination of the structure of the flow guide device in the main flow direction by 2D simulation can greatly reduce 3D flow field adjustment times.

### 2.2.  3D flow field numerical simulation optimization

3D geometric modeling is built according to the whole drawing of SCR denitrification reactor. The gas flow distribution is optimized in the 3D simulation process, and then the ammonia spraying process is optimized.

During gas flow distribution optimization, the whole DeNOx device is divided into three sections: the flue gas inlet to AIG, AIG to the first catalyst and the bottom catalyst to the flue gas outlet. The flow distribution in the three sections is optimized respectively. Since the velocity distribution will be uniform when the flue gas flows from the first layer catalyst to the bottom layer catalyst, it is not necessary to optimize the flow field from the first layer catalyst to the bottom layer after the optimization of the upstream flow field of the first layer catalyst. The specific optimization process is:

- Based on the 3D structure of SCR DeNOx reactor, the 3D geometric models of the sections from the flue gas inlet to AIG, AIG to the 1st catalyst layer and the bottom layer catalyst to the flue gas outlet are respectively established and the guide vanes in the main flow direction are set according to the 2D optimization;
- For the section from flue gas inlet to AIG, guide vanes are set in the  direction perpendicular to the main flow direction in the size-varied duct, and numerical simulation is carried out until the velocity Cv above the AIG is less than 10%;
- For the section from AIG to the 1st catalyst layer, the rectifiers in the direction perpendicular to the main flow direction are arranged upstream the first catalyst and numerical simulation is carried out until the velocity profile Cv upstream the first layer catalyst is less than 10%;
- For the section from bottom catalyst to the flue gas outlet, the flow guide vanes in the direction perpendicular to the main flow direction is set in the downstream duct of the catalyst and the numerical simulation is carried out until the outlet cross-section velocity distribution Cv is less than 15%，in order to improve the uniformity of the inlet velocity distribution of the air preheater downstream the SCR DeNOx reactor to ensure the normal operation of the air preheater;

After the gas flow distribution of the three sections are optimized, a complete 3D structure model of the SCR DeNOx reactor is established, and numerical simulation is carried out by arranging the guide device according to the above three section flow distribution optimization. If the flue gas velocity Cv upstream of AIG or the first layer catalyst are greater than 10%, small adjustment of the guide vanes is required until Cv is less than 10%. Theguide device structure of SCR DeNOx reactor can be determined if the flow distribution of the 3D flow field satisfies the requirement of Cv less than 10%.

After the optimization of the gas flow distribution in 3D simulation, the species transport model is added to simulate the gas and ammonia mixing process, and the ammonia concentration Cv upstream

the 1st layer catalyst is calculated. If ammonia concentration upstream the 1st layer catalyst is larger than 5%, it requires to adjust ammonia flowrate of each AIG nozzle or install static mixer behind AIG to strengthen the mixture of ammonia and flue gas, until the ammonia concentration $C_v$ upstream the 1st layer catalyst is less than 5%.When the ammonia concentration $C_v$ is less than 5%, the optimal structure of SCR DeNOx reactor can be determined, and the numerical simulation is finally completed.

In the 3D flow field simulation process, the optimization of gas flow distribution is carried out step by step to reduce the number of each case grids, which can reduce the calculation time of each case. Finally, the optimization of ammonia injection process is carried out by adding the component transport model after gas flow distribution optimization. The calculation will converge quickly, and the simulation time of ammonia injection process is greatly shortened.

"Method of multi-dimension numerical simulation optimization for SCR DeNOx flow field" can reduce the frequency of 3D flow field adjustment by 2D numerical simulation and the computational time of the three-dimensional flow field by 3D segmentation numerical simulation. Therefore, the time of flow field optimization for a single SCR DeNOx project can be reduced greatly, and the optimization efficiency of the flow field can be improved remarkably.

## 3. Engineering Application Example

The optimizing process of SCR DeNOx flow field for 350 MW Unit in a Power Plant will be used as an example to illustrate the specific application of "Method of multi-dimension numerical simulation optimization for SCR DeNOx flow field".The entire numerical calculation process is completed based on the commercial CFD software -ANSYS-FLUENT.

The structure of the SCR DeNOx reactor without arrangement of flow field optimization device is shown in Figure 2.
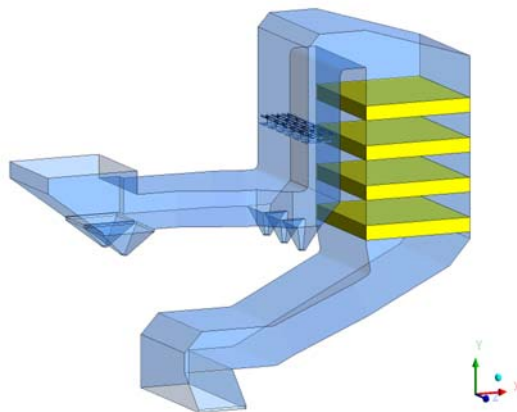


**Figure 2.** Structure of the SCR DeNOx reactor without flow field optimization device

According to the "Method of multi-dimension numerical simulation optimization for SCR DeNOx flow field", the 2D and 3D flow fields are optimized respectively.

### 3.1. 2D flow field numerical simulation optimization

2D geometric modeling is built based on the main view without AIG. After flow guiding device is installed in the main flow direction and several adjustments are taken, velocity distribution $C_v$ upstream AIG and the 1st catalyst layer in 2D flow field can be 5.6% and 4.5% respectively, both less than 10%, indicating that the velocity distribution is sufficient uniform. At this time, the flow guide device in the main flow direction is determined (Figure 3), and the corresponding numerical simulation results are shown in Figure 4.The number of 2D grids of the SCR DeNOx reactor is about 50,000, which consumes little computation time in the process of 2D numerical simulation of flow field optimization, and the flow guiding device in main flow direction can be determined quickly.
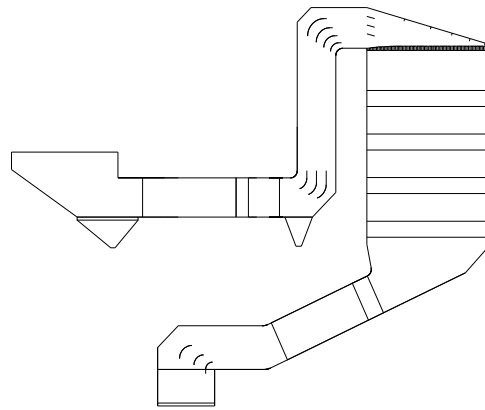
**Figure 3.** Flow guiding device in the main flow direction



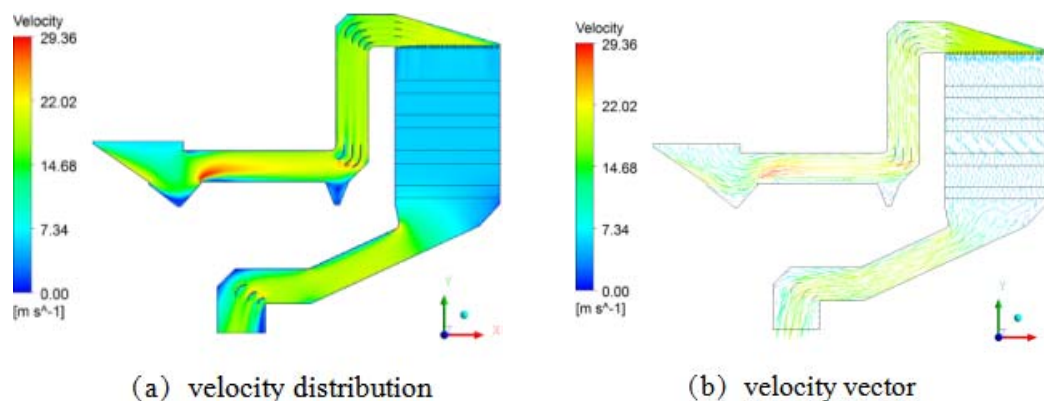(a) velocity distribution                    (b) velocity vector

**Figure 4.** Numerical simulation results of 2D flow field

*3.2. 3D simulation of flow field optimization*

The 3D geometric models of the sections from flue gas inlet to AIG, AIG to the 1st catalyst layer and the bottom catalyst layer to the flue gas outlet are built based on the 3D structure of SCR DeNOx reactor. Meanwhile, the flow guide vanes in the main flow direction, such as the turning duct guide vanes and rectifier, are arranged according to the 2D flow field optimization results.

For the section from flue gas inlet to AIG, guide vanes are arranged in the direction perpendicular to the main flow direction in the size-varied duct. By adjusting several times, the velocity distribution Cv upstream AIG is 6.5% ultimately, less than 10%, indicating that the velocity distribution is uniform enough to determine the guide vanes arrangement in the section from the flue gas inlet to AIG (as shown in Figure 5) The corresponding simulation results are shown in Figure 6.
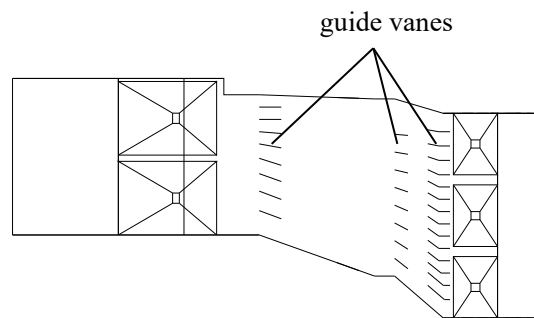
**Figure 5.** The guide vanes arrangement in the section from flue gas inlet to AIG
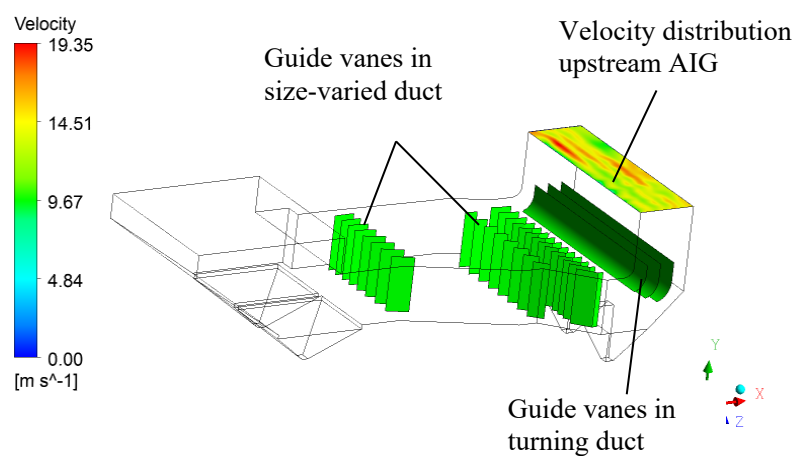


**Figure 6.** Numerical simulation results in the section from flue gas inlet to AIG

For the section from AIG to the first catalyst layer, the rectifier perpendicular to the main flow direction is arranged upstream of the first catalyst layer. By adjusting the rectifying grids several times, the velocity Cv upstream the 1st layer catalyst reaches 5.0%, indicating that the velocity distribution is uniform sufficiently, and the rectifier in the section from AIG to the first catalyst layer can be determined, as shown in Figure 7. The corresponding numerical simulation results are shown in Figure 8.
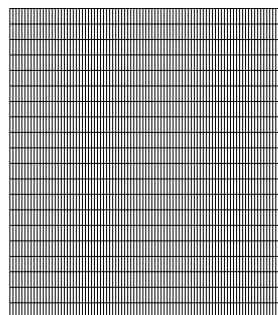


**Figure 7.** Rectifier arrangement in the section from AIG to the bottom layer catalyst
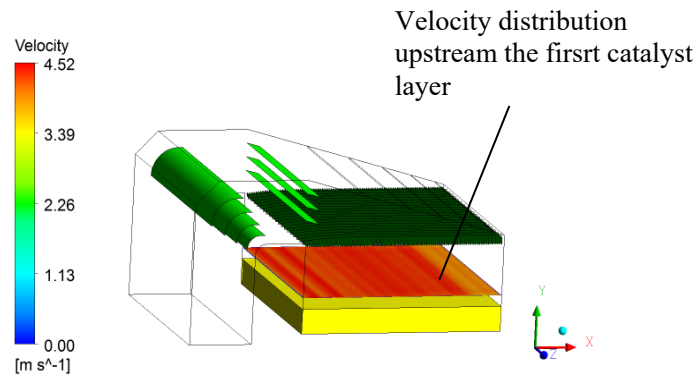
**Figure 8.** Numerical simulation results of the flow field in the section from AIG to the first catalyst layer

For the section from the bottom catalyst to the flue gas outlet, guide vanes in the direction perpendicular to the main flow direction are arranged in the size-varied duct and are adjusted by several times. The final velocity $C_v$ upstream the outlet is 13.8%, less than 15%, indicating velocity distribution upstream the outlet is uniform, and the guide vanes in the section from the bottom catalyst to the outlet can be determined, as shown in Figure 9. The corresponding simulation results are shown in Figure 10.
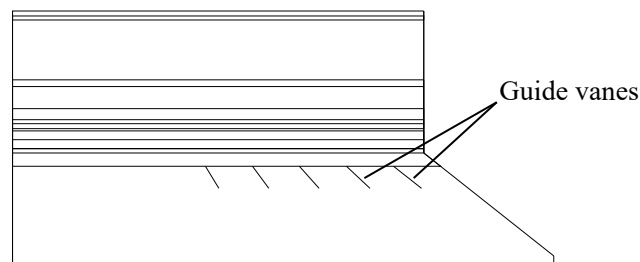


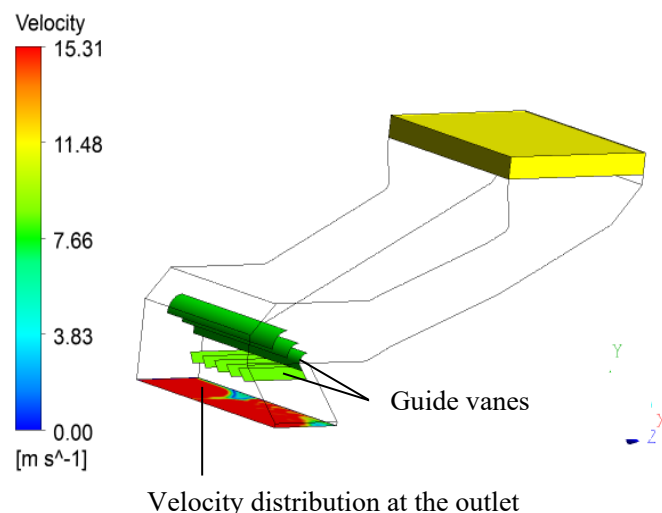**Figure 9.** guide vanes arrangement in size-varied outlet duct



**Figure 10.** Numerical simulation results of flow field from the bottom catalyst layer to the outlet

The 3D geometric model of the whole SCR DeNOx reactor is established according to the flow guide device optimized by the segmented flow distribution, as shown in Figure 1. Then the flow field

of the whole SCR DeNOx reactor is simulated. It shows that the velocity Cv upstream AIG and the first catalyst layer are 8.6% and 5.5%, respectively, which are both less than 10%. The results reveal that the velocity distribution upstream AIG and the first layer catalyst, so it is not necessary to adjust the guide device determined by the segmented flow distribution optimization.

Simulation of gas flow distribution and ammonia spraying is carried out by adding the component transport model to the 3D flow field calculation case. The results are shown in Figure 11.The ammonia concentration Cv upstream the first  catalyst layer is 6.9%, which is larger than 5%. Therefore, it is necessary to adjust ammonia injection flow rate of each nozzle of AIG or add static mixers behind AIG to enhance ammonia and gas mixing.
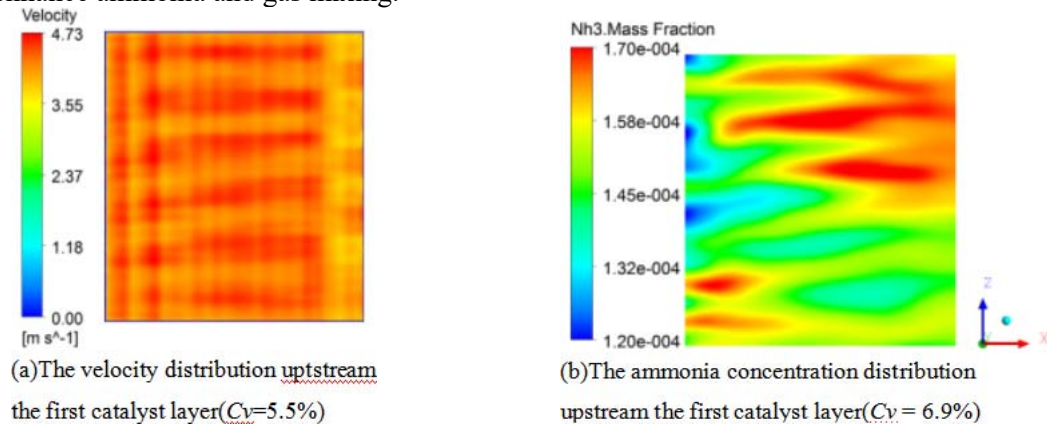


(a)The velocity distribution uptstream the first catalyst layer($Cv$=5.5%)

(b)The ammonia concentration distribution upstream the first catalyst layer($Cv$ = 6.9%)

**Figure 11.** simulation results of 3D flow field

By adding a static mixer behind AIG (the ammonia flow rate is not adjusted in each nozzle in this case), as shown in Figure 12, velocity and ammonia concentration upstream the first catalyst layer obtained by simulation is 6.4% and 3.5% respectively. It shows that the ammonia concentration distribution is improved obviously, and the flow field of the SCR DeNOx reactor can satisfy the requirement of flue gas velocity distribution and ammonia concentration distribution upstream the first catalyst layer. Therefore, Overall optimization structure of the SCR DeNOx reactor can be determined (as shown in Figure 12). The corresponding simulation results are shown in Figure 13. Thus, SCR DeNOx flow field simulation has been finished.
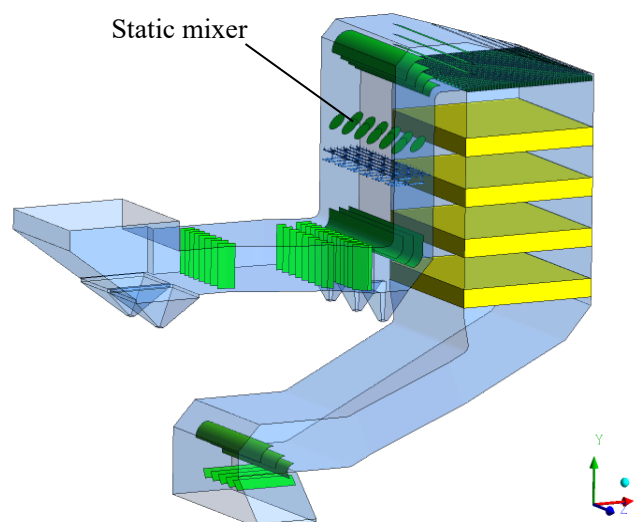


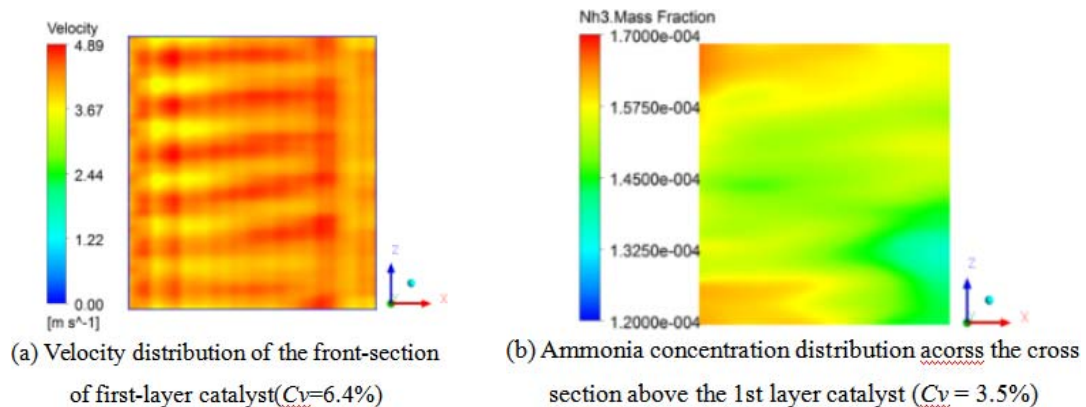**Figure 12.** Optimized structure of SCR DeNOx device

(a) Velocity distribution of the front-section of first-layer catalyst($Cv$=6.4%)

(b) Ammonia concentration distribution acorss the cross section above the 1st layer catalyst ($Cv$ = 3.5%)

**Figure 13.** Simulation results of SCR DeNOx flow field optimization

## 4. Physical model test

In order to verify the accuracy of the simulation results, a scale ratio of 1:10 is selected for the scale model of cold flow field according to the fluid mechanics similarity theory (geometry similarity, dynamic similarity, motion similarity). The scale model is shown in Figure 14. Nine testing holes are uniformly arranged upstream the first catalyst layer and 9 testing points are evenly set in each testing hole. There are 90 testing points in total upstream the first catalyst layer, as shown in Figure 15. The velocity and concentration distributions upstream the first layer catalyst are 6.7% and 3.6%, respectively. The average dimensionless value of velocity and concentration (the ratio of the mean measured data in each hole to the average data in the whole cross-section) for each hole is compared with the numerical simulation results as shown in Figure 16. The numerical simulation results agree well with the model test results. Therefore, the numerical simulation results are accurate and reliable.
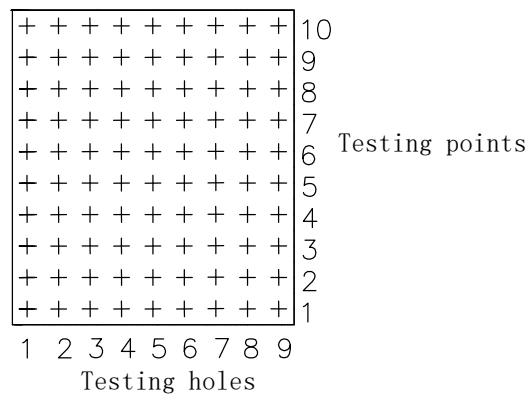


**Figure 14.** The physical model

**Figure 15.** The testing holes and points layout in the corss-section upstream the first catalyst layer
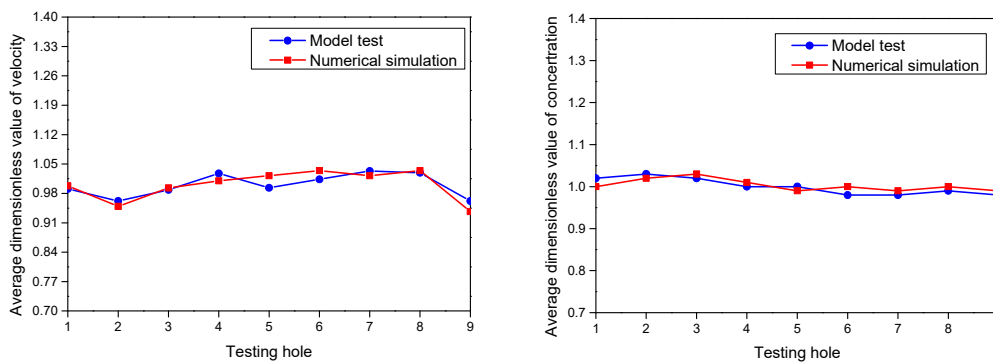


**Figure 16.** Comparison between the results of model test and numerical simulation

## 5. Summary

To solve the difficulty and time-consuming problem of SCR DeNOx flow field optimization, "method of multi-dimension numerical simulation optimization for SCR DeNOx flow field" is put forward. 2D and 3D flow field in SCR DeNOx reactor are optimized step by step. The flow field is adjusted to meet the SCR DeNOx flow optimization index by the idea of adopting least adjustment times and shortest calculation time for each case. This method can greatly shorten the flow field optimization period for each SCR DeNOx project, and provide guidance for optimizing the SCR denitrification flow field.

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