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Study on Flow Field Optimization of SCR Denitrification Reactor Based on CFD Numerical Simulation Technology

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Abstract. CFD numerical simulation method was used to simulate and diagnose the flow field in SCR reactor and connecting flue. The characteristics of the smoke flow field in the system before and after the layout of the guide plate were studied. The flow field distribution and data at different positions in the calculation model were obtained, and the flow field in the system before and after the layout of the guide plate was compared. By optimizing the setting of the flow guide plate in the system, it is proved that: due to the lack of flow guide plate to correct the airflow, the flue gas velocity distribution in the flue duct section and reactor section is uneven. The uniform velocity of flue gas in SCR system can be significantly improved by proper distribution of guide plate, and the relative standard deviation of the velocity of the inlet surface of the first layer catalyst can be reduced to 4.47\%. Most of the speed relative to the standard deviation of the reference section shows different degree of decrease. Layer 1 catalyst entrance section (500 mm) above the first layer of catalyst average velocity angle of absolute value reduced to 4.39\(^\circ\), while local position angle was still slightly larger, but had no significant effect on the whole flow field.

1. Introduction
In order to meet the "ultra-low emission" standard of NO\textsubscript{X} concentration less than 50mg/Nm\textsuperscript{3} \textsuperscript{[1]}, most coal-fired power stations need to carry out ultra-low emission transformation of denitrification system \textsuperscript{[2]}. In order to avoid the problems of local catalyst passage flue gas overspeed, catalyst wear and uneven flow field caused by improper design of guide plate after the modification \textsuperscript{[3]}, it is necessary to grasp the flow field characteristics of SCR reactor in advance and adjust the flow field by placing guide plate in the flue to improve the flow field uniformity \textsuperscript{[4]}. However, the reasonable setting of the flow guide plate requires the re-simulation experiment of the reactor and inlet and outlet flue, and according to the simulation experiment results, the top cover plate of the corresponding reactor and the flow guide plate of the flue are set \textsuperscript{[5,6]}. In this paper, CFD numerical simulation software was used to model the flow field inside the flue of a denitrification reactor. Three-dimensional CFD numerical simulation was carried out on the flow field inside the flue of a denitrification reactor. The characteristics of the flow field before and after the distribution of the flow guide plate in the flue were studied.
2. Scheme and Procedure of Numerical Simulation

Fluid dynamics calculation software FLUENT6.3.26 and modeling and mesh division software GAMBIT2.3.16 were used for numerical simulation [8].

(1) According to the specific structural data of SCR reactor and connected flue, the corresponding geometric model of reactor and flue was established in GAMBIT2.3.16;

(2) In GAMBIT2.3.16, the geometric model was meshed and divided into regions according to different structures;

(3) In GAMBIT2.3.16, boundary conditions such as inlet, outlet, porous media and internal reference surface were set for the mesh model.

(4) Import the grid file into FLUENT for grid check and setting of relevant parameters;

(5) Select the default relaxation factor and SIMPLE algorithm;

(6) The flue gas inlet flow field is initialized and iterative calculation is started;

(7) After the calculation is completed, the cloud diagram of data and calculation results is displayed in FLUENT, and the calculated data is analyzed by Excel software;

(8) Carry out multiple calculations according to different design schemes, compare and analyze the calculation results, and finally choose the design scheme that meets the standards.

3. Calculation Parameter Determination

Table 1 Calculation of Flue Gas Parameters at 100% Load

| Name                                | Load  | 100%      |
|-------------------------------------|-------|-----------|
| Flue gas temperature                | °C    | 404.4     |
| Flue gas amount                     | Nm³/s | 323.46    |
| Flue gas volume (actual temperature)| m³/s  | 802.34    |
| Inlet velocity of the lower section of the economizer | m/s | 6.18    |
| Flue gas temperature                | K     | 677.55    |
| Flue gas density                    | kg/m³ | 0.53      |
| Dynamic viscosity of flue gas       | Pa·s  | 3.15116×10⁻⁵ |
| Kinematic viscosity of smoke        | m²/s  | 5.94327×10⁻⁵ |
| Turbulence intensity at cross section inlet at lower end of economizer | %   | 2.913   |
| Concentration of ammonia gas mixed with air | % | 5.00  |

4. Numerical Simulation and Result Analysis

4.1. Reference Section Setting

In order to obtain the velocity field data and distribution at different positions in the calculation model so as to facilitate the flow field comparison in the system before and after the guide plate layout, the reference section must be set in the calculation model. The reference section position set for this model is shown in FIG. 1.
4.2. 100% Load without Guide Plate Simulation Results
The flue gas velocity distribution in flue gas was analyzed by simulating the reactor and flue gas flue without any guide plate. According to the simulation results, the flow guide plate is arranged pertinently so that the technical indexes can meet the performance assessment requirements.

4.2.1. Velocity Field

![Figure 2 Distribution Diagram of Total Velocity Field under 100% Load without Deflector Plate](image)

The FIG. 2 shows that in the case of no guide plate, the flue gas is more affected by the inertia tilted movement, vertical flue side movement towards reactor, the reactor at the top to the lateral movement, the roof because of a lack of diversion threatening the airflow to correct, cause flue section and reactor section of flue gas flow velocity distribution, cause catalyst partial wear, NH$_3$ mixing effect is poor and the denitration reaction efficiency is low.

![Figure 3 Velocity Distribution Diagram of Refer2 (left) and Refer3 (right) at 100% Load without Deflector.](image)

RSD relative standard deviation: 29.22% (Refer2)、20.57% (Refer3)

FIG. 3 shows that the flue gas tends to move towards the wall near the reactor side in the vertical flue gas in accordance with the reaction of the whole longitudinal section of the flue gas flue. Refer2 also shows that the uneven distribution of airflow in the Y direction is caused by the existence of the reducing deflection section. It is the existence of the reducing deflection section at the front and bottom ends of the horizontal intake flue and the vertical flue that causes the airflow in the vertical flue to move to the outer side of the boiler center line. Therefore, when it reaches the Refer4 at the end of the vertical flue, the gas velocity on the expansion side is on the high side [9].
Because reactor entrance guide plate position is not set, the single rely on rectifying grating meets the requirement of the reactor inlet cross section velocity uniformity, can be seen in figure 5, before the incident catalyst airflow in reactor in central position, and velocity distribution from the upper figure 2 shows, the airflow is by inclined top deflection. The velocity deviation distribution of 0.5m above the inlet section of the first-layer catalyst and directly above the first-layer catalyst was 22.91% and 11.32%, both exceeding the design requirements. As the catalyst layer has a large resistance loss, it can play a role of flow uniformity to some extent. Therefore, as shown in FIG. 6, the gas velocity distribution of the reactor section has been significantly improved after passing through the catalyst layer, so the velocity distribution after passing through the catalyst layer will not be discussed in the subsequent simulation results.
FIG. 7 shows the air preheater gas velocity changes above the entrance, because after 90 ° corner, in the case of no guide plate, airflow due to the inertia will turn to the side of the boiler, into the air preheater airflow distribution. There is also a reducer section at the inlet of the air preheater that expands by 10000mm from 8800mm, so the speed deviation from Refer10 to the Y direction of Outlet position is also caused.

Table 2 Mean Velocity and Relative Standard Deviation of Velocity of Each Reference Surface at 100% Load without Deflector

| No. | Description                                           | Average Speed (m/s) | Velocity Relative Standard Deviation |
|-----|-------------------------------------------------------|---------------------|-------------------------------------|
| Refer2 | End position of vertical flue reducer               | 17.19               | 29.22%                              |
| Refer3 | Section of inlet flue of ammonia spray grate       | 17.04               | 20.57%                              |
| Refer4 | Vertical flue end position                          | 16.17               | 18.49%                              |
| Refer6 | 500mm above the inlet section of the first layer catalyst | 5.15               | 22.91%                              |
| Refer7-1 | The first layer catalyst inlet surface       | 4.68                | 11.32%                              |
| Refer7-2 | The first layer catalyst outlet surface       | 3.87                | 3.51%                               |
| Refer8-1 | The second catalyst outlet surface             | 3.88                | 0.33%                               |
| Refer10 | The end of SCR system bend to the               | 12.85               | 22.37%                              |
Calculation results show that without layout guide plate and the flue adjustment, under the condition of the flow field in the system of relative standard deviation is higher, the flow field uniformity is poorer, there are local dead zones at low speed and high velocity and high pressure area, results in a loss of pressure deviation in the system is larger, uneven distribution of NH$_3$ / NO$_X$ mole ratio, especially the ammonia injection grid flow field at the entrance of inhomogeneity will directly affect the effect of NH$_3$ and NO$_X$ in flue gas mixture\[^{10}\]. As shown in Table 2, the velocity deviation in front of the ammonia spraying grating reached 20.57% without the addition of the guide plate, which seriously affected the NH$_3$ mixing effect. However, the high velocity deviation above the first layer of catalyst (the relative deviation is 22.91%) will definitely lead to obvious differences in the working air velocity of catalysts in different regions, which will have a negative impact on the efficiency of the denitrification system\[^{11}\]. In addition, the relative standard deviation of the flow velocity at the outlet of the model reached 52.05%, which was relatively high and would affect the heat transfer effect of the downstream air preheater. Therefore, it is necessary to improve the uniformity of the flow field in the system by reasonable arrangement of baffles.

4.2.2. Velocity Vector at the Inlet of the First Layer Catalyst

![Figure 8](image1.png)

**Figure 8 Flue Gas Velocity Vector Diagram of the First Layer Catalyst Inlet Area at 100% Load without Deflector Plate**

![Figure 9](image2.png)

**Figure 9 Schematic Diagram of the Flow Line in the First Layer of Catalyst at 100% Load without Baffle**

By the figure 8 and figure 9 you can see, the first layer of catalyst entrance area of flue gas deflection degree is higher, the condition of the return parts, catalyst at the entrance to the flue gas flow rate is 37.5° angle, on average, maximum angle 82°, far cannot achieve the indexes stipulated in the technical agreement. Excessive flue gas incidence Angle at the top of the catalyst for the first time is
likely to cause wear and blockage of the catalyst and seriously affect the performance and service life of the catalyst [12-14]. Therefore, the flue gas incidence angle must be reduced by setting up a guide plate.

Table 3 reference section Refer6 incident catalyst angle at 100% load without Deflector Plate

| Section Name | Average angle of incidence | Maximum angle of incidence | Incidence angle >10° ratio |
|--------------|---------------------------|---------------------------|---------------------------|
| Refer 6      | 37.5°                     | 82°                       | 94.86%                    |

4.3. Optimum Baffle Setting Scheme

![Figure 10 Layout of Flow Guide Plate in SCR Denitrification System](image)

Table 4 Distribution Method of Flow Guide Plate in SCR Denitrification System

| No./Name       | Description                                                                 |
|----------------|-----------------------------------------------------------------------------|
| Vane 1 (Flow guide plate 1) | Horizontal reducer expansion section, 7 straight flow guide plates           |
| Vane 2 (Flow guide plate 2)  | 90° bend guide plate at horizontal flue (arc plate + two groups of straight board) |
| Vane 3 (Flow guide plate 3)  | Vertical flue reducer deflection guide plate, 6 straight guide plate         |
| Vane 4 (Flow guide plate 4)  | Vertical flue rectifying guide plate, 38 pieces                             |
| Vane 5 (Flow guide plate 5)  | 90° bend guide plate of vertical flue at end position (arc plate + straight five groups) |
| Vane 6 (Flow guide plate 6)  | 90° corner at the back of the reactor outlet, 2 pieces of arc plate          |

4.4. Simulation Results of 100% Load Optimal Baffle Setting

4.4.1. Velocity Field

![Figure 11 Distribution Diagram of Total Velocity Field at 100% Load with Baffle Added](image)

As it is can be seen from FIG. 11, the uniformity of airflow can be significantly improved by adding baffles to curves and reducing diameters. The change of the inclined roof structure of the reactor makes the airflow deflect from the beginning when it enters the reactor site. The inclined roof structure combined with the rectifying grid can well distribute the airflow on the 2500mm flue to the
reactor section uniformly. Refer 2, 3, 4 section velocity distribution diagram shows that the deflecting position of the diameter of the guide plate is a good solution to the vertical upward flue Y direction velocity distribution problem.

Figure 12 Speed Distribution of Refer 2 (left) and Refer 3 (right) at 100% Load with Guide Plate
RSD: 17.10% (Refer 2)、14.84% (Refer 3)

Figure 13 Velocity Distribution of Refer 4 (left) and Refer 5 (right) at 100% Load with Guide Plate
RSD: 9.13% (Refer 4)、9.20% (Refer 5)

Figure 14 Velocity Distribution of Refer 6 (left) and Refer 7-1 (right) at 100% Load with Guide Plate
RSD: 4.47% (Refer 6)、0.77% (Refer 7-1)
The airflow guide plate from the reactor outlet to the air preheater inlet bend can solve the problem of airflow inertia deflection to the boiler side and improve the uniformity of airflow at the air preheater inlet. The low speed zone in the positive Y direction of Outlet section is caused by the reducer at this location. Considering the effect of less deflection and the flow uniformity of components inside the air preheater, the guide plate is not set at this reducer section.

Table 5 Relative Standard Deviation of Velocity at 100% Load with Guide Plate

| No.     | Average Speed (m/s) | Velocity Relative Standard Deviation | Relative standard deviation of speed compared with 100% load without guide plate |
|---------|---------------------|-------------------------------------|--------------------------------------------------------------------------------|
| Refer2  | 15.75               | 17.10%                              | -12.12%                                                                        |
| Refer3  | 15.78               | 14.84%                              | -5.73%                                                                         |
| Refer4  | 15.87               | 9.13%                               | -9.36%                                                                         |
| Refer5  | 3.88                | 9.20%                               | -                                |
| Refer6  | 3.89                | 4.47%                               | -18.44%                                                                        |
| Refer7-1| 3.89                | 0.77%                               | -10.55%                                                                        |
| Refer10 | 12.22               | 18.16%                              | -4.21%                                                                         |
| Outlet  | 10.53               | 24.09%                              | -27.96%                                                                        |

The results show that the uniformity of the flow field in the SCR system is significantly improved after the guide plate is added and the flue is adjusted, and most of the velocity relative to the standard deviation in the set reference section area is reduced to different degrees. Among them, the inlet surface of the first layer catalyst (500mm above the first layer catalyst, Refer6) that was paid special attention to decreased the relative standard deviation of velocity to 4.47% (Reduce 18.44%). The speed of the Outlet of the SCR system (air preheater inlet, outlet) decreases to 24.09% (Reduce 27.96%) relative to the standard deviation, which improves the uniformity of the air flow field into the air preheater to some extent. In general, the setting of the guide plate achieves the goal of expected flow field homogenization.

4.4.2. Velocity Vector at Inlet of the First Layer Catalyst
As it is can be seen from FIG. 17, the smoke flow direction in the inlet area of the first layer catalyst is basically perpendicular to the inlet surface. Calculated according to the entrance of the first layer of the catalyst surface set up 7275 computing nodes, the regional average streamline angle of absolute value is 4.39 °, is less than the conventional technical agreement standard of plus or minus 10 °, can meet the engineering need [16]. The speed of the differences in the local area makes the angle is bigger (maximum of 20.7 °), but no obvious impact on finishing the flow field in the system.

Table 6 Refer to Refer 6 Incident Catalyst angle at 100% Load with Diversion Plate

| Section Name | Average angle of incidence | Maximum angle of incidence | Incidence angle >10° ratio |
|--------------|----------------------------|----------------------------|---------------------------|
| Refer 6      | 4.39°                      | 20.7°                      | 7.61%                     |

5. Conclusion

CFD numerical simulation technology was used to diagnose and analyze the flow field in SCR denitrification system, and the simulation results of flow field without adding guide plate (flue adjustment) were compared and analyzed under 100% load condition. The results of 100% load calculation show that the uniformity of smoke flow field in the SCR system is significantly improved with the addition of baffles, and the velocity relative to the standard deviation in the set reference section area is mostly reduced to different degrees. The relative standard deviation of the inlet velocity of the first layer catalyst reached 4.47%, meeting the technical index of 5%. The first layer of catalyst entrance (500 mm) above the entrance to the catalyst layer average velocity angle of absolute value reduced to 4.39 °, lower than ± 5 ° index, while the angle of local position angle was a little big, but had no significant effect on the whole flow field, which could meet the design needs[17-18]. The calculation results show that the design of the diversion plate layout and the flue adjustment scheme can meet the requirements of engineering design.
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