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Numerical Simulations of SCR DeNOx System for a 660MW coal-fired power station

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Abstract.Aimed at the selective catalytic reduction (SCR) DeNOx system of a 660 MW coal-fired power station, which is limited by low denitrification efficiency, large ammonia consumption and over-high ammonia escape rate, numerical simulations were conducted by employing STAR-CCM+ (CFD tool). The simulations results revealed the problems existed in the SCR DeNOx system. Aimed at limitations of the target SCR DeNOx system, factors affecting the denitrification performance of SCR, including the structural parameters and ammonia injected by the ammonia nozzles, were optimized. Under the optimized operational conditions, the denitrification efficiency of the SCR system was enhanced, while the ammonia escape rate was reduced below 3ppm. This study serves as references for optimization and modification of SCR systems.

1 Introduction

Owing to the "poor in oil and gas, rich in coal" characteristic of China, the coal-fired power generation dominates the domestic power industry [1]. In 2012, the domestic power generation was 4.97 trillion kW·h and the coal-fired power generation was 3.91 trillion kW·h (78.6%) [2]. The dominant role of coal-fired power generation makes significant reductions of NOx by coal-fired furnaces extremely challenging. Nevertheless, optimization methods of coal-fired furnaces reported previously do not meet requirements by current standards [3]. Among various NOx treatment methods, the SCR denitrification technology is one of the most widely applied and most effective methods [4]. The mechanism of SCR denitrification is that reducers (e.g., NH_3 and urea) selectively react with NOx to generate N_2 and H_2O under prescribed catalysts.

In denitrification processes by the selective catalytic reduction (SCR), the concentration distribution of reducers in SCR reactor and airflow distribution has a direct effect on its denitrification efficiency. Currently, the flow fields of the system were analyzed using computational fluid dynamic (CFD) methods [5-6].

2 Equipment

The denitrification of the target coal-fired station was achieved by SCR with double flue, double reactor, and 2+1 catalyst layers (one spare layer). Liquid ammonia was used as reducer and the denitrification rate was no less than 80% (NOx at standard status, 6% oxygen content, dry basis). Each reactor in the denitrification system has a size of 13950mm (L) ×11200 mm (W) ×19080mm (H) (requirements by flue gas under 50%BMCR working conditions). Table 1. summarizes key design parameters of the proposed SCR denitrification system.

Table 1. Key design parameters of the SCR DeNOx system.

NOx concentration at denitrification system inlet	350mg/Nm^3
Denitrification efficiency	80%
Reducer	liquid ammonia
NH_3 escape rate	<3 ppm
SO_2/SO_3 conversion rate	<1%
Systematic resistance of SCR	≤1100 Pa(with spare catalyst)
NH_3/NOx mole ratio	0.81
Flow velocity in reactor	~5m/s
Number of catalyst layers	2+1 (one spare layer)

3 Numerical simulations of SCR DeNOx system

3.1 Establishment of numerical simulations model

A 1:1 model from the economizer outlet to the air preheater inlet was established according to the structure of the SCR reactor. The SCR reactor has a length of 13950mm, width of 11200mm, and height of 19080mm, and it contains two catalyst layers. Deflectors were designed according to the actual arrangement, ammonia injection mixer and AIG were designed at the flue inlet, and rectifier grills were designed on top of the catalyst layer.

Owing to the complicated structure of SCR, which contains various deflectors and rectifier grills, the model was divided into seven areas and the 3D model was divided by polyhedral grid [7]. Meshes at certain locations (e.g., small AIG nozzles) were encrypted to observe flow fields and ammonia injections around nozzles. Boundaries at deflectors and side walls are divided into two layers to enhance the accuracy of numerical simulations.

For numerical simulations of SCR, several assumptions should be proposed. First, the hot flue gas is assumed to be Newtonian fluid and uniformly distributed at the model inlet. Second, the catalyst layer of the reactor is assumed to be porous medium. Third, chemical reactions (ammonia and NOx) are assumed to be negligible as the temperature is below the critical value. The standard k-Epsilon model[8], which has been widely used for calculations of Reynolds number of high turbulence and fluid flows far from side walls[9], was selected. The boundary conditions at the flue gas inlet were aligned with those at the velocity inlet and the compositions of flue gas at inlet were designed accordingly. The boundary conditions at AIG were aligned with those at the velocity inlet and the compositions of flue gas at inlet were designed according to actual ammonia/air ratio (see Table 2.).

Table 2. SCR boundary conditions.

Temperature of flue gas at inlet (°C)		38.4
Flue gas velocity of flue gas at inlet (m/s)		17.3
Compositions of flue gas at inlet	O_2(Vol%)	3.2
	N_2(Vol%)	74.1
	H_2O(Vol%)	8.4
	CO_2(Vol%)	14.2
Temperature at ammonia nozzle (°C)		320
Velocity at ammonia nozzle (m/s)		15.0
Compositions of flue gas at ammonia nozzle	NH_3(Vol%)	5.0
	O_2(Vol%)	74.8
	N_2(Vol%)	20.2

3.2Numerical simulation results and discussion

As the distributions of ammonia concentration and flue gas velocity at the first catalyst layer inlet have significant effects on denitrification by SCR, the first catalyst layer is the focused area for study of flow field. Moreover, the set-up contains two catalyst layers and distributions of flue gas velocity and ammonia concentration at the second catalyst layer outlet should also be paid attention. Herein, the standard deviation coefficient (C_V) was used to evaluate performance of the SCR system. C_V is defined as the percentage of standard deviation over average for velocity/concentration at different cross sections in the SCR reactor. It can be calculated by Eq (1) and (2):

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where σ_V 错误!未找到引用源。 refers to the standard deviation,

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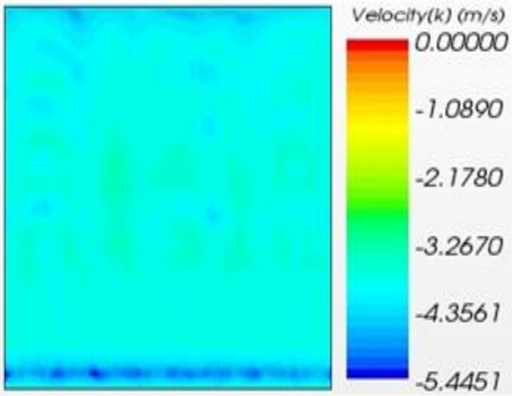
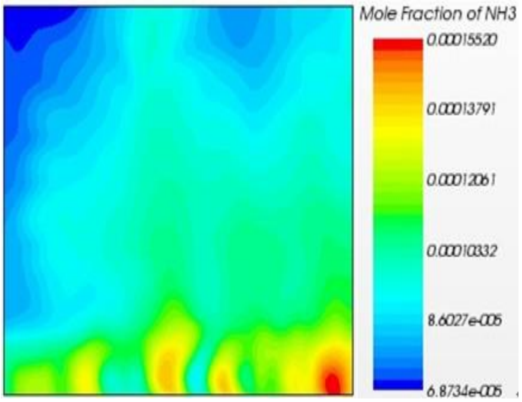
Fig. 1 shows distributions of flue gas velocity and concentration at the first catalyst layer inlet under BMCR working conditions obtained by numerical simulations. As observed, C_V of flue gas velocity at the first catalyst layer inlet was 8.30%, which is lower than the critical value(15%). As shown in Fig. 1 (b), the ammonia concentration field was high at the region close to X-axis. Indeed, C_V of ammonia concentration at this location was 14.9%, while the critical C_V of ammonia concentration is lower than 10.0%.



(a) flue gas velocity distribution at the first catalyst layer inlet.

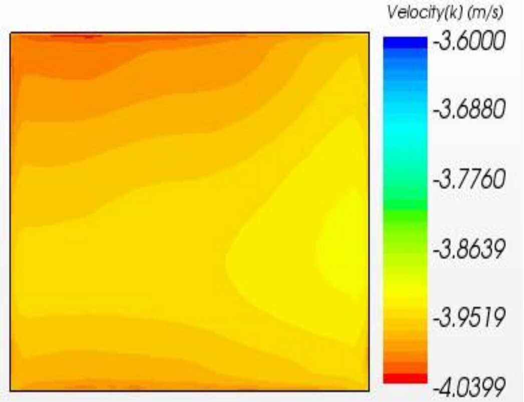


(b) ammonia concentration distribution at the first catalyst layer inlet (gas volumetric ratio).

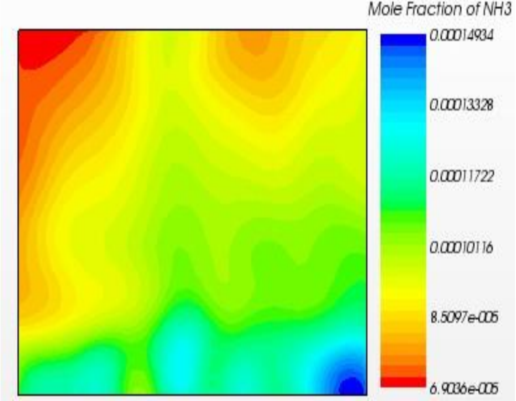
Fig 1. Flow field at the first catalyst layer inlet in initial design.

Fig 1. (a) shows the distribution of flue gas velocity at the first catalyst layer inlet. As observed, the flue gas velocity at the nozzle was up to 4.5m/s, which can be attributed to the angle of the static mixer.

Fig 1. (b) shows the distribution of ammonia concentration field at the first catalyst layer inlet. As observed, the ammonia concentration was high at bottom nozzle which can be attributed to the angle of the static mixer. More specifically, the flue gas flow in this area was relatively high, resulting in high ammonia injections and ammonia concentrations in this area as the gas involved was a mixture of ammonia and flue gas.



(a)flue gas velocity distribution at the second catalyst layer outlet.



(b)ammonia concentration distribution at the second catalyst layer outlet.

Fig. 2 Flow field at exit of the second catalyst layer in initial design.

Fig 2. shows numerical simulations of flue gas velocity distribution and ammonia concentration distribution at the second catalyst layer outlet. As observed, flue gas velocity was uniformly distributed, while slightly high at the top. Meanwhile, ammonia concentration uniformly distributed, although it was relatively high at top left corner and relatively low at bottom left corner.

The distributions of velocity and concentration obtained by the actual operational data of the SCR DeNOx system were consistent with those obtained by numerical simulations, despite slight errors induced by equipment. Owing to this phenomenon, potential problems in the design of SCR system can be predicted by numerical simulations. In other words, non-uniform distributions of flue gas in the catalyst layer can be relieved in design, thus optimizing the performance of the SCR DeNOx system. Additionally, vector diagrams of numerical simulations velocity illustrate flow field distributions, thus avoiding non-uniform flue gas distribution and unexpected wear of the catalyst layer.

It is, therefore, can be concluded that the distributions of concentration and velocity in SCR are affected by factors such as structure and angle of the mixer, location and angles of deflectors, and ammonia injections by each nozzle.Hence, these factors are optimized by numerical simulations to obtain optimized design parameters. In this study, ammonia injections by each nozzle were optimized with the overall ammonia injection staying constant.

4 Ammonia injection optimization

Before entering AIG, the flue gas distribution was non-uniform and the flow of ammonia was determined by the flue gas velocity and the flue gas/ammonia ratio. Therefore, ammonia injection by each nozzle in AIG was adjusted to achieve uniform mixing of flue gas and ammonia in AIG. With constant overall ammonia injection, define the upper and lower nozzles before AIG as nozzles in Row A and B, respectively; adjust ammonia injections by nozzles in Row A and B successively. In order to enhance denitrification efficiency and reduce ammonia consumption and ammonia escape rate, C_V of ammonia concentration field at the first catalyst layer inlet of SCR should be minimized and C_V of velocity field should be no larger than15%.

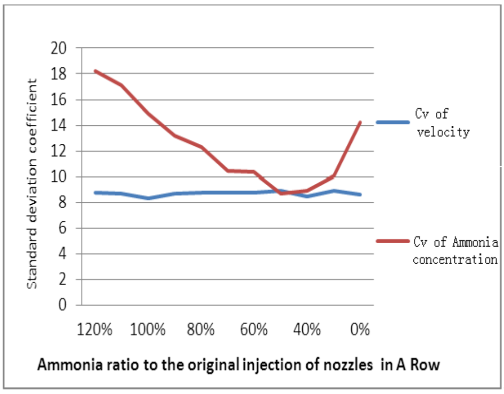
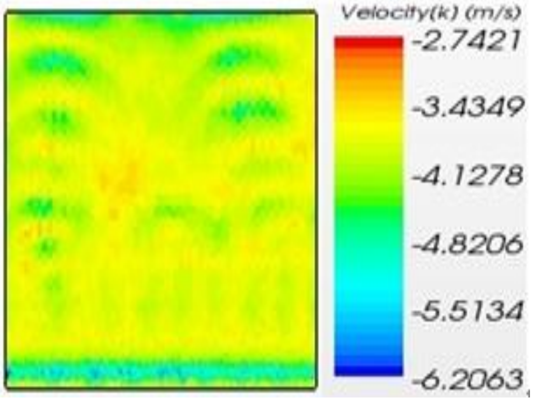
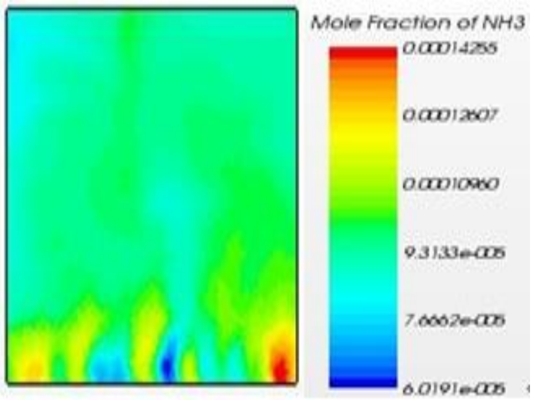


Fig 3. C_V of ammonia injections by nozzles in Row A and B.



(a)Flow field at the first catalyst layer.



(b)concentration field at the first catalyst layer.

Fig 4. Flow field and concentration field at the first catalyst layer inlet after optimization.

Under BMCR working conditions, the ammonia injections by nozzles in Row A and B were adjusted. Fig 3. summarizes the results of numerical simulations. As observed, denitrification by SCR is optimized by adjusting ammonia injections by nozzles in Row A and Row B to 55% and 145% of the initial values, respectively.

Under BMCR working conditions of ammonia injection optimization, the ammonia concentration distribution at the first catalyst layer inlet was uniform (see Fig 4.). Indeed, CV of ammonia concentration distribution was reduced from 14.9% to 8.7% and CV of flue gas velocity was 8.2%, which was slightly enhanced.

5 Hot tests

With constant overall ammonia injection, optimizations of ammonia injections by nozzles in Row A and B were adjusted successively. Table 3. summarizes results of hot tests in this thermal power set under conventional working conditions.

Table 3. Performances of Furnace 1.

Item	Unit	Working Conditions 1	Working Conditions 2
Electrical load	MW	652	666
NOx A at SCR inlet	mg/m^3	449	456
NOx B at SCR inlet	mg/m^3	445	450
NOx A at SCR outlet	mg/m^3	88	84
NOx B at SCR outlet	mg/m^3	85	82
SCR denitrification efficiency A	%	80.40	81.58
SCR denitrification efficiency B	%	80.90	81.78
NH_3 at SCR outlet A	ppm	3.92	2.93
NH_3 at SCR outlet B	ppm	3.33	2.85
Ammonia consumption A	kg/h	137.5	135.9
Ammonia consumption B	kg/h	136.2	135.2

To verify the ammonia injection optimization, under typical working conditions, NOx concentration distributions at Outlet A before (see Table 4) and after ammonia injection optimization (see Table 5) were obtained. Under working conditions 1 (before ammonia injection optimization), the average NOX at Outlet A of the SCR system was 87.7mg/Nm3 (deviation = 16.86%), resulting in large ammonia consumption, high ammonia escape rate, and low denitrification efficiency. Under working conditions 2 (after ammonia injection optimization), the average NOx at Outlet A of the SCR system was 83.95mg/Nm3 (deviation = 9.89%) and concentration distributions (<10%) meet requirements. Indeed, the ammonia consumption was reduced from 137.5kg/h to 135.9kg/h, the ammonia escape rate was reduced from 3.92ppm to 2.93ppm, and the denitrification efficiency was enhanced from 80.4% to 81.58%.

Table 4. NOx concentration distribution at SCR system Outlet A under working conditions 1.

Location	Hole 1	Hole 2	Hole 3	Hole 4
1	92.4	61.2	87.1	101.7
2	94.2	62.8	85.9	102.1
3	91.4	62.4	86.3	105.2
4	94.9	65.2	88.3	105.4
5	98.2	66.3	89.4	102.1
6	99.5	67.7	75.8	104.3
7	96.6	65.6	70.5	102.1
8	97.7	63.4	88.4	108.6
9	98.4	66.8	89.3	105.3
10	97.5	68.5	91.1	108.2
Average (mg/Nm^3)	87.7	Mean square deviation (%)	16.86	

Table 5. NOx concentration distribution at SCR system Outlet A under working conditions 2.

Location	Hole 1	Hole 2	Hole 3	Hole 4
1	82.5	72.2	85.5	96.5
2	83.6	73	83.2	96.4
3	83.5	74.5	84.7	95.2
4	85.2	75.8	86.9	97.2
5	85	70.2	88.1	95.3
6	87.5	72.9	87.3	96.5
7	86.6	71.6	83.1	93.1
8	82.8	70.9	84.4	97.6
9	81.5	68.9	81.1	92.9
10	83.5	69.5	78.5	93.6
Average (mg/Nm^3)	83.95	Mean square deviation (%)	9.89	

6 Conclusions

In this study, flue gas velocity field and concentration field distributions of SCR DeNOx system for a 660MW coal-fired power station were simulated ,the results of the proposed SCR system before and after optimization were compared with each other. The following conclusions can be obtained:

(1) Field distributions obtained by numerical simulations are consistent with the actual operational data, indicating that numerical simulations can predict distributions of flue gas in the catalyst layer for design of SCR systems, thus facilitating optimization of denitrification by SCR systems by eliminating non-uniform flue gas distribution and unexpected wear.

(2) With a constant overall ammonia injection, denitrification by SCR is optimized by adjusting ammonia injections by nozzles in Row A and Row B to 55% and 145% of the initial values, respectively. As a result, Cv of concentration distribution was reduced from 14.9% to 8.7% and that of flue gas velocity was 8.2%.

(3) Hot tests indicated that the mixing of ammonia and flue gas is affected by the ammonia injection ratio. With a constant overall ammonia injection, optimization can be further enhanced by adjusting ammonia injection by each nozzle and the denitrification efficiency of the SCR system is improved. Indeed, the ammonia escape rate was reduced below 3ppm and the denitrification ammonia consumption was reduced. This study provides references for optimization of SCR systems.

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