The Open Mechanical Engineering Journal, **2014**, *8*, 643-647

Numerical Simulation to Reduce NO_x of Diesel Engine Urea-SCR System

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Abstract: By using computational fluid dynamics and chemical reaction dynamics method, the mathematical model of SCR (selective catalytic reduction) system was established. On the basis of the verified feasibility, by CFD numerical analytical method, the reducing agent inside the catalysts concentration distribution was compared under different added urea schemes. Jet direction and the form of fuel injector were studied on the basis of the effects of reducing agent concentration distribution. The simulation result shows good agreement with the experimental data. The simulated results can be utilized in optimization design of the diesel SCR catalyst.

Keywords: NO_x, numerical simulation, Urea-SCR, Grid Model, AVL exhaust gas analyzer, SCR catalyst.

1. INTRODUCTION

Selective Catalytic Reduction (SCR) has been applied to stationary source, fossil fuel fire, combustion units for emission control since the early 1970's and is currently being used in Japan, Europe, and the United States. There has been limited application of SCR to other combustion devices and processes such as simple cycle gas turbines, stationary reciprocating internal combustion engines, nitric acid plants, and steel mill annealing furnaces. SCR can be applied as a stand-alone NOx control or with other technologies such as combustion controls. SCR systems have experienced relatively few operational or maintenance problems [1].

SCR is typically implemented on stationary source combustion units requiring a higher level of NOx reduction than achievable by SNCR or combustion controls. Theoretically, SCR systems can be designed for NOx removal efficiency by up to 100 percent (%). Commercial coal, oil and natural gas-fired SCR systems are often designed to meet control targets of over 90%. However, maintaining this efficiency is not always practical from a cost standpoint. In practice, SCR systems operate at efficiency in the range of 70% to 90%.

Like SNCR, the SCR process is based on the chemical reduction of the NOx molecule. The primary difference between SNCR and SCR is that SCR employs a metal-based catalyst with activated sites to increase the rate of the reduction reaction. A nitrogen-based reducing agent (reagent), such as ammonia or urea, is injected into the post combustion flue gas. The reagent reacts selectively with the flue gas NOx within a specific temperature range and in the presence of the catalyst and oxygen to reduce the NOx into molecular nitrogen (N2) and water vapor (H_2O).

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Urea-SCR technology can effectively reduce diesel engine exhaust gas nitrogen oxide (NOx) emissions. Urea - SCR is the most promising technology which meets emission standards of the diesel engine to meet the Euro IV and V regulations [2]. According to the Eley-Rideal mechanism, finished urea catalyzed reduction NOx three-dimensional numerical simulation [3], by using the AVL FIRE software, can provide reference for optimization design of catalysts. Depending on the use of reducing agent which can be roughly divided into two categories, NH_3-SCR and HC-SCR, this study mainly introduces NH_3-SCR technologies using NH3 as reducing agent.

2. UREA-SCR REACTION MECHANISM

Urea-SCR principle is the reducing agent that is sprayed into the exhaust pipe, and in the SCR catalytic converter, NO_x is reduced by the presence of ammonia (NH_3) into water and nitrogen (N_2). The NH_3 is obtained from urea by hydrolysis at high temperatures (see Eq. (1)). The SCR system currently adopted the reducing agent as aqueous solution containing 32.5% urea:

$$NH_2CONH_2 + H_2O \rightarrow 2NH_3 + CO_2 \quad (1)$$

NO_x emissions in diesel exhaust gas are usually composed of more than 90% NO [4]. Thus, the standard SCR reaction is dominated by NO_x reduction progress (see Eq. (2)) [5, 6]. When the temperature ranges from 250 to 450°C, the standard SCR reaction is useful.

$$4NO + O_2 + 4NH_3 \rightarrow 4N_2 + 6H_2O \quad (2)$$

The reaction rate of the equivalent molar mixtures of NO and NO_2 is faster than the reaction involving only NO as shown in Eq. (2). The reaction as shown in Eq. (3) is called the fast reaction [7]. The effect of this reaction is pronounced when the temperature is below 300°C.

$$NO + NO_2 + 2NH_3 \rightarrow 2N_2 + 3H_2O \quad (3)$$

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Taking into account the leakage of ammonia during the operation of the engine,, in the ammonia catalytic converter with SCR catalyst, NH_3 reacts with O_2 to form N_2 and H_2O (see Eq. (4)):

$$4NH_3 + 3O_2 \rightarrow 2N_2 + 6H_2O \tag{4}$$

Although there are several ammonia oxidation reactions that have been studied by researchers, it is assumed that ammonia is only converted to NO for the sake of facilitating model validation [8]. The ammonia oxidation is an undesirable reaction, as shown in Eq. (5) [9]. In this reaction, the ammonia is oxidized to NO, which limits the maximum NO_x conversion. The effect of this reaction is pronounced when the temperature is higher than 500°C.

$$5O_2 + 4NH_3 \rightarrow 4NO + 6H_2O \tag{5}$$

At high temperatures (>400°C), the commonly used catalysts based on TiO_2-WO_3-V_2O_5 tend to form nitrous oxide. One of the possible reactions leading to nitrous oxide is shown in Eq. (5) [10].

$$4NO + 3O_2 + 4NH_3 \rightarrow 4N_2O + 6H_2O \tag{6}$$

The two reactions seriously affect the NO_x conversion rate. When temperature is below 200 °C, explosive material NH_4NO_3, NH_3 and NO_2 react (see Eq. (7)):

$$2NO_2 + 2NH_3 \rightarrow NH_4NO_3 + N_2 + H_2O \tag{7}$$

NH_4NO_3 can be adhesive on the surface of the catalyst in the form of a liquid or solid, which poisons the catalyst temporarily, but NH_4NO_3 automatically decomposes in reaction temperature higher than 300°C [11].

The reaction principle of Urea - SCR system is shown in (Figs. **1** & **2**).

Oxidation catalyst at the front of SCR catalysts device was not chosen in the study of this subject.

3. CFD MODELING AND VALIDATION SCR SYSTEM

Analysis and comparison of experimental and numerical simulation model of the temperature- NO_x conversion rate relationship are conducted to verify the accuracy and feasibility of numerical simulation.

3.1. The Establishment of the Grid Model

Three-dimensional simulations are carried out with the commercial CFD simulation package, FLUENT 6.3, ANSYS Inc. [12, 13], in two steps: first, by using three-dimensional modeling software, Pro/E establishes lean combustion NO_x catalysts system geometric model, and transfers to the STL file format output; then it makes use of the FIRE mesh generator to generate the mesh (Fig. **3**).

3.2. Calculation Model and Boundary Conditions

Simulation of coupling the material transport model, the spray model, porous media model, gas phase reaction model and catalytic reaction model, the model parameters were set up under different working conditions, but the boundary condition varies due to the different nature of the exhaust. Four points were selected as sites in the process of simulation experiment as shown in Table **1**. For the inlet boundary using the given mass flow mode and for the turbulent parameter setting, 5% average velocity square is imported as the turbulent kinetic energy, with the characteristic length being the inlet diameter of 10% [6]; The outlet boundary condition parameters were set to static pressure, which is a standard atmospheric pressure; the wall boundary condition parameters were the same, the velocity components were 0. The concentration of imported components and other conditions were based on engine test

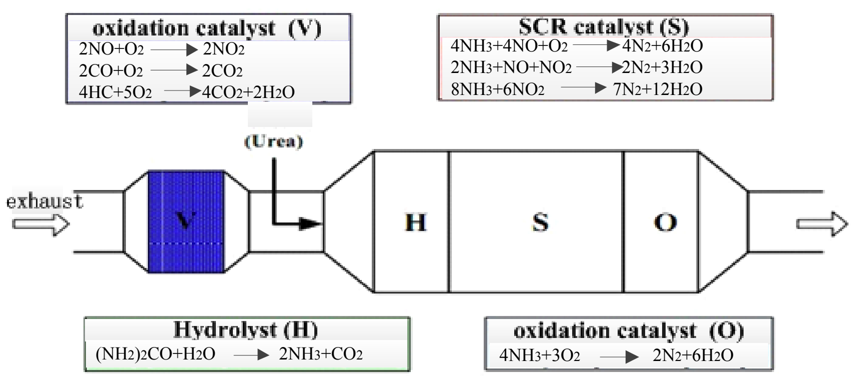


Fig. (1). The reaction principle of Urea - SCR system.

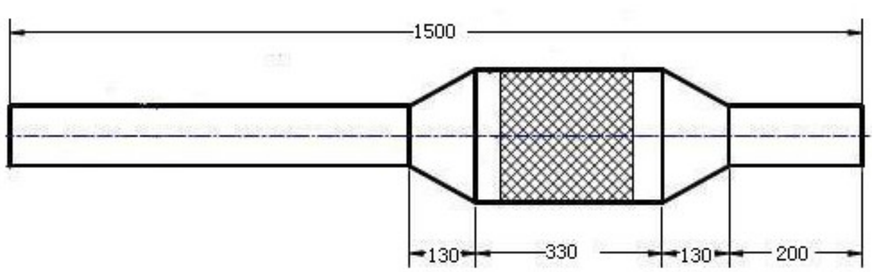


Fig. (2). The simplified schematic Urea - SCR system size.

bench measurements. Urea reducing agents were according to weight ratio and NO_x material for 1.2:1 injection.

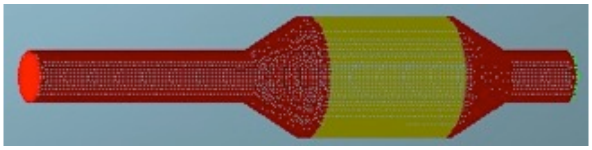


Fig. (3). Catalysts geometric model.

Table 1. Stable working condition of engine test data table.

Working Condition	1	2	3	4
load	37	45	61	71
Exhaust temperature(K)	476	553	670	710
Exhaust gas flow(kg/h)	237	266	338	378
entrance φ(NO_x) /10-6	443	854	1153	1168
export φ(NO_x) /10-6	284	340	220	220

3.3. Urea-SCR Test

The experimental device utilizes the YC4F115-40 high pressure common rail engine experiment bench (Fig. **4**), having the main technical parameters of the engine according to Table **2**. By using AVL exhaust gas analyzer to measure NO_x emission concentration from the engine body without Urea-SCR system, the test was conducted to determine NO_x emission levels of the original machine when without Urea-SCR system [14, 15]. Then portion of the SCR system was installed post-processing, renewing the corresponding conditions test, to determine NO_x emission levels of the machine with Urea-SCR system, and verify the four standards. The NO_x conversion rate of the aqueous urea as reducing agent was acquired by relative four standards of NO_x emission concentration of the original machine. This engine test bench is shown in Fig. (**4**). The dosing pump of Urea aqueous on test bench is shown in Fig. (**5**), and the jet entrance of Urea aqueous is shown in Fig. (**6**). The test provides initial boundary conditions for numerical simulation.

Fig. (4). YC4F115-40 high pressure common rail engine experiment bench.

Table 2. The main technical parameters of the engine.

Specifications	Parameter
Form	Four stroke, water cooled, inline four cylinder
engine displacement	2660(mL)
The intake form	intercooler engine
fuel system	high pressure common rail
rated output	85kW
net power	3400r/min
torque	285 N.m
torque speed	1800—2400r/min
emission standard	the national standard stage IV

Fig. (5). Dosing pump of Urea.

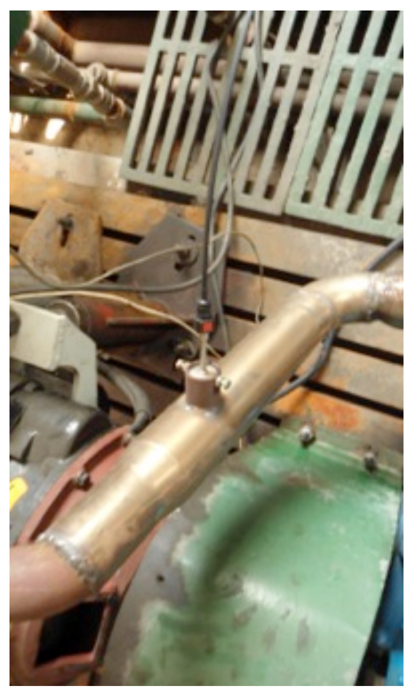


Fig. (6). The jet of Urea.

3.4. The Feasibility of the Model Validation

In order to verify the feasibility of numerical simulation of SCR catalytic converter model, the tests were conducted on the experimental bench. The simulation results and the experimental result are shown in Fig. (**7**). Fig. (**3**) shows that the result obtained by the conversion efficiency of simulation is higher than the actual, and this result and the prediction results are consistent, but the trends on the two are the same. The simulation results are in good agreement with the experimental results, and can predict the actual results effectively.

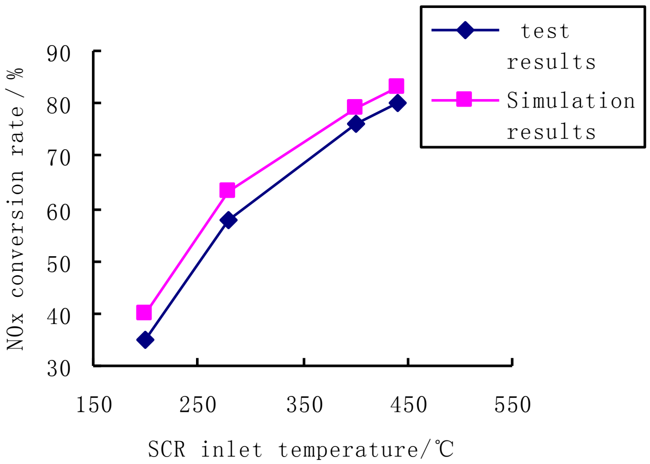


Fig. (7). The contrast of Simulation results and test results.

4. SIMULATION RESULTS AND ANALYSIS

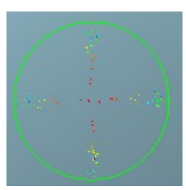
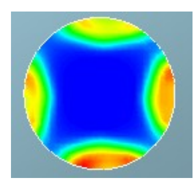
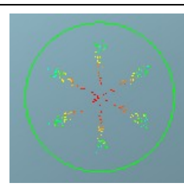
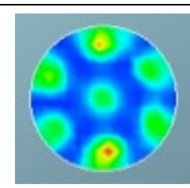
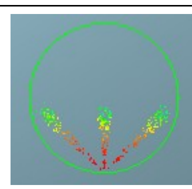
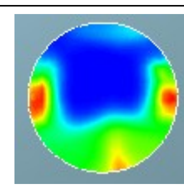
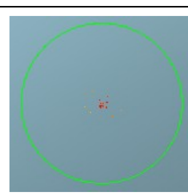
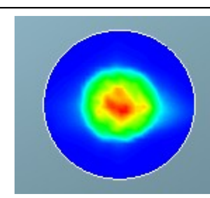
As shown in Table **3,** four kinds of urea added scheme and simulation are implemented for the mixing process of urea of diesel engine NO_x catalysts reducing agents and the exhaust gas. Through analyzing NH_3 concentration distribution of 4 different schemes under reducing agents, the study was conducted on an injector and its injection direction affected the reducing agents concentration distribution.

Through comparing the distribution of spray droplet scheme 1 and scheme 2, it can be seen that the number of different holes injection can give different distribution ranges of reducing agent; 6 injector hole distribution ranged larger than 4 hole and was more uniform for the reducing agent.

Through comparing the distribution of spray droplet scheme 1 and scheme 3, for the two kinds of urea injection modes, along the direction of the center line of the exhaust pipe injection cases, reducing agent concentration distribution exhibited more uniformity than the vertical direction of exhaust pipe wall case. In scheme 3, reducing agents are not evenly distributed, as being only distributed on the lower half circle, while the other half is rarely distributed.

Through comparing the distribution of spray droplet scheme 1 and scheme 4, compared to the shaft type injector needle, hole type injector is conducive to reducing agent from a larger scope. In scheme 1, on the edge of the area of section near the pipe wall exists thick and thin alternating

Table 3. Adding urea schemes.

	Scheme Features	Different Droplet Distribution of Urea Injection Scheme	Different Schemes NH_3 Concentration Distribution
1	4 holes injector, along the reverse jet of the exhaust pipe center line direction		
2	6 holes injector, along the reverse jet of the direction of the center line of the exhaust pipe		
3	6 holes injector, perpendicular to the pipe wall jet		
4	Shaft needle type injector, reverse jet		

regions, and the concentration distribution close to a series of concentric circles in the scheme 4. Thus, Shaft needle type injector can get better circumferential distribution uniformity, as the Shaft needle type injector is superior to the hole type injector.

CONCLUSION

(1) Research on Urea-SCR system suggests that under steady state conditions, NO_x conversion is related to the temperature of the catalyst. That is, the higher the temperature, the better the performance of the catalyst. The higher conversion rate of the catalyst at temperature of 400°C, makes NO_x conversion rate higher than 80%.

(2) Nozzle type choice: compared with the shaft needle type injector, hole type injector is conducive to reducing agent dispersed to a larger range, thus improving the reducing agent concentration distribution can have a significant effect. But using hole type injector is difficult to obtain uniform distribution in circumferential direction.

(3) Jet direction choice: by comparing jet along the exhaust pipe axis direction in the middle of the exhaust and jet along exhaust pipe axis direction in the vertical exhaust pipe wall, the uniformity of the reducing agent concentration distribution is better than the latter.

(4) Using three-dimensional CFD can accurately simulate exhaust gas after-treatment systems under steady state and can provide reference for optimization design of catalysts.

CONFLICT OF INTEREST

The authors confirm that this article content has no conflict of interest.

ACKNOWLEDGEMENTS

This paper belongs to the project of the "National Natural Science Foundation of China", No. 51376113.

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Received: January 8, 2015 Revised: January 15, 2015 Accepted: January 16, 2015