Dynamic Model Parameter Identification and Simulation of SCR Based on Genetic Algorithm[§]

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Abstract: The Selective Catalytic Reduce (SCR) is studied. The unknown parameters of the SCR kinetic model equations are fitted based on the Genetic Algorithm (GA), which is in the range of the allowable error, compared to the experimental data. Then in AVL Boost software, the simulation results of SCR reaction are obtained. Compared to the test data, the simulation results prove that the parameter identification is effective. At last, the SCR reaction is simulated in AVL Boost, and at the same exhaust temperature, the effect of GHSV and NSR on the SCR reaction is studied.

Keywords: AVL boost, GA, parameter identification, SCR.

1. INTRODUCTION

Diesel engine is widely used because of its excellent dynamic performance and fuel economy, and CO, HC emission is better than that from gasoline engine. But NO_X and PM emission from diesel engine is a problem, thus it is a main research direction in the field of engine to reduce NOX and PM emission from diesel engine effectively [1]. SCR as an effective method to reduce NO_X emissions has been widely applied in foreign countries. Scholars from home and abroad have researched on reaction mechanism of SCR, reaction catalyst, SCR system structure and so on by means of experiments and simulations [2-9]. Simulations have aroused the attention of researchers due to its ability to reduce the test cost and accelerate research process. One of the key factors is to determine the kinetic parameters of simulation of SCR reaction, which will affect the accuracy of simulation results directly. At present, some researchers have calculated the kinetic parameters of SCR with different methods [10, 11]. But these methods are based on the SCR catalyst preparation test, and this test needs more basic SCR catalyst parameters which are difficult to be obtained. In this paper SCR reaction is simulated with AVL Boost software, and the dynamic parameters of the chemical reaction are identified using the genetic algorithm, because of its the rapid convergence. After the results are calibrated, the effect of impact factors on the SCR reaction is studied.

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2. SCR CHEMICAL REACTION AND REACTION MODEL

2.1. SCR Chemical Reaction

Diesel engine SCR reaction principle is that at a certain temperature and under the action of catalyst, the emissions NO_X from diesel combustion take place the selective oxidation reduction reaction with reducing substance NH_3 or urea, which generates H_2O and N_2.

Oxidation chemical reaction of typical Urea-SCR system includes urea pyrolysis and hydrolysis, NO_X and NH_3 reduction reaction, NH_3 oxidation reaction. Among them NO_X and NH_3 reaction includes four types: fast SCR reaction (1), standard SCR reaction (2), Slow NO SCR reaction (3) and Slow NO_2 SCR reaction (4).

Standard SCR $\quad 4NH_3+4NO+O_2 \rightarrow 4N_2+6H_2O \quad$ (1)

Fast SCR $\quad 4NH_3+2NO+2NO_2 \rightarrow 4N_2+6H_2O \quad$ (2)

Slow NO SCR $\quad 4NH_3+6NO \rightarrow 5N_2+6H_2O \quad$ (3)

Slow NO_2 SCR $\quad 4NH_3+3NO_2 \rightarrow 3.5N_2+6H_2O \quad$ (4)

When the concentration of oxygen is over 2% in the reaction, the reaction progress is standard SCR reaction and fast SCR reaction, and in diesel engine exhaust NOx mainly exists in the form of NO, so this research mainly consider standard SCR.

2.2. SCR Reaction Model

At present there are a lot of research on the mechanism of SCR reaction, and the catalyst of SCR is V_2O_5 that is carried on TiO_2 [12-15]. Comparing these mechanisms, the public have accepted the mechanism proposed by TopsØe. The mechanism considers that $-NH_4^+$ is formed with NH_3 by being adsorbed on Brönsted acid sites (also known as adsorption sites) V^{5+}-OH firstly, then it is oxidized to NH_3^+ by adjacent oxidation potential V^{5+}=O, while V^{5+}=O is restored to the tetravalent state V^{4+}-OH. The combination of -NH_3^+ and NO from gas phase format -NH_3^+NO which is decomposed into N_2 and H_2O instantly. V^{4+}-OH is decomposed into V^{3+}, V^{5+}=O and H_2O through the same responses among species, V^{3+} is oxidized to form V^{5+}=O under the function of O_2, thus the catalytic cycle process is completed [12].

From this analysis, the SCR reaction is accordance with the Eley-Rideal mechanism, the standard reaction rate equation in SCR [16]:

$$-r = k_1 \cdot C_1 \cdot \emptyset_{NH_3} \quad (5)$$

$\emptyset_{NH_3}$ is the rate of adsorption of NH_3 [16]

$$\emptyset_{NH_3} = \frac{k_2 C_2}{1+k_2 C_2} \quad (6)$$

Combined with the Arrhenius equation [17], the reaction rate equation can be expressed as：

$$r_{NO} = k_1 \cdot \exp\left(\frac{-E_1}{RT}\right) \cdot C_1 \cdot \frac{k_2 \cdot \exp\left(\frac{-E_2}{RT}\right) \cdot C_2}{1 + k_2 \cdot \exp\left(\frac{-E_2}{RT}\right) \cdot C_2} \quad (7)$$

Among them, r_{NO}: the reaction rate of NO, kmol · s^{-1} · m^{-3}, k_1: the pre-exponential factor of NO reaction， s^{-1}, E_1: the activation energy of the reaction of NO, J · mol^{-1}, C_1: the molar concentration of NO in the reactor, kmol · m^{-3}, k_2: the pre-exponential factor of the NH_3 adsorption reaction, m^3kmol^{-1}, E_2: the activation energy of adsorption reaction of NH_3, J · mol^{-1}, C_2: the molar concentration of NH_3 in the reactor, kmol · m^{-3}, T : the reaction temperature, K, R: ideal gas constant, 8.314J · mol^{-1} · K^{-1}.

3. SCR DYNAMIC PARAMETER IDENTIFICATION

3.1. Basic Principle of Genetic Algorithm (GA)

In the natural evolution, each species become to be more adaptable to the environment. The basic characteristics of the individual species is inherited by their offspring, but they are not entirely same with their parents. The nature of the individual is decided by the chromosome which is composed by ordered arrangement gene. Individuals decided by chromosome have different adaptability to the environment, through gene hybridization and gene mutation produce the individual of strong adaptability. In the development of generation, the natural selection "the survival of the fittest" has the forces to make the individual feature be adapted for the environment.

GA is the search algorithm which is based on natural selection and natural genetic mechanism, the search space of optimization problems is mapped for the genetic space, each solution is coded as a binary string (also have other coding methods) chromosomes. Each chromosome position is called genes. Each chromosome (corresponding to an individual) represents a solution and a certain number of individuals forming a group. GA first randomly generate initial population consisted of some individuals (a group of candidate), the fitness function on the problem of environmental adaptation is determined according to the objective function. According to the fitness function of the objective function the fitness of each individual to the problem of environment is computed, then the corresponding individual chromosomes is chosen according to the individual fitness. At last genetic operation such as crossover and mutation has evolved into the generation of groups. So the generation continuously evolves towards a more optimal solution, and finally some convergence condition of adapting environment is met, and the optimal solution of the problem is obtained.

3.2. Dynamic Parameters Identification

3.2.1. SCR Test Results

This paper takes a heavy duty diesel engine SCR as a research object, the dynamics parameters of SCR in equation (1) k_1, E_1, k_2, E_2 are solved. When the four kinetic parameters are solved, the test results of other parameters in the SCR are shown in Table **1**. The reaction temperature of these tests is 300℃-350℃， so the applicable temperature scope of the kinetic parameters is 300℃-350℃。

3.2.2. Dynamic Parameter Identification

The SCR dynamics parameter identification process based on genetic algorithm is shown in Fig. (**1**).

The genetic algorithm parameters are set in the Table **2**.

The calculation results obtained by genetic algorithm are taken into the standard SCR kinetic equation, and the NO reaction rate is obtained. Compared to the experimental

Table 1. Relevant parameter values.

Data Group	Catalyst Reaction time/s	Concentration of NO kmol．m^{-3}	Reaction Rate of NO kmol．m^{-3}．s^{-1}	NH_3 Concentration kmol．m^{-3}
1	0.1092	58.514	510.8011	61.1279
2	0.1139	63.4353	241.3488	33.1317
3	0.1140	63.4353	400.2720	53.4208
4	0.1142	63.4353	494.5784	66.0062
5	0.1142	63.4353	505.1675	70.7168
6	0.1808	55.5763	131.2798	25.9943

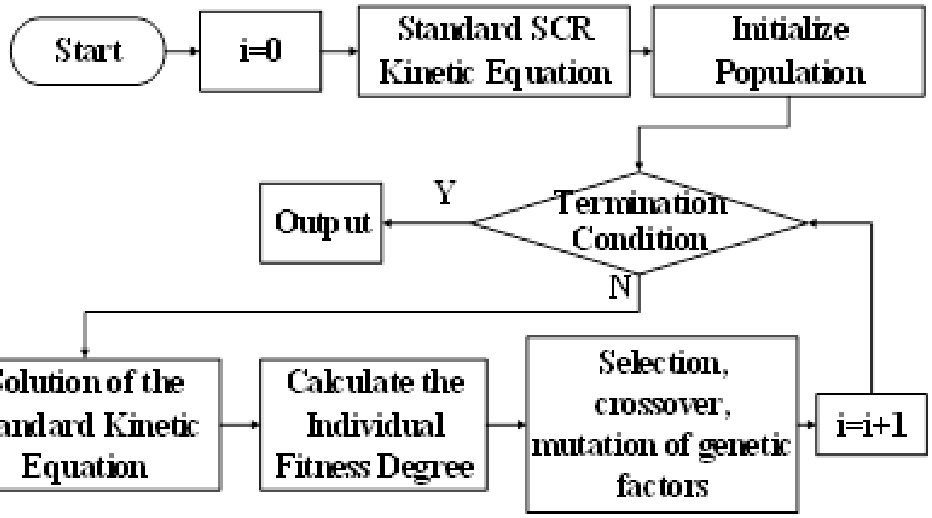

Fig. (1). Flow-chart of identification process of standard scr model.

Table 2. Relevant parameter values of GA.

Parameters of the Algorithm	Parameter Setting
Number of Population	50
Crossover Probability	0.65
Mutation Probability	0.01
Convergence of Allowable Error	1×10^{-9}
Convergence Allows Decision Error number	1000
Maximum Allowable Number of Iterations	20000

Table 3. Results of the kinetic parameters identification.

Parameters	Value	Unit
Pre-exponential factor of NO-k_1	57.220170	s^{-1}
Pre-exponential factor of NH_3-k_1	0.002710	$m^3 \cdot kmol^{-1}$
Activation energy of NO-E_1	-0.210367	$J \cdot mol^{-1}$
Activation energy of NH_3-E_2	996.80537	$J \cdot mol^{-1}$

data, the effect of fitting error is within 5%, which can be accepted.

Kinetic parameters of SCR based on genetic algorithm are shown in Table **3**.

3.3. The Simulation and Calibration of SCR

AVL Boost is used for the simulation of automobile engine. SCR could be simulated by the software, but the process of simulation need to input dynamic parameters. The kinetic parameters obtained by genetic algorithm are plugged into the SCR simulation model built in AVL Boost. The simulation results of SCR model are compared to the experimental results to verify the correct of reaction kinetic parameters obtained with genetic algorithm. The comparison result is shown in Fig. (**2**). The data issued by simulation are in line with the experimental data. The error was less than 5%. The result shows that the kinetic model of SCR reaction obtained by genetic algorithm is closed to the actual chemical reaction process, so these kinetic parameters can be used for further study.

4. SIMULATION OF SCR INFLUENCE FACTORS

The obtained parameters are applied into kinetic model in AVL BOOST software. The variation curve of NO conversion rate is obtained by adjusting GHSV or NSR, When the reaction temperature is in the range of 300℃to 350℃, which provides a theoretical basis for studying the influence factors of SCR reaction and improving the conversion rate of NO.

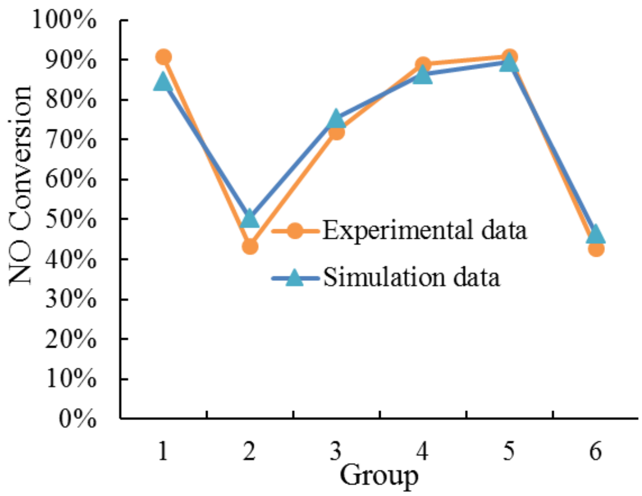

Fig. (2). NO conversion rate of experiment and simulation.

4.1. Effect of GHSV on Reaction of SCR

GHSV is defined as volume flow of exhaust gas through an unit volume catalyst under standard conditions. Reaction time is the inverse of GHSV. Keeping exhaust temperature and volume unchanged, GHSV is controlled well by adjusting exhaust gas. Fig. (**3**) shows the maximum of NO conversion rate when GHSV was $10000h^{-1}$, $20000h^{-1}$, $30000h^{-1}$, $40000h^{-1}$, $50000h^{-1}$ and $60000h^{-1}$ by the simulation. NO conversion rate decreases as GHSV increases, which is because of the less reaction time. The contact time between gas and catalyst become shorter, a part of gas cannot be adsorbed completely and mass transfer has been discharged, so the low conversion rate is caused.

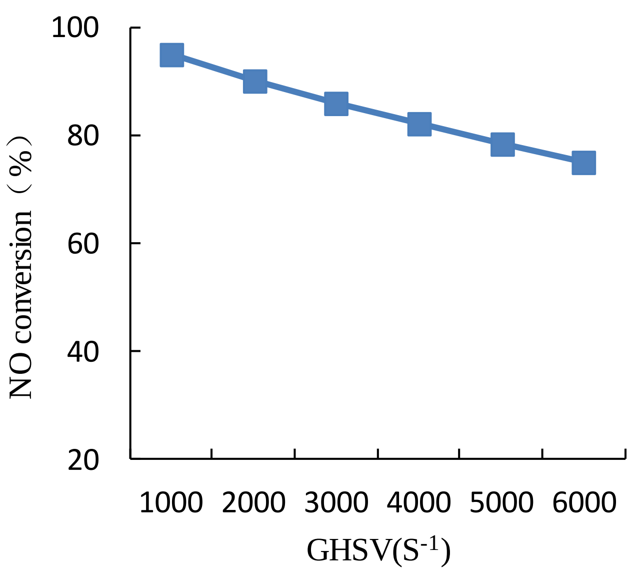

Fig. (3). NO conversion ration with GHSV.

4.2. Effect of NSR on Reaction of SCR

Keeping exhaust temperature and GHSV unchanged, NSR is controlled well by adjusting the amount of urea injected. The rate of NO conversion is shown in Fig. (**4**). The conversion rate of NO increases with NSR increasing. While NSR is greater than 1, the increase trend slow down, and it is close to a fixed value. This is largely because that the concentration of NH_3 increases with urea injected increasing. The conversion rate of NO improves with the ratio of NH_3 to NO increasing. While when the ration is bigger than 1, the NO conversion will be closed to limit value and no longer increases.

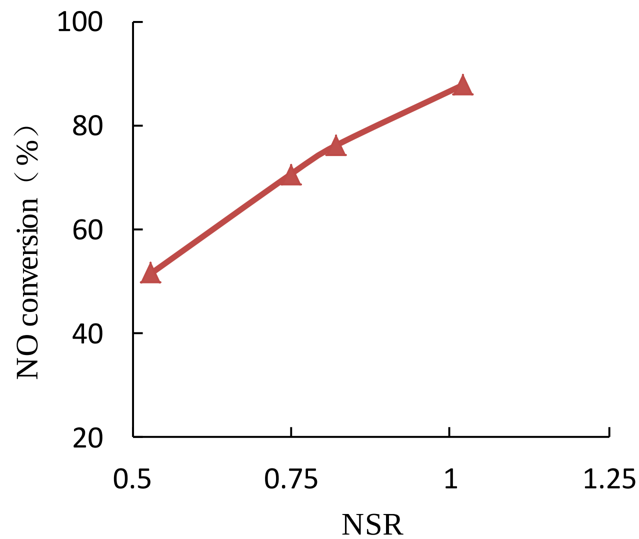

Fig. (4). NO conversion ratio with NSR.

CONCLUSION

1) Compared to the experimental data, it is proved that it is a right way to identify the kinetic parameters of SCR with genetic algorithm. The pre-exponential factor of NO reaction is $57.22s^{-1}$, the activity energy of NO is -0.21037J . mol^{-1}. The pre-exponential factor of NH_3 adsorption is $0.0027m^3$. $kmol^{-1}$, the activity energy of NH_3 is 996.81J . mol^{-1}.
2) NO conversion rate is calculated with the simulation model of SCR assigned with identified parameters in AVL Boost software. The results are in well agreement with experimental results, and the error is in under 5%.
3) Through the simulation in AVL BOOST software, it is proved that the conversion rate of NO decreases significantly with GHSV increasing, and it increases gradually when NSR is raised, which provides a new way to research SCR.

CONFLICT OF INTEREST

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

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