Optimization Analysis of Various Parameters Based on Response Surface Methodology for Enhancing NO\textsubscript{x} Catalytic Reduction Performance of Urea Selective Catalytic Reduction on Cu-ZSM-13 Catalyst

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Abstract: While selective catalytic reduction (SCR) has long been indispensable for nitrogen oxide (NO\textsubscript{x}) removal, optimizing its performance remains a significant challenge. This study investigates the combined effects of structural and intake parameters on SCR performance, an aspect often overlooked in previous research. This paper innovatively developed a three-dimensional SCR channel model and employed response surface methodology to conduct an in-depth analysis of multiple key factors. This multidimensional, multi-method approach enables a more comprehensive understanding of SCR system mechanics. Through target optimization, we achieved a simultaneous improvement in three critical indicators: the NO\textsubscript{x} conversion rate, pressure drop, and ammonia slip. It is worth noting that the NO\textsubscript{x} conversion rate has been optimized from 17.07\% to 98.25\%, the pressure drop has been increased from 3454.62 Pa to 2558.74 Pa, and the NH\textsubscript{3} slip has been transformed from 122.26 ppm to 17.49 ppm. These results not only advance the theoretical understanding of SCR technology but also provide valuable design insights for practical applications. Our findings pave the way for the development of more efficient and environmentally friendly SCR systems, potentially revolutionizing NO\textsubscript{x} control in various industries.

Keywords: diesel engine; SCR system; ammonia storage characteristics; NO\textsubscript{x} conversion efficiency

1. Introduction

The position of traditional internal combustion engines in the industry remains unshakable [1]. The composition of diesel engine exhaust emissions is very complex, including approximately 150–200 substances [2]. The most difficult pollutants to remove are nitrogen oxides (NO\textsubscript{x}), hydrocarbons (HCs), carbon monoxide (CO), and particulate matter (PM), which directly cause photochemical smog and haze weather, posing great harm to human health [3]. At present, researchers are trying to use oxygen-containing fuels (methanol, ethanol, dimethyl ether, furan, etc.) and no-carbon fuels (hydrogen, ammonia, etc.) to replace traditional fossil fuels to reduce pollutant emissions [4]. Although various alternative fuels have many advantages, they still produce a certain amount of NO\textsubscript{x} emissions and have many limitations in practical applications [5,6]. The operation mode of a four-stroke diesel engine involves the injection of diesel into the cylinder, causing the piston to compress the gas when it reaches the compression top dead center, thereby creating a high-temperature environment and promoting the spontaneous combustion of the fuel–air mixture [7,8]. The mixing rate of diesel and air affects the combustion rate and products [9,10]. Due to the high cetane number and high viscosity of diesel, its volatility is poor, resulting in a low
pre-mixing amount of the mixture. This easily leads to high temperatures over concentration zones and high-temperature flame zones [11]. In the high-temperature flame zone, an oxygen-rich environment is conducive to the generation of NO\textsubscript{x}. So, recently, using after-treatment technology to reduce NO\textsubscript{x} emissions from diesel engine exhausts has become an inevitable choice [12]. NO\textsubscript{x} generally refers to the combination of nitric oxide (NO) and nitrogen dioxide (NO\textsubscript{2}), mainly produced in high-temperature and oxygen-rich areas. NO accounts for the vast majority of NO\textsubscript{x} (approximately 95%). Under a high temperature, O\textsubscript{2} decomposes into individual oxygen atoms and reacts with N\textsubscript{2} entering the cylinder air to form N and NO [13]. N\textsubscript{2} decomposes into individual nitrogen atoms and reacts with O\textsubscript{2} to form O and NO. At present, common after-treatment technologies for controlling diesel engine pollutant emissions include lean burn NO\textsubscript{x} capture technology, passive NO\textsubscript{x} capture technology, and selective catalytic reduction (SCR) technology [14]. The use of a urea injection device can effectively control the amount of urea injected. When urea enters the exhaust pipe, the temperature in the exhaust pipe is used to evaporate, hydrolyze, and pyrolyze it. Under the action of a catalyst, it reacts with NO\textsubscript{x} in the exhaust gas to reduce emissions [15]. The conversion efficiency of SCR catalysts is related to temperature, space velocity, ammonia storage capacity, and so on [16]. SCR technology has become a highly effective means of reducing NO\textsubscript{x} emissions from heavy-duty diesel engines [17]. The most widely used SCR technology currently is urea selective catalytic reduction (urea-SCR) [18]. Under the action of a catalyst, NH\textsubscript{3} can efficiently and selectively reduce NO\textsubscript{x}. The principle of urea-SCR technology is to use urea aqueous solution as the precursor of the reducing agent [19]. When urea solution is sprayed into high-temperature exhaust gas, it will decompose into ammonia and carbon dioxide. The generated ammonia undergoes a selective catalytic reduction reaction with nitrogen oxides in exhaust gas under the action of specific catalysts (such as vanadium-based or copper-based catalysts), converting harmful nitrogen oxides into harmless nitrogen gas and water [20]. The widespread use of urea-SCR is mainly due to its three advantages [21]. Firstly, the NO\textsubscript{x} conversion efficiency of urea-SCR is relatively high, generally reaching over 90% [22]. In addition, the use of this technology can ensure the good fuel economy of the engine, with a minimal impact on its performance [23]. Secondly, as a carrier for urea-SCR, NH\textsubscript{3} has the advantages of being non-toxic and cost-effective [24,25]. At present, a large number of urea replenishment base stations have been established both domestically and internationally, making urea-SCR more convenient and efficient for urea replenishment [26]. The generation of NH\textsubscript{3} from urea aqueous solution mainly includes three steps: evaporation, pyrolysis, and hydrolysis. The specific chemical reaction formulae are as follows:

\begin{align} 
(1) \quad \text{CO(NH}_2\text{)}_2 \text{ evaporation reaction:} \\
\text{NH}_2 - \text{CO} - \text{NH}_2(\text{aq}) \rightarrow \text{NH}_2 - \text{CO} - \text{NH}_2(1 \text{ or } g) + x\text{H}_2\text{O} 
\end{align}

\begin{align} 
(2) \quad \text{CO(NH}_2\text{)}_2 \text{ pyrolysis:} \\
\text{NH}_2 - \text{CO} - \text{NH}_2(1 \text{ or } g) \rightarrow \text{NH}_3(g) + \text{HCO}(g) 
\end{align}

\begin{align} 
(3) \quad \text{Isocyanate hydrolysis:} \\
\text{HNCO}(g) + \text{H}_2\text{O}(g) \rightarrow \text{NH}_3(g) + \text{CO}_2(g) 
\end{align}

After mixing NO\textsubscript{x} and NH\textsubscript{3} in diesel engine exhaust, standard, fast, and slow SCR reactions mainly occur [27]. When NO/NO\textsubscript{x} = 1, the standard SCR reaction mainly occurs; when NO/NO\textsubscript{2} = 1, that is, when the concentrations of NO and NO\textsubscript{2} are the same, rapid SCR reactions mainly occur, and the reaction rate is significantly faster than the standard SCR reaction; when NO\textsubscript{2}/NO\textsubscript{x} = 1, a slow SCR reaction mainly occurs, with a reaction rate slower than that of standard and fast SCR [28,29]. The specific chemical reaction formulae are as follows:
(1) **Standard SCR reaction:**

\[ 4\text{NO} + 4\text{NH}_3 + \text{O}_2 \rightarrow 4\text{N}_2 + 6\text{H}_2\text{O} \]  

(4)

(2) **Rapid SCR response:**

\[ 4\text{NH}_3 (\theta) + 2\text{NO} + 2\text{NO}_2 \rightarrow 4\text{N}_2 + 6\text{H}_2\text{O} \]  

(5)

(3) **Slow SCR reaction:**

\[ 8\text{NH}_3 (\theta) + 6\text{NO}_2 \rightarrow 7\text{N}_2 + 12\text{H}_2\text{O} \]  

(6)

(4) **Possible side reactions on catalyst support:**

\[ 4\text{NH}_3 (\theta) + 3\text{O}_2 \rightarrow 2\text{N}_2 + 6\text{H}_2\text{O} \]  

(7)

where, \( \theta \) represents the adsorption state of \( \text{NH}_3 \).

The function of an SCR catalyst is to provide a catalyst for the catalytic reduction reaction between \( \text{NO}_x \) and \( \text{NH}_3 \) [30]. This catalyst is coated on the surface of a cordierite support [31]. Although the catalyst itself does not directly participate in the reaction, it is a core component of the SCR system [32]. At present, three mainstream catalysts with different materials are mainly used domestically and internationally: vanadium-based catalysts, iron zeolite molecular sieve catalysts, and copper zeolite molecular sieve catalysts [33]. Copper zeolite molecular sieve catalysts exhibit high selectivity between \( \text{NH}_3 \) and \( \text{NO}_x \) [34]. This can effectively promote the catalytic reduction reaction between \( \text{NO}_x \) and \( \text{NH}_3 \), reduce the adverse effects of side reactions, and improve the efficiency of SCR systems [35].

This catalyst has good low-temperature catalytic activity, is relatively easy to regenerate, and can reduce maintenance costs and environmental pollution [36]. Zang et al. [37] demonstrated in their research that copper zeolite molecular sieve catalysts had a wider SCR activity temperature window and better hydrothermal stability. Shin et al. [38] used urea-SCR as a copper zeolite molecular sieve catalyst in their research. They found that compared to iron zeolite molecular sieve catalysts, copper zeolite molecular sieve catalysts could maintain a higher \( \text{NO}_x \) conversion efficiency and lower \( \text{N}_2\text{O} \) generation at temperatures above 450 \( ^\circ \text{C} \).

Sun et al. [39] changed the load through experiments to achieve an effect of the ammonia/nitrogen ratio (ANR), spatial velocity, and \( \text{NO}_x \) component on the conversion efficiency of a Cu-SSZ-13 catalyst at different intake temperatures (temperature range of 180–450 \( ^\circ \text{C} \), with an increase of 20–50 \( ^\circ \text{C} \)). They found that the duration of the catalyst’s action was a significant factor affecting the catalytic efficiency in intake environments below 250 \( ^\circ \text{C} \). Therefore, optimizing the catalyst structure is very necessary. In addition, Zhong et al. [40] established an integrated post-treatment system model for catalyzed diesel particulate filters (CDPFs) and SCR based on Cu-ZSM-5 catalysts. Their research results indicated that the inlet temperature had an impact on the catalytic performance of SCR. In addition, after the passive regeneration of CDPF, the conversion efficiency of SCR was mainly affected by the concentration of \( \text{NO}_2 \) at the inlet. When actively regenerating, the conversion efficiency was mainly affected by the oxygen concentration. Xu et al. [41] studied the effects of catalysts with different structures on the \( \text{NO}_x \) conversion efficiency and \( \text{NH}_3 \) slip rate at different airspeeds on a six-cylinder four-stroke water-cooled engine. The research results indicated that the catalytic effect of urea-SCR was optimal when the ANR was 1. In addition, they believed that the \( \text{NO}_x \) emissions were influenced by the airspeed and catalyst volume. The larger the catalyst volume and the lower the airspeed, the higher the \( \text{NO}_x \) conversion efficiency. Zhao et al. [42] studied a catalyst with a corrugated substrate and explored the effects of the ammonia/nitrogen ratio on the \( \text{NO}_x \) conversion rate, \( \text{NH}_3 \) slip rate, and \( \text{N}_2\text{O} \) selectivity. After urea-SCR, there was also a copper-based catalytic ammonia slip catalyst (ASC). Their research results indicated that as the ammonia/nitrogen ratio increased from 1.0 to 1.2, the \( \text{NO}_x \) emissions from urea-SCR and ASC both decreased to a certain extent, but the \( \text{N}_2\text{O} \) emissions and \( \text{NH}_3 \) slip rate increased. Liang et al. [43] studied the effects of catalyst structure on the \( \text{NO}_x \) conversion rate, catalyst volume, and pressure drop before...
and after SCR. They established a one-dimensional copper-based catalyst NH\textsubscript{3}-SCR model using AVL-Boost and validated the model on a six-cylinder two-stroke marine diesel engine. Subsequently, they used the response surface methodology (RSM) to search for the optimal solution with structural parameters such as wall thickness, catalyst length, and coating thickness as independent variables. Their simulation optimization results on NH\textsubscript{3}-SCR showed that the channels per square inch (CPSI) of the catalyst had a significant impact on the internal pressure drop of the catalyst. A smaller catalyst volume was beneficial for reducing unnecessary fuel loss and improving the endurance of ship engines.

While previous studies have primarily focused on NO\textsubscript{x} conversion rates in urea-SCR systems, this research breaks new ground by simultaneously addressing the critical, yet often overlooked, aspects of the NH\textsubscript{3} storage capacity and NH\textsubscript{3} slip rate prediction across various temperatures. This innovative approach integrates these multiple performance indicators into a comprehensive analysis, providing a more holistic understanding of SCR dynamics. This article developed a novel four-stroke urea-SCR diesel engine model based on copper zeolite molecular sieve catalyst technology. This model uniquely incorporates a wide array of parameters, including catalyst length, cross-sectional diameter, NO/NO\textsubscript{2} ratio, and intake temperature, to evaluate their combined effects on the NH\textsubscript{3} slip, NO\textsubscript{x} conversion efficiency, and pressure drop. Notably, we employed the advanced response surface methodology to conduct an in-depth, multidimensional analysis of these parameters’ impacts on three key target variables. This sophisticated approach not only enhances our theoretical understanding of SCR systems but also yields optimized parameters with practical implications for industry applications.

2. Experimental Setup and Methods

2.1. Catalyst

The small sample catalyst used in this chapter was obtained on a commercial full-size Cu-SSZ-13 diesel engine molecular sieve SCR catalyst. Cu-SSZ-13 catalyst with a Cu content of 2.7% and a Si/Al molar ratio of 10.5 was used. The catalyst powder coated a support with a pore density of 300 CPSI to obtain a full-size catalyst. Before all experiments, the fresh Cu-SSZ-13 catalyst was treated for 3 h at 450 °C and at standard SCR conditions (350 ppm NH\textsubscript{3}, 350 ppm NO, 10% O\textsubscript{2}, 7% H\textsubscript{2}O, N\textsubscript{2} as equilibrium gas). This stabilized the performance of the catalyst. Afterward, the catalyst was pretreated for 1 h at 450 °C in a mixed atmosphere of 10% O\textsubscript{2}, 7% H\textsubscript{2}O, and N\textsubscript{2} as equilibrium gases to eliminate impurities remaining on the catalyst surface during this process.

2.2. Mathematical Model

When applying a model, it is usually necessary to test these basic assumptions and adjust and improve the model according to the characteristics of the data. The establishment of the urea-SCR model in this article requires a certain degree of simplification, assuming the following:

1. The internal catalyst of SCR only adsorbs one substance, which conforms to the Eley–Rideal mechanism. The Eley–Rideal mechanism can be represented as:

\[ \frac{d\theta}{dt} = k_a \times C_{NH_3} \times (1 - \theta) - k_d \times \theta \]  

where, \( \theta \) is the surface coverage of adsorbed NH\textsubscript{3}; \( k_a \) is the adsorption rate constant; \( k_d \) is the desorption rate constant; \( C_{NH_3} \) is the concentration of NH\textsubscript{3} in the gas phase.

2. The complete conversion of the urea aqueous solution to NH\textsubscript{3};

3. Considering movement and changes only along the \( x \)-axis, it can use a one-dimensional convection–diffusion–reaction equation:

\[ \frac{\partial C_i}{\partial t} + u \times \frac{\partial C_i}{\partial x} = D_i \times \frac{\partial^2 C_i}{\partial x^2} + R_i \]

(9)
where, $C_i$ is the concentration of species $i$; $u$ is the gas velocity; $D_i$ is the diffusion coefficient of species $i$; $R_i$ is the reaction rate of species $i$.

(4) Not considering the heat exchange between the catalyst and the external environment, which can use an adiabatic energy balance:

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \frac{\partial T}{\partial x} = -\Sigma \Delta H_{rxn,i} R_i$$

(10)

where, $\rho$ is the density of the gas; $C_p$ is the heat capacity of the gas; $T$ is the temperature, $^\circ\text{C}$; $\Sigma \Delta H_{rxn,i}$ is the heat of reaction for reaction $i$.

### 2.3. Simulation Model and Grid Independence Analysis

The urea-SCR system is a honeycomb-like structure composed of multiple identical and independent pore structures. The three-dimensional channel can truly reflect the flow, mass transfer, and reaction process of flue gas in it. It can be used as an object for SCR denitrification performance research. The results (denitrification efficiency and NH$_3$ slip rate) obtained are more accurate under the condition of the uniform distribution of the inlet parameters. This article is based on a small amount of sample experimental data and uses AVL-Fire2014 software to establish a three-dimensional reaction kinetics model of Cu-SSZ-13 molecular sieve urea-SCR. The geometric parameters of the catalyst’s single channel are shown in Table 1.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Numerical Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Catalyst volume</td>
<td>L</td>
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<tr>
<td>Catalyst length</td>
<td>mm</td>
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<tr>
<td>Catalyst density</td>
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<tr>
<td>Thermal conductivity</td>
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<tr>
<td>CSPF</td>
<td>1/in$^2$</td>
<td>400</td>
</tr>
<tr>
<td>Specific heat</td>
<td>J/(kg·K)</td>
<td>1200</td>
</tr>
<tr>
<td>Wall thickness</td>
<td>mm</td>
<td>0.01</td>
</tr>
</tbody>
</table>

Table 1. Urea-SCR geometric structure parameters.

The SCR catalyst model in AVL-Fire2014 software is mainly used for performance analysis and structural optimization design of diesel engine SCR systems. This model can not only be used as part of the overall diesel engine simulation, but can also be independently used to establish catalyst simulation research. It has good flexibility and allows input of various key parameters including exhaust temperature and exhaust components, ensuring more accurate and practical simulation results. In addition, the model helps developers optimize catalyst design and improve the efficiency and performance of the SCR system by simulating the chemical reactions and thermodynamic processes in detail. Figure 1 shows the partitioning structures for three different grid scenarios. Considering the calculation time, a medium grid is selected for the simulation.

![Figure 1. Cont.](image-url)
2.4. Various Parameters of Diesel Engine

This article takes the SCR test bench of an R6105AZLD diesel engine Cu-SSZ-13 molecular sieve catalyst as the research object, and the diesel engine models are shown in Table 2. The diesel engine needs to reach a stable operating state during the testing process and be able to accept the input of urea solution. The experimental flowchart is shown in Figure 2. In this system, components such as the urea storage tank, delivery pipeline, and injection system are responsible for delivering the urea aqueous solution to the SCR catalyst for chemical reactions. The exhaust gas analyzer can accurately measure the volume fractions of NO\textsubscript{x} and ammonia in the exhaust gas.

![Figure 1. Three-dimensional simulation model of urea-SCR system. (a) Rough; (b) moderate; (c) meticulous.](image)

![Figure 2. Experimental process.](image)
Table 2. Diesel engine parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Numerical Value</th>
</tr>
</thead>
<tbody>
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<td>Maximum power</td>
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<tr>
<td>Number of cylinders</td>
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<td>6</td>
</tr>
<tr>
<td>Cylinder diameter × stroke</td>
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</tr>
<tr>
<td>Speed</td>
<td>r/min</td>
<td>1500</td>
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<tr>
<td>Total cylinder displacement</td>
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</tr>
<tr>
<td>Compression ratio</td>
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<tr>
<td>Fuel consumption rate</td>
<td>g/(kW h)</td>
<td>218</td>
</tr>
</tbody>
</table>

2.5. Model Validation

By adjusting the engine load, the intake temperature can change between 200 °C and 450 °C. Figure 3 shows the comparison between simulated and experimental values of the NO\textsubscript{x} conversion rate at different intake temperatures. From the figure, it can be seen that the error between the simulation values and the experimental values is less than 5%, indicating that the established 3D model can predict the performance of SCR.

![Figure 3. Comparison between simulated and experimental values of NO\textsubscript{x} conversion rate.](image)

3. Results and Discussion

3.1. Catalyst Diameter

Under the boundary conditions of a catalyst length of 200 mm, inlet temperature of 300 °C, CPSI of 300 1/in\textsuperscript{2}, NH\textsubscript{3}/NO\textsubscript{x} of 0.8, NO/NO\textsubscript{2} of 1, inlet flow rate of 0.6 kg/s, and coating thickness of 0.01 mm, the catalyst diameter gradually increases from 150 mm to 400 mm. The simulation results show that the effects of different catalyst lengths on the NO\textsubscript{x} conversion rate, pressure drop, and NH\textsubscript{3} slip are shown in Figure 4. In this figure, it can be seen that within the reaction temperature range, the denitrification performance of SCR increases with the increase in the catalyst diameter, while the pressure drop and NH\textsubscript{3} slip decrease with the increase in the catalyst diameter. The NO\textsubscript{x} conversion rate, pressure drop, and NH\textsubscript{3} slip of SCR do not increase linearly with the increase in the catalyst diameter. When the diameter of the catalyst varies between 150 mm and 300 mm, the three curves show significant changes. Among them, the NO\textsubscript{x} conversion rate increased from 52.9% to 83.77%, with an increase of 58.36%; the pressure drop decreased from 6072.66 Pa to...
1558.63 Pa, with a decrease of 74.33%; the NH3 slip decreased from 90.04 ppm to 40.34 ppm, with a decrease of 55.19%. When the diameter of the catalyst varies from 300 mm to 400 mm, the NOx conversion rate increases by 9.97%, the pressure drop decreases by 43.48%, and the NH3 slip decreases by 43.54%. This is because an increase in the catalyst diameter will increase the contact area of the gas and solid, thereby increasing the reaction rate, increasing the reaction rate of SCR and promoting the conversion of NOx. Increasing the diameter of the catalyst can increase the contact area between the gas and solid, thereby increasing the reaction rate. As the diameter increases, the diffusion effect gradually saturates, and the amplitude of the increase or decrease will gradually decrease. In addition, when the diameter of the catalyst increases to a certain extent, the reaction rate reaches an equilibrium point and begins to stabilize.

Figure 4. The influence of catalyst diameter.

3.2. Catalyst Length

Figure 5 shows the effect of the catalyst length on the NOx conversion rate, pressure drop, and NH3 slip. It can be seen that the NOx conversion rate and pressure drop increase with the increase in the catalyst length, while the NH3 slip decreases with the increase in the catalyst length. When the catalyst length varies between 200 mm and 450 mm, the NOx conversion rate increases by 26.15%, the pressure drop increases by 120.86%, and the NH3 slip decreases by 41.70%. This is because an increase in the catalyst length will increase the surface area of the catalyst, increase the chance of contact between the various substances in SCR, and more reactions occur on the catalyst. This can increase the reaction rate of SCR and promote the conversion of NOx. Increasing the length of the catalyst can increase the contact time of NH3 within the catalyst, which is conducive to a sufficient reaction between NH3 and NOx, reducing the situation where NH3 penetrates the catalyst layer without a reaction, thereby reducing the NH3 slip. However, increasing the length of the catalyst will increase the resistance of gas passing through the catalyst, leading to an increase in gas flow resistance and thus an increase in pressure drop. The increase in the catalyst length will increase the contact area between the gas and solid, thereby increasing the frictional resistance. This will increase the resistance of gas passing through the catalyst and increase the pressure drop.
Processes 2024, 12, 1519

200 250 300 350 400 450
40 45 50 55 60 65 70 75 80

Figure 5. The influence of catalyst length.

3.3. Intake Temperature

The changes in the engine operating parameters directly affect the changes in the exhaust gas temperature, and the temperature is an important influencing factor in catalytic reactions. In order to better understand the influence of the SCR inlet temperature on the catalytic reaction, this paper uses an inlet flow rate of 0.6 kg/s as the boundary condition at the inlet to study the SCR reaction characteristics when the inlet temperature changes between 200 °C and 450 °C. Figure 6 shows the variation curves of the NOx conversion rate, pressure drop, and NH3 slip at the outlet of the reactor at different inlet temperatures. From the figure, it can be seen that as the intake temperature increases, the NOx conversion rate and pressure drop both show an upward trend. At a temperature of 450 °C, the NOx conversion rate reached 75.06% and the pressure drop reached 5106.64 Pa. This is because the higher the temperature, the faster the catalytic conversion reaction rate, resulting in an increase in the NOx conversion rate and pressure drop. A higher intake temperature promotes the adhesion and adsorption of reactants on the surface of the ammonia molecules, thereby reducing the NH3 slip.

Figure 6. The influence of intake temperature.
3.4. CPSI

CPSI refers to the number of channels per square inch. In this section, a catalyst diameter of 200 mm, a catalyst length of 200 mm, an inlet temperature of 300 °C, NH3/NOx of 0.8, NO/NO2 of 1, an inlet flow rate of 0.6 kg/s, and a coating thickness of 0.01 mm are used. Figure 7 shows the effect of 250–500 1/in² CPSI on the NOx conversion rate, pressure drop, and NH3 slip. It can be seen that with the increase in CPSI, the NOx conversion rate and pressure drop increase. At 500 1/in² CPSI, the NOx conversion rate is 77.13% and the pressure drop is 6500.31 Pa. The NH3 slip decreases with the increase in CPSI. At 500 1/in² CPSI, the NH3 slip is at a minimum value of 50.98 ppm. A higher number of CPSI can improve the NOx conversion rate. This is because increasing the number of CPSI can increase the surface area of the catalytic conversion reaction inside the SCR. This increases the opportunity for the catalyst to react with the reactants, promotes the progress of the reaction, and thus increases the NOx conversion rate. In addition, with the increase in CPSI, the gas flow resistance inside the SCR catalyst will increase, leading to an increase in the overall pressure drop through which the SCR gas passes. A higher CPSI will result in the more uniform diffusion and distribution of ammonia in the SCR catalyst, leading to a decrease in the NH3 slip. Therefore, the higher the CPSI, the greater the NOx conversion rate and pressure drop, and the smaller the NH3 slip.

![Figure 7. The influence of CPSI.](image)

3.5. NH3/NOx

Figure 8 shows the effects of different NH3/NOx ratios on the NOx conversion rate, pressure drop, and NH3 slip. As the NH3/NOx ratio increases in the figure, the NOx conversion rate and pressure drop decrease, and the NH3 slip increases. However, compared with other factors, it can be found that the size of the NH3/NOx ratio has little effect on the NOx conversion rate and pressure drop, but still has a certain influence on the NH3 slip. When the NH3/NOx ratio increases from 0.8 to 1.3, the NOx conversion rate decreases by 2.08% and the pressure drop decreases by 5.96 Pa. This is because the SCR reaction is related to parameters such as the NH3 concentration, NOx concentration, temperature, and O2 concentration. The O2 concentration at the inlet has an inhibitory effect on the SCR catalyst reaction. Under high temperature conditions, NH3 tends to undergo its own oxidation reaction with O2, thereby reducing the NOx conversion rate and pressure drop during SCR. When the NH3/NOx ratio increases from 0.8 to 1.3, the ammonia slip increases by approximately 28.27 ppm. An excessively high NH3/NOx ratio can prevent NH3 from
fully reacting with NO\textsubscript{x} and being removed outside the catalyst. Therefore, the magnitude of the NH\textsubscript{3}/NO\textsubscript{x} ratio still has a certain impact on the NH\textsubscript{3} slip.

![Figure 8. The influence of NH\textsubscript{3}/NO\textsubscript{x}](image)

**3.6. NO/NO\textsubscript{2}**

Figure 9 shows the effects of different NO/NO\textsubscript{2} ratios on the NO\textsubscript{x} conversion rate, pressure drop, and NH\textsubscript{3} slip. In this section, the NO/NO\textsubscript{2} ratio is set to 1–10. It can be seen that the NO\textsubscript{x} conversion rate and pressure drop decrease with the increases in the NO/NO\textsubscript{2} ratio, while the NH\textsubscript{3} slip increases with the increases in the NO/NO\textsubscript{2} ratio. When the NO/NO\textsubscript{2} ratio increases from 1 to 4, the NO\textsubscript{x} conversion rate decreases significantly, reaching 54.78%. Generally speaking, a NO/NO\textsubscript{2} ratio of 9 in the exhaust is more prone to standard SCR reactions. Increasing the concentration of NO\textsubscript{2} in the SCR reactor is beneficial for the occurrence of rapid SCR reactions during SCR. At a temperature of 300 °C, as the NO/NO\textsubscript{2} ratio increases from 1 to 10, the chemical reactions during SCR transition from rapid SCR reactions to standard SCR reactions.

![Figure 9. The influence of NO/NO\textsubscript{2}](image)
3.7. Intake Flow Rate

Figure 10 shows the comparison of the NO\textsubscript{x} conversion rate, pressure drop, and NH\textsubscript{3} slip when the intake flow rate varies from 0.4 kg/s to 0.9 kg/s. From the figure, it can be seen that the NO\textsubscript{x} conversion rate, pressure drop, and NH\textsubscript{3} slip are greatly affected by the intake flow rate. The NH\textsubscript{3} slip and pressure drop increase with the increase in the intake flow rate, while the NO\textsubscript{x} conversion rate decreases with the increase in the intake flow rate. When the intake flow rate is 0.9 kg/s, the NO\textsubscript{x} conversion rate, pressure drop, and NH\textsubscript{3} slip are 56.9%, 5149.6 Pa, and 84 ppm, respectively. A larger intake flow rate allows more gas molecules to pass through the catalytic layer, increasing resistance and thus increasing the pressure drop. A high inlet flow rate can lead to an excessive supply of NH\textsubscript{3} molecules during SCR, resulting in the saturation of the catalytic reduction chemical reactions during SCR, reducing the NO\textsubscript{x} conversion rate and promoting the NH\textsubscript{3} slip. In some studies, the NO\textsubscript{x} conversion rate was less affected by the intake flow rate. This is because the temperature of the control group in this section is 300 °C, which is relatively low. Generally speaking, within the optimal temperature range, the NO\textsubscript{x} conversion rate and pressure drop are less affected by the intake flow rate.

![Figure 10. The influence of intake flow rate.](image)

3.8. Coating Thickness

Figure 11 shows the effect of the coating thickness on the NO\textsubscript{x} conversion rate, pressure drop, and NH\textsubscript{3} slip on the catalysts. From the figure, it can be seen that as the coating thickness increases, the NO\textsubscript{x} conversion rate decreases, while the pressure drop and NH\textsubscript{3} slip increase. This is because the increase in the coating thickness leads to an increase in the path length of the SCR catalyst layer, which reduces the reaction rate and thus lowers the NO\textsubscript{x} conversion rate. In addition, the research results indicate that compared with other parameters, the influence of the coating thickness on the NO\textsubscript{x} conversion rate and NH\textsubscript{3} slip is also relatively small. This may be because an increase in the coating thickness does not significantly alter the density of active sites or surface characteristics of the SCR catalyst. Therefore, although an increase in the coating thickness can affect the mass transfer performance and reaction rate, its impact is relatively small and may not be the main factor compared to other factors such as the catalyst formulation and structure.
3.39
d = 0.005 0.010 0.015 0.020 0.025 0.030

\text{NO}_x \text{ conversion rate} = 58.76 + 18.974A + 7.94B + 33.6C + 4.37D - 19.01E + 1.26AB + 3.20AC + 0.2253AD + 6.04AE + 0.8482BC + 0.2728BD + 3.49BE + 1.28CD + 15.29CE + 0.9835DE - 4.02A^2 - 1.02B^2 - 5.30C^2 - 0.7165D^2 + 13.19E^2  \tag{11}

\text{Pressure drop} = 4260.19 - 6218.98A + 1768.79B + 2267.39C + 2061.70D - 6.56E - 2057.73AB - 3717AC - 2227.01AD + 8.56AE + 347.27BC + 635.88BD - 1.98BE + 589.95CD + 3.34CE - 2.20DE + 3930.37A^2 - 60.71B^2 + 674.49C^2 - 125.42D^2 - 221.99E^2  \tag{12}

\text{NH}_3 \text{ slip} = 39.16 - 41.32A - 15.33B - 20.04C - 13.19D + 9.70E + 5.51AB + 12.30AC + 4.32AD - 10.87AE + 3.56BC + 2.85BD - 5.06BE + 5.12CD - 7.52CE - 3.39DE + 15.97A^2 + 2.94B^2 - 1.05C^2 + 3.62D^2 - 6.78E^2  \tag{13}

where, A is the diameter, mm; B is the length, mm; C is the intake temperature, °C; D is CPSI, 1/in²; E is NO/NO₂.
Table 3. Top 20 optimization experiment designs.

<table>
<thead>
<tr>
<th>Group</th>
<th>Diameter (mm)</th>
<th>Length (mm)</th>
<th>Intake Temperature (°C)</th>
<th>CPSI (1/in²)</th>
<th>NO/NO₂</th>
<th>NOₓ Conversion Rate (%)</th>
<th>Pressure Drop (Pa)</th>
<th>NH₃ Slip (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>275</td>
<td>325</td>
<td>200</td>
<td>375</td>
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<td>2839.4</td>
<td>33.5</td>
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<tr>
<td>2</td>
<td>275</td>
<td>450</td>
<td>325</td>
<td>250</td>
<td>5.5</td>
<td>61.7</td>
<td>3583.5</td>
<td>38.1</td>
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<tr>
<td>3</td>
<td>150</td>
<td>200</td>
<td>325</td>
<td>375</td>
<td>5.5</td>
<td>23.5</td>
<td>8499.1</td>
<td>126.1</td>
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<tr>
<td>4</td>
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<td>325</td>
<td>200</td>
<td>375</td>
<td>10</td>
<td>7.1</td>
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<tr>
<td>5</td>
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<td>325</td>
<td>325</td>
<td>250</td>
<td>5.5</td>
<td>59.2</td>
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<tr>
<td>6</td>
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<td>200</td>
<td>325</td>
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<td>17</td>
<td>400</td>
<td>325</td>
<td>375</td>
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<td>1</td>
<td>97.9</td>
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<td>375</td>
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<tr>
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<td>375</td>
<td>375</td>
<td>10</td>
<td>72.6</td>
<td>8253.3</td>
<td>14.6</td>
</tr>
<tr>
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<td>325</td>
<td>375</td>
<td>375</td>
<td>10</td>
<td>74.9</td>
<td>2014.9</td>
<td>11.3</td>
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</tbody>
</table>

To further verify the accuracy of the model, the significance of the optimization process is analyzed. Table 4 presents the significance evaluation criteria for the RSM. The NOₓ conversion rate, pressure drop, and F-value of the NH₃ slip for this model are 38.04, 23.33, and 59.41, respectively. Their p-values are all <0.0001, and the R² and Adjusted R² are close to 1. The difference between the Adjusted R² and Predicted R² is less than 0.2. These evaluation indicators indicate that the predictive equation has good significance and can be used to predict the NOₓ conversion rate, pressure drop, and NH₃ slip under different conditions. Figure 12 shows the relationship curve between the predicted and actual values of the NOₓ conversion rate, pressure drop, and NH₃ slip.

Table 4. Significance evaluation criteria for RSM.

<table>
<thead>
<tr>
<th>Evaluating Indicator</th>
<th>F-Value</th>
<th>p-Value</th>
<th>R²</th>
<th>Adjusted R²</th>
<th>Predicted R²</th>
<th>Adeq Precision</th>
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</thead>
<tbody>
<tr>
<td>NOₓ conversion rate (%)</td>
<td>38.04</td>
<td>&lt;0.0001</td>
<td>0.97</td>
<td>0.94</td>
<td>0.90</td>
<td>23.32</td>
</tr>
<tr>
<td>Pressure drop (Pa)</td>
<td>23.33</td>
<td>&lt;0.0001</td>
<td>0.95</td>
<td>0.91</td>
<td>0.81</td>
<td>19.65</td>
</tr>
<tr>
<td>NH₃ slip (ppm)</td>
<td>59.41</td>
<td>&lt;0.0001</td>
<td>0.98</td>
<td>0.96</td>
<td>0.93</td>
<td>28.82</td>
</tr>
</tbody>
</table>

Figure 12. Cont.
4.2. NO\textsubscript{x} Conversion Rate

The response surface can determine the degree of influence of two factors on the response value, and the degree of inclination of the response surface refers to the magnitude of the influence. The plotted response surface and the third factor in the contour map are all at the zero level. Figure 13a,b show the response surface and contour plots of the diameter and intake temperature to the NO\textsubscript{x} conversion rate. At this point, the length is 325 mm, CPSI is 375 1/in\textsuperscript{2}, and NO/NO\textsubscript{2} is 5.5. Figure 13c,d show the response surface and contour plots of the intake temperature and NO/NO\textsubscript{2} to NO\textsubscript{x} conversion rate. At this point, the diameter is 275 mm, the length is 325 mm, and the CPSI is 375 1/in\textsuperscript{2}. From the figures, it can be seen that the NO\textsubscript{x} conversion rate is directly proportional to the diameter and intake temperature, and inversely proportional to the NO/NO\textsubscript{2} ratio. In addition, the NO\textsubscript{x} conversion rate is greatly affected by the diameter. This is because the diameter affects the surface area of the catalyst in contact. The larger the surface area, the more active sites can be provided for the catalyst reaction, so the NO\textsubscript{x} conversion rate is higher.

Figure 13. Cont.
Figure 13. Response surface and contour plots of two factors to NO\textsubscript{x} conversion rate. (a) Response surface diagram of diameter and intake temperature to NO\textsubscript{x} conversion rate; (b) contour plot of the effect of diameter and intake temperature on NO\textsubscript{x} conversion rate; (c) response surface diagram of intake temperature and NO/NO\textsubscript{2} to NO\textsubscript{x} conversion rate; (d) contour plot of the effect of intake temperature and NO/NO\textsubscript{2} on NO\textsubscript{x} conversion rate.

4.3. Pressure Drop

Figure 14a,b show the response surface and contour plots of the diameter and length to the pressure drop. At this time, the intake temperature is 325 °C, CPSI is 375 1/in\textsuperscript{2}, and NO/NO\textsubscript{2} is 5.5. Figure 14c,d show the response surface and contour plots of the diameter and length to the pressure drop. At this point, the length is 275 mm, CPSI is 375 1/in\textsuperscript{2}, and NO/NO\textsubscript{2} is 5.5. Based on Figure 14 and the F-value of the quadratic model variance analysis, it can be seen that the order of influencing factors on the pressure drop is diameter > intake temperature > CPSI > length > NO/NO\textsubscript{2}. In the above analysis, it can be seen that the diameter affects the number of active sites in the catalyst. Higher temperatures can enhance the activity of catalysts. This will lead to a strong increase in the pressure drop.

4.4. NH\textsubscript{3} Slip

Figure 15a,b show the response surface and contour plots of the diameter and length to the NH\textsubscript{3} slip. At this time, the intake temperature is 325 °C, CPSI is 375 1/in\textsuperscript{2}, and NO/NO\textsubscript{2} is 5.5. Figure 15c,d show the response surface and contour plots of the intake temperature and NO/NO\textsubscript{2} to NH\textsubscript{3} slip. At this point, the diameter is 275 mm, the length is 325 mm, and the CPSI is 375 1/in\textsuperscript{2}. It can be seen that the influence of the diameter on the NH\textsubscript{3} slip is greater than that of the length on the NH\textsubscript{3} slip. The NH\textsubscript{3} slip will decrease with the increasing diameter. Smaller diameters result in smaller internal surface areas. This is not conducive to the contact between NH\textsubscript{3} molecules and active sites, resulting in an increase in the NH\textsubscript{3} slip amount.

Figure 14. Cont.
4.4. NH$_3$ Slip

Figure 15a,b show the response surface and contour plots of the diameter and length to the NH$_3$ slip. At this time, the intake temperature is 325 °C, CPSI is 375 1/in$^2$, and NO/NO$_2$ is 5.5. Figure 15c,d show the response surface and contour plots of the intake temperature and NO/NO$_2$ to the NH$_3$ slip. At this point, the diameter is 275 mm, the length is 325 mm, and the CPSI is 375 1/in$^2$. It can be seen that the influence of the diameter on the NH$_3$ slip is greater than that of the length on the NH$_3$ slip. The NH$_3$ slip will decrease with the increasing diameter. Smaller diameters result in smaller internal surface areas. This is not conducive to the contact between NH$_3$ molecules and active sites, resulting in an increase in the NH$_3$ slip amount.

Figure 15. Cont.
Figure 15. Response surface and contour plots of two factors on NH₃ slip. (a) Response surface diagram of diameter and length to NH₃ slip; (b) contour plot of NH₃ slip with respect to diameter and length; (c) response surface diagram of intake temperature and NO/NO₂ to NH₃ slip; (d) contour plot of the effect of intake temperature and NO/NO₂ on NH₃ slip.

4.5. Optimal Solution Set

In the subsequent target study, the maximum NOₓ conversion rate, minimum pressure drop, and minimum NH₃ slip were set as targets. Finally, a total of 100 sets of optimal solution sets were obtained. Considering the actual situation, a diameter of 300 mm, a length of 349.99 mm, an intake temperature of 378.92 °C, a CPSI of 286.475 1/in², and 1.01 NO/NO₂ are selected. The NOₓ conversion rate reached 98.25%, with a pressure drop of 2558.74 Pa and an NH₃ slip of 17.49 ppm. Based on the optimized results, a new simulation was conducted, and the comparison between the simulation and optimization results is shown in Figure 16. The error of the NOₓ conversion rate, pressure drop, and NH₃ slip is less than 5%, indicating the reliability of the optimization results.

Figure 16. Comparison between optimized values and simulated values.
5. Conclusions

This article establishes a three-dimensional SCR channel model and analyzes the effects of intake and structural parameters on the SCR performance. Subsequently, response surface design experiments are conducted to investigate the effects of the catalyst diameter, length, inlet temperature, CPSI, and inlet NO/NO₂ ratio on the NOₓ conversion rate, pressure drop, and NH₃ slip. The following conclusion is drawn:

(1) An SCR 3D channel model is established using AVL-Fire2014 and the accuracy of the model is verified through experiments. The established model can predict the performance of SCR for subsequent experiments.

(2) The diameter of the catalyst and the ratio of NO/NO₂ at the inlet has a more significant impact on the NOₓ conversion rate. As the diameter increases, the NOₓ conversion rate gradually increases. The NO/NO₂ ratio at the entrance exhibits an opposite effect on the NOₓ conversion rate. Compared to the pressure drop, the NO/NO₂ ratio at the inlet is the least significant influencing factor. For the NH₃ slip, the catalyst diameter and intake temperature are the most significant influencing factors. The NH₃ slip decreases with increasing diameter and intake temperature. The diameter of the catalyst and the inlet temperature can affect the number of active sites and the activity of the catalyst.

(3) Through RSM optimization design, 100 sets of optimal solution sets are obtained. The optimized SCR system achieved a remarkably high NOₓ conversion rate of 98.25%, contributing significantly to reducing vehicular emissions and improving air quality. This study successfully balances multiple performance criteria (NOₓ conversion, pressure drop, and NH₃ slip), providing a comprehensive solution that addresses the key challenges in SCR system design.

The limitation of this article is that it only involves laboratory-scale experiments and simulations. The research on other parameters is not comprehensive enough, and further research will continue to advance. In addition, NH₃ emissions can be further reduced by fine-tuning the urea injection amount while maintaining a high NOₓ conversion rate in practical applications.

Author Contributions: Conceptualization, W.L. and J.W.; methodology, W.L. and J.W.; software, W.L. and J.W.; validation, W.L.; formal analysis, D.Y.; investigation, W.L. and F.W.; resources, L.W.; data curation, H.L.; writing—original draft preparation, W.L.; writing—review and editing, W.L. and H.H.; visualization, W.L. and J.W.; supervision, J.H.; project administration, W.L. and J.W.; funding acquisition, J.H. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest: The authors declare no conflicts of interest.

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