On the Influencing Factors of Integrated Aftertreatment System in Diesel Engine

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Abstract. In order to reduce the pollutants of diesel exhaust, DOC, DPF, SCR, AOC, etc. are mainly used for off-machine after-treatment technology, but it is difficult to meet the requirements of the newest emission regulations simply by relying on a certain aftertreatment technology. Therefore, the use of integrated aftertreatment system has become a necessary choice. In this paper, the research object is one of the integrated aftertreatment systems (DOC+DPF+ SCR+AOC). Then, the effects of the different exhaust parameters, the different structural parameters and different chemical reaction parameters on the catalytic conversion efficiency of NOx, HC, CO, and PM are studied.

Keywords: Diesel Engine, Aftertreatment System, Conversion Efficiency, Simulation

1. Introduction
It was recognized soon after the discovery and development of the compression-ignition engine by Rudolph Diesel more than a century ago that those engines emitted high concentrations of particulate matter (PM), nitrogen oxides (NOx), Hydrocarbons (HC) and carbon monoxide (CO) [1]. Pollutants such as NOx, PM, CO, and HC emitted from diesel engines also cause serious air pollution. Many countries have formulated corresponding emission regulations to limit the emission of pollutants [2]-[4]. According to the "China Vehicle Environmental Management Annual Report of 2017" issued by the Ministry of Environmental Protection, [5], in 2016, the national automobile emissions pollutants were initially accounted for 44.725 million tons. According to the relevant regulations of the automobile emission standards formulated by the Ministry of Environmental Protection in 2016 [6]: From January 1, 2020, new vehicles that do not meet the “national VI” emission standards will not be produced, sold or registered.

To reduce the pollutants emitted by diesel engines, the off-board after-treatment technologies mainly include DOC, DPF, SCR, AOC, etc., but relying on a certain aftertreatment technology alone, it is difficult to meet the requirements of the “National Sixth” emission regulations. Therefore, the use of integrated aftertreatment systems has become a necessary choice.

Based on this, this paper uses the technical parameters of the aftertreatment system provided by the self-provided system to apply the GT simulation software to build the diesel engine GT-Power
simulation model and each aftertreatment system (including DOC subsystem, DPF subsystem, SCR subsystem and AOC subsystem). And the integrated aftertreatment system GT-Power simulation model to study the catalytic conversion of NOx, HC, CO and particulates in the “Self-integrated aftertreatment system” under different exhaust parameters, different pollutant concentrations, different structural parameters and different chemical reaction parameters. The changing characteristics of efficiency.

2. Simulation Model of Integrated Aftertreatment System

The research object of this paper is "Zhongzi integrated aftertreatment system" (DOC+DPF+SCR+AOC) system is divided into four parts: DOC, DPF, SCR and AOC.

The chemical reactions occurring in the catalytic converter are very complex, and many reactions can be carried out simultaneously; these reactions are related to the composition of the exhaust gas, the temperature, and the active components of the catalyst coating. Since the DPF used in this system mainly plays a role in physical filtration of particles, it does not involve chemical screening. Therefore, this paper mainly considers the reaction equation defined in the DOC, SCR, and AOC models established by GT-Power.

The following four reaction equations are defined in the DOC model:

\[ 2CO + O_2 \rightarrow 2CO_2 \]

\[ [HC] + O_2 \rightarrow CO_2 + H_2O \]  \hspace{1cm} (2)

\[ 2H_2 + O_2 \rightarrow 2H_2O \]  \hspace{1cm} (3)

The following four reaction equations are defined in the SCR model:

\[ 2NO + O_2 \rightarrow 2NO_2 \]  \hspace{1cm} (4)

\[ 4NH_4 + 4NO + O_2 \rightarrow 4N_2 + 6H_2O \]  \hspace{1cm} (5)

\[ 4NH_3 + 6NO \rightarrow 5N_2 + 6H_2O \]  \hspace{1cm} (6)

\[ 4NH_3 + 2NO + 2NO_2 \rightarrow 4N_2 + 6H_2O \]  \hspace{1cm} (7)

\[ 8NH_3 + 6NO_2 \rightarrow 7N_2 + 12H_2O \]  \hspace{1cm} (8)

\[ 4NH_3 + 4NO + 3O_2 \rightarrow 4N_2O + 6H_2O \]  \hspace{1cm} (9)

\[ 4NH_4 + 5O_2 \rightarrow 4NO + 6H_2O \]  \hspace{1cm} (10)

\[ 2NH_3 + 2NO \rightarrow NH_4NO_3 + N_2 + H_2O \]  \hspace{1cm} (11)

The following four reaction equations are defined in the AOC model:

\[ 4NH_3 + 3O_2 \rightarrow 2N_2 + 6H_2O \]  \hspace{1cm} (12)

The kinetic rate of the above chemical reaction can be expressed as [7]:

\[ r = \frac{A \exp \left( - \frac{E}{RT} \right) C_i}{G \left( T_s, c \right)} \]  \hspace{1cm} (13)

where A is the pre-factor; E is the activation energy; Ts is the surface temperature of the carrier; Ci is the concentration of each component, and G is the inhibition term.

In the calculation, according to the technical parameters and physical parameters of the aftertreatment system provided by Zhongzi, as shown in Table 1, the simulation model of the subsystem working process is established by using GT simulation software and according to the layout scheme of the aftertreatment system (DOC+DPF+SCR+AOC) The simulation model of the working process of each subsystem is combined into the integrated aftertreatment as shown in Fig.1.
Table 1. Integrated Aftertreatment System Subsystem Parts Technical Parameters

| Subsystem | Carrier material / (mm) | Carrier diameter / (mm) | Carrier length / (mm) | Carrier volume / (L) | Hole density / (cps) | Wall thickness / (mil) |
|-----------|------------------------|-------------------------|-----------------------|----------------------|----------------------|------------------------|
| DOC       | Cordierite             | 143.8                   | 101.6                 | 1.65                 | 400                  | 4                      |
| DPF       | SiC                    | 143.8                   | 228.6                 | 3.71                 | 300                  | 9                      |
| SCR       | Cordierite             | 172                     | 101.6+101.6           | 4.72                 | 400                  | 4                      |
| AOC       | Cordierite             | 172                     | 50.8                  | 1.18                 | 400                  | 4                      |

Figure 1. "Integrated Post Processing System" (DOC+DPF+SCR+AOC) GT-Power Simulation Model.

3. Influencing Factors of Integrated Aftertreatment System

This section uses the simulation model of the integrated aftertreatment system that has been established to change the gas flow, gas temperature and pollutant concentration in the inlet gas of the aftertreatment system, simulate the catalytic conversion process in the catalytic converter, analyze and study the exhaust parameters and structural parameters. And the influence of chemical reaction parameters on the catalytic conversion characteristics of the integrated aftertreatment system.

The approximate range of diesel exhaust flow, exhaust temperature, NOx emission concentration, HC emission concentration, CO emission concentration, and particulate emission concentration is determined by consulting relevant literature [8-10], the exhaust parameter value table is made according to the parameter range, as shown in Table 2.

Table 2. Exhaust parameter value table

| Parameters                  | Value |
|-----------------------------|-------|
| Mass Flow / (g s⁻¹)         | 20    |
| Exhaust gas temperature / (K) | 550  |
| NOx concentration / (10⁻⁶)  | 300   |
| HC concentration / (10⁻⁶)   | 50    |
| CO concentration / (10⁻⁶)   | 150   |
| Soot concentration / (10⁻⁶) | 200   |

The variable parameters were studied by the control variable method, with the intermediate amount of each parameter in the table: exhaust flow rate 45g/s, exhaust gas temperature 685K, NOx concentration 500×10⁻⁶, HC concentration 150×10⁻⁶, CO concentration 250×10⁻⁶ and the particle concentration of 400×10⁻⁶ are quantitative, and the parameter values of the integrated aftertreatment system are not changed with time. The simulation is carried out by changing different independent variables to study different exhaust parameters for the integrated aftertreatment system. The effect of catalytic conversion characteristics.

3.1. Effect of Exhaust Parameters on Conversion Characteristics of Integrated aftertreatment System

Fig.2 and Fig.3 show the effect of exhaust mass flow and exhaust gas temperature on the catalytic conversion characteristics of an integrated aftertreatment system.
As shown in Fig.2, the CO conversion rate does not change much as the exhaust gas flow increases. There is a large reduction in HC and NOx conversion. As the flow rate of the exhaust gas increases, the active site of the catalyst is completely covered, and the reaction is saturated, resulting in a low conversion rate of the contaminant. The particle purification rate increases slightly with increasing exhaust gas flow rate. Because the filter mechanism of the filter is related [11]. As the exhaust flow rate increases, the inertia of the particles increases, and the DPF's filtration effect on the particles is better.

As shown in Fig.3, the CO conversion rate does not change much as the exhaust gas temperature increases. HC conversion rate has increased. Because the higher the exhaust gas temperature, the greater the activity of the catalyst, the higher the conversion of HC. The NOx conversion rate first rises and then decreases slightly. This is because when the temperature in the catalytic converter is too high, the activity of the catalyst is rather lowered, and too high a temperature causes the catalyst to be overheated. The particle purification rate has increased slightly, and the overall impact is small.

The effect of integrated aftertreatment system on the conversion efficiency of various pollutants under different emission concentrations, as shown in the Fig.4.

As shown in Fig.4(a), with the increase of NOx concentration, the CO conversion rate of the integrated aftertreatment system does not change much. The HC conversion rate has dropped slightly, and the overall impact is small. The NOx conversion rate increases. The particle purification rate is almost unchanged. This indicates that the inhibition of CO oxidation by NO in NOx is not obvious, but slightly inhibits the oxidation of HC.

As shown in Fig.4(b), with the increase of HC concentration, the CO conversion rate of the integrated aftertreatment system does not change much. The HC conversion rate increased slightly. The NOx conversion rate has increased slightly. The particle purification rate has increased slightly, and the overall impact is small.

As shown in Fig.4(c), the increase of CO concentration, the CO, HC, NOx and particulate conversion efficiency of integrated aftertreatment systems are not obvious.
As shown in Fig.4(d), the conversion rates of CO, HC and NOx are almost unchanged with the increase of particle concentration. The particle conversion rate increases, but the increase rate gradually decreases as the particle concentration increases.

3.2. Effect of Structural Parameters on Conversion Characteristics of Integrated aftertreatment System

In this section, the technical parameters such as catalyst pore density and catalyst carrier length provided by the company are used as benchmarks to simultaneously change the pore density and carrier of four subsystems in the integrated aftertreatment system (DOC+DPF+ SCR+AOC) at the same rate of change. Length, study the effect of different structural parameters on the catalytic conversion characteristics of integrated aftertreatment systems.

The effect of structural parameters on the catalytic conversion characteristics of the integrated aftertreatment system is shown in Fig.5(a) and Fig.5(b) during the change of carrier pore density and carrier length change from -50% to +50%.

![diagram](image_url)

**Figure 5.** Effect of emission concentrations on conversion efficiency

As shown in Fig.5(a), the CO conversion rate of the integrated aftertreatment system increases slightly with the increase of the carrier pore density. The HC conversion rate increases, but the increase rate decreases as the rate of change in pore density increases. This may be because as the pore density of the catalyst increases, the pressure loss after the gas passes through the catalyst increases to promote the oxidation reaction [11], and the effective reaction of HC on the catalyst surface increases with the increase of the pore density. The area also increases, the chemical reaction proceeds more fully, and the difference in HC concentration before and after the catalyst increases, so that the HC conversion rate increases. The NOx conversion rate increased slightly (for reasons similar to the above changes in HC conversion rate). Since the DPF adopts a wall-flow filtering structure, as the pore density increases, the combination of the particles and the filter mesh is more sufficient under the premise of the porosity, and the particle purification rate of the integrated aftertreatment system is slightly increased.

As shown in Fig.5(b), the CO conversion rate of the integrated aftertreatment system is almost unchanged with the increase of the length of the carrier. HC conversion rate has increased. An increase in the length of the carrier means that the contact area of the HC in the exhaust gas with the catalyst carrier is increased, and the oxidation reaction proceeds more sufficiently. The NOx conversion rate rises, possibly for reasons similar to the above-mentioned changes in HC conversion. The particle purification rate decreased slightly. An increase in the length of the carrier means that the flow rate of the particles in the filter becomes small, the inertia of the particles is smaller, and the filtration effect is deteriorated.

3.3. Effect of Chemical Parameters on Conversion Characteristics of Integrated Aftertreatment System

In this section, the technical parameters such as the catalyst activation energy in the chemical reaction module of the GT software and the pre-exponential factor in the Arrhenius equation are used as
benchmarks to simultaneously change the integrated aftertreatment system (DOC+DPF+SCR+ AOC) at the same rate of change. The catalyst activation energy of the four subsystems and the pre-exponential factor in the Arrhenius equation were used to study the effects of different chemical parameters on the catalytic conversion characteristics of the integrated aftertreatment system.

The effect of chemical reaction parameters on the catalytic conversion characteristics of the integrated aftertreatment system is shown in Fig.6(a) and Fig.6(b) during the change of reactant activation energy and pre-exponential factor change rate from -50% to +50%.

![Figure6](image)

**Figure6.** Effect of chemical parameters on conversion efficiency

As shown in Fig.6(a), with the increase of activation energy, the conversion rates of CO, HC and NOx decrease to different degrees when the activation energy exceeds a certain value. Since the filtration of the particles is a physical process, the particle purification rate does not change significantly.

As shown in Fig.6(b), the CO conversion rate of the integrated aftertreatment system has no significant change with the increase of the pre-exponential factor. The HC conversion rate increased slightly. The NOx conversion rate increases. However, the increase rate gradually decreases as the rate of change of the pre-exponential factor increases. Since the filtration of the particles is a physical process, the particle purification rate does not change significantly.

4. Conclusions

In this paper, taking DOC+DPF+SCR+AOC as the research object, by changing different diesel engine exhaust parameters, the integrated aftertreatment system was used to convert NOx, HC, CO and PM under different exhaust parameters, different catalytic converter structural parameters and chemical reaction parameters, conclusions are drawn from the research:

(1) Through research, it is found that the larger the exhaust gas flow rate, the saturated reaction, the unreacted pollutants in the exhaust gas, the lower the pollutant conversion rate; the activity of the catalyst increases as the exhaust gas temperature increases, thus The conversion rate of pollutants increases, but too high temperature will cause overheating damage of the catalyst and reduce the conversion rate of pollutants; NO, CO and HC in NOx have mutually inhibiting oxidation, and the conversion rate of particles is relatively different by different pollutant and less affected.

(2) The increase of the pore density and the length of the carrier promotes the catalytic conversion of the integrated aftertreatment system;

(3) The effects of activation energy and pre-exponential factor on the catalytic conversion of the integrated aftertreatment system are more complicated, and the activation energy is more effective than the pre-exponential factor.

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References

[1] Imad A. Khalek, Matthew G. Blanks, Patrick M. Merritt & Barbara Zielinska (2015) Regulated and unregulated emissions from modern 2010 emissions-compliant heavy-duty on-highway diesel engines, Journal of the Air & Waste Management Association, 65:8, 987-1001, DOI: 10.1080/10962247.2015.1051606.

[2] Guan, B., Zhan, R., Lin, H., & Huang, Z. (2015). Review of the state-of-the-art of exhaust particulate filter technology in internal combustion engines. Journal of environmental management, 154, 225-258.

[3] Bonnel, P., Carriero, M., Forni, F., Alessandrini, S., Montigny, F., Demircioglu, H., Giechaskiel, B., 2010. EU-PEMS PM Evaluation Program-first Report, EU Joint Research Centre (JRC) Scientific and Technical Reports.

[4] Mamakos, A., Carriero, M., Bonnel, P., Demircioglu, H., Douglas, K., Alessandrini, S., Forni, F., Montigny, F., Lesueur, D., 2011. EU-pems PM Evaluation Programsecond Report-study on Post DPF PM/PN Emissions, EU Joint Research Centre (JRC) Scientific and Technical Reports.

[5] State Environmental Protection Administration, China Vehicle Environmental Management Annual Report, 2017.

[6] Chen Daying, et al, Summaries and viewpoints about emission from diesel engine, Lubricating oil, 23.1(2008):10-15.

[7] Kandylas I P, Koltsakis G C. NO2-Assisted Regeneration of Diesel Particulate Filters: A Modeling Study, Ind. Eng. Chem. Res, 41.9(2002): 2115-2123.

[8] Liu Tingting, Analysis on Diesel After-treatment System Fault Diagnosis for CRT ageing and failure, Diss. Beijing Jiaotong University, 2012.

[9] Xu Wenjie, Development of Model Based Virtual Calibration Platform for Diesel Engine Emission, Shandong University, 2019.

[10] Jinhao Ning, Fengjun Yan, IMC based Iterative Learning Control of DOC Temperature during DPF Regeneration. 2016 European Control Conference (ECC) June 29 - July 1, 2016. Aalborg, Denmark.

[11] Li Xinghu, Exhaust Aftertreatment Technologies for Diesel Vehicles, 2016.