Numerical Simulation of Internal Flow Field and Structural Optimum Design for the diesel engine SCR Catalytic Converter

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Abstract. A three-dimensional model and finite element model of the diesel engine SCR catalytic converter were established by using ANSYS software. The numerical simulation of the internal flow field for the diesel engine SCR catalytic converter was performed. The results show that the pressure loss of the catalytic converter is larger and the velocity distribution in the front of substrate is nonuniform. On this base, the effects of the diameters and lengths of the substrate on the catalytic converter's internal flow field characteristic were studied. The results show that when the substrate's length increases, the pressure loss increases and the velocity distribution uniformity in the front of substrate becomes worse. When the diameter of substrate increases, the pressure loss decreases and the velocity distribution uniformity in the front of substrate becomes better. Therefore, the structure of catalytic converter was optimized. Through the optimization of the structure, the velocity distribution in the front of substrate is more uniform. The passing capacity of substrate is increased. The conversion efficiency of catalytic converter is improved. The back pressure is reduced.

1. Introduction

The environment problem has become one of the most serious social problems in the modern world. The catalytic converter is an effective device for auto emission reduction. The Urea-SCR is presently considered the most promising technique for the removal of nitrogen oxides from the exhaust of heavy-duty diesel vehicles. The catalytic converter is an important part of the SCR system. With the increasingly strict emission regulations, the performance requirements on the catalytic converter are also getting higher and higher. Not only to have a high conversion efficiency, but also to have a long life, and at the same time, the flow resistance is small. Therefore, it is necessary to understand the internal flow law of catalytic converter and analyzes the factors of affecting the flow characteristic [1]. In the early 1970s, the internal flow of catalytic converter was researched. It was found that the uniformity of velocity distribution in carrier and pressure loss of catalytic converter had greatly effect on catalytic converter performance [2]. Therefore, the key of catalyst structure design is to reduce the inhomogeneity of gas velocity distribution in carrier and decrease the pressure loss of the catalytic converter. The structure of catalytic converter need to be optimized. With the rapid development of computer technology and computational fluid dynamics (CFD), the structure design and optimization of the catalytic converter was provided guidance by using CFD software to simulate the flow characteristics of catalytic converter. It also reduce the test workload and greatly shorten the design period [3-4]. In this paper, the three-dimensional numerical simulation of the catalytic converter's internal flow field was performed by using computational fluid dynamic method. The effect of the length and diameter of the carrier on the performance of catalytic converter was analyzed. On this base, the carrier of the catalytic converter structure has been optimized. The velocity distribution inside the carrier became more uniform. The pressure loss of the catalytic converter was reduce. The conversion efficiency of the catalytic converter was improved. The energy loss was reduced during emission.

2. Performance evaluation index of catalytic converter

2.1. Pressure Loss of Catalytic Converter

The back pressure of exhaust system has important influence on engine power and fuel economy. In the exhaust system, the pressure loss of the catalytic converter accounted for about one-third. Therefore, reduction the pressure loss of the catalytic converter is one of the main purpose of studying on catalytic converter.

2.2. Uniformity of Flow in Carrier

If the flow velocity distribution in Carrier is nonuniform, Not only affects the flow resistance but also lead to the carrier temperature distribution nonuniform. Furthermore, resulting in catalyst carrier in the radial direction of deterioration degree is uneven and reduces the service life of the catalyst. The catalytic efficiency of the whole is reduced. The flow uniformity index in the carrier is an important index to evaluate the uniformity of the flow. In this paper, the criteria for evaluating the flow distribution characteristics of the carrier by using the uniformity index defined by Welt ens et al [5]:

$$\gamma = 1 - \frac{1}{2n}\sum_{i=1}^{n}\frac{\sqrt{(v_i - v_{mean})^2}}{v_{mean}} \tag{1}$$

In the formula: $\gamma$is uniformity index. Its value varies between 0 and 1, 1 represents the ideal uniform flow, 0 indicates that the gas only flow through a single channel, n is the number of the channels of carrier, v_i and v_{mean} represent the velocity of the i pipe and the average velocity of the carrier cross section, respectively.

3. Mathematical model

Research shows that the prediction of flow velocity in the catalytic converter without considering reaction conditions and the existence of chemical reaction the deviation is less than 10%. So the chemical reactions in the catalytic converter wasn't to be considered in this paper. The gas flow of SCR catalytic converter was in the following simplifications and assumptions [5]: (1) the engine exhaust was considered as ideal gas; (2) the gas flow in catalytic converter was steady flow; (3) the gas flow in the catalytic converter was incompressible flow; (4) the gas properties were regard as constants. In order to qualitative analyze the internal flow characteristics of catalytic converter, the internal flow was simplified as adiabatic three-dimensional steady flow without chemical reaction.

3.1. Control Equations

In the catalytic converter free flow region (except the carrier region), for the incompressible three-dimensional steady flow, Reynolds averaged conservation equations are as follows:

- mass conservation equation

$$\frac{\partial}{\partial x_j}(\rho u_j) = 0 \tag{2}$$

- momentum conservation equation

$$\frac{\partial}{\partial x_j}(\rho u_j u_i - \tau_{ij}) = -\frac{\partial p}{\partial x_{ij}} + s_i \tag{3}$$

Where, s_i is source item, express the resistance of catalytic converter carrier; τ_{ij} is stress tensor, for Newton fluid satisfies:

$$\tau_{ij} = -\mu(s_{ij} + \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}) + \bar{\rho}\cdot\overline{u_i' u_j'} \tag{4}$$

Where, δ_{ij} is Kroneker number; $\bar{\rho}\cdot\overline{u_i' u_j'}$ is Reynolds stress tensor; s_{ij} is fluid deformation rate tensor. Given by formula (5):

$$s_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \tag{5}$$

3.2. Turbulent Model

Due to the gas flow state in the catalytic converter was turbulence flow (except carrier). So the standard k-e turbulence model was used to calculate Reynolds stress and close the above control equation, namely:

$$\bar{\rho}\cdot\overline{u_i' u_j'} = -\mu_t s_{ij} + \frac{2}{3}(u_t\frac{\partial u_k}{\partial x_k} + \rho k)\delta_{ij} \tag{6}$$

Where, u_t is turbulent viscosity coefficient. Given by formula (7):

$$\mu_t = \frac{C_\mu \rho k^2}{\varepsilon} \tag{7}$$

Where, k is turbulent kinetic energy. The transport equation is the formula (8). ε is turbulent dissipation rate. The transport equation is the formula (9).

$$\frac{\partial}{\partial x_j}(\rho u_j k - \frac{u_t}{\sigma_k}\frac{\partial k}{\partial x_j}) = u_t s_{ij}\frac{\partial u_i}{\partial x_j} - \rho\varepsilon - \frac{2}{3}(u_t\frac{\partial u_t}{\partial x_i} + \rho k)\frac{\partial u_i}{\partial x_i} \tag{8}$$

$$\frac{\partial}{\partial x_j}(\rho u_j \varepsilon - \frac{u_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_j}) = C_{\varepsilon 1}\frac{\varepsilon}{k}u_t s_{ij}\frac{\partial u_i}{\partial x_j} - \rho\varepsilon - \frac{2}{3}(u_t\frac{\partial u_i}{\partial x_i} + \rho k)\frac{\partial u_i}{\partial x_i} - C_{\varepsilon 2}\frac{\varepsilon^2}{k} + C_{\varepsilon 4}\rho\varepsilon\frac{\partial u_i}{\partial x_i} \tag{9}$$

The empirical coefficients in the formula are [6]: σ_k=1, σ_ε=1, $c_{\varepsilon 1}$=1.44, $c_{\varepsilon 2}$=1.44, $c_{\varepsilon 4}$=-0.33, c_μ=0.09.

3.3. Carrier Flow Model

The carrier of catalytic converter is ceramic honeycomb carrier. The carrier is composed of many of the same size of square pipes. As carrier pipes are too small, too much. So the exact multidimensional simulation of the carrier gas flow is very difficult. From the view of engineering, the research is mainly focus on the overall performance of the carrier and its influence on the flow. Therefore, the carrier is treated as the porous medium in the simulation. and the equivalent continuum method is used to simulate [7]. Due to the carrier pipe size is very small and Reynolds number in the carrier channel is less than 1000, so the flow in the carrier is steady incompressible laminar flow. When the porous medium has great resistance, momentum equation of convection and diffusion terms can be ignored in the carrier. The momentum equation is simplified as:

$$\frac{\partial p}{\partial x_{ij}} = -K_i u_i \tag{10}$$

$$K_i = \alpha_i |V| + \beta_i \tag{11}$$

Where, K_i is permeability, it is proportional to the local velocity. α_i and β_i are the empirical constant. The axial value of α_i and β_i are determined by the test. In the radial and circumference, α_i and β_i are 1×10^5. Namely, the gas flows along the axial and in the other two directions, there are no mass exchange [8].

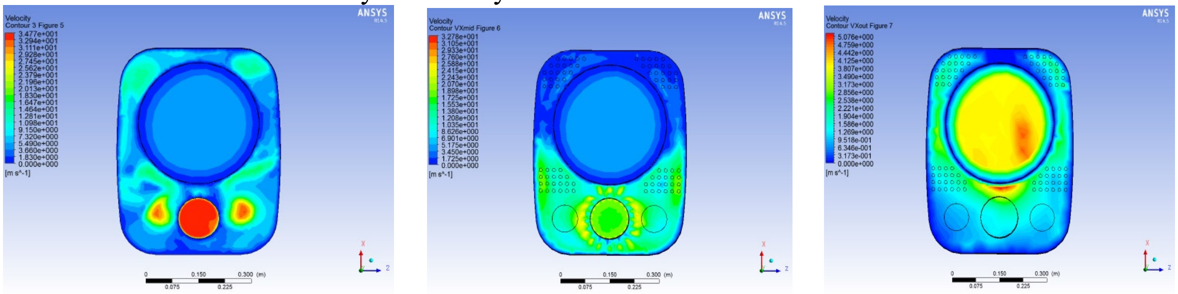
4. Numerical simulation

Inlet: Hypothesis of the velocity distribution of inlet is uniform. Within the scope of conventional engine flow rate, the mass flow rate of inlet is 0.443kg/s. The turbulent kinetic energy and its dissipation rate are respectively calculated according to the 0.5% turbulence intensity and 120mm hydraulic diameter. The temperature of inlet is 440°C.Outlet: The outlet is pressure outlet. The outlet pressure is 97400Pa. It was measured by experiment. The turbulent kinetic energy and its dissipation rate are respectively calculated according to the 5% turbulence intensity and 134 mm hydraulic diameter. The temperature of outlet is 440°C.Wall: The wall velocity is no slip boundary and the heat exchange with gas is not considered. Utilizing the computational fluid dynamics software FLUENT to solve the governing equations, the finite volume difference method is used to discrete the governing equations. The SIMPLE algorithm is used to calculate the steady incompressible flow.

5. Results and analysis

5.1. Velocity Distribution

The velocity distribution contour of different position in the carrier was shown in Fig.1. It can be seen that the velocity distribution of the exhaust gas was relatively uniform and the velocity gradually decreased during the whole process of flow. The carrier velocity distribution uniformity index was 0.9832. It shows that the velocity uniformity at the entrance of the carrier is better.



(a) Front cross section (b) Middle cross section (c) Rear cross section

Figure 1. Velocity distribution contours of carrier

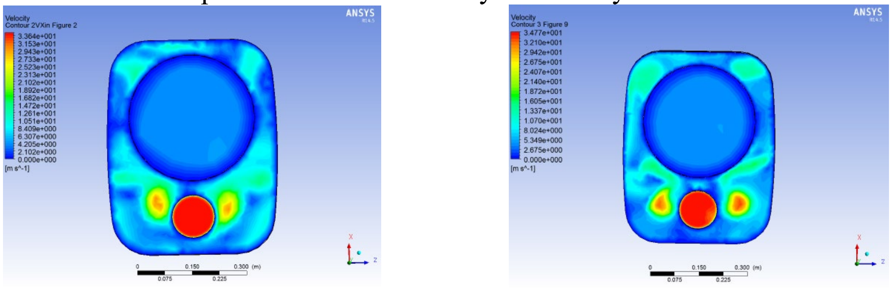
5.2. Pressure Distribution

The pressure drop of SCR catalytic converter is mainly the pressure drop in the carrier. The pressure loss is 9.0531E+05Pa. The back pressure of catalytic converter was relatively larger.

6. Analysis of the influence of SCR catalytic converter structure parameters on Performance

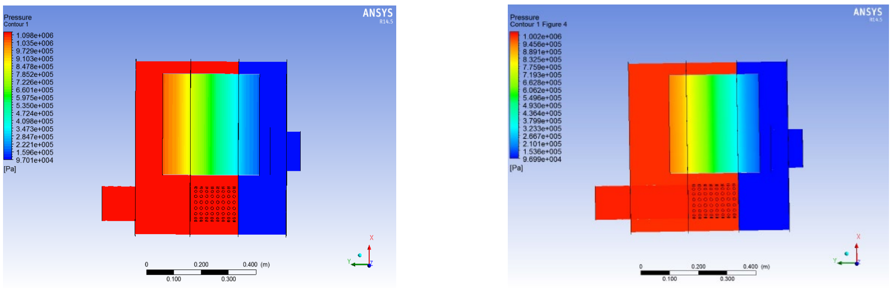
6.1. The Influence of Carrier Length on Catalytic Converter's Performance

The length on the left side of the carrier is increased by 40mm and the position of the carrier is unchanged, the flow field of the catalytic converter was simulated under the same boundary conditions.The velocity distribution and pressure distribution contrast contour of new model and the original model is respectively shown in Fig. 2 and Fig. 3.However, The carrier velocity distribution uniformity index of new model was 0.97927. It can be concluded that with the increase of the carrier length, the uniformity of the velocity distribution is slightly decreased. With the increase of carrier length,the pressure loss of catalytic converter increased significantly.Therefore, the length of the carrier has effect on the exhaust back pressure and the velocity uniformity.



(a) Length changed (b) original

Figure 2. Comparison of velocity distribution contour for different lengths

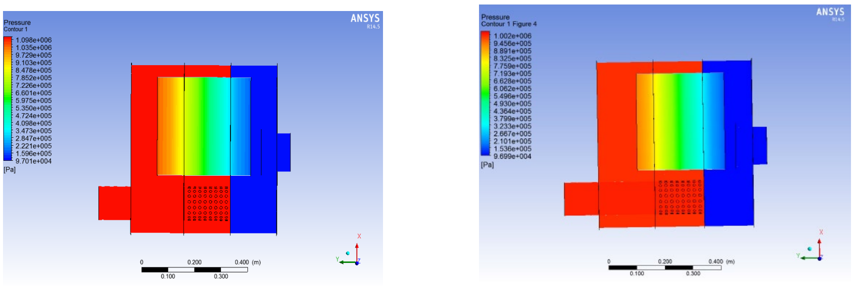


(a) Length changed (b) original

Figure 3. Comparison of pressure distribution contour for different lengths

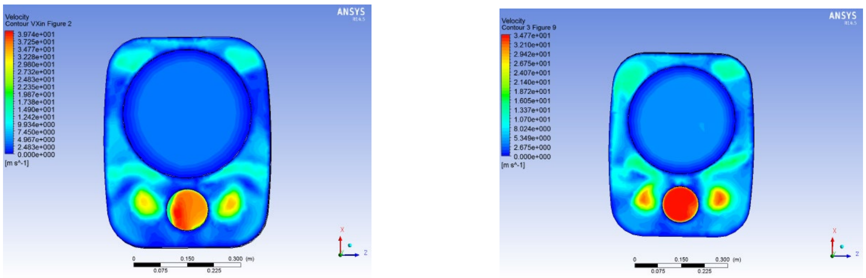
6.2. The Influence of Carrier Diameter on Catalytic Converter's Performance

The position of the carrier is unchanged and the diameter of carrier is changed to 360mm, the flow field of the catalytic converter was simulated under the same boundary conditions.The velocity distribution and pressure distribution contrast contour of new model and the original model is respectively shown in Fig. 4 and Fig. 5. Fig. 4 shows that the velocity distribution becomes more uniform.The carrier velocity distribution uniformity index of new model was 0.98349. Fig.5 shows that with the increase of carrier diameter, the pressure loss of catalytic converter decreased.So the velocity distribution uniformity and pressure loss are affected by the diameter of the carrier.



(a) Length changed (b) original

Figure 4. Comparison of pressure distribution contour for different lengths



(a) Diameter changed (b) original

Figure 5. Comparison of velocity distribution contour for different diameter

7. Catalytic converter structure optimized

From the above analysis, the carrier length and diameter will impact on the flow field characteristics of catalytic converter. So by using ANSYS software, the carrier length and diameter are used as optimization parameters, the carrier velocity distribution uniform index and catalytic converters pressure loss are utilized as the optimization target, the structure of catalytic converters was optimized. By calculation, in the optimal design point of catalytic converter, the pressure loss is 7.9121E+05Pa, the velocity distribution uniformity index is 0.98367. The catalytic converter optimized structural parameters values is shown as table1.

Table 1. Optimized structural parameters

Structural parameters	Optimized value
Carrier length	220mm
Carrier diameter	360mm

8. Conclusion

In this paper, By using fluid dynamics (CFD) technology, the catalytic converter internal flow field was simulated. On the basis of, the structure parameters of the catalytic converter influence on the carrier velocity distribution uniformity and the catalytic converter pressure loss were analyzed, the structure parameters of catalytic converter has been optimized. The conclusion is as follows: With the carrier's length increases, the pressure loss increases and the velocity distribution uniformity in the front of carrier becomes worse; When the diameter of carrier increases, the pressure loss decreases and the velocity distribution uniformity in the front of substrate becomes better; Optimizing the structure parameters of the catalyst can improve the performance of the catalyst.

Acknowledgments

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