

# Analysis Vehicle TWC Light-off Characteristics on AMESim Platform

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## Abstract

Though building an AMESim physical model of vehicle three-way catalytic converter (TWC), this article aims to study the light-off characteristics of TWC. By solving the energy and mass conservation equations of gas-solid two phase of the model, this article obtains the emissions conversion rate, such as CO, unburned hydrocarbons (CaHb) and nitrogen oxides (NOx) under different parameters. The results show that, the TWC light-off characteristics can be affected by the engine control strategy, allocation of TWC and the structure of TWC carrier.

**Keywords:** vehicle, TWC, light-off, simulation

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## 1. Introduction

CO, NOx, CaHb in vehicle emissions have gradually increased, and easy cause to photochemical smog and the secondary pollution on the human environment [1]. Studies have shown that harmful gases accounted 50% to 80% of the entire European Energy Test Cycle (EETC) during the cold start (1 to 2min) [2-3]. Many engine manufacturers constantly updated technology to reduce emissions to meet the listing requirements, such as lean-burn technology cooler, EGR, turbo technology, multi-valve technology. But, because of the factors such as structural design and manufacturing cost, cold start emission control effect failed to be highlighted [1, 4, 5].

TWC is developed in order to meet the vehicle emission standards and a key equipment to reduce exhaust pollution, but only when the catalyst reaches a certain temperature it can begin to work (i.e. ignition). So it's important to shorten the catalytic converter light-off time [4]. Rapid light-off of the catalytic converter technology has become an effective way to reduce cold start emissions. To identify the factors and impact of TWC light-off characteristics, the light-off characteristics of vehicle cold starting process of TWC is simulated by this article on AMESim platform, which can make some references for the engine designers.

## 2. TWC Physical Model

A model using the inline four-cylinder multi-point injection engine, whose bore is 83mm, and the stroke is 83mm, compression ratio is 10:1, front and rear oxygen sensor are used. TWC is built by ceramic (basic materials, MgO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub> and SiO<sub>2</sub>) coated with  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>. The simulated TWC wall thickness is 0.16mm, the porosity of the wall is 77%, internal surface area of the wall is 1.957m<sup>2</sup>/L, and the proportion of the wall is 435g/L. the physical model of TWC on AMESim software platform shown in Figure1 [6, 7].

## 3. Simulation

In this article, the simulation using the single-hole, heat and mass transfer model, combined with the chemical reaction to simulate the concentration distribution of the gas exhaust components within the carrier center channel. According to the carrier material and the physical and chemical properties of the coating material, it is assumed that the exhaust gas temperature, concentration and speed on the same cross section of the hole is uniform in the

carrier channel, and it's laminar flow in the channels. Because of tiny channel, gas flow along the radial direction is ignored. the exhaust gas along the axial mass diffusion and heat diffusion, radiation, heat exchanger on the heat transfer process and pore body diameter to heat transfer are also ignored because of the cold start exhaust.

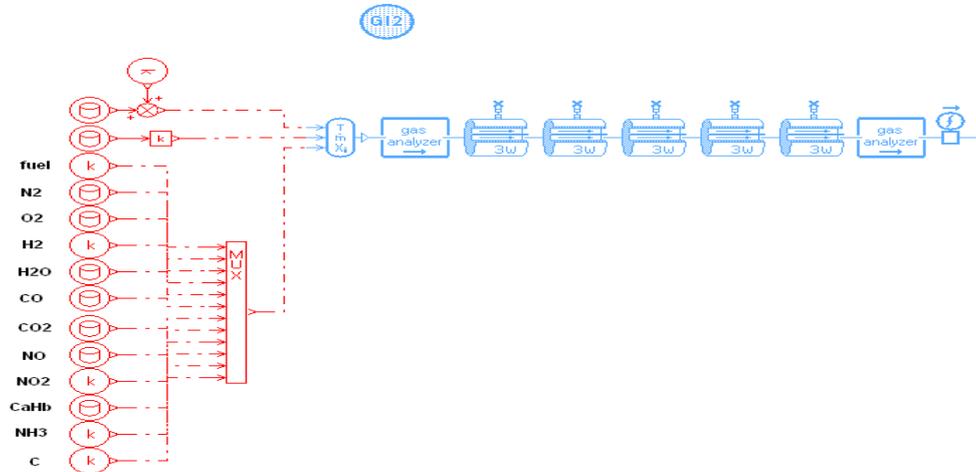


Figure 1. TWC AMESim Simulation Model

Based on those assumptions, accord to the law of conservation of energy and mass of gas and solid, mathematical model of gas-solid in the TWC can be built [3].

**3.1. Controlling Equations.**

Based on the assumption that the ceramic substrate in the single-hole channel, the gas mass conservation mathematical model can be written as [8]:

$$\epsilon \frac{\partial C_{g,k}}{\partial t} + \frac{\rho_p v_p}{\rho_g} \frac{\partial C_{g,k}}{\partial x} = K_{f,k} S (C_{s,k} - C_{g,k}) \tag{1}$$

where: the subscript 1 to 6 represent CO, C<sub>3</sub>H<sub>6</sub>, CH<sub>4</sub>, NO, H<sub>2</sub>, O<sub>2</sub> six gases respectively; *t* is time;  $\epsilon$  is carrier aperture ratio;  $C_{g,k}$  is the concentration of components in the exhaust;  $\rho_p$  is the end of the exhaust gas density;  $v_p$  is exhaust axial velocity;  $\rho_g$  is exhaust concentration. *x* is axial coordinate;  $K_{f,k}$  is exhaust components of the mass transfer coefficient; *S* is the geometry of the unit volume of carrier concentration;  $C_{s,k}$  is the concentration of the surface of the catalyst components.

And the Single Hole Road mathematical model of gas energy conservation can be written as:

$$\epsilon \rho_g \frac{\partial T_g}{\partial t} + \rho_p v_p \frac{\partial T_g}{\partial x} = h_x \frac{S}{C_{p,g}} (T_g - T_s) \tag{2}$$

where:  $T_g$  is exhaust temperature;  $T_s$  is vectors temperature;  $h_x$  is heat transfer coefficient between the carrier and exhaust;  $C_{p,g}$  is exhaust heat at constant pressure. The solid mass conservation mathematical model can be written as:

$$S_{cat} R_k(\bar{C}_s, T_s) = \frac{\rho_g}{M_g} K_{f,k} S(C_{g,k} - C_{s,k}) \quad (3)$$

where:  $S_{cat}$  is the unit vector volume of activity of the catalyst surface area;  $R_k$  is the composition of the reaction rate;  $M_g$  is exhaust molecular weight.

And the solid energy conservation mathematical model can be written as:

$$(1-\varepsilon)\rho_s C_{p,s}^M \frac{\partial T_s}{\partial t} = (1-\varepsilon) \left( \lambda_{s,x} \frac{\partial^2 T_s}{\partial x^2} \right) + h_x S(T_g - T_s) + S_{cat} \sum_{k=1}^n (-\Delta H)_k R_k(\bar{C}_s, T_s) \quad (4)$$

where:  $\rho_s$  is the carrier material density;  $C_{p,s}^M$  is ceramic carrier component of the specific heat;  $\lambda_{s,x}$  is thermal conductivity of the ceramic substrate in the  $x$  direction;  $(-\Delta H)_k$  is the reaction heat of the  $k$ -st reaction.

### 3.2. Calculation Conditions

Set 12m/s to velocity inlet boundary conditions, radial velocity is zero, the gas density is approximately 2.5kg/m<sup>3</sup>, the concentration of the exhaust of entrance is generated by physical model signal. Set the engine initial speed is 800rpm, the simulation calculation time step is set to 0.2s, the total duration is 150s.

## 4. Results and Analysis

Simulation values in Figure 2 are the simulation results of NO<sub>x</sub>, and the test values is the results in the reference [2] through a real car three-conditions-cycle conversion rate. The comparison chart of the two tests shows that in the cold start (ie, start in the first 120s), the CO, C<sub>a</sub>H<sub>b</sub> and NO<sub>x</sub> conversion rate of the simulated values and experimental values are basically the same, so the previously built simulation model is reasonable, and it can be used to TWC light-off characteristics study.

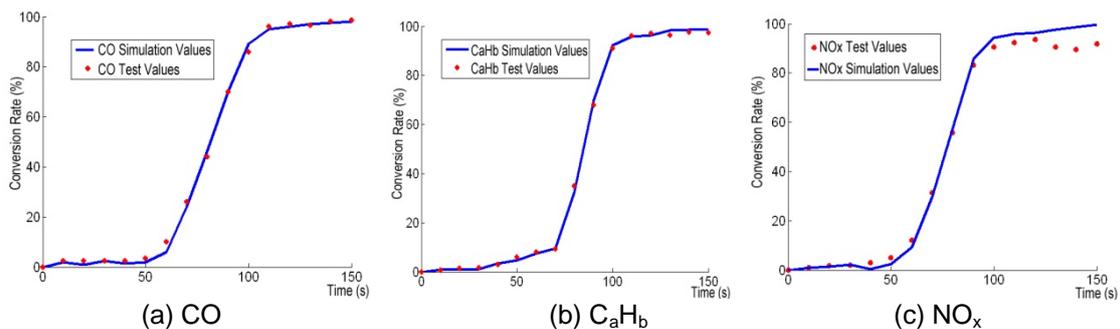


Figure 2. Exhaust Comparison of Simulation Results and Measurement Values

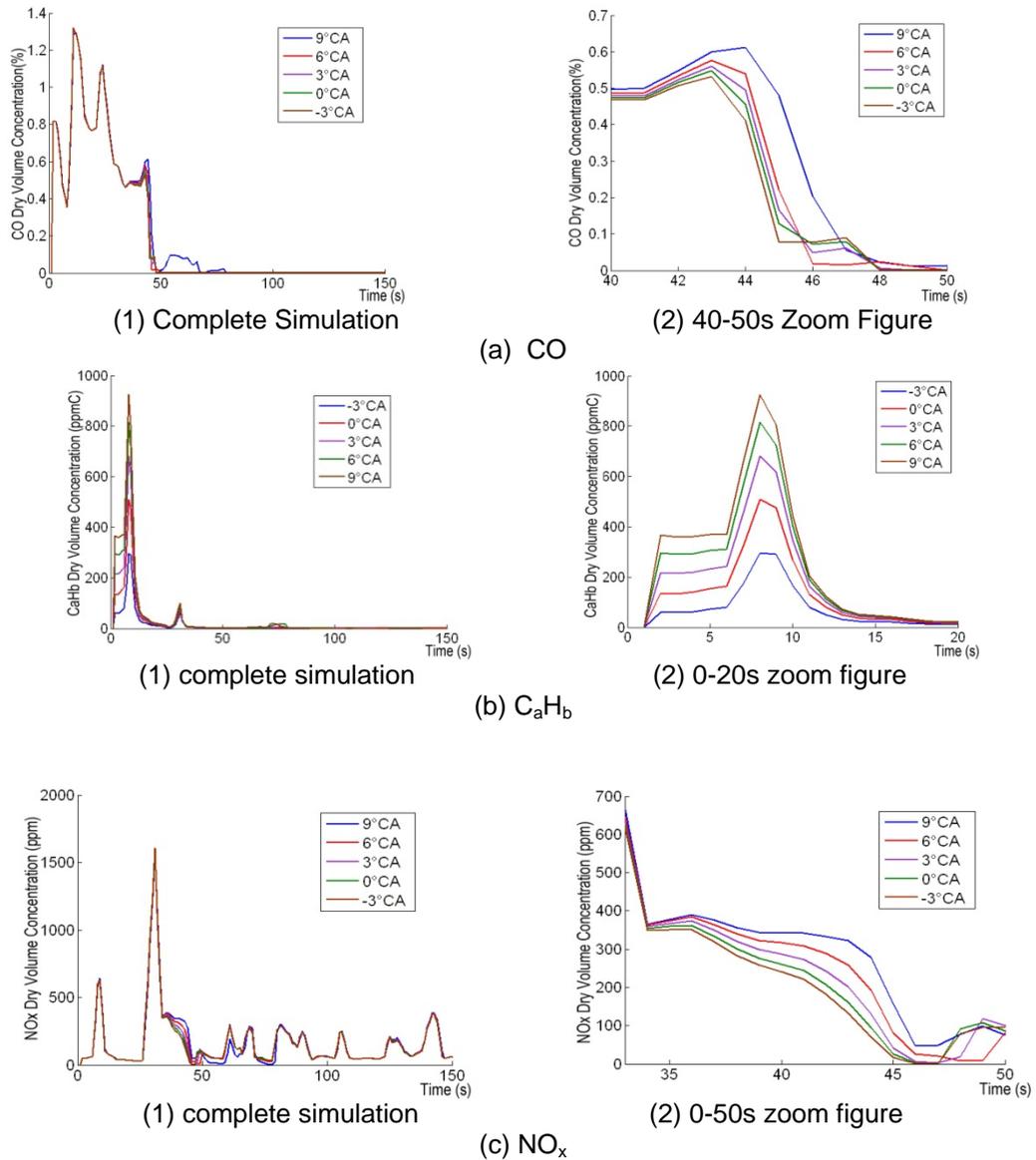


Figure 3. Exhaust Dry Volume Concentration in Different Light-off Advance Crankshaft Angle

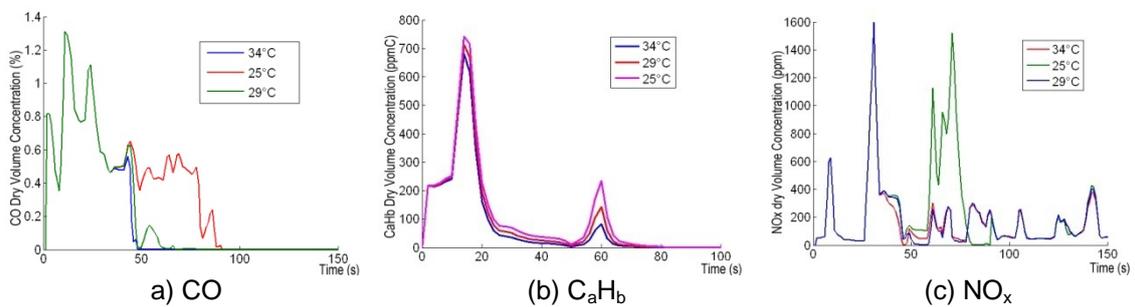


Figure 4. Exhaust Dry Volume Concentration In Different Intake Air Temperature

Figure 3 shows CO, C<sub>a</sub>H<sub>b</sub>, NO<sub>x</sub> dry volume concentration in TWC of different light-off advance CA. The figures show that the longer the light-off advance angle increases, the longer the catalyst light-off, the higher the exhaust dry volume concentration, and the poorer the light-

off characteristics. So, it should be to reduce the light-off advance CA during cold start phase. Figure 4 shows the TWC light-off characteristics under different intake air temperature (which can simulate the TWC and the engine at different distances [6]). The figure shows that the lower the intake air temperature (equivalent to the distance increases), the higher the exhaust dry volume concentration, the worse the light-off characteristics. Therefore, if there are no active heating measures, the installation location of the TWC should be appropriately close to the engine or take dual catalytic converters, which help to improve the cold start light-off characteristics.

Exhaust dry volume concentration in different carrier length shown in Figure 5. These figures show that, the longer the carrier length, the shorter the TWC reached burning time, the lower concentration the emission of each component, and the better the ignition characteristics. As the carrier length is further increased, the steady-state conversion efficiency of the further increased part of the carrier decreased to some extent due to the density decrease of catalyst distribution, and the combustion characteristics are also decreased. This means that, for the same amount of noble metal catalyst carrier, there is an optimum value of the carrier length. TWC combustion characteristic influence of wall thickness is shown in Figure 6. The figure shows that, with the carrier wall thickness increased, the temperature of the carrier rises slowed, the exhaust gas component concentration increased, and the burning time of the catalyst is longer. Therefore, it should be as far as possible to reduce the wall thickness of carrier when designing a TWC.

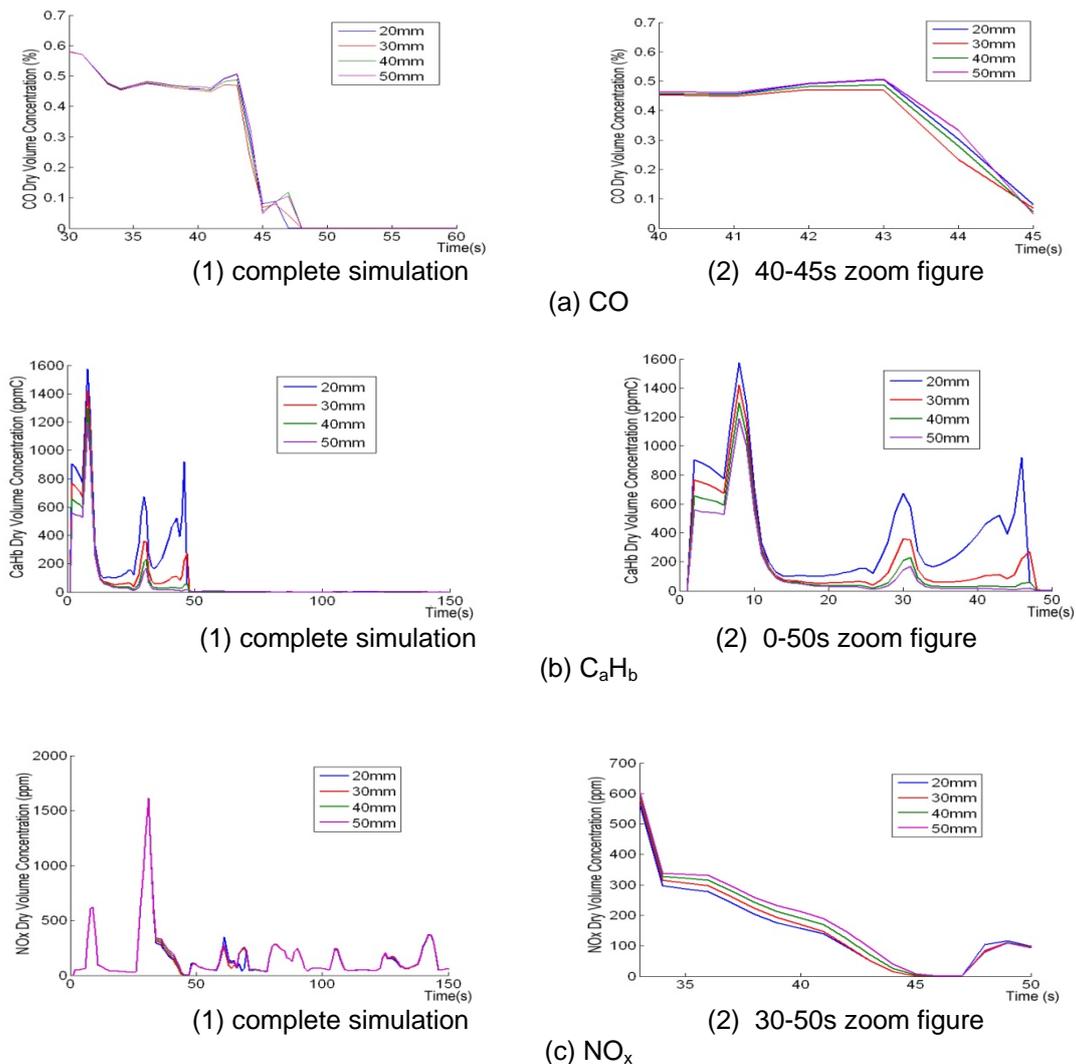


Figure 5. Exhaust Dry Volume Concentration in Different Carrier Length

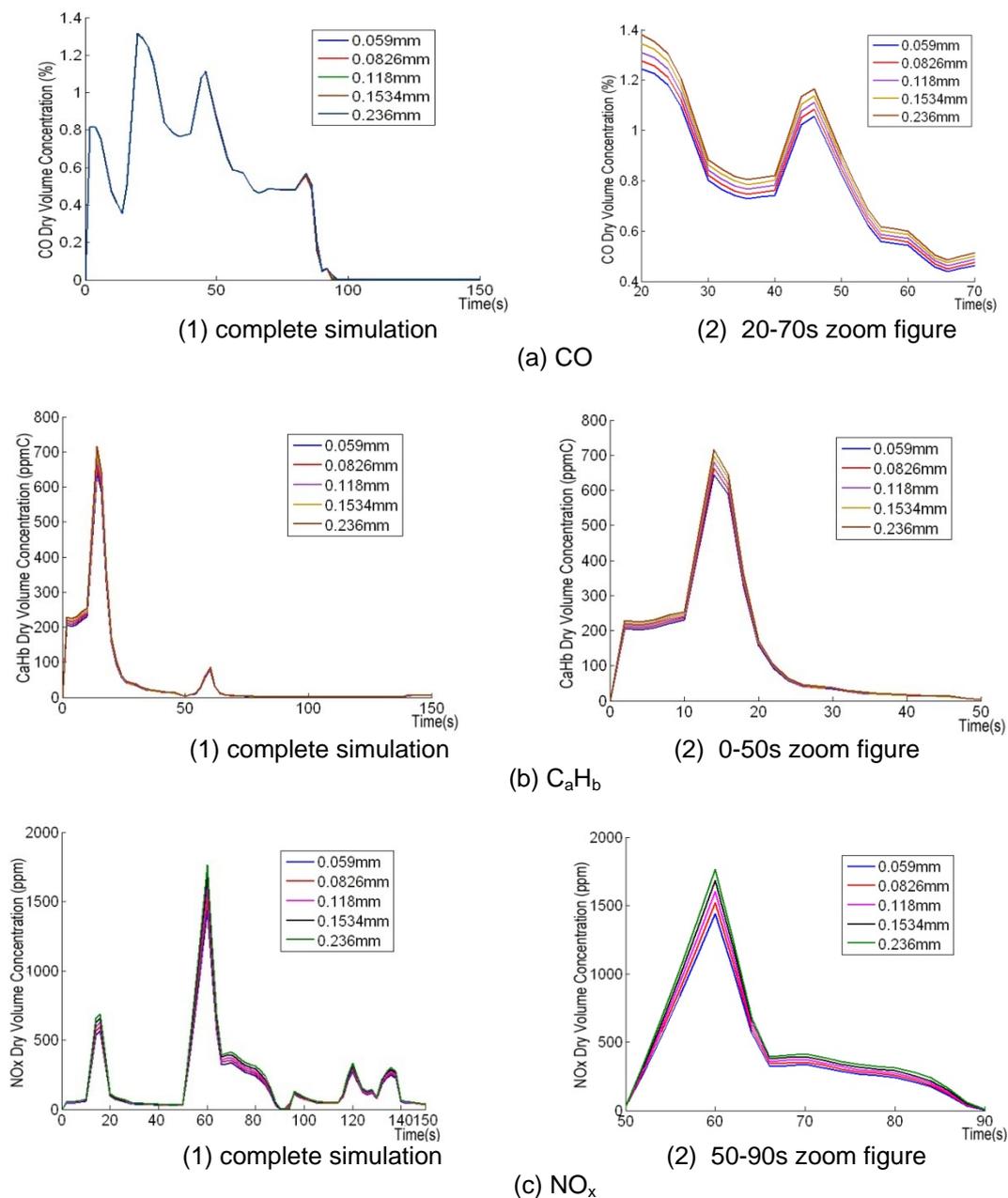


Figure 6. Exhaust dry volume concentration in different wall thickness

## 5. Conclusion

Through building the AMESim model of TWC, solving gas-solid mass and energy conservation equations, and simulating TWC light-off characteristics by changing the light-off advance CA and the distance between TWC and engine, this article gains the TWC light-off characteristics under different factors. Analysis of the simulation results shows that:

1. Model tested by real vehicle fitted the experiment well, so that the model is reasonable;
2. The engine control strategies have an impact on the light-off characteristics of TWC, and reduce the light-off advance CA during cold starting can improve the light-off characteristics;
3. under the same conditions, the closer the distance between TWC and the engine, the thinner the carrier wall, the better the light-off characteristics.
4. This article is calculated a single catalytic converter influencing factors, actually, pairs of the catalytic converter is more complex, and can be subsequently further simulation analysis.

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