

# Numerical Study on Catalytic Reaction and Catalytic Mechanism of Ceramic Catalytic Turbine Technology under Variable Operating Conditions during Vehicle Warm-up

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## ABSTRACT

In this paper, numerical simulation methods are adopted to explore the influencing factors of a Ceramic Catalytic Turbine (CCT) for reduced exhaust pollution from vehicles during the warm-up stage. Also, an analysis is conducted regarding the potential effects of turbulence on the catalytic reaction mechanism and the sensitivity of relevant parameters to the Arrhenius equation. It is found out that the air-fuel ratio inside the engine has a considerable effect on the reactions of CCT, with the conversion efficiency of each emission species sharply reduced under fuel-rich conditions. At 600K, the conversion efficiency declines by 11.3% for C<sub>3</sub>H<sub>6</sub>, 12.26% for CO, and 3.64% for NO. At 700K, the conversion efficiency is reduced by 6.7% for C<sub>3</sub>H<sub>6</sub>, 11.56% for CO, and 6.44% for NO. Despite increasing the concentration of reaction gas components, a high flow rate makes little difference to the reaction itself. At the same rotational speed of the turbine, the conversion rate of harmful components drops with an increase in flow rate due to the increase in space velocity. When the flow rate is constant and the temperature is kept in the control zone of chemical kinetics, the conversion efficiency of the catalytic reaction is enhanced at a higher rotational speed. Differently, when the temperature is in the control zone of mass transport and the flow rate is constant, the conversion efficiency decreases as the turbine accelerates. In practical terms, reducing activation energy within a controllable range is equivalent to further reducing the light-off temperature of the catalyst. Meanwhile, this may disrupt the convergence of numerical calculations because the catalytic reactions could occur at around the light-off temperature.

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## 1. INTRODUCTION

The use of a three-way catalytic converter (TWC) plays a crucial role in reducing the emissions of various harmful substances present in exhaust gases, such as HC, CO, and NO<sub>x</sub> (Twigg, 2003). To a large extent, the efficiency of the catalytic converter depends on the exhaust temperature reached during the warm-up stage of a specific vehicle (Crane et al., 1997; Yamamoto et al., 2000; Harikrishnan et al., 2018). Once the catalyst reaches a normal working temperature of over 400°C, the conversion rate of harmful exhaust components approaches 100%. However, a prolonged warm-up time of an automotive turbocharger and catalytic converter can have a significant adverse effect on tailpipe emissions

from the engine (Chen & Chang 2015). Prior studies have confirmed that during the warm-up period (1~2min) of a typical driving route, the emissions of HC and CO account for as high as 60-80% of the total in one test cycle (Gottberg et al., 1991; Moore & Mondt 1993; Summers et al., 1993).

In a study on transient warm-up characteristics of the catalyst, it was found out that the characteristics of catalyst in chemical kinetics were significantly affected by the non-uniformity of its flow inside the channels of the catalytic converter, which was particular the case at lower inlet temperatures (Chakravarthy et al., 2003). Moreover, the non-uniform flow of catalyst with high velocity was found to reduce the light-off performance of the inner core

NOMENCLATURE			
<i>CCT</i>	three-way catalytic converter	<i>O</i>	original turbine (without catalyst)
<i>E<sub>A</sub></i>	original activation energies of the reaction about C <sub>3</sub> H <sub>6</sub> and CO	<i>R</i>	inlet condition in a fuel-rich state
<i>E<sub>B</sub></i>	original activation energies of the reaction about NO	<i>S</i>	ideal stoichiometric condition
<i>TWC</i>	catalytic ceramic turbine		

in a catalytic reactor (Zygorakis, 1989). Thus, improving the outcome of mass transportation was suggested as a solution to the enhancement of conversion efficiency. It was also indicated that the occurrence of turbulent flow significantly improved the efficiency of catalytic conversion, particularly at high inlet temperatures and space velocities (Santos & Costa 2009). Therefore, it is presumed that increasing turbulence is effective in improving the conversion efficiency of a catalyst relative to a laminar flow through the TWC.

As a critical component of diesel engines, turbocharger has been increasingly applied in various gasoline engines. The flow inside the turbine is of turbulent nature. Also, it is located in close proximity to the engine, which causes the inlet temperature of the turbine to increase faster than the downstream catalysts during the warm-up period. Given the exothermic catalytic reactions, it is conceivable that a turbine rotor functioning as a catalytic could undergo a significant catalytic reaction. This technology is known as Ceramic Catalytic Turbine (CCT). In practical applications, the ceramic coating of a catalyst can be attracted by other components of a turbine, such as turbine housing and nozzle guide vanes, which thus accelerates the light-off of downstream catalyst and reduces emissions from the engine during the warm-up period.

## 2. ESTABLISHMENT OF THE NUMERICAL MODEL AND THE SETTING OF CALCULATION

Introduced in a previous paper (Wang et al., 2021), the method of numerical CCT modelling and simulation intended for the turbine of gasoline engines is applied in this paper and summarized below.

### 2.1 Establishment of the Numerical Model

The turbine used in this study consisted of 9 rotor blades and a round-shaped volute outlet with a diameter of 37.8mm. The grid of the volute was established using the commercially available mesh generator IGG. Derived from the software NUMECA, this mesh generator relied on butterfly technology to improve mesh quality. The total mesh volume was 1,459,289, and the first mesh boundary layer was 0.005mm in thickness. The model of a single-channel rotor was constructed using the Turbo-grid package from the software ANSYS. To prevent the risk of outlet backflow without increasing the total mesh volume, the shroud and hub lines were extended by 26mm along the axial direction at the rotor outlet. With the assistance of the ICEM package from ANSYS, the model of the rotor with full passages was established by replicating the single-channel rotor grid in a circular pattern. Finally, the turbine grid was incorporated into the rotor and the volute grids.

Previously, a discussion has been conducted about the grid independence verification for the simulation of performance and catalytic reaction in the volute and single-channel rotor grid (Wang et al., 2021).

#### (1) Volute grid independence verification

There were three densities of volute grids selected for grid independence verification: coarse, medium, and fine meshes. Accordingly, the total number of grid cells was 700,329, 1,459,289, and 3,003,069 for coarse, medium, and fine meshes, respectively. The grid independence was verified numerically by examining the total pressure loss coefficient between the inlet and outlet of the volute at a normal rotational speed of 80,000rpm and three different mass flow rates respectively: 0.031, 0.027, and 0.024kg/s.

According to the simulation results, the total pressure loss coefficients as obtained with the medium and fine meshes were clearly comparable, with a maximum difference of less than 1.5% in all scenarios. However, the total pressure loss coefficient as obtained with the coarse mesh differed significantly from the other two. For this reason, the medium mesh volume was selected for further analysis.

#### (2) Rotor grid independence verification for turbine performance

Three single-channel rotor grids were used, whose mesh volume was 522,231, 1,106,467, and 2,186,428, respectively. Besides, their boundary layer was 0.002 mm in thickness. The number of grid layers in the blade tip clearance exceeded 17, and their y plus values were less than 3.5.

The expansion ratio and efficiency of the rotor were compared under three different working conditions. As indicated by the simulation results, the expansion ratios of all three grids were almost consistent. Although the efficiency of medium mesh was closely matched by that of fine mesh, the efficiency of coarse mesh was much higher compared to fine mesh (Zhao et al., 2018).

To evaluate rotor performance of the turbine, grid independence verification was also carried out at low rotational speed (11,600rpm) and low inlet temperature (450K) during the warm-up period. As revealed by the results, the expansion ratio versus mass flow curves were not significantly different between the three grids. Also, the simulation results obtained with medium and fine meshes showed a high degree of overlapping. For the curves of expansion ratio versus efficiency, the simulation results obtained with medium mesh and fine meshes were consistent at a high expansion ratio, despite the maximum difference of about 2.5% at a low expansion ratio.

(3) Grid independence verification for catalytic reactions

This section was conducted at a low rotational speed (11,600rpm) and a low mass flow (0.0086kg/s), while the inlet temperature varied at 700K, 600K, and 450K, respectively. The performance of the catalytic combustion turbine (CCT) was evaluated using the conversion rate of catalytic reactions and the variation in outlet temperature.

The three single-channel rotor grids as mentioned above were also used to verify the grid independence of catalytic reactions. The results showed that the medium mesh was more suitable for the calculation. In this medium grid, the effect of boundary layer thickness on catalytic reactions was investigated. Three additional models were constructed by maintaining the similar mesh density. Meanwhile, the thickness of the first boundary layer and their y plus values were increased or decreased. The comparison involved conversion efficiency, the changes in exhaust temperature, and the convergence curves of C<sub>3</sub>H<sub>6</sub> (with the highest content in the exhaust).

To sum up, the medium mesh satisfies the requirement on grid independence and can be used for computational analysis.

(4) Computational formula

Proposed and modified by MENTER in 1994 according to a standard  $k-\omega$  model, the SST( $k-\omega$ ) turbulence model is a two-equation model. The model adopts a formula for simulation calculation near the boundary layer but a different one in the fully developed fluid region, which eliminates the possibility that the formula is overly sensitive to inlet turbulent flow. The general governing equations of SST( $k-\omega$ ) turbulence model are as follows:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho \bar{u}_i k) = \frac{\partial}{\partial x_i}(\Gamma_k \frac{\partial k}{\partial x_j}) + F_k - Y_k \quad (1)$$

$$\frac{\partial}{\partial t}(\rho \omega) + \frac{\partial}{\partial x_i}(\rho \bar{u}_i \omega) = \frac{\partial}{\partial x_i}(\Gamma_\omega \frac{\partial \omega}{\partial x_j}) + F_\omega - Y_\omega + D_\omega \quad (2)$$

where  $k$  represents turbulence kinetic energy;  $t$  stands for time;  $\rho$  indicates the density;  $\bar{u}_i$  and  $\bar{u}_j$  are referred to as the average of turbulent velocity;  $x_i$  and  $x_j$  are referred

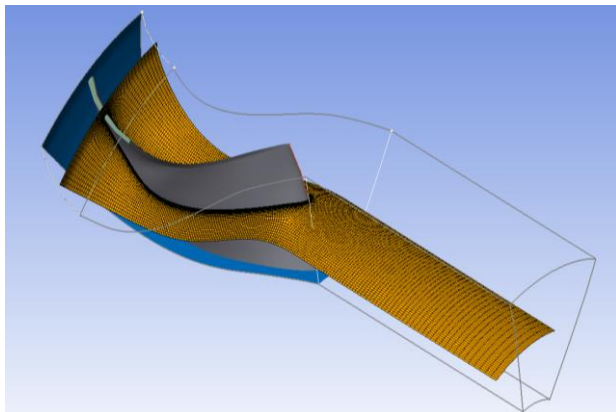


Fig. 1 Grid topology of the single-channel rotor

to as the coordinate components;  $\omega$  denotes specific turbulence dissipation rate;  $\Gamma_\omega$  and  $\Gamma_k$  represent the effective diffusion coefficients;  $F_k$  and  $F_\omega$  are referred to as turbulence generation terms;  $Y_\omega$  and  $Y_k$  are used to represent the dissipation terms for  $k$  and  $\omega$ , respectively;  $D_\omega$  denotes the diffusion term. The turbulent dynamic viscosity coefficient [ $\mu_1$ ] of the model was modified as follows:

$$\mu_1 = \frac{\rho k}{\omega} \cdot \frac{1}{\max\left[\frac{1}{\alpha^*}, \frac{SF_2}{\alpha_1 \omega}\right]} \quad (3)$$

where  $\alpha^*$  represents the low Reynolds number correction coefficient;  $\alpha_1$  indicates an empirical constant term;  $S$  denotes a constant term of shear stress;  $F_2$  refers to a mixing function.

As shown in Fig.1, the mesh volume of the single-channel rotor grid was 1,106,467 and the thickness of the first mesh boundary layer was 0.002 mm. The number of grid layers in the blade tip gap exceeded 17, and the y value was below 3.5.

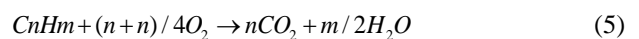
2.2 Setting of Calculation

Numerical calculation was performed using the FLUENT package from ANSYS 19.2. First of all, the performance of the entire turbine stage was evaluated through calculation based on the turbo flow bench test, with the resulting flow field conditions at the inlet and outlet of the rotor as the initial field for simulating the single-channel rotor model. The turbulence was modeled using the (SST) model, and the coupled algorithm was applied to solve the equations of pressure and velocity. Space discretization was performed using the Least Squares Cell-based Gradient Scheme, with the pressure term discretized by a second-order scheme and the remaining terms discretized by the Second-order Upwind scheme. The catalytic reaction was modeled using the CHEMKIN mechanism, with the rotor hub and blade surface as the catalyst surface. The CHEMKIN-CFD Solver and Eddy-Dissipation Concept were used for Chemistry Solver and Turbulence-Chemistry interaction, respectively.

2.3 Catalyst and Reaction Mechanism

The catalyst used in this paper had a precious metal composition of Pt/Rh at a ratio of 5:1. The surface-active site densities of Pt and Rh were  $2.04 \times 10^{-9} \text{mol/cm}^2$  and  $0.68 \times 10^{-9} \text{mol/cm}^2$ , respectively.

The chemical reaction model based on the Pt/Rh catalyst of multi-element reaction as established by Chatterjee et al. (2002) was adopted for the catalytic reactions as follows:



**Table 1** Volume concentration of exhaust components in different air-fuel ratios of the engine

Species		C <sub>3</sub> H <sub>6</sub>	CO	NO	O <sub>2</sub>
Mole Fraction (%)	S	0.045	1.420	0.100	0.770
	R	0.045	1.420	0.100	0.400
Species		CO <sub>2</sub>	H <sub>2</sub> O	H <sub>2</sub>	N <sub>2</sub>
Mole Fraction (%)	S	10.000	10.000	0	77.665
	R	10.000	10.000	0	78.035

### 3. EFFECT OF AIR-FUEL RATIO ON CATALYTIC REACTIONS

In the study of Wang et al. 2021, a narrow range of air-fuel ratios under the stoichiometric condition was selected for the engine to validate CCT. This fuel enrichment is a popular approach for quick engine warm-up, which inevitably leads to high emissions. Within this range, the concentration ratios of C<sub>3</sub>H<sub>6</sub>, CO, and NO can be converted most effectively because they are more adaptable to a three-way catalyst. During the warm-up stage, combustion usually occurs in the cylinder in a fuel-rich state, thus reducing the concentration of O<sub>2</sub> in the exhaust and resulting in incomplete combustion. As a result, the effectiveness of catalytic reactions would also be beneficial when the exhaust passes through the CCT to mitigate the excessive HC/CO emissions caused by fuel enrichment.

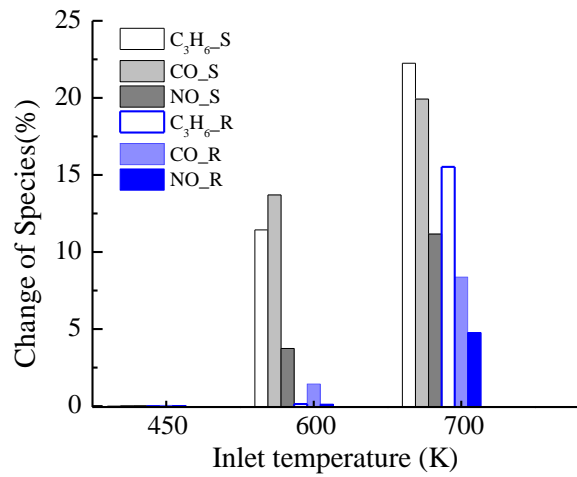
As pointed out previously (Wang et al., 2021), the chemical reactions in CCT can be divided into three stages: non-reaction, reaction light-off, and violent reaction. On this basis, the three typical turbine inlet temperatures, 450K, 600K, and 700K, were selected for further analysis. In addition, as shown in the "R" row of Table 1, an inlet boundary condition in a fuel-rich state was selected for comparison with the results obtained under the ideal stoichiometric condition indicated by "S" in Table 1.

In all the calculation process, the turbine was kept at a low level in terms of rotational speed (11600RPM) and mass flow (0.00776kg/s). Only the reactions involving harmful substances C<sub>3</sub>H<sub>6</sub>, CO, and NO were under consideration. Figure 2 and Fig. 3 show the conversion efficiencies achieved as the temperature of the catalytic reaction varied when the exhaust gas passed through CCT at the two selected air-fuel ratios. The conversion efficiency is expressed as Equation 1.

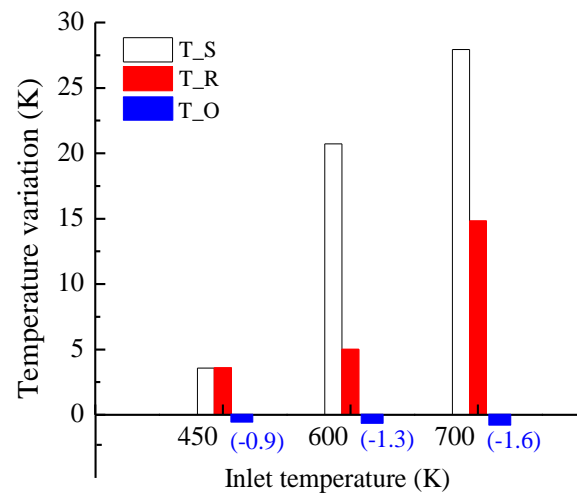
$$\eta_i = (C_{i\_inlet} - C_{i\_outlet}) / C_{i\_inlet} \times 100\% \quad (7)$$

where  $\eta_i$  represents the conversion efficiency of harmful exhaust components  $i$ ;  $C_{i\_inlet}$  and  $C_{i\_outlet}$  are referred to as the mass fraction of harmful exhaust components at the inlet and outlet of the turbine, respectively.

Figure 2 shows that under the fuel-rich condition, the conversion efficiency of the harmful exhaust components was fairly low (all less than 0.04%) at a turbine inlet temperature of 450K, suggesting that the catalytic reaction was not significantly affected by the change in exhaust concentration at low inlet temperatures. However, at an



**Fig. 2** Effect of air-fuel ratio on the conversion efficiency of CCT



**Fig. 3** Effect of air-fuel ratio on the exhaust temperature of CCT

inlet temperature of 600K and in the presence of air-fuel mixture enriched, the conversion efficiency of the harmful components was low, reaching 2.5% at maximum. At an inlet temperature of 700K, the conversion efficiency of each harmful component was significantly lower in the fuel-rich condition than under the stoichiometric condition, despite the optimal reaction temperature reached for the catalyst.

In Fig. 3, T<sub>O</sub> indicates the decrease in temperature when the exhaust passes through the original turbine (without catalyst). However, the temperature increases when the exhaust gas passes through the CCT at either of the above-mentioned two air-fuel ratios (T<sub>S</sub> and T<sub>R</sub>). It is implied that the efficiency of catalytic conversion declined due to diminishing exothermic reaction. As a result, the change in temperature of the exhaust gas across the CCT was less significant under the fuel-rich condition. The temperature rise in the turbine outlet as caused by the exothermic reaction was only 15K when the turbine inlet temperature reached 700K under fuel-rich conditions. It is also demonstrated that the catalytic performance of the CCT can be reduced by a relative decrease of O<sub>2</sub> or an increase in the content of harmful exhaust components.

#### 4. INFLUENCE OF TURBINE OPERATING CONDITIONS ON CATALYTIC REACTIONS

In the study of TWC, it has been found out that the properties of harmful exhaust components, the activity of the catalyst, operating temperature, space velocity, turbulent length scale, and its spatial distribution can all affect the performance of the catalyst converter (Wei & Chen, 1999). Similarly, the performance of CCT inevitably varies between different conditions under which the turbine operates.

##### 4.1 Effect of Mass Flow on Catalytic Reactions

With the mass flow rate increasing, the concentration of exhaust gas rises, which thus leads to an increase in the amount of exhaust substances involved in the reaction. Nevertheless, the increase in mass flow rate can also shorten the duration of contact between various exhaust components and the catalyst. It is thus necessary to better understand the impact of exhaust gas flow on CCT by exploring the effect of space velocity on catalytic reactions.

Allowing for the characteristics of the engine regarding cold start, the rotational speed was set to 11,600rpm. Also, there were four relatively lower mass flow points selected: 0.008, 0.012kg/s, 0.029kg/s, and 0.055 kg/s. Thus, the turbine inlet temperature was 450K, 600K, and 700K, respectively. Under these conditions, a comparison was performed in the conversion efficiency of catalytic reactions at a time when the harmful exhaust gas passed through CCT, as shown in Fig.4. The changes in exhaust temperature are shown in Fig.5, respectively.

At the same flow rate, the conversion efficiency of harmful exhaust components was improved with the rise in inlet temperature, as shown in Fig. 4. However, there was a reduction in this efficiency with a rise in mass flow. Even when the inlet temperature reached as high as 700K, the effect of increasing mass flow remained significant. It is suggested that, in the presence of turbulent flow, the increase of mass flow would have a considerable impact on the catalytic reaction. When the mass flow rate increased with turbine inlet temperature, the extent of temperature rise diminished due to a decrease in the efficiency of catalytic conversion, as shown in Fig. 5.

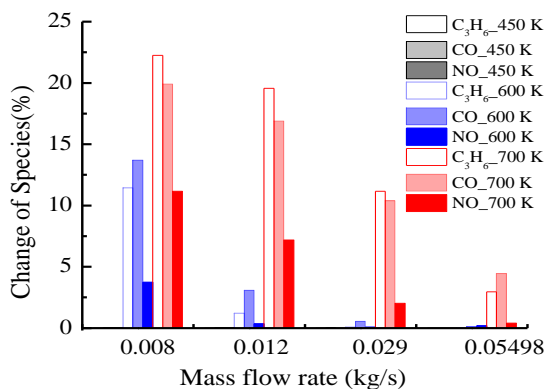


Fig. 4 Effect of mass flow on the conversion efficiency of CCT

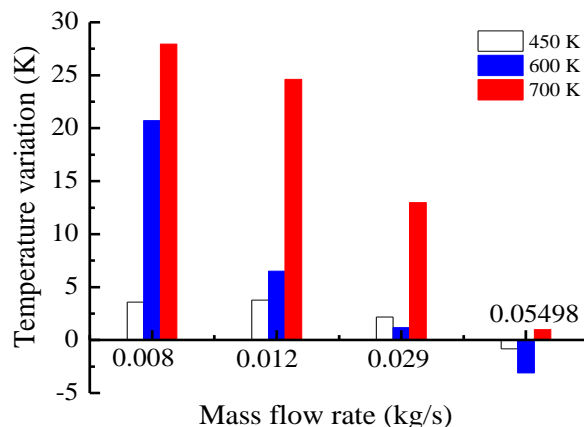


Fig. 5 Effect of mass flow on the exhaust temperature of CCT

When the inlet temperature reached 450K or 600K and the flow rate fell below 0.029kg/s, temperature rise remained observable due to the exothermic reaction, despite the low conversion efficiency of harmful exhaust components and the occurrence of turbine expansion. As shown in Fig. 5, an increase in flow rate suppressed temperature rise. Especially, when the inlet temperature reached 450K and 600K at a flow rate of 0.055kg/s, the temperature was lower in the outlet than in the inlet. There may be two reasons for this finding. On the one hand, a faster flow rate reduced the conversion efficiency of harmful exhaust components due to shortened residence time. Consequently, the release of thermal energy from the exothermic reaction was inhibited. On the other hand, at a constant rotational speed, the expansion ratio increased as the flow rate rose, which improved the outcome of heat transfer while mitigating thermal expansion loss across the turbine.

##### 4.2 Effect of Turbine Rotational Speed on Catalytic Reactions

In addition to 11,600rpm, 0rpm, 3000rpm, and 6000rpm were considered at the constant minimum flow rate of 0.008kg/s. At each speed, a simulation was performed respectively at the inlet temperature of 450K, 600K, and 700K, the results of which are presented in Figs. 6 and 7.

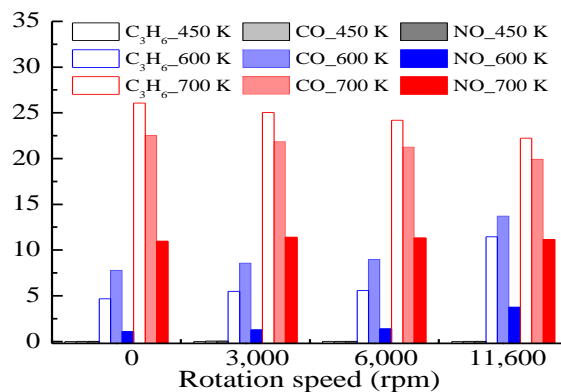
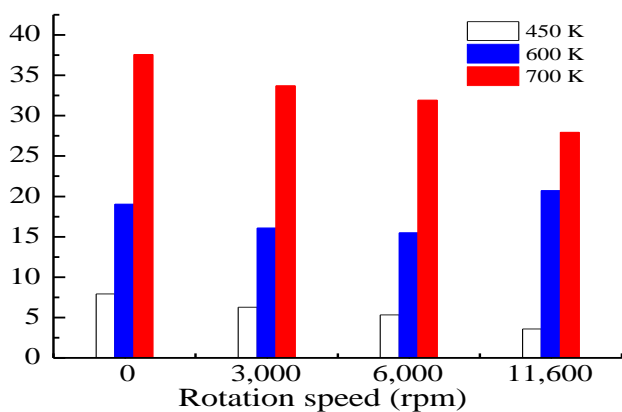


Fig. 6 Effect of turbine rotational speed on the catalytic reaction



**Fig. 7** Effect of turbine rotational speed on the exhaust temperature

When the inlet temperature reached 450K, the conversion efficiency was still very low (less than 0.05%) regardless of the rotational speed, with little difference observed. However, at an inlet temperature of 600K, to increase the rotational speed enhanced the conversion efficiency. Differently, given the inlet temperature of 700K, the conversion efficiency seemingly stabilized as the rotational speed varied. The extent of temperature rise from the inlet to the outlet declined as the rotational speed was raised. When the inlet temperature was 600K, the conversion efficiency of all harmful components was improved at a higher rotational speed. However, the extent of temperature rise showed no obvious pattern as the rotational speed changed.

Given the combined calculation results obtained at the above two turbine inlet temperatures (600 and 700K), a conclusion can be drawn that the conversion efficiency of the catalytic reactions is improved with the rotational speed when the inlet temperature is close to that under the light-off condition. The reason for this is suspected to be that the sufficient mixing of the reaction gas improves the uniformity of contact between the harmful exhaust components and the catalyst surface when the reaction occurs in the Control Zone of Chemical Kinetic. Meanwhile, the thermal energy released by the reaction with a low overall conversion at a low inlet temperature is not as significant as when the temperature drops due to turbine expansion.

As shown in Fig. 6, when the inlet temperature of the turbine reached 700K, the conversion efficiency of  $C_3H_6$  and CO was significantly reduced with an increase in the rotational speed. At this inlet temperature, the reaction occurred in the Control Zone of Mass Transport when the rate of reaction was determined by the rate of mass transport. Therefore, the rotor blades with a high rotational speed may reduce the mass transfer rate due to the shortened residence time. Consequently, the conversion efficiency of  $C_3H_6$  and CO diminished. However, the conversion efficiency of NO was barely affected by the rotational speed of the turbine, as shown in Fig. 6. A potential reason for this is that the reaction of NO still occurred in the Control Zone of Chemical Kinetics where the conversion efficiency was largely determined by the temperature (see Fig. 14 in a prior study (Wang et al.,

2021)). The red bars in Fig. 7 indicate that the difference of exhaust temperature decreased with the increase in rotational speed of the turbine. Nonetheless, the increase of exhaust temperature as caused by the release of reaction heat was far more significant than that caused by turbine expansion. It is indicated that the overall conversion efficiency at an inlet temperature of 700K was relatively higher than at other temperatures. In reality, the improved conversion efficiency would translate into the increase in exothermic energy inside the turbine or the reduction in operating speed of the turbine to drive the same boost out of the compressor.

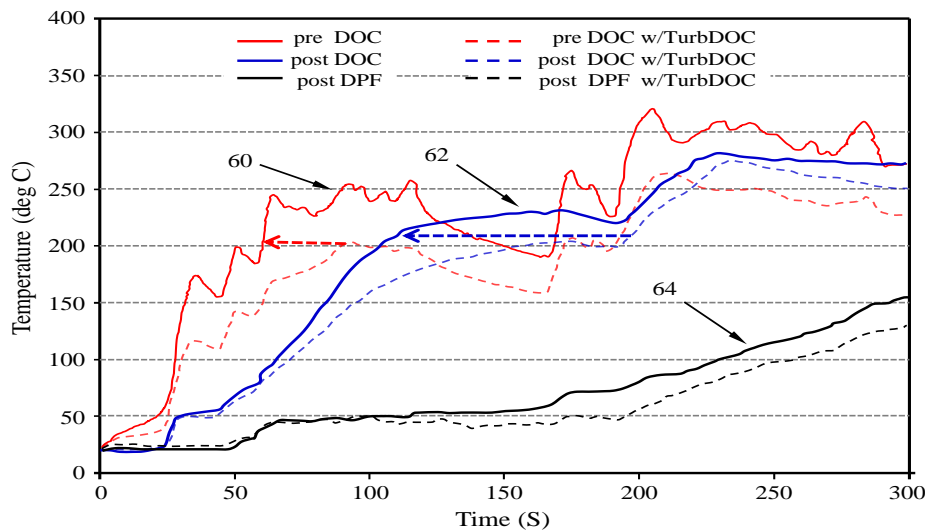
## 5. DISCUSSION ON THE CATALYTIC MECHANISM

### 5.1 Development of a Limitation on the Mechanism of Catalytic Reaction

So far, plenty of research has been conducted on the chemical reaction modeling of TWC. However, it remains difficult to obtain reaction kinetics equations accurately given the complex and transient working environment of catalyst coating. Therefore, various hypotheses and theories have been put forward regarding the mechanism of catalytic reaction.

In 1973, Voltz et al. proposed to quantify the reaction rate through the surface reaction concentration of a catalyst and the Langmuir-Hinshelwood mechanism, and to express the catalytic reaction rate as the intrinsic reaction rate, which had a profound impact on the following research. In the 1980s, Oh and Cavendish (1982) proposed a three-reaction mechanism, only considering the oxidation reactions of CO, HC, and  $H_2$ . This is considered the prototype of the modern reaction mechanism models. Subramaniam and Varma (1985) developed another 3-reaction mechanism, involving only CO, NO,  $O_2$ , and  $H_2O$ , and predicted some of the chemical reaction kinetics data, which laid a foundation for introducing chemical kinetics into emission control. In the 1990s, Montreuil et al. (1992) established an experimental database related to CO, NO,  $C_3H_8$ ,  $C_3H_6$ ,  $H_2$ , and  $O_2$ , with a model of 13 reaction mechanisms constructed. Pattas et al. (1994) devised a simple transient simulation program for the catalyst converter. Sugiura et al. (1995) proposed a 5-reaction model for 6 components (CO,  $CH_4$ ,  $C_3H_6$ , NO,  $H_2$ , and  $O_2$ ), and others. Since 2000, there have been numerous new reaction models and mechanisms developed regarding the change of hydrocarbon structure, the increase of oxygen storage and release reaction, water gas conversion and steam reforming reaction, and the addition of  $NH_3$  and  $N_2O$  to the reactants, etc. (Tsinoglou & Koltsakism 2002; Wu & Song 2005; Tsinoglou & Koltsakism 2009; Kwon et al., 2007)

In 2001, Chatterjee et al. (2002) established a detailed chemical reaction model of multi-elementary reactions based on a Pt/Rh catalyst converter, where  $C_3H_6$  represented the hydrocarbon of various structures and NO represented the nitrogen oxides. Proposed for surface active components, this heterogeneous catalytic reaction mechanism involves 8 gas components, 23 surface components, and a total of 61 elementary reactions requiring



**Fig. 8 Effect of a diesel CCT on the exhaust temperature (Wang et al. 2018)**

three process: adsorption, reaction, and desorption. The conversion efficiency and surface component coverage of TWC were simulated under steady state to obtain the results consistent with the experimental results. This reaction mechanism has already been adopted in many other studies.

Through the above discussion, a full understanding of catalytic reactions presently is still required, leaving various theories incomplete and catalytic reaction mechanisms unreliable. In future research, experiments will be conducted to verify the rationality and accuracy of the catalytic mechanism. In this way, the mechanism of catalytic reaction can also be dynamically calibrated according to the experimental results.

### 5.2 Effect of the Turbulence on the Catalytic Reaction Mechanism of CCT

Figure 8 shows the results obtained from an experiment conducted on the catalytic reaction of a diesel CCT during the warm-up stage (Wang et al., 2018), in which the catalyst was coated on the surface of the rotor. The red dash line of #60 in the figure shows the exhaust temperature before the Diesel Oxidation Catalyst (DOC) was coated on the rotor surface, while the red solid line of #60 indicates the exhaust temperature after it was coated. To some extent, the difference between the two curves reflects the intensity of the catalytic reaction. By comparing the two curves of #60, it can be found out that the catalyst started to react in 6~7s after the cold start, given a lower temperature of exhaust from the engine than 30°C (about 303K). When the temperature of exhaust from the engine was around 150°C (423K), the temperature rose by about 50°C due to the release of reaction heat, indicating the significant catalytic reaction. The above phenomenon evidences that the turbulence in the turbine significantly reduces the activation energy and light-off temperature of the catalyst.

Due to similarity in the structure of turbulence inside the turbine, the principles of oxidation, and the reduction reactions of the catalyst converter, it can be inferred that

the above phenomenon may occur to the CCT of a gasoline engine as well. In the present study, the reaction mechanism proposed in literature (Chatterjee et al., 2002) was applied. According to the simulation results of CCT in literature (Wang et al., 2021), the reaction mechanism still plays a critical role in the efficiency of catalytic conversion for the turbulent flows in a gasoline engine with a stoichiometric air-fuel ratio. Compared with a traditional TWC with laminar flows inside honeycomb channels, the activation temperature of the catalyst shows no significant reduction, and the light-off temperature remains between 250 and 340°C. Therefore, the mechanism of catalytic reaction in laminar flow does not apply directly to the catalytic reaction in turbulent flow between turbine blades. Instead, only the turbulence model, transport equation, and chemical reactor solver are applied to carry out numerical calculation. Meanwhile, the catalytic reaction mechanism obtained from the simulation results, in reference to prior experimental study (Wang, et al. 2018), determines the reaction rate thus the conversion efficiency of CCT. In summary, the conventional laminar flow based mechanism of catalytic reaction should be further adapted to a turbulent state in a turbine.

### 5.3 Effect of the Parameters of Reaction Mechanism on the Catalytic Reactions of CCT

In respect of chemical reaction kinetics, the chemical reaction rate constant is usually used to represent the reaction rate and it determines the conversion efficiency of a substance in the reaction. The chemical reaction rate constant can be expressed as the exponential form of the Arrhenius equation in Formula 8, which is the most widely used empirical correlation (Laidler, 1987; Connors 1990).

$$k = A \cdot \exp(-E_a / RT) \quad (8)$$

where  $k$  represents the reaction rate constant (frequency of collisions);  $A$  denotes the pre-exponential factor related to the collision frequency and the reaction rate of activated molecules that are converted into product;  $R$  represents the universal gas constant;  $T$  indicates the

thermodynamic temperature;  $E_a$  is referred to as the activation energy of the reaction that indicates the energy difference between different molecular energy levels. At a specified temperature, a lower activation energy means a larger number of activated molecules and a higher rate of the reaction.

The Arrhenius equation indicates the relationship between the chemical reaction rate constant and temperature, which is experimentally correlated within a certain range of temperature, under the assumption that the activation energy is independent of temperature. Within a wider range of temperature, Adams (Laidler, 1996) corrected the formula by introducing a temperature index  $m$  to further clarify the dependence of the pre-exponential factor on temperature. It is called the three-parameters equation, as shown in Formula 9.

$$k = A \cdot T^m \cdot \exp(-E_a / RT) \quad (9)$$

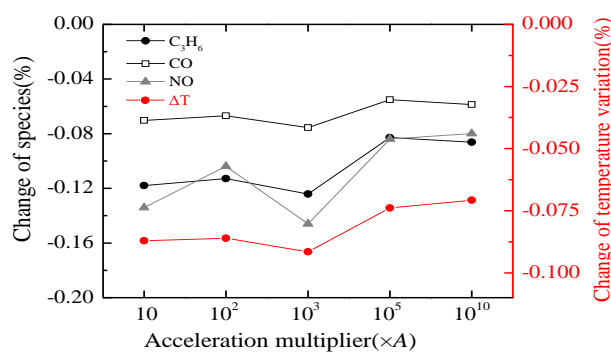
where  $m$  is a constant, which is independent of temperature, e.g.,  $m=0$  in the original Arrhenius equation. In general,  $m$  is an integer or a half-integer (no more than 4) when the vibration effect is ignored (Zhao et al. 1984).

To ensure that the mechanism of catalytic reaction is reliable, it is necessary to adjust the above-mentioned three parameters through experimentation for CCT. If necessary, the content of the reaction mechanism can also be changed as appropriate by removing or introducing some process like adsorption, surface reaction, and desorption. The mechanism of catalytic reaction as used in this paper involves the thermophysical parameters of each reaction gas component with assumed intermediate products. It also reveals three processes: adsorption, surface reaction, and desorption, including the detailed process of reaction and the value of each variable of the Arrhenius equation. To study the catalytic reactions, the reaction steps and substances are ignored in this paper to discuss only how to adjust the relevant parameters to this reaction mechanism in numerical simulation for obtaining the results that are better correlated with future experiments.

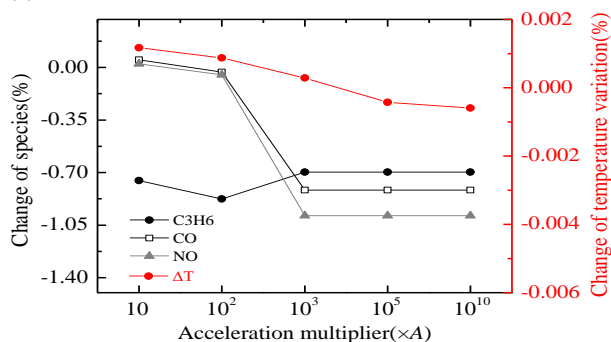
(1) Effect of the pre-exponential factor ( $A$ ) on the catalytic reactions of CCT

According to the Law of Guldberg and Waage, turbulence is supposed to promote the mixing of reactant gases to increase the concentration near the catalyst surface in a chemical reaction, which is equivalent to increasing the number of activated molecules per unit volume, thereby increasing the frequency of effective collisions between molecules and the reaction rate. It is effectively to increase the pre-exponential factor ( $A$ ) for the Arrhenius equation.

Therefore, the first study is to observe the effect of increasing the pre-exponential factor  $A$  on catalytic reaction at lower inlet temperatures. The value of  $A$  was increased by 10, 102, 103, 105 and 1010 times, respectively, to calculate the catalytic reaction. For each value of  $A$ , there were two conditions considered at the



(a) Inlet T= 600K



(b) Inlet T= 475K

**Fig. 9 Effect of the pre-exponential factor ( $A$ ) on catalytic reactions**

turbine inlet temperature of 600K and 475K, respectively, including the corresponding conversion efficiency of harmful exhaust components and the variation in temperature relative to the original value of  $A$  as shown in Fig. 9.

From Figs. 9(a) and (b), it can be found out that, despite the value of  $A$  increasing within a considerable range, the change in conversion rate of related harmful exhaust components was less than 0.15% and the change of temperature rise was less than 0.1% compared with the results of catalytic reaction. It is implied that the effect of increasing the chemical reaction rate by adjusting the  $A$  value was extremely limited in the presence of turbulence flow. Therefore, the amount of activation energy determines the rate of catalytic reaction.

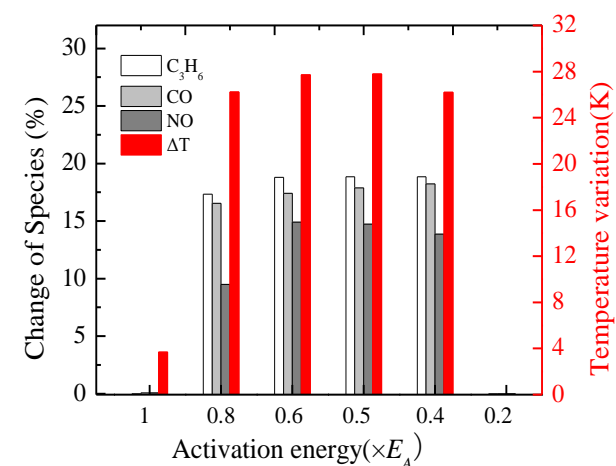
(2) Effect of the constant  $m$  being independent of temperature on the catalytic reactions of CCT

In Formula 3, the position of  $T^m$  is the same as the pre-exponential factor  $A$ , while the range of variation in  $m$  and the temperature in the inlet of the turbine is known. Therefore, it can be inferred that the change of the parameter  $m$  would have little effect on the chemical reaction constant.

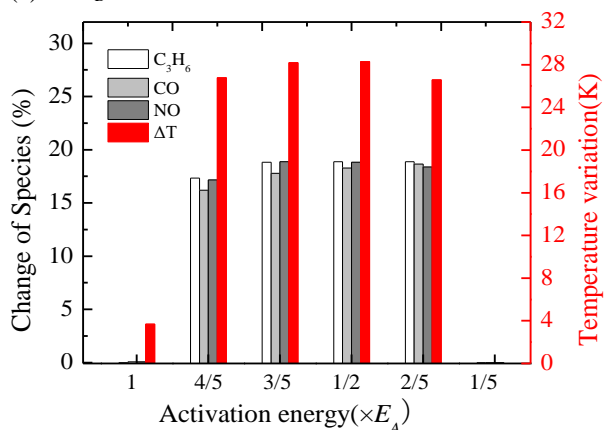
(3) Effect of the activation energy  $E_A$  on catalytic reactions of CCT

There is no measurement of the activation energy performed in the presence of turbulence and little discussion around the relationship between turbulence and activation energy in literature. Herein, turbulence characteristics, molecular motion, and activation energy are investigated.





(a) 0.8E<sub>B</sub> for NO



(b) 0.6E<sub>B</sub> for NO

**Fig. 10 Effect of the activation energy E<sub>A</sub> on catalytic reaction (1)**

Temperature is usually considered to be a measure of average kinetic energy for molecular thermal motion. The dissipation of kinetic energy occurs in the presence of turbulence, and a significant velocity gradient results from the random change of turbulence velocity in space. Due to turbulent viscous force, the kinetic energy of turbulence is converted into the kinetic energy of molecular motion through constant internal interaction, which increases the molecular energy, thus leading to an increase in the number of activated molecules. It can be found out that the turbulent state of the gas at a given temperature causes an increase in the number of activated molecules, which is equivalent to reducing the activation energy of the reaction. To verify the impact of activation energy on the catalytic effect, the numerical model of CCT was tested by reducing the activation energy of each reaction. In a previous study (Wang et al., 2021), the conversion rate of NO in the three-way catalytic reaction was relatively low. For this reason, the activation energy of the catalytic reaction involving NO was maintained at a relatively high level in this paper.

In the calculation of activation energy adjustment, the turbine inlet temperature was set to 475K, the rotational speed of the turbine was set to 11,600 rpm, and the mass flow rate was set to 0.008kg/s. The original activation energy of the reaction involving C<sub>3</sub>H<sub>6</sub> and CO was denoted as E<sub>A</sub>, and the initial activation energy of the reaction

involving NO was denoted as E<sub>B</sub>. Thus, 0.8 and 0.6 of the initial E<sub>B</sub> value were studied. Under each condition and given the reduction in E<sub>B</sub>, E<sub>A</sub> was adjusted to 0.8, 0.6, 0.5, 0.4, and 0.2 of its initial value, respectively. A different catalytic reaction mechanism was revealed and inputted into the FLUENT Software for re-simulation. Figure 10 shows the results of harmful exhaust components and temperature changes.

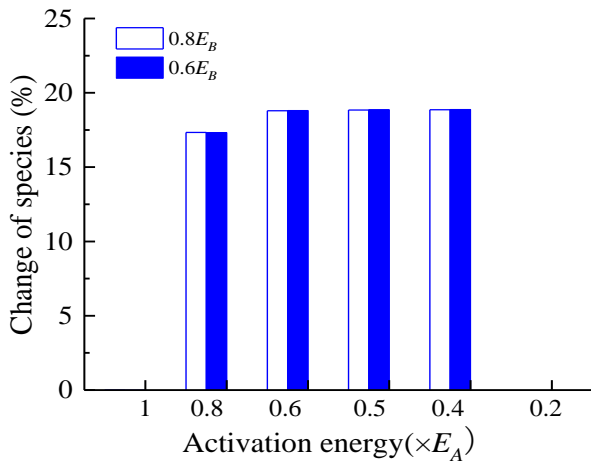
According to the simulation results, when E<sub>A</sub> was 0.2 of its initial value, no convergence occurred during the numerical simulation. Thus, no results were obtained at the position shown in Figs. 10 and 11. It is indicated that there is a lower limit on the adjustment of activation energy with the current simulation method. As shown in Fig. 10, given a turbine inlet temperature of 475K, the reaction of harmful exhaust components was clearly insignificant when the activation energy remained unchanged. By reducing activation energy, the conversion efficiency of the reaction and exhaust gas temperature were considerably improved, because the reduced activation energy reduced the light-off temperature of the catalyst effectively.

To better understand the impact of activation energy in each harmful component on itself and other gases, Fig. 11 is presented to show the data extracted from Fig. 10. As shown in Fig. 11, reducing the activation energy of one harmful gas while keeping others constant improved the conversion rate of this gas effectively. In addition, as can be seen from Figs. 11(a) and (b), with E<sub>A</sub> reduced to a certain level, such as 0.6 E<sub>A</sub>, the conversion rate of C<sub>3</sub>H<sub>6</sub> and CO stabilized as the activation energy further increased. This is because the reaction temperature had

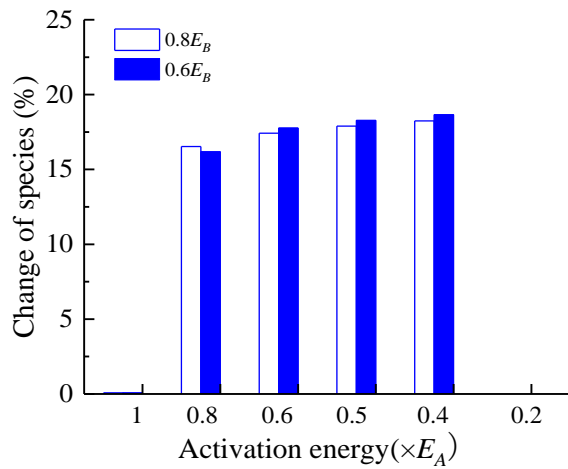
entered the control zone of mass transfer by reducing the activation energy. According to Fig. 11(c), the conversion rate of NO was significantly improved by the reduction of E<sub>B</sub> and constant E<sub>A</sub>, indicating that the reaction temperature for NO remained in the control zone of chemical kinetics where the reaction was relatively more sensitive to the change in activation energy.

In addition, it can be seen from Fig. 11 that reducing the activation energy of a harmful gas component not only improved its conversion rate effectively, but also affected the conversion rate of other harmful gas components. As shown in Fig. 11(a), C<sub>3</sub>H<sub>6</sub> did not react with NO. Therefore, the change in E<sub>B</sub> made no difference to the conversion rate of C<sub>3</sub>H<sub>6</sub>. According to Fig. 11(b), since CO reacted with O<sub>2</sub> and NO simultaneously and the rate of reaction between CO and O<sub>2</sub> as well as between CO and NO varied by E<sub>A</sub>, the conversion rate of CO did not necessarily increase when E<sub>B</sub> was reduced, such as when E<sub>A</sub> was 0.8 of its initial value. Similarly, it can be seen from Fig. 11(c) that the conversion rate of NO showed no linear increase as E<sub>A</sub> decreased. The conclusions drawn from Figs. 11(b) and (c) can also explain why the exhaust temperature showed non-linear changes with E<sub>A</sub> decreasing, as can be seen from Fig. 10.

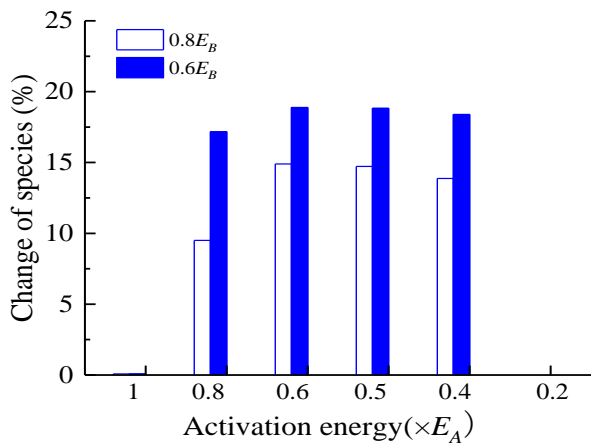
From the above discussion, it is known that the activation energy remains the key factor affecting the catalytic reaction rate in the presence of turbulence. At an appropriate lower temperature, the chemical reaction rate



(a) Effect of the activation energy EA on C<sub>3</sub>H<sub>6</sub> catalytic reaction



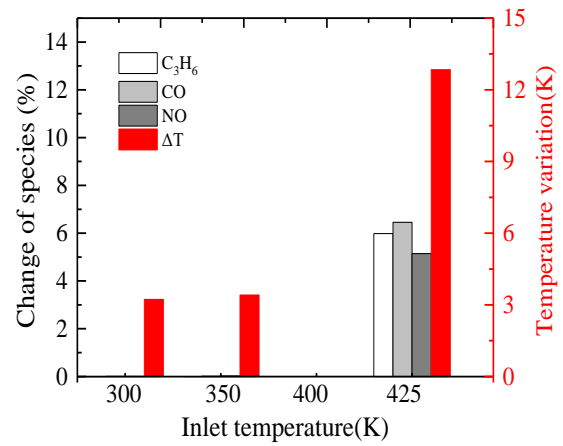
(b) Effect of the activation energy EA on CO catalytic reaction



(c) Effect of the activation energy EA on NO catalytic reaction

**Fig. 11 Effect of the activation energy EA on catalytic reaction (2)**

increases with the decrease of activation energy, and the conversion rate of harmful exhaust components is improved. In reality, the adjustment of activation energy is a more complex process. The activation energy in the catalytic mechanism may be affected differently by turbulence, and other relevant reactions may also be



**Fig. 12 Catalytic reaction at lower inlet temperature with the reduced activation energy (0.8EA and 0.8EB)**

affected after the adjustment, which needs to be confirmed by conducting further experiments.

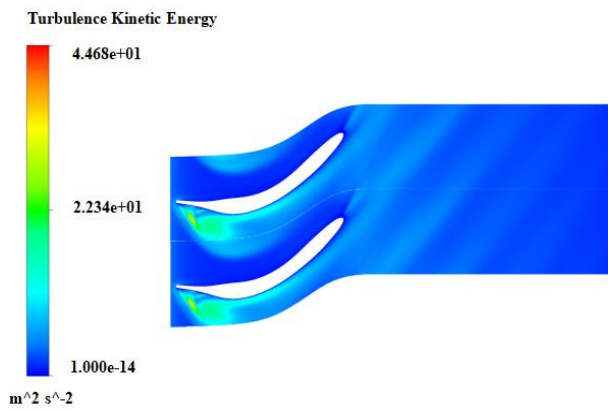
It is worth noting that the initial lower inlet temperature may become identical to the light-off temperature of the catalyst after a reduction in the activation energy in catalytic reactions, which may impede the calculation of catalytic reactions from convergence. Given a reduction in the EA and EB to 0.8 of the initial value, the conversion efficiency of the harmful exhaust components and the change in exhaust temperature at four lower turbine inlet temperatures were calculated for CCT, as shown in Fig. 12. Obviously, the change of exhaust temperature indicates that the catalytic reaction occurred at an inlet temperature of 300K and 350K, respectively, despite the extremely low conversion efficiency. When the inlet temperature was 425K, there was a sharp rise in conversion efficiency and temperature change for the catalytic reactions, which indicated that the inlet temperature approached the light-off point of the catalyst. Additionally, it was found out that the catalytic reaction did not converge at the inlet temperature of 400K as calculated, which might be attributed to the residual fluctuation caused by the catalyst when it was just involved in the intense reaction after activation (Wang et al. 2021).

#### 5.4 The Relationship Between Turbulence and Catalytic Reaction

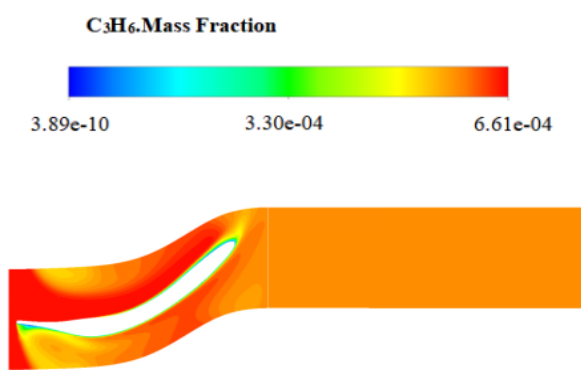
Allowing for the potential impact of turbulent flow on activation energy in catalytic reaction kinetics as discussed in Section 5.3, catalytic reactions are more likely to occur in the region with high turbulent kinetic energy. To verify this inference, the changes of C<sub>3</sub>H<sub>6</sub> in the turbine rotor flow field were investigated when the CCT inlet temperature was 700K, given a constant speed of 11,600 rpm and a single-channel gas flow rate of 0.008kg/s.

The turbulent kinetic energy can be estimated by using the turbulence intensity, and it is expressed as follows:

$$k = \frac{3}{2}(UI)^2 \quad (10)$$



**Fig. 13** Distribution of turbulent kinetic energy in the flow field of a typical turbine rotor



**Fig. 14**  $C_3H_6$  material distribution in CCT turbine rotor flow field

where  $U$  represents the average velocity of the gas, and  $I$  refers to the intensity of turbulence.

Figure 13 shows the distribution of turbulent kinetic energy at 50% of the blade height in a complete single channel of a typical turbine rotor under certain working conditions. It features a region of high turbulent kinetic energy at the leading edge of the blade suction face that results from the complex state of flow such as gas expansion and acceleration in the turbine.

Figure 14 shows the distribution of  $C_3H_6$  around the blade at 50% of the blade height of the CCT rotor. Through a comparison with Fig. 1, it can be found out that the pattern of  $C_3H_6$  distribution is closely associated with the distribution of turbulent kinetic energy in the rotor, with low material content in the areas of high turbulent kinetic energy. It is implied that the turbulent flow in the turbine promotes catalytic reaction, and the conversion rate of the catalytic reaction may be improved with a rise in the intensity of turbulent flow.

## 6. CONCLUSION

There is innovation in the use of CCT to mitigate the exhaust pollution by an automobile engine during the warm-up period. In this study, a numerical method is adopted to explore the impact of engine air-fuel ratios and

turbine operating conditions on the catalytic reactions of CCT. Similar to the existing experimental results obtained for the catalytic turbine of a diesel engine in the cold-start stage, the potential effects of turbulence on the mechanism of catalytic reaction are revealed and analyzed.

The major conclusions of this study are presented as follows:

(1) The air-fuel ratio of the engine plays a crucial role in CCT performance. Under the fuel-rich condition, a slight decrease in the  $O_2$  concentration or an increase in the concentration of exhaust components significantly reduces the conversion efficiency of each exhaust component.

(2) In a turbulent state of CCT, the increase of mass flow rate is accompanied by the less residence time allowed for reactive gases to be in contact with the catalytic surface on the turbine blades. The residence time has a greater effect on the conversion rate of exhaust components. Specifically, at a constant rotational speed of the turbine during the warm-up period, the conversion rate of exhaust components declines with an increase in mass flow. This effect remains significant when the inlet temperature of the turbine rises.

(3) During the warm-up period at a constant flow rate, the conversion efficiency of the catalytic reaction is improved with the rotational speed at a relatively low inlet temperature. The reason for this may be that such low temperatures are in the control zone of chemical kinetics and the increase of rotational speed enhances the mixing of the reactants, thus promoting the surface catalytic reaction. When the inlet temperature reaches the control zone of mass transfer, the conversion efficiency decreases with an increase in rotational speed. The high-speed flow leads to a short residence time.

(4) Due to the turbulent state of the gas at a specified temperature, there is an increase in the number of activated molecules near the catalyst surface, promoting a kinetic chemical reaction, which is equivalent to reducing the activation energy of the reaction. The activation energy under turbulent flow is found to be the determinant of reaction rate for CCT. The appropriate reduction of activation energy can help significantly improve the conversion efficiency and increase the exhaust temperature, which is consistent with prior experimental study (Wang, et al., 2018). Nevertheless, the numerical simulation of catalytic reaction would be hindered from convergence at low temperatures when the existing simulation method is applied.

(5) Turbulence can promote catalytic reactions. The greater the intensity of turbulence in a turbine, the higher the conversion rate of catalytic reaction occurring in the corresponding region.

Although there is no experiment data to correlate with current numerical study on CCT for gasoline application at the moment, the Arrhenius equation was carefully tuned to demonstrate the effectiveness of activation energy reduction, or the molecular motion enhancement, in the presence of turbulence flow, with reference to prior experiment of a CCT for a diesel application.

It is concluded that such a catalyst-coated turbine blade could accelerate the light-off of a downstream catalyst with exothermic energy from the surface chemistry, which is basically coherent with prior study.

Like many hypothetical studies, a further experiment correlation should be conducted as the next step before a more credible model of catalytic surface chemistry in the presence of turbulent flow can be widely accepted and applied.

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## CONFLICT OF INTEREST

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## AUTHOR CONTRIBUTION:

All authors contributed to the study conception and design. The numerical analyses were conducted by both **L. L. Wang** and **Z. P. Li**; The paper was written by **L. L. Wang**; The project was initiated and the paper edited by **H. Sun**; The numerical analyses and paper drafting was assisted by **Z. Tan**; The whole project was guided and organized by **A. Engeda**; All authors commented on previous versions of the manuscript. All authors read and approved the final manuscript

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