Numerical Study of NOx Generation in a Trapped Vortex Combustor Fuelled by Kerosene Blended with Ethanol

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Abstract. The study of alternative fuels is of great importance, and the study of ethanol blended with kerosene is necessary. The trapped vortex combustor is a new type of combustor and NOx emissions are important in the study of trapped vortex combustors. In this article, the NOx generation rate of trapped vortex combustor was studied using kerosene blended with ethanol in different mass fractions as fuel. The results show that the thermal NOx is the main source of NOx in the combustor, which is mainly generated at the back of the combustor, and the thermal NOx generation rate decreases with the increase of ethanol mass fraction. The prompt NOx generation rate decreases with the increase of ethanol mass fraction. NOx is also easily produced near the sidewall of the combustor.

1. Introduction
At present, many new structural schemes have been proposed for the combustion chamber of aero-engines, and the trapped vortex combustor is one of the new types of combustion chambers [1]. Trapped vortex combustion method is a staged combustion method, which refers to adding a cavity structure on the side of the main flow area, and separate air and fuel supply in the cavity area. The combustion in the cavity is not affected by changes in the working environment of the main flow, which lead to a stable combustion.

Many studies have been carried out on the trapped vortex combustor, the numerical simulation study of a low-emissions trapped vortex combustor shows that the equivalence ratio of the main flow, the position and the flow injection angle in the cavity has significant impact on the emissions [2]. The lean blow-out [3], the dome structure effects [4] and the vortex stability [5] of a trapped vortex combustor have also been studied.

Ethanol, as a clean renewable fuel, is considered as one of the promising alternative fuels to kerosene. [6] [7] Previously, researchers have studied the combustion and emission performance of ethanol as an alternative fuel, Zhang [8] and Schifter [9] did research on ethanol diesel and ethanol gasoline, and received some results that can be applied to engineering practice.

At present, there are many researches on the combustion of alternative fuels in the combustion chamber of aero-engines. Patra [10] studied the emission performance of kerosene fuel blended with ethanol on the combustion chamber. Song [11] studied the influence of injection pressure on the atomization and combustion characteristics of kerosene-ethanol mixed fuel.

For the research of alternative fuels, it is an indispensable research in the field of gas turbine combustion. In this paper, the combustion effect of ethanol-blended aviation kerosene in the trapped vortex combustor is numerically simulated, which will help clean fuels application in aero engines in the future.

2. Mathematical methods and combustor structure
2.1. Mathematical method
The combustion in the trapped vortex combustor can be considered stable, turbulent and compressible. Therefore, the general form of the governing equations for continuity, momentum, energy, and composition is

$$\frac{\partial (\rho \varphi)}{\partial t} + \frac{\partial (\rho \varphi u)}{\partial x} + \frac{\partial (\rho \varphi v)}{\partial y} + \frac{\partial (\rho \varphi w)}{\partial z} = \frac{\partial}{\partial x} \left( \Gamma_\varphi \frac{\partial \varphi}{\partial x} \right) + \frac{\partial}{\partial y} \left( \Gamma_\varphi \frac{\partial \varphi}{\partial y} \right) + \frac{\partial}{\partial z} \left( \Gamma_\varphi \frac{\partial \varphi}{\partial z} \right) + S_\varphi \tag{1}$$

In the control equations, the meaning of $\varphi$, $\Gamma_\varphi$, $S_\varphi$ are shown in Table 1.

| Equation Type                  | $\varphi$ | $\Gamma_\varphi$ | $S_\varphi$ |
|--------------------------------|-----------|------------------|-------------|
| Continuity equation            | 1         | 0                | $S_m$       |
| momentum equation in x-direction | u         | $\mu_e$          | $S_x$       |
| momentum equation in y-direction | v         | $\mu_e$          | $S_y$       |
| momentum equation in z-direction | w         | $\mu_e$          | $S_z$       |
| Energy equation                | h         | $\mu_e/\sigma_h$ | $S_h$       |
| Component equation             | Y         | $\mu_e/\sigma_Y$ | $S_Y$       |

Among the equations, $S_\varphi$ represents the source term, $\sigma_h$ and $\sigma_Y$ are model constants, $\mu_e$ is the effective viscosity, $Y$ is the element concentration, and $h$ is the convective heat transfer coefficient.

The combustion in the trapped vortex combustor is a typical turbulent activity with relatively high Reynolds number. In this paper, the $k$-$\varepsilon$ two-equation turbulence model is selected, and the wall enhancement function is used

$$\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_j} (\rho ku_j) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon - Y_M + S_k \tag{2}$$

$$\frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_j} (\rho \varepsilon u_j) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + \rho C_1 S \varepsilon - \rho C_2 \varepsilon \frac{\varepsilon^2}{k + \sqrt{\varepsilon^2}} + C_1 \varepsilon \frac{\varepsilon}{k} C_3 \varepsilon G_b + S_\varepsilon \tag{3}$$

Where $G_b$ is turbulence kinetic energy caused by the buoyancy force, $G_k$ is the turbulence kinetic energy caused by the mean velocity gradient, $k$ is the turbulent kinetic energy, $Y_M$ is the fluctuation effect of the total dissipation rating in compressible turbulence flow, $\varepsilon$ is the turbulent energy dissipation rate, $C$ is the model constant, and $\sigma$ is the surface tension.

In the trapped vortex combustor, the combustion method is mainly diffusion combustion, so this paper uses the probability density function PDF (probability density function) model for combustion calculation. The PDF model can simplify the detailed mechanism calculation while maintaining the calculation accuracy.

Fuel spray is described using a discrete phase model. In this paper, the most commonly applied Rosin-Rammler distribution is used to describe the particle size of the fuel droplets by the formula

$$Y_d = 1 - e^{-\left(\frac{d}{d_o}\right)^n} \tag{4}$$

Where $d$ is the droplet diameter and $n$ is the size distribution parameter.

2.2. Combustor structure
The main structure and specific parameters of the trapped vortex combustor used in this article are shown in Figure 1. Air inlets are arranged on the front and rear wall surfaces of the cavity, and a flame
stabilizer is installed at the centre of the inlet end of the combustor. In this paper, the same model that the research group has previously verified [12] is used for numerical simulation.

![Structure of combustor model](image1)

![Mesh of combustor model](image2)

**Figure 1.** Schematic diagram of the combustor model [12].

3. Results and discussion

NOx is produced in three ways, thermal NOx, prompt NOx and fuel NOx. The simulations in this paper assume that the kerosene molecule is C\textsubscript{12}H\textsubscript{23}, which contains no N atoms, and that ethanol molecules do not contain N atoms either. The analysis of fuel-based NOx is therefore removed. The thermal NOx as well as prompt NOx are studied in this paper. The Z0 plane is the centre section of the nozzle as well as the centre section of the combustion chamber. The Z1 and Z2 plane are 40 mm and 80 mm in front of the Z0 plane, respectively, and the Z0 plane is used in the analysis in this paper unless otherwise specified.

3.1. Thermal NOx analysis

In this paper, ethanol fuel is blended according to mass fraction. The mass fractions of ethanol are 20\%, 60\% and 100\%, respectively. The air velocity of mainstream and cavity is 40m/s and 50m/s. The air and fuel temperature are 700K and 341K, respectively, and the fuel mass flow is 0.002kg/s.

The generation of thermal NOx is mainly generated by reactions of N and O atoms in the high temperature zone of the flame and in the air behind the flame. Typically, the generation rate of the thermal NOx is exponentially related to the flame temperature, and the generation rate is generally larger when temperature is higher than 1850K. In addition, an increase in residence time increases the generation of thermodynamic NOx. In this paper, the generate rate of NOx with three different mass fractions of ethanol is analysed.
As can be seen in Figure 2, the main area of thermal NOx generation is in the area behind the combustor and increases with the distance from the combustion zone, whereas thermal NOx is rarely generated in the cavity. Thermal NOx is hardly produced in the middle of the model combustor and is re-generated close to the walls, as the vicinity of the walls is also flame prone and therefore NOx is produced.

![Figure 2. Thermal NOx generation rates (20% ethanol) for different sections (a)Z0 (b)Z1 (c)Z2.](image)

As can be seen in Figure 3, as the mass fraction of ethanol increases, there is a decreasing trend in the generation of thermal NOx. This is due to the fact that the same mass of ethanol can release less heat than kerosene, resulting in a lower temperature rise inside the combustor, and the production of thermal NOx is closely related to the temperature rise.

![Figure 3. Thermal NOx generation rates for different ethanol mass fractions (a)20% (b)60% (c)100%.](image)

**3.2. Prompt NOx analysis**

NOx could be found pretty early in the flame region [13], the structure of which is the oxidation of HCN molecules and N atoms in fuel or intermediate products, although the production of prompt NOx
is small relative to the generation of thermal NOx, it has a greater impact on the production of NOx for lean premix combustion. The research of the prompt NOx cannot be ignored.

It can be seen from Figure 4 that the generation area of prompt NOx includes the cavity and the mainstream area. With the reaction going on, the generation rate of prompt NOx decreases. This is consistent with the region where prompt NOx is often produced. Also, the prompt NOx generation region of the trapped vortex combustor continues to the mainstream region. In addition, Prompt NOx also appears near the wall. It can be seen from Figure 5 that the prompt NOx produces more under the condition of small ethanol mass fraction.

![Figure 4. Prompt NOx generation rates (20% ethanol) for different sections (a)Z0 (b)Z1 (c)Z2.](image)

![Figure 5. Prompt NOx generation rates for different ethanol mass fractions (a)20% (b)60% (c)100%.](image)

4. Conclusions
In this paper, the NOx generation of kerosene mixed with different mass fractions of ethanol is analysed in the vortex combustor, and the following conclusions are obtained
(1) Thermal NOx is mainly generated in the back of the combustor, and the generation rate is reduced by increasing the proportion of ethanol.
(2) The generation rate of prompt NOx decreases with the increase of ethanol mass fraction.
(3) The generation of thermal NOx is the main factor affecting the generation of NOx in the trapped vortex combustor.
(4) NOx is also generated near the wall of the model combustor.

5. References
[1] D Zhao, E Gutmark, P de Goey. 2018. A review of cavity-based trapped vortex, ultra-compact, high-g, inter-turbine combustors, *Prog. Energ. Combust.* 66 42-82.
[2] YB Deng, FM Su. 2016. Low emissions trapped vortex combustor, *Aircr. Aerosp. Tec.* 88 33-41.
[3] F Xing, P Wang, et al. 2012. Experiment and simulation study on lean blow-out of trapped vortex combustor with various aspect ratios. *Aerosp. Sci. Technol.* 18 48-55.
[4] M Li, X He, et al. 2017. Dome structure effects on combustion performance of a trapped vortex combustor. *Appl. Energ.* 208 72-82.
[5] S Vengadesan, C. Sony. 2010. Enhanced vortex stability in trapped vortex combustor. *Aeronaut. J.* 114 333-337.
[6] I S Blakey, L Rye, C W Wilson. 2011. Aviation gas turbine alternative fuels: A review. *P. Combus. Inst.* 33(2):2863-2885.
[7] J I Hileman, R W. Stratton 2014. Alternative jet fuel feasibility. *Transp. Policy*, 34 52-62.
[8] R Zhang, H He, C Zhang. 2003. Preparation of ethanol-diesel fuel blends and exhausts emission characteristics in diesel engine. *Chinese J. Environ. Sci.*, 24 (4) 1-6.
[9] I Schifter, L Diaz, R Rodriguez. 2011. Combustion and emissions behavior for ethanol-gasoline blends in a single cylinder engine. *Fuel*, 90(12) 3586-3592.
[10] J Patra, P Ghose, A Datta. 2015. Studies of combustion characteristics of kerosene ethanol blends in an axisymmetric combustor. *Fuel*. 144 205-213.
[11] L Song, T Liu, W Fu. 2016. Experimental study on spray characteristics of ethanol-aviation kerosene blended fuel with a high-pressure common rail injection system. *J. Energy Inst.*, 91(2) 203-213.
[12] R Zhang, Q Xu, W Fan. 2018. Effect of swirl field on the fuel concentration distribution and combustion characteristics in gas turbine combustor with cavity. *Energy* 162 83-98.
[13] Arthur H Lefebvre and Dilip R. Ballal 2010 *Gas Turbine Combustion*. P378

Acknowledgments
The authors would like to acknowledge for the financial support from National Science and Technology Major Project (2017- II-0008-0034).