Numerical simulation of NO emission characteristics of a high-speed and high-temperature heat-airflow test system

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Abstract. In this paper, the distributed parameter calculation model of the combustor of the high-speed and high-temperature heat-airflow test system is presented. The three-dimensional geometric model of combustor is established by using commercial software ANSYS 15.0, and the grids are divided. In order to understand the NO emission characteristics of the combustor of the high-speed and high-temperature heat-airflow test system, the combustion of fuel in the combustor is simulated by using the computational fluid dynamics simulation module of ANSYS 15.0. The simulation results show that the combustor produces the most thermodynamic NO near the theoretical oil-gas ratio, but less thermodynamic NO when the air is insufficient or excessive. Therefore, in order to effectively control the production of thermodynamic NO, it should be considered from lean or rich oil combustion.

1. Introduction
High-speed and high-temperature heat-airflow simulation refers to the combustion of aviation kerosene and high-speed air flow to produce high-speed and high-temperature gas flow field in a hot wind tunnel, so as to simulate the heating condition of the specimen in actual work. Its most typical application is to measure the thermal strength of aeroengine’s blades and to dynamically calibrate high temperature thermocouples [1]. The high-speed and high-temperature heat-airflow test system is a ground simulation system which is established to satisfy the thermal test in the case of high-speed and high-temperature air flow. NO emission is an important technical index for evaluating the performance of combustor of high-speed and high-temperature heat-airflow test system. Predicting concentration distribution of NO and obtaining NO emission characteristics is one of the main purposes of numerical simulation of combustion in combustor [2]. Therefore, the study of NO emission characteristics of combustor of the high-speed and high-temperature heat-airflow test system is not only important to improve the performance of the system, but also important to energy saving and emission reduction.

In view of the emission characteristics and distribution of NO in the combustor, a lot of research work has been done by relevant scholars. Park described various technologies to reduce NOx emission from DME-fueled engines, such as the multiple injection strategy and premixed combustion [3]. The co-combustion characteristics and the NO emission characteristics of pulverized coal/biomass blends at constant temperature were studied by Wang [4]. Ma applied a new combustion system to a 600 MW WeFoster Wheeler (FW) down-fired boiler to reduce NOx emissions without increasing the carbon content of fly ash [5]. The effect of fuel-air equivalence ratio, ignition advance angle, engine speed and exhaust gas recirculation on NOx emission were studied by Sun [6]. In order to reduce NOx emissions, Ren introduced an overheated air (OFA) system on a 300 MW boiler [7].
2. Geometric model and mesh generation of combustor

The combustor of the high-speed and high-temperature heat-airflow test system is a cylindrical burner with a diameter of 0.2m and a length of 0.5m. Although the structure of the cylindrical burner is not very complicated, the three-dimensional model of the combustor can reflect the actual combustion situation more clearly. Therefore, this paper directly establishes the three-dimensional geometric model of the system combustor in ANSYS 15.0, as shown in Figure 1.

![Figure 1. The geometry model of combustor.](image)

The nozzle for injecting kerosene in the combustor is located on the central line of the combustor and the diameter of the nozzle is 5 mm. Air enters the combustor from both sides of the nozzle and is fully mixed with the kerosene injected. The two-dimensional model of the combustor is shown in Figure 2.

![Figure 2. Two dimensional model structure of combustor.](image)

For the mesh generation of three-dimensional geometric model, the usual mesh elements are tetrahedron, hexahedron, triangle and so on. In addition, many scholars have conducted in-depth research on polyhedral meshes in numerical simulation, and obtained many important results[8-11]. In this study, on the one hand, the flow in the combustor varies greatly, on the other hand, in order to improve the automation of mesh generation and the fitness of the mesh, so unstructured tetrahedron mesh is used to mesh the combustor. Mesh module in ANSYS 15.0 is used to mesh the geometric model, and the results are imported into Fluent as shown in Figure 3. The number of meshes in the whole calculation area is 17131. After checking, the mesh quality meets the requirements and can be used for the following numerical simulation of combustor.

![Figure 3. The meshing of combustor.](image)
3. Computational models and boundary conditions

3.1. Computational models

3.1.1. Combustion flow control equation. In order to simulate the combustion of kerosene in the combustor under different conditions, a one-step lump reaction model is used to simulate the combustion of kerosene, and the mixture gas is regarded as ideal gas. At the same time, the shape of kerosene liquid is considered as ideal sphere, and there is no friction and collision between the kerosene droplets. The flow control equations include gas phase control equation and liquid phase control equation.

The gas phase control equations include mass conservation equation, momentum conservation equation and energy conservation equation, which can be obtained from reference [12].

$$\frac{\partial \rho}{\partial t} + \text{div}(\rho \mathbf{u}) = 0$$  (1)

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \text{div}(\rho \mathbf{u}) = \text{div}(\mu \text{grad} \mathbf{u}) - \frac{1}{\rho} \frac{\partial p}{\partial x} + S_u$$  (2)

$$\frac{\partial (\rho v)}{\partial t} + \text{div}(\rho \mathbf{u}) = \text{div}(\mu \text{grad} v) - \frac{1}{\rho} \frac{\partial p}{\partial y} + S_v$$  (3)

$$\frac{\partial (\rho w)}{\partial t} + \text{div}(\rho \mathbf{u}) = \text{div}(\mu \text{grad} w) - \frac{1}{\rho} \frac{\partial p}{\partial z} + S_w$$  (4)

$$\frac{\partial (\rho T)}{\partial t} + \text{div}(\rho \mathbf{u} T) = \text{div} \left( \frac{\lambda}{c_p} \text{grad} T \right) + \frac{S_T}{c_p}$$  (5)

where \( t \) is time; \( \rho \) is fluid density; \( p \) is fluid pressure; \( \mathbf{u} \) is velocity vector; \( u, v, w \) is the component of velocity vector \( \mathbf{u} \) in \( x, y, z \) directions; \( S_u, S_v, S_w \) is the generalized source term of momentum conservation equation; \( T \) is the temperature of fluid; \( c_p \) is the specific heat capacity of fluid; \( \lambda / c_p \) is the heat transfer coefficient of fluid, \( S_t \) is the viscous dissipation term.

Liquid phase control equations include particle orbit model, spray model, droplet evaporation model and two-phase coupling model, which can be obtained from reference [13].

$$\frac{d\mathbf{x}}{dt} = \mathbf{V}_p$$  (6)

$$\mathbf{V}_p = \frac{m_p}{\rho_p A}$$  (7)

$$m_p c_p \cdot dT_p / dt = h A_p (T_{\text{ad}} - T_p) + dm_p / dt \cdot h_g$$  (8)

$$S_{d,m} = m_{p,0} \cdot \Delta m_p / m_{p,0}$$  (9)

$$S_{d,v} = ((u_p - \bar{u}) \cdot (18 \mu C_D \text{Re}) / (24 \rho_p D^2) + \bar{F}_{\text{other}}) m_p \Delta t$$  (10)

$$S_{d,h} = (c_p \Delta T_p \cdot m_p / m_{p,0} + (-h_g + h_{\text{prot}} + \int_{r_0}^{r_f} c_p(T) \cdot \Delta m_p / m_{p,0} \cdot m_{p,0}) \Delta t$$  (11)

where \( \mathbf{V}_p \) is the particle velocity, \( A \) is the cross-section area of the nozzle exit, \( \rho_p \) is the liquid density, \( m_p \) is the liquid flow-rate, \( A_p \) is the surface area of the droplet, \( T_{\text{ad}} \) is the local gas temperature, \( h \) is the convective heat transfer coefficient, \( dm_p / dt \) is the rate of evaporation, \( h_g \) is the latent heat of the droplet evaporation, \( m_{p,0} \) is the initial mass of the droplet, \( \Delta m_p \) is the change of the droplet mass, \( u_p \) is the velocity of droplets, \( \bar{u} \) is fluid velocity, \( \mu \) is fluid viscosity, \( C_D \) is drag coefficient, \( \text{Re} \) is
Reynolds number, $d_p$ is the diameter of droplet, $\overline{F}_{inter}$ is the interaction force between other phases, $\Delta t$ is time step, $\overline{m}_p$ is the average mass of droplets, $h_{pyro}$ is the heat required for pyrolysis when volatilization occurs, $T_p$ is temperature of droplet, $T_{ref}$ is the reference temperature corresponding to enthalpy, $c_{p,v}$ is the specific heat of volatile precipitation; $\dot{m}_{p,0}$ is the initial mass flow-rate of tracked particles.

### 3.1.2. Turbulence model
Since the RNG $k-\varepsilon$ model is more accurate than the standard $k-\varepsilon$ model, the RNG $k-\varepsilon$ model is selected to simulate the turbulent flow in the combustor of the high-speed and high-temperature heat-airflow test system. Its control equations can be obtained from reference [14].

\[
\frac{\partial (\rho k)}{\partial t} + \nabla \cdot (\rho k \mathbf{u}) = \nabla \cdot \left( \alpha_k \mu_{eff} \nabla k \right) + G_k - \rho \varepsilon \tag{12}
\]

\[
\frac{\partial (\rho \varepsilon)}{\partial t} + \nabla \cdot (\rho \varepsilon \mathbf{u}) = \nabla \cdot \left( \alpha_\varepsilon \mu_{eff} \nabla \varepsilon \right) + \frac{C_{\varepsilon \varepsilon}^\prime}{k} G_k - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} \tag{13}
\]

where $G_k$ is the production term of turbulent kinetic energy $k$, $\mu_{eff} = \mu + \mu_t$, $\mu_t$ is turbulent viscosity, $\alpha_k = 1.39$, $C_{\varepsilon \varepsilon}^\prime = 1.68$.

### 3.1.3. Combustion model
Because the combustion process in the combustor of the high-speed and high-temperature heat-airflow test system is carried out under atmospheric pressure and the Mach number is not high, so the simplified PDF-rapid reaction model of non-premixed turbulent combustion is selected as the combustion model for simulation from reference [15].

### 3.1.4. Radiation model
In this paper, P1 radiation model is used to consider the influence of the thermal radiation effect on the wall temperature and gas temperature of the combustor of the high-speed and high-temperature heat-airflow test system. Its control equation as follows.

\[
a = \frac{1}{3(a + \sigma_s) - C\sigma_s} \nabla G \tag{14}
\]

$a$ is the absorption coefficient, $\sigma_s$ is the scattering coefficient, $G$ is the incident radiation, and $C$ is the linear attenuation coefficient.

### 3.1.5. Fuel injector
The injection angle, diameter, injection speed, static temperature and mass of fuel droplets are given.

### 3.2. Boundary conditions
High-speed and high-temperature heat-airflow is produced by combustion of aviation kerosene and high-speed airflow. In order to study NO emission characteristics in combustor by numerical simulation, it is necessary to understand the reaction mechanism. Using C$_8$H$_{18}$ to represent aviation kerosene, the equation of reaction can be expressed as

\[
2\text{C}_8\text{H}_{18} + 25\text{O}_2 \Leftrightarrow 16\text{CO}_2 + 18\text{H}_2\text{O} \tag{15}
\]

The boundary conditions considered in this paper include the inlet of kerosene and air, the outlet of combustor and the wall conditions.

### 3.2.1. Inlet boundary conditions
In order to study the effect of different oil-gas ratio on NO concentration in the combustor, the inlet condition is set as mass flow-rate inlet. At the same time, the working pressure in the combustor is set to be atmospheric pressure 101325Pa, the inlet gas composition is 79% N$_2$ and 21% O$_2$, and the liquid fuel is C$_8$H$_{18}$(ISO). Because the evaporation temperature of aviation kerosene(C$_8$H$_{18}$) is 292 K, so the inlet temperature of the liquid fuel is set to
292 K, and the air inlet temperature is set to 500 K. In the calculation process, the droplets of aviation kerosene are regarded as ideal spherical particles, and the deformation of droplets is not considered. For determining the hydraulic diameter of the inlet turbulent size, it is set to two times the diameter of the cylindrical combustor. For the calculation of PDF, it is necessary to define the mixing fraction at the inlet and its variation. The fuel studied in this paper is injected into the system in the form of discrete phase and evaporated. Therefore, the gas mixing fraction at the inlet is set to 0.

3.2.2. Outlet boundary condition. The boundary condition of the combustor outlet is set as the pressure outlet, the outlet static pressure (the relative static pressure) is set to zero, and the total reflux temperature is set at 1800 K [16].

3.2.3. Wall condition. For the wall condition of the combustor, the wall is set as a non-slip solid boundary, the standard wall function is selected, the wall temperature of the combustor is kept at 500 K, the boundary of the droplet impinging on the wall is set as elastic reflection, and there is no momentum loss of the droplet after the collision.

4. Simulation results and analysis

In the test system, the emissions from the combustor mainly include NOx, CO₂, CO, smoke and some unburned hydrocarbons. Because it is difficult and important to control NOx emission effectively, and it is also an important index to reflect the performance of combustor, this paper mainly studies the influence of different oil-gas ratio on NOx emission. NO produced in the combustor mainly includes NO and NO₂, and NO is the main, it mainly includes thermodynamic NO, rapid NO and fuel NO. Because the temperature of the studied system is higher, the NOx produced is mainly thermodynamic NO. Therefore, this paper mainly studies the influence of different oil-gas ratio on the emission of thermodynamic NO. Selecting the cross section of z=0, the mass fraction diagram of NO at different oil-gas ratio can be obtained as shown in Figure 4.

According to the data in Figure 4, the statistical results shown in Table 1 can be obtained through analysis and calculation.

As can be seen from Figure 4 and Table 1, when the oil-gas ratio is lower than the theoretical oil-gas ratio and the oil-gas ratio is 0.0333, the mass fraction of thermodynamic NO produced in the combustor is the lowest. With the increase of the oil-gas ratio, the mass fraction of thermodynamic NO increases gradually, and the high mass fraction of NO keeps approaching the outlet of the combustor, which is because when the actual oil-gas ratio is less than the theoretical oil-gas ratio, with the actual oil-gas ratio increasing, the temperature at the combustor outlet increases continuously until the highest temperature of the combustor is reached, while the thermodynamic NO is produced under high temperature conditions, and the concentration will increase with the temperature rising, at this time it is also in the stage of excessive air, that is, in the combustion process, the oxygen concentration in the combustor is also higher, so the mass fraction of NO produced is also larger. When the oil-gas ratio equals the theoretical oil-gas ratio, almost all of the high mass fraction of NO concentrates at the outlet of the combustor. Although the mass fraction of NO decreases and the range of high mass fraction of NO decreases correspondingly, the mass fraction of NO is still large, which may be related to the higher temperature in the combustor. When the oil-gas ratio is larger than the theoretical oil-gas ratio and the oil-gas ratio is 0.08, 0.0824, 0.0941 and 0.1 respectively, the mass fraction of NO decreases suddenly in the stage of insufficient air. With the increase of the oil-gas ratio, the mass fraction of NO decreases continuously, and the high concentration of NO moves to the combustor. It can be seen from the analysis that the thermodynamic NO produced in the combustor will generally reach a higher value near the theoretical oil-gas ratio, but it will be less when the air is insufficient or excessive, that is, in the lean or rich oil combustion state. Therefore, in order to effectively control the generation of thermal NO, it should be considered from lean or rich fuel combustion.
(a) Oil-gas ratio is 0.0333                                      (b) Oil-gas ratio is 0.0462

(c) Oil-gas ratio is 0.0571                                       (d) Oil-gas ratio is 0.068

(e) Oil-gas ratio is 0.08                                         (f) Oil-gas ratio is 0.0824

(g) Oil-gas ratio  is 0.0941                                          (h) Oil-gas ratio is 0.1

**Figure 4.** The mass fraction of NO under different oil-gas ratios
Table 1. The statistical results of NO mass fraction under different oil-gas ratios.

| working condition | fuel flow-rate (kg/s) | airflow-rate (kg/s) | oil-gas ratios | maximum mass fraction of outlet | maximum mass fraction in combusor |
|-------------------|-----------------------|---------------------|----------------|---------------------------------|-----------------------------------|
| 1                 | 0.004                 | 0.12                | 0.0333         | 3.82e-5                         | 6.23e-5                           |
| 2                 | 0.006                 | 0.13                | 0.0462         | 1.1e-4                          | 1.39e-4                           |
| 3                 | 0.008                 | 0.14                | 0.0571         | 1.42e-4                         | 1.43e-4                           |
| 4                 | 0.01                  | 0.147               | 0.068          | 1.31e-4                         | 1.31e-4                           |
| 5                 | 0.012                 | 0.15                | 0.08           | 8.34e-5                         | 8.47e-5                           |
| 6                 | 0.014                 | 0.16                | 0.0824         | 5.13e-5                         | 5.26e-5                           |
| 7                 | 0.016                 | 0.17                | 0.0941         | 3.2e-5                          | 3.34e-5                           |
| 8                 | 0.018                 | 0.18                | 0.1            | 2.16e-5                         | 2.55e-5                           |

5. Conclusions

In this paper, a three-dimensional geometric model of the combustor of the high-speed and high-temperature heat-airflow test system is established, and the meshing of the model is carried out. The distributed parameter calculation model of the combustor of the high-speed and high-temperature heat-airflow test system is given, and the boundary conditions of the numerical simulation of the combustor are set up. Computational fluid dynamics (CFD) simulation module in ANSYS 15.0 is used to simulate the combustion of fuel in the combustor and the effects of different oil-gas ratios on NO emission of the combustor are studied. The following conclusions are drawn:

(1) When the actual oil-gas ratio is close to the theoretical oil-gas ratio, the mass fraction of thermodynamic NO produced in the combustor is high, but when the actual oil-gas ratio is large or small, the mass fraction of thermodynamic NO produced will be reduced.

(2) In order to control the emission of thermodynamic NO, the amount of air can be increased or reduced appropriately, that is, combustion should be considered from lean or rich oil.

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