Estimation of NOx emissions from the combustion chamber of heavy-duty gas turbines

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Abstract: In order to study the estimation of NOx emission, numerical optimization and data fitting methods are used to study the NOx emission law of the combustion chamber of heavy-duty gas turbines. The inlet pressure $P_{in}$, air mass flow $m_a$, and average temperature in the combustion zone $T_{pz}$ are used for the fitting of NOx emission estimation formula under the multi-parameter impact. The results show that this is a fast and effective research method for the estimation of NOx emissions in the combustion chamber under the condition of ensuring the accuracy, which can obtain the NOx emission far below the average level under the condition of optimal inlet pressure.

1. Introduction

Due to the importance attached to environmental protection, the requirements for the emission standards of combustion chamber pollution have become more stringent in China. As one of the important standards for examining gas turbine combustion chambers, NOx emission has become the main monitoring parameter in the design stage of combustion chambers. Therefore, it is an important direction for the development of the combustion chamber of gas turbines in China to develop the NOx emission estimation model of strong universality[1].

The test of gas turbine combustion chambers has high demands on the environment and is also time-consuming and of high cost, which poses a great challenge to the research on pollutant emission of combustion chambers[2]. This paper uses the numerical simulation instead of part of experiments to study and analyze the combustion chamber of heavy-duty gas turbines. Also, the numerical simulation results of multi-parameter optimization are compared with traditional estimation models to study the relationship between three main parameters, namely inlet pressure, air mass flow and the average temperature in the combustion zone and NOx emission. The fitting formula suitable for these three parameters is obtained based on the numerical simulation results and the multi-parameter impact database of the pollutant emission of gas turbine combustion chambers is constructed and supplemented, which provides a reference basis for the design of the same type of the combustion chamber of heavy-duty gas turbines. Also, it provides a reliable research method for the quick estimation of NOx emissions in the combustion chamber of heavy-duty gas turbines.

2. Physical Model and Calculation Method

The CFD calculation method is used in this paper to study the pollutant emission of the combustion chamber of heavy-duty gas turbines and to calculate the change in parameters such as temperature and pressure of combustion chambers under different operating conditions; the Latin square design[5] and statistical analysis method are used to calculate the change law of different parameters to construct the
pollutant emission database of the combustion chamber of heavy-duty gas turbines; the least square method is used for the fitting of the research parameter and NOx emission formula in the database to show the relationship between parameter change and NOx emission.

2.1 Boundary Conditions
In this paper, the numerical simulation of the combustion process in a single flame tube of a gas turbine under the no-loading condition is performed. The calculation parameter of this gas turbine is shown in Table 1.

| Parameter                  | Value   |
|----------------------------|---------|
| Fuel temperature/K         | 610.5   |
| Inlet temperature/K        | 610.5   |
| Operation pressure/Pa      | 1.2159×106 |
| Fuel inlet/(kg/s)          | 1.525   |
| Primary air inlet/(kg/s)   | 3.2895  |
| Secondary air inlet/(kg/s) | 5.3649  |

2.2 Physical Model and Mesh Generation
One of the 20 flame tubes of a heavy-duty gas turbine is selected as the calculation domain, and the full-scale periodic numerical analysis model is established (as shown in Figure 1). This flame tube consists of 20 primary air inlets, 6 secondary air inlets, 20 small holes of backup fuel and 8 rows of cooling holes.

Figure 1. Physical model of the flame tube

Figure 2 shows the simplified physical model and the computational grid of the flame tube. The hybrid grid is selected. After the independent verification of grids, the final grid number is determined as 5,920,786. On the basis of ensuring the calculation accuracy, it is necessary to minimize the use of mesh to ensure efficient and accurate calculation. The global mesh generation of the flame tube is shown in (a) in Figure 2.

3. Simulation Results and Formula Fitting
3.1 Numerical Results of Design Points

The basic design data of the combustion chamber is used for the numerical analysis of the combustion chamber and the temperature distribution of the longitudinal section of the combustion chamber is shown in Figure 3.

![Temperature Distribution](image)

It can be seen from Figure 3 that the jet depth of the secondary air is about one quarter of the height of the flame tube, which cuts off the boundary of the recirculation zone of the head; the secondary airflow generates a recirculation zone in the rear region of the flame tube, which plays the role of supporting the combustion and blending so as to achieve sufficient combustion of fuels; with the increase of pressure, the flame front becomes shorter and the flame boundary tends to be closer to the flame tube wall[6][7].

3.2 NOx Estimation Experience / Semi-Empirical Formula

Through the reference to previous literature and comparison with numerical simulation calculation results, it is found that the following six empirical formulas have significant reference value for the research in this paper, as shown in Table 2.

| Author       | Experience formula                                                                 |
|--------------|-------------------------------------------------------------------------------------|
| Lefebvre[3]  | \[ NO_x = 9 \times 10^4 \frac{P_i^{0.3} V_c \exp(0.01T_e)}{m T_{pe}} \] g/kg         |
| Odgers[8]    | \[ NO_x = 29 \exp\left(\frac{-21670}{T_{pe}}\right)^{0.65} \left[1 - \exp(-250r)\right] g/kg \] |
| Rizk[9]      | \[ NO_x = 0.15 \times 10^6 \left(\tau - 0.5 \tau_{cr}\right)^{0.5} \exp\left(\frac{-71100}{T_{u}}\right) \] g/kg |
| Rokke        | \[ NO_x = 18.1 \times P_{in}^{1.42} m_a^{0.3} q^{0.72} \times 10^{-6} \]            |
| Lewis[10]    | \[ NO_x = 3.3192 \times 10^{-6} \exp\left(0.0079777T_{pe}\right) P_{in}^{0.5} \times 10^{-6} \] |
| Lin Qinghua[4] | \[ NO_x = e^{0.00258T_e + 0.00747P_{in} - \left[17.31927X_{R50} + 16.95517X_{C2} + 17.69844X_{C1}\right]} \] |

The above six empirical formulas of NOx emission are used as a reference in this research. By comparing these formulas with the NOx emission change under the impact of three main parameters in this paper, namely inlet pressure, air mass flow, and the average temperature in the combustion zone, the change law and its main reason are analyzed and relevant NOx emission law and estimation method are summarized.
3.3 NOx Prediction Based on Inlet Pressure

The relationship between NOx emission and inlet pressure is shown in Figure 4. This result indicates that the impact of inlet pressure on NOx emission is not significant. Within the same pressure range, the empirical formula trend of Odges and Lefebvre is similar. With the increase of inlet pressure, the NOx emission also shows an increasing trend and the reason for this phenomenon is that these two empirical formulas are greatly affected by the inlet pressure; the NOx emission obtained by the Odgers's empirical formula is high at about 0.4g/kg, which is higher than the simulation result; the NOx emission obtained by Lefebvre's empirical formula is low at about 0.25g/kg, which is lower than the simulation result, indicating that the range selected for this numerical simulation is suitable. Under the condition of the same inlet pressure, the numerical simulation results are similar to the empirical formula results of Rizk and the trend is the same. The estimation formula of Rizk derives from the combustion chamber of heavy-duty gas turbines. Also, the experimental verification proves that the calculation results of this formula are approximately the same as the measured NOx emission of five 1.5-34MW natural gas-fired industrial gas turbines, indicating that the use of numerical simulation for the research is reliable and scientific.

![Figure 4. Impact of inlet pressure on NOx emissions](image)

3.4 NOx Estimation Based on Mass Flow

The relationship between the NOx emission and air mass flow is shown in Figure 5. The numerical simulation results are opposite to the results obtained by the empirical formula of Rokke. The reason for this formula is that Rokke has strictly stipulated that the experiment is performed at the optimal fuel-air ratio (1: 14.7). With the increase of air mass flow, the fuel flow and the average temperature in the combustion zone will increase accordingly, thus leading to the increase in NOx emission; the numerical simulation results are consistent with the results obtained by the empirical formula of Lefebvre. The NOx emission decreases with the increase of air mass flow, which indicates that the numerical simulation has achieved good results and is reliable. The simulation results can be used as a reference for the NOx emission in the combustion chamber of heavy-duty gas turbines.
Figure 5. Impact of air mass flow on NOx emission

It can be seen from the comparison and analysis of the variation trend of the data curve of numerical simulation and empirical formula that the results obtained from the numerical simulation are consistent with the overall trend of the calculation results using Lefebvre's empirical formula, indicating that replacement of experiment with numerical simulation and its results are of certain reference and research value.

3.5 NOx Prediction Based on Average Temperature in the Combustion Zone

The relationship between the NOx emission and average temperature in the combustion zone is shown in Figure 6. The fitting formula of Lin Qinghua is mainly based on the synthesis gas combustion chamber and this formula is related to the outlet temperature and the percentage of diluent. Within the same average temperature range in the combustion zone, the NOx emission increases with the average temperature in the combustion zone, and the variation range is relatively large, indicating that this prediction model is relatively sensitive to this parameter; the empirical formula of Lewis is applicable to lean and homogeneous fuel combustion chambers. The NOx emission obtained within the same temperature range is lower, which is more in line with national NOx emission standards, within the same temperature variation range, the NOx emission obtained by the prediction formula of Lefebvre is similar to the numerical simulation results but the overall trend is opposite. However, it can still be seen that the NOx emission is affected by the average temperature in the combustion zone and the trend is consistent with the calculation results based on the empirical formula of Lewis and Lin Qinghua, which indicates that the NOx emission obtained using the numerical simulation method is of certain research value.
3.6 NOx Emission Fitting Formula

The coefficient determination is obtained by the fitting of the variation curve between the NOx emission obtained by the numerical simulation and three parameters. The least-square method is used for this fitting formula, and the final formula is as follows.

\[
NOx = 0.3704e^{-0.18T_p} + 1.2318e^{-0.299\rho_c} + 0.1213e^{0.0015T_c} 
\]  

(1)

One of the application conditions of the fitting formula is the combustion chamber of heavy-duty gas turbines. For formula (4), when the parameter selection range is consistent with the selection range in this paper, the formula will be relatively reliable; when the parameter selection range is inconsistent, the fitting formula needs to be further verified before using.

4. Conclusion

(1) The use of numerical simulation in the research on the pollutant emission of the combustion chamber of heavy-duty gas turbines is an efficient estimation method, and the research results are scientific.

(2) In the study of pollutant emission of the combustion chamber of heavy gas turbines, the optimization algorithm and least squares method are used to enrich the database content, which provides convenient conditions for the database establishment.

(3) For the combustion chamber of heavy-duty gas turbines, with the increase of the average temperature in the combustion zone, the NOx emission also increases accordingly. As the temperature does not reach 1850K, the increase is mainly fast NOx.

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