Numerical study of the processes of co-combustion of pulverized coal and gas fuel based on nonstationary methods of turbulence modeling

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Abstract. In this work, a numerical study of the combustion of pulverized coal in a gas flame is carried out on the basis of the proposed mathematical model of combustion processes, using a nonstationary method for modeling turbulence, complex heat transfer and a reduced mechanism for chemical kinetics. The calculation results show acceptable agreement with the experimental data on the main characteristics of the flame, make it possible to qualitatively correctly determine the structure of the dust and gas flow and derive such parameters as the gas composition, the temperature of particles and gas, the degree of carbon burnout, etc.

1. Introduction

Coal is the most common type of fuel. It can be found on all continents, in many countries around the world. Coal-fired power plants generate nearly 40% of the world's electricity. As the reserves of this fuel are large, it is expected that coal will continue to play a leading role in the energy sector.

Mathematical modeling of heat and power devices is today one of the most important ways to obtain representative information about processes. Mathematical modeling based on a stationary approximation using turbulence models based on averaged transport equations is widely and successfully used to optimize and design burner-furnace devices for pulverized coal boilers. [1-5]. However, this approach does not allow one to study the stability of combustion, processes of local ignition, flame blowout, transient processes and processes when changing the load, type of fuel, etc. For this purpose, it is proposed to develop nonstationary modeling methods for the conditions of co-combustion of pulverized coal and gas fuel.

The paper [6] provides an overview of the latest advances in modeling the combustion of pulverized coal. Computational fluid dynamics can be divided into Reynolds-averaged Navier-Stokes (RANS) simulation, large eddy simulation (LES) and direct numerical simulation (DNS). The work [6] focuses on the latest achievements in the high-fidelity DNS and LES of pulverized coal combustion. Much attention has been paid to various models of the release of volatile matter, since this process is critical for the ignition and stabilization of the combustion of pulverized coal. Simulation of homogeneous combustion is also an important point in calculating the pulverized coal combustion, since the velocity distribution, gas composition, temperature, etc., depend on it. Typically more accurate and complex models / methods are computationally expensive. Therefore, the optimal use of each approach depends on the specific research objective.
2. Problem statement and research methods

To simulate an open turbulent flame of co-combustion of methane and coal, a burner with a nozzle diameter of 15 mm was chosen (figure 1). The outflow of the fuel jet and its combustion were carried out into an open space. The oxidizing agent for combustion came from the surrounding area. The dimensions of the computational area behind the nozzle exit were selected based on methodological calculations. As a result, the following dimensions were set: the diameter of the computational domain was 40 cm, the height was 40 cm.

As the boundary conditions at all outlet boundaries of the computational domain, the outlet conditions with a fixed pressure were specified. Solid wall conditions were set on the outer and inner surfaces of the nozzle. At the nozzle inlet, the fixed flow rate of the mixture of methane (25-40% vol.) and nitrogen (60-75% vol.), which was \( Q = 0.174 \text{ g/s} \). When coal was supplied, the percentage of methane increased to 40%. The coal consumption was 0.055 g/s. In the calculations, long-flame coal from the Kuznetsk deposit was used, technical characteristics and elemental analysis are presented in table 1. Half of the supplied coal particles have a size of <50 microns, the rest of the particles - 50 ÷ 100 microns.

![Figure 1. Geometry and an example of an unstructured computational mesh in the nozzle area.](image)

| \( W_g \), % | \( A_d \), % | \( V_{daf} \), % | \( C_{daf} \), % | \( H_{daf} \), % | \( N_{daf} \), % | \( S_{daf} \), % | \( O_{daf} \), % | \( Q_{daf} \), MJ/kg |
|---|---|---|---|---|---|---|---|---|
| 5,4 | 22,3 | 44,7 | 75,57 | 5,66 | 1,78 | 0,55 | 16,44 | 27,7 |

The proposed complex mathematical model for describing the processes of co-combustion of methan and pulverized coal combustion includes: model of motion of a multicomponent non-isothermal gas medium (carrier phase) based on the URANS and hybrid RANS/LES turbulence models; radiation transfer model based on the discrete ordinate method; model of particle motion based on the Lagrange approach; a one-stage kinetic model is used to calculate the release rate of volatiles; model of combustion in the gas phase based on a eddy-dissipation model (EDC); and model of coke residue burnout calculated according to the provisions of the classical diffusion-kinetic theory. In the model, the process of ignition and combustion of a particle occurs in stages. To describe coal burning, a model of ignition and combustion of coal particles is used. According to this model, the particles are heated, the internal moisture and volatile components of fuel are released, and the coke residue is burned. Volatile components burn out in the gas phase. Testing of the combustion model of pulverized coal is presented in the work [5].

The problem was solved in a three-dimensional non-stationary setting taking into account the forces of gravity. An unstructured computational grid (2 mil. cells) was used with local concentration near the nozzle and the region of the flame formation. The transfer equations were discretized using the control volume method. The time step met the condition: average CFL <2. The studies were carried out using the universal Ansys Fluent CFD package.
The authors of the article previously tested a mathematical model of the gas combustion process for different modes and burners, including for this nozzle [7-9]. On the basis of these data, a eddy-dissipation model (EDC) model with a four-stage methane reaction mechanism was chosen (table 2). Coke residue combustion is described by a three-stage reaction mechanism (table 3).

**Table 2.** Kinetic constants of homogeneous reactions [10].

| Reaction                      | $A$, kmol/m$^3$/s | $E$, J/kmol | $\beta$ | Components degree $\gamma$ |
|-------------------------------|------------------|-------------|---------|----------------------------|
| $\text{CH}_4+0.5\text{O}_2\rightarrow\text{CO}+2\text{H}_2$ | $4.4\cdot10^4$  | $1.26\cdot10^8$ | 0       | $\gamma_{\text{CH}_4}=0.5$, $\gamma_{\text{O}_2}=1.25$ |
| $\text{CH}_4+\text{H}_2\text{O}\rightarrow\text{CO}+3\text{H}_2$ | $3.1\cdot10^8$  | $1.26\cdot10^8$ | 0       | $\gamma_{\text{CH}_4}=1$, $\gamma_{\text{H}_2\text{O}}=1$ |
| $\text{CO}+0.5\text{O}_2+\text{H}_2\text{O}\rightarrow\text{CO}_2$ | $2.5\cdot10^8$  | $6.69\cdot10^7$ | 0       | $\gamma_{\text{CO}}=1$, $\gamma_{\text{O}_2}=0.3$ |
| $\text{H}_2+0.5\text{O}_2\rightarrow\text{H}_2\text{O}$ | $7.9\cdot10^8$  | $1.46\cdot10^8$ | 0       | $\gamma_{\text{H}_2}=1$, $\gamma_{\text{O}_2}=0.5$ |

**Table 3.** Kinetic constants of heterogeneous reactions [11].

| Reaction                      | $A$, kmol/m$^3$/s | $E$, J/kmol | $\beta$ | Components degree $\gamma$ |
|-------------------------------|------------------|-------------|---------|----------------------------|
| $\text{C}+0.5\text{O}_2\rightarrow\text{CO}$ | 2.3              | $9.23\cdot10^7$ | 1       | $\gamma_{\text{O}_2}=0.4$ |
| $\text{C}+\text{CO}_2\rightarrow2\text{CO}$ | 4.4              | $1.62\cdot10^8$ | 1       | $\gamma_{\text{CO}_2}=0.6$ |
| $\text{C}+\text{H}_2\text{O}\rightarrow\text{CO}+\text{H}_2$ | 1.33             | $1.47\cdot10^8$ | 1       | $\gamma_{\text{H}_2\text{O}}=0.6$ |

3. Results and discussion

Figure 2 shows the results of calculating the combustion of CH$_4$-N$_2$ gas based on the RANS approach. The simulation results are qualitatively compared with the experimental data obtained at the stand of the IT SB RAS. The photograph of the experiment shows that the combustion of methane occurs at the interface of mixing the fuel with the oxidizer. As a result, the burnout of methane does not occur instantaneously, therefore the shape of the flame has an elongated shape. Since hydrogen is an intermediate element in the methane oxidation reaction, it can be assumed that the hydrogen concentration in the calculations corresponds to the position of the flame front. Comparing the calculation results obtained using different turbulence models, it can be seen that the shape of the flame is significantly different for the three options. The results obtained using the RSM are in better agreement with the experiment on the location of the flame front and the degree of fuel burnup. From the results obtained using the k-w SST, it can be seen that there is demolition of the flame at a distance of two nozzle diameters. On the basis of the results obtained, the RSM model was chosen for further research in the nonstationary formulation of the problem.

Below are the results of nonstationary calculations obtained using DES and URANS RSM. The photographs from the experiment show that when CH$_4$-N$_2$ gas is supplied through the nozzle, the flow rate pulsates. As a result, the air swirls periodically inside the fuel jet. A mushroom-shaped flame is formed. Further, with an increase in the temperature and speed of the combustible gases, the flame is separated. Figure 3 shows that the chosen calculation method allows qualitatively correct description of the processes. When using the DES method in calculations, the flame is demolition a distance of two nozzle diameters. A more similar flame shape was obtained with the URANS RSM.
Figure 2. Flame shape during combustion of CH$_4$ (25%): a) RANS k-e, b) RANS k-w SST, c) RANS RSM, d) experiment (left - methane concentration, right - hydrogen concentration).

Figure 3. Flame shape during combustion of CH$_4$ (40%): a) DES k-w SST, b) URANS RSM, c) experiment (left - hydrogen concentration, right - oxygen concentration).
The URANS RSM method was chosen for the numerical description of the processes of co-combustion of coal and methane. Figure 4 shows a comparison of calculation results with experiment. The calculation results show that when coal is supplied, a local increase in hydrogen concentration occurs due to the release of volatile matter from coal (figure 4a). Burnout of solid carbon begins at a distance of 6-7 cm from the nozzle. It is worth noting that the coal particles are carried away by the gas flow and fall into the vortices described earlier. As a result, the combustion of particles occurs in annular structures. Figure 4c shows the calculation results in the form of the temperature distribution on the coal particles. Coal particles getting into the gas flame begin to warm up, moisture and volatile matter come out. Then solid carbon is ignited, and the temperature of the particles reaches 1000 °C and above. The distribution of particles in the flame corresponds to the experimental data (figure 4c, d).

![Figure 4](image_url)

**Figure 4.** Flame at co-combustion CH4 (40%) and coal: a) hydrogen concentration, b) carbon residue burnup rate, c) temperature of coal particles, d) experiment.

4. Conclusion
A numerical study of the combustion of pulverized coal in a gas flame is carried out on the basis of the proposed mathematical model of combustion processes, using a nonstationary method for modeling turbulence, complex heat transfer and a reduced mechanism for chemical kinetics. The results of the calculations indicate that the mathematical model of the processes makes it possible to qualitatively correctly solve three-dimensional nonstationary problems, such as co-combustion of methane and coal in an open flame. The proposed model will make it possible to analyze the stability of combustion of gas-coal flames and transient processes accompanying a change in the supply modes of the fuel-oxidizing medium.
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