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NUMERICAL STUDY OF DIFFUSION COMBUSTION

OF PULVERIZED COAL IN A GAS JET

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Abstract: Adaptation of a mathematical model of gas diffusion combustion for different flow rates of $CO-H₂$ and a constant coal flow rate is carried out. It is shown that the results of calculating the main characteristics of the flame are in satisfactory agreement with experimental data and can be used to determine the structure of pulverized coal–gas flow, gas composition, particle and gas temperature, carbon combustion efficiency, etc. The proposed model is suitable for analyzing the stability of coal– gas flame and the transient processes accompanying changes in the mode of supply of the fuel-oxidizer medium.

Keywords: flame, pulverized coal combustion, ignition, mathematical model.

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INTRODUCTION

Coal is one of the key energy resources; its world production in 2019 increased by 1.5% and was 7953 million tons [1]. Coal power is still a major contributor to power generation (approximately 38% of the total energy consumption), and according to forecasts, in the next decades, the share of coal will make up the main part in the global energy balance [2]. This is primarily due to the large world reserves of coal (approximately 1055 billion tons) and its competitive low prices [3].

Combustion is the main way to obtain energy from coal. Among existing coal combustion technologies, flame combustion is the most common [4, 5]. However, burning coal leads to an increase in harmful emissions into the environment, so that the problem of reducing them with a minimal loss of process efficiency becomes more and more important [6, 7]. The problem of efficient and environmentally friendly combustion of coal has received great attention all over the world [8, 9].

Various types of vortex burners for burning coal have been developed that make it possible to reduce harmful emissions, increase the completeness of fuel combustion, and ensure combustion stability over a wide range of loads [7–12]. To optimize and design pulverized coal boiler furnaces, it is common to apply mathematical modeling using a steady-state approximation and turbulence models based on averaged transport equations [13–17]. However, this approach cannot be used to investigate combustion stability, localized ignition, flameout, transients,

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and the processes occurring with a change in load, type of fuel, etc. For this purpose, unsteady methods for modeling the co-combustion of pulverized coal and gas fuels have been developed.

A review of papers devoted to modeling pulverized coal combustion is given in [18]. There are the following methods of computational fluid dynamics: the method involving the solution of the Reynolds-averaged Navier–Stokes equations (RANS), the large eddy method (LES), and direct numerical simulation (DNS). In [18], modifications of the methods such as high-accuracy of DNS and LES of pulverized coal combustion (PCC) are mainly considered. In addition, in [18], much attention is paid to the study of different models of volatile release since this process has a significant effect on the ignition of pulverized coal and the stabilization of its combustion. Modeling of homogeneous combustion is an important step in PCC calculations since velocity, gas composition, temperature, etc. distributions depend on this. Usually, the development of more accurate and complex models (methods) has high computational costs.

MATHEMATICAL MODEL

To adapt the mathematical model based on the results of studying the combustion of pulverized coal in CO–H² gas flame, we use a burner with flow swirling (due to built-in blades) (Fig. 1). In the central channel, a combustible gas (50 vol.% CO and 50 vol.% H_2) was supplied with a flow rate of 3 liter/min. In the annular channel, oxidizer (air) with added coal were supplied; the flow rate of air was was 1.6 kg/h, and the air flow rate was 8 m³/h. Half of the supplied coal particles have size less than 50 μ m, and the size of the other particles is $50-100 \mu$ m. The calculations were performed for long-flame coal from the Kuznetsk Basin which has the following technical characteristics and composition: mass fraction of moisture determined in an analytical sample $W_a = 2\%$, ash content of the dry fuel $A_d = 21\%$, yield of volatiles in the dry ash-free state $W_{Vdaf} = 41\%$, mass fraction of carbon in the dry ash-free state $W_{Cdaf} = 74.5\%$, mass fraction of hydrogen in the dry ash-free state $W_{Hdaf} = 4.9\%$, mass fraction of oxygen in the dry ash-free state $W_{O^d} = 17.7\%$, mass fraction of nitrogen in the dry ash-free state $W_{N\,dd} = 2.2\%$, and the mass fraction of total sulfur in the dry state $W_{S\,dd} = 0.6\%$. The calculation was carried out in an unsteady full-scale 3D formulation taking into account gravity. An unstructured computational grid containing 1.5 million cells with local refinement in the nozzle region and in the region of flame formation (Fig. 2).

The mathematical formulation of the problem of pulverized coal combustion includes a set of interrelated models describing turbulent gas motion, heat and radiant energy transfer, combustion, gasification, and motion of coal particles, etc. For the numerical simulation of the unsteady turbulent flow of the burning medium, URANS RSM, URANS (k–w)-SST, and DES models were used. Particle motion is described by the equations of dynamics of a material point taking into account the resistance and gravity forces. Flow turbulence during particle motion is taken into account by introducing random fluctuations of gas velocity into the equation of particle motion. The solution of the equation of radiant energy transfer is based on the P1-approximation of the spherical harmonics method for a two-phase two-temperature gray medium. The combustion of a coal particle includes the following successive stages: evaporation of moisture from the fuel, release and combustion of volatile components, and combustion of the coke residue. The release of $C_xH_yO_z$ volatiles is considered in a single-component approximation, and the rate of release is calculated using a two-stage approximation based on the Kobayashi model. To calculate the combustion of gaseous components, the eddy dissipation concept (EDC) model was used. The burning rate of the coke residue was calculated in accordance with classical diffusion-kinetic theory.

The pulverized coal combustion model was tested in [17]. The mathematical model of gas combustion was previously tested for various modes and burners, including for the nozzle considered [19–21]. Based on these data, an eddy dissipation concept (EDC) model with a four-stage mechanism of methane reaction was chosen (Table 1). The combustion of the coke residue is described using a three-stage reaction mechanism (Table 2). In Table 1, 2 A is the pre-exponential factor, E is the activation energy, β is the temperature exponent, and γ is the degree of concentration of the components.

The calculation was carried out in a full-scale unsteady three-dimensional formulation taking into account gravity. The transfer equations were discretized using the control volume method. The relationship between the velocity and pressure fields for incompressible fluid was implemented using the SIMPLEC procedure. The convective terms of the equations describing turbulent characteristics and the equations of fluid dynamics were approximated using a second-order upwind scheme in URANS models and a central difference scheme in the DES method. The dif-

Fig. 1. Diagram of the burner: (1) swirler, (2) CO and H_2 gas supply channel, (3) air and coal supply channel; arrows show the flow direction.

Fig. 2. Geometry of the computational domain and computational grid (the enlarged fragment is the region of blades).

Table 1. Values of the kinetic constants of homogeneous reactions [22]

Reaction	A, kmol/ $(m^3 \cdot s)$	E, J/kmol		
$CH_4 + 0.5O_2 \rightarrow CO + 2H_2$	$4.4 \cdot 10^{11}$	$1.26 \cdot 10^8$	θ	$\gamma_{\text{CH}_4} = 0.5, \gamma_{\text{O}_2} = 1.25$
$CH_4 + H_2O \rightarrow CO + 3H_2$	$3.1 \cdot 10^8$	$1.26 \cdot 10^8$		$\gamma_{\text{CH}_4} = 1, \gamma_{\text{H}_2\text{O}} = 1$
$CO + 0.5O2 + 0H2O \rightarrow CO2$	$2.5 \cdot 10^8$	$6.69 \cdot 10^{7}$		$\gamma_{\rm CO} = 1, \gamma_{\rm O_2} = 0.3$
$H_2 + 0.5O_2 \rightarrow H_2O$	$7.9 \cdot 10^{10}$	$1.46 \cdot 10^8$		$\gamma_{\text{H}_2} = 1, \gamma_{\text{O}_2} = 0.5$

Table 2. Values of kinetic constants of heterogeneous reactions [23]

Fig. 3. Gas flow structure: (a) streamlines, (b) velocity field, (c) field of the velocity component along the x axis.

Fig. 4. Flame shape: (a, b) calculation (a) $O₂$ concentration (volume fraction) field, (b) CO concentration (volume fraction) field, (c) experiment.

Fig. 5. Trajectory (a) and concentration field (b) of flame particles.

fusion terms were approximated using a second-order scheme, and unsteady terms using an implicit second-order scheme. The time step satisfied the Courant–Friedrichs–Levy (CFL) condition of convergence: the average value of the parameter $CFL < 2$.

CALCULATION RESULTS AND THEIR ANALYSIS

Figures 3–5 show the results of calculating the combustion of pulverized coal fuel in a $CO-H₂$ gas flame. Figure 3 shows the structure of the gas flow in the central section. It can be seen that in the flame combustion, the flows have swirling structure and the maximum speed (swirling) along the y coordinate reaches 1.9 m/s. At a height approximately equal to three diameters, the swirling speed begins to decrease significantly, and the flow is lifted up due to the low density of the gas.

Figures 4 and 5 show the calculated and experimental results for pulverized coal–gas combustion. It is seen that in the experiment and calculations, the combustion front of the gas and coal particles is at the oxidizer–fuel interface. The flame front starts from the annular channel of small diameter. The concentration of carbon oxide in the calculation characterizes the degree of combustion of the combustible gas and the flame shape (see Fig. 4b). The bright lines in Fig. 4c show the direction of motion of burning coal particles entrained in the swirling flow and moving along a helical path. Similar results were obtained in the calculations (see Fig. 5b). In addition, the calculation results show that, due to the centrifugal and gravity forces, some coal particles scatter and fall down.

CONCLUSIONS

Adaptation of the mathematical model was performed based on the results of studying pulverized coal combustion in CO–H² gas flow in the range of experimentally investigated parameters. The calculation results indicate that the mathematical model of the processes can be used to solve three-dimensional unsteady problems such as the co-combustion of CO–H₂ gas and coal in naked flame.

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