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HEAT AND MASS TRANSFER AND PHYSICAL GASDYNAMICS

Modeling of Heat Mass Transfer in High-Temperature Reacting Flows with Combustion

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Abstract—A multiprocessor computer system suitable for physical, mathematical, and chemical models, as well as an exact method for the solution of a system of differential equations that describe the actual combustion of a pulverized coal flare, are necessary to study the numerically complex, physicochemical processes occurring in the combustion chambers of power plants. The results of numerical simulation can provide quite a high accuracy. However, the task of setting up a physical and mathematical model with the correct initial and boundary conditions has yet to be completed. In this paper, we studied heat and mass transfer in high-temperature reacting flows during the burning of Karaganda coal in the combustion chamber of an actual power boiler of a thermal power plant in Kazakhstan. The optimal conditions for computational experiments that correspond to real combustion processes are determined.

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INTRODUCTION

Urgent problems of the current stage of the development of thermal power engineering include the need to optimize solid fuel combustion; the development and implementation of "clean" technologies to protect the environment; and the efficiency of thermal power plants (TPPs) [1–7]. This requires an in-depth study of the methods for burning solid fuels and studies of the technological processes in combustion boiler chambers so that it is possible to optimize processes at coal- burning TPPs when combining physical, scientific, applied, technological, and engineering-design studies. Thus, computational experiments on the ignition, heat transfer, and mechanisms of burnout of a pulverized coal torch in the combustion chambers of power plant boilers are an indispensable tool for efficiency [8–10].

At present, the intensive development of computer technologies and methods of numerical simulation provides a sufficiently high accuracy, convergence of numerical results, and agreement with the results of field experiments [11, 12]. The use of computational technologies with adequate initial and boundary conditions makes it possible to obtain data without in-situ experiments that can later be used to justify the parameters and regimes of thermophysical processes in the preparation of subsequent experimental studies on actual energy objects.

Thus, the goal of the present paper is to conduct computational experiments on the selection of optimal initial conditions for the temperature of the combustion chamber walls in order to study heat mass transfer in high-temperature reacting flows during the combustion of coal fuel.

PHYSICAL MODEL OF FUEL COMBUSTION IN HIGH-TEMPERATURE REGIONS

Complex structural changes occur in combustion in high-temperature regions. They are accompanied by chemical reactions in the gas phase and solid states [13–15]. Coal combustion is known to consist of three stages: the drying and removal of volatile components with the release of volatile substances due to rapid heating of the coal particle; the oxidation of coke residue via heterogeneous combustion of solid coke after the removal of gaseous components; and the reaction of volatile substances via the of a homogeneous gas phase of combustion products.

The removal of volatile substances occurs in the initial phase of particle heating. The temperature rises due to radiation and convection during coal combustion within a certain furnace volume. At elevated temperatures, coal is separated and converted to gaseous, semicoke, and bituminous compounds. When the particle reaches a certain temperature, the volatiles begin to be released, and they ignite rapidly in the presence of sufficient oxygen at high temperatures.

Volatile substances are organic decomposition products that arise as a gas or water vapor when coal is heated in air. In this case, the initial temperature is

900°C. Volatile components consist of various hydrocarbons, such as carbon oxides (CO and CO_2), H_2O, methane, ethane, ethylene, and resins. With an increase in the degree of coal carbonization, the content of volatile components associated with the carbon particle decreases and, as a logical result, the fraction of elementary fixed carbon increases. Based on this, we can conclude that the coal rank reflects its property of coalification, which means that the fraction of volatiles is usually proportional to the coal age.

After the volatile combustion products are released, a porous coke matrix remains. It has a high carbon content with respect to the other particles. This coke burns unevenly in the secondary zone behind the flame. When coal of a higher rank is burned, more volatile substances appear as released components, the further burning and cracking of which generates a large amount of hydrocyanic acid HCN and ammonia NH_3, which are usually an indicator of increased NO_x emissions [16].

In coke residue oxidation, oxygen diffuses into the particle pores and reacts with the bound carbon. This transformation is proportional to the inner surface area of the particle. The main factor for the rate of the chemical reaction is the temperature, since, the reaction rate below 600°C is relatively slow and oxygen can completely penetrate the pores of the carbon particles. At high temperatures, the diffusion rate of oxygen into the pores becomes a limiting factor and, during combustion, the outer particle surface contracts over time due to the oxidation of bound carbon [17].

MATHEMATICAL STATEMENT OF THE PROBLEM OF PULVERIZED COAL COMBUSTION

The main influence on the course of burning in the combustion chamber is the aerodynamic movement of gases, air, and polydisperse fuel particles, as well as the heat and mass exchange and combustion stability. The mathematical model characterizing combustion includes a large number of fundamental physical laws, various approaches, and methods that describe heat and mass transfer in the combustion chamber [18–23]. Below, the basic equations used in the mathematical model of the problem are presented.

The equation of mass conservation can be written in the following form:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = S_i, \qquad (1)$$

where S_i is the source that determines the mass added to the continuous phase and any other sources that depend on a particular physical task. Since, the transformation of the constituent components occurs only in this paper, there are no mass sources. In this case, equation (1) takes the form

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0.$$

The equation of momentum conservation can be written in the form of the Navier-Stokes equation as follows:

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i + F_i. \qquad (2)$$

The first term on the left in (2) describes the flow nonstationarity and the second is convective transport, while the first and second terms on the right are surface forces (pressure gradient and molecular diffusion), the third is the mass forces (gravity), and the fourth is external mass forces.

The equation of energy conservation includes the energy transfer due to conductivity, diffusion as well as viscous dissipation:

$$\frac{\partial(\rho h)}{\partial t} + \frac{\partial}{\partial x_i}(\rho h u_i) = \frac{\partial p}{\partial t} + u_i \frac{\partial p}{\partial x_i} - \frac{\partial}{\partial x_i}\left(k_{\text{eff}} \frac{\partial T}{\partial x_i}\right) - \frac{\partial}{\partial x_{ij'}} h_{j'} J_{j'} + (\tau_{ij'})_{\text{eff}} \frac{\partial u_j}{\partial x_j} + S_h.$$

Here, S_h takes into account the heat due to chemical reactions and other volumetric energy sources (radiation, convective exchange between particles and the gas phase, combustion heat). The transport equation for the generalized φ variable indicating the mass or kinds of components and momentum or energy can be written as a generalized transport equation for turbulent flows:

$$\frac{\partial(\rho\varphi)}{\partial t} + \frac{\partial}{\partial x_i}(\rho\varphi u_j) = \frac{\partial}{\partial x_i}\left(\Gamma_\varphi \frac{\partial \varphi}{\partial x_i}\right) + S_\varphi,$$

where S_φ is the source term that takes into account the contribution of chemical reactions to the change in the transfer by the variable $\varphi(u, v, w, T, C, k, \varepsilon)$.

The combustion proceeds with hundreds of intermediate reactions that cannot be actually calculated in detail. Therefore, some simplifications or assumptions should be made. In this paper, we take only the key reactions into account, while the chemical model is described in detail elsewhere [1–6]. To describe pressure and velocity, we used the effective method of the Simple algorithm, which solves the problem of discretization of the momentum and continuity equations [24].

In turbulent flows in high-temperature media, it is necessary to take into account the velocity pulsations. In this paper, we used a standard k–ε model in which the kinetic energy of turbulence k and the dissipation of energy ε can be obtained using the following equations:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i k) = \frac{\partial}{\partial x_i}\left(\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_i}\right) + G_k + G_b - \rho\varepsilon,$$

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i \varepsilon) = \frac{\partial}{\partial x_i}\left|\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_i}\right| + G_{1\varepsilon}\frac{\varepsilon}{k}(G_k + (1 - C_\mu)G_b - C_{2\varepsilon}\rho\frac{\varepsilon^2}{k},$$

where G_k is the generation of k (the production of turbulent kinetic energy) relative to the turbulent stress and G_b is the generation of k due to buoyancy. The constants of the k–ε turbulence model have the following values: $C_{1\varepsilon} = 1.44$, $C_{2\varepsilon} = 1.92$, $C_\mu = 0.09$, $\sigma_k = 1.0$, and $\sigma_\varepsilon = 1.3$ [25].

In the flame zone, the contribution of radiant heat transfer is 90% or more. The change in the radiation intensity on the path segment is due to the following processes: a decrease is due to absorption, emission in the medium, and scattering loss, while an increase is due to the incoming scattered energy in the chosen direction. To describe heat transfer due to radiation, we used a six-flux model proposed elsewhere [26]. In this model, the distribution of the radiation energy flux is approximated by power series and spherical functions at the corresponding sections of the spatial angles.

MODELING OF THERMAL ASSOCIATION PROCESSES IN HIGH-TEMPERATURE REACTING FLOWS

For the 3D modeling of heat and mass transfer in high-temperature reacting streams, the FLOREAN (FLOwREActioN) software package was used [27–29]. This software package was modified and adapted by the authors to study the combustion processes at Kazakhstan thermal power plants. The equations describing heat and mass transfer in a gas-fuel mixture are solved by the control volume method with the standard k–ε model of turbulence and the corresponding initial and boundary conditions.

The combustion chamber of the BKZ-75 boiler (Shakhtinskaya TPP, Kazakhstan), in which low-grade Karaganda coal is burnt (the ash content exceeds 35%), was chosen as the object of study. Figure 1 shows the combustion chamber of the boiler used for computational experiments with its sampling for control volumes. In accordance with the given geometry, the finite difference grid of the combustion chamber volume is divided into 126 496 control volumes.

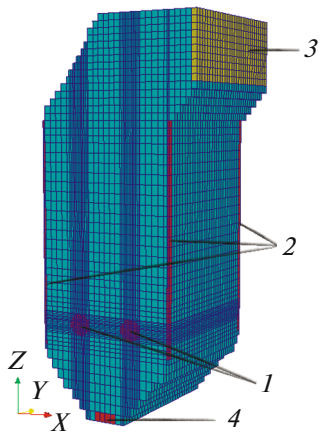

Fig. 1. Sampling for the control volumes of the combustion chamber of the BKZ-75 boiler: (*1*) burner area, (*2*) chamber outlet section, (*3*) air sucker in the chamber, and (*4*) cold funnel.

BOUNDARY CONDITIONS FOR THE TEMPERATURE OF THE COMBUSTION CHAMBER WALLS

Insufficient knowledge of the behavior of the heat flow and heat and mass transfer during the combustion of pulverized coal makes the choice of a realistic model of the boundary conditions of chamber wall temperature almost arbitrary. An improperly chosen boundary condition for the chamber wall temperature in the furnace volume of the boiler can give erroneous results, which, if they are used at real TPPs, will lead to various discrepancies and incorrect judgments about heat and mass exchange processes. However, with knowledge of the degree of discrepancy in the results of the studies, they could serve as an effective tool for the primary qualitative and/or quantitative assessment in determining the parameters and characteristics of heat and mass transfer at a new or reconstructed energy facility.

The used computer package allowed a more detailed study of the effect of the boundary condition for the temperature of the combustion chamber walls on heat and mass transfer. Convective heat exchange between the hot fuel–air stream and the wall at a given temperature is determined by the flow in the wall region [30, 31]. For adiabatic walls, the heat flux is zero ($q_{\text{surf}} = 0$ and $T_{\text{surf}} = \text{const}$), and the boundary conditions as in the plane of symmetry are used in this case.

In the case of heat exchange between the wall and the reacting flow, the wall temperature or heat flux is set ($q_{\text{surf}} \neq 0$ and $T_{\text{surf}} \neq \text{const}$). The surface temperature of the chamber wall T_{surf} can be calculated as follows:

$$\dot{q} = \lambda(T_{\text{surf}} - T_{\text{steam}}) \quad \text{and} \quad T_{\text{surf}} = \frac{\dot{q}}{\lambda} + T_{\text{steam}},$$

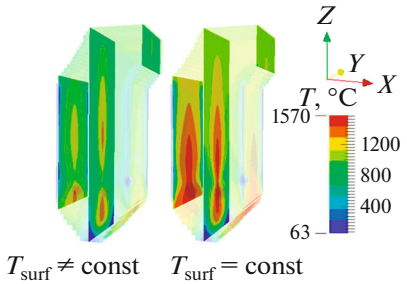

Fig. 2. Temperature fields in three longitudinal sections of the combustion chamber of the BKZ-75 boiler: $X = 0.2$, 3.19, and 7 m.

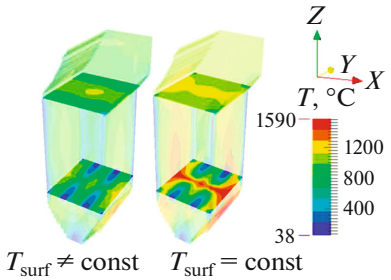

Fig. 3. Temperature distributions in two cross sections of the combustion chamber in height: $Z = 4$ and 12.65 m.

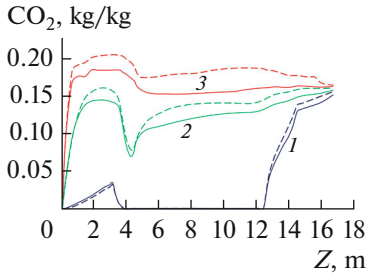

Fig. 4. CO_2 concentration distribution along the height of the combustion chamber of the BKZ-75 boiler ((*1*) minimum, (*2*) medium, and (*3*) maximum concentrations) at two boundary conditions for the wall temperature: solid curve is at $T_{surf} \neq$ const and dashed curve is at $T_{surf} =$ const.

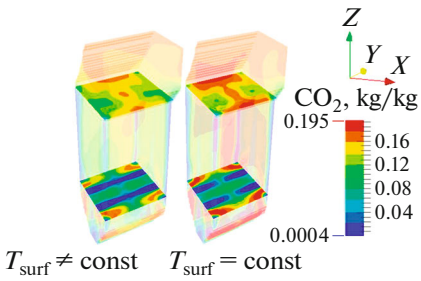

Fig. 5. CO_2 concentration distributions in two cross sections of the combustion chamber: $Z = 4$ and 12.65 m.

where λ is the thermal conductivity between the walls and the pipelines, W/(m^2 K).

The surface temperature of the chamber wall T_{surf} affects the heat flux as a whole, so its calculation is performed by iteration procedures: (a) calculation of the heat flux, (b) calculation of the surface temperature T_{surf}, (c) recalculation of the heat flux with a new surface temperature T_{surf}, and (d) recalculation of the new surface temperature T_{surf}.

RESULTS OF NUMERICAL SIMULATION

Figures 2 and 3 show the temperature distributions over the selected sections of the combustion chamber for two cases of the boundary conditions on the combustion chamber walls: $T_{surf} =$ const and $T_{surf} \neq$ const. In the absence of heat transfer between the wall and combustion products in the chamber ($T_{surf} =$ const), the temperature is higher everywhere: in vertical ($X =$ 0.2, 3.19, and 7 m) and horizontal ($Z = 4$ and 12.65 m) sections. On the temperature scale, the difference in their values for the two boundary conditions can be determined to be about 200°C.

The main reaction in the solid fuel combustion at high temperatures is the chemical reaction of air oxygen with the carbon of pulverized coal, which results in the formation of carbon monoxide CO (in case of incomplete combustion) or carbon dioxide CO_2 (in case of complete combustion).

Figure 4 shows the distribution of minimum, average, and maximum relative concentrations of carbon dioxide CO_2 along the combustion chamber height. The qualitative nature of these distributions in two cases of boundary conditions for the temperature of the combustion chamber walls is almost the same while the quantitative discrepancies in the results with respect to the combustion chamber height are significant. For two variants of boundary conditions, the carbon dioxide concentration along the combustion chamber height has higher values than that in the region of burners. This is explained by the fact that carbon dioxide, as a product of complete combustion, does not have time in the furnace zone to react with air oxygen.

Figures 5 and 6 show the distributions of CO_2 concentrations along the cross sections for two variants of boundary conditions for the temperature of the BKZ-75 combustion chamber walls. The regions with minimal CO_2 concentrations correspond to the fuel supply zones from the burners at $Z = 4$ m (Fig. 5). As the height advances to the outlet of the combustion chamber, the CO_2 concentration increases in both cases of the boundary conditions and, at the output, has the following average values: 0.14 kg/kg at $T_{surf} \neq$ const and 0.16 kg/kg at $T_{surf} =$ const (Fig. 6).

Based on a comparison of the results of computational experiments on the distribution of CO_2 concen-

trations for the two boundary conditions of the temperature of the combustion chamber walls, the greatest (~7%) discrepancies for its mean values are observed in the region of ignition, the formation of a torch, and the zone of the burner belt. This is due primarily to ignition instability, combustion stabilization inside the torch, oxidation intensity, and the formation of combustion products. At the exit from the furnace, where combustion is mostly completed, the differences in the CO_2 concentration profiles for different boundary conditions on the furnace walls are smoothed out and are only ~1.2%.

To select the boundary conditions for the combustion chamber wall temperature that describes best the actual technological process, the results of numerical simulation and experimental data obtained directly at TPP were compared. Figure 7 shows such a comparison. The figure shows the results of numerical calculations and measurements carried out directly at TPP [32], as well as the calculated temperature at the outlet of the combustion chamber obtained by the standard method for the BKZ-75 boiler [33]. We note that the change in the boundary conditions for the chamber wall temperature significantly affects the character of the temperature distribution in the combustion chamber. In the initial sections along the furnace height (up to 1 m), the differences are insignificant because the temperature values are distributed evenly due to the presence of a cold funnel at the bottom of the combustion chamber. However, significant differences in temperature distributions occur in the regions of the burner device arrangement (Fig. 7, zone I) and further along the torch length in the direction to the combustion chamber output (Fig. 7, zone II). This is due to the fact that, when the air mixture is blown from the burners, the fuel ignites and burns and some fraction of the heat is transferred to the walls of the combustion chamber, the temperature of which is constantly changing.

Due to the absence of heat exchange with the medium in the screen tubes at a constant wall temperature T_{surf} = const, the level of turbulent pulsations rises throughout the entire volume of the combustion device, thereby raising the temperature. Analyzing the distributions of the average temperature T over the furnace height, the difference for the two cases of boundary conditions can be seen to be approximately 152°C, which is about 14%. At the same time, the qualitative temperature behavior for the two boundary conditions is the same.

However, only the results of a computational experiment with the boundary condition $T_{surf} \neq$ const coincide with the chamber wall temperature values measured directly at TPP [32], where the average temperature at the combustion chamber outlet is 922°C; at T_{surf} = const, the temperature value is 1074°C. The difference in the calculated temperature at the chamber outlet [33] with the results of our computational experiment for the boundary condition on the chamber walls is only 45°C (4.6%) at $T_{surf} \neq$ const and 106°C (10.9%) at T_{surf} = const. Consequently, the condition for the variability of the temperature of the combustion chamber walls corresponds to the actual conditions of the technological process of burning coal in the combustion chamber of the BKZ-75 boiler at Shakhtinskaya TPP.

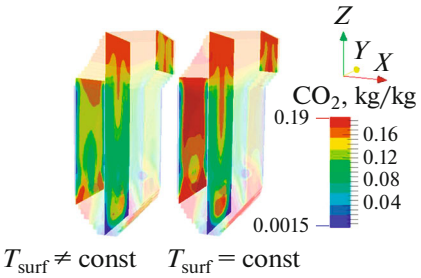

Fig. 6. CO_2 concentration fields in the three longitudinal sections of the combustion chamber of the BKZ-75 boiler: X = 0.2, 3.19, and 7 m.

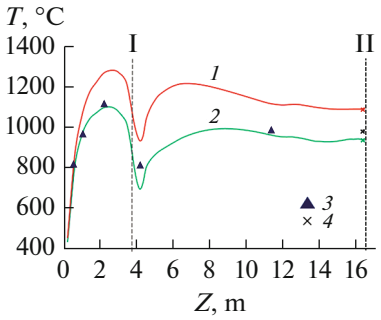

Fig. 7. Comparison of the numerical modeling results ((*1*) T_{surf} = const, (*2*) $T_{surf} \neq$ const) for the combustion chamber of the BKZ-75 boiler with (*3*) full-scale data [32] and (*4*) the calculated value [33].

Analysis of the results showed that the boundary conditions for the temperature of the combustion chamber walls have a significant effect on the data of the computational experiments. At the same time, it should be noted that the choice of the constant temperature T_{surf} = const of the chamber walls in the numerical simulation of the pulverized coal combustion significantly reduces the computational time, as experience has shown. Thus, in performing numerical studies of heat and mass transfer in high-temperature regions, the boundary conditions for the wall temperature must be selected proceeding from the goal (the determination of exact values of unknown quantities or the rapid determination of their approximate values).

CONCLUSIONS

In this work, we performed computational experiments to burn low-grade Kazakhstan pulverized coal under various boundary conditions for the tempera-

ture of the combustion chamber walls. We showed that, when the wall temperature is constant, the thermal (T) and CO_2 concentration characteristics differ significantly from the results of a numerical calculation with temperature variability on the furnace walls. At the furnace outlet, the temperature is $T = 922$°C in the case of a variable wall temperature and $T = 1074$°C at a constant wall temperature. Comparison of the obtained data with the results of field experiments performed directly at TPP and with the calculated temperature at the combustion chamber outlet showed that the obtained temperature at the chamber outlet with variability of the chamber wall temperature is closer to the experimental data and to the temperature calculated by the normative method ($T = 968$°C). This is confirmed by the fact that the boundary condition for wall temperature variability better describes the combustion and should be a priority in carrying out computational experiments.

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