The computational study of heat and mass transfer processes at combustion of pulverized Kazakh coal in real conditions of energy objects

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The article is devoted to the complex research processes of heat and mass transfer occurring during combustion of solid fuel (coal) in the real conditions in the boiler. The methods of numerical 3D modelling were used to describe the aerodynamic and heat-mass transfer processes characteristics and investigate their exact numerical values. Formation of high-speed flows, its temperature and concentration fields were found during the burning of pulverized low-grade Kazakh coal in the volume of the real combustion chamber. So temperature values increased at core of torch to 1370ºC and monotonically decreased to 922ºC at the outlet of boiler. Carbon dioxide CO₂ has its maximal values ~ 0.16 kg/kg at the outlet of the chamber, and the nitrous oxide NOx have their maximal amount of ~ 1200 mg/m³ (at normal conditions) at the burners’ zone. Obtained results have great practical importance; it will allow improving the operating energy objects and design new combustion chambers of energy boilers and also-burners, finally optimize the whole process of fossil fuel combustion.

Keywords: aerodynamic, combustion, heat exchange, numerical experiment

INTRODUCTION

Solid fuel combustion is a complex physical and chemical phenomenon, which occurs at high temperatures with rapid and complete oxidation of combustible matter (carbon) by atmospheric oxygen while accompanied by a large amount of heat release [1-2]. Due to the low quality of Kazakh coal deposits the exploitation of its coal has many challenges associated with the growth of scientific and applied research. Conducting in-depth research on coal combustion in real conditions can ensure the efficient technological process [3-5]. Increased interest observed in particular in the study of heat and mass transfer processes at combustion of pulverized Kazakh coal with high ash content [6-10]. Combustion processes take place under conditions of strong turbulence and non-isothermal flow, multiphase medium with a significant impact of nonlinear effects of thermal radiation, interfacial interaction and multistage proceeding with chemical reactions [11-12]. Such phenomena have an important role in studying of the natural phenomenon of low-grade coal combustion. So investigations of turbulent chemically reacting media are extremely important to deepen the knowledge of physical and chemical properties and understanding of possibilities for application.

THE STATE OF THE ART

In the context of depletion of natural energy resources and environmental pollution increasing the efficiency of energy generation and solution of environmental problems are urgent and important task to solve [13-15]. Development of technological processes with economic and ecological advantages are the main purpose for many researches in this area. The complex processes of heat and mass transfer in the presence of combustion are non-stationary, strongly non-isothermal with a constant change in the physical and chemical state of the environment. It greatly complicates their experimental study. In this case, studying of heat and mass transfer in high-reacting media with simulation of physical and chemical processes occur during combustion of pulverized coal is important for the solution of modern power engineering industry and ecology problems. In this regard, a comprehensive study of heat and mass transfer processes at high-temperature media is observed. Research based on the achievements of modern physics using numerical methods of 3D modelling are cost-effective and does not require a lot of manpower and a lot of time as in full-scale studies. Applying of computational technology allow us to describe the actual physical processes that occur during combustion of energy fuel as accurate as possible [16-19]. Finally, the objective of this paper focused on numerical experiments and

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studying of heat and mass transfer processes occurring in the areas of real geometry of the combustion chamber during the burning of fuel. A mathematical model of physical-chemical combustion process has been established.

**PROBLEM STATEMENT**

Study of processes of heat and mass transfer during coal combustion is possible only based on a complete knowledge of combustion physics. It includes a wide range of physical and chemical effects and its formulation of a mathematical model. The fundamental laws of conservation of mass, momentum and energy are used for the simulation of heat and mass transfer in the presence of physical and chemical processes [20-23]. As it known the heat and mass transfer processes in the presence of physical and chemical transformations are the interaction of turbulent flows. Therefore, the chemical processes here should take into account the law of conservation of components of the reacting mixture, multiphase medium, its turbulence degree, heat generation due to the radiation of heated fluid and chemical reactions.

**Basic equation**

The law of conservation of substance written in the form of the law of conservation of matter as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = q_{\text{n}} \tag{1}$$

The law of conservation of momentum and the equation of motion expressed as:

$$\frac{\partial}{\partial t} (\rho u_i) = -\frac{\partial}{\partial x_j} (\rho u_i u_j) + \frac{\partial}{\partial x_j} (\rho P) + \rho f_i \tag{2}$$

Law of energy conservation:

$$\frac{\partial}{\partial t} (\rho h) = -\frac{\partial}{\partial x_j} (\rho u_j h) + \frac{\partial}{\partial x_j} (\rho q_{\text{n}}) + \frac{\partial P}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_i u_j) + \tau_{ij} + S_i \tag{3}$$

The conservation law for the components of the reaction mixture:

$$\frac{\partial}{\partial t} (\rho C_{\beta}) = -\frac{\partial}{\partial x_j} (\rho C_{\beta} u_j) + \frac{\partial}{\partial x_j} (\rho \dot{C}_{\beta}) + S_\beta \tag{3}$$

For technical flame matter transfer is taken into account only by diffusion. Transfer of substance due to the pressure gradient, the action of external forces (electric and magnetic fields) and thermal diffusion are small and they be neglected. Then the last equation is written as follow:

$$\frac{\partial}{\partial t} (\rho C_{\beta}) = -\frac{\partial}{\partial x_j} (\rho C_{\beta} u_j) + \frac{\partial}{\partial x_j} \left( \frac{\mu_{\beta}}{\sigma_{\beta \rho_{\beta}}} \frac{\partial C_{\beta}}{\partial x_j} \right) + S_\beta \tag{4}$$

the standard $k$-$\varepsilon$ turbulence model is used in this paper for modelling of turbulence flows excluding the effect of lift or “twist” of flow, which is represented by the equation of turbulent kinetic energy transfer:

$$\frac{\partial (\rho k)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j k) = \frac{\partial}{\partial x_j} \left( \frac{\mu_{\text{eff}}}{\sigma_k} \frac{\partial k}{\partial x_j} \right) + \left( \frac{\varepsilon^2}{k} - \varepsilon \right) P - \rho \varepsilon \tag{5}$$

In addition, the equation of dissipation (turbulent kinetic energy conversion into internal) turbulent kinetic energy $\varepsilon$:

$$\frac{\partial (\rho \varepsilon)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j \varepsilon) = \frac{\partial}{\partial x_j} \left( \frac{\mu_{\text{eff}}}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_j} \right) + C_{\varepsilon} \frac{\varepsilon}{k} \rho \varepsilon - \frac{C_{\varepsilon}}{k} \rho \frac{\varepsilon^2}{k} \tag{6}$$

Here the kinetic energy production:

$$P = \mu_{\text{turb}} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) = \frac{2}{3} \rho \varepsilon \frac{\partial u_i}{\partial x_j} \tag{7}$$

In addition, the rate of dissipation of turbulent energy:

$$\rho \varepsilon = \mu_{\text{turb}} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \tag{8}$$

If $k$ and $\varepsilon$ are known, the turbulent viscosity determined by the Prandtl-Kolmogorov relationship is:

$$\mu_{\text{turb}} = \frac{\text{c}}{\rho} \frac{k^2}{\varepsilon} \tag{9}$$

Empirical constants like $c_{\rho}$, $c_{\varepsilon}$, $c_{\mu}$, $C_{\mu}$ and $C_{\varepsilon}$ in previous equations are determined experimentally. For our case, they are taken as $c_{\rho} = 0.09$; $c_{\varepsilon} = 1.00$; $c_{\mu} = 1.30$; $C_{\mu} = 1.44$; $C_{\varepsilon} = 1.92$. For the turbulent numbers of Prandtl and Schmidt taken 0.9 [24].

A generalized equation of the transport value in a turbulent flow will then be:

$$\frac{\partial}{\partial t} (\rho \Phi) = -\frac{\partial}{\partial x_j} (\rho u_j \Phi) + \frac{\partial}{\partial x_j} \left( \frac{\mu_{\text{turb}}}{\sigma_{\rho \Phi}} \frac{\partial \Phi}{\partial x_j} \right) + S_{\text{Phi}} \tag{10}$$

High-temperature media emits heat during combustion. As a result, this thermal energy is transformed into radiant energy on the surface of the heated body. Thus, the energy equation in the study of heat and mass transfer during combustion considered the heat exchange by radiation. On the heat-exchange by radiation has a major influence of the water vapor and carbon dioxide. Heat exchange by radiation can be treated in modeling of flows at temperatures $500 \, K < T < 2000 \, K$ in the region of the visible and infrared parts of the spectrum. The emissivity of the gas mixture consists of components emissivity, and depends on the partial pressure, temperature and wavelength.
The six-flow model [25] is used to determine the intensity of the radiation in this study.

Physical and chemical processes occurring in the combustion chamber are rapid and complete processes of oxidation of the fuel (in this case high-ash content coal). These processes take place at high temperatures, accompanied by a large release of energy due to chemical reactions and changes in the concentrations of all substances interact. To describe real physical transformations that occur during combustion of fuel, and to avoid mistakes that can lead to a physically meaningless result, an adequate initial and boundary conditions corresponding to real physical process are given, while an adequate numerical model [26-27] of physical process is also chosen. Chemical reactions, which in turn determines the source terms in the equations for energy and the substance components. A chemical model is adopted in this paper it takes into account only the key components of the reaction. A Mitchell-Tarbell model was used [28], which takes into account the rank of coal for modelling nitrogen-containing components (in this case for the Kazakh coal ash content is 35.1%). The Mitchell-Tarbell model demonstrates the formation of nitrogen oxides NOx by the oxidation of fuel bound nitrogen. The kinetic scheme takes into account the reaction of the primary pyrolysis, homogeneous combustion of hydro carbonaceous compounds, heterogeneous combustion of coke and formation of nitrogen compounds by thermal and fuel NOx mechanisms.

The Florean software package were used for computational simulations of heat and mass transfer processes during combustion of pulverized coal. And as an object of research was chosen the combustion chamber of the real energy boiler BKZ-75 Shakhtinsk TPC, Kazakhstan). All conditions taken into account describe real processes of solid fuel combustion. Control volume method were used for conducting numerical modelling, where the chamber has been divided into 126 496 cells in computational experiment.

RESULTS OF NUMERICAL MODELLING

The following results show three-dimensional modelling of heat and mass transfer processes during combustion of pulverized low-grade coal in real conditions of combustion chamber of boiler. Aerodynamic pattern of motion of two-phase turbulent flow of pulverized coal combustion causes the heat and mass transfer process in general [29-30]. Fig.1 shows a two-dimensional graph of the full velocity vector, determined by the relationship:

$$\overrightarrow{V} = \sqrt{U^2 + V^2 + W^2}.$$ (11)

Flows’ speed decreased in the direction of camera output. The peak area values with maximum speed of 20 m/s is clearly visible. The burners were located at 4 m by height of chamber burners, they fed fuel and oxidant mixture into the camera at maximum speed. Distribution character of full velocity vector in Fig.1a depends on the geometrical design of the chamber and due to the vortex transfer of reacting medium. At the outlet region of chamber \((Z\sim16\,\text{m}, \text{Fig.1b})\), it is seen that velocity has a maximum value 8.76 m/s, while an average value does not exceed 5 m/s by height.

![Fig.1. Distribution of full velocity vector](image)

The maximum perturbation of turbulence characteristics notably in the vortex region, this cause the highest change of velocity (Fig.2). The presence of a stream of vortices in the central region of the combustion chamber is advantageous for the combustion of pulverized coal (heat transfer and mass transfer).

Fig.3a shows the distribution of maximum, minimum and average values of the temperature field in the combustion chamber.

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Fig. 2. 2D distribution of turbulence characteristics

Fig. 3. Distribution of temperature fields and its verification with known data

A sharp decrease in temperature observed at fuel feeding zone—because the fuel supplied there by a lower temperature. It can be seen that temperature values reach their maximum in the area below the burner’s zone where torch core is located (approximately at 3 m). This was caused with the eddy currents (from installed four burners: on two burners on two opposite tiers) that have a maximum convective transfer. This increases the residence time of coal particles here. As a result, the temperature rise to \(\sim 1370^\circ C\) in this area. Moreover, maximum value of temperature is about 900-950\(^\circ C\) at the output of the chamber. This is clearly seen from the 3D view of temperature in Fig. 3b. The point of the theoretically calculated value of the temperature of exhaust gases for this boiler defined according to the normative method of thermal calculation [31] data from the natural experiments held in real TPP of RK [32] are presented in Fig. 3a.

Fig. 4. 3D temperature distribution by the chamber sections

The method of thermal calculation in power engineering is still the most reliable for finding the temperature at the outlet of the combustion chamber. It is seen that the difference between results of numerical calculation and known data is only 4.7\%. This proves that the method of 3D modelling gives us a good description of real processes of heat and mass transfer fuel combustion.

The following Fig. 4, which shows the 3D temperature distribution by the chamber sections, observed the same character as in the previous
Temperature values are monotonically fall by the height of the combustion chamber.

From 3D view of temperature it is seen that the core of flame is located in the lower part of chamber (section Y=3.19 m, Fig.4a). The maximal value of temperature is equal to 1340°C there and they decreased by the height of camera. So temperature has the value 940°C in average in section Z=12.65 m (Fig.4b), when it has 922°C at the section Z=7 m (the output of chamber, Fig.4b).

Below the results of 3D modeling of carbon dioxide CO and nitrogen oxides NOx concentration distributions are shown.

![Fig.5](image1.png)

**Fig.5.** 3D distribution of the carbon dioxide concentrations on sections of the chamber (CO₂, kg/kg)

Carbon monoxide CO completely react with oxygen O₂ and further form carbon dioxide CO₂. Concentrations of carbon dioxide CO₂ have their largest amount at the top areas of chamber (Fig.5a, section Y=3.19 m). In addition, the minimal values are observed at the region, where the burner equipments are set.

Analyzing the Fig.5a it is seen that concentration of carbon dioxide CO₂ has the minimal value equal to 0.0089 kg/kg at the section Y=3.19 m. In average it is raised to ~ 0.13 kg/kg at the Z=12.65 m section by height and ~ 0.15 kg/kg at the outlet of the chamber (section X=7.0 m, Fig.5b).

Nitrous oxides NOx are formed by seven main nitrous compounds, but it is considered to negligible others except of nitrous monoxides NO and dioxides NO₂ (in total NOx). The NOx formation mechanism is caused mainly with the fuel-N compound. The maximal amount of nitrous oxides NOx concentration is presented at the burners zone and equal to 0.0109 kg/kg (Fig.6a, see section Y=3.19 m). As it shown in Fig.6 the decreasing of nitrous oxides concentration is observed with height of boiler. It has the average value equal to 5.09·10⁻¹² kg/kg at the output of the combustion volume (section X=7.0 m, Fig.6b).

![Fig.6](image2.png)

**Fig.6.** 3D distribution of the nitrogen oxides concentrations on sections of the chamber (NOx, kg/kg)

Obtained results of computational simulation of carbon dioxide CO₂ and nitrous oxides NOx concentration distributions were verified with the known data as shown in Fig.7.
Concentrations of carbon dioxide CO$_2$ (Fig. 7a) and nitrous oxides NOx (Fig. 7b) are in a good agreement with experimental data, received from real thermal power plant equipment [32]. Moreover, nitrous oxide NOx concentrations meet the requirements of limit value for Kazakhstan Republic TPP [33]. By comparison of numerical experiment results held in this work with natural data from TPP, it can be noticed that the difference is for carbon dioxide CO$_2$ is 4% and for nitrous oxides NOx is 5%. Finally we can confirm the observed method of research of heat and mass transfer processes is fairly reliable and efficient. Also, the method of computer simulation can be useful in studying the technological processes of low-grade coal combustion in energy objects.

CONCLUSIONS

In conclusion, velocity characteristics of turbulent flows, their turbulent kinetic energy and dissipation energy are determined via computational modelling experiments on heat and mass transfer processes during combustion of Kazakh coal. Aerodynamic characteristics of flow shows the intensive mixing of fuel and oxidant, which is held in the central part of the chamber. It caused the increasing of temperature values at core of torch to 1370°C and monotonically decreasing to 922°C at the outlet. Formation of hazardous substances as carbon and nitrous oxides (CO$_2$, NOx) are depends on their chemical interaction with oxygen. Carbon dioxide has its maximal values at the outlet of the chamber (~ 0.16 kg/kg), and the nitrous oxides have its maximal amount of ~ 1200 mg/Nm$^3$ ($N$ means normal conditions) at the burners’ zone. Obtained results of numerical experiments have great theoretical and practical importance. It allow to improve design of combustion chambers and burners, to optimize the process of burning of high-ash content energy coal of Kazakhstan Republic.

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