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Numerical Modeling of Pulverized Coal Combustion at Thermal Power Plant Boilers

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The paper deals with development and application the numerical model for solution of processes at combustion chamber of the thermal power plant boiler. Mathematical simulation is based on solution of physical and chemical processes occuring at burning pulverized coal in the furnace model. Three-dimensional flows, heat and mass transfer, chemical kinetics of the processes, effects of thermal radiation are considered. Obtained results give quantitative information on velocity distributions, temperature and concentration profiles of the components, the amount of combustion products including harmful substances. The numerical model becomes a tool for investigation and design of combustion chambers with high-efficiency and reliable operation of boiler at thermal power plants.

Keywords: combustion, emission, modeling, thermal power plant

Introduction

Combustion is undoubtedly complex physical and chemical process of burning of fuels in combustion chambers at attendance of access of an oxydizer. Investigation effort for preparation, development and application of numerical models solving three-dimensional flows, heat and mass transfer, chemical kinetics of the combustion processes, and effects of thermal radiation in combustion chambers gives possibilites to obtain knowledge on complex combustion processes [1]. The system of balance equations - balance of mass, momentum, and energy – is theoretical basis for physical description of three-dimensional fluid flow [2]. The numerical task is formulated. Numerical solution of this system can be solved by means of finite volume method to obtain flow parameters, namely velocity vector distributions. Results of calculations of motion and heat and mass transfer in gas phase obtained by means of the Eulerian approach are expressed in the form for Lagrangian approach for solution of heat and mass transfer and chemical processes of individual fuel particles. Obtained results at application of the computational model of pulverized combustion in combustion chamber are expressed as distributions of velocity vector in solved domain, as streamlines and trajectories of particles. Tempertature profiles in the combustion chamber can be depicted. Important information on combustion proces is given by means of data on distribution of concentration of combustion products in the solved domain, namely carbon oxides (carbon monooxide CO, carbon dioxide CO_2), nitrogen oxides (nitrogen monoxide NO, and others).

The numerical model of pulverized coal combustion is applied for investigations in the field of thermophysics but also for design of new boilers of thermal power plants (particularly in Kazakhstan) and for replacement of obsolete equipment by new boiler instalations for thermal power plants working on existing and new depo-

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sits of coal.

Models of physical and chemical processes

The study of heat and mass transfer in high-temperature environments occurring in physical and chemical processes is performed and fundamentals are used in the chemical, mathematical and physical models. These models include a system of three-dimensional Navier-Stokes equations of heat and mass transfer with the source terms, which are determined by the chemical kinetics of the process, nonlinear effects of thermal radiation, the interfacial interaction and multistage chemical reactions. The basic equations used to solve the problem are the following:

– The law of conservation of mass (continuity equation):

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0; \tag{1}$$

– The law of conservation of momentum (Navier-Stokes):

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

where ρ – density, t – time, $u_{i,j}$ – velocity in direction i, j, $x_{i,j}$ – Cartesian coordinates, $\tau_{i,j}$ – viscous stress tensor, P – pressure, f_i – the external force;

– The law of conservation of energy (the first law of thermodynamics):

$$\frac{\partial}{\partial t}(\rho h) = \frac{\partial}{\partial x_i}(\rho u_i h) - \frac{\partial q_i^{\text{res}}}{\partial x_j} + \frac{\partial P}{\partial t} + u_i \frac{\partial P}{\partial x_i} + \tau_{ij} \frac{\partial u_j}{\partial x_i} + S_h, \tag{3}$$

where h – specific enthalpy, q_i^{res} associated with energy transfer by conduction and diffusion flux of matter, S_h - a source of energy due to chemical reactions and radiative heat transfer;

– The conservation of components of the mixture:

$$\frac{\partial}{\partial t}(\rho C_\beta) = -\frac{\partial}{\partial x_i}(\rho C_\beta u_i) + \frac{\partial j_i}{\partial x_i} + S_\beta, \tag{4}$$

where C_β - mass concentration of the components β, j_i - a weight average flow in the i-th direction, S_β - components of source term β.

To describe the motion and heat and mass transfer of gas phase, the numerical method is used, which is based on the Euler approach. This method uses the spatial balance equations of mass, momentum, energy to the gas mixture, concentrations of gaseous components, Eqs.(1) to (4), respectively. To describe the motion and heat and mass transfer of individual particles of fuel along their trajectories Lagrangian approach [3] is used. The turbulent flow pattern is described by means of a two-equation k-ε turbulence model, where k - turbulent kinetic energy, ε - turbulent energy dissipation. Radiation heat transfer is determined by six-flux radiation model [4, 5].

The above system of equations describing fluid dynamics and thermal aspects of gases moving in combustion chamber is solved numerically.

In the simulation of the formation of the products of combustion in coal-dust flame, kinetic model of chemical reactions is used, which is valid for a wide range of temperatures and concentrations of the reactants. However, due to the high computational cost or due to lack of information about all the intermediate reactions, detailed modeling of the reactions can be performed only in simple cases, e.g. for the combustion of carbon monoxide.

Used integrated model of the reaction is based on the fact that most chemical reactions occur in several stages, while the slowest reaction step determines the speed of the reaction. A plurality of multistage reactions can be modeled using one-step reaction patterns and kinetic data are determined by the slowest stage of the reaction. Model of pulverized coal used in this study takes into account the integral component of the fuel oxidation reaction to the stable end products of the reaction [6]. In this case, the reaction intermediate, education and changing unsustainable intermediates are not included.

In operation the combustion model is considered as the following steps:

- Pyrolysis with the release of volatile substances and the formation of coke,
- The combustion of the volatile products and carbon monoxide,
- Burning coke.

Modeling of pyrolysis

Combustion model should describe only the local heat from the combustion products of combustion and influence on heat transfer. Therefore, the choice of models of pyrolysis and combustion renounced the use of bulky systems with many components.

A single stage pyrolysis model described in references [1, 2, 6] is used, as in this case the stechiometric coefficients of the pyrolysis reaction can be deduced from expression data analysis, which is important and preferred. In addition, this model works quite accurately, and in many cases is a good compromise to reduce computational cost.

Modeling of burning the volatile substances

Pyrolysis products mixed with air form a reactive mixture. Reaction rate of combustion of gaseous products are so high that approximation of diffusion combustion is acceptable. In describing the process of pyrolysis, volatiles are treated as fictitious hydrocarbons. Since the interest is primarily only the velocity and heat by oxidation at high temperatures, sufficient oxygen combustion of

volatile substances can be represented as a two-step reaction, assuming that first oxidizes the volatile substances to CO and H_2O [2]:

$$C_xH_y + (\frac{x}{2} + \frac{y}{4})O_2 \rightarrow xCO + \frac{y}{2}H_2O,$$

and the second step - the oxidation to CO_2 [1]:

$$xCO + \frac{x}{2}O_2 \rightarrow xCO_2 \cdot$$

Modeling cokes burning

The heterogeneous reaction of combustion of solid carbon on the surface of the coke particles is determined by the diffusion of oxygen from the environment into the boundary layer of a porous medium and in the particles, as well as the reaction between carbon and oxygen on the surface of the particle. The slowest of these processes determines the rate of burning coke. Depending on the diameter and the temperature of the particles, carbon monoxide or carbon dioxide will be formed [10]:

$$C+O_2 \rightarrow 2CO, \quad 2CO + O_2 \rightarrow 2CO_2 \cdot$$

It is assumed that the combustion of coke fuel particle diameter ranges from d_1 to d_2. When the particle size of the volatile components is not changed, and the fuel density changes only - the density of the dry coal ρ_1 coke to a density ρ_2:

$$d_2 = d_1 \left[\frac{A_p}{(1-W_p)(1-f_n)} \right]^{0.333}, \qquad (5)$$

where A_p, W_p – fraction of ash and moisture after grinding coal, respectively, f_n – mass fraction of volatiles in the dry coal.

The change in the concentration of carbon coke ξ_C is defined by the equation:

$$\frac{d\xi_C}{dt} = -K_C A_{sp} \xi_C, \qquad (6)$$

where K_C – rate constant of the oxidation of carbon coke, and A_{sp} – specific surface area of particles, referred to its mass.

For the reaction of order n we have the relation:

$$K_C = K_{kin} \left(p_{O_2} - \frac{K_C}{K_d} \right)^n \cdot \qquad (7)$$

There K_{kin} - the kinetic rate constant of carbon combustion reaction component coke, K_d - diffusion constant velocity oxidant, p_{O_2} - relative partial pressure of oxygen. Reaction order n has the following values: for coal – 1.0, for brown coal - 0.5. Then, for example, to have a relation of coal:

$$K_C = \frac{p_{O_2}}{\frac{1}{K_d} + \frac{1}{K_{kin}}} \cdot \qquad (8)$$

The contribution is determined by the diffusion of oxygen through the effective diffusion coefficient according to [7]:

$$K_d = \frac{ShM_C f_m D_{O_2}}{Rd_p T_{GS}}, \qquad (9)$$

where M_s – molar mass of carbon; Sh - number of Schwarzschild (for spherical particles accept Sh = 2); $T_{GS} = \frac{T_G + T_P}{2}$ – an average temperature of the mixture; T_G and T_P – temperature of gas and solid particles, respectively; $D_{O_2} = D_{0,O_2} \left(\frac{T_{GS}}{T_0} \right)^{1.75}$ – the diffusion coefficient of oxygen to the surface of the particle [7], $D_{0.O2} = 3.49 \times 10^{-4}$ m^2/s – self-diffusion coefficient at $T_0 = 1600$ K [8].

The contribution of chemical reactions is determined by the rate constant of a chemical reaction, which is expressed by the relation [9]:

$$K_C = k_{0,C} e^{-\frac{E_{a,C}}{RT_p}} \cdot \qquad (10)$$

Kinetic parameters $k_{0,C}$ and $E_{a,C}$ used in the calculations are taken from [9]. Their values are $k_{o,C} = 2.22 \cdot 10^{12}$ 1/s and $E_{a,C} = 1.69 \cdot 10^5$ kJ/kmol.

Thus, in general, for the chemical reaction of combustion of coke formed of order n we have the expression:

$$\frac{d\xi_C}{dt} = -\xi_C A_{sp} p_{O_2}^n K_{kin} \left(1 - \frac{k_C}{K_d p_{O_2}} \right)^n \cdot \qquad (11)$$

Nitrogen oxides (NO and NO_2) cause photochemical air pollution, acidification of atmospheric moisture and the depletion of the ozone layer and are considered the most toxic emissions. Reducing the concentration of nitrogen oxides at the outlet of the combustion chamber is a very important task in the organization and optimization of the combustion process of coal in the power station.

Formation of nitrogen oxides

The calculation of NO_x formation was based on the proposed model in references[10, 11]. When burning coal has greatest contribution to the formation of nitrogen oxides, nitrogen gives fuel (fuel nitrogen oxides). Nitrogen oxides are also formed from molecular nitrogen air (thermal nitrogen oxides). The proposed kinetic model takes into account the evolution reaction volatiles coal, homogeneous combustion of hydrocarbon compounds, heterogeneous combustion of coke formation of thermal NO_x and fuel.

The process of formation of nitrogen oxides can be represented as follows: the thermal decomposition of coal particles exits, the nitrogen contained in the fuel, and about 80% of bound nitrogen in the fuel is gasified as cyanides (HCN).

The resulting transformed into amines cyanides which either react with oxygen to form NO, N_2, or from reduced NO:

$$HCN+H_2O+0.5O_2 \rightarrow NH_3+CO_2,$$

$$NH_3+O_2 \rightarrow NO+H_2O+0.5H_2,$$

$$NH_3+NO \rightarrow N_2+H_2O+0.5H_2.$$

The remaining 20% of the nitrogen is oxidised to NO at once at a speed proportional to the rate of coke burning residue:

$$N+0.5O_2 \rightarrow NO.$$

Furthermore, the following reaction in the formation of HCN by reacting hydrocarbons with NO is:

$$NO+\frac{1}{m}C_mH_B+\frac{3-\frac{B}{m}}{2}H_2 \rightarrow HCN+H_2O$$

where C_mH_B is – the yield of volatile from coal [11].

and heterogeneous reaction between NO and coke particles:

$$C+2NO \rightarrow CO_2+N_2.$$

To close the model of formation of nitrogen oxides it is sufficient to determine the values of the rates of chemical reactions responsible for the change in concentrations of NH_3, HCN, NO, O_2, coke and volatile substances, which were taken from [11].

Simulation of pulverized coal combustion in an industrial boiler

The theoretical model of combustion process described above was applied at numerical simulation fluid dynamics, heat transfer and chemical processes in an industrial boiler. Calculation domain is proposed according to power boiler BKZ-75 Shakhtinskaya thermal power station (Kazakhstan). The domain is depicted in Fig.1, where dimensions and discretization of structured grid are shown. Combustion chamber is equipped with four vortex dust burners, established two on the front ant two on the rear side in one layer. The sheme of the vortex burner is shown in Fig.2.

The fuel is pulverized coal is from Karaganda and has ordinary 35.1% of coal ash, volatile 22.0%, 10.6% moisture content and calorific value of 18.55kJ/kg.

Following initial and boundary conditions were defined for the task :

for the velocity:

$\left.\frac{\partial u_i}{\partial x_i}\right|_{normA} = 0$ - derivative of velocity normal to the exit plane;

$u_i|_{normS} = 0$ - velocity normal to the plane of symmetry;

$\left.\frac{\partial u_i}{\partial x_i}\right|_{normS} = 0$ - derivative of velocity normal to the plane of symmetry;

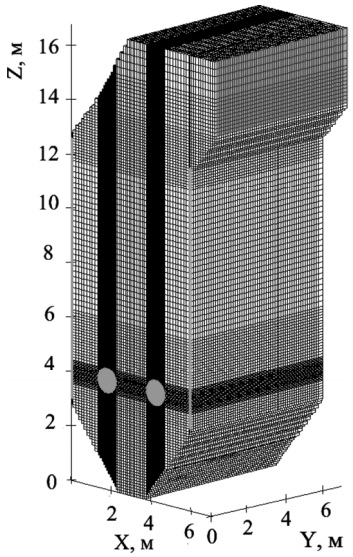

Fig. 1 Computational domain and finite volume discretization grid of the combustion chamber

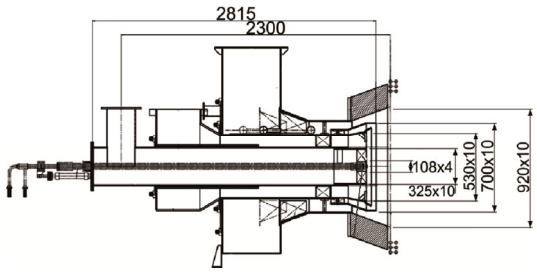

Fig. 2 Scheme of pulverized coal burner.

$u_i|_{normW} = 0$ - velocity normal to the wall, no mass flow;

$\left.\frac{\partial u_i}{\partial x_i}\right|_{normW} = 0$ - derivative of velocity normal to the walls;

$u_i|_{tang} = 0$ - tangential to the wall speed, slip condition;

for pressure:

$\partial p|_{rand} = 0$ - correction to the pressure at the border;

for energy:

$h = C_pT$ - specific enthalpy, T - inlet temperature;

$\left.\frac{\partial h}{\partial x_i}\right|_{normA} = 0$ - derivative of enthalpy normal to the exit plane;

$\left.\frac{\partial h}{\partial x_i}\right|_{normS} = 0$ - derivative of enthalpy normal to the plane of symmetry;

$\left.\frac{\partial h}{\partial x_i}\right|_{\tan gS} = 0$ - derivative of enthalpy tangential to the

plane of symmetry;

for the components of the mixture:

c_k - the initial concentration of component k at the input;

$\left.\frac{\partial c_k}{\partial x_i}\right|_{normA} = 0$ - derivative of c_k normal to the exit plane;

$\left.\frac{\partial c_k}{\partial x_i}\right|_{normS} = 0$ - derivative of c_k normal to the plane of symmetry;

$\left.\frac{\partial c_k}{\partial x_i}\right|_{normW} = 0$ - derivative of c_k normal to the solid surface.

The numerical experiments and the creation of a database for the simulation were carried out in several stages using software systems and application control volume method. A 3-dimensional computational fluid dynamics code was used to analyze the performance of boiler with pulverized coal combustion. As an effective method for design, optimization and problem solved in power plant operation, the FLOREAN – code, which predicts thermal and hydrodynamic aspects of flue gases mixing in the near wall region and inside the furnace was chosen. Program FLOREAN is based on the numerical solution of the Reynolds averaged balance equations for mass, species, energy and momentum [12]. This program was used on other boilers of thermal plants and shows believable results with good accuracy of 2% [13-15].

The used software package needs to create source files that contain physical and geometrical data of the test process. For the calculation the entire computational domain is divided into 1 500 000 unit control cells (volumes), the nodes in the region of furnace of size 6× 6.6×16.75 m. It enables to solve the system of nonlinear equations for heat- and mass transfer processes in each control volume of investigated furnace.

From calculations it was possible to find the changes of flow velocities in the central section of combustion chamber, see Fig.3. Area of the fuel mixture flow through the burner are clearly visible and maxima are observed. At the distance 3 meters from the level of the burner, velocity is reduced, and the velocity field is leveled, evenly distributed over the cross section of the combustion chamber. In the field of coal-fired burners intense eddy currents are observed. They evolve into a parallel flow towards the exit of the combustion products from the furnace.

Figure 4 depicts temperature conditions, characteristic of combustion of coal dust in the combustion chamber, created in turbulent jets. They are determined by intensity of heat and mass transfer in the jets and the nature of their spread in the furnace. Therefore, the physical conditions of combustion in turbulent jets are determined by the laws of the distribution of temperature and velocity. Lots of convective transport in the furnace is observed in pulverized coal feed mixture. Consequently, the most intensive combustion takes place in the central part of the furnace, as indicated by the maxima in the temperature distribution in the various sections of the combustion chamber Fig.4(c).

Combustion reactions occur in those areas most intensively. They are associated with significant changes in temperature in the region close to the reaction zone in the flame peaks detected in the temperature distribution and its gradient. Temperature is gradually decreased to exit from the combustion chamber Fig.4(b,c).

The chemical and the mechanical completeness of combustion can be judged from the concentrations of products in the fields of chemical reactions in the combustion chamber between the fuel (coal) and the oxidant (oxygen from the air). It can be carried out according to the chemical model scheme described above. Carbon oxides (CO and CO_2) in Fig.5 and nitrogen oxide (NO) in Fig.6 are the main pollutants of the environment. Figure 5(a) shows the distribution of concentration of carbon monoxide in the furnace section at the location of the burners. The maximum value of the concentration is observed at the mouth of the burner ($2\cdot10^{-2}$kg/kg). Figure 5(b) shows the distribution of the CO concentration at the outlet of the furnace, where there is a deficiency of oxygen, and the temperature substantially lower than the flame kernel (Fig.4). It can be seen that the chemical processes associated with the formation of intense CO damped. At the exit of the furnace average CO concentration is $4.47\cdot10^{-4}$kg/kg, which corresponds to the maximum allowable concentrations taken at thermal power plants, and chemical evidence of the completeness of fuel burnup.

The concentration distributions of CO_2 are shown in Fig.4(c, d). Differences in the formation of CO_2 and CO are evident. It can be seen that the main formation of carbon dioxide takes place at the distance from the center

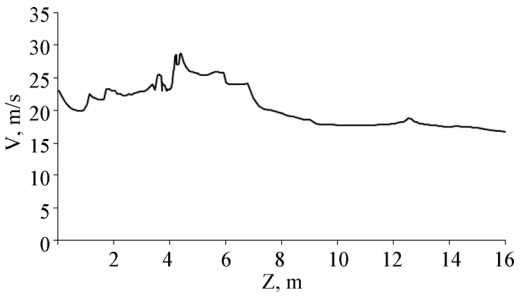

Fig. 3 Distribution of velocity in the central section along the furnace height.

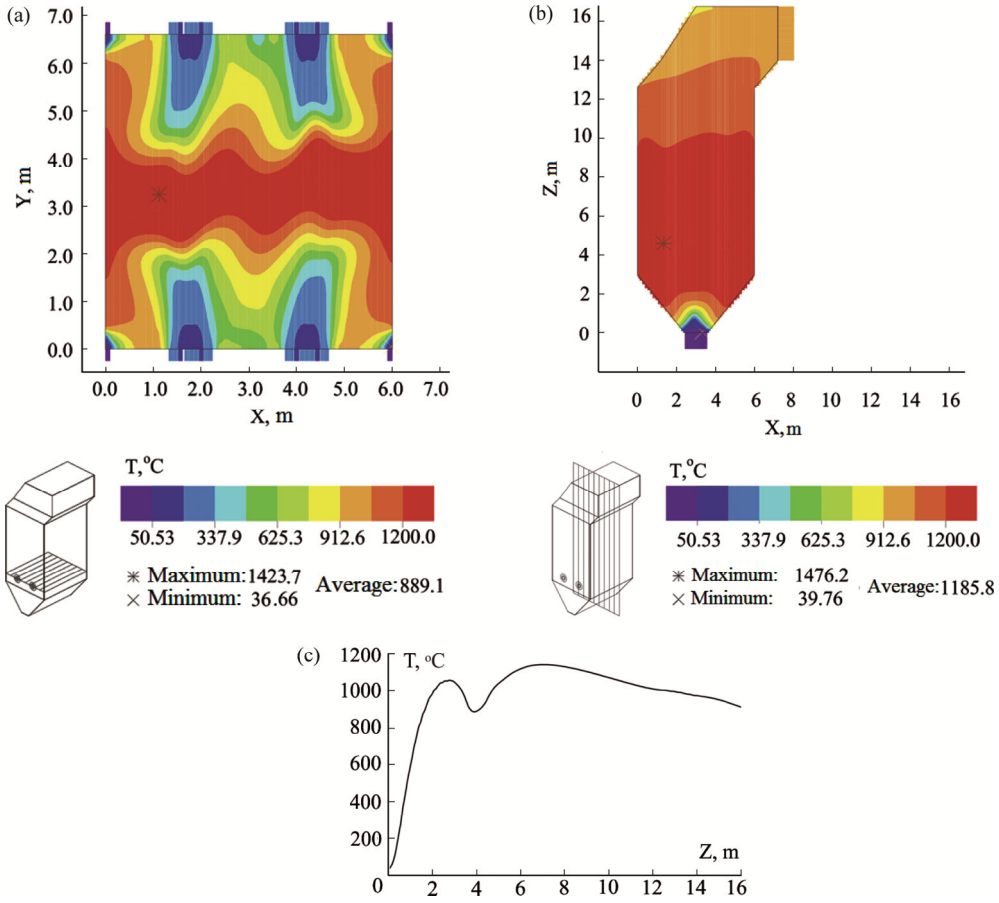

Fig. 4 Temperature profiles at the location of the burner (a), and in a longitudinal section of the furnace (b), and the average of the temperature distribution along the height of the furnace (c).

of the furnace, i.e. at collision region of the fuel and oxidant jets from opposite burners.

This indicates that the formation of carbon oxides is dependent not only on transport phenomena and the kinetics of the process. The fact that carbon and oxygen can react in different ways, is extremely important in the design of combustion chambers. Combustion technology should ensure thorough mixing of the fuel with oxygen and its complete burning to form CO_2, and not to form CO. Otherwise, the heat will fall sharply, in the formation of CO only 28% of the energy released compared to that in the formation of CO_2.

Figure 6 shows the distribution of the NO concentration in the furnace. The highest values of NO concentrations occur in the zone of the burners, where the core of the plume and the highest concentrations of oxygen appear. Thus, the maximum concentration of NO is 3675.4 mg/Nm^3. At the output, the minimum value of the concentration of NO is 565.3 mg/Nm^3, aand the average value of NO at the exit cross section is 609.8 mg/Nm^3. This is quite acceptable for adoption at thermal power station emission standards.

Conclusions

Swirling stream supplying fuel burners through the furnace counter create a vortex flow volume in its central part. In the corners of the furnace due to the direct impact on its wall, flow is distributed into two parts. The main part of the flow is directed upwards, and the other at a slight angle directed downward, evolving into two vortices. Due to the intensity of the vortex motion of dust and gas flows within the furnace significantly increases the residence time of the fuel particles in the furnace, which allows for a more complete burning, even by burning coarser coal dust.

The most intense combustion occurs in the central portion of the furnace, wherein the flow temperature reaches about 1200°C. Due to the fact that the coal particles in this area radiate more intensely and have a higher density, the total surface temperature reaches a maximum near the location of the burner section. Exactly in this area the combustion of fuel occurs more intensively.

The maximum concentrations of the products of combustion in the furnace are observed in the installation of

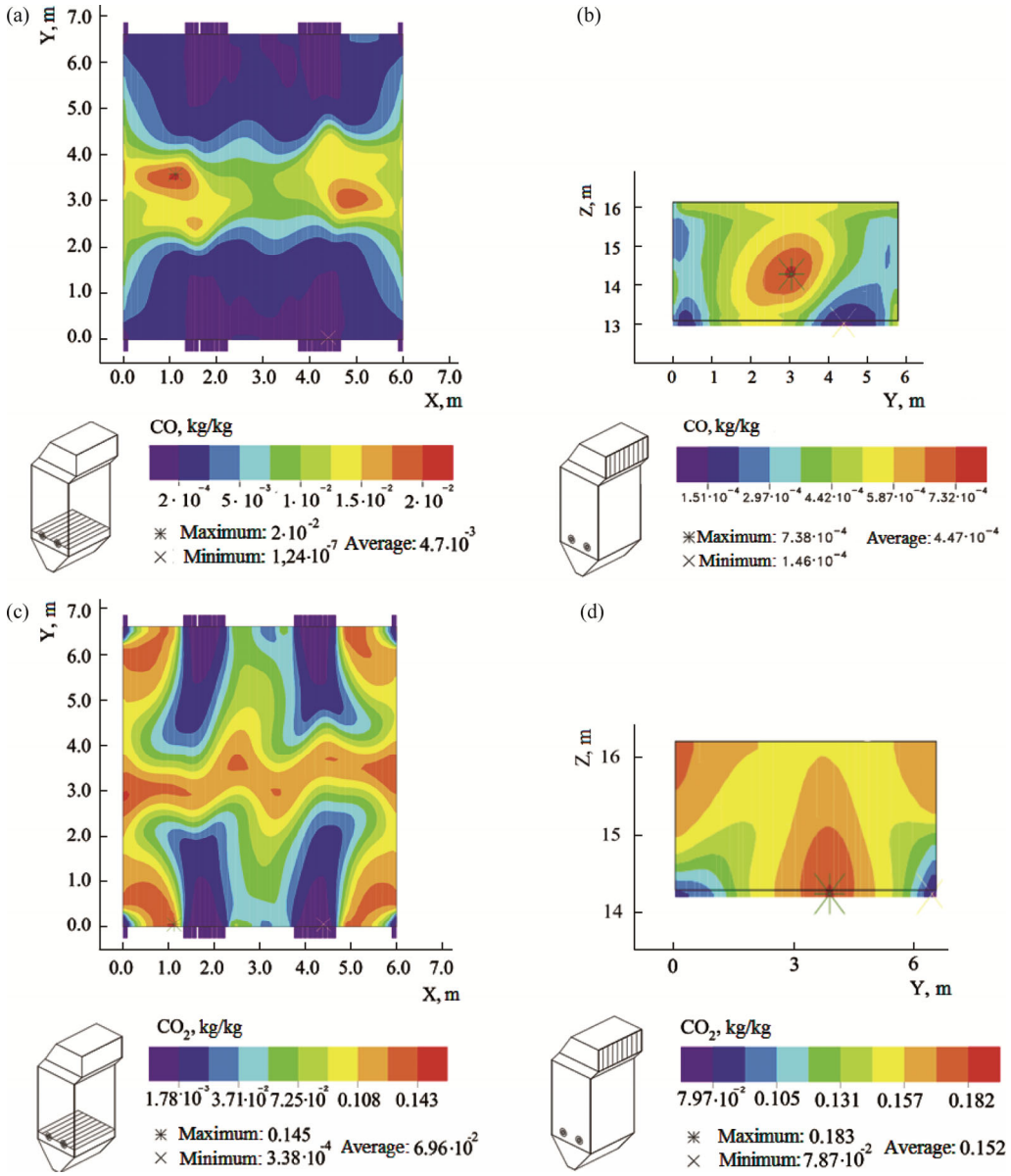

Fig. 5 The distribution of CO and CO_2 concentrations in the cross section at the location of the burner (a), (c), and at the outlet of the furnace (b), (d)

burners, in a section of the nucleus of the torch. At the furnace outlet concentration of harmful emissions do not exceed the maximum permissible concentrations established for coal-fired thermal power stattions in Kazakhstan.

Numerical model of pulverized coal combustion is proposed, verified and applied for solution of flow parameters, heat and mass transfer, and chemical processes at thermal power plant boiler. The model becomes an efficient tool for solving important data needed for design and operation of efficient combustion chambers.

The numerical model can solve special thermophysical problems where air flows in three-dimensional domain and heat and mass transfer processes take place and chemical reactions (namely combustion) are going on.

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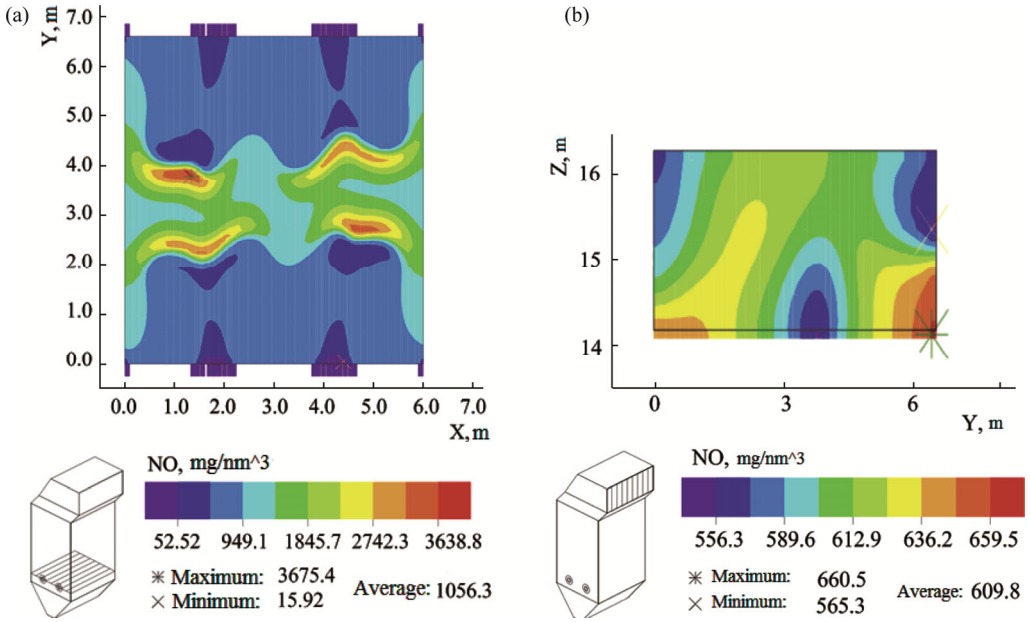

Fig. 6 NO concentration distribution in the cross section at the location of the burners (a), and at the outlet of the furnace (b).

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