3D computer simulation of heat and mass transfer processes to improve the energy efficiency of combustion chambers

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Thermal power plants are the main producers of electricity in the most countries of the world and will remain so for at least the next 50 years. To optimize the combustion of solid fuels, to develop and implement "clean" technologies and to protect the environment and ensure the efficiency of power plants, research of the complex physical and chemical processes in combustion chambers is required. It is also necessary to build adequate physical, mathematical, and chemical models and develop an accurate method for solving the system of differential equations that describes the real technological process of pulverized coal combustion. The results of 3D computer simulation make it possible to obtain data without conducting full-scale experiments, which can be used to substantiate the parameters and modes of thermal and hydro aerodynamic processes in the preparation of subsequent experimental studies on real energy facilities.

Keywords: computer simulation, heat and mass transfer, energy efficiency, combustion

INTRODUCTION

To ensure the energy efficiency of combustion chambers and reduce emissions of harmful substances into the atmosphere, it is necessary to study the problems of solid fuel combustion in heating chambers of thermal power plants (TPPs). Numerical simulation of heat and mass transfer processes in high-temperature reactive media is the main tool for theoretical study of nonlinear heat and mass transfer processes, taking into account various physical phenomena. For numerical simulation of complex physicochemical processes occurring in combustion chambers of operating TPPs, it is necessary to have: an adequate mathematical and physical-chemical model; an exact method for solving a system of differential equations that describe a real technological process of pulverized flame combustion in an existing power plant; a multiprocessor computing system [1-8].

MATHEMATICAL MODEL

Since most practical flows are turbulent, the conservation equations must be considered in averaged and time-filtered or spatial forms, which must be closed using additional turbulent models.

To formulate a mathematical model, we consider the basic equations.

The mass conservation equation can be written:

$$\frac{\partial p}{\partial t} + \frac{\partial}{\partial x_i}(pu_i) = S_i \tag{1}$$

where

S_i - the source of mass. It determines the mass added to the continuous phase and any other sources determined by a specific physical task.

The *mass conservation equation* or the continuity equation takes the form:

$$\frac{\partial p}{\partial t} + \frac{\partial}{\partial x_i}(pu_i) = 0 \tag{2}$$

The momentum conservation equation can be written by the Navier-Stokes equation in the form:

$$\frac{\partial(pu_i)}{\partial t} + \frac{\partial}{\partial x_j}(pu_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \tag{3}$$

$$+pg_i + F_i$$

The stress tensor can be expressed as:

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\mu\frac{u_l}{\partial x_l}\delta_{ij} \tag{4}$$

The energy conservation equation takes into account energy transfer due to conductivity, diffusion, and viscous dissipation:

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$$\frac{\partial(ph)}{\partial t} + \frac{\partial}{\partial x_i}(phu_i) = \frac{\partial p}{\partial t} + u_i\frac{\partial p}{\partial t} - \qquad (5)$$

$$-\frac{\partial}{\partial x_i}\left(k_{eff}\frac{\partial T}{\partial x_i}\right) - \frac{\partial}{\partial x_{ij}}h_iH_j + \left(\tau_{ij}\right)_{eff}\frac{\partial u_j}{\partial x_j}$$

where

$h = \sum_{j'} m_{j'}h_{j'}$ – heat content for ideal gases;

$h = \sum_{j'} m_{j'}h_{j'} + \frac{\rho}{p}$ for incompressible gas flows;

$h_{j'}{}_{T_{ref}}^{T}C_{p,j'}dT$ – j'substance heat content of $J_{j'}$ diffusion flow;

$k_{eff} = k_l + k_t$– effective thermal conductivity (the sum of laminar and turbulent thermal conductivity);

$\left(\tau_{ij}\right)_{eff}$– effective stress tensor;

S_h– source member, which takes into account heat from chemical reactions and other bulk energy sources (heat from radiation, convective exchange between particles and the gas phase and calorific value) [9-17].

When solving the problem, the mathematical model should include specific initial and boundary conditions for the desired functions (velocity, temperature, concentration of the mixture components, etc.) corresponding to the geometry of the selected combustion chamber and the actual technological process of fuel combustion at TPPs.

To solve the problem, the following boundary conditions for the velocity were chosen:

– Input: u_i –input velocity,
– Exit: $-\frac{\partial u_i}{\partial x_i}\Big|_\infty = 0$
– Symmetry plane: $u_i|_{no} = 0, \frac{\partial u_i}{\partial x_i}\Big|_\infty = 0$
–Hard surface: $u_i|_{no} = 0, \frac{\partial u_i}{\partial x_i}\Big|_\infty = 0, \frac{\partial u_i}{\partial x_i}\Big|_{no} = 0, u_i|_{ta} = 0$

The following relation was used for the friction stress on the wall:

$$\tau_W = \frac{\rho C_\mu^{0.25}k_{WP}^{0.5}k}{ln[EE_{y_*}]}u_{i,WP}|_{ta} \qquad (6)$$

To solve the energy equation, we chose the following boundary conditions:

– Input: $h = C_pT$– inlet flow temperature is set,

– Exit: $\frac{\partial h}{\partial x_i}\Big|_{no} = 0,$

– Symmetry plane: $\frac{\partial h}{\partial x_i}\Big|_{no} = 0, \frac{\partial h}{\partial x_i}\Big|_{ta} = 0$

On solid walls, various types of boundary conditions for temperature can be specified. For adiabatic walls, the heat flux q_w is equal to zero; in this case, boundary conditions are used as in the plane of symmetry. In the case of heat exchange between the wall and the liquid, you can set the wall temperature or heat flux. If the convective heat transfer coefficient a is experimentally or analytically determined, then we can use the condition:

$$q_W = \alpha(T_{WP} - T_W) \qquad (7)$$

For the equation for the transfer of the concentration of components, the following boundary conditions can be specified:

– Input: C_p - component concentration value,
– Exit: $\frac{\partial c_\beta}{\partial x_i}\Big|_{no} = 0$
– Symmetry plane: $\frac{\partial c_\beta}{\partial x_i}\Big|_{no} = 0$
– Hard surface: $\frac{\partial c_\beta}{\partial x_i}\Big|_{no} = 0.$

PHYSICAL-CHEMICAL MODEL

Due to the consumption of huge amounts of coal, coal-burning objects annually emit various pollutants into the atmosphere - oxides of sulfur and nitrogen, particulate matter, trace elements (including arsenic, lead, mercury, fluorine, selenium and radionuclides) and organic compounds - that can cause health problems [18-20].

Describing the process of CO formation, the combustion of volatile components, which also include CO and CO_2, can be represented as a two-step reaction. Then the direct reaction between CO and O_2 will be:

$$CO + O_2 \rightarrow CO_2 + O \qquad (8)$$
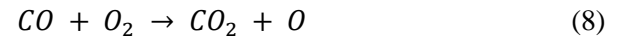
The formed oxygen atom O does not lead to any fast chain branched reactions, but even with the minimal presence of hydrogen, OH radicals form. In this case, the formation of CO_2 occurs through the reaction:

$$CO + OH \rightarrow CO_2 + H \qquad (9)$$
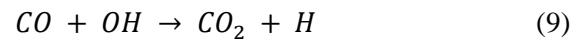
When carbon burning, two primary direct heterogeneous oxidation reactions are possible:

$$C + O_2 = CO_2 \qquad (10)$$

$$xC + O_2 = xCO \qquad (11)$$

As a result of the formation of CO_2 and CO, two secondary reactions can take place:

a) carbon monoxide oxidation

$$xCO + O_2 = xCO_2 \qquad (12)$$

carbon dioxide reduction

$$CO_2 + C = xCO \qquad (13)$$
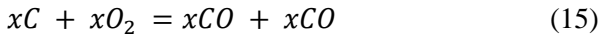
The ratio between CO and CO_2 at the surface of a particle depends on the temperature of gases in this region. For example, according to experimental studies, the reaction proceeds at 1200°C:

$$xC + xO_2 = xCO + xCO_2, \qquad (14)$$
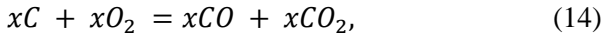
at temperatures above 1500°C, the reaction is:

$$xC + xO_2 = xCO + xCO \qquad (15)$$

CO will be formed in large amount if there is a lack of oxygen required for complete combustion, if the temperature range is not enough to fully respond CO to CO_2, and if the residence time in the combustion zone with the appropriate temperature and sufficient oxygen content for complete combustion is not enough.

In numerical calculations, since only velocity and heat release during oxidation are in the main interest, at high temperatures and sufficient oxygen the formation of CO can be represented as a generalized reaction of hydrocarbon components with oxygen, assuming that the decomposition of the fuel molecules to CO and H_2O occurs:

$$C_xH_y + \left(\frac{x}{2} + \frac{x}{4}\right)O_2 \rightarrow xCO + \frac{y}{2}H_2O \qquad (16)$$
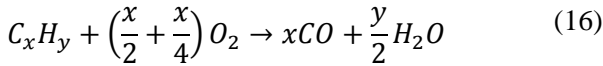
The velocity of CO formation is determined by the ratio:

$$\left(\frac{d\xi_{CO}}{d\tau}\right) = \xi CO * 10^{-3} * \left(\frac{\xi_{O_2}}{M_{O_2}}\right)^{\frac{1}{2}} \qquad (17)$$

$$* \left(\frac{\xi_{H_2O}}{M_{H_2O}}\right)^{\frac{1}{2}} * 1.3 * 10^{14}$$

$$* \exp(-\frac{15155}{T})$$

The expression of complete reaction, taking into account the law of Arrhenius and the entry of water vapor into the reaction, will look as follows:

$$\frac{d\overline{c_{x,CO}}}{dt} = -k_{0.co} * \overline{c}_{x,CO}^{-1.0} * \overline{c}_{x,H_2O}^{-0.5} \qquad (18)$$

$$* \overline{c}_{x,O_2}^{-0.25} * e^{-\frac{E_{\alpha,CO}}{RTG}} * p_{gem}^{0.75}$$

where

$k_{0.co} = 2.2179 \cdot 10^{12}$ 1/s;
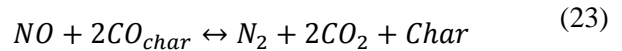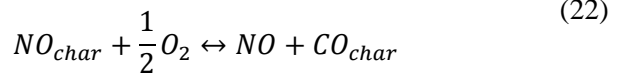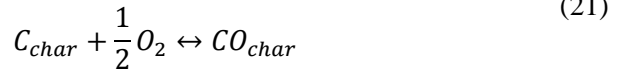
$E_{\alpha,CO} = 1.6914 \cdot 10^5$ kJ/kmol.

During coal combustion, nitrogen oxides are produced by dozens of species. The total amount of NO_x emissions from burning solid fuels can be described by summing up the three main identified ways of reactions: thermal NO_x, fuel NO_x, and fast NO_x.

Thermal NO_x results from the oxidation of nitrogen present in the air at high temperatures available in the combustion zone. They typically range from 20% to 50% of the total generated NO_x. For this purpose, the necessary temperatures prevail predominantly in the secondary combustion zone. Zeldovich described the oxidation of nitrogen and revealed the following mechanism:

$$O + N_2 \leftrightarrow NO + N \qquad (19)$$

$$N + O_2 \leftrightarrow NO + O \qquad (20)$$

The first reaction requires high activation energy, so it is slow at low temperatures. The burning of stable bound nitrogen N_2 requires a very high activation energy, which needs a temperature above 1200°C. Therefore, the main formation of thermal NO_x. occurs in parts of the flame close to the burner, where the peak temperature of the flame is highest in combination with the available oxygen [21-25].

During the formation of fuel NO_x, fuel-bound organic nitrogen reacts with existing hydrocarbons (C_xH_y). Organic nitrogen, which is chemically bound to fuel, is the main source for total NO_x emissions from coal flame. The production of nitrogen oxides NO and molecular nitrogen N_2 can form either as a homogeneous gas phase reaction or as a result of a heterogeneous reaction that includes the surface of the char. In this regard, the most important reactions on the surface of coke are described by the following reaction equations:

$$C_{char} + \frac{1}{2}O_2 \leftrightarrow CO_{char} \qquad (21)$$

$$NO_{char} + \frac{1}{2}O_2 \leftrightarrow NO + CO_{char} \qquad (22)$$

$$NO + 2CO_{char} \leftrightarrow N_2 + 2CO_2 + Char \qquad (23)$$

In order to implement the mechanism of fast NO_x formation, bound nitrogen reacts with hydrocarbons or available hydrocarbon fragments, which are formed as a result of thermal

decomposition in a reducing atmosphere. There is another chemical mechanism of rapid NO_x at temperatures of 1600-2100°C. Formation is initiated by various fragments of hydrocarbon fuels, such as CH and CH_2, which appear during the release of volatile substances. Molecular nitrogen is attacked by these hydrocarbons. Fenimore [26] described this phenomenon as follows:

$$N_2 + CH \leftrightarrow HCN + N \qquad (24)$$

This reaction takes place mainly in fuel-rich areas where hydrocarbon radicals increase the formation of HCN using the following reactions:

$$N_2 + CH_2 \leftrightarrow HCN + NH \qquad (25)$$

$$N + CH_3 \leftrightarrow HCN + H_2 \qquad (26)$$

Nitrogen is oxidized in the composition of the fuel and becomes oxides of nitrogen NO_x when burned, as well as fuel NO_x, and HCN is oxidized to NO depending on conditions. A significant part of nitrogen compounds is formed during the fast mechanism of conversion to diatomic nitrogen (N_2) inside the boiler. It is assumed that part of the rapid NO_x is less than 5% of the total amount of NO_x generated during coal combustion.

Thus, nitrogen oxides are formed as a result of atmospheric nitrogen oxidation at high temperatures (thermal NO_x) and the oxidation of fuel nitrogen compounds (fuel NO_x). In the case when hydrocarbon components in the flame zone react with nitrogen with the appearance of a nitrogen atom, forming NO, fast NO_x are formed [27-33].

COMPUTATIONAL EXPERIMENTS

The boiler chamber BKZ-75 of the Shakhtinsk TPP operated in the Karaganda region was selected as the object of research [34-35].

To carry out computational experiments, the geometry of the research object was constructed according to a real scheme, and its finite-difference grid was compiled for numerical simulation of solid fuel combustion in the combustion chamber of the BKZ-75 boiler. The finite-difference grid has steps along the X, Y, Z axes: 59×32×67, which is 126.496 control volumes (Fig.1).

Figs.2-6 show the aerodynamic characteristics of the process (distribution of the total velocity along the height of the furnace, three-dimensional distributions of the total velocity vector in longitudinal and cross sections of the combustion chamber, at the exit from it, and in the region of the rotating chamber).

a)   b)
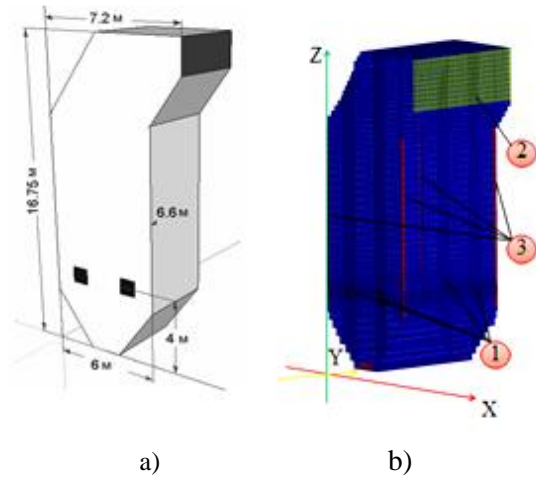
1- burners, 2-chamber outlet area, 3-suction cups; X-width of the furnace, Y-depth of the furnace, Z-height of the combustion chamber

Fig.1. General view of the boiler BKZ-75 of the Shakhtinsk TPP (a) and its discretization for control volumes (b)

Fig.2 shows the curves of the maximum, minimum and average values of the full velocity vector along the height of the combustion chamber of the BKZ-75 boiler. It clearly shows the region of maximum values (~ 20 m/s) of the flow velocity, which falls on the places where the burner devices are installed (Z = 4 m), from which an air mixture is injected with the primary air.
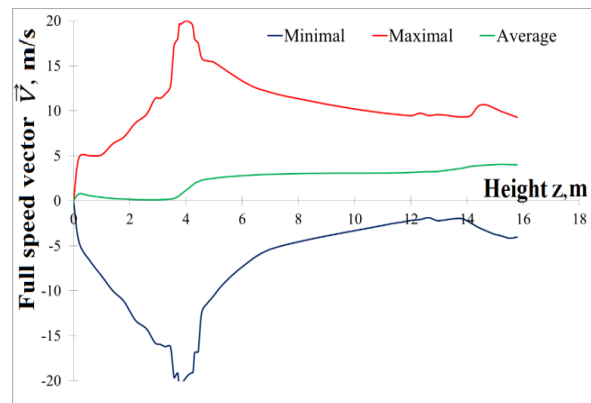

Fig.2. Distribution of full velocity at the height of the combustion chamber of the boiler BKZ-75 Shakhtinsk TPP

From the analysis of Fig.2 that as the flow of the air mixture and combustion products moves towards the exit, the velocity monotonously decreases, except for the turning area (Z=14.6m) of the boiler combustion chamber, where its surge is observed. This is due to the fact that at this height the geometry of the combustion chamber

changes, and the flow, due to a change in its direction, becomes unsteady, forming an additional vortex, increasing the flow turbulence, which leads to a velocity change in this area of the furnace space.

Fig.3 shows the three-dimensional distributions of the full velocity vector over the cross sections: longitudinal sections of the first and second pair of burners (X = 1.76 and 4.22 m); in cross section at the outlet of the furnace (X=7m); longitudinal radial-central section (Y=3.19m); in the cross section of the burner area (Z=4m) and in the turning area (Z=12.65m). From the analysis of Fig.3, it can be said that the flow of the air mixture with combustion products has a vortex character in the region of the burners and in the lower part of the combustion chamber at a height of Z from 2 m to 8 m. It can be seen that the full velocity vector has its maximum values (~ 16 m/s) in the region of the burner (Fig.3a).
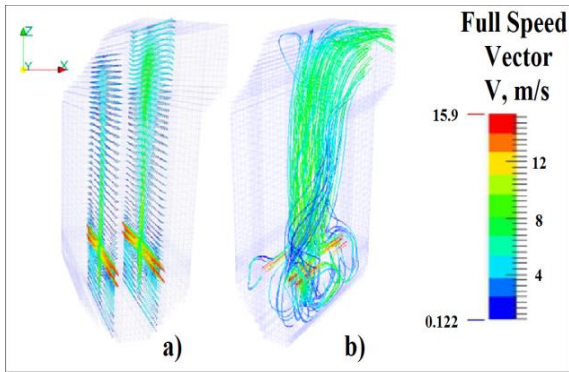

Fig.3. Three-dimensional distribution of the overall velocity in longitudinal sections (X = 1.76 and 4.22 m) and over the volume of the combustion chamber of the boiler BKZ-75 of the Shakhtinsk TPP

This is explained by the fact that the countercurrent flows injected from the burner devices, heading towards the center of the furnace space, with maximum velocity, collide. And here, dissipating into several whirlwinds, they form a reverse flow up and down (Fig.3b) along the heating space. Such a nature of vortices arises due to turbulence due to the interaction of the air mixture with the oxidizing agent. Above Z=8m in height, towards the exit from the furnace space, there is a gradual smoothing of the currents, the velocity of which lies in the range of 4-8 m/s.

Fig.4 shows the three-dimensional distribution of the full velocity vector over the depth of the combustion chamber (Y=3.19 m) in its central region. In the figure you can see how the threads collide in the center of the furnace, here the velocity is greatest. A part of the flows with maximum velocity (about 11 m/s) descends to the

area of the cold funnel, forming eddy currents, and the other part goes up to the exit from the combustion chamber.
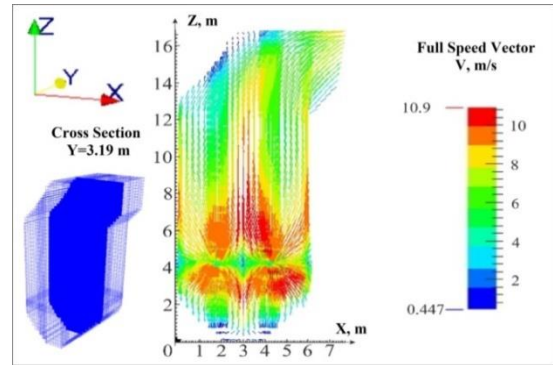

Fig.4. Three-dimensional distribution of the full-velocity vector in the longitudinal central section over the depth of the combustion chamber (Y=3.19 m) of the BKZ-75 boiler at the Shakhtinsk TPP

Fig.5 shows the aerodynamics of the flow in cross section in the area of the burners (Z=4m), it can be seen that some flow symmetry is preserved, which confirms the distribution of the full velocity over the height of the combustion chamber (Fig.2).
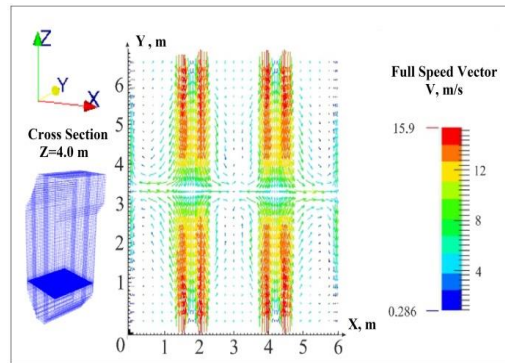

Fig.5. Three-dimensional distribution of the full velocity vector in the cross section in the burner area of the combustion chamber (Z = 4m) of the BKZ-75 boiler at the Shakhtinsk TPP

Fig.6 shows the field of the overall velocity in the area of the rotating chamber (Z=12.65 m) and in the outlet section (X=7m) from the boiler combustion chamber. Analysis of Fig.6 shows that as the turbulent flow moves towards the exit from the combustion chamber, the vortex nature of the flow weakens, then it increases in the region of the rotating section of the boiler and an almost uniform velocity profile is observed at the exit from the chamber.

It is noticeable that in the cross section of the furnace's turning area the maximum velocity (9 m/s) are concentrated in the central part and in the near-wall area, which to some extent can be

explained by the asymmetric geometry of the furnace in this area. At the exit from the furnace space, the velocity is practically equalized, no mixing of the flows is observed and its average value is ~ 4 m/s.
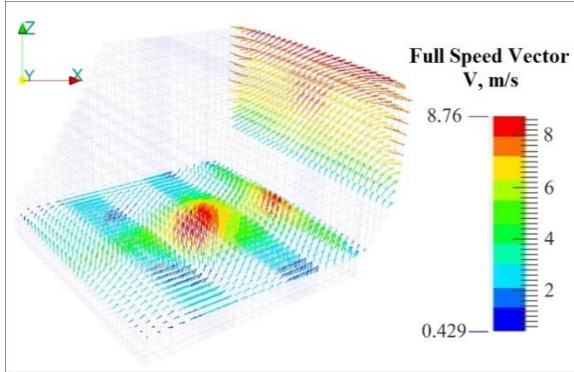

Fig.6. Three-dimensional distribution of the full velocity vector in the rotary region of the combustion chamber (Z = 12.65 m) and at the exit from the furnace (X = 7 m) of the BKZ-75 boiler at the Shakhtinsk TPP
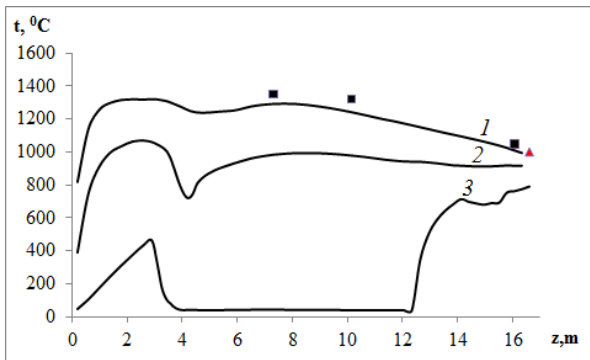

Fig.7. Distribution of the temperature T along the height of the combustion chamber of the BKZ-75 boiler:1-maximum; 2-average; 3- minimum;

■ - experimental data at TPPs [36]; ▲- is theoretical values obtained by the method of thermal calculation (CBTI – Central Boiler-and-Turbine Institute) [37]

The analysis of the curves in Fig.7 shows that the behavior of the temperature curves and the measured temperature values coincide qualitatively, however, the experimental data have higher values in the torch region, as well as at the outlet from the furnace space. The temperature at the outlet of the combustion chamber (base version) is confirmed by experimental data at TPPs and theoretical value calculated by the method of CBTI (Central Boiler-and-Turbine Institute) for direct-flow supplying of air mixture [37].
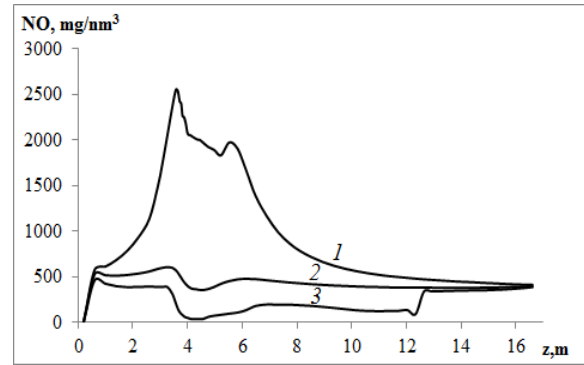

Fig.8. Distribution of concentration nitrogen oxide NO along the height of the combustion chamber of the BKZ-75 boiler: 1-maximum; 2-average; 3- minimum

Fig.8 shows the distribution curves of the maximum, minimum and average values of the concentrations of nitrogen oxide NO over the height of the combustion chamber of the boiler BKZ-75. From the analysis of the figure it is seen that the maximum values of the concentration of nitrogen oxide NO are in the area of the burners. This is due to the fact that in the studied problem, coal dust combustion occurs at a temperature of 1000-1700K; therefore, the main source of formation of nitrogen oxides is nitrogen NO contained in the fuel.

At the outlet nitrogen oxide NO concentrations are less than the maximum permissible concentration (MPC) accepted in Kazakhstan. Thus, we can conclude that the vortex method of supplying air mixtures in the combustion chambers of energy boilers significantly improves the environmental performance of thermal power plants.

CONCLUSIONS

• Using modern numerical 3D computer simulation methods, the research of thermal processes, aerodynamic and concentration characteristics of the combustion chamber of the boiler BKZ-75 of the Shakhtinsk TPP (Kazakhstan) were carried out.

• Physical and chemical processes were investigated during the combustion of high-ash energy fuel in the combustion chamber of an industrial energy facility, taking into account the main stages of coal combustion, the formation and destruction of harmful dust and gas emissions.

• Geometric and technical characteristics for 3D computational experiments on the combustion of low-quality high-ash Kazakhstan coal in the combustion chambers of existing power plants were determined. A program Preproz for introducing the initial parameters for conducting

3D computational experiments on the combustion of high-ash coal was created. The chemical composition of low-quality high-ash Karaganda coal has been studied.

ACKNOWLEDGEMENTS

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