

Influence of boundary conditions to heat and mass transfer processes

Aliya S. Askarova, Saltanat A. Bolegenova, Symbat A. Bolegenova, Valeriy Yu. Maximov, and Meruyert T. Beketayeva

Abstract — Investigation of heat and mass transfer processes in the area of combustion chamber during fuel burning is the one of the most difficult task for solving. Combustion processes accompanied with difficult physical and chemical reactions of two-phase flow at high temperatures. In this regard it's effective and preferable using of computational technologies. Computational modelling of pulverized coal combustion is an actual problem that needed to be solved. During combustion processes there occurring highly reactive flows that interact with each other, and release hazardous components to the environment. It is difficult to find any decisions to minimize their amount. Holding natural experiments nowadays are very problematic regarding of economic issues. So the best way to study these problems is computational experiments. It helps to determine results that can help to find and offer special activities to improve ecological and economic situation of energy objects. So in cooperating with engineers of combustion institute in this paper were carried out computational experiments on modelling of heat-mass transfer processes during combustion of pulverized coal.

Keywords — computational experiment, boundary conditions, reacting flow, heat-mass transfer.

I. INTRODUCTION

Due to the scenario of development of Kazakhstan Republic to improve the efficiency of the energy sector while maintaining its economic benefits and environmental safety set goals [1], which can be solved only by deep and thorough in joint research engineers in the field of technical physics, thermal energy, and information technologies [2]-[6]. In this regard an importance has the task of carrying out computational experiments, which can give full information about the nature of complex processes occurring in boilers while burning in it fuel. This kind of investigations conducted with holding researches of flow characteristics and particularly their heat and mass transfer characteristics.

To carry out computational experiments in this paper were

A. S. Askarova is with Al-Farabi Kazakh national University, Almaty, Kazakhstan Republic (e-mail: aliya.askarova@kaznu.kz).

S. A. Bolegenova is with Al-Farabi Kazakh national University, Almaty, Kazakhstan Republic (e-mail: saltanat.bolegenova@kaznu.kz).

S. A. Bolegenova is with Al-Farabi Kazakh national University, Almaty, Kazakhstan Republic (e-mail: bolegenova.symbat@kaznu.kz).

V. Yu. Maximov is with Al-Farabi Kazakh national University, Almaty, Kazakhstan Republic (e-mail: maximov.v@mail.ru).

M. T. Beketayeva is with Al-Farabi Kazakh national University, Almaty, Kazakhstan Republic (corresponding author to provide phone: +7 707 611 15 86; e-mail: meruyert.beketayeva@kaznu.kz).

used 3D modeling technology applied to combustion chamber of the boiler BKZ-75 in Shakhtinskaya CHP. As a base of computer modelling were used computer package FLOREAN [7], this has widely application for calculation in the field of highly reactive processing flows during combustion of fuels. The accuracy and adequacy of expected results defined by program are provided by the correct formulation of the physical, mathematical and chemical models of combustion processes [8]-[9].

II. PROBLEM FORMULATION

Pulverized coal flame is a complex heterogeneous system, i.e., its heat radiation is associated not only with CO₂ gas emission, H₂O and soot particles, but also ash and coke. The latter have a larger size and a mass concentration in the plume. Radiation ash strongly influences the radiation properties of the flames throughout the volume of the combustion chamber. It is therefore necessary to hold experiments on studying of heat and mass transfer processes thorough research process by burning coal with high ash content.

Computational experiments are based on a correct set of mathematical models of physical processes, which consist of a system of differential equations, algebraic relations and the closing boundary (initial and boundary) conditions [9]-[12]. Inadequate study of determining the behavior of the heat flow and mass transfer processes in the combustion chamber during the burning of pulverized coal at different boundary conditions of temperature on the walls of the chamber focuses on realistic model of choice is almost arbitrary.

Convective heat transfer process between hot fuel-air flows and the wall defined by the wall region flow. For adiabatic walls (when wall temperature of the combustion chamber is constant), the heat flux is zero ($q_w=0$) in this case is used as a boundary conditions in the plane of symmetry.

In the case of heat exchange between the wall and the reactive flux can specify the wall temperature or heat flux (for the problem when the furnace wall temperature variable). Assuming known convective heat transfer coefficient α , the heat flux can be expressed as follows:

$$q_w = \alpha(T_{wp} - T_w) \quad (1)$$

When the wall temperature of combustion chamber is variable heat flux \dot{q} can be calculated by the formula:

$$\dot{q} = \underbrace{\alpha(T_{FG} - T_{Surf})}_{\text{convection}} + \underbrace{C_{12}(T_{FG}^4 - T_{Surf}^4)}_{\text{radiation}}, \quad (2)$$

where, $C_{12} = \varepsilon_{12}\sigma$; T_{FG} - flue gas temperature;

T_{Surf} - the temperature of the surface of the wall of the chamber;

α - the coefficient of heat transfer by convection, $\text{W/m}^2\cdot\text{K}$;

ε_{12} - emissivity of the wall;

σ - the Boltzmann constant, $\text{W/m}^2\cdot\text{K}$.

The computational application can investigate two ways of accounting of changes in the boundary conditions of the surface temperature of the wall (Fig. 1):

- 1) fixed constant surface temperature $T_{surf} = const$;
- 2) the estimated surface temperature of a constant heat transfer and evaporation fixed constant temperature inside the tubes $T_{steam} = const$.

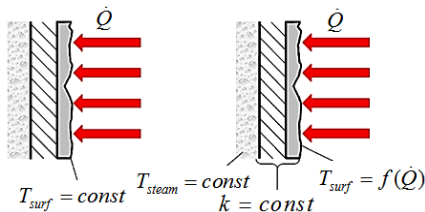


Fig. 1 Model of the boundary condition for the temperature of the wall of the combustion chamber

The surface temperature T_{surf} of the chamber wall can be calculated as follows:

$$\dot{q} = k(T_{surf} - T_{steam}), \quad (3)$$

$$T_{surf} = \frac{\dot{q}}{k} + T_{steam}, \quad (4)$$

here k - the thermal conductivity between the walls and pipes, $\text{W/m}^2\cdot\text{K}$.

The temperature of the wall surfaces of the combustion chamber T_{surf} affect the flow of heat, so its calculation procedure is performed iteration: calculation of the heat flow; calculation of the surface temperature T_{surf} ; recalculate heat flux to the new value of surface temperature; recalculate a new surface temperature T_{surf} .

To carry out computational experiments with the use of 3D modeling was selected combustion chamber of the boiler BKZ-75, operating in Shakhtinsk CHP (Fig. 3). Boiler has a block vertical tube design, U-shaped pattern of motion of the working environment based on natural circulation.

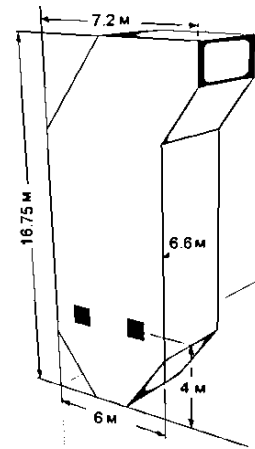


Fig. 3 General View of the boiler BKZ-75 of Shakhtinsk CHP

Combustion chamber completely shielded pipe diameter of 60×3 mm and consists of 12 separate circulation circuits. The combustion chamber of the boiler BKZ-75 is equipped with four-bladed axial swirl coal dust burners arranged in one tier on the side walls of the chamber.

The Karaganda coal burned in this thermal power station has the following characteristics: C - 79.57%, H_2 - 6.63%, O_2 - 9.65%, S_2 - 1.92%, N_2 - 2.23%, W - 10.6%, A - 35.1%. Q - $3.4162 \cdot 10^4$ kJ/kg. To carry out computational experiments was built by the geometry of the object according to the real circuit, and was composed of 126 496 control volumes.

Technical parameters of the combustion chamber of the boiler BKZ-75 are shown in Table below.

Table Technical parameters of the combustion chamber of the boiler BKZ-75 of Shakhtinsk CHP

Designation	Value
Number of burners on the boiler, N_b , ps.	4
Capacity of one burner in fuel, B_b , t/h	3.2
Primary air flow to the boiler, V_{pa} , Nm^3/h	31797
Secondary air flow to the boiler, V_{sa} , Nm^3/h	46459
Hot air temperature, t_{ha} , $^\circ\text{C}$	290
Air ratio in the furnace, α	1.2
Calculated fuel consumption for the boiler, B_c , t/h	12.49
Cold air temperature, t_{ca} , $^\circ\text{C}$	30
Pressure at inlet, P , mbar	$1.013 \cdot 10^3$
Pressure drop of the fuel mixture burner channel, ΔP , mm.w.c.	67.1
Fuel mixture temperature, t_{fm} , $^\circ\text{C}$	140
Wall temperature, t_w , $^\circ\text{C}$	430.15

In case of simulation of combustion processes in order to determine the formation of harmful substances in the

combustion chambers, a model to describe the transfer of heat energy must be as accurate as possible to predict the temperature distribution in the combustion space, since the kinetic processes of chemical reactions in very strong function of temperature.

In combustion chambers of the boiler, with the proviso that all known emitting properties and the temperature distribution in the reaction medium and on the walls, it is possible prediction radiant heat from the flame and products of combustion to the walls and the heating surfaces. However, in most cases the temperature itself - unknown option so the laws of conservation of the total energy and radiation energy equation together in one system.

III. MATH

The mathematical description of the physical system takes into account the impact of physical and chemical processes, such as combustion of fuel aerodynamic movement of the gases, air and poly disperse particles of fuel, as well as heat and mass transfer. Description of the numerical model is based on a number of physical laws of conservation of mass, momentum, energy and others [13].

Program application is based on the solution of heat and mass transfer equations for gas fuel mixture by control volume method, the standard k-ε turbulence model. Used program consists of sub-models of momentum balance, energy and components of the substance, also SIMPLE pressure correction method, six-flux model of radiation.

Computational experiment was carried out in several stages, which include the setting of the geometric data of the investigated boiler, the initial and boundary conditions for the simulation of heat and mass transfer process in reacting flows, complete mathematical description of the physical processes.

The equation of conservation of mass can be written as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = S_i, \quad (5)$$

where, S_i – the source of supply. It determines the mass added to the continuous phase, and any other sources, certain specific physical problem.

The equation of conservation of momentum can be written in the form:

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i + F_i. \quad (6)$$

The 1st term describes the unsteady flow, the 2nd - convective transfer, the 3rd and 4th terms - surface forces (pressure gradient and molecular diffusion), the 5th - the mass forces (gravity), the 6th - the external mass forces. Energy conservation equation takes into account the transfer of energy by conduction, diffusion and viscous dissipation:

$$\frac{\partial (\rho h)}{\partial t} + \frac{\partial}{\partial x_i} (\rho h u_i) = \frac{\partial p}{\partial t} + u_i \frac{\partial p}{\partial x_i} - \frac{\partial}{\partial x_i} (k_{eff} \frac{\partial T}{\partial x_i}) - \frac{\partial}{\partial x_{ij}} h_j J_j + (\tau_{ij})_{eff} \frac{\partial u_j}{\partial x_j} + S_h. \quad (7)$$

Generalized transport equation for variable flow, means the mass, or the kinds of components, the momentum or energy can be written in the form of a generalized transport equation in turbulent flows:

$$\frac{\partial (\rho \phi)}{\partial t} + \frac{\partial}{\partial x_i} (\rho \phi u_i) = \frac{\partial}{\partial x_i} (\Gamma_\phi \frac{\partial \phi}{\partial x_i}) + S_\phi. \quad (8)$$

IV. PROBLEM SOLUTION

Hydrodynamics of two-phase turbulent flows from the combustion of pulverized coal determines the character of the entire combustion process. Aerodynamic basis of all of the combustion process in the combustion device is a vortex transfer. The main role of the aerodynamic vortex flow pattern - perfect mixture formation of pulverized fuel and an oxidant (oxygen O_2 in the air), without which it is impossible to achieve any desired intensity of processes, no valid figures on emissions or a high level of efficiency of combustion. Results of computational experiments of the aerodynamic characteristics of the combustion process are shown in Fig. 5.

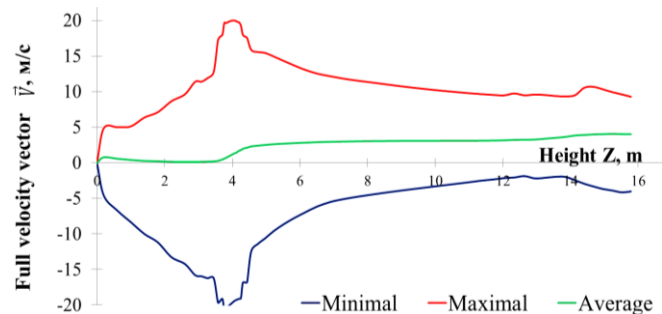


Fig. 5 Full velocity vector of flows by height of the boiler

Fig. 5 shows the curves of maximum, minimum and average values of the full velocity vector by height of the combustion chamber of the boiler BKZ-75. The figure clearly shows the maximum values of the flow rate ~20 m/s in the area where observed placed burners (at $Z = 4$ m) from which injected the air mixture with the primary air. As the flow of fuel mixture and the combustion products moves to the exit of chamber velocity decreases monotonically, except of a field ($Z = 14.6$ m) of the combustion chamber of the boiler, where it is observed surge. It is due to the fact that the height of the geometry of the combustion chamber changes, and the flow due to the change of the direction becomes unsteady, so additional vortex forming while increasing the flow turbulence [14]-[17], leading to a change of the velocity.

Figure 6 shows the distribution plots of average values of the temperature in height of the furnace volume of the boiler BKZ-75 for two cases of changing of boundary conditions for the temperature of the furnace walls.

Minimal temperatures in the burners are obtained for two cases of boundary conditions due to the low temperature of the injected fuel mixture (140°C). As can be seen from the curves change of boundary conditions for the temperature of the walls greatly affect the nature of the temperature distribution in the combustion chamber.

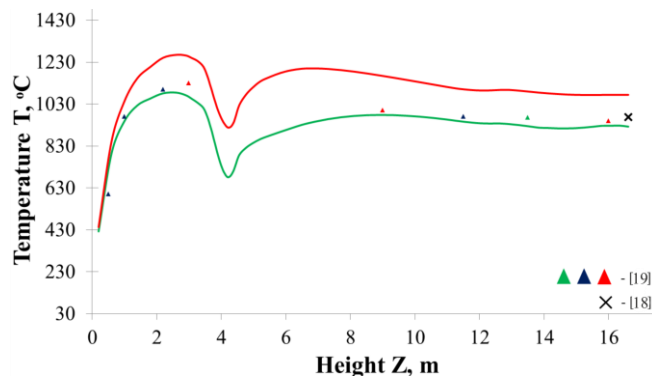


Fig. 6 Comparison of the results of computer simulations in the combustion chamber of the boiler BKZ-75 from the field data and theoretically calculated value

To select a boundary condition for the temperature of the walls of the combustion chamber, that best describes conditions close to the CHP and the actual process were compared results of numerical simulations with the theoretically calculated value of the temperature at the outlet of the combustion chamber of the boiler BKZ-75 (Fig. 6) obtained by normative method [18], also with the experimental data [19]. It may be noted a good agreement with the data. Where theoretical point of numerical results output from the furnace using the boundary condition of impermanence of wall temperature. The temperature at the outlet of the combustion chamber when the computational experiment is equal to $T = 922^{\circ}\text{C}$, and theoretically calculated value for the boiler BKZ-75 is equal to $T = 968^{\circ}\text{C}$.

Fig. 4 shows that although the distribution of the average temperature values along the Z axis of the combustion chamber for both boundary conditions are qualitatively similar, it can be seen that at constant temperature chamber walls all temperatures higher than in the case where the wall temperature variable and determined by the heat flow. Based on the mean temperature is not impossible to notice that the difference for the two cases is about 14%.

Significant differences occur in the temperature distribution at the location of burners and forth along the length of the torch towards the outlet of the combustion chamber. This is because by blowing fuel mixture from the burner, the ignition of the fuel and its combustion heat is given to the emerging part of the combustion chamber walls, the temperature of which changes all the time.

To the exit of the combustion chamber, the physical process with chemical transformations between the hot combustion gases and oxidant are weakened, and leads to a lowering of the temperature at the outlet of the furnace. Thus, at the outlet of the combustion chamber when the temperature of the variable temperature chamber walls has an average value 922°C , and in the case of constant wall temperature, the average temperature is equal 1074°C .

By analyzing the three-dimensional temperature distributions in Fig. 7-8, it is possible to make a similar conclusion: the temperature in all selected sections of the combustion chamber at a value which can be determined by the temperature scale, everywhere above for boundary conditions, when the temperature of the chamber walls is maintained constant.

In the field of burning devices temperature values reach 1252°C for the case of $T_{surf} = const$, and reaches values 1585°C for the case of $T_{surf} = f(q)$ (Fig. 7). At the section of camera rotation zone ($Z=12.65\text{ m}$) temperature fields differ only quantitatively.

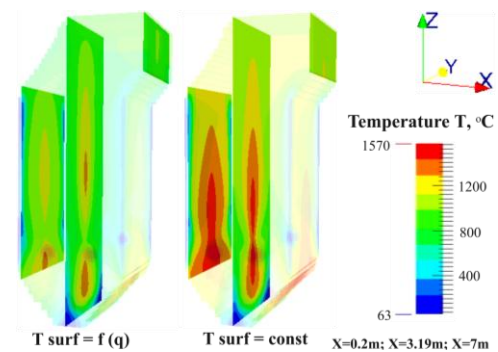


Fig. 7 Three-dimensional temperature distribution in the longitudinal sections of the combustion chamber of the boiler BKZ-75

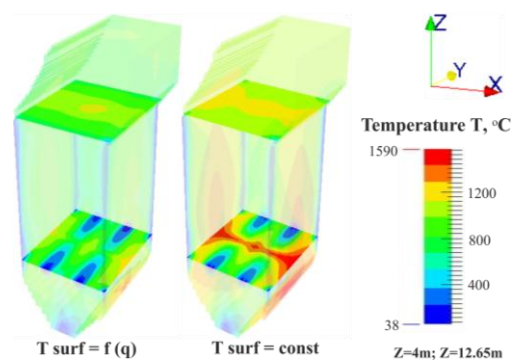


Fig. 8 Three-dimensional temperature distribution in the cross-sections of the combustion chamber of the boiler BKZ-75

It's known that main product of the combustion of the solid fuel at high temperatures with the oxygen of air are carbon oxides CO, carbon dioxides CO_2 (Fig. 9-10) and nitrous oxides [20]-[23]. Comparing the results of numerical experiments to determine the concentrations of CO_2 for two boundary conditions the temperature of the combustion chamber wall

can be said that they are also quite different.

The largest differences for the average concentration of carbon dioxide observed about ~7% in the ignition, and the formation of the flame in the burner zone.

This is due to the instability of ignition, combustion stabilization processes within the plume, an intensive process of oxidation and the formation of the combustion products. At the exit of the furnace, where the combustion process substantially completed, the differences in the profiles the concentration of CO₂ for different boundary conditions on the walls of the furnace are smoothed and are only ~1.2%.

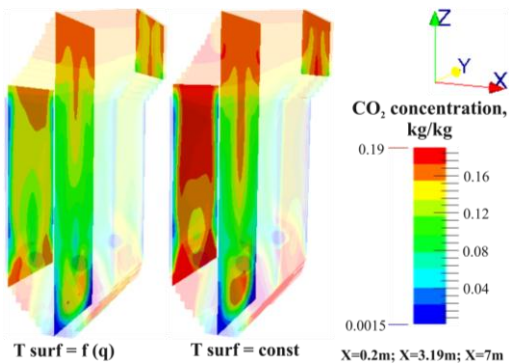


Fig. 9 Distribution of the CO₂ concentrations in the longitudinal section of the combustion chamber of the boiler

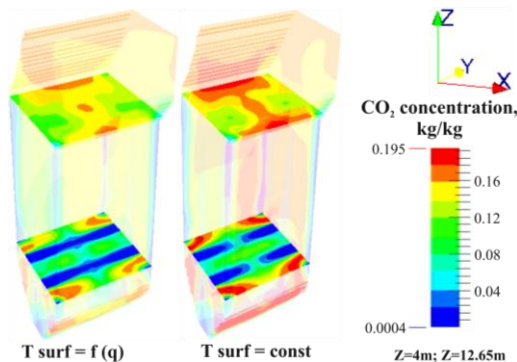


Fig. 10 Distribution of the CO₂ concentrations in the cross-sections of the combustion chamber of the boiler

Thus comparing two cases of the boundary conditions for the temperature of the wall has been determined the adequacy of the results for the case when temperature of the wall surface is impermanence. Therefore further been found in more detail the characteristics of the combustion process taking into account the heat exchange between the combustion chamber wall and reacting flow.

V. CONCLUSION

The energy sector of Kazakhstan Republic characterized by combustion of low-grade (A ~30-50%) coal at industrial CHP [24]-[26]. As ash content known as mineral matter of coal particle it makes the burning process more difficult and inefficiency. In this paper investigated combustion process of

low-grade Karaganda coal in the model of real boiler placed in Central Kazakhstan.

The methodology used numerical calculations makes it possible to obtain a complete picture of the processes occurring in the combustion chamber and to determine the values of the unknown quantities at any point of the combustion chamber, which is not always possible in conducting of field experiments. The difference between the theoretically calculated values at the outlet of the furnace with the result of a computational experiment is only ~4.6% for the boundary conditions, when the temperature of the chamber walls of the variable. However, at a fixed temperature of the surface of the walls of the combustion chamber for computational experiment requires less computer time. This means that the increased power requirements and computing (processor frequency and RAM of the computer). Accordingly, when performing such complex computational experiments on burning low-grade coal in the boiler furnaces actual operating purposes must take into account these two conditions to select the optimum ratio: the time and resources expended and the accuracy of the experiment and produce results that are in agreement with the real data.

REFERENCES

- [1] N.Nazarbayev, *Strategii ustoychivoy energetiki budushchego Kazakhstana do 2050 goda*. Astana: Ekonomika, 2011, ch 1.
- [2] A. S. Askarova, E. I. Karpenko, Yu. E. Karpenko, V. E. Messerle, A. B. Ustimenko, "Mathematical modelling of the processes of solid fuel ignition and combustion at combustors of the power boilers (Published Conference Proceedings style)," in Proc. *7th International Fall Seminar on Propellants, Explosives and Pyrotechnics*, Xian, 2007, pp. 672-683.
- [3] A. S. Askarova, V. E. Messerle, A. B. Ustimenko, S. A. Bolegenova, V. Yu. Maksimov, "Numerical simulation of the coal combustion process initiated by a plasma source," *Thermophysics and aeromechanics*, vol. 21, iss. 6, pp. 747-754, 2014.
- [4] S. A. Bolegenova, V.Y. Maximov, A. Bekmukhamet, M.T. Beketayeva, Z.K. Gabitova, etc., "Computational method for investigation of solid fuel combustion in combustion chambers of a heat power plant," *High temperature*, vol. 5, iss. 5, pp. 751-757, 2015.
- [5] A. S. Askarova, S. A. Bolegenova, S. Bolegenova, A. Bekmukhamet, V. Yu. Maximov, M.T. Beketayeva, "Numerical experimenting of combustion in the real boiler of CHP," *International Journal of Mechanics*, vol. 7, iss. 3, pp. 343-352, 2013.
- [6] R. Leithner, *Numerical Simulation. Computational Fluid Dynamics CFD: Course of Lecture*. Braunschweig: IWBT, 2006.
- [7] R. Leithner, H. Müller, CFD studies for boilers, *Second M.I.T. Conference on Computational Fluid and Solid Mechanics*, Cambridge, 2003, pp. 172-180.
- [8] W. Pauker, *Creating data sets for Florean using the tool PREPROZ*. IWBT, 1997.
- [9] Y. Heierle, R. Leithner, H. Müller, etc., "CFD Code FLOREAN for Industrial Boilers Simulations," *WSEAS Transactions on heat and mass transfer*, vol. 4, iss. 4, pp. 98-107, 2009.
- [10] A. De Marco, F. Lockwood, "A new flux model for the calculation of radiation furnaces," *Italian Flame Days*, Sanremo, 1975, pp. 1-13.
- [11] D. Spolding, "The calculation of combustion processes: Future application of combustion theory (Report style)," Report RF/TN/A/8, 1971.
- [12] S. Patankar, *Numerical heat transfer and fluid flow*. New York: Hemisphere Publishing Corporation, 1980.
- [13] V. E. Messerle, A. B. Ustimenko, A. S. Askarova, A. O. Nagibin, "Pulverized coal torch combustion in a furnace with plasma-coal system," *Thermophysics and aeromechanics*, vol. 17, iss. 3, pp. 435-44, 2010.

- [14] M. Gorokhovski, A. Chtab-Desportes, I. Voloshina, A. Askarova, "Stochastic simulation of the spray formation assisted by a high pressure (Published Conference Proceedings style)," in *AIP Conference Proceedings*, Xian, 2010, pp. 66-73.
- [15] A. S. Askarova, S. A. Bolegenova, A. Bekmukhamet, V. Yu. Maximov, "Mathematical simulation of pulverized coal in combustion chamber," *Procedia Engineering*, vol. 42, pp. 1259-1265, 2012.
- [16] A. Askarova, S. Bolegenova, A. Bekmukhamet, V. Maximov, M. Beketayeva, Sh. Ospanova, Z. Gabitova, "Investigation of turbulence characteristics of burning process of the solid fuel in BKZ 420 combustion chamber," *WSEAS Transactions on Heat and Mass Transfer*, vol. 9, pp. 39-50, 2014.
- [17] *Teplovoi raschet kotlov: normativnyi metod*. Moscow: NPO CKTI, 1998.
- [18] B. K. Aliyarov, M. B. Aliyarova, Shhiganiye kazakhstanskikh ugley na TES i na krupnykh kotel'nykh: opyt i perspektivy. Almaty, 2011.
- [19] S. Vockrodt, R. Leithner., A. Schiller, et al. "Firing technique measures for increased efficiency and minimization of toxic emissions in Kasakh coal firing," in *19th German Conference on Flames*, Germany, 1999, pp. 93.
- [20] A. Askarova, M. A. Buchmann, "Structure of the flame of fluidized-bed burners and combustion processes of high-ash coal," *Combustion and incineration*, vol. 1313, pp. 241-244, 1997.
- [21] V. Maximov, S. Bolegenova, M. Beketayeva, P. Safarik, et al., "Numerical Modeling of Pulverized Coal Combustion at Thermal Power Plant Boilers," *Journal of thermal science*, vol. 24, iss. 3, pp. 275-282, 2015.
- [22] A. S. Askarova, V. E. Messerle, A. B. Ustimenko, S. A. Bolegenova, V. Yu. Maximov, Z. Kh. Gabitova, "Numerical simulation of pulverized coal combustion in a power boiler furnace," *High temperature*, vol. 53, iss. 3, pp. 445-452, 2015.
- [23] E. I. Karpenko, V. E. Messerle, et al., "Plasma enhancement of combustion of solid fuels," *Journal of High Energy Chemistry*, vol. 40, iss. 2, pp. 111-118, 2006.
- [24] V. E. Messerle, Ye. I. Lavrishcheva, E. I. Karpenko, A. B. Ustimenko, et al., "Plasma-supported coal combustion in boiler furnace," *IEEE Transactions on Plasma Science*, vol. 35, iss. 6, pp. 1607-1616, 2007.
- [25] A. S. Askarova, A. Bekmukhamet, S. A. Bolegenova, M. T. Beketayeva, Yu. V. Maximov, Sh. S. Ospanova, Z. K. Gabitova, "Numerical modeling of turbulence characteristics of burning process of the solid fuel in BKZ-420-140-7c combustion chamber," *International Journal of Mechanics*, vol. 8, pp. 112-122, 2014.

Aliya S. Askarova, Doctor of Physical and Mathematical Sciences, corresponding member of the Academy of Sciences of the Republic of Kazakhstan, Professor, is a successor of the well-known scientific school of thermal physics in Kazakhstan. A. S. Askarova was awarded the Order "Kurmet", breast signs "Honorary Worker of Education of the Republic of Kazakhstan", "For merits in development of science of RK", "Altynsarin", is the owner of the state scientific grants for scientists and experts who have made outstanding contributions to the development of science and technology. At the time, she formed own scientific school, whose work aimed at solving the fundamental problems of thermal physics, combustion physics, computational fluid dynamics and have a practical value for the heat power industry and the environment.