# Mathematical modeling of heat and mass transfer in the presence of physical-chemical processes

A.S. Askarova[1], S.A. Bolegenova[2], Symbat Bolegenova[2], V.Yu.Maximov[1], R. Manatbayev[2*], Zh.K. Shortanbayeva[2], A.M. Maksutkhanova[2], A.N. Aldiyarova[2], A.E.Boranbayeva[2]

[1] *SRI of Experimental and theoretical physic, Al-Farabi Kazakh National University, 71, al-Farabi ave., 050040, Almaty, Kazakhstan*

[2] *Faculty of Physics and Technology, Al-Farabi Kazakh National University, 71, al-Farabi ave., 050040, Almaty, Kazakhstan*

At the present time there is an increased interest to the study of heat-and-mass transfer in high temperature environments in the presence of burning. These processes occur in strong turbulent and non-isothermal flows, multiphase fluids, in the conditions of significant impact of nonlinear effects of thermal radiation, interfacial interactions and multistage chemical reactions. To solve the problems of modern power engineering and ecology it is especially important to study the processes of heat-and-mass transfer in the high-temperature reacting media and to simulate physical and chemical processes that occur during the combustion of pulverized coal. These problems are related, on the one hand, to the concept of "energy safety" of the country and, on the other hand, to the development of processes of "clean" fuel combustion under strict standards of emission of harmful substances into the environment. Consider 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 occurring 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, heat and mass transfer, emission, modeling, thermal powerplant

## INTRODUCTION

The power system of Kazakhstan is presented mostly by thermal power stations more than 70 % of total amount of the electric power are generated. Thermal power stations work on solid fuel when pulverized coal combustion is predominant. Also natural gas and black oil can be used. Tendency of low grade coals usage to increase in domestic industry, it becomes especially important to develop and introduce new energy-saving technologies of solid fuel consumption and reduction in pollutant substance emissions. Applied technology of direct burning of low-grade coals in furnaces does not provide demanded reliability of working equipment and protection of environment from harmful combustion products due to approximately 50 % of pollutant emissions from stationary sources comes from thermal power enterprises and about 33 % are emitted by ferrios and non-ferrious metallurgy and mining.

Industrial implementation of any new technology is not possible without preliminary analysis of advantages and disadvantages of suggested method. The rapid development in computer sciences gives the advance to computational techniques to be used for simulation of complex combustion processes in industrial furnaces.

Products of combustion contain different harmful substances and the emission of this components grows in to a great problem. Industrial development causes an increase in hydro carbonaceous fuels' consumption. These fuels contain harmful and poisonous components such as carbonic oxide (CO), nitric oxide (NO), sulphur dioxide, acid sulphate, lead combinations and different hydrocarbons etc.

To decrease emissions of harmful substances various methods are applied, including special fire regimes (organization of combustion process), which suppresses the formation of harmful substances in flame and two-stage burning, when the burners work with low air surplus. In this way numerical experiments became one of the most effective and suitable means for detail analysis and in-depth study of physical and chemical phenomena.

In contrast to construction of an operating reduced model of the chamber, the three-dimensional modeling with the application of modern computer technology enables to carry out deep analysis of all chamber's parameters and save

* To whom all correspondence should be sent:
  rustem1977@mail.ru

time and finances. At the same time, without additional inputs, it is possible to obtain the full set of characteristics of a convective heat and mass transfer process in reactive media, intervene flexibly in the process at any stage and reproduce separate technical solutions (the configuration of the fire chamber and assembly and construction burners), to model the formation of harmful dust and gaseous emissions and to investigate the influence of previous preparation of coal on its ignition and combustion stabilization.

Thus the development of "clean" combustion process when the discharge of harmful substances is minimal is extremely important. That is why all constructive and regime parameters of such process must be optimized both in way of maximal effective energy production and high ecological safety. In this relation usage of computed aided complex for modeling of combustion process and prediction of main characteristics behavior in furnace volume and on the furnace outlet is of great interest for research.

## MATHEMATICAL MODEL

The computer simulation experiment was fulfilled with the help of the computer code FLOREAN [1-3] valid for the three-dimensional simulation of coal fired furnaces. This code is based on the solution of the conservative equations of the flue gas mixture by finite volume method. It includes a submodels of momentum and energy balances, SIMPLE-method for pressure corrections, k-ε turbulence model, six-flow model for radiation heat transfer calculations and balance equation for the components of substance. This computer code allows to extract the velocity components {u,v,w}, the temperature T, the pressure P, the concentration of combustion products and other characteristics of the process.

Pulverized coal flames are turbulent reacting two–phase flows. In pulverized coal flames, the volumetric fraction of the particle phase is typically less than 0.001. Therefore, the particle cloud is approximated as continuum and the mean particle velocity is assumed to be approximately equal to the gas phase velocity. Additional transport equations for the oxidant, coal, volatiles, char and combustion products are solved. The pollutant formation is calculated de- coupled from the calculation of the flow and temperature field. Using a global model, the NOx–concentrations are post–calculated by means of the previously predicted values (velocity, temperature, species

concentration) in the furnace chamber.

For description of chemistry simplified models were used. They account only chemical reactions of the main components and integral reactions of fuel components oxidizing up to stable end-products of the reactions. At that intermediate reactions and also the formation and alteration of unstable intermediate products are not taken into consideration.

The formation of nitrogen oxides from the nitrogen-containing fuel can be approximately calculated by a simplified process scheme. According to this scheme these substances are mainly decomposed during the combustion of the volatile matters down to active atomic nitrogen which partially recombines into molecular nitrogen $(N+N \rightarrow N_2)$ and partially oxidizing to the mixture of nitrogen oxides $(mN+O_2 \rightarrow mNO_X)$. The concentration of resulting molecular nitrogen and mixture of nitric oxides in the combustion gas is found by the solution of the equation of homogeneous kinetics. Different combinations of possible reaction ways serve as a basis of various models. The choice of one of them is associated with capabilities of the available computer [4-7].

For simulation of nitrogen oxides formation in combustion it is assumed that the main re- action are the oxidation of molecular nitrogen (thermal $NO_X$) and the oxidation of the fuel bounded nitrogen (fuel $NO_X$). The detailed kinetic models for fuel NO prediction with 29 elementary reactions are used [8-11].

At the same time selection criteria of a model are the minimum number of reactions and participating components with simultaneous precision of carrying calculations and their satisfactory agreement with experimental data.

## RESULTS

Computational experiments have been carried out for low-rank Kuuchekinskij bitumi- nous coal incinerated at the boiler BKZ-160 with steam capacity of 160 t/h. This furnace has jet type burners in tangential firing system The boiler is installed in Almaty Thermal Power Plant (Kazakhstan). The cross section of the furnace is 7,1 m x 6,5 m and the height is 21 m (Fig.1). Eight jet burners are placed in the corners, 4 burners on two levels, directed to a fictive combustion cycle (Fig.2).
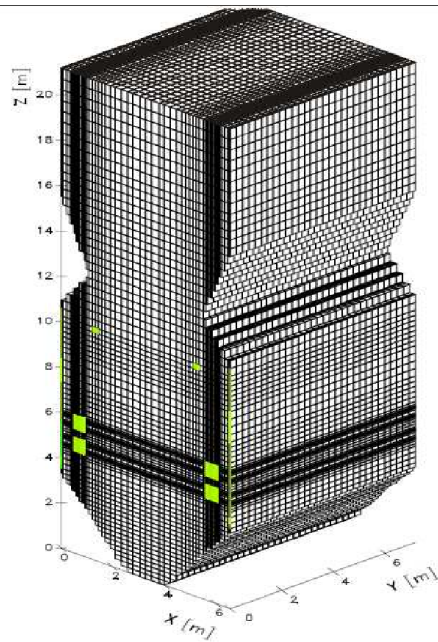
**Fig.1.** Scheme of the furnace BKZ160

the level of the burners. Here the intensive combustion took place.

The existing of minima in presented temperature field caused by low temperature of fuel and transporting gas supplied to furnace through the burners nozzles.
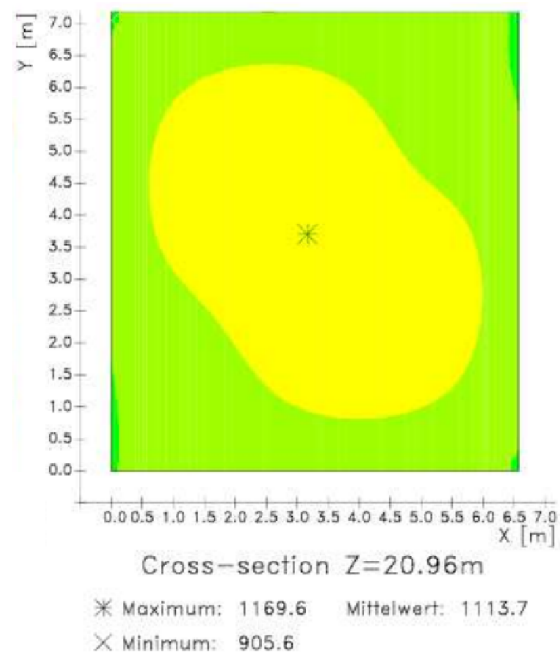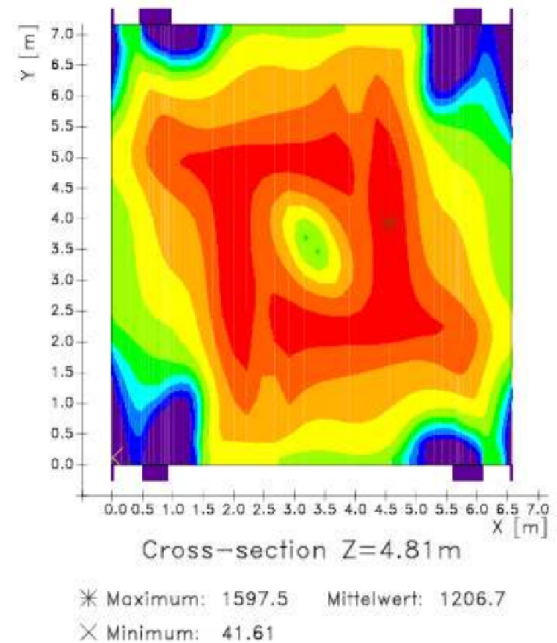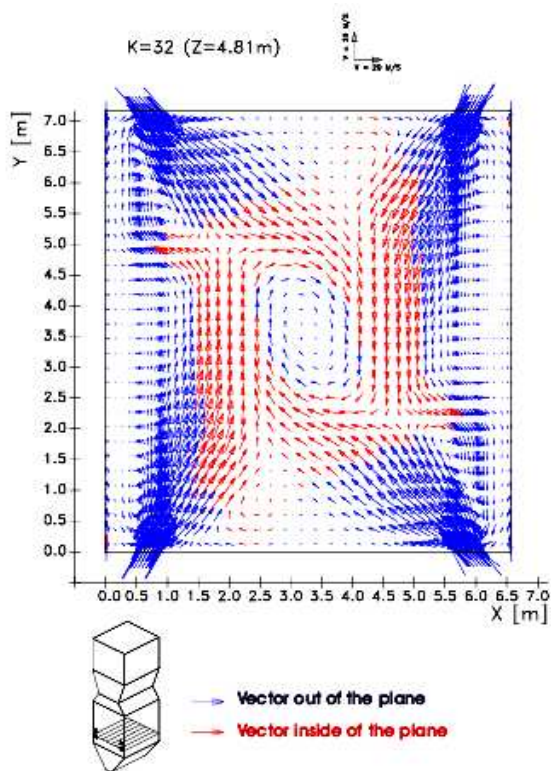


Cross-section Z=4.81m

✳ Maximum: 1597.5    Mittelwert: 1206.7
✕ Minimum:  41.61





**Fig.2.** Scheme of burners location

Fig.3 and Fig.4 shows the temperature distribution in cross section of the furnace in the lower level of the burners and furnace outlet and temperature distribution in the middle vertical sections of the furnace. It's seen that maximum temperatures is in the center of the fire-chamber on
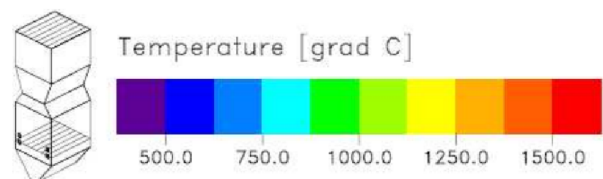


Cross-section Z=20.96m

✳ Maximum: 1169.6    Mittelwert: 1113.7
✕ Minimum:  905.6

Temperature [grad C]



500.0    750.0    1000.0    1250.0    1500.0

**Fig.3.** Temperature distribution in cross section of the furnace in the level of the burners and furnace outlet
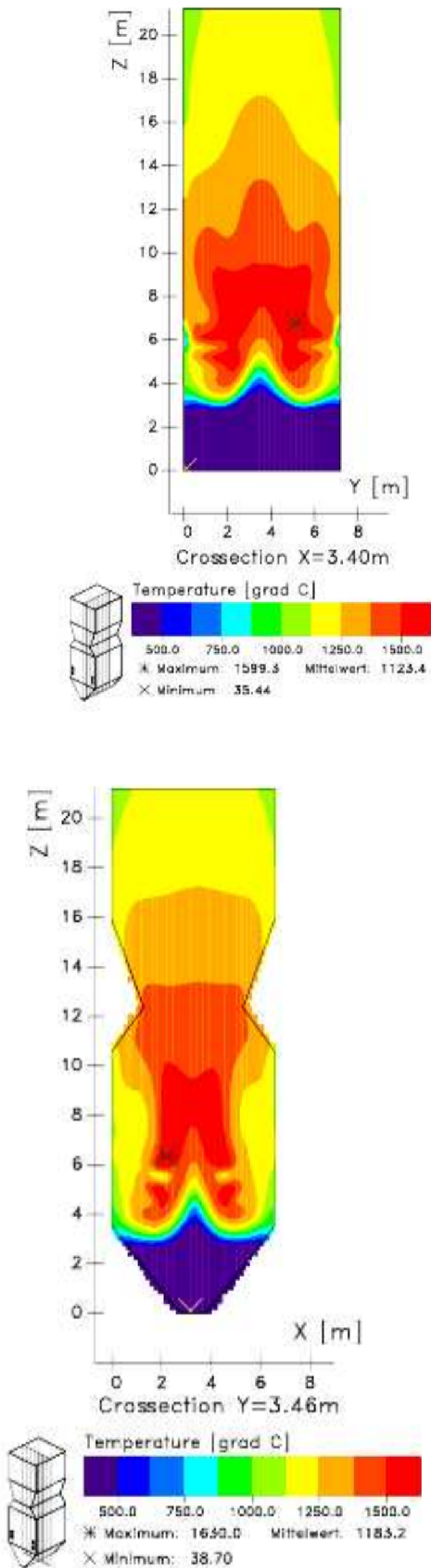
**Fig.4.** Temperature distribution in the middle vertical sections of the furnace
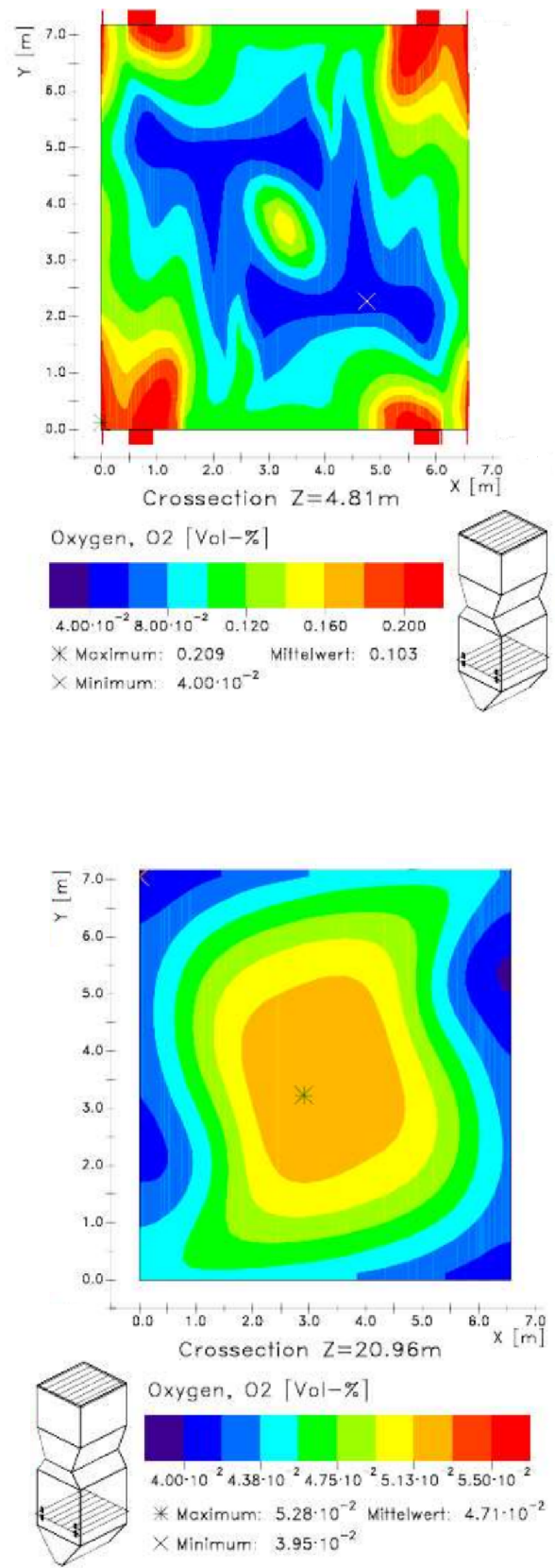
**Fig.5.** Oxygen distribution in cross section of the furnace in the level of the burners and furnace outlet
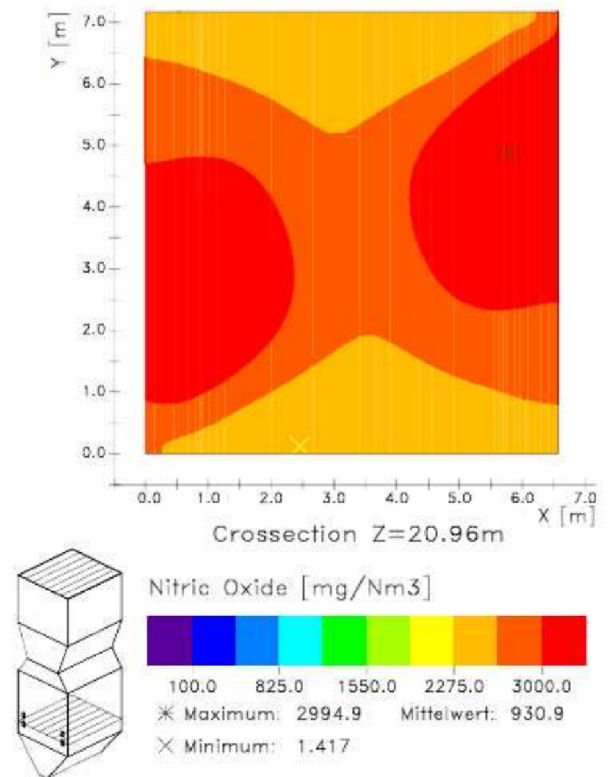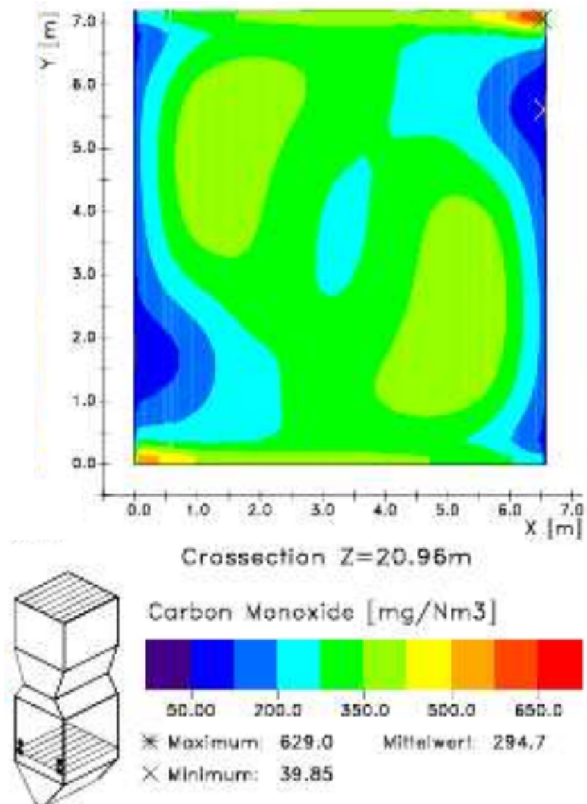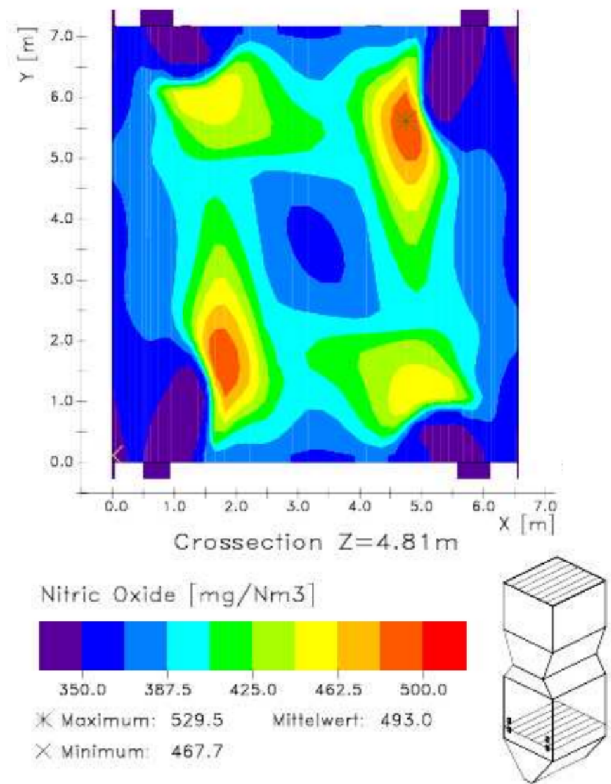
**Fig.6.** Carbon monoxide distribution in cross section of the furnace in the level of the burners and furnace outlet

**Fig.7.** Nitric oxide distribution in cross section of the furnace in the level of the burners and furnace outlet
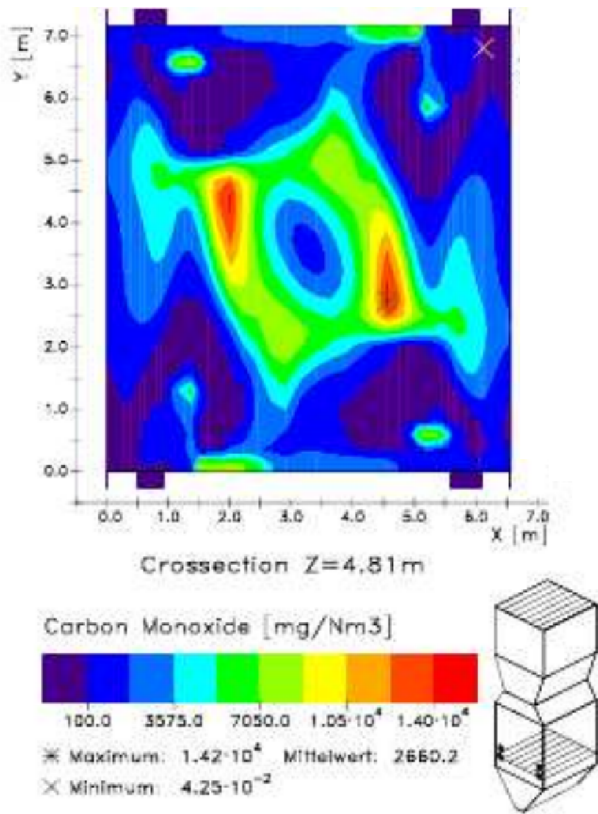
The picture of fuel burning out is shown in Fig.5 to Fig.7 by fields of concentration change of oxygen $O_2$ (Fig.5), carbon monoxide CO (Fig.6) and nitric oxide NO (Fig.7) in cross section of the furnace in the level of the burners and furnace outlet. The analysis of these figures shows, that main gas formation in a torch occurs in a zone of burners, and in general it is typical for all kinds of combustion chambers.

Fig.5 and Fig.6 show the oxygen and carbon monoxide distributions in cross section of the furnace in the lower level of the burners.

The carbon monoxide (Fig.6) is concentrated mainly in a zone of jets collision of fuel from opposite torches, i.e. there, where carbon exists. Let's note that the zone of its formation begins and comes to an end before exothermic zone of torch. Concentration of $O_2$ and CO at the outlet of the furnace (Fig.6 and Fig.7) depends not only on the transport phenomena but also on kinetics. In the upper space of the combustion chamber rate of burning out decreases.

Nitrogen oxide distribution in cross section of the furnace in the lower level of the burners and furnace outlet is displayed in the Fig.7.

## ACKNOWLEGEMENT

## CONCLUSION

Results obtained by means of computer modeling of gas flows behavior, species concentrations, temperature fields due to combustion, radiation and convective heat transfer and the pollutant formation and destruction in furnace of real boiler BKZ-160 can be used to predict main characteristic of combustion process and to provide recommendations for effective boiler performance. Results from CFD simulation can be useful for engineers to choose an appropriate boiler performance for successful furnace and overall combustion process optimization.

## REFERENCES

1 A. Askarova, E. Karpenko, Yu. Karpenko, E. Messerle, A. Ustimenko Mathematical modelling of the processes of solid fuel ignition and combustion at combustors of the power boilers 7th International Fall Seminar on Propellants, Explosives and Pyrotechnics. Xian, Vol. 7, 672, (2007).

2 A. Askarova, V Messerle, A Ustimenko, S Bolegenova, V Maximov, Z Gabitova Numerical simulation of pulverized coal combustion in a power boiler furnace, High temperature, Vol. 53, issue 3, 445, (2015).

3 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, issue 3, 275 (2015).

4 V. Messerle, A. Ustimenko, A. Askarova A. Nagibin Pulverized coal torch combustion in a furnace with plasma-coal system, Thermophysics and aeromechanics, Vol. 17, issue 3, 435, (2010).

5 E. Karpenko, V. Messerle et al. Plasma enhancement of combustion of solid fuels, Journal of High Energy Chemistry, Vol. 40, Issue: 2, 111, (2006).

**6** V. Messerle, Ye. Lavrishcheva, E. Karpenko, A. Ustimenko et al. Plasma-supported coal combustion in boiler furnace, **IEEE Transactions on Plasma Science,** Vol. **35,** Issue **6, 1607, (**2007).

7 A. Askarova, V Messerle, A. Ustimenko, S. Bolegenova, V. Maksimov Numerical simulation of the coal combustion process initiated by a plasma source, Thermophysics and aeromechanics, Vol. 21, issue 6, 747, (2014).

8 S. Bolegenova, V. Maximov, A. Bekmukhamet, M. Beketayeva, Z. Gabitova etc. Computational method for investigation of solid fuel combustion in combustion chambers of a heat power plant, High temperature, Vol. 5, issue 5, 751, (2015).

9 A. Askarowa, M. Buchmann Structure of the flame of fluidized-bed burners and combustion processes of high-ash coal, Gesell Energietech, Combustion and incineration - eighteenth dutch-german conference on flames, VDI Berichte, v. 1313, 241, (1997).

10 S. Vockrodt, R. Leithner, A. Schiller et al. Firing technique measures for increased efficiency and minimization of toxic emissions in Kasakh coal firing, VDI, 19th German Conference on Flames, Germany, VDI Gesell Energietechn; Verein Deutsch Ingn., Combustion And Incineration, VDI Berichte, v. 1492, 93, (1999).

11 M. Gorokhovski, A. Chtab-Desportes, I. Voloshina, A. Askarova Stochastic simulation of the spray formation assisted by a high pressure, AIP Conference Proceedings, Xian, Vol. 1207, 66, (2010).