

## Optimization of the design and operating characteristics of a boiler based on three-dimensional mathematical modeling

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Currently, ANSYS Fluent software is widely used as an alternative engineering tool for describing the physical processes that occur in boiler furnaces and burners. Studies of the fuel preparation and combustion characteristics in the KVTK-100-150-4 boiler using the ANSYS Fluent program were performed. The characteristics of the combustion process in the combustion chamber were calculated. The analysis of methods for reducing the pollutant formation showed the rationality of using staged combustion to reduce NO<sub>x</sub> emissions. The performance of the proposed modeling method in MATLAB was demonstrated by using Type I and Type II error functions, followed by higher statistical performance such as error variance and correlation analysis. A comparative analysis was carried out to substantiate the superiority of the proposed modeling technique.

**Keywords:** burner, boiler plant, volatile substances, nitrogen oxide, combustion process.

### INTRODUCTION

The structure of the carbon soot preparation and burner devices, equipment of the KVTK-100-150-4 boiler of Ekibastuz CHP were studied. Energy characteristics of the Ekibastuz coal were determined and analysis of methods of reduction and generation of harmful substances was performed.

The causes of mechanical deterioration and nitrogen oxides formation in the CHP were determined. The main areas of reducing and preventing the occurrence of nitrogen oxide emissions were considered. Various thermal profiles of thermal preparation of burning fuel using chemical reactors, air-flow and process furnaces, pyrolysis of coal dust with reduction of nitrogen oxides in combustible products, as well as surface and contact heat exchangers were compared.

Preconditions for clean concepts of habitat protection of boiler units to be redesigned and updated were created for the focal phenomena and thermal circuits. Proposals were made to significantly reduce emissions of nitrogen oxides in

the CHP with minimal changes of burners and coal preparation systems.

A simulation of Ekibastuz coal and generator gas combustion in the KVTK-100-150-4 boiler unit was performed. The temperature and velocity contours were obtained inside the hearth. Concentrations of nitrogen oxide at the burners' level and at the outlet of the hearth were calculated.

The advanced boiler plant modeling strategy includes experiment-based modeling [1, 2] and first-principle-based modeling. Experimental modeling is utilized for control designing and reflecting the major non-linear dynamics. First-principle-based modeling shows the relationship between engineering principles and physics and true plant parameters, and it can control the algorithm evaluation. For better boiler efficiency, innovative methods have to be developed with advanced optimization approaches. The optimization of boiler operation parameters can be achieved by two broad methodologies, namely (a) traditional method and (b) intelligent method. In the traditional method, the design value, experimental value, historically optimum value and actual data

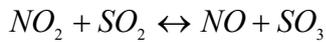
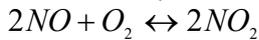
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are used to optimize the boiler operational parameters. The method has advantages such as real-time updating at good probability, while it has disadvantages such as difficulty in handling multiparameters, high investment of work force and resource, survey and installation errors, equipment aging issues, and limitations in mining strategies. The intelligent method is based on data mining technology and intelligent technologies.

Based on the detailed analysis of the problem carried out in the interim report, the most effective method of preventing the formation of nitrogen oxides is the organization of fuel combustion in a three-stage manner, as shown in Fig. 1.

During the fuel combustion, sulfur dioxide  $SO_2$  is formed, due to the burning of  $FeS_2$  pyrite. Oxide accelerates the synthesis between  $SO_2$  and  $O_2$  [3]:



Chemically active  $NO_2$  accelerates the transformation of sulfuric oxide into more toxic sulfuric anhydride.

formation of nitrogen oxides requires comprehensive consideration of its secondary results (with the consequences of incomplete combustion): formation of carcinogenic substances and environmentally dangerous CO, increase in consumption of chemical and mechanical incomplete combustion, high-temperature hydrogen sulfide oxidation.

Therefore, it is worth saying that the reduction of harmful gas emissions from the combustion of organic fuel is necessary for habitat protection and resource saving (which leads to the reduction of vegetation and oxygen, which in turn affects the human life due to the harmful radioactive waste of nuclear power plants and lack of energy (which is independently equivalent to global causal conditions such as heat deaths) is an urgent task.

Based on sufficiently effective measures to prevent nitrogen oxides formation, nitrogen is converted into inert matter by pyrolysis until air is introduced, this phenomenon being explained by the preliminary re-compression of active nitrogen in matter.

The thermal profiles of thermal preparation of fuel with a conventional hearth and chemical reactor, with a nitrogen oxide recovery pyrolyzer, with surface heating of dust in the designed boiler, as well as in Fig. 1 with recuperative heating of coal dust in an upgraded boiler were compared and implemented. The coefficient of flue gas recirculation with a temperature of  $1200^\circ C$  up to  $900^\circ C$  used for pyrolysis and drying of coal dust has values from 0.149 to 0.35. According to Bleyer [3], the degree of gasification of bibastuz coal was about 50%. Then, the amount of nitrogen oxides released into the environment decreases by 3.3 times and is about  $0.210 \text{ g/m}^3$  for KVTK-100-150-4 boiler. See Fig. 1 for the layout of a nitrous oxide recovery pyrolyzer, i.e., the performance is expected to be even better for the layout of the dual avoidance of nitrous oxides. Heat exchange of two-phase flows is performed according to [5]. The characteristics of the injector for aeration of coal dust of the KVTK-100-150-4 boiler with fuel and gas consumption of  $8.194 \text{ kg/s}$  and  $62 \text{ kg/s}$ , operating flow  $400^\circ C$  and mixture heat  $900^\circ C$  were calculated [4].

A numerical study of the process of formation of nitrogen oxides during the combustion of Ekibastuz coal by the dust method was performed using the method of mathematical modeling at various values of oxygen concentration, temperature and process time, taking into account the kinematics of the formation of fuel oxides of nitrogen. Drying and transportation take place with air, and hot flue gases are taken from flue gas channels, at a temperature of

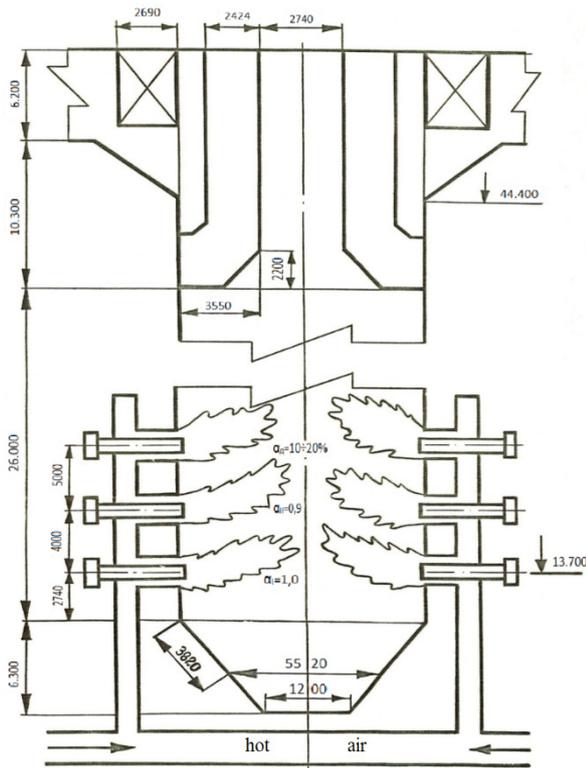


Fig.1. Three-staged burning

Under the influence of hydrogen and carbon oxides, sulfur dioxide turns into a corrosive active hydrocarbon. Carcinogenic active benz(a)pyrene is formed due to reduction of local coefficient of excess air and increase of  $C_2H_2$  and  $C_2H_4$  concentration. Ultimately, prevention of the

about 400°C. In such an uncomplicated reconfiguration of the air duct and the replacement of the air-drying agent with a gaseous one, the burners remain structurally unchanged. Their stable operation is ensured by maintaining the gas flow rate in the primary channel (not less than 25 m/s [6]) and air flow rates in the secondary channel (not less than 15 m/s) at the same level. The level of emissions of nitrogen oxides and the phenomenon of combustion are regulated by changing the primary and secondary airflow and the consumption of additional primary air.

*General characteristics of the KVTk-100-150 boiler*

The KV-TK-100-150 boiler has a capacity of 116 MW and operates on crushed stone and brown coal. Boilers of the KBTK-100-150 type are designed to operate in the main mode (when installed for industrial heating), in some cases in peak mode (when installed to cover the peak thermal load at the TPP (Thermal Power Plant). The boiler is single-hull and has a U-shape.

The main technical indicators of the boiler are presented in Table 1. The boiler diagram is shown in Fig. 1.

**Table 1.** Technical indicators of hot water boiler KVTk-100-150

Technical indicators of hot water boiler	Numerical value
Thermal power, MW	116.3
Water inlet temperature (main/peak mode), °C	70/100
Hot water outlet temperature, °C	150
Hot water pressure, MPa	2.35
Water flow rate (main/peak mode), t/h	1 236/2 460
Fuel consumption (calculated), t/h	17.8
Width along the column axis, mm	12 300
Depth along the column axis, mm;	18 000
Height of the boiler, mm	29 680

*Description of the physical model*

It is believed that all combustion processes, in particular aerodynamics, chemical reaction, combustion, heat and mass exchange and the formation of nitrogen oxides are interrelated in the ANSYS fluent complex. The gas introduced in the burners has the following components: carbon dioxide CO<sub>2</sub>, molecular nitrogen N<sub>2</sub>, water vapor H<sub>2</sub>O and oxygen O<sub>2</sub>. the description of the turbulence characteristics of the flow is carried out by the modified standard turbulence model k [4].

In this work, a model was adopted that considers the main stages of combustion, namely: evaporation of moisture, heating, ignition, combustion of volatile substances and combustion of coke residues. in the

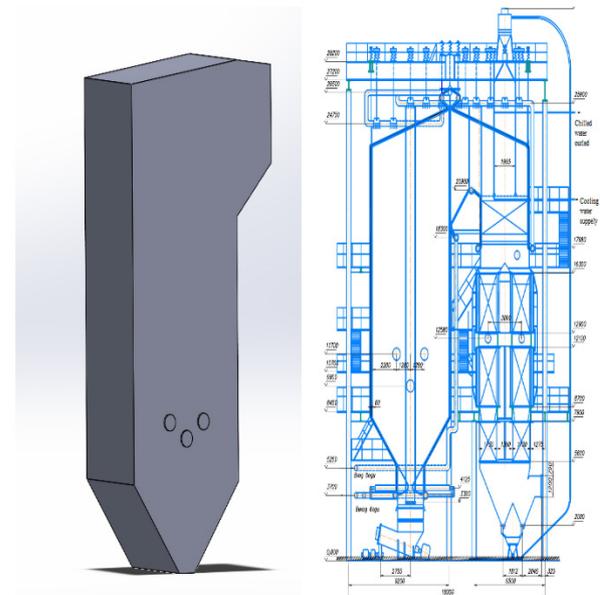
combustion chamber, the coal particle undergoes heat treatment due to thermal radiation (Fig. 1). The calculation was made for ash content of Ekibastuz coal [5]. The composition of the fuel and lower heating value (LHV) is shown in Table 2.

**Table 2.** Elemental composition and lower heating value of Ekibastuz coal [4]

Rank	Units	Value
Carbon, C <sup>r</sup>	%	44.8
Hydrogen, H <sup>r</sup>	%	3.0
Nitrogen, N <sup>r</sup>	%	0.8
Oxygen, O <sup>r</sup>	%	7.3
Sulfur, S <sup>r</sup>	%	0.70
Water, W <sup>r</sup>	%	6.5
Ash, A <sup>r</sup>	%	36.9
LHV	kJ/kg	16 493

*Mathematical modeling of the transformation of the furnace and burner processes of the KVTk-100-150 boiler*

At the initial stage of the research, a lattice model of the combustion chamber of the KVTk-100-150 boiler unit was built (Fig. 2), fuel and air inlets were fixed. The mesh model consists of 250,000 cells.

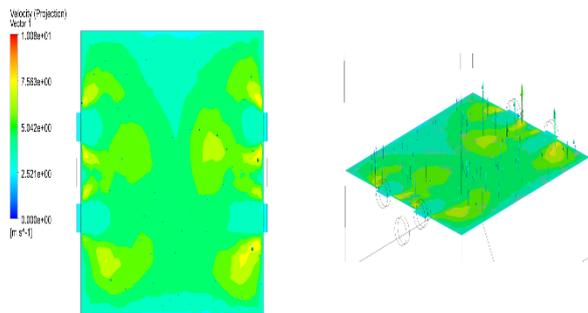


**Fig. 2.** Calculation model of KVTk-100-150 steam boiler

Boundary conditions were the speed of fuel in burners, temperature values as shown in Table 2 and elemental mass of fuel. The initial temperature of air was 750 K, and the initial temperature of fuel was 450 K. The reason for this is that fuel and air are preheated in boiler units, so their temperatures are assumed to be higher than atmospheric. Six burners in the form of an inverted triangle are located on the surface wall of the KVTk-100-150 boiler shown in Fig. 2.

Three-dimensional calculations performed in the ANSYS Fluent program allow obtaining the rate of formation of nitrogen oxides, temperature and concentration distribution in the horizontal and vertical sections of the combustion chamber, as well as tracking the trajectory of coal particles.

Fig. 3 shows the velocity vectors at the burner level of the boiler. The following can be drawn from the pictures - the direction of the velocity vectors is vertical, the main reason for this is that the direction of the gases is toward the outlet of the combustion chamber; there are no vectors showing the vortex.



**Fig. 3.** Velocity vector field at the burner level of the KVTk-100-150 boiler unit (m/s)

Fig.4 shows the distribution of temperatures at the burner level of the boiler. As can be seen in the picture, the high-temperature zone is located at the inlet of the burners, that is, in the part where the coal particles meet the air and burn.

Fig. 5 shows the movement trajectory of solid fuel particles in the KVTk-100-150 boiler. It can be seen from the general trajectories that when the fuel particles leave the two fuel groups, they meet in the geometric center of the furnace and move further vertically.

Turbulence modelling was performed by using the k-ε turbulence model. Input parameters include air and fuel parameters, as well as domain parameters. The initialization procedure checks the correctness of the model and prepares it for calculation (2000 iterations are given in the calculation).

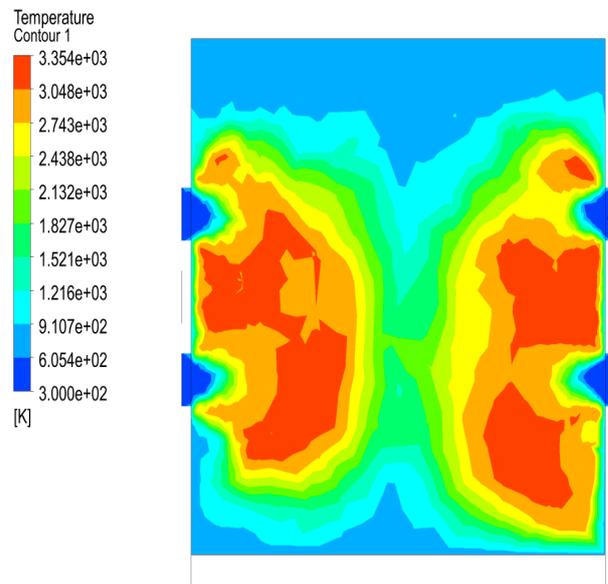
Fig. 6 shows temperature contours (fields) in the vertical section of the boiler. As can be seen in the picture, the main part of the gases burns in the upper part of the boiler furnace. Therefore, their temperature reaches 1770 K.

The main reason for this is the intensity of mixing of gases with air, that is, in a diffusion flame, the combustion of gases is limited only by the order of mixing.

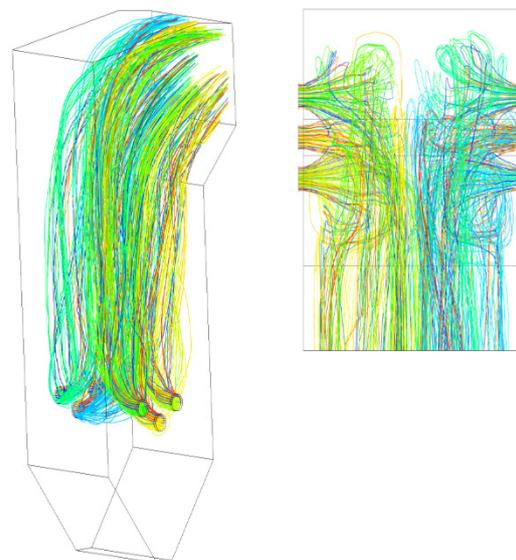
The obtained results show that the selected mathematical model implemented in the ANSYS Fluent program, as a whole, shows similar values with the thermal calculations of

the boiler plant and shows the current picture of the combustion processes. Analysis of the results of mathematical modeling of the KVTk-100-150 boiler unit confirms the presence of slag-increasing zones of the combustion chamber in the pinch zone of the boiler.

High values of the temperature of flue gases leaving the combustion chamber of the KVTk-100-150 steam boiler intensify the process of formation of primary and secondary ash and slag deposits on the heating surfaces. At the same time, the concentration of nitrogen oxides is 443.8 mg/m<sup>3</sup>, almost 1.5 times higher than standard indicators. Thus, the conducted calculations confirm the existence of problems in boiler plants.



**Fig. 4.** Field of temperatures (K) at the burner level of the KVTk-100-150 boiler



**Fig. 5.** Distribution of coal particles in the furnace of the KVTk-100-150 boiler unit

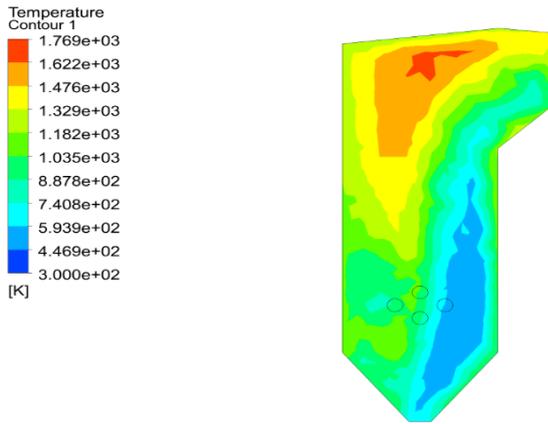


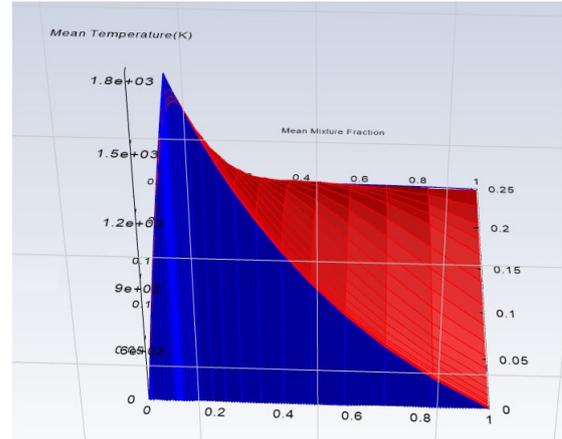
Fig. 6. Temperature field (K) in the vertical section of the KVTk-100-150 boiler

Since the conversion of the KWTK-100-150 boiler from solid fuel to generator gas is envisaged, it is necessary to calculate the generator gas. Generator gas can be obtained from a variety of solid fuels. This paper is based on the literature on the composition of generator gas, which is produced from the Ekibastuz coal. The composition and LHV of the generator gas is shown in Table 3. In this simulation, a three-dimensional simulation of the gas generator was performed.

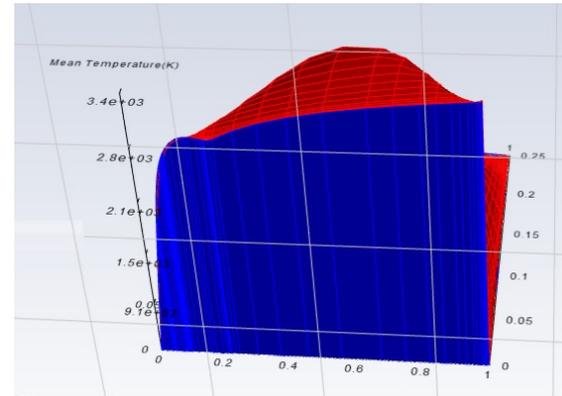
Table 3. Elemental composition and lower heating value of generator gas

Rank	Units	Value
Hydrogen, H <sub>2</sub>	%	30.0
Nitrogen, N <sub>2</sub>	%	50.4
Oxygen, O <sub>2</sub>	%	7.3
Sulphur, S	%	0.70
Carbon monoxide, CO	%	30.0
Carbon dioxide, CO <sub>2</sub>	%	5.0
Methane, CH <sub>4</sub>	%	2.0
Hydrogen sulphide, H <sub>2</sub> S	%	0.2
Total	%	125.6
LHV	kJ/kg	6 400

To ignite the gas generator, it is necessary to provide its composition in the ANSYS Fluent program. The composition of the gas generator will depend on the composition of coal. The elementary composition and LHV of generator gas is shown in Table 3. Since the LHV of the generator gas is 5 times less than that of coal, its maximum temperature will be much lower. Therefore, in addition to these calculations, work was carried out to determine the maximum temperatures. The results are shown in Fig. 7. It was found that the adiabatic combustion temperature of Ekibastuz coal and generator gas has the following values: 3000 K and 1800 K, respectively [7-12].



a) Maximum temperature level for generator gas



b) Maximum temperature level for Ekibastuz coal

Fig. 7. Comparison of the maximum temperature level for the Ekibastuz coal and generator gas

#### Analysis of the results obtained by modeling

Nitrogen concentrations and temperature levels at the furnace outlet are shown graphically in Fig. 8. From the results obtained, we can conclude that the generation of nitrogen oxide occurs through two mechanisms: first, the high temperature inside the furnace – that is, thermal NO<sub>x</sub> formation mechanism, and the second is the fuel NO<sub>x</sub> formation mechanism. In the case of Ekibastuz coal combustion, whose LHV (LHV=16 493 kJ/kg) is 2.57 times higher than that of generator gas (LHV=6 400 kJ/kg) it is obvious that the mass fraction of NO<sub>x</sub> is much higher. At the same time, the values given in Table 1 clearly indicate that the fuel contains nitrogen (N<sup>F</sup>= 0.8%), which of course affects the formation of fuel nitric oxide.

In order to study the distribution of temperature levels, temperature and velocity contours at heights of 9.2, 11.2, 13.2, 15.2 meters of the boiler furnace, were considered. The results are shown in Fig. 8.

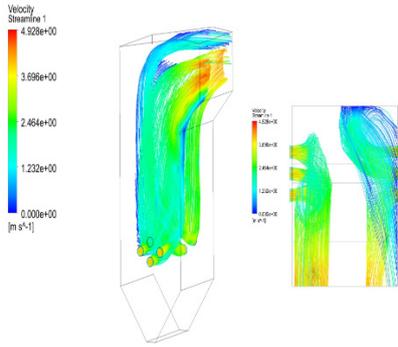


Fig. 8. Temperature and speed values in the vertical section of the KWTK-100-150 boiler

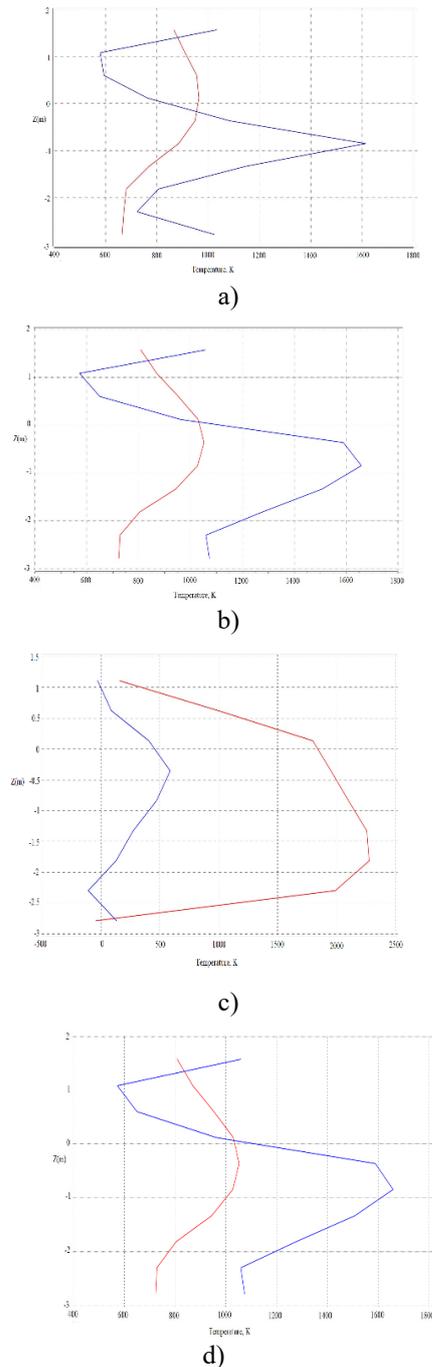


Fig. 9. Temperature distribution by altitude, K (red line for generator gas; blue line for coal)

Fig. 9 shows the temperature distribution for Ekibastuz coal and generator gas in the vertical section of the KWTK-100-150 boiler. As it can be seen, the temperature of coal has a low value at altitudes between 9.2 and 11.2. The main reason for this is the length of the combustion time of a coal particle relative to the gas. However, in the upper radiation part of the boiler, it is clear that the temperature of coal is much higher when compared with generator gas. It is clear that when switching the boiler to gas, it is necessary to take into account the location of the screen pipes and the modes of water circulation.

It is obvious that a decrease in the concentration of the oxidizing agent leads to a decrease in temperature in the combustion zone, due to the lack of oxygen to initiate the combustion reaction. At minimum values of oxygen concentration in the combustion zone, the highest temperatures were between 1500K and 1600K.

The decrease in the concentration of oxygen leads to insufficient combustion of fuel, which, in turn, reduces the temperature in the combustion zone. It was noted that an increase in the oxygen concentration from 16% to 18% leads to a sharp increase in the concentration of nitrogen oxides.

The same character has the dependence of the concentration of soot on the oxygen concentration in combustion chamber. A sharp increase in the concentration of soot at 18% indicates that there is no sufficiently complete burning out of pulverized coal.

"Rebening-process" - three-stage combustion. Suppression of nitrogen oxides to molecular nitrogen.

However, as was previously shown in the works, this method to reduce emissions of nitrogen oxides has a fundamental disadvantage. The resulting reduction zones in the form of carbon monoxide and hydrogen contribute to significant corrosion of metals, as well as the occurrence of carcinogenic substances.

The paper [8] notes the feasibility of less costly measures to suppress the formation of nitrogen oxides through the appropriate organization of combustion processes.

The above results clearly demonstrate the fairly high efficiency of the proposed method of initial gasification of Ekibastuz coal in the mechanism for suppressing the formation of nitrogen oxides without increasing the yield of products of incomplete combustion of fuel.

The essence of the proposed phase shift method with the reduction of nitrogen oxide to molecular nitrogen, due to the carbon of the fuel and the phase

shift of the air supply, consists in preliminary gasification of coal particles with a temporary delay in supplying air to the gasification products before entering the combustion zone in the flue volume itself [8].

This technique allows, in our opinion, to ensure the reduction of nitrogen oxide emissions to the level of modern requirements without increased emission of carcinogenic substances, high-temperature corrosion of metals, chemical and mechanical underburning, and with the lowest capital and operating costs.

## CONCLUSIONS

The performed mathematical modeling of combustion in a boiler allowed us to draw the following conclusions:

- the NO<sub>x</sub> emission is significantly affected by the temperature of the fuel and air. The study of combustion and mixing processes made possible to determine the optimal combination of fuel consumption with an oxidizer in terms of the formation of nitrogen oxides;

- the process of flame stabilization and the formation of harmful substances is largely affected by the excess air, which is determined in inverse proportion to the concentration (consumption) of fuel;

- the results obtained by the mathematical modeling of combustion processes make it possible to explain the processes under study in more detail than when conducting experiments alone, since real combustion processes are rather transient.

The results of the simulation of burning Ekibastuz coal and generator gas in the KWTK-100-150 boiler led to the following conclusions:

- owing to the high heating value of Ekibastuz coal, at the same fuel consumption, the temperature level inside the furnace is much higher.

- the temperature distribution directly depends on the combustion rate of the coal particle. That is, the temperature of coal particles above the level of the burners is much higher.

The error deviation has been evaluated, and it is noted that the error is decreased with definite parameters. The obtained results prove the efficiency of the proposed modeling technique. The proposed boiler plant model has advantages such as flexibility, accuracy, and the ability without the knowledge of experts. However, the proposed model has not been

experimented for its accuracy under external disturbance. In such cases, the precision shall be uncertain, which should be compensated for in the future.

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