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Numerical simulation of the coal dust process to the emission of nitrogen oxides

B. Ongar[1], I. K. Iliev[2]

[1]*Almaty University of Power Engineering and Telecommunications, Department of Heat Engineering Installations, 126, A. Baitursynov Str., 050013 Almaty, Kazakhstan*

[2]*University of Ruse, Department of Thermotechnics, Hydraulics and Ecology, 8 Studentska Str., 7017, Ruse, Bulgaria*

In the experiment, the influence of the shift of the oxidant feed on the processes of formation of nitrogen oxides was studied. In order to do so, a vertical tubular furnace with electric heating was used. The flow of dust of Ekibastuz coal in all experiments was kept constant to 0.042 g/s, the grinding factor was 18% and the excess air ratio 1.2. The temperature in the furnace varied from 500°C to 700°C at an 11% oxygen concentration inside.

As a result of the experiments, it is shown that by pyrolysis of coal dust from Ekibastuz coal at temperatures of 500-700°C and the delay of time of air supply to the combustion zone by 0,1 s, under experimental conditions, we were able to reduce the concentration of nitrogen oxides by 3 times, including a 1.25 and 1.9 times reduction due to pyrolysis at temperatures ranging from 500 to 700°C , in addition to a 2.7 and 1.9 times reduction owing to the delay of the air supply introduced.

In the numerical simulation, the effect parameters such as fuel consumption, fuel temperature and air temperature on the nitrogen oxides' formation processes is investigated. Increasing the concentration of oxygen from 16 to 18% significantly increases both the temperature and the formation of thermal nitrogen. The increase in the concentration of coal dust has a complex nature of dependence, for instance at values higher than 40 kg/h, there was a reduction in the formation of nitrogen oxides.

Keywords: Combustion processes, concentration of nitrogen oxides, nitrogen oxides, torch, recombination, burner device

INTRODUCTION

In world energy consumption, coal accounts for about a quarter. For the most part, coal is used to generate electrical and heat energy for the pulverized combustion of large power plants in boilers. Large energy enterprises on coal are the main source of nitrogen oxide emissions into the atmosphere. The use of low-emission burners and step-by-step combustion schemes allows a significant reduction in nitrogen oxide emissions at relatively low costs for the reconstruction of the furnace.

As shown by experiments and data [1], noticeable pyrolysis of coal dust and the formation of nitrogen oxides begin at temperatures above 500° C.

From previous adjustment experiments [1], it is known that pyrolysis of Ekibastuz coal dust occurs without the formation of nitrogen oxides, which confirms the position known from the absence of the influence of fuel oxygen on the formation of nitrogen oxides. During gasification of Ekibastuz coal dust in the air, the concentration of nitric oxide NO increases with increasing temperature. Thus, when the furnace temperature changed from 500 to 900°C, the concentration of nitric oxide changed from 340 to 670 mg/m^3.

However, this is only a simplified scheme. In fact, modernization projects include a full range of changes in the combustion system. First of all, it is necessary to study in detail:

- combustion chamber for calculating heat exchange and residence time of fuel particles in it;
- equipment for air supply;
- elemental composition of fuels, their thermal and physical properties and granulometric characteristics;
- method of burning fuel;
- operating conditions of the boiler, including its load, the composition of the fuel mixture, the distribution of air and gas streams, the boiler control system, etc. All these components are very important and not strongly related to each other. Therefore, they can be modelled separately [2].

Questions of numerical modelling of combustion devices, construction of a mathematical model of the combustion process in the combustion chamber of a boiler unit are relevant.

THE RESULTS OF STUDY AND THEIR DISCUSSION

Suppression of the formation of nitric oxide in the combustion of dust from Ekibastuz coal is mainly dependent on the kinetics of the chemical processes taking place in the mixture. The purpose of this paper is to develop experimental studies on

* To whom all correspondence should be sent:
iiliev@enconservices.com

the determination of effective ways to suppress the formation of nitric oxide, taking into account the concentrations of the components of the mixture. Such studies are carried out using mathematical modelling. The formulation of the problem of mathematical modelling is carried out in the form of a system of algebraic equations, compiled based on the laws of conservation of mass, momentum and energy.

Analysis of the results of well-known experimental studies allow us to draw the following unambiguous conclusions for building a model:

The formation of heat occurs in the initial part of the torch at the stage of ignition and combustion of volatile substances.

The output of fuel NO_X according to this data is in the range of maximum temperature values $T_M = 1200 \div 1800\,\mathrm{K}$ and is proportional to $(T_M - 1025)^{0,33}$ with oxygen concentration in the reaction zone $\sim O_2^2$.

$T_M < 1800$

The type of nitrogen-containing compound and the oxygen content in the fuel do not affect the yield of nitrogen fuel oxides.

The effect of fuel oxides from nitrogen on the total emissions of nitrogen oxides is more significant at low temperatures of the combustion process ($T_M < 1800\,\mathrm{K}$).

The kinetic mechanism in the formation of fuel oxides of nitrogen has not yet been fully studied, therefore, when building a mathematical model, two trends can be observed. Some researchers [3] are trying to take into account all sorts of elementary combustion reactions and the formation of nitrogen oxides of all kinds, as well as decomposition reactions of nitrogen oxides.

The kinetic constants of reactions, which are taken from literature data [4], as a rule, are very approximate and do not take into account the possible mutual influence of reactions in such a complex system.

In an experimental study of the formation of nitrogen oxides in the pulverized coal flare of Ekibastuz coal, the results of the study are shown in the form of the recombination graphs N_{exit} и N_2 (pic. 1) and experimental points of the experiments, which show the dependence of the concentration of nitrogen oxides on the concentration of molecular oxygen and temperature in a one-dimensional flow. It can be seen that a decrease in the oxygen concentration in the carrier stream leads to a sharp decrease in NO_x formation and a decrease in the final yield of nitrogen oxides.

Experimental data (Fig. 1) shows that the main formation of nitrogen oxides occurs when volatiles leave the coal. At very low temperatures (less than 900 K), volatiles do not ignite, and fuel oxides of nitrogen are almost not formed.

Figure 1 shows the graphs in the moment of release of atomic nitrogen from the fuel and its recombination into molecular nitrogen at different values of oxygen concentration (curves 1, 2, 3, 4, 5 correspond to oxygen concentrations of 1.3, 7, 10, 14% and process temperature in limits T = 800 - 1800 K).

Curve 1 in this figure indicates that in the absence of oxygen, atomic nitrogen fully recombines into molecular nitrogen under temperature conditions corresponding to energetic flue processes. Nitrogen oxides with the highest values of $O_2 = 14\,\%$ and $T = 1800\,\mathrm{K}$, are less than $7\,\%$ from fuel. If, after complete recombination of atomic nitrogen, oxygen is introduced into the molecular nitrogen region of the reaction, nitrogen oxide is not formed. This is the advantage of the proposed method of phase shift processes (MFSP).

Also from curves 2-5 shown in Figure 1, it can be seen that, the greater the oxygen concentration, the less atomic nitrogen recombines into molecular nitrogen at the same temperature values T. This can be explained by the fact that with increasing oxygen concentration, chemically active atomic nitrogen reacts with oxygen to increase the degree of formation of nitric oxide.

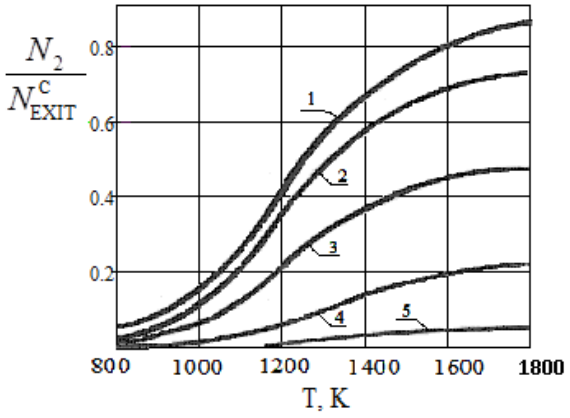

Fig.1. Recombination in for various 1, 2, 3, 4, 5 - ($N_2 = N_{EXIT}$), 1, 3, 7, 14 (%), ($N_{EXIT}^C = 2{,}10^{-4}, kg/nm^3$), 1, 2, 3, 4, 5 - $T = 800, 1000, 1200, 1400, 1600, 1800\ K$

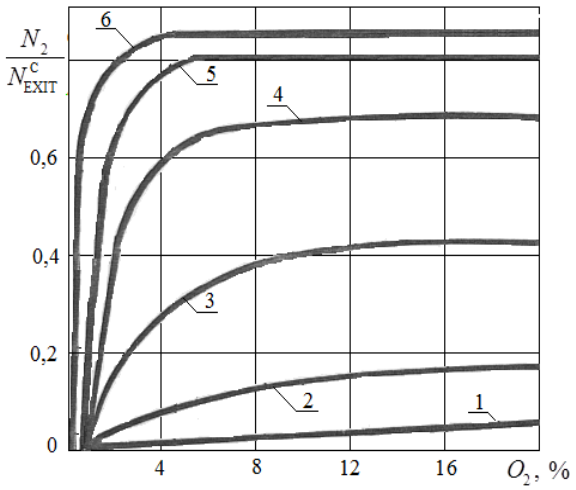

Fig.2. A recombination of N in N_2 depending on the temperature level of process at various values of concentration of oxygen 1 % (1), 2 % (2), 3 % (3), 4 % (4) and 5 % (5) of oxygen

Based on the data presented in Figure 2, it can be seen that the higher the temperature of the gasification process, the faster the release of atomic nitrogen and its recombination into molecular nitrogen. In this case, the indicated recombination ends at lower values of the oxygen concentration.

The recombination of atomic nitrogen into molecular nitrogen occurs, as can be seen from Fig.2, in a very short time and under ordinary energy conditions: $T = 1800 \div 1600$ K; O_2 no more 3% in flue gases (recirculation to the root of the flare), this recombination ends in a time less than c (see curves 6 in Fig.2). Consequently, the recombination of atomic nitrogen into molecular nitrogen occurs at a distance of at most one meter from the cut-off of the burner. According to Figure 1, the possible recombination of atomic nitrogen into molecular nitrogen occurs in a very short time, less than 0,4s, over a wide range of oxygen concentration changes. For example, if in the gasification of the Ekibastuz coal dust in the environment of the combustion products ($T = 1200$ K and $O_2 = 3\%$) the degree of this possible recombination is less 20%, then during its pyrolysis at T = 1800 K this ratio increases to 74%, that is almost 4 times. The degree of formation (concentration) of nitric oxide decreases so many times.

It is therefore evident, that the realization of such a high pyrolysis temperature of coal dust, close to 1800 K, is most likely possible in the furnace itself due to the powerful radiation of the torch, incendiary belt and lining. Another task is to provide this gasification temperature of coal dust with possible minimization of oxygen access, at least during the 0,4s.

In order to solve the different tasks, it is proposed to organize furnace processes with a phase shift in the supply of fuel and air to the combustion zone.

Modelling the formation of nitrogen oxides

To predict NO_x emissions, ANSYS Fluent solves the transport equation (equation 1). In cases where fuel nitrogen is specified, ANSYS Fluent solves additional transport equations for intermediate compounds such as HCN, NH_3. The transport equation NO_x is solved on the basis of data on flows and solutions to the equations of the combustion process. In other words, NO_x is processed after solving the combustion equations. Obviously, the accuracy of obtaining data on NO_x emissions are higher the higher the accuracy of the solutions of the combustion equations.

ANSYS Fluent solves the mass transfer equations for NO taking into account convection, diffusion, formation and decomposition of NO and related compounds. This general approach is based on the laws of conservation of mass. The influence of the time of finding on the mechanisms of formation of nitrogen oxides is taken into account through the convection variables in the determining equations. For the equation of the mechanism for the formation of thermal and fast NO_x, only one equation is needed:

$$\frac{\partial}{\partial t}(\rho Y_{NO}) + \nabla \cdot (\rho \vec{v} Y_{NO}) = \nabla \cdot (\rho D Y_{NO}) + S_{NO} \qquad (1)$$

where, Y_{NO} is the mass fraction of NO, S_{NO} is a constant set by the user.

The formation of thermal NO_x is determined by a group of chemical equations that depend significantly on temperature, called the extended Zeldovich mechanism.

Influence of the temperature of coal dust on the emission of nitrogen oxides

To calculate the temperature of the particle, taking into account the convective and radiative heat exchange of the particle with the surrounding gas, a mathematical model with a number of empirical expressions was used, which made it possible to correct the heat transfer taking into account the mass exchange processes occurring during the heating and burning of the coal particle [5].

Conducting computational studies, a model of the volume of a fresh charge located in the inlet channels and in the cylinder was created (Fig.3).

The process is a simultaneous flow of interrelated processes: aerodynamic, chemical and thermal.

The pulverized flare in the combustion chamber is a two-phase medium. We use equations for a continuous medium, into which corrections are introduced for the presence of solid dust particles of coal. In such technical flows that occur in combustion chambers, as a rule, the effect of the second phase is neglected and it is believed that the pulverized-coal flare is a two-phase gaseous dispersion medium in which the influence of the solid phase on the flow aerodynamics can be neglected [6-8].

The experience of mathematical modelling of furnace processes is disclosed in an experimental study of the formation of nitrogen oxides in a pulverized-coal flare, so we describe the models used in the study.

For the description of turbulent characteristics, a two-parameter κ-ε turbulence model, which has proved itself for developed turbulent flows, is used. This model, as noted in accuracy in conjunction with relatively low requirements for computing facilities. Tab.1 shows the data for the simulation.

Table 1, Initial parameters

Parameter	Unit. Measurement	Digital value
Air consumption	kg/s	0,08
Coal dust consumption	kg/s	0,005
Argon flow rate	kg/s	0,001
Air temperature	K	300
Coal dust temperature	K	300-700
Argon temperature	K	500

During modelling, the temperature of coal dust varied from 500 K to 700 K in steps of one hundred degrees. The isometric view of the simulated area is shown in Fig.3.

In the simulated region, coal was fed from the upper part, and heated argon was fed tangentially. The air was fed by a counter flow to the coal dust.

Heated carrier (argon) is an inert medium in the form of argon that is used to heat the particles to the required temperature before supplying air to the mixing zone and increasing reliability in achieving adequate conditions for the mixing process and ignition of pulverized coal in physical and numerical experiments.

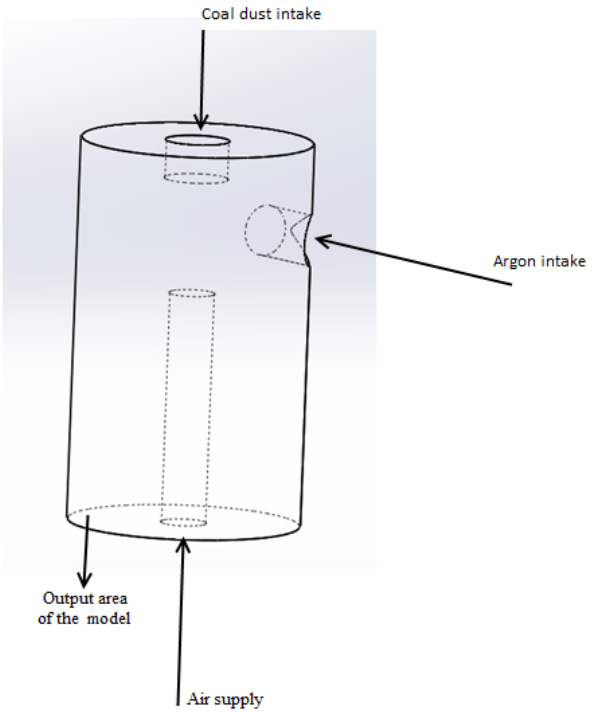

Fig.3. Modelling area

Fig.4 shows the contours of longitudinal velocities at different temperatures of coal dust. As can be seen from the picture, as the temperature increases, the air velocity from the nozzle increases, which indicates a lesser resistance to coal dust.

Second, it can be seen that the tangential velocity component created by argon tends to decrease, which is highlighted by the red circle.

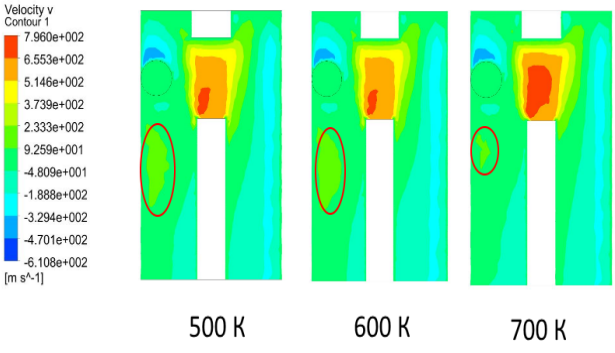

Fig.4. Contours of axial velocities at various temperatures of coal dust

Fig.5 shows the temperature profiles as a function of the temperature of the coal dust. As can be seen from the picture, with an increase in the

temperature of coal dust, the high-temperature zone shifts to the output of the model. This can be explained by the velocity flows shown in Fig.4. Air having a lower resistance pushes out high-temperature gases towards the exit region.

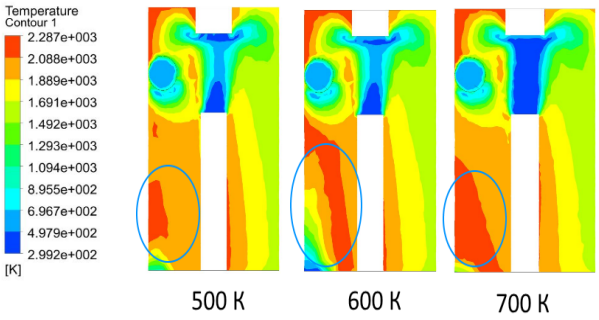

Fig.5. Temperature contours depending on the temperature of coal dust

Fig.6 shows the dependence of the concentrations of nitrogen oxides on the temperature of coal dust. It can be seen from the figure that an increase in the temperature of coal dust leads to an increase in the formation of nitrogen oxides, which is natural, in view of the fact that an increase in the temperature in the combustion zone increases the formation of nitrogen oxides.

An increase in the temperature of coal dust by 100 K leads to a twofold increase in the concentrations of nitrogen oxides, which explains the exponential dependence of the concentrations of nitrogen oxides and temperature.

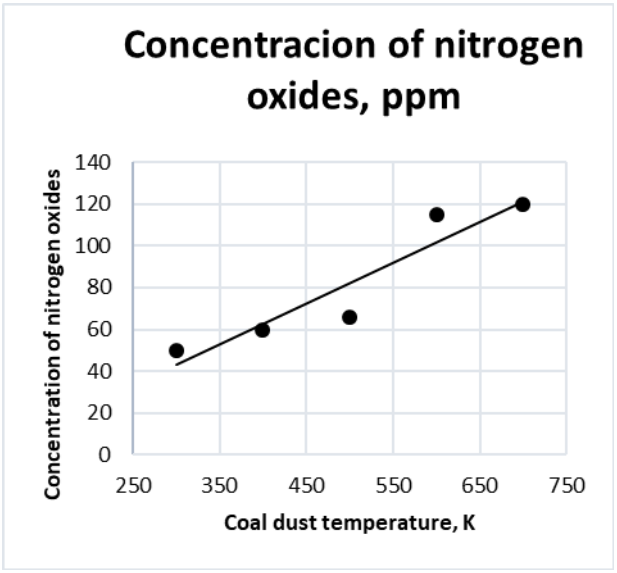

Fig.6. Dependence of concentrations of nitrogen oxides on the temperature of coal dust

Influence of air temperature

In these numerical experiments, the temperature of the initial air varied from 300 to 700 K.

Table 2, Parameters in the study

Parameter	Unit. Measurement	Digital value
Air consumption	kg/s	0,08
Coal dust consumption	kg/s	0,005
Argon flow rate	kg/s	0,001
Air temperature	K	300-700
Coal dust temperature	K	500
Argon temperature	K	500

Fig.7 shows the temperature contours for different initial air temperatures. An increase in air temperature leads to an increase in the temperature in the combustion zone. It is seen that, in comparison with the increase in fuel temperature, an increase in air temperature leads to a significant increase in the emission of nitrogen oxides. This is due to the fact that with an increase in temperature, which in the mass composition is greater than the composition of the fuel.

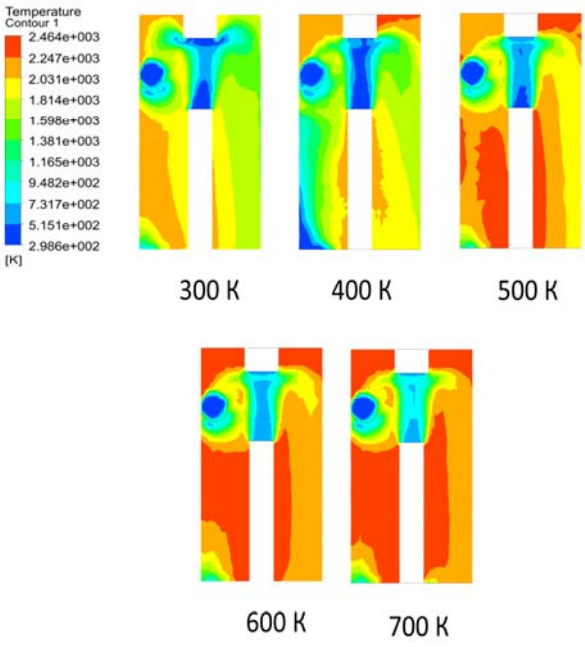

Fig.7. Dependence of temperature on the initial air temperature

Separately, it can be noted that the combustion process starts earlier, which indicates that an increase in temperature leads to an earlier ignition of the fuel.

It should be noted that the high-temperature zone with increasing air temperature approaches asymmetrical form. This is especially noticeable with an initial air of 700 K.

Fig.8 shows the dependence of the concentration of nitrogen oxides on the initial air temperature. An increase in the initial air temperature leads to a sharp increase in the emission of nitrogen oxides. Moreover, an increase in the initial air temperature until leads to an exponential increase in the concentration of nitrogen oxides. When the difference between 600 K and 700 K is almost 150 ppm, which is twice as much.

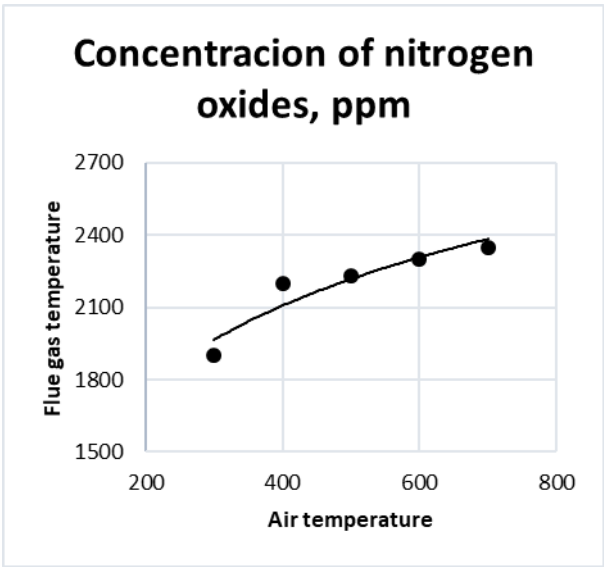

Fig.8. Dependence of the concentration of nitrogen oxides on the initial air temperature

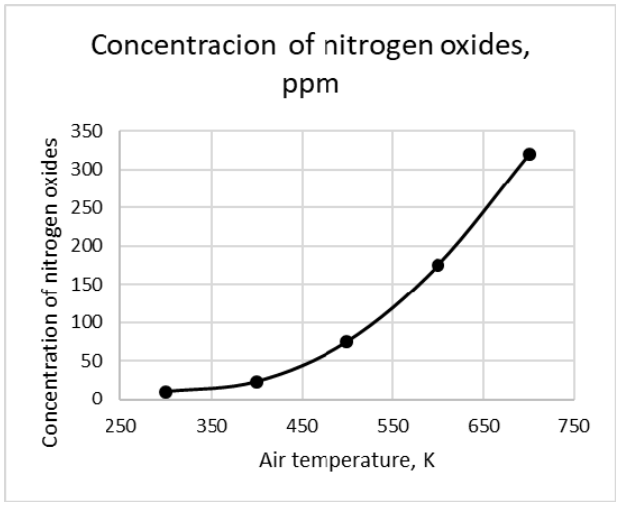

Fig.9. Temperature dependence of outgoing gases as a function of air temperature

An increase in the initial air temperature increases the average temperature at the exit from the experimental zone. Given that most of the nitrogen oxides are thermal, we can assume that despite an insignificant increase in the mean temperature, zones with local concentrations of fuel grow, which ensures a high growth of nitrogen oxide concentrations, as shown in Fig. 9.

CONCLUSIONS

The numerical simulation allowed to draw the following conclusions:

1. The temperature of fuel and air significantly influences the process of emissions of harmful substances. The numerical simulation of the combustion and mixing processes allowed us to determine the optimal combination of fuel consumption.

2. The process of flame stabilization and formation of harmful substances is significantly influenced by the excess air factor, determined in inverse relationship to the concentration of fuel (flow).

3. Numerical modelling of combustion processes, allow more detailed explanation of the combustion processes during the experiments, in view of the fact that the actual combustion processes are short-lived.

4. The optimal parameters for the fuel mass and pressure in the combustion chamber have previously been identified in the works of scientists, specializing in the modelling of two-phase flows [9-12]. Various types of solid fuels are used by these authors, especially coals from Kazakhstan of various grades and ash content, which are burnt in thermal power stations at the different thermal power plants of the country [13-15].

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NOMENCLATURE

HHV - Higher heating value of fuel at 273 K, 0.1 MPa basis, MJ/m^3;

LHV - Lower heating value of fuel at 273 K, 0.1 MPa basis, MJ/m^3;
NO_X - nitrogen oxides;
NO - concentration of an oxide of nitrogen;
N_2 - molecular nitrogen, %;
O_2 - oxygen in air, %;
R - universal gas constant, R=8.314 J/(mol.K);
T - absolute temperature, K.

Subscripts

NO - concentration of an oxide of nitrogen.

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