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# Numerical investigation of the influence of operating conditions on the formation of nitrogen oxides in the combustion chamber of a low-power boiler during the combustion of coal-water fuel

**Viktor Kuznetsov**[1,2], **Leonid Maltsev**[2], **Alexander Dekterev** [1,2] **and Mikhail Chernetskiy**[2]

[1] Siberian Federal University, 79 Svobodny, Krasnoyarsk, 660041, Russia
[2] Kutateladze Institute of Thermophysics, Novosibirsk, 630090, Russia

E-mail: victor_partner@mail.ru

**Abstract.** The paper presents verification of the mathematical model and the results of a numerical research of the influence of operating conditions on the formation of nitrogen oxides during the combustion of coal-water fuel in a promising low-capacity boiler. For the numerical simulation of turbulent flow of an incompressible liquid, we used the approach of Reynolds-averaged Navier–Stokes equations (RANS) taking into account the interfacial interactions. To solve the equation of thermal radiation transfer, the P1 approximation of spherical harmonics method was employed. The optical properties of gases were described based on the sum of gray gases model. To describe the motion of coal particles we used the method of Lagrange multipliers. The combustion process of coal-water fuel is considered in terms of the following consecutive steps: evaporation of the water part of the droplet, evaporation of moisture from the fuel, devolatilization and the combustion of the volatile components, and the combustion of the coke residue. Comparative analysis has shown that the selection of the operating conditions of the boiler has a significant influence on the oxygen concentration in combustion chamber and the temperature of the flue gases. This leads to significant differences in the formation of nitrogen oxides during the combustion of coal-water fuel.

## 1. Introduction

The improvement of technologies for the use of various fuels for the development of the energy sector is now an important task. Concerning, coal energy at this stage requires the use of innovative technologies - energy-efficient, resource-saving and environmentally friendly. One of the ways to ensure large-scale involvement of coal, at least in low-capacity energy, can be the use of coal combustion technology in the form of a coal-water suspension (coal-water fuel, CWF) [1-4]. The technology of coal combustion in the form of CWF is one of the most environmentally friendly, economically viable and promising. It allows the use of low-calorie and lean coals and by-product coal for the preparation of CWF, as well as the creation of composite water-peat-coal, water-oil-coal and other fuel compositions on their basis.

Mathematical description of coal-water fuel combustion includes a set of interrelated models describing turbulent gas motion, the transfer of thermal and radiant energy, combustion, movement of the coal particles, etc.

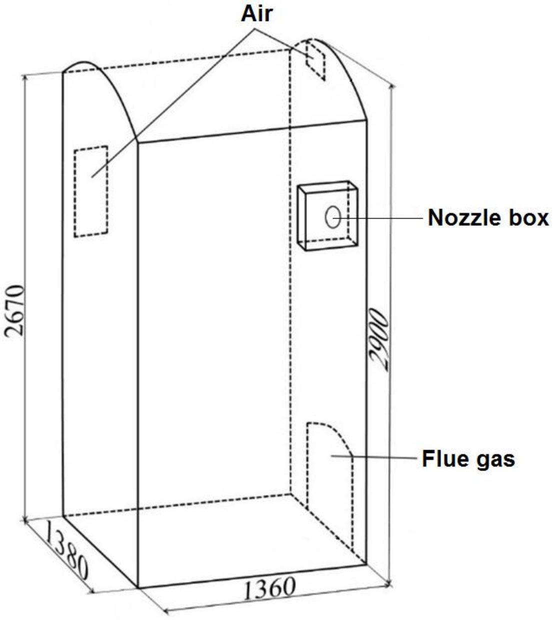

**Figure 1.** Scheme of boiler furnace (in mm).

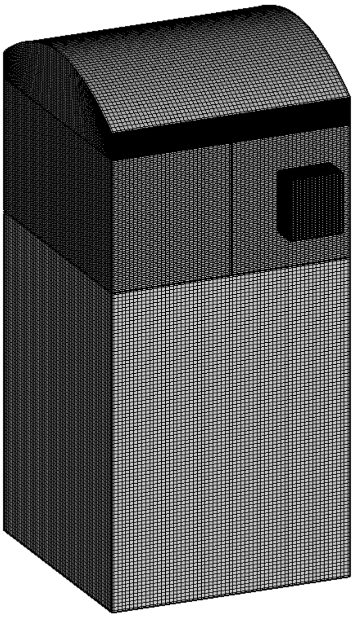

**Figure 2.** Computation mesh of combustion chamber.

The aim of this work is the verification of a complex mathematical model and a numerical research of the influence of operating conditions on the description of the nitrogen oxides formation during the combustion of coal-water fuel in a perspective low-capacity boiler.

## 2. Problem statement and research methods

For numerical studies and verification of the mathematical model we used experimental data on the combustion of coal-water fuel in a water-heating boiler with a nominal power of 1 MW [5]. The sketch of the boiler is presented in figure 1. To ensure high economic characteristics of the boiler, its design envisaged air heater and a system of liquid ash removal. Fuel in the furnace is supplied by a pneumatic nozzle [6], which has good indicators of efficiency and reliability in operation. In the furnace there are two windows for air supply (figure 1) which provide a swirling flow of the fuel-oxidizer and allow the intensification of the heat-mass-exchange processes of combustion. The nozzle for spraying coal-water fuel is located on the front wall of the furnace and is directed towards the air ducts located in the rear and right side walls of the furnace. In the combustion chamber, there are no heating surfaces, which contribute to the adiabatic combustion process. Flue gases from a cyclone furnace are removed through a window located in the lower part of the side wall of the furnace (figure 1).

We investigated the effect of the amount and temperature of the supply air on the nitrogen oxides formation during the combustion of coal-water fuel. The operating conditions and flow characteristics during the calculations are shown in table 1. The studies were carried out using coal-water fuel, which is a mixture of coal "K" (table 2) and water with a mass ratio of 50/50.

For numerical simulation of the turbulent flow of incompressible liquid, the approach of Reynolds-averaged Navier–Stokes equations (RANS) were used taking into account the interphase interaction [7,8]. Reynolds equations closure was provided by the popular two equation k−ε turbulence model [7,8]. The wall function approach was used to simulate wall boundary conditions. To describe the motion of particles, we used the Lagrange multiplier method. The particle motion is described by the dynamics equations for material point inclusive of the drag force and gravity. Accounting for flow turbulence in the particle motion is produced by the introduction of random fluctuations of the gas velocity in the motion equation for the particles. The solution to the equation of radiant energy transport is based on the P1 approximation of spherical harmonics for a two-phase two-temperature

**Table 1.** The operating conditions and flow characteristics.

| Variant | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| Fuel consumption, kg/s | 0.097 | 0.097 | 0.097 | 0.097 | 0.097 | 0.12 | 0.12 | 0.12 | 0.12 | 0.12 |
| Air consumption through nozzle, kg/s | 0.045 | 0.045 | 0.045 | 0.045 | 0.045 | 0.045 | 0.045 | 0.045 | 0.045 | 0.045 |
| Total air consumption, kg/s | 0.369 | 0.369 | 0.369 | 0.336 | 0.401 | 0.345 | 0.345 | 0.345 | 0.317 | 0.372 |
| Air temperature through air ducts, °C | 25 | 280 | 400 | 280 | 280 | 25 | 280 | 400 | 280 | 280 |
| Excess air ratio, $\alpha$ | 1.7 | 1.7 | 1.7 | 1.55 | 1.85 | 1.25 | 1.25 | 1.25 | 1.15 | 1.35 |

**Table 2.** Technical and elemental analysis of coal grade "K" (daf - dry ash-free state).

| $W^r$,% | $A^{daf}$,% | $V^{daf}$,% | $C^{daf}$,% | $H^{daf}$,% | $S^{daf}$,% | $N^{daf}$,% | $Q^r$, MJ/kg |
|---|---|---|---|---|---|---|---|
| 50.86 | 22.41 | 28.86 | 83.62 | 4.397 | 0.52 | 0.01 | 10.8 |

gray medium. As shown by previously performed computational studies [9, 10, 11], this integrated model gives good correlation with the experimental data, when burning solid fossil fuel in a pulverized form. The combustion process of coal-water fuel is considered in terms of the following consecutive steps: evaporation of the water part of the droplet, evaporation of moisture from the fuel, devolatilization and the combustion of the volatile components, and the combustion of the coke residue. Yield of volatiles is considered in the single-component approximation in the form of $C_xH_yO_z$ substance. The rate of devolatilization was calculated using a single-stage kinetic model with constants appropriate to the studied grade of coal [12]. Calculation of the gaseous components combustion was carried out with due account for the reactive power and concentration of fuel and oxidizer, as well as the rate of turbulent mixing of fuel and oxidizer. The combustion rate of coke residue was calculated in accordance with the provisions of the classical diffusion-kinetic theory. Kinetic constants of chemical reaction for the oxidation of coke residue were taken from [12].

A mathematical model of NOx formation during coal combustion involves consideration of three mechanisms taking into account the influence of temperature fluctuations: thermal NOx calculated based on the known dependence of Zeldovich [13], prompt NOx and fuel NOx calculated using a model proposed in [14], as well as the supplement of the “reburning”, proposed by Chen [15]. The calculation of the nitrogen oxides formation was conducted after obtaining the convergent solution for the basic parameters of two-phase reacting flow in the "postprocessing" regime.

To solve the conservation equations for the gas phase, we used the well known control volume method. For calculation of diffusion fluxes on the faces of the control volume, we used the central-difference approximation of the second-order accuracy. When approximating convective terms, we used the second-order accuracy scheme. To solve the resulting system of equations, we used the incomplete factorization method, in which just the diagonal terms were factored out. To link the pressure and velocity fields, in the present work we used the SIMPLE-like algorithm with collocated grids. The proposed model and solution methods were previously tested for solving problems on pulverized coal combustion and gasification [10, 11], and showed a satisfactory agreement with the experimental data in terms of the basic process parameters in the combustion chamber. The task is solved in a three-dimensional formulation. The grid was 864,140 nodes (figure 2), in the nozzle area the grid was constructed in more detail in order to describe the process of spraying coal-water fuel more qualitatively.

**Table 3** Parameters flue gas at the outlet of the combustion chamber.

| Variant | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| Flue gas temperature (calculation), °C | 1037 | 1133 | 1197 | 1196 | 1098 | 1236 | 1382 | 1422 | 1390 | 1327 |
| Flue gas temperature (experiment [5]), °C | - | 1134 | - | - | - | - | 1412 | - | - | - |
| Carbon losses (calculation), % | 5.9 | 4.5 | 4.1 | 4.9 | 4.3 | 9.8 | 8.6 | 8.4 | 12.6 | 7.0 |
| NOx, ppm (calculation) | 57 | 80 | 84 | 82 | 75 | 78 | 101 | 114 | 90 | 151 |
| NOx, ppm (experiment [5]) | - | 83.6 | - | - | - | - | 104.4 | - | - | - |

## 3. Results and discussion

Table 3 and figures 3, 4 present the results of a calculation study of the combustion of coal-water fuel in a promising boiler. Note that the calculated concentration of nitrogen oxides in flue gases and temperature of the flue gases at the exit of the combustion chamber is in good agreement with the experiment (variant 2, 7).

We can see that, when the supply air temperature increases from 25°C to 400°C, the NOx concentration in the flue gas increases by 27 ppm for variant 1-3 and by 39 ppm for variant 6-8. This is primarily due to the growth of the thermal NOx [16], since the temperature in the combustion chamber and the temperature of the flue gases increase.

Figures 3, 4 show the results of a calculation study in the form of oxygen concentration and nitrogen oxides in the center of the combustion chamber. As is well known, a decrease in the concentration of the oxidant in the combustion zone affects the formation of NOx in two ways: on the one hand, their concentration decreases as a consequence of the smaller formation of the fuel NOx, on the other hand, the concentration of the thermal NOx increases due to the temperature increase with decreasing excess air ratio. For variants 2 and 5 (table 3, figures 3, 4), when the excess air factor is increased, the concentration of the thermal NOx decreases due to a decrease in temperature. The fuel

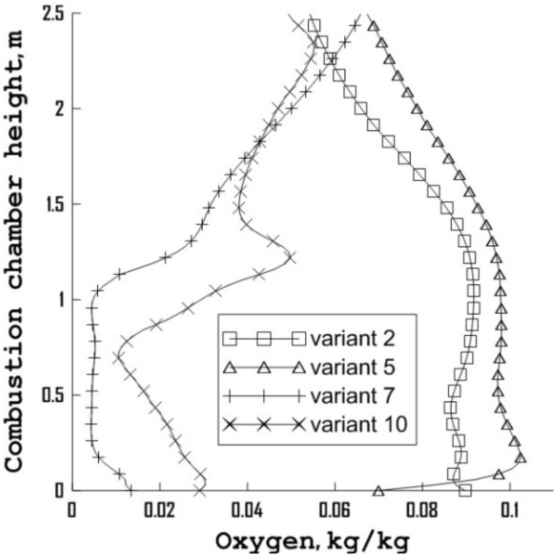

**Figure 3.** Concentration of oxygen.

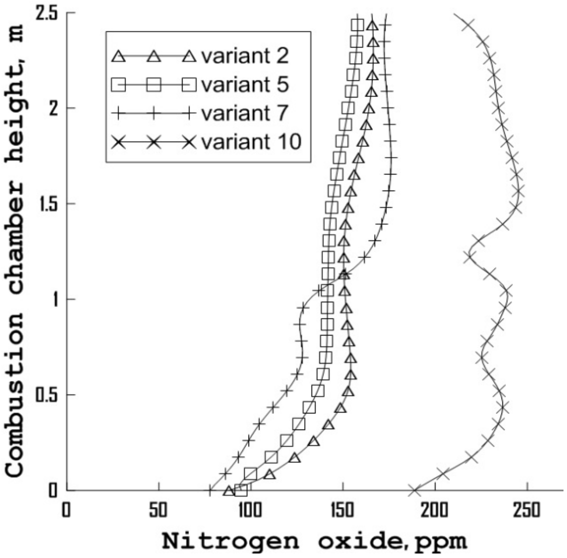

**Figure 4.** Concentration of nitrogen oxides.

NOx does not change significantly, because for this regime, excess air is ballast and does not take part in the oxidation reaction.

For variants 7 and 10, with an increase in the excess air ratio from 1.25 to 1.35, the concentration of nitrogen oxides in the flue gases increases by 50 ppm (table 3). This is due to the increase in the fuel NOx (figure 4) due to the increase in oxygen in the combustion chamber (figure 3), since for this regime the excess air ratio is close to the stoichiometric value and added oxygen actively participates in oxidative reactions. Reduction of carbon losses by 1.6% (table 3) with increasing amount of air confirms this.

## 4. Conclusion

We have performed verification of the complex mathematical model of burning of coal-water fuel in the combustion chamber, based on a comparison of the calculated and experimental data obtained on the same boiler. We have performed numerical investigation of the influence of the operating conditions of the boiler on the formation of nitrogen oxides during the combustion of coal-water fuel. It is shown that the mathematical model of fuel combustion satisfactorily describes the processes occurring inside the furnace. Selection of the operating conditions of the boiler, when calculating the combustion of coal-water fuel, significantly influences the distribution of oxygen concentration and temperature. It is shown that for different operating conditions of the boiler on coal-water fuel, an increase in the excess air ratio can both increase and decrease the concentration of nitrogen oxides.

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