Journal of Engineering Science and Technology Review
Special Issue on Telecommunications, Informatics, Energy and Management 2019

Conference Article

JOURNAL OF
Engineering Science and Technology Review

www.jestr.org

Numerical Simulation of the Formation of Nitrogen Oxides in Pulverized Furnaces

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Received 25 September 2019; Accepted 11 February 2020

Abstract

The object of research is the area of generation of nitrogen oxides of a pulverized coal torch.
Theoretical and experimental studies of the combustion process in the combustion chamber of the boiler were performed. Multiparametric calculations using numerical simulation methods make it possible to obtain results that are fully compatible with experimental data, as well as to visualize the solutions obtained. Consideration of alternative technical solutions, analysis of existing methods to reduce the formation and emission of nitrogen oxides and consideration of the possibility of applying an integrated approach to the issue of reducing the formation of nitrogen oxides using the method of mathematical modelling in combination with experiment – all together represents a tool of this study. Based on a comparison of the results of theoretical calculations with experimental data, important conclusions on the formation of nitric oxide in pulverized furnaces were obtained.
In the numerical simulation, the effect parameters such as fuel consumption, fuel temperature and air temperature on the nitrogen oxides' formation processes are 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: Numerical simulation, mathematical model, torch, recombination, atomic nitrogen, molecular nitrogen.

1. Introduction

Theoretical and experimental studies of the combustion process in the combustion chamber of the boiler were performed. Multiparametric calculations using numerical simulation methods make it possible to obtain results that are fully compatible with experimental data, as well as to visualize the solutions obtained. Consideration of alternative technical solutions, analysis of existing methods to reduce the formation and emission of nitrogen oxides and consideration of the possibility of applying an integrated approach to the issue of reducing the formation of nitrogen oxides using the method of mathematical modelling in combination with experiment – all together represents a tool of this study. Based on a comparison of the results of theoretical calculations with experimental data, important conclusions on the formation of nitric oxide in pulverized furnaces were obtained.

In the numerical simulation, the effect parameters such as fuel consumption, fuel temperature and air temperature on the nitrogen oxides' formation processes are 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.

2. The results of study and their discussion

Taking into consideration the complex nature of the harmful effects of nitrogen oxides on the environment, it is the processes of their formation that are identified in this paper as the subject of study. The object of research is the area of generation of nitrogen oxides of a pulverized coal torch.

The formation of harmful substances is modelled using reaction-kinetic models and models of burning coal dust. The criteria for choosing a kinetic scheme is the optimal number of reactions and the components involved in them, as well as the accuracy of the reproduction of experimental data by calculations.

Studies of the processes of combustion and heat transfer of a torch are possible by the methods of mathematical modelling of these processes since it allows studying the fields of velocity, pressure, temperature and concentrations of substances in the torch. The mathematical model consists of a system of differential equations in partial derivatives and boundary conditions. For rotating flows of fuel and air,

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ISSN: 1791-2377

in general, the solution of a complex three-dimensional problem is required.

Classical engineering methods of calculation, as a rule, are applicable only to bodies of simple configuration and often cannot provide the necessary accuracy in the calculations of a complex real structure. For many engineering problems, the mathematical model includes systems of differential equations. Differential equations, which describe real physical processes, can be complex, in many cases, they are not solved by methods of classical mathematics. It turns out, when classical methods are unsuitable or for their application or it is necessary to greatly simplify computational models, which leads to significant errors in the obtained results, numerical methods are increasingly used to solve complex physical problems. They make it possible to reduce the solution to the implementation finite number of arithmetic operations, even if it is large and provided only an approximate solution with specific values of parameters and initial data. The main thing in this is that the allowable calculation error is acceptable. Many numerical methods have been known for a long time, but the volume of calculations did not allow them to be widely used for solving practical problems. The emergence of computing technology has significantly reduced the complexity of the calculations. As a result, today numerical methods are one of the main tools along with experiment at various stages of creating new technology.

Questions of numerical simulation of combustion devices, construction of a mathematical model of the combustion process in the combustion chamber of a boiler unit are extremely important for increasing the efficiency of the combustion process. In addition, in recent years, domestic heat and power engineering are increasingly in need of improving the means and methods of optimizing existing furnaces in order to improve their technical, economic and environmental performance. The development of modern computing, numerical simulation methods and specialized software packages greatly facilitate the solution of many complex problems. It became possible to carry out multi-parameter calculations that cannot be done analytically and to obtain results that are fully compatible with the experimental data, and also to visualize the solutions obtained. The software uses the physical principles of heat transfer calculation, takes into account a large number of influencing factors in the form of physically sound dependencies between them.

During the combustion of solid fuel in a pulverized state, in the combustion chamber occurs with turbulent processes of transferring heat and mass of reacting components and products of their interaction. Such processes are described by equations based on the laws of conservation of mass and momentum. For reacting streams in which heat transfer processes and chemical reactions occur, it is necessary to additionally solve the energy conservation equation and add the conservation equation for the mixture components or the conservation equation for the mixture fractions and their changes. Turbulence is described by transport equations for turbulent characteristics [1, 2].

A feature of the oxidation reaction NO is that in the Arrhenius equation, the reaction rate of the activation energy is negative E = -7.5 kJ/mol. According to the classical theory of the reaction rate with increasing temperature should grow, whereas the above numbers show that the oxidation rate of NO slows down with increasing temperature. Some authors try to explain this paradox on the basis of a possible multiphase mechanism of the reaction, for example, by equations:

$$NO + O_2 \leftrightarrow NO_3$$
$$NO_3 + NO \leftrightarrow 2NO_2 \quad (1)$$

It is assumed that with increasing temperature, the rate of the reaction of the formation increases NO_3 with an equilibrium shift to the left. An indirect confirmation of the correctness of the proposed explanations is the detection of in reacting mixtures by a spectrograph method.

The total concentration of nitrogen oxides in terms of dioxide (we emphasize that the combustion products of boilers of thermal power plants before the chimney contain 95-99% nitric oxide NO and 1÷5% dioxide NO_2) is determined by the formula [3].

$$C_{NO_X} = A(1+n)^{0.415} d_Э^{0.8} \alpha_T^3 (1-k_r r)(1-k_\delta \delta) k_Э, \quad (2)$$

where A = 0.18 - coefficient of proportionally; $d_Э = \frac{4F}{U}$ - the equivalent diameter of the combustion chamber, m; q_T - furnace thermal stress, mW/m^3; α_T - the coefficient of excess air in the furnace (burner); $r = \frac{100V_{PST}}{V_B}$ - gas recirculation rate usually 10-20%; k_r - recirculation efficiency coefficient ($k_r = 0.01$ when gas is fed into the slots under the burner; 0.015 through the annular channel around the burner;) 0.025 – in the blast air; 0.030- in the chopping of two air streams; β = 1.4 in liquid slag removal in other cases β = 1; δ- of the total supplied as (usually 20÷25%); k_δ - the efficiency ratio of the two-stage combustion (Table 1).

Table 1. The dependence of the efficiency coefficient of two-stage combustion on the proportion of secondary air

δ, %	5	10	15	20	fuel
k_δ	0.020 0.028	0.020 0.026	0.019 0.024	0.018 0.020	gas, fuel oil,

k_{eff}- The coefficient of efficiency of the joint action of two or more methods of suppressing nitrogen oxides ($k_{eff} = 1.3 \div 2$):

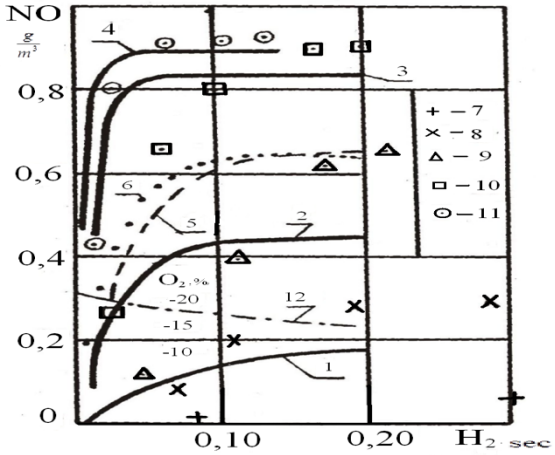
$$n = \frac{d_k(d_k - a)}{ab} \quad (3)$$
$$n = \frac{d_k(a + d_k + 2P_n)}{ab} \quad (4)$$

n - the intensity of the twist of the air flow for tangential and snail-tangential supplies, respectively; P_n- the shortest distance between the burner cylindrical channel and the inlet pipe wall nearest to the axis; a and b – width and length of the tangential approach.

For vortex burners approximately $(1+n)^{0.415} = \frac{1}{0.85} = 1.15$, and for direct-flow burners $(1+n)^{0.415} = \frac{1}{0.85} = 1.0$.

The formula is applicable in the range of changes in the coefficient of excess air $\alpha = 1{,}03 \div 1{,}16$.

In the figure 1, the calculation results are compared with experimental data. [4]. Overall, their agreement with each other is satisfactory. Due to the kinetic nature of chemical reactions, taken into account in the mathematical model some value is higher according to the results of the calculation of the formation of a nitric oxide than according to experimental data. In fact, the rate of a given chemical reaction is somewhat slow due to not considered factors associated with the nature of the organization and the diffusion nature of the mixture formation processes. Comparison of curves 2, 5 and 6 (see figure 1), related to the same temperature of 1200K, but to different values of oxygen concentration (3 and 14%) and coefficient γ (0,26; 0,8; 0,38), taking into account according to the proportion of nitrogen in the fuel passing into the gas phase. The main calculated curves 1, 2, 3 and 4 in the figure 5.5 correspond to the value $\gamma = 0{,}26$, which occupies an intermediate position between the values of 0.2 and 0.3, related to stone and brown coal, respectively.



Curves 1, 2, 3, 4 (T = 1000, 1200, 1600, and 1800 K); pyrolysis completeness coefficient: 0.26 at O_2= 14%; curve 5 (the coefficient of completeness of pyrolysis: 0.8 at O_2= 3% and T = 1200K); curve 6 (the coefficient of completeness of pyrolysis is 0.38 at O_2= 14% and T = 1200K); curves 7,8,9,10,11,12 (T = 950, 1050, 1220, 1570, and 1740K [5])

Fig 1. Comparison of calculation results with experimental data

When comparing the calculated and experimental data, it should be taken into consideration that the formation of nitrogen oxides is influenced by such a difficultly controlled factor as the polydispersion of particles of coal dust.

From the calculation data presented in the 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.

As can be seen from the above calculation results in a very short time and under normal conditions of the combustion process $T = 1800 \div 1600$ K; with O_2 no more than 3% in the flue gases, this recombination ends in less than 0.4s. (see the curves 6 and 5 in the figure 2).

Consequently, the recombination of atomic nitrogen into molecular nitrogen under normal conditions of a natural combustion process occurs in the furnace at a distance of not more than one meter from the burner cut, which corresponds to a dimensionless distance from the burner nozzle about one caliber.

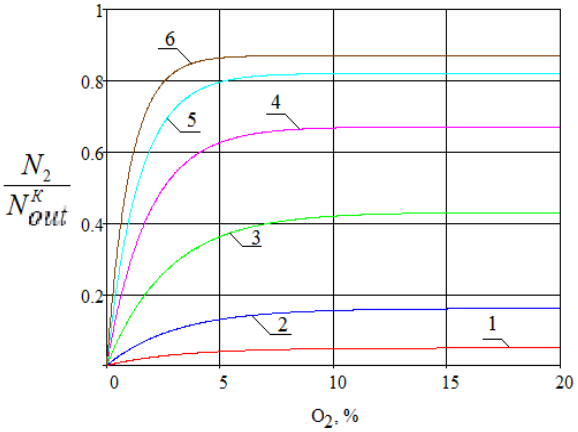


Fig 2. Recombination of atomic nitrogen N in N_2 at various concentrations of oxygen O_2 = 1,5,10,15,20% and temperature: - $T = 800, 1000, 1200, 1400, 1600, 1800\ K$ (curves 1, 2, 3, 4, 5, 6 – respectively)Estimated energy savings distributed by measures

3. The effect of oxygen concentration on the formation of nitrogen oxides in the gasification zone.

The figure 3 shows the temperature profiles in the model depending on the oxygen concentration.

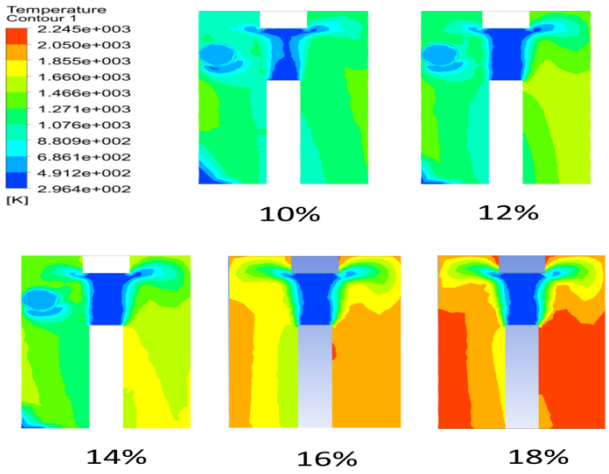


Fig 3. Temperature profiles in the model depending on the oxygen concentration

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 air in the combustion zone, the highest temperatures were 1500-1600K.

The figure 4 shows the dependence of the concentration of nitrogen oxides on the concentration of oxygen in the air.

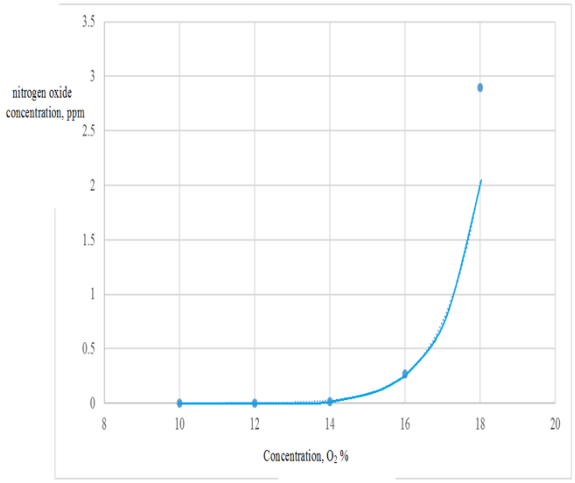


Fig 4. The dependence of the concentration of nitrogen oxides on the oxygen concentration in the supply air

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 in the feed air from 16 to 18% leads to a sharp increase in the concentration of nitrogen oxides.

The same character is the dependence of the concentration of soot from the oxygen concentration in the fuel (figure 5). A sharp increase in the concentration of soot at 18% indicates that up to 16% there is no sufficiently complete burning out of pulverized coal.

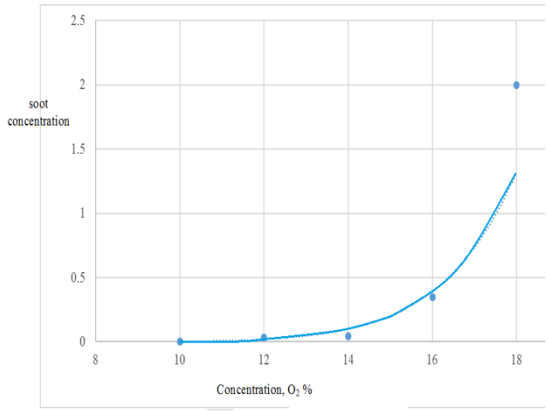


Fig 5. The dependence of the concentration of soot from the oxygen concentration in the air

The recommended application of the MACT method with the supply of secondary fuel to the zone of the start of ignition of pulverized coal contributes to the formation of a reducing zone in the horizontal plane with the subsequent afterburning of the fuel particles by alternating oxidizing and reducing zones in the firebox.

However, as was previously shown in the works [6-10], 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 [11] notes the feasibility of mass introduction 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 nitric 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 [12,13].

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

4. Conclusion

The conducted mathematical modelling led to the following conclusions:

- The temperature of fuel and air has a significant effect on the amount of nitrogen oxide emissions;
- A study of combustion and mixing processes made it possible to determine the optimal combination of fuel consumption with an oxidizing agent from the point of view of the formation of nitrogen oxides;
- The process of flame stabilization and the formation of harmful substances is largely influenced by the coefficient of excess air, which is determined in inverse relation to the concentration (consumption) of fuel;
- The results obtained by the method of mathematical modelling of combustion processes allow us to explain in more detail the processes under study than with the conduct of experiments alone, since the actual combustion processes are rather transient.

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