

Research of Formation and Destruction of NO_x During Combustion of Low-Grade Coal in CHP

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Abstract. The emissions of harmful substances such as sulphur and nitrogen oxides from thermal power plants are major source of adverse impact on the environment. In this regard, it remains be urgent the deeper studying of the solid fuel combustion processes. In this paper, two global schemes of formation and destruction of harmful nitrogen compounds NO_x studied during combustion of low-grade Kazakh coal in a real industrial boiler BKZ-75.

Introduction

The World Energy Outlook presents that global energy demand will continue to rise over the coming decades, with solid fossil fuels will continue to dominate as a raw material for the energy industry. Worldwide annual production of about 5 billion tons of coal, 70% of which are located in the United States, China and the CIS countries, including Russia and Kazakhstan. Most of the stocks (~63%) in Kazakhstan are fossil fuels, which has high ash-content [1-2].

Ensuring environmental safety requires a comprehensive study of operational processes in power plants. The deep study of complex nonlinear processes like combustion occurring in the combustion chamber of TPP is almost impossible without computational experiments [3-8]. In addition, it is profitable by financial and time costs. Meanwhile, the results of computational experiments can give full information about the nature of heat and mass transfer processes. The accuracy and adequacy of the expected results provided by the correct formulation of the physical, mathematical and chemical models of combustion processes [9].

The State of the Art

As the object, the proposed work used combustion chamber of the real industrial boiler BKZ-75 (Shakhtinskaya CHP, Kazakhstan). The burnt coal was Karaganda coal which has a composition: C - 33.87%, H₂ - 6.63%, S - 1.92%, N₂ - 2.23%, O₂ - 9.65%. W - 10.60%, A - 35.1%, Q - 34162 kJ/kg, R₉₀ - 20%. The modeling of combustion chamber worked out with the finite-difference grid, which consists of 126496 control volumes.

Numerical study of combustion processes based on the solution of convective heat transfer equations, taking into account convective and radiative heat transfer, chemical kinetics and the two-phase medium equations [10]. These equations consist of non-linear equations of the law of conservation of mass and momentum (the Navier-Stokes equations), the law of conservation of energy and matter. The law of conservation of mass has the form:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = 0 \quad (1)$$

Total Navier-Stokes equation, which describes the law of conservation of momentum:

$$\frac{\partial (\rho u_i)}{\partial t} = - \frac{\partial (\rho u_i u_j)}{\partial x_j} + \frac{\partial}{\partial x_j} \left(\mu \cdot \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \cdot \delta_{ij} \frac{\partial u_l}{\partial x_l} \right) \right) - \frac{\partial p}{\partial x_i} + \rho g_i \quad (2)$$

The equation describing the law of conservation of energy:

$$\frac{\partial (\rho E)}{\partial t} = - \frac{\partial (\rho u_j E)}{\partial x_j} - \frac{\partial q_j^{res}}{\partial x_j} - \frac{\partial (p u_i)}{\partial x_i} + \frac{\partial (u_i \tau_{ij})}{\partial x_j} + \rho u_i g_i + S_Q \quad (3)$$

The equation describing the law of conservation of matter:

$$\frac{\partial (\rho c_\beta^*)}{\partial t} = - \frac{\partial (\rho c_\beta^* u_i)}{\partial x_i} + \frac{\partial}{\partial x_i} \left(\rho \cdot D_{c_\beta^*} \cdot \frac{\partial c_\beta^*}{\partial x_i} \right) + S_\beta \quad (4)$$

Formation and destruction of harmful substances containing nitrogen modeled by two kinetic schemes [11] in the paper. The kinetic model by De Soete explains that key reaction mechanism for NOx formation consist by 90% of nitrogen oxide NO formed through hydrocyanic acid HCN, where much importance has the atomic nitrogen N:

$$\frac{dY_{NO}}{dt} = 1 \cdot 10^{10} Y_{HCN} Y_{O_2}^b \exp(-33700/T) ; \frac{dY_{N_2}}{dt} = 3 \cdot 10^{12} Y_{HCN} Y_{NO}^b \exp(-30100/T) \quad (5)$$

When the other scheme of NO formation takes into account the ammonia NH3:

$$\frac{dY_{NO}}{dt} = 4 \cdot 10^6 Y_{NH_3} Y_{O_2}^b \exp(-16100/T) ; \frac{dY_{N_2}}{dt} = 1.8 \cdot 10^8 Y_{NH_3} Y_{NO}^b \exp(-13600/T) \quad (6)$$

The second conducted Mitchell Tarbell model describes the nitrogen oxides NO formation by the oxidation of fuel bound nitrogen. There the kinetic scheme takes into account the reaction of the primary pyrolysis, homogeneous combustion of hydro-carbonaceous compounds, and heterogeneous combustion of coke; thermal-fuel formation of nitrogen compounds. Mitchell Tarbell model provides the first reaction step in the conversion of hydrogen cyanide HCN to ammonia NH₃ (Eq. 7). A formed ammonia NH₃ generates and destroys nitric oxide NO in the two parallel reactions as in Eq. (8).

$$\frac{dY_{HCN}}{dt} = -1.94 \cdot 10^{15} Y_{HCN} Y_{O_2} \exp(-39500/T) \quad (7)$$

$$\frac{dY_{NO}}{dt} = \frac{3.48 \cdot 10^{20} Y_{NH_3} Y_{O_2} \exp(-50325/T)}{1 + 6.90 \cdot 10^{-6} \exp(21140/T)} ; \frac{dY_{NH_3}}{dt} = -6.22 \cdot 10^{14} Y_{NH_3} Y_{NO} \exp(-27680/T) \quad (8)$$

The Mitchell-Tarbell model also takes into account recirculation of nitrogen oxides NO back to hydrogen cyanide HCN by reacting with hydrocarbons:

$$\frac{dY_{NO}}{dt} = -1.0 \cdot 10^4 Y_{NO} Y_{C_{xH_y}} \quad (9)$$

To carry out a computational experiment were used the following initial and boundary conditions.

For the velocity (derivative normal to the exit plane, velocity normal to the plane of symmetry, derivative, normal to the plane of symmetry, velocity normal to the wall, i.e. no mass flow, derivative, normal to the walls, speed, tangential to the walls sticking condition):

$$\left. \frac{\partial u_i}{\partial x_i} \right|_{normA} = 0 ; u_i|_{normS} = 0 ; \left. \frac{\partial u_i}{\partial x_i} \right|_{normS} = 0 ; u_i|_{normW} = 0 ; \left. \frac{\partial u_i}{\partial x_i} \right|_{normW} = 0 ; u_i|_{tang} = 0 \quad (10)$$

For energy (inlet temperature, derivative normal to the exit plane, derivative, normal to the plane of symmetry, derivative, tangential to the plane of symmetry):

$$h = C_p T ; \left. \frac{\partial h}{\partial x_i} \right|_{normA} = 0 ; \left. \frac{\partial h}{\partial x_i} \right|_{normS} = 0 ; \left. \frac{\partial h}{\partial x_i} \right|_{tangS} = 0 \quad (11)$$

For the components of the mixture (the initial concentration of component k at the input, derivative normal to the exit plane, derivative normal to the plane of symmetry, derivative normal to the solid surface):

$$c_k ; \left. \frac{\partial c_k}{\partial x_i} \right|_{normA} = 0 ; \left. \frac{\partial c_k}{\partial x_i} \right|_{normS} = 0 ; \left. \frac{\partial c_k}{\partial x_i} \right|_{normW} = 0 \quad (12)$$

Results of Numerical Modeling

The results of conducted computational experiments on the formation and destruction of NOx by two models of formation shown below.

Figures 1-3 shows field concentrations of nitrogen oxides NOx in the combustion chamber. From the analysis, it seen that the NOx concentration for the two models are differ from each other. This is because of the fact that by De Soete model the NOx formation performed mainly by the idealized kinetic scheme of chemical reactions when combusted the fuel with high quality. Whereas the kinetic scheme of Mitchell-Tarbell model of NOx formation based on chemical reactions, which takes into account the whole properties of fuel.

Figure 1 shows the distribution of NOx concentrations in the region of the burners (opposite placed 2 burners in one tier), where fuel-N and air-N (approximately in air 79%) is oxidized. From the analysis of NOx concentration fields by two models (De Soete – DS and Mitchell-Tarbell – M&T) shown that maximum concentrations by M&T model appeared in the boundary areas (approximately 5000 mg/Nm³) and in center (3000-4000 mg/Nm³) of combustion volume.

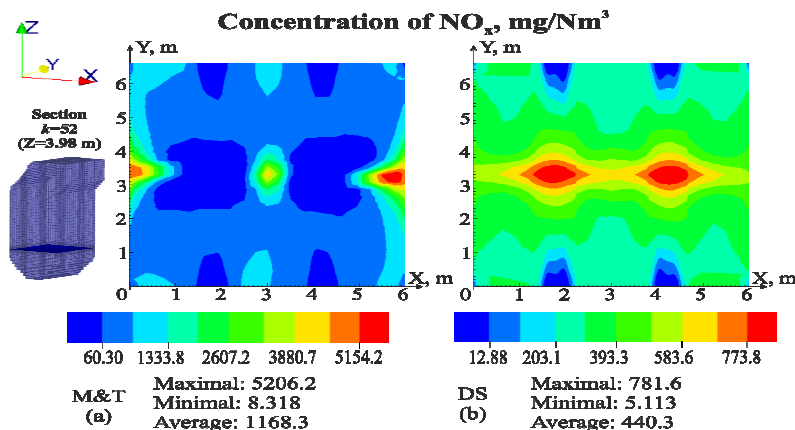


Figure 1. Distribution of the concentration of NOx in the region of the burners of the combustion chamber (Z=3.98 m) of the boiler BKZ-75.

In addition, by DS model the highest concentration of NOx obtained in the central area of combustion chamber (comparing to M&T model there is lower concentration equal to 800 mg/Nm³). The average NOx concentration in this section is 1168.3 mg/Nm³ by M&T model, and 440.3 mg/Nm³

by DS model. This difference rated as 60 %, which can have awesome influence on the accuracy of the results and subsequently, in whole research.

Figure 2 shows the three-dimensional distribution of the NO_x concentration at the outlet of the combustion chamber (X=7.14 m) by two models of formation and destruction of NO_x. This section has a mainly significance for the engineers who cares about the environmental task of the TPP's exploitation. The maximal value of NO_x there is not more than 700 mg/Nm³ for both model. This kind of decreasing is due to the weak of chemical interactions of nitrogen oxides. The difference in the mean concentration of nitrogen oxides NO_x on these models is ~ 25%.

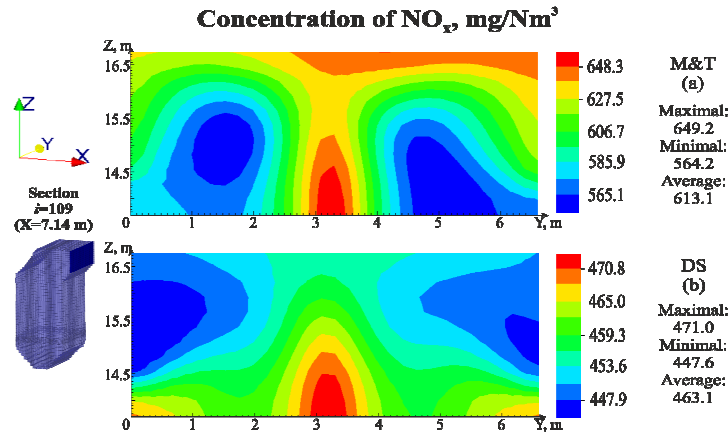


Figure 2. Distribution of concentration of NO_x at the outlet of the combustion chamber of the boiler BKZ-75.

For holding the computational experiments in our task, it is need to choose the most appropriate and adequate model for modeling the NO_x formation when burning the native high-ash content coal. For this purpose, in figure 3 shown the verification of average values of NO_x concentrations by Mitchell-Tarbell and De Soete models with values of nitrogen oxides NO_x obtained directly on CHP of Kazakhstan [12], as well as limit values (MPC) [13] for a coal-fired power plants of republic.

Analyzing these data, we can see that the experimental points and the value of the MPC (640 mg / Nm³) is closer to the values that were obtained using the model Mitchell-Tarbell, while for the second case (model De Soete) values are clearly underestimated.

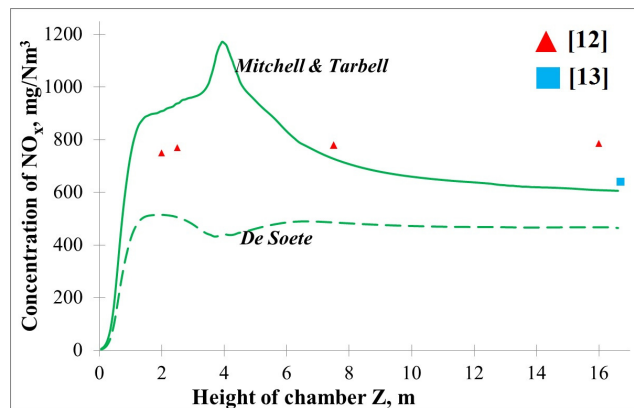


Figure 3. Distributions of the mean values of the concentration of NO_x by the height of the furnace of the boiler BKZ-75 for two models and its verification.

Thus, during the computational experiments on burning of Kazakhstan high ash content coal (30-50%) we can talk about the adequacy of the results when using the Mitchell-Tarbell model, which takes into account the stages comprising a primary pyrolysis, burning hydrocarbons and volatiles CH and burning of coke, which are recorded during the combustion of low grade coals.

Conclusion

In the energy sector of the Kazakhstan Republic dominated the use of low-grade coal with high ash content (~ 30-50%). It leads exceeding the maximum permissible emissions into the environment and thus the deterioration of the ecological situation in the country. To propose ecological clean and economic effective ways of work of TPPs it is best to hold computational research. This needs to choose the most adequate numerical methods of solution of tasks. In this regard, it chosen the right kinetic model for the formation of the most harmful component – NO_x.

In conclusion, it was marked that the De Soete model can greatly boost the numerical calculation process, so reduce computational time and resources. While the Mitchell-Tarbell model lasts longer and demanded more calculation resources. However, when carrying out computational experiments to study the characteristics of formation and destruction of the nitrogen compounds NO_x in boilers of Kazakhstan TPP where used (burned) low-grade native coal it is better and preferable to use the Mitchell-Tarbell model to obtain the adequate results. It shown and proven with verification given above.

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