Selection of the optimal kinetic scheme for the formation of nitrogenous substances in the simulation of low-quality coal combustion in the furnace chamber of a real heat-power facility

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Introduction

In conditions of depletion of natural energy resources and environmental pollution, the rational use of energy fuel, increasing the efficiency of energy production and solving environmental problems are an urgent and important task that needs to be solved. The main energy fuel in Kazakhstan is coal. The poor quality of coal from the main Kazakh coal deposits leads to industrial and environmental problems during its operation. In this regard, studies of the processes of burning low-grade coals are relevant.

Conducting detailed and in-depth research in real conditions is much more expensive than conducting computational experiments using computer modeling methods. At the same time, the results obtained by computational methods can also ensure the development of effective technological solutions [1-3]. However, it is worth emphasizing here that the correct formulation of the problem in modeling plays a crucial role. Currently, there are various software packages and approaches being developed to obtain adequate and most realistic results. Unfortunately, there are no universal approaches yet. Therefore, it is important to consider and study each task separately, thereby at least grouping the main points.

The choice of the most optimal scheme

Combustion processes occur under conditions of strong turbulence and non-isothermal flow, multiphase medium with significant influence of nonlinear effects of thermal radiation, interphase interaction and multistage flow of chemical reactions. Such phenomena play an important role in the study of the natural phenomenon of low-grade coal burning. All these factors must be taken into account in the formulation of the physical, mathematical and chemical model of the problem. A number of kinetic schemes based on global reaction rates have been developed to describe the processes of formation and destruction of nitrogen oxides [4-5].

The choice of the most optimal scheme for the formation of nitrogen oxides during the combustion of low-grade pulverized coal fuel will provide adequate research results. This will give a chance to really estimate the amount of nitrogen oxide emissions, as well as design and implement various approaches to minimize it. In the process of burning coal, nitrogen oxides are formed during homo- and heterogeneous reactions of air, volatile substances and charcoal. The complex mechanisms of nitrogen oxide formation during coal combustion are classified using a nitrogen source and divided into two main groups:

- fuel processes: oxidation of nitrogen compounds that are chemically bound to the organic matter of the fuel;
- thermal processes: reactions of atmospheric nitrogen with atomic oxygen, which is formed at high temperatures.

In the proposed article, the processes of formation of nitrogen oxides are considered, according to two kinetic models of their formation – the Mitchell Tarbell model and the De Soet model. De Soet was the first researcher to develop a heterogeneous model of the formation and decomposition of NO and N2O based on surface reactions with active centers [CN] and [CNO]. In the case of coal combustion, the Mitchell Tarbell kinetic model of fuel NO formation takes into account coal pyrolysis, homogeneous combustion of hydrocarbons and heterogeneous coke burning.

Based on the kinetic mechanism of the formation of nitrogen oxides NOx according to the models of De Soete and Mitchell Tarbell, computational experiments were carried out to determine the concentration characteristics of the formation and destruction of nitrogen oxides (NO and NO2) in the furnace chamber (Fig.1) of the boiler BKZ 75 Shakhtinskaya CHP when burning high-ash Kazakh coal in it.

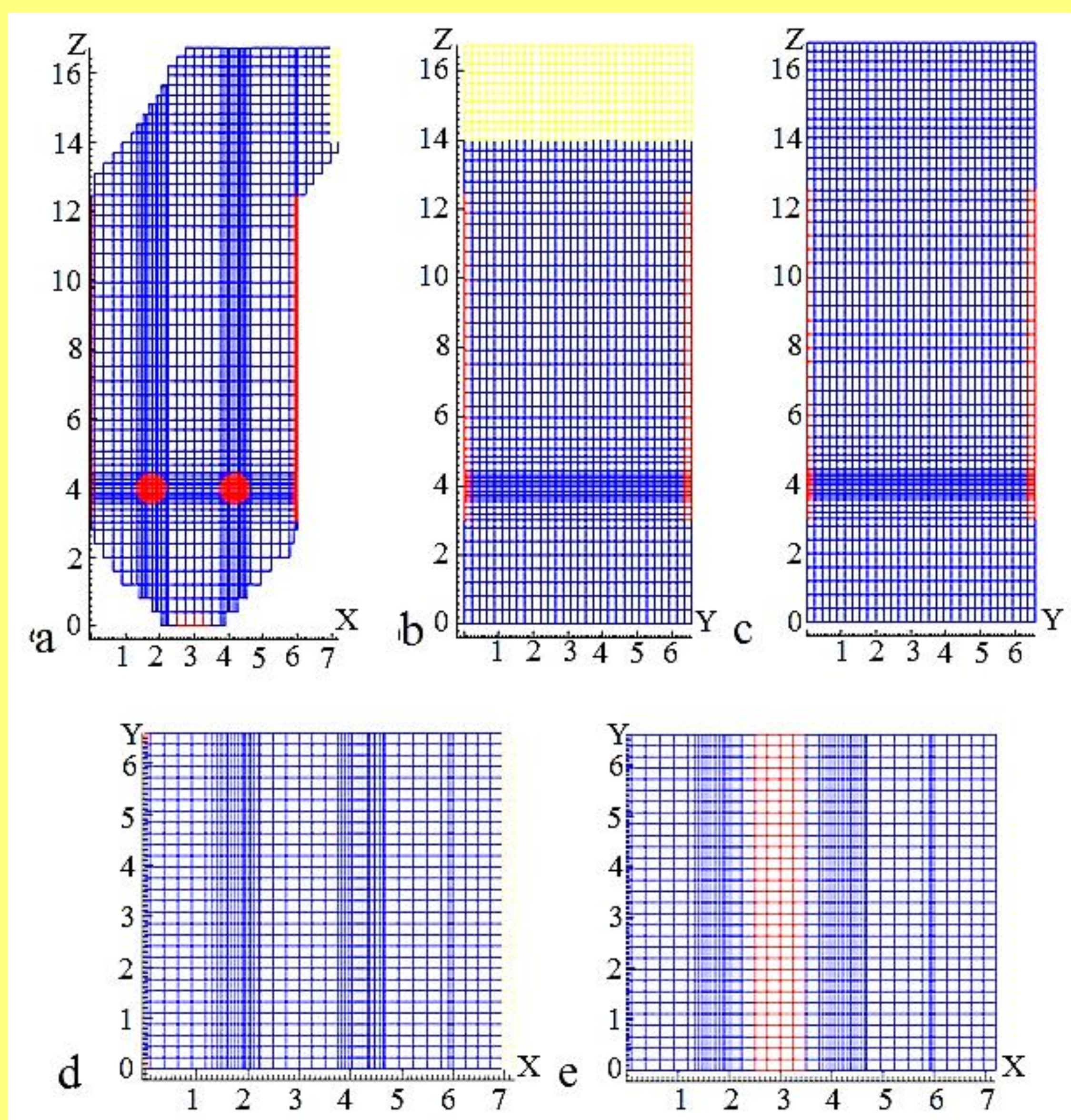

Fig. 1. Grid breakdown of the combustion chamber into control volumes
(a - front side, b - right side, c - left side, d - ceiling, e - bottom).

Results

A comparison of the results of the study using two models and field experimental data allows us to conclude that the Mitchell-Tarbell model is the most adequately describing model. From the analysis of the concentration fields of nitrogen oxides shown in Fig.2, it can be noted that the results of calculating NO concentrations during computational experiments for the two models are significantly different.

From the distribution of the average concentrations of nitrogen oxides NO according to the results of the computational experiment, it was determined that the data of known field experiments are more close to the values obtained by the Mitchell-Tarbell model.

At the output, the average concentration of nitrogen oxides NO for the Mitchell-Tarbell model is 613 mg/nm3, for the De Soete model is 463 mg/nm3. At the same time, in the work, the experimental value (full-scale experiment at a thermal power plant) of the NO concentration at the output is 530 mg/nm3.

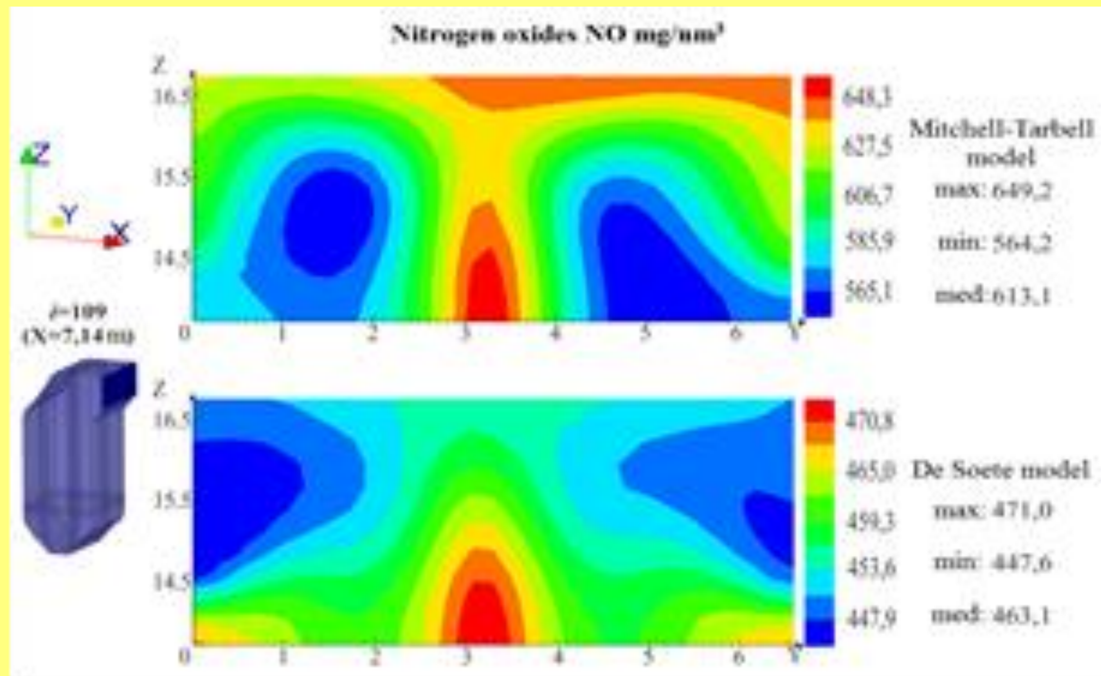

Fig. 2. Three-dimensional distribution of the concentration of nitrogen oxides NO in the longitudinal section at the outlet (X= 7 m) from the furnace chamber of the boiler BKZ-75 according to two models of NOx formation: Mitchell-Tarbell and De Soete.

Conclusions

Thus, as a result of the conducted computational experiments, the high efficiency and adequacy of the Mitchell Tarbell kinetic model was noted in relation to the high-ash coal under study. This allows us to conclude that the use of the Mitchell Tarbell model to reproduce the process of burning low-grade coals is more preferable. The results obtained will help to realistically estimate the amount of nitrogen oxide emissions, as well as to design and implement various approaches to their minimization.

Acknowledgements

This work was supported by the Ministry of Education and Science of the Republic of Kazakhstan (No AP14870834).

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