Comparative analysis of the influence of turbulence models on the description of the nitrogen oxides formation during the combustion of swirling pulverized coal flow

V Kuznetsov[1,*], N Chernetskaya[2], M Chernetskiy[1,2]

[1]Siberian Federal University, 79 Svobodny, Krasnoyarsk, 660041, Russia
[2]Kutateladze Institute of Thermophysics, Novosibirsk, 630090, Russia
[*]victor_partner@mail.ru

Abstract. The paper presents the results of numerical research on the influence of the two-parametric k-ε, and k-ω SST turbulence models as well as Reynolds stress model (RSM) on the description of the nitrogen oxides formation during the combustion of pulverized coal in swirling flow. For the numerical simulation of turbulent flow of an incompressible liquid, we used the Reynolds equation 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. Burning of coke residue was considered based on diffusion – kinetic approximation. Comparative analysis has shown that the choice of turbulence model has a significant impact on the root mean square (RMS) values of the velocity and temperature pulsation components. This leads to significant differences in the calculation of the nitrogen oxides formation process during the combustion of pulverized coal.

1. Introduction

Nitrogen oxides are one of the dangerous pollution from coal combustion at thermal power stations. Influencing the combustion process, i.e. applying technological methods, it is possible to reduce significantly the concentration of nitrogen oxides in exhaust gases [1-3]. One of the effective technological methods to reduce NOx concentration is the use of low NOx swirl burners [4]. The optimization of their operation is largely based on numerical experiment [5-7]. Despite the great strides achieved in the development of the numerical experiment, as well as large variety of various numerical techniques, the complicated structure of coal, yet not fully understood, and the complex chemical processes occurring during coal fuel combustion and gasification, do not allow creating universal models. Therefore, search for mathematical models that would describe more accurately the combustion processes of pulverized coal and the formation of nitrogen oxides in furnace-burner units still remains quite urgent.

Mathematical description of pulverized fuel combustion includes a set of interrelated models describing turbulent gas motion, the transfer of thermal and radiant energy, combustion, gasification, movement of the coal particles, etc. When considering vortex burners with a swirling flow, it is important to select turbulence model, which would accurately describe the averaged fields and the large-scale pulsations of the swirling flows. As shown by existing works, $k–\varepsilon$ and $k–\omega$ turbulence models poorly describe the swirling flow. To improve the description of swirling flows it is proposed to use modifications of the two-parameter turbulence models, for example, $k–\omega$ SST model of Menter,

Reynolds stress transfer models, as well as eddy-resolving methods, such as for example, large-eddy simulation (LES) method.

At that, it can be assumed that the choice of turbulence model will affect also the description of the pulverized coal combustion processes and eventually to predict the formation of nitrogen oxides.

The aim of this work is to conduct comparative analysis of the effect of the two-parametric $k–\varepsilon$ turbulence model and Menter's $k–\omega$ *SST* model, as well as Reynolds stress transfer models on the results of the simulation of nitrogen oxides formation during the combustion of swirling pulverized coal torch.

2. Problem statement and research methods

For numerical studies and verification of the mathematical model we used experimental data on pulverized coal torch combustion involving flow swirl. The data were obtained from 2.4 MW firing stand [8]. The sketch of the firing stand is presented in Fig. 1. Flow characteristics when conducting experimental studies and calculations were as follows: the primary (dry) air - 0.117 kg/s, the temperature - 343.15 K, the average axial velocity - 23.02 m/s, and the (dry) coal consumption - 0.073 kg/s. The secondary (dry) air flow rate - 0.745 kg/s, the temperature - 573.15 K, the average axial velocity - 43.83 m/s, the average tangential velocity - of 49.42 m/s. Technical content of coal (wt. %, dry): volatile matter - 37.4, fixed carbon - 54.3, Ash - 8.3. Chemical composition of coal (wt. % daf): C - 80.36, H - 5.08, N - 1.45, S - 0.94, O - 12.17. Qv = 32.32 MJ/kg.

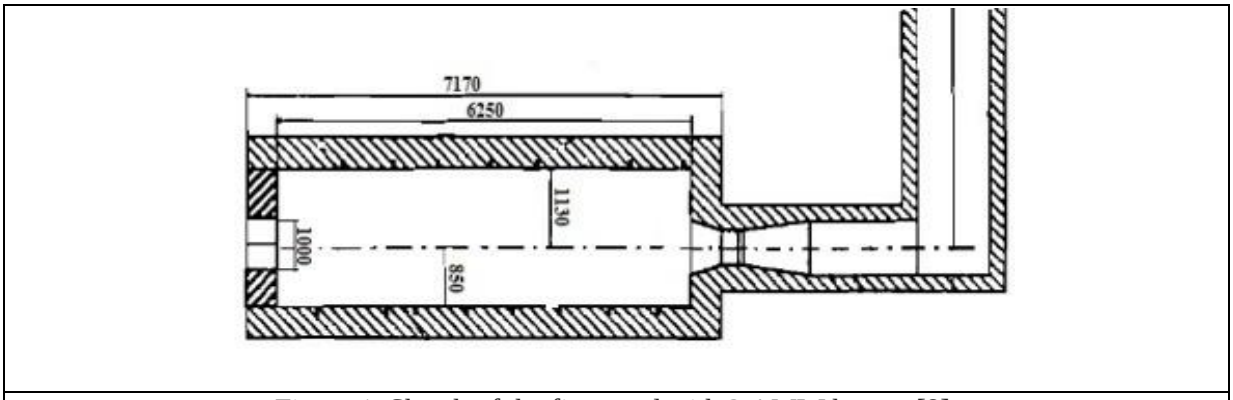

Figure 1. Sketch of the fire stand with 2.4 MW burner [8].

For the numerical simulation of turbulent flow of an incompressible liquid we used the Reynolds equations with due account for the interphase interaction. The Reynolds equations were closed by the following two-parametric turbulence models: standard $k–\varepsilon$ turbulence model [9], and $k–\omega$ SST model of Menter [10]. In Reynolds stress transfer model components $\overline{u_i' u_j'}$ of the Reynolds stress tensor are found by solving the transport equations:

$$\frac{\partial}{\partial x_l}\left(\rho u_l \overline{u_i' u_j'}\right) = \rho\left(P_{ij} + Diff_{ij} - \varepsilon_{ij} + \phi_{ij}\right),$$

where P_{ij} - is the term describing the Reynolds stress generation, $Diff_{ij}$ - is the transfer due to diffusion, ε_{ij} - is the dissipation rate, ϕ_{ij} - is the pressure cross-term.

To describe the right hand side terms of the equation we take several hypotheses. Diffusion term is modeled by a generalized gradient diffusion hypothesis (GGDH) [11]. Pressure cross-term may be modeled on the basis of [12, 13]. In the present work to describe the motion of particles we used 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 gray medium. As shown by previously performed computational studies [6, 14, 15], this integrated model gives good correlation with the experimental data, when burning solid fossil fuel in a pulverized form. The combustion process of coal particle is considered in terms of the following consecutive steps: 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 [8]. 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 [8].

A mathematical model of NOx formation during coal combustion involves consideration of three mechanisms taking into account the influence of temperature fluctuations: the thermal NOx calculated based on the known dependence of Zeldovich [16], prompt NOx and fuel NOx calculated using a model proposed in [17] with reactions (1, 2), as well as the supplement of the "reburning" reaction (3), proposed by Chen [18].

$$dx_{HCN} / dt = -3.5*10^{10} \exp(-3370 / T) x_{HCN} x_{O_2}^{a}, \quad (1)$$

$$dx_{HCN} / dt = -3*10^{12} \exp(-30200 / T) x_{HCN} x_{NO}, \quad (2)$$

$$dx_{NO} / dt = -2.7*10^{6} \exp(-9466 / T) x_{NO} x_{C_nH_m} \quad (3)$$

where x – is the molar fraction of the respective component, a – is the order of reaction with respect to oxygen.

The reaction rate of NO formation is strongly temperature dependent due to the large activation energy values. Consequently, temperature fluctuations can greatly increase the concentration of nitric oxide formed in turbulent flows. To account the effect of turbulent fluctuations on the nitric oxide formation process, we produced the solution to the equation for temperature variation, when solving the transfer equations for NO and HCN concentrations. To determine the average rate of NO formation reaction, we carried out integration between the upper and lower temperature limits using the probability density function of the β distribution.

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, we used in the present work the SIMPLE-like algorithm with aligned grids. The proposed model and solution methods were previously tested for solving problems on pulverized coal combustion and gasification [14, 15], and showed a satisfactory agreement with the experimental data in terms of the basic process parameters in the combustion chamber.

3. Results and discussion

Previously conducted computational studies on the influence of computational mash refinement on the calculation results of pulverized coal torch burning in the combustion chamber of fire stand with swirling burner have shown [19] that for the mesh size of more than 500,000 cells, no significant differences were noted in the calculation results. Therefore, in this paper, we have used a computational mesh with 500,000 cells. It was shown previously [19] that for the distribution of axial and tangential velocity components over the sections of the combustion chamber, Reynolds stress model and the two-parameter k-ε and Menter's k- ω SST turbulence models give similar results for

pulverized coal combustion. At the same time, there are significant differences in the fluctuating velocity component depending on the selected turbulence model (Fig. 2). From Fig. 2 we can see that the RMS velocity fluctuation, common to axial and tangential velocity, and calculated from the expression $(2k/3)^{0.5}$, has a lower level and better agreement with the experimental data for Reynolds stress model. This in turn affects the calculation of burnout rate of the volatile component. It is obvious from Fig. 3 that higher values of pulsations in the initial section of the torch lead to more rapid burnout of volatile component and, accordingly, to higher temperatures. The temperature differences at the initial section of the torch amount to about 10% when using the two-parameter k-ε turbulence model and Reynolds stress model, respectively.

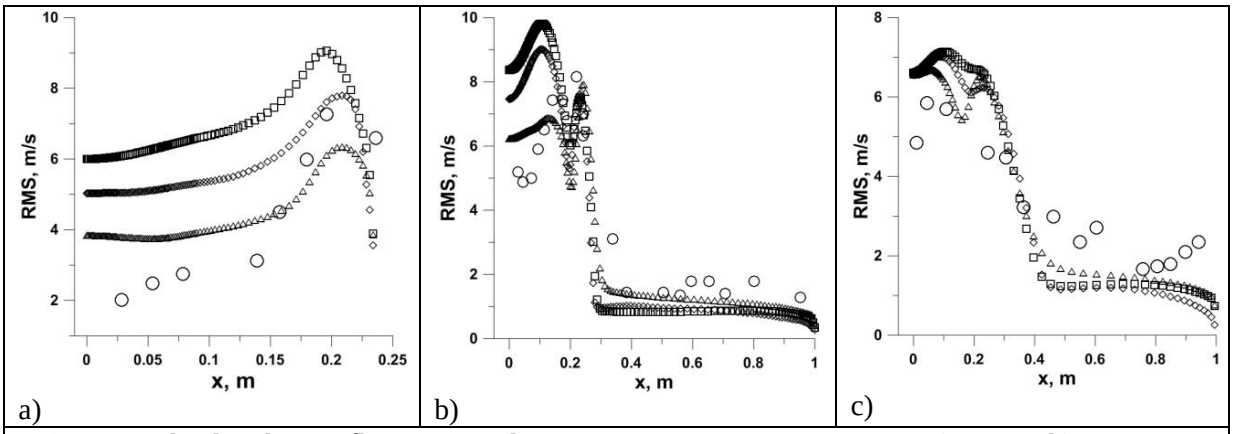

Figure 2. The distribution fluctuating velocity component in cross sections. a) z=0 m; b) z=0.25 m; c) z=0.85 m. Circle - experiment, rhombus – k-w SST, square – k-e, triangle -RSM.

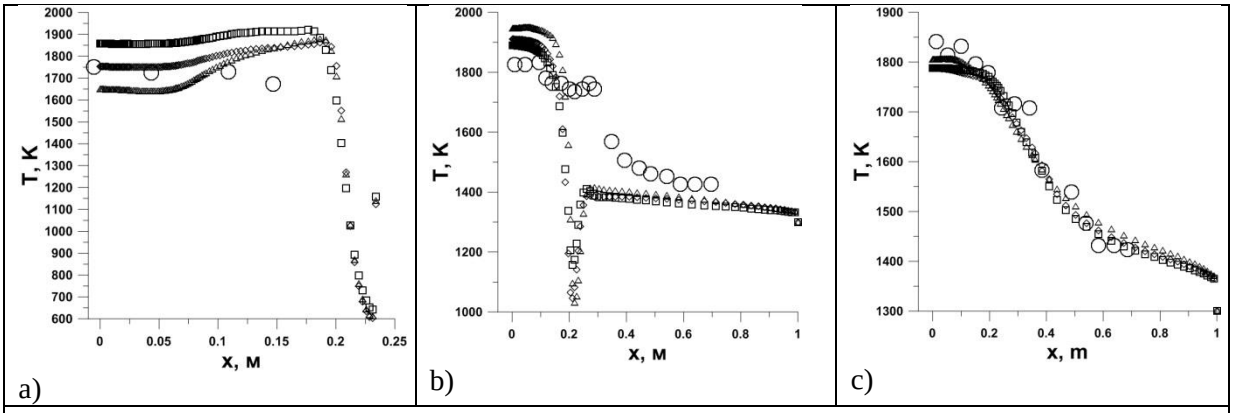

Figure 3. Temperature distribution in the cross sections: a) z=0 m; b) z=0.25 m; c) z=0.85 m. Circle - experiment, rhombus – k-w SST, square – k-e, triangle -RSM.

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. At that, we solved the additional equation for the temperature variation to take into account the influence of the pulsation components of the flow on the nitrogen oxides formation. Figure 4 presents the nitrogen oxides concentrations in the sections of the combustion chamber, while Fig. 5 shows RMS for temperature.

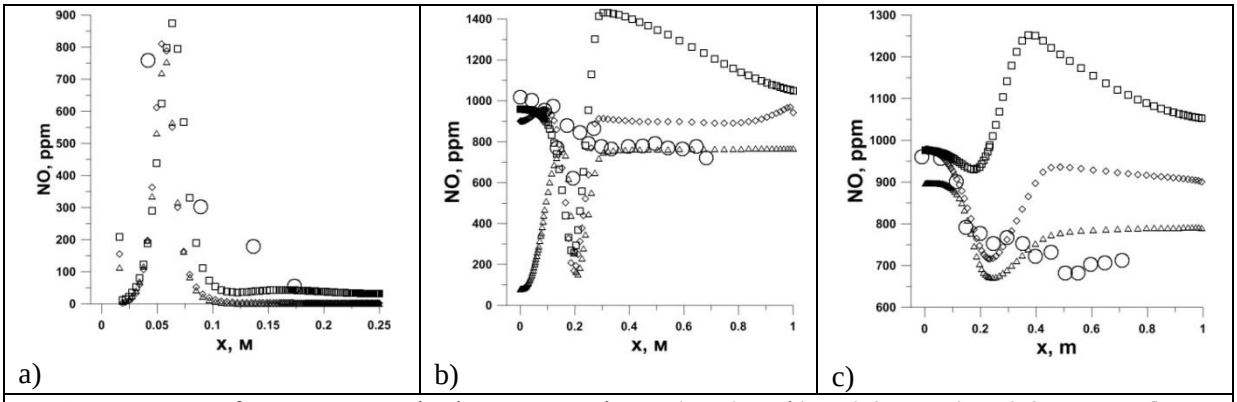

Figure 4. NO of concentration in the cross sections: a) z=0 m; b) z=0.25 m; c) z=0.85 m. Circle - experiment, rhombus – k-w SST, square – k-e, triangle -RSM.

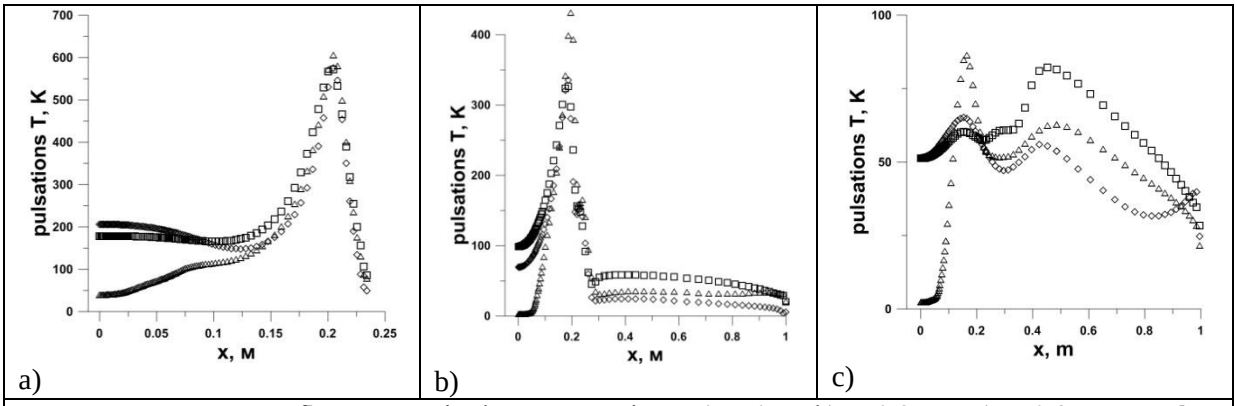

Figure 5. Temperature fluctuations in the cross sections: a) z=0 m; b) z=0.25 m; c) z=0.85 m. Circle - experiment, rhombus – k-w SST, square – k-e, triangle -RSM.

We can see that, when using Reynolds stress model as a turbulence model, nitrogen oxides concentration values are lower than those obtained for the two-parameter turbulence model, and are in satisfactory agreement with the experimental data. For Menter's k-ω SST model and the standard k-ε turbulence model, concentrations of nitrogen oxides exceed the experimental values by more than 25 and 50%, whereas for the Reynolds stress model, deviation of the NO concentration does not exceed 10% in comparison with the experimental data.

This is primarily due to higher values of RMS for both the velocity (Fig. 3) and the temperature (Fig. 5). Deviation of the RMS values for temperature according to the selected model is about 10-30% depending on the considered section of the combustion chamber. Given the exponential dependence of the fuel NO formation reaction rate on the temperature (formulas 1-3), which in this case make the main contribution to the formation of NO, this is one of the major factors explaining the difference in calculation results.

Conclusion

We have performed numerical study on the influence of the two-parametric k-ε, and k-ω SST turbulence models, as well as Reynolds stress transfer model, on the description of the nitrogen oxides formation during the combustion of pulverized coal in the swirling flow. It is shown that the choice of turbulence model when calculating combustion of pulverized fuel in the swirling flow significantly influences the distribution of the RMS values of velocity and temperature fluctuations. This leads to a difference in the description of burning process of the gaseous components, especially at the initial part of the torch, and, accordingly, the difference in temperatures that accounts for more than 10% at the initial part of the torch, depending on the choice of turbulence model.

It is shown that the use of two-parametric turbulence models results in satisfactory agreement of the calculation with the experimental data on the averaged parameters of velocity, temperature and concentration of the gas components (discrepancy does not exceed 5%), though gives a significant deviation (more than 50%) in the nitrogen oxides concentration within the combustion chamber space in comparison with the experimental data. Reynolds stress model gives a deviation in distribution of the nitrogen oxides concentration no more than 10% as compared to experimental data, with underlying slight difference in the distribution of the axial and tangential velocities, temperatures and concentrations of gases as compared to the two-parametric turbulence models.

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