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Modeling of Combustion Processes in Cylindrical Chambers Using Modern Package Programs

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Abstract. The main problem of mathematical modeling of gas fuel combustion processes within the framework of the ANSYS Fluent software package is the choice of a turbulence model. As part of the study, to describe the turbulence phenomenon, the standard and modified $k-\varepsilon$ models, the Spalart-Allmaras model, the $k-\varepsilon$ model and the RNG $k-\varepsilon$ model were tested for describing the mixing and combustion of methane in a cylindrical channel according to the Arrhenius law. The control volume method embedded in ANSYS Fluent was used in the calculations, where the velocity and pressure fields are linked by the PISO algorithm. A satisfactory agreement between the results of calculation and experiment was obtained when implementing the modified $k-\varepsilon$ model by the axial distribution of temperature and longitudinal velocity.

INTRODUCTION

At present, software products are actively used in scientific and technical organizations and universities for modeling various processes. Their use in the study of heat engineering processes observed in machinery and technology has become relevant.The utilization of fire played a key role in the development of civilization. Fire opened up the possibility of heat treatment of food and heating of dwellings, and subsequently - the development of metallurgy, energy, and the creation of new, more advanced tools and technologies, where solid, liquid, and gaseous substances were used as fuel. The control of combustion processes underlies the creation of modern engines for cars, aircraft, ships, and rockets, where the combustion of pre-mixed and unmixed mutually reacting substances is practiced.

Combustion is a complex physicochemical process of transformation of initial materials into combustion products during chemical reactions accompanied by intense heat release. Its complexity lies not only in the most complex mathematical description of the process but also in the complexity of its experimental study. Due to the importance of the combustion process in technical devices, together with the high cost of full-scale experiments, computer simulation is developing.

To study and analyze gas dynamics and thermos-physical processes in power plants, ANSYS CFD, ANSYS Fluent, ANSYS CFX, Star-CD, Flow 3D, Open Foam, Flow Vision, VP2/3, Sigma Flow, and FIRE 3D application program packages are currently actively used; they operate under various simulation conditions using mesh methods with improved convergence.

The purpose of this study is to simulate the combustion process in the ANSYS Fluent software package. ANSYS Fluent is a full-fledged CFD package that is not inferior in functionality to ANSYS CFX and specializes in modeling multi-phase flows and combustion processes. The development of computer technology has made it possible to bring engineering calculations to a whole new level. When solving computational problems, an engineer considers various methods and approaches that allow obtaining a high-quality result in the shortest possible time. Modern practice proves that the use of software systems based on the finite difference method (FDM) and finite element method (FEM) makes it possible to achieve the goals posed.

Numerical study of gas combustion is a complex task of thermal physics since it requires an account for a large number of complex interrelated factors and phenomena. Therefore, the computational experiment is becoming an increasingly important element in the study of combustion processes and the design of various devices that use the combustion process. It is safe to say that its role will continue to grow in the future. In this regard, the methods of

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computational fluid dynamics are becoming more widespread in thermal physics, when there appears a possibility to optimize an experiment based on its virtual prototype.

Many publications [1-14] are devoted to the study of combustion processes, and the resulting substances. The authors of reference [3] studied the diffusion combustion of methane and propane in a square-section combustion chamber with fuel supplied through a porous cylinder. As results, the fraction profiles of the fuel components, the oxidizer, CO and CO_2 are given. In [4], a numerical and experimental study of the combustion of a partially mixed methane-air mixture in a cylindrical combustion chamber was conducted. The distributions of temperatures and fractions of components N_2, O_2, CH_4, CO_2, H_2O, CO, H_2, OH, NO were presented. The study of diffusion combustion with the concurrent supply of methane and air was performed in [5, 6], where the results of numerical calculations and experimental data were presented: temperature and fraction profiles of CH_4, CO_2, H_2O, CO.

The need for efficient and effective mathematical descriptions of turbulent reacting flow systems has led to significant research interest in turbulent models based on turbulent spectrum resolution [7] and combustion models [8] that take into account complex chemical reactions without involving too large computational resources. The Large Eddy Simulation (LES) approach [9] is known as one of the most popular turbulent models due to one of its most important features. In it, large-scale turbulent eddies that dominate turbulent dynamics and motions are directly resolved by applying the filter method based on cell size [10]. However, this well-known superiority of LES in describing large eddy motions also leads to one drawback of the model - high computational power required for LES simulation due to the use of small grid cells to fill the computational domain. As such, the LES modeling approach is more commonly used in academic research rather than in industry, due to the complex and large-scale components often required in the latter. On the other hand, in academia, the focus is on physical phenomena in small to medium-scale configurations, which allows for a more computationally expensive LES approach.

Due to this disadvantage of LES, alternative mathematical methods such as Detached Eddy Simulation (DES) [11] and Scale Adaptive Simulation (SAS) are attracting more attention from engineers (in applied fields) due to their lower processing power requirements and their ability to resolve a turbulent spectrum. In particular, the DES method uses the Reynolds-averaging Navier–Stokes (RANS) modeling approach near boundary layer domains and the LES modeling approach – near the basic domain; in addition, the SAS method uses an additional von Karman length scale to provide an accurate energy distribution over the turbulent spectrum and improve the performance of the RANS model [12]. In fact, DES is often considered a hybrid RANS-LES modeling method of the first generation, while SAS is considered a method of the second generation. This is because, compared to DES, SAS has two additional advantages that allow it to be quickly adapted to practical tasks. First, SAS (unlike DES) does not have an explicit local dependence on the grid spacing in each direction [13]. Second, SAS can be easily incorporated into an existing experimentally adapted RANS model.

In [14], the modeling of the combustion processes of pulverized coal fuel is considered and a technique for engineering calculations in the power boiler BKZ-500 is presented using the ANSYS Fluent software package. ANSYS Fluent allows the authors of the article to simulate the combustion process, taking into account turbulence, heat transfer, and chemical reactions. To design the computational grid in the combustion chamber area, the ICEM CFD package, which is a grid preprocessor for ANSYS Fluent, was used. A hexahedral grid consisting of 2 million elements was formed in the area of the combustion chamber of the power boiler. The flow was described by a system of stationary Reynolds-averaged Navier-Stokes equations of conservation of mass and energy. Turbulent viscosity was calculated using the $k-\varepsilon$ model. Radiative heat transfer in a two-phase flow was taken into account within the P1 approximation of the spherical harmonics method.

The presence of well-studied mechanisms of combustion reactions of some types of gases makes it possible to obtain a detailed description of a large number of ongoing processes and a wide range of chemical radicals and reacting components.

Among the numerous combustion modeling techniques, the approach based on the mixing proportion of fuel and oxidizer, the “flamelet model”, stands out separately. At present, the flamelet model has been seriously modified compared to its original version.

FORMULATION OF THE PROBLEM

A jet of combustible gas is considered, which flows out of a cylindrical nozzle of diameter $1.2\ cm$ and propagates in a cocurrent oxidizer flow at a finite chemical rate. The velocity distribution in the outlet section of the nozzle and in the concurrent flow, as well as the initial (at $x=0$) distributions of temperature and fractions of fuel and

oxidizer, are considered given, uniform, and homogeneous. It is assumed that a nozzle of a thickness of 0.5 *mm* protrudes by 1 *cm* to the calculation domain (Figure. 1).

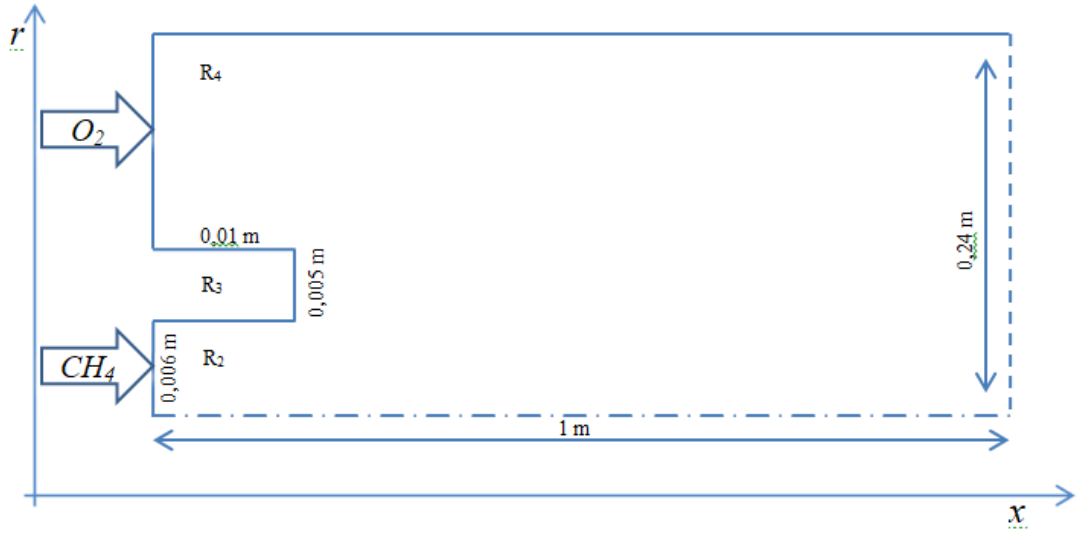

FIGURE 1. Scheme of the axisymmetric computational domain

In parallel with the turbulent mixing of two flows, a chemical reaction occurs between the interacting components - fuel and oxygen from the composition of the air. The domain of mixing gradually expands.

The purpose of this study is to develop a method for calculating the mixing, combustion, and propagation of various compositions of combustible mixtures in a cylindrical chamber, which makes it possible to conduct a computational experiment to study the processes of heat and mass transfer. First of all, it is necessary to choose an adequate turbulence model for describing a jet flow with intense chemical transformation.

MATHEMATICAL MODEL

Most flows are turbulent in nature and the state of turbulence during the movement of the medium strongly affects such flow parameters as momentum transfer, temperature and fractions of substances in the mixture. A general view of the system of equations describing the turbulent flow of a multicomponent reacting gas is presented below. The system of Navier-Stokes equations, which includes the laws of conservation of mass, momentum, concentration, and energy of an unsteady spatial flow, is written for a Cartesian coordinate system:

$$\begin{cases} \dfrac{\partial \rho}{\partial t}+\dfrac{\partial}{\partial x_i}\left(\rho \bar{u}\right)=0, \\ \dfrac{\partial}{\partial t}\left(\rho \bar{u}_i\right)+\dfrac{\partial}{\partial x_j}\left(\rho \bar{u}_i \bar{u}_j\right)=\dfrac{\partial}{\partial x_j}\left(\sigma_{ij}\right)-\dfrac{\partial \bar{p}}{\partial x_i}-\dfrac{\partial \tau_{ij}}{\partial x_j}, \\ \dfrac{\partial \rho \overline{h_i}}{\partial t}+\dfrac{\partial \rho \overline{u_i}\,\overline{h_s}}{\partial x_i}-\dfrac{\partial \bar{p}}{\partial t}-\overline{u_j}\dfrac{\partial \bar{p}}{\partial x_i}-\dfrac{\partial}{\partial x_i}\left(\lambda \dfrac{\partial \bar{T}}{\partial x_i}\right)=-\dfrac{\partial}{\partial x_j}\left[\rho\left(\overline{u_i h_s}-\overline{u_i}\,\overline{h_s}\right)\right], \\ \dfrac{\partial}{\partial t}\left(\rho c_n\right)+\dfrac{\partial}{\partial x_i}\left(\rho u_i c_n\right)=\dfrac{\partial}{\partial x_i}\left(\dfrac{\mu_{eff}}{\sigma_{c_{n,eff}}}\dfrac{\partial c_n}{\partial x_i}\right)+S_n. \end{cases}$$

The tensor of viscous shear stress is defined as:

$$\sigma_{ij} \equiv \left[\mu\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) \right] - \frac{2}{3}\mu \frac{\partial \overline{u}_l}{\partial x_l}\delta_{ij}, \quad \tau_{ij} \equiv \rho\overline{u_i u_j} - \rho\overline{u}_i\overline{u}_j,$$

$$\rho\left(\overline{u_i h_s} - \overline{u}_i\overline{h}_s\right) = -\frac{\mu_{SGS}C_p}{\mathrm{Pr}_{SGS}}\frac{\partial \overline{T}}{\partial x_j}, \qquad S_n = \sum \omega_n,$$

$$-\rho\overline{u_i' u_j'} = \mu_t\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3}\left(\rho k + \mu_t \frac{\partial u_k}{\partial x_k} \right)\delta_{ij};$$

μ_{eff} represents the total dynamic viscosity.

$$h = c_p T + c_2 h_2^*, \; c_p = \sum_{n=1}^{N} c_{pn} c_n$$

In the process of solving the problem, the following turbulence models are used to describe turbulence.

Modified $k-\varepsilon$ **model.** In contrast to [15], here it is proposed to use the modified $k-\varepsilon$ model [13-16] to describe turbulent exchange; this contributes to a more adequate description of the heat and mass transfer process:

$$\begin{cases} \dfrac{\partial}{\partial t}(\rho k) + \dfrac{\partial}{\partial x_j}(\rho k u_j) = \dfrac{\partial}{\partial x_j}\left[\left(\mu + \dfrac{\mu_t}{\sigma_k} \right) \dfrac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho\varepsilon - 2\rho\varepsilon M_t^2 + S_k, \\ \dfrac{\partial}{\partial t}(\rho\varepsilon) + \dfrac{\partial}{\partial x_j}(\rho\varepsilon u_j) = \dfrac{\partial}{\partial x_j}\left[\left(\mu + \dfrac{\mu_t}{\sigma_\varepsilon} \right) \dfrac{\partial \varepsilon}{\partial x_j} \right] + \rho C_1 S\varepsilon - \rho C_2 \dfrac{\varepsilon^2}{k + \sqrt{\nu\varepsilon}} + C_{1\varepsilon}\dfrac{\varepsilon}{k} C_{3\varepsilon} G_b + S_\varepsilon. \end{cases}$$

The following notation is used

$$C_1 = \max\left[0.43, \frac{\eta}{\eta+5} \right], \; \eta = S\frac{k}{\varepsilon}, \; S = \sqrt{2S_{ij}S_{ij}}, \; \mu_t = \rho C_\mu \frac{k^2}{\varepsilon}, \; C_\mu = \frac{1}{A_0 + A_S \dfrac{kU^*}{\varepsilon}}, U^* \equiv \sqrt{S_{ij}S_{ij} + \tilde{\Omega}_{ij}\tilde{\Omega}_{ij}},$$

$$\Omega_{ij} = \overline{\Omega_{ij}} - 2\varepsilon_{ijk}\omega_k, \; A_S = \sqrt{6}\cos\phi, \; \phi = \frac{1}{3}\cos^{-1}\left(\sqrt{6}W\right), \; W = \frac{S_{ij}S_{jk}S_{ki}}{\tilde{S}^3}, \; \tilde{S} = \sqrt{S_{ij}S_{ij}}, \; S_{ij} = \frac{1}{2}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right),$$

$$G_k = -\rho\overline{u_i' u_j'}\frac{\partial u_j}{\partial u_i}, \; S \equiv \sqrt{2S_{ij}S_{ij}}, \; G_b = \beta g_i \frac{\mu_t \partial T}{\mathrm{Pr}_t \partial x_i}., \; \mathrm{Pr}_t = 1/a_t, \; a_0 = 1/\mathrm{Pr} = k/\mu c_p, \; \beta = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T} \right)_p,$$

$$G_b = -g_i \frac{\mu_t}{\rho\,\mathrm{Pr}_t}\frac{\partial \rho}{\partial x_i}, \; M_t = \sqrt{\frac{k}{a^2}}, \; a = \sqrt{\gamma RT}.$$

The empirical constants of the $k-\varepsilon$ model take standard values: $C_{1\varepsilon} = 1.44$, $C_2 = 1.9$, $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.2$, $A_0 = 4.04$.

Spalart-Allmaras model. This model belongs to the class of one-parameter linear turbulence models. Here, only one additional differential equation appears for calculating the kinematic coefficient of eddy viscosity. This low Reynolds number turbulence model, which describes the entire flow region, is given by the following equation:

$$\frac{\partial}{\partial t}\left(\rho\tilde{\nu}\right) + \frac{\partial}{\partial x_i}\left(\rho\tilde{\nu}u_i\right) =$$

$$G_\nu + \frac{1}{\sigma_{\tilde{\nu}}}\left[\frac{\partial}{\partial x_j}\left\{ \left(\mu + \rho\tilde{\nu}\right)\frac{\partial \tilde{\nu}}{\partial x_j} \right\} + C_{b2\rho}\left(\frac{\partial \tilde{\nu}}{\partial x_j} \right)^2 \right] - C_{w1\rho} f_w \left(\frac{\tilde{\nu}}{d} \right)^2 + S_{\tilde{\nu}}.$$

Turbulent eddy viscosity is calculated by formula $\mu_t = \rho\tilde{\nu} f_{\nu 1}$, additional definitions are given by the following dependencies:

$$f_{v1}=\frac{\chi^3}{\chi^3+C_{v1}^3},\quad \chi=\frac{\tilde{\nu}}{\nu},\quad \tilde{S}\equiv S+\frac{\nu}{\kappa^2 d^2}f_{v2},\quad f_{v2}=1-\frac{\chi}{1+\chi f_{v1}},\quad S\equiv\sqrt{2\Omega_{ij}\Omega_{ij}},\quad \Omega_{ij}=\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j}-\frac{\partial u_j}{\partial x_i}\right),$$

$S_{ij}=\frac{1}{2}\left(\frac{\partial u_j}{\partial x_i}+\frac{\partial u_i}{\partial x_j}\right)$, $r=\frac{\tilde{\nu}}{\tilde{S}\kappa^2 d^2}$

closure constants for the model are: $C_{prod}=2.0$, $C_{b1}=0.1355$, $C_{b2}=0.622$, $\sigma_{\tilde{\nu}}=\frac{2}{3}$, $C_{v1}=7.1$, $C_{w1}=\frac{C_{b1}}{\kappa^2}+\frac{(1+C_{b2})}{\sigma_{\tilde{\nu}}}$, $C_{w2}=0.3$ $C_{w3}=2.0$, $\kappa=0.4187$.

Standard $k-\varepsilon$ model.

$$\begin{cases}\frac{\partial}{\partial t}(\rho k)+\frac{\partial}{\partial x_i}(\rho k u_i)=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]+G_k+G_b-\rho\varepsilon-Y_M+S_k,\\ \frac{\partial}{\partial t}(\rho\varepsilon)+\frac{\partial}{\partial x_i}(\rho\varepsilon u_i)=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right]+C_{1\varepsilon}\frac{\varepsilon}{k}(G_k+C_{3\varepsilon}G_b)-C_{2\varepsilon\rho}\frac{\varepsilon^2}{k}+S_\varepsilon.\end{cases}$$

Turbulent eddy viscosity is calculated by formula $\mu_t=\rho C_\mu\frac{k^2}{\varepsilon}$, closure constants for the standard $k-\varepsilon$ model are $C_{1\varepsilon}=1.44$, $C_{2\varepsilon}=1.92$, $C_\mu=0.09$, $\sigma_k=1.0$, $\sigma_\varepsilon=1.3$.

RNG $k-\varepsilon$ model [10].

$$\begin{cases}\frac{\partial}{\partial t}(\rho k)+\frac{\partial}{\partial x_i}(\rho k u_i)=\frac{\partial}{\partial x_j}\left(\alpha_k\mu_{eff}\frac{\partial k}{\partial x_j}\right)+G_k+G_b-\rho\varepsilon-Y_M+S_k,\\ \frac{\partial}{\partial t}(\rho\varepsilon)+\frac{\partial}{\partial x_i}(\rho\varepsilon u_i)=\frac{\partial}{\partial x_j}\left(\alpha_\varepsilon\mu_{eff}\frac{\partial \varepsilon}{\partial x_j}\right)+C_{1\varepsilon}\frac{\varepsilon}{k}(G_k+C_{3\varepsilon}G_b)-C_{2\varepsilon\rho}\frac{\varepsilon^2}{k}-R_\varepsilon+S_\varepsilon.\end{cases}$$

Turbulent eddy viscosity is calculated by formula $\mu_t=\rho C_\mu\frac{k^2}{\varepsilon}$, closure constants for the RNG $k-\varepsilon$ model are $C_\mu=0.0845$, $R_\varepsilon=\frac{C_\mu\rho\eta^3(1-\eta/\eta_0)}{1+\beta\eta^3}\frac{\varepsilon^2}{k}$, $\eta\equiv Sk/\varepsilon$, $\eta_0=4.38$, $\beta=0.012$, $\eta\approx 3.0$, $C_{2\varepsilon}^*\approx 2.0$, $C_{1\varepsilon}=1.42$, $C_{2\varepsilon}=1.68$.

The $k-\omega$ model is the very first high-Reynolds number model with two differential equations [15]. It does not contain terms reflecting the effect of molecular viscosity on turbulence. Now rarely used.

$$\begin{cases}\frac{\partial}{\partial t}(\rho k)+\frac{\partial}{\partial x_i}(\rho k u_i)=\frac{\partial}{\partial x_j}\left[\Gamma_k\frac{\partial k}{\partial x_j}\right]+G_k-\rho\beta^* f_{\beta^*}k\omega+S_k,\\ \frac{\partial}{\partial t}(\rho\omega)+\frac{\partial}{\partial x_i}(\rho\omega u_i)=\frac{\partial}{\partial x_j}\left[\Gamma_\omega\frac{\partial \omega}{\partial x_j}\right]+G_\omega-\rho\beta f_\beta\omega^2+S_\omega.\end{cases}$$

Turbulent eddy viscosity is calculated by formula $\mu_t = \alpha^* \frac{\rho k}{\omega}$, model constants are defined as function of $\Gamma_k = \mu + \frac{\mu_t}{\sigma_k}$, $\Gamma_\omega = \mu + \frac{\mu_t}{\sigma_\omega}$, $\alpha^* = \alpha_\infty^* \left(\frac{\alpha_0^* + \mathrm{Re}_t / R_k}{1 + \mathrm{Re}_t / R_k} \right)$, $\mathrm{Re}_t = \frac{\rho k}{\mu \omega}$, $G_k = -\rho \overline{u_i' u_j'} \frac{\partial u_j}{\partial x_i}$, $\Omega_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right)$, $G_\omega = \alpha \frac{\omega}{k} G_k$, $\alpha = \frac{\alpha_\infty}{\alpha^*} \left(\frac{\alpha_0 + \mathrm{Re}_t / R_\omega}{1 + \mathrm{Re}_t / R_\omega} \right)$, $\chi_k \equiv \frac{1}{\omega^3} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}$, $\beta^* = \beta_i^* \left[1 + \zeta^* F(M_t) \right]$, closure constants for the $k - \omega$ model are $\alpha_0^* = \frac{\beta_i}{3}$, $\mathrm{R}_k = 6$, $\beta_i = 0.072$, $\alpha^* = \alpha_\infty^* = 1$, $R_\omega = 2.95$, $\alpha = \alpha_\infty = 1$, $\beta_i^* = \beta_\infty^* \left(\frac{4/15 + \left(\mathrm{Re}_t / R_\beta \right)^4}{1 + \left(\mathrm{Re}_t / R_\beta \right)^4} \right)$, $\zeta^* = 1.5$, $R_\beta = 8$, $\beta_\infty^* = 0.09$, $\chi_\omega = \left| \frac{\Omega_{ij} \Omega_{ij} S_{ij}}{\left(\beta_\infty^* \omega \right)^3} \right|$, $\beta = \beta_i \left[1 - \frac{\beta_i^*}{\beta_i} \zeta^* F(M_t) \right]$, $M_t^2 \equiv \frac{2k}{a^2}$, $M_{t0} = 0.25$, $a = \sqrt{\gamma R T}$, $\alpha_\infty^* = 1$, $\alpha_\infty = 0.52$, $\alpha_0 = \frac{1}{9}$, $\beta_\infty^* = 0.09$, $\beta_i = 0.072$, $R_k = 6$, $R_\omega = 2.95$, $\zeta^* = 1.5$, $M_{t0} = 0.25$, $\sigma_k = \sigma_\omega = 2.0$.

The system of Navier-Stokes equations, reduced to two nonlinear diffusion equations that take into account fluctuations in the average rate of turbulent flows, is a family of $k - \varepsilon$ and $k - \omega$ models where $k -$ is the mass density of turbulent energy, ε - is its dissipation rate; $\omega -$ is the energy dissipation rate per unit volume and time. A feature of this system is the cascading of its solution, which is most convenient for use in software packages for modeling processes in cylindrical coordinates.

Here and below, u, v are the averaged longitudinal and transverse (radial) components of the velocity vector $\left(m\, s^{-1} \right)$ in cylindrical coordinates; ρ, T are the density $\left(kg\, m^{-3} \right)$ and absolute temperature (*K*) of the gas mixture; p is the hydrostatic pressure (*Pa*); Pr, Sc_n are turbulent analogs of the Prandtl and Schmidt numbers; c_n is the mass concentration of the n-th gas component in the mixture (kg kg-1); ω_n is the mass rate of formation or disappearance of the n-th gas component $\left(kg\, m^{-3}\, s^{-1} \right)$; $c_p = \sum_{n=1}^{N} c_{pn} c_n$ and c_{pn} – are the heat capacities of the gas mixture and n-th component at constant pressure $\left(J\, kg^{-1}\, K^{-1} \right)$; h_n^* is the calorific value of the n-th component $\left(J\, kg^{-1}\, K^{-1} \right)$; ν, ν_t are the kinematic coefficients of laminar and turbulent viscosity $\left(m^2\, s^{-1} \right)$.

The gas mixture is assumed to be perfect, therefore its state satisfies the Mendeleev-Clapeyron equation:

$$p = \rho R_0 T / m.$$

COMBUSTION MODEL

Special attention is paid to the issue of modeling sources in the equations of energy and fraction transfer related to chemical reactions occurring in the combustion process.

The rate coefficient of the direct reaction according to Arrhenius is determined as follows [15-22]:

$$\tilde{\omega}_2 = -A_{fk} n_1 n_2 \exp\left(-\frac{E_k}{R_0 T} \right),$$

where $A_{fk} -$ is the pre-exponential factor; $E_k -$ is the activation energy.

Methane is considered a combustible gas; the one-stage combustion kinetics of methane in air is given by the following stoichiometric equation [17-19]:

$$\nu'_{CH_4} CH_4 + \nu'_{O_2} O_2 \rightarrow \nu''_{CO_2} CO_2 + \nu''_{H_2O} H_2O + h_2^*,$$

where $\nu'_{CH_4} = 1;\ \nu'_{O_2} = 2;\ \nu''_{CO_2} = 1;\ \nu''_{H_2O} = 2.$

The rate of the combustion reaction of methane with oxygen in the fuel mass conservation equation, according to the data given in [15], has the following form:

$$\tilde{\omega}_2 = -A_{r1}\frac{c_1 c_2 \bar{\rho}^2}{\bar{u}}\exp(-A_{r2}/T),$$

where $A_{r1} = 8.6\cdot 10^9$, $\frac{E_a}{R} = 18,05 = A_{r2}$.

CALCULATION ALGORITHM

The equations described above are integrated by the finite volume method in the ANSYS Fluent package. Convective and diffusion flows are calculated with the second-order approximation. Due to the fact that all the problems modeled below are quasi-stationary, the first-order approximation in time is used. The PISO algorithm links the velocity and pressure fields. Solution algorithms, depending on the selected combustion model, have distinctive features.

CALCULATION RESULTS

The problem is solved in a two-dimensional formulation; the cylindricity is taken into account due to the computational grid built in the form of a sector. To simplify the presentation, in the section describing the boundary conditions, hereinafter, the parameters are given both for the flamelet model and for models of the kinetic reaction rate.

The boundary conditions for the computational domain are set as follows [15-21]:

$$r = 0:\ \frac{\partial F}{\partial r} = 0,\quad F = \{U, T, c_i, k, \varepsilon, \omega, \tilde{\nu}\},\quad \vartheta = 0;$$

$$r = R_0:\ \frac{\partial F}{\partial r} = 0,\quad F = \{T, c_i, k, \varepsilon, \omega, \tilde{\nu}\},\quad \vartheta = 0,\quad u = 0;$$

$$x = 0:\ r < R_2:\quad \vartheta = 0,\quad u = 82\,m/s,\quad T = 300\,K,\quad c_2 = 1;$$

$$x = 0:\ R_2 < r < R_3:\ \frac{\partial F}{\partial x} = 0,\quad F = \{T, c_i, k, \varepsilon, \omega, \tilde{\nu}\},\quad u = \vartheta = 0;$$

$$x = 0:\ R_3 < x < R_4:\quad \vartheta = 0,\quad u = 0.6\,m/s,\quad T = 300\,K,\quad c = 1.$$

The computational grid is condensed in logarithmic form. Grid convergence was studied on various finite-volume meshes with non-uniform steps: $30\times100\times1$ (No. 1), $50\times160\times1$ (No. 2), $60\times200\times1$ (No. 3). Significant quantitative differences in the results are observed in the calculations on grids No. 1 and No. 2. However, when calculating on grids No. 2 and No. 3, the differences in the distribution of parameters are small. Therefore, the main calculations are conducted on grid $50\times160\times1$.

Below, we compare the calculation results for the presented turbulence models with the experimental data given in [1].

Figure 2 shows the curves of the axial temperature of the gas mixture, and Figure 3 shows the mass fraction of the combustion component CO_2. As seen from the figures, the modified $k-\varepsilon$ turbulence model gives results close to the experiment.

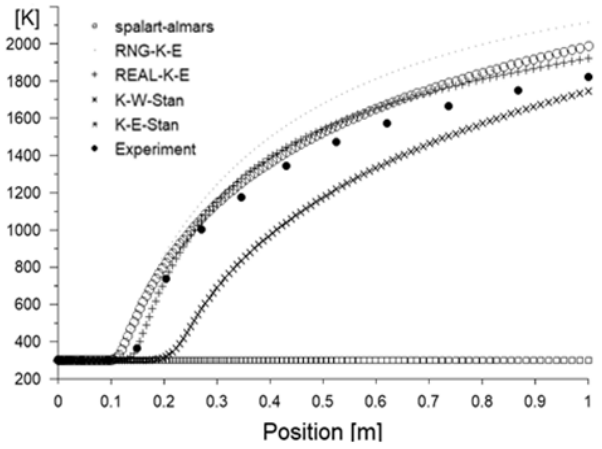

FIGURE 2. Axial temperature

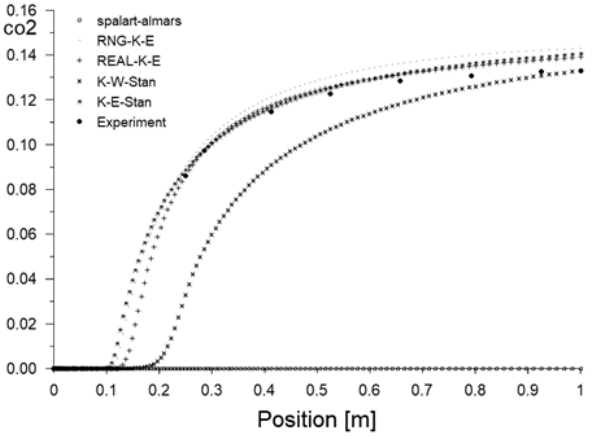

FIGURE 3. Mass fraction of combustion component CO_2

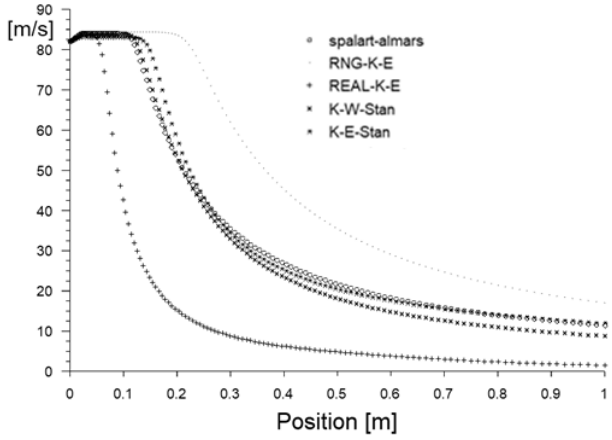

FIGURE 4. Axial distribution of longitudinal velocity

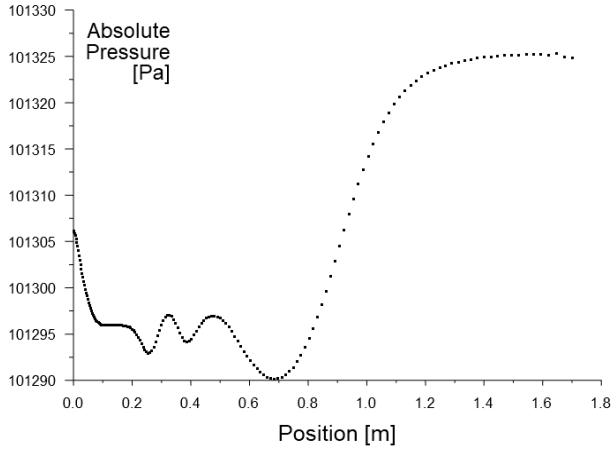

FIGURE 5. Absolute Pressure. Real $k-\varepsilon$ model

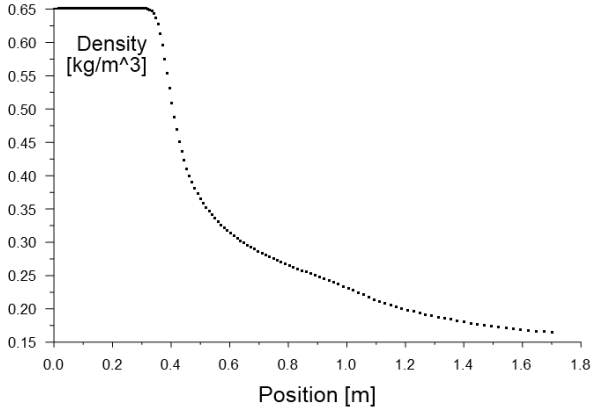

FIGURE 6. Density. Real $k-\varepsilon$ model

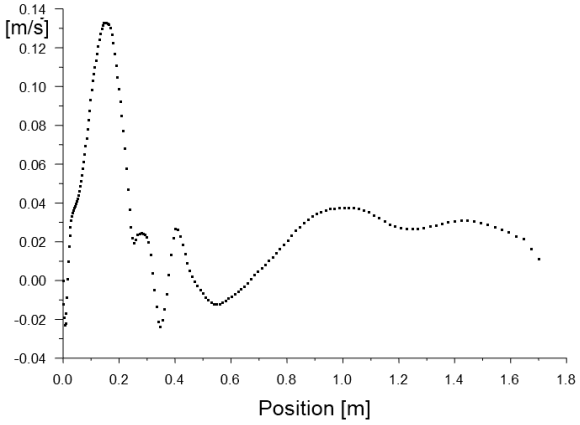

FIGURE 7. Radial velocity. Real $k-\varepsilon$ model

CONCLUSION

The results obtained in the article demonstrate the possibility of using the ANSYS Fluent software package for the efficient calculation of the gas combustion process in a power boiler. So, according to the results of a comparative analysis of the experimental and program package of five turbulence models, the calculated values of the axial temperature and carbon dioxide fraction presented in Figures. 2 and 3, it can be noted that the maximum difference between the values of mathematical modeling and experiment does not exceed 10% [1].

From the analysis of the results, it can be seen that the modified $k-\varepsilon$ model matches the experiment more qualitatively than the other four turbulence models.

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