Numerical simulation of combustion processes

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Abstract. In this paper, we propose a numerical method for solving the problem of the propagation and combustion of a methane jet in an axisymmetric satellite air flow. Within the framework of the modified turbulence model and the Arrhenius law, mathematical and numerical models of the problem of a turbulent axisymmetric methane jet in an infinite cocurrent air flow at a finite reaction rate have been developed. By introducing functions and generalized Schwab-Zel'dovich functions, as well as the stream function, ten differential equations for the conservation of substances are represented by differential equations equivalent to them. The equations of the turbulent boundary layer of a multicomponent gas for an axisymmetric jet are transformed with the transition to dimensionless variables and the introduction of a stream function. The dimensionless equations of the turbulent boundary layer of reacting gases in von Mises coordinates are used for modeling. For the numerical solution of the combustion problem according to the Arrhenius law, an implicit finite-difference scheme was used, which provides the second order of approximation accuracy in longitudinal and transverse coordinates. This made it possible to significantly reduce the calculation time as a result of using a large calculation step for the longitudinal coordinate. In connection with the nonlinearity of the equations of conservation and transfer of substances, an iterative process was organized. Some results of the computational experiment are presented. Comparison of the results of calculating the change in the temperature of the axial flow according to the turbulence models modified by $k-\varepsilon$ and Prandtl with experimental data. The adequacy of the results was verified by the implementation of the laws of conservation of mass, momentum and total enthalpy, as well as by comparing the results with experimental data from other authors with the largest 5% deviation. This means that the previously presented algorithm and calculation program can be used for practical purposes. The results obtained with both turbulence models were compared with experimental data. Analyzing the results, one can notice that the $k-\varepsilon$ model coincides more qualitatively with the experiment than the Prandtl turbulence model.

1 Introduction

Combustion is a complex physico-chemical process of transformation of starting substances

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into combustion products during exothermic reactions, accompanied by intense heat release.

In the world, jet flows of reacting media are widely used in everyday life, in the production of thermal and electrical energy, in internal combustion chambers, in chemical lasers, in the production of mercury and building materials, in power plants of rocket engines and many other branches of technology and production. Depending on the purpose of the organization and the design of gas combustion devices, various problems of object management arise. In particular, the gas component in the global energy balance accounts for about 70%. Despite the constant improvement in the performance of gas combustion devices, their efficiency is still very low.

One of the possible options for studying the regularities of intensive heat and mass exchange with gorenje is mathematical modeling and computational experiment. To do this, you need to have an adequate mathematical model of the object and an effective numerical algorithm. There are some serious problems in describing the gorenje kinetics and flow turbulence. In addition, the number of equations is quite large and there are computational problems for multidimensional problems. The present work is devoted to the solution of these problems, the purpose of which is to develop numerical methods for solving problems of turbulent jet flow of gases and their application in the study of heat and mass exchange processes under conditions of chemical transformations.

Combustion problems are formed by involving systems of complex nonlinear partial differential equations and closing relations [1-3].

In the work of Vasiliev A. A. [4], the differential equations of energy and diffusion were solved using the integral method, taking into account the Reynolds analogy. The model of the diffusion front combustion was used to calculate the distribution of temperatures and concentrations [5]. A ratio is proposed for calculating the efficiency of a two-phase cooler, which gives 25-30 % higher than the efficiency of a single-phase curtain.

The method of calculating a turbulent diffusion torch based on the statistical theory of turbulent diffusion, presented in [6], is also semi-empirical. The main physical parameter used in this method for calculating the size of the torch-the dispersion of the jet, is also borrowed from experience. As can be seen, the role of the experiment in determining the length of a turbulent diffusion torch remains decisive to this day. The approaches to determining the shape and length of a turbulent flare developed in [7] are of interest. In order to highlight the general properties of the phenomena associated with turbulent diffusion flames, while maintaining a simple analytical description, an axisymmetric turbulent diffusion flame was considered. The main goal was to achieve an understanding of the phenomenon, taking into account the possibility of obtaining practical conclusions. Simplifying assumptions were made that did not lead to the loss of essential properties of the flame.

In [8], the problem of the kinetic combustion of a methane jet flowing into a satellite subsonic air flow in an axisymmetric channel is considered. A "narrow channel" model and a differential oneparameter turbulence model are used to describe the flow. The kinetics of methane combustion in air is described by a one-stage stoichiometric gross reaction. The influence of the initial turbulent viscosity and the location of the artificial ignition cross-section on the development of the combustion process is investigated.

In the article [9], a simulation of turbulent combustion methane in areas with complex geometry is carried out. The parameters for one-stage and two-stage models of chemical kinetics are selected. The parameters of chemical kinetics significantly affect the correctness of the mathematical combustion model used to calculate the characteristics of the explosion of a methane-air mixture in a residential building. A comparison with the results of experimental measurements is carried out.

The article [10] presents a model of the combustion of a carbon particle of high

porosity in oxygen, which takes into account the course of heterogeneous and homogeneous chemical reactions inside the particle and heat exchange by radiation. The boundaries of the region to which the combustion dependence on the particle temperature belongs are determined. The possibility of the existence of two combustion modes is shown: high-speed, in which the reaction of carbon with oxygen occurs in the layer near the surface of the particle, and low-speed, in which the reaction occurs in the entire volume of the particle.

An analysis of the literature [1-10] shows that the processes of homogeneous combustion of fuel gases, the main component of which is methane, are insufficiently studied. Combustion Due to the imperfection of the theoretical foundations of chemical exothermic reactions under turbulent flow conditions, theoretical work in this area continues. Taking into account these aspects, the article discusses the distribution of methane in the air satellite flow and the problem of flare control.

2 Methods

A jet of combustible gas is considered, which flows out of a circular nozzle with a diameter of $2a$ and propagates in a satellite flow of an oxidizer at a finite chemical velocity. The velocity distribution in the outlet section of the nozzle and in the satellite flow, as well as the initial (at x=0) distributions of temperature and concentration of fuel and oxidizer, will be considered given, uniform, homogeneous. There is a tangential gap of indicators at the nozzle boundary.

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Modeling of combustion processes is one of the most difficult tasks of computational thermophysics. This is due to the combination of three main processes that require a joint solution – turbulence, chemical reactions and radiant heat transfer. There are a large number of mathematical models for each of the physical phenomena under consideration, which does not allow us to formulate a universal, unambiguous approach to modeling combustion.

Currently, despite the fact that scientific groups in Russia, the USA, India and China have been engaged in the problem of numerical modeling of processes in vortex countercurrent burner modules, there is no generally accepted approach to modeling vortex countercurrent burner devices. There are almost no works where the influence of turbulence and combustion models on the results of calculating processes in countercurrent burner modules is studied. At the same time, success in the creation of burner devices has been achieved by a combination of theoretical and experimental approaches.

Numerical studies, as a method for studying and optimizing processes in vortex countercurrent burner devices, were practically not used until the early 2000s. Apparently, this is due to the complexity of the experimental study of the processes inside the burner modules and, as a result, the lack of experimental data necessary for verification of the numerical model. Therefore, numerical studies were mainly carried out to find optimal geometric parameters and study the effects that occur during combustion fuel.

Given $k-\varepsilon$ the turbulence model was used to solve the problem under consideration. Model $k-\varepsilon$ it is used for modeling a wide range of tasks, its strengths are simplicity, good convergence of calculation, versatility while maintaining good accuracy. The known disadvantages of this model are manifested in insufficiently accurate modeling: the points of separation of the flow from smooth surfaces, the flow in the boundary layer, strongly swirled currents and currents with a large curvature of the current lines. The model consists

of two transport equations for the kinetic energy of turbulent pulsations k and its dissipation ε, as well as an equation for calculating the turbulent viscosity:

$$\begin{aligned}
&\frac{\partial \rho k}{\partial t}+\frac{\partial}{\partial x_j}\left(\rho U_j k\right)=\frac{\partial}{\partial x_j}\left(\left(\mu+\frac{\mu_t}{\delta_k}\right)\frac{\partial k}{\partial x_j}\right)+P_k-\rho\varepsilon,\\
&\frac{\partial \rho \varepsilon}{\partial t}+\frac{\partial}{\partial x_j}\left(\rho U_j \varepsilon\right)=\frac{\partial}{\partial x_j}\left(\left(\mu+\frac{\mu_t}{\delta_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right)+\frac{\varepsilon}{k}\left(C_{\varepsilon 1}P_k-C_{\varepsilon 2}\rho\varepsilon\right),\\
&\mu_t=C_\mu\rho\frac{k^2}{\varepsilon},\quad P_k=\mu_t\left(\frac{\partial U_i}{\partial x_j}+\frac{\partial U_j}{\partial x_i}\right)\frac{\partial U_i}{\partial x_j}-\frac{2}{3}\frac{\partial U_k}{\partial x_k}\left(3\mu_t\frac{\partial U_k}{\partial x_k}+\rho k\right).
\end{aligned} \tag{1}$$

where P_k- turbulence generation term from the action of viscosity forces; $C_{\varepsilon 1}, C_{\varepsilon 2}, \delta_k, \delta_\varepsilon-$ constants.

A constant model for describing the flow of a reacting gas can be obtained on the basis of a joint solution of the equations of motion of a viscous gas and the transport equations for individual components of the mixture [8].

$$\begin{cases}
div\left(\rho\bar{\vartheta}\right)=0,\\
div\left(\rho\bar{\vartheta}\bar{\vartheta}\right)=\rho\bar{F}-grad\,P+div\,\tau,\\
div\left(\rho\bar{\vartheta}H\right)=\rho\bar{F}\bar{\vartheta}+div\left(\tau\bar{\vartheta}\right)-div\left(\rho\bar{\vartheta}\right)-div\,\bar{q}-\rho Q,\\
div\left(C_i\bar{\vartheta}\right)=div\,\bar{I}_i+W_i^*,\ i=1,.....N,\\
H=\sum_{i=1}^{N}h_i c_i+\frac{\bar{\vartheta}^2}{2},\\
p=\rho RT\mu_\Sigma^{-1}.
\end{cases} \tag{2}$$

Here $\bar{F}$ - vector of external forces, Q- the influx of radiant energy, W^* - the rate of formation i-th components as a result of chemical reactions, τ — viscous stress tensor.

Due to the specifics of the presented gas flow: the flow is weakly or does not depend at all on the conditions at one of the boundaries, it is advisable to use a parabolic approximation of the complete system of Navier-Stokes equations to describe a viscous jet flow. Since it is convenient to use a system of uicoordinates associated with current lines when describing the jet flow of a viscous gas, the question of the parabolization procedure in different coordinate systems was considered when constructing a mathematical model of the flow. The essence of the problem is that the parabolization of the complete system of equations, performed formally in a particular coordinate system, leads not only to different types of parabolized equations, but also to the" loss " of some terms, for example, if the rejection of the second derivatives along the march coordinate is performed in a cylindrical coordinate system.

This system is closed by the following dependencies:

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

The gas mixture is assumed to be perfect, so its state satisfies the Mendeleev-Clapeyron equation: $p = \rho R_0 T / m$

where $m = \left(\sum_{n=1}^{N} c_n / m_n \right)^{-1}$ and m_n – molecular weights of the gas mixture and n is gas component $\left(kg\ mol^{-1} \right)$; R_0 is universal gas constant $\left(8.34141\ Dj\ mol^{-1} K^{-1} \right)$.

Since direct-flow free expanded jets are considered, it is assumed that $p = const$.

Using the example of the Mises coordinates defined as

$$\frac{\partial \psi}{\partial x} = -\frac{\rho \vartheta r}{\psi};\ \frac{\partial \psi}{\partial r} = -\frac{\rho u r}{\psi}. \qquad (3)$$

The parabolization of the complete Navier-Stokes system describing the spatial turbulent combustion of a gas flare is carried out, and the estimation of most of the mixed derivatives that are actually lost in the cylindrical coordinate system is performed. Combustion-Stokes it is shown that the form of parabolized equations depends on the order of execution of two transformations: the transition to a curved coordinate system and the direct deletion of the second derivatives along the march coordinate.

For practical application, the system of Navier-Stokes equations in the viscous layer approximation, parabolized in the Mises coordinates, is used:

$$\begin{cases} \frac{\partial}{\partial x}(\rho u r) + \frac{\partial}{\partial r}(\rho \vartheta r) = 0; \\ \frac{\partial u}{\partial x} = -\frac{1}{\rho}\frac{\partial P}{\partial x} + \frac{\vartheta r}{u \psi}\frac{\partial P}{\partial \psi} + \frac{1}{\psi}\frac{\partial}{\partial \psi}\left(\frac{\mu \rho u r^2}{\psi}\frac{\partial u}{\partial \psi} \right); \\ \frac{\partial H}{\partial x} = \frac{1}{\psi}\frac{\partial}{\partial \psi}\left(\frac{\mu}{\Pr}\frac{\rho u r^2}{\psi}\frac{\partial H}{\partial \psi} \right); \\ \frac{\partial C_i}{\partial x} = \frac{1}{\psi}\frac{\partial}{\partial \psi}\left(\frac{\mu}{Sc}\frac{\rho u r^2}{\psi}\frac{\partial C_i}{\partial \psi} \right) + \omega_i;\ \mathrm{i} = 1 \ldots . \mathrm{N}, \\ P = \rho R T \mu_{\Sigma}^{-1},\ \frac{\partial r}{\partial \psi} = \frac{\psi}{\rho u r}; \\ H = \sum_{i=1}^{N} h_i(T) C_i + \frac{u^2 + \vartheta^2}{2}. \end{cases} \qquad (4)$$

Here and further u, v is averaged longitudinal and radial components of the velocity vector $(m \cdot s^{-1})$ in cylindrical coordinates; ψ is Mises coordinates $(m,\ kg^{1/2} \cdot s^{-1/2})$; ρ, T is density $(kg \cdot m^{-3})$ and the absolute temperature (K) gas mixture; p is hydrostatic pressure (Pa); $\Pr$, Sc is hydrostatic pressure Turbulent analogs of the Prandtl

and Schmidt numbers; C_i is mass concentration the i-th component of the gas in the mixture ($kg\ kg^{-1}$); ω_i is mass rate of formation or disappearance of the I isth gas component $(kg \cdot m^{-3} \cdot s^{-1})$; h_i^* is calorific value of the i-th component $j \cdot kg^{-1} \cdot K^{-1}$; $\mu,\ \mu_t$ is kinematic coefficients of laminar and turbulent viscosity $m^2 \cdot s^{-1}$; H is total gas enthalpy $\left(J\ kg^{-1}\right)$;

Methane is considered as a combustible gas, the one-stage kinetics of methane combustion in the air of which is given through the stoichiometric equation

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O + h_2^*. \qquad (5)$$

The indices 1, 2, 3, 4 and 5 highlight the parameters of the components – oxygen, methane, carbon dioxide, water vapor and nitrogen, respectively.

We introduce the Schwab-Zeldovich functions. With a known value of the reaction rate of the fuel, the rates of chemical transformations of the remaining components in dimensional form are represented as

$$\omega_1 = \frac{\nu_1 m_1}{\nu_2 m_2}\omega_2,\ \omega_3 = -\frac{\nu_3 m_3}{\nu_2 m_2}\omega_2,\ \omega_4 = -\frac{\nu_4 m_4}{\nu_2 m_2}\omega_2,\ \ \omega_5 = 0\ \ (\nu_5 = 0).$$

The rate of the combustion reaction of methane with oxygen in the fuel mass conservation equation, according to the proposals of works [12, 17], in dimensionless Mises coordinates has the form:

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

where

$$A_{r1} = 1.35 \cdot 10^{20},\ \frac{E_a}{R} = 15,05\,K = A_{r2}\,K. \qquad (6)$$

Method of casting N differential equations of conservation of components to two equations (with respect to the combustible component and the Schwab-Zeldovich function) for $n = 1..5$ and the formulas for the reverse transition to mass concentration are given in the article [11-13].

The process of combustion of gas fuel in the furnace process is carried out at rather low speeds relative to the speed of sound. Therefore, the kinetic energy of the gas can be neglected in the simulation. Then a substitution similar to that introduced for the concentration can also be used for the total enthalpy, which leads to the normalization of the total enthalpy.

$$\bar{\bar{H}} = \frac{H - H_1}{H_2 - H_1}. \qquad (7)$$

Here $H_1 = \left(c_p\right)_1 T_1 + \left(c_2\right)_1 h_2^*,\ \ H_2 = \left(c_p\right)_2 T_2 + \left(c_2\right)_2 h_2^*.$

In this case, the value of the mixture temperature is calculated by the formula

$$T = \left(H - c_2 h_2^*\right) / c_p = \left[H_1 + \left(H_2 - H_1\right)\bar{\bar{H}} - c_2 h_2^*\right] / \sum_{n=1}^{N} c_{pi} c_i \cdot \qquad (8)$$

The necessary value for further calculations of the density of the gas mixture is found by the formula

$$\rho = \frac{p}{R_0 T \sum_{i=1}^{N} c_i / \mu_i} \qquad (9)$$

At the entrance $x = 0$ the following conditions are imposed on the calculation area:

by $0 \le \psi < 1$: $u = 1,\ \bar{\bar{H}} = 1,\ C_2 = \left(c_2\right)_2,\ k = 1,\ \varepsilon = 1.$

by $1 \le \psi < \psi_\infty$: $u = \left(u\right)_1,\ \bar{\bar{H}} = 0,\ c_2 = \left(c_2\right)_1,\ \bar{k} = \left(k\right)_1,\ \bar{\varepsilon} = \left(\varepsilon\right)_1.$

By $x > 0$ we have

by $\psi = 0$: $\frac{\partial u}{\partial \psi} = 0,\quad \frac{\partial \bar{\bar{H}}}{\partial \psi} = 0,\quad \frac{\partial C}{\partial \psi} = 0,\quad \frac{\partial k}{\partial \psi} = 0,\quad \frac{\partial \varepsilon}{\partial \psi} = 0.$

when $\psi \to \psi_\infty$: $u = \left(u\right)_1,\ \bar{\bar{H}} = 0,\ C_2 = \left(c_2\right)_1,\ k = \left(k\right)_1,\ \varepsilon = \left(\varepsilon\right)_1.$

The right-hand sides of the equations involve the square of a dimensionless radial coordinate r^2. Let's calculate it with the second order of accuracy

$$\left(r_{i,j}^s\right)^2 = \left(r_{i,j-1}^s\right)^2 + 2\frac{\psi_j^2 - \psi_{j-1}^2}{\rho_{i,j-1}^{s-1} u_{i,j-1}^{s-1} + \rho_{i,j}^{s-1} u_{i,j}^{s-1}} \cdot$$

This r^2 - the formula for the *i*-th section; S – the sequence number of the iteration for the i -th section. For $i-1$- th section $\tilde{r}^2$ calculated according to the data of the previous section.

To solve the problem in the Mises coordinates, a two-layer, six-point implicit finite-difference scheme is used, which provides a second-order accuracy of approximation by coordinates. Due to the nonlinearity of the equations of conservation and transfer of substances, an iterative process was organized.

3 Results and discussion

According to the presented material, a program was compiled and calculations were carried out. The mass composition of the air was set as $\left(c_1\right)_1 = 0.232, \left(c_5\right)_1 = 0.768$. Methane without impurities was considered as a fuel. The speed of the main flow was 61 *m/s*, a of the satellite stream – 18.3 *m/s*. Air temperature – $T_1 = 293.15\ K$. Thermophysical parameters of the components and the lowest heat of combustion of methane (50.2 *Mj/kg*) borrowed from [11-13, 17]. The kinetic energy of pulsation motion and the rate of

dissipation of turbulence energy at the fuel nozzle section were $k_2 = 0.007u_2^2 \left(м^2/c^2\right)$ и $\varepsilon_2 = \frac{0.001k_2^{3/2}}{0.3} \left(м^2/c^3\right)$, and in the satellite stream is $k_1 = 0.007u_1^2 \left(м^2/c^2\right)$ и $\varepsilon_1 = \frac{0.001k_1^{3/2}}{0.3} \left(м^2/c^3\right)$ accordingly. The molar masses of the components are $m_1 = 32.000\ г/моль$, $m_2 = 16.043\ г/моль$, $m_3 = 44.011\ г/моль$, $m_4 = 18.020\ г/моль$, $m_5 = 28.016\ г/моль$. The stoichiometric coefficients for the presented gross reaction were $\nu_1 = 5\ моль$, $\nu_2 = 1\ моль$, $\nu_3 = 3\ моль$, $\nu_4 = 4\ моль$, $\nu_5 = 0\ моль$. Lower heat of combustion of methane – 50.2 *MDj/kg* [12].

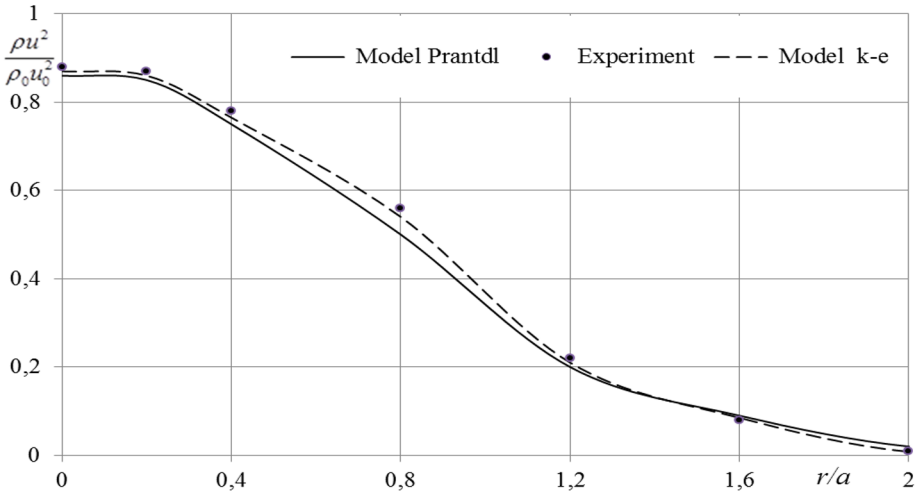

Fig. 1. Comparison of the distribution of the pulse flux density in the flow field with the experiment [1]. When $x/d = 6,\ T_2 = 600\,K,\ c_{22} = 0.085\,кg/кg.$

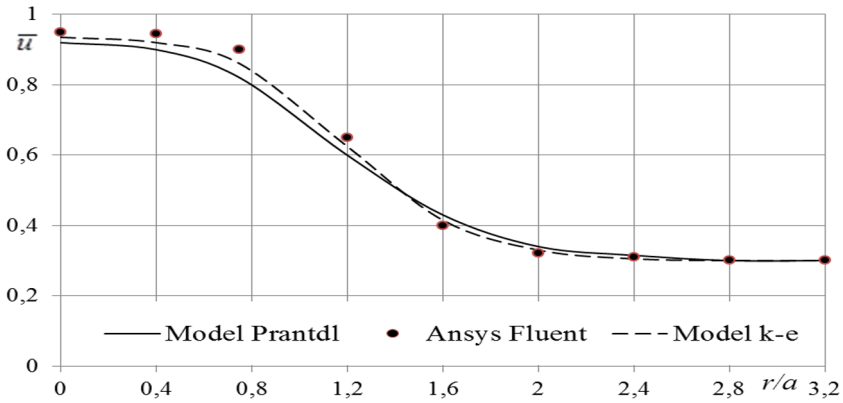

Fig. 2. Comparison of the results. Radial velocity distribution at $x/d = 7,\ T_2 = 1100\,K,\ c_{22} = 0.085\,кg/кg.$

Ansys Fluent is a powerful tool for optimizing the process of design, engineering and technological training in the field of computational dynamics of liquids and gases. The Ansys Fluent software module has a wide range of possibilities for modeling the flows of liquids and gases for industrial tasks, taking into account turbulence, heat transfer, and chemical reactions.

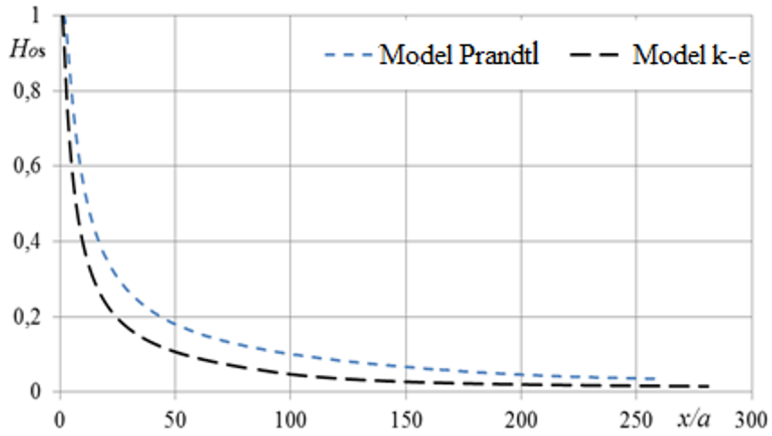

Fig. 3. Curves relative to the excess enthalpy of the gas

The program demonstrates that an intense reaction takes place at the initial part of the jet up to about 100 calibers. The reaction rate gradually decreases, so at the end of the conditional length of the torch, 0.03996 part of the mass of the injected methane remains.

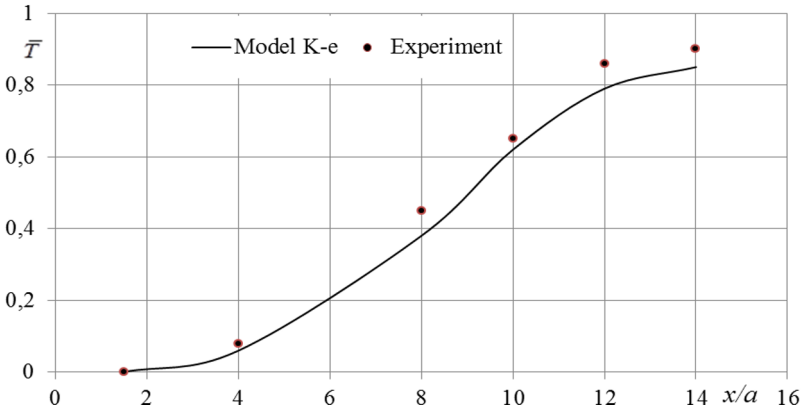

Fig. 4. Comparison of the calculation of the axial excess temperature with the experiment [1]: here $\bar{T} = \frac{T - T_1}{T_2 - T_1}$

In Fig. 4 the axial values of the gas temperature, which were obtained by the previously proposed method and by the Ansys Fluent program, are compared. The picture is qualitatively similar: first a kind of "incubation zone" is formed for combustion, then the axial value of temperature increases. The term "incubation zone" may not be very successful, but it suggests an analogue of the combustion process of a gas mixture in a limited volume, where combustion requires "incubation time" for the development of the combustion process.

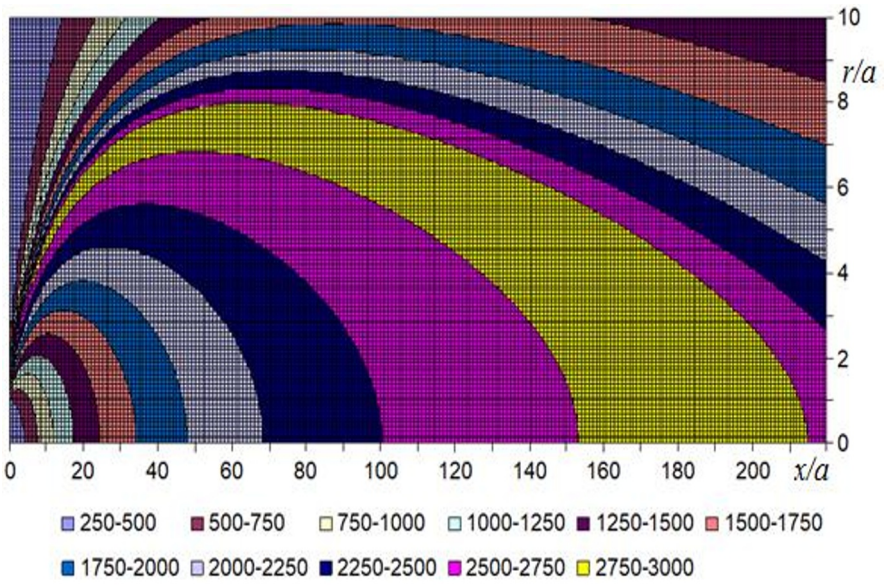

Fig. 5. Isotherms in the process of methane diffusion combustion at $T_1 = 400K$, $T_2 = 293K$, $a = 0.01м$

When applying the Arrhenius law, a monotonous temperature change in the cross-section of the jet is also observed after the closure of the" conditional " flame front on the axis of the jet. Its greatest value is reached on the axis of the jet, then, with distance from the axis of the jet, it monotonically falls. The highest temperature according to the Burke-Schumann model $T^* = 2910.44\ K$ it remains constant along the entire length of the front, and it is much larger than when using a model with a finite reaction rate. This is due to the fact that according to the BSHZ at the end of the torch ($l^* = 203.74$) the entire mass of fuel burns, at the same time, in the Arrhenius model, the condition $\tilde{\tilde{H}}(\bar{x},0) \le 0.02$ performed in a cross section $\bar{x} = 712.0$.

4 Conclusions

Within the framework of the work, methods of introducing the Schwab-Zeldovich functions and relatively excessive enthalpy for the case of methane combustion in a satellite air stream with a finite velocity were demonstrated. A numerical method has been developed for solving the problem of the propagation of an axisymmetric jet of fuel in a satellite air flow in Mises variables using a modified $k-\varepsilon$ model for the turbulence coefficient.

For the numerical solution of the problem, an approximation scheme of the second order of accuracy was used for both coordinates, which gives a more accurate picture of the object. An algorithm and a calculation program with internal and external iteration for the longitudinal velocity and other indicators of heat and mass transfer processes have been developed.

The adequacy of the results was verified by the implementation of the laws of conservation of mass, momentum and total enthalpy, as well as by comparing the results with experimental data from other authors with the largest 5% deviation. This means that the previously presented algorithm and calculation program can be used for practical purposes.

The results obtained with both turbulence models were compared with experimental data. Analyzing the results, one can notice that the $k-\varepsilon$ model coincides more qualitatively with the experiment than the Prandtl turbulence model.

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