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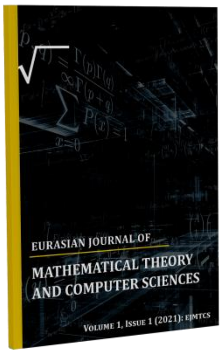

NUMERICAL SIMULATION OF THREE-DIMENSIONAL TURBULENT JETS OF REACTING GASES

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ABSTRACT

In this paper, a method and an effective algorithm for calculating the study of the outflow of a three-dimensional turbulent jet of reacting gases from a rectangular nozzle and propagating in a cocurrent (flooded) air flow are presented. To describe the flow, three-dimensional parabolized systems of Navier-Stokes equations for multicomponent chemically reacting gas mixtures are used. To calculate the turbulent viscosity, a modified model of the first moments of turbulence is proposed, taking into account molecular transfer, three-dimensionality and temperature inhomogeneity of the jet, and a two-parameter "k-ε" turbulence model is used.

On the basis of the developed method, the influence of the ratio of the temperature of the combustible jet and the oxidizer, as well as the pressure gradient on the configuration of the diffusion flame, was investigated.

The main tool for studying gas dynamics, heat and mass transfer of turbulent jet flows of multicomponent gas mixtures is mathematical modeling, which, unlike a physical experiment, is often more cost-effective and is often the only possible research method. In general, the simulation of turbulent jet flows of reacting gas mixtures is based on the generally accepted system of coupled partial differential equations expressing the laws of conservation of mass, momentum, energy, and matter [1÷4].

In works [5–12,16,17,18], mainly the results of experimental and theoretical - numerical calculations are given, devoted to the study of the outflow of air flowing out of a rectangular nozzle.

At the same time, the problem of mathematical modeling of three-dimensional jet flows of reacting gas mixtures remains one of the most difficult in mechanics. The complexity of the problem under consideration is associated, on the one hand, with the incompleteness of the theory of turbulence, and, on the other hand, with the specific features of turbulent flows in the presence of chemical reactions.

This paper presents modified models for calculating the turbulent effective viscosity, a calculation method, and some numerical results of studying three-dimensional turbulent jets of reacting gases flowing from a rectangular nozzle and propagating in a flooded (cocurrent) air flow during diffusion combustion.

Formulation of the problem. Consider a reacting jet flowing from a rectangular nozzle and propagating in a cocurrent (flooded) air flow. As the origin of coordinates of the Cartesian system, we will choose the center of the initial section of the jet: the OX axis is directed along the jet, and the OY and OZ axes are parallel to the sides of the nozzle, with dimensions 2a and 2b, respectively. Let us assume that the flow is symmetric about the OX axis and the YOX, ZOX planes, which form the boundary of the integration region and allow considering only one quarter of the rectangular jet.

Such a flow is described by the following parabolized system of equations [1,3,4,11,12, 16]:

$$\frac{\partial pu}{\partial x}+\frac{\partial pv}{L\partial y}+\frac{\partial pw}{\partial z}=0 \qquad (1)$$

$$pu\frac{\partial u}{\partial x}+pv\frac{\partial u}{L\partial y}+pw\frac{\partial u}{\partial z}=\frac{\partial p}{\partial x}+\frac{\partial}{L^2\partial y}\left(\mu\frac{\partial u}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mu\frac{\partial u}{\partial z}\right), \qquad (2)$$

$$\rho u\frac{\partial v}{\partial}+\rho v\frac{\partial v}{L\partial y}+\rho w\frac{\partial v}{\partial z}=-\frac{\partial p}{L\partial y}+\frac{4}{3L^2}\frac{\partial}{\partial y}\left(\mu\frac{\partial v}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mu\frac{\partial v}{\partial z}\right)-\frac{2}{3L}\frac{\partial}{\partial y}\left(\mu\frac{\partial w}{\partial z}\right)+\frac{\partial}{L\partial z}\left(\mu\frac{\partial w}{\partial y}\right), \qquad (3)$$

$$\rho u\frac{\partial w}{\partial x}+\rho v\frac{\partial w}{L\partial y}+\rho w\frac{\partial w}{\partial z}=-\frac{\partial p}{\partial z}+\frac{4}{3}\frac{\partial}{\partial z}\left(\mu\frac{\partial w}{\partial z}\right)+\frac{\partial}{L^2\partial y}\left(\mu\frac{\partial w}{\partial y}\right)+\frac{\partial}{L\partial y}\left(\mu\frac{\partial v}{\partial z}\right)-\frac{2\partial}{3L\partial z}\left(\mu\frac{\partial v}{\partial y}\right) \qquad (4)$$

$$\rho u\frac{\partial H}{\partial x}+\rho v\frac{\partial H}{L\partial y}+\rho w\frac{\partial H}{\partial z}=\frac{1}{L^2Pr_T}\frac{\partial}{\partial y}\left(\mu\frac{\partial H}{\partial y}\right)+\frac{1}{Pr_T}\frac{\partial}{\partial z}\left(\mu\frac{\partial H}{\partial z}\right)+\left(1-\frac{1}{Pr_T}\right)\left[\frac{\partial}{L^2\partial y}\left(\mu\,u\frac{\partial u}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mu\,u\frac{\partial u}{\partial z}\right)+\frac{\partial}{\partial z}\left(\frac{\partial v}{\partial z}\right)+\frac{\partial}{L^2\partial y}\left(\mu\,w\frac{\partial w}{\partial y}\right)\right]+\left(\frac{4}{3}-\frac{1}{Pr_T}\right)\left[\frac{\partial}{L^2\partial y}\left(\mu\,v\frac{\partial v}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mu\,w\frac{\partial w}{\partial z}\right)\right]-\frac{\partial}{L\partial y}\left(\frac{2}{3}\mu\,v\frac{\partial w}{\partial z}\right)+\frac{\partial}{L\partial z}\left(\mu\,v\frac{\partial w}{\partial y}\right)+\frac{\partial}{L\partial y}\left(\mu\,w\frac{\partial v}{\partial z}\right)-\frac{\partial}{L\partial z}\left(\frac{2}{3}\mu\,w\frac{\partial v}{\partial y}\right), \qquad (5)$$

$$\rho u\frac{\partial\bar{\bar{C}}}{\partial x}+\rho v\frac{\partial\bar{\bar{C}}}{L\partial y}+\rho w\frac{\partial\bar{\bar{C}}}{\partial z}=\frac{\partial}{L^2Sc_T\partial y}\left(\frac{\mu\,\partial\bar{\bar{C}}}{\partial y}\right)+\frac{\partial}{Sc_T\partial z}\left(\frac{\mu\,\partial\bar{\bar{C}}}{\partial z}\right), \qquad (6)$$

$$H=c_pT+\frac{u^2+v^2+w^2}{2}+\sum_{i=1}^{N}c_ih_i \qquad (7)$$

$$P=\rho T\sum_{i=1}^{N}\frac{c_i}{M_i} \qquad (8)$$

To calculate the effective turbulent viscosity, we use a modified algebraic model that takes into account molecular transfer, three-dimensionality, and temperature inhomogeneity of the jet in the form

$$\mu=\mu_\tau+ae\rho l^2\sqrt{\left(\frac{\partial u}{L\partial y}\right)^2+\left(\frac{\partial u}{\partial z}\right)^2+\left(\frac{\partial w}{L\partial y}\right)^2}\left(\frac{T}{T_2}\right)^{\propto} \qquad (9)$$

and also by connecting the equation of kinetic and dissipation of kinetic energy of turbulence to calculate turbulent viscosity ("k-ε" model), which has the following form:

$$\rho u\frac{\partial k}{\partial x}+\rho v\frac{\partial k}{L\partial y}+\rho w\frac{\partial k}{\partial z}=\frac{\partial}{L^2\partial y}\left(\frac{\mu_T}{\sigma_k}\frac{\partial k}{\partial y}\right)+\frac{\partial}{\partial z}\left(\frac{\mu_T}{\sigma_k}\frac{\partial k}{\partial z}\right)+G-\rho\varepsilon, \qquad (10)$$

$$\rho u\frac{\partial\varepsilon}{\partial x}+\rho v\frac{\partial\varepsilon}{L\partial y}+\rho w\frac{\partial\varepsilon}{\partial z}=\frac{\partial}{L^2\partial y}\left(\frac{\mu_T}{\sigma_\varepsilon}\frac{\partial\varepsilon}{\partial y}\right)+\frac{\partial}{\partial z}\left(\frac{\mu_T}{\sigma_\varepsilon}\frac{\partial\varepsilon}{\partial z}\right)+(C_1G-C_2\rho\varepsilon)\frac{\varepsilon}{k}, \qquad (11)$$

где $G=\mu_T\left[\left(\frac{\partial u}{L\partial y}\right)^2+\left(\frac{\partial u}{\partial z}\right)^2\right]$, $\mu_T=C_\mu\rho k^2/\varepsilon$ (12)

In equations (1 ÷ 12, 16) and, v, w are the components of the speed along the x, y, z axes; k, ε - kinetic energy of turbulence and its dissipation; p, P, T are the density, pressure and temperature of the mixture, R is the universal gas constant; PrT, ScT - turbulent Prandtl and Schmidt numbers; μ-coefficient of dynamic effective turbulent viscosity; cp is the heat capacity of the mixture at constant *pressure; ci, hi * -concentration and heat of formation of the i -th component; N is the number of mixture components; ae is Karman's empirical constant; α-exponent taking into account the temperature heterogeneity of the jet; μ_τ = const • T0.64 (const- is determined taking into account the collision diameter, characteristic temperature, parameter of the potential function of intermolecular interaction, as well as the collision integral for momentum transfer [13]); The* l-length of the mixing path is defined as √ (b ^ 2 (Ly) + b ^ 2 (z)); C_1, C_2, C_μ, σ_k, σ_ε -empirical constants "k-ε" of the turbulence model. Systems of equations (1 ÷ 12) are given in dimensionless form, choosing the value -b as the length scale, for velocities -u_2 (hereinafter, index 2 refers to the initial values of the combustible jet), density- p_2, pressure- p_2 u_2 ^ 2 , total enthalpy and heat of formation of the i-th component-u_2 ^ 2, effective turbulent viscosity-bρ_2 u_2 ^

1) 0 ≤ y ≤1, 0 ≤ z ≤ 1: *u=l, v=0, w=0,* $H=H_2$, $P=P_2$, $\bar{\bar{c}} = 1$, ($k=k_2$, $E=E_2$)

$E=E_1$)

II: $x > 0$:

l) $z=0$, $0 \le y < y_{+\infty}$: $w=0$, $\frac{\partial f}{\partial z} = 0$ ($f=u,v,H,\bar{\bar{c}},k,E$) (13)

$y \to y_{+\infty}$: $u=u_1$ $v=0$, $w=0$, $H=H_1$, $P=P_1$ $\bar{\bar{c}} = 0$, $k=k_1$, $E=E_1$

Here, the subscripts "1", "2", and "+ ∞" mark respectively the dimensionless quantities of the oxidizer and the combustible jet, as well as their values

2, heat capacity at constant pressure- (R / M1), temperature-u_2 ^ 2 / (R / M1), molecular weights- M1 (M1 is the molecular weight of the oxidizer), the kinetic energy of turbulence and its dissipation, respectively, u_2 ^ 2 and u_2 ^ 3 / b, as well as the dimensionless inlet section of the nozzle into the square region using the formula y = y¯ / L (L = a / b, y¯ - dimensionless coordinate).

The concentration equation (6) is written in the form of the conservative Schwab-Zeldovich function with respect to the mass concentration of the i-th components, which makes it possible to reduce the number of equations with sources of terms to one, for a four-component mixture [14]. It is assumed that the reaction takes place in the zone of contact of the fuel with the oxidizer, i.e. diffusion combustion is considered.

The function $\bar{\bar{c}}$ at the nozzle exit of the fuel value is 1, and in the air zone 0.

For this setting, the systems of equations (1 ÷ 9) or (1 ÷ 8, 10 ÷ 12) can be solved using the following dimensionless boundary conditions:

$x = 0$:

2) $1 < y < y_{+\infty}$, $1 < z < z_{+\infty}$: $u=u_1$ $v=0$, $w=0$, $H=H_1$, $P=P_1$, $\bar{\bar{c}} = 0$, ($k=k_1$

2) $y=0$, $0 \le z < z_{+\infty}$: $v=0$, $\frac{\partial f}{\partial y} = 0$ ($f=u,v,H,\bar{\bar{c}},k,E$).

3) $z \to z_{+\infty}$,

at infinity.

The system of equations (1 ÷ 9) is partially parabolized, therefore their elliptical effects are manifested through the pressure field and their elliptical properties associated with the field of motion are preserved [2 ÷ 3]. When a subsonic free jet outflows through a rectangular nozzle into a medium, the pressure gradient in the longitudinal direction and small changes in it in the transverse plane can be neglected, which sometimes makes it possible to perform calculations with a given pressure [1÷3]

Solution method. For the numerical integration of the system of equations (1 ÷ 9) [or (1 ÷ 8, 10 ÷ 12), 16] with the boundary conditions (13), we use a spatial two-layer ten-point finite-difference scheme of alternating directions [8] with an accuracy of the order of 0 (Δx, Δy2, Δz2).

Most of the solutions to three-dimensional parabolized equations are obtained according to the segregated method proposed in the SIMPLE procedure [2] and a slightly different formulation, which also leads to the Poisson equation for pressure renewal [1].

In this paper, an efficient method similar to SIMPLE is presented, the Poisson equation is solved directly to determine the correction to the velocities. The supposedly redundant continuity equation is used to calculate the mass imbalance. In contrast to [2,3], corrections are given for three velocity components; the found solutions u, v, w in the new iteration are expressed as calculated (ir, vp, wp) and plus correction (is, vc., wc) in the form

$u = u_p + u_c,\ v = v_p + v_c,\ w = w_p + w_c.$

The correction rates are determined from the continuity equation by introducing the potential Q,

$$\rho u_c = \frac{\partial Q}{\partial x},\ \rho v_c = \frac{\partial Q}{L\partial y},\ \rho w_c = \frac{\partial Q}{\partial z}, \qquad (15)$$

which is the solution to the Poisson equation:

$$\frac{\partial^2 Q}{\partial x^2} + \frac{\partial^2 Q}{L\partial y^2} + \frac{\partial^2 Q}{\partial z^2} = Q_p \qquad (16)$$

where Qp is the source term.

1) Difference equation (16) can be written for the potential Q at each grid point across the flow in the plane along i (numbering of i-sections along the Ox axis, j-along Oy, k-along Oz) and use a tridiagonal system of equations with the following reasonable assumptions:

2) *Qi-1, j, k = 0, Qi, j, k-1 = 0-means that the corrections to the velocity in the plane (i-1) and in the section (k-1), in which the conservation of mass is already ensured ...*

3) *Qi + 1, j, k = 0, Qi, j, k + 1 = 0- means that the corrections to the velocity will be equal to zero, as in the plane (i + 1) and in the section (k + 1) their convergence, in this plane and in the section, respectively.*

Let us briefly describe the algorithm for solving the problem:

1. Setting the first approximation of the unknown unknowns.
2. Solution of equation (2) to calculate ir.
3. Solving equation (3) to calculate vp using the value of u_p.
4. Solving equation (4) to calculate wp using the values of u_p and vp
5. Solution of equation (16) to calculate Q, taking into account the assumptions 1) and 2)
6. Calculate uc, vc, wc from the equation (15). (14).
7. Calculation of u, v, w by the formula (14).
8. The corrected values of the velocities solve the energy equations (5) and the concentration equations with respect to excess concentrations (6) for calculating

H and $\bar{\bar{c}}$, respectively, and are calculated from the equations (10.11) of the kinetic energy and dissipation of the kinetic energy of turbulence (10 ÷ 11) if used -ε "turbulence model, and then the individual concentration components are calculated.

9. The temperature is calculated from the relation (7) and the density from 8).

10. The viscosity is calculated by the formula (9), if the "k-ε" model is used, then by the formula (12).

The expansion of the computational domain (expansion of the jet boundary) along the Oz and Oy axes was carried out according to the condition: $\max_{i,j,k}|F_{ijk} - F_{BH}| > \delta$, where F= {u, H}, F_{BH} = {u_1, H_1 } a - small number.

If this condition is met, then the number of calculated points is increased by one point.

For, in the nonisobaric case, in addition to relation (14), we assume that the true pressure is expressed as the calculated pressure plus the correction pressure, i.e. as

$$P = P_p + \beta P_C \qquad (17)$$

where β - relaxation coefficient.

Further, the proposed method is based, as in the original approach of Patankar and Spalding [2, 3], that the corrections to the velocity are determined by corrections to the pressure in accordance with very approximate equations of motion, but we use for all equations of motion in which the longitudinal convective terms are balanced by pressure terms. Discretizing the left-hand sides of these equations, taking into account the assumption that in the plane (i-1) the corrections to the velocity are equal to 0, we obtain

$$u_c = -\frac{\Delta x \partial P_c}{\rho u \partial x},\quad v_c = -\frac{\Delta x \partial P_c}{L\rho u \partial x},\quad w_c = -\frac{\Delta x \partial P_c}{\rho u \partial z}, \qquad (18)$$

Taking into account that the corrected velocities (18) must satisfy the continuity equation, we obtain the Poisson equation for Pc, and it can be easily solved in each section. If we introduce some reasonable assumptions like 1) and 2), and in this case, the calculation algorithm is similar to that described above, with the only difference that after finding Pc, the true pressure value and correction velocities are calculated using formulas (14).

Numerical results. To check the performance and reliability of the given numerical calculation, let us consider a free air jet flowing from a rectangular nozzle and experimentally investigated in [6].

The calculations were carried out with a variable step along the longitudinal coordinate and, at the same time, in the initial section, the step did not exceed 0.02. Comparison of the results (Fig. 1) with the experimental results [6] on the distribution of the flux density in the cross sections x = 80 mm (experiments are marked by dots) and x = 300 mm (- along the OZ axis) show that they are in satisfactory agreement. Further, the combustion of a propane-butane mixture in air is considered with the initial values taken from [14,16,17], respectively, as:

Oxidizer zone	Fuel zone
$u_1=0$;	
$T_1=300K$;$(k=k_1, \varepsilon=\varepsilon_1)$	
$u_2=61м/с$; $T_2=1200 K$;$(k=k_1, \varepsilon=\varepsilon_1)$	
$(C_1)_1=0{,}232$; $(C_2)_1=0$	$(C_1)_2=0$; $(C_2)_2=0{,}12$

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$(C_3)_1=0$; $(C_4)_1=0,768$ *$(C_3)_2=0$; $(C_4)_2=0,88$*

$P_1=P_2=1$ атм; Pr=0.7; Sc=0.7; a:в=1:1

Here, internal indices show the components of the mixture (1-oxidant, 2-fuel, 3-reaction product, 4-inert gas). This process, with the same initial data of the jet and the oxidizer, was numerically investigated in different modifications of the algebraic model (9) to calculate the effective viscosity.

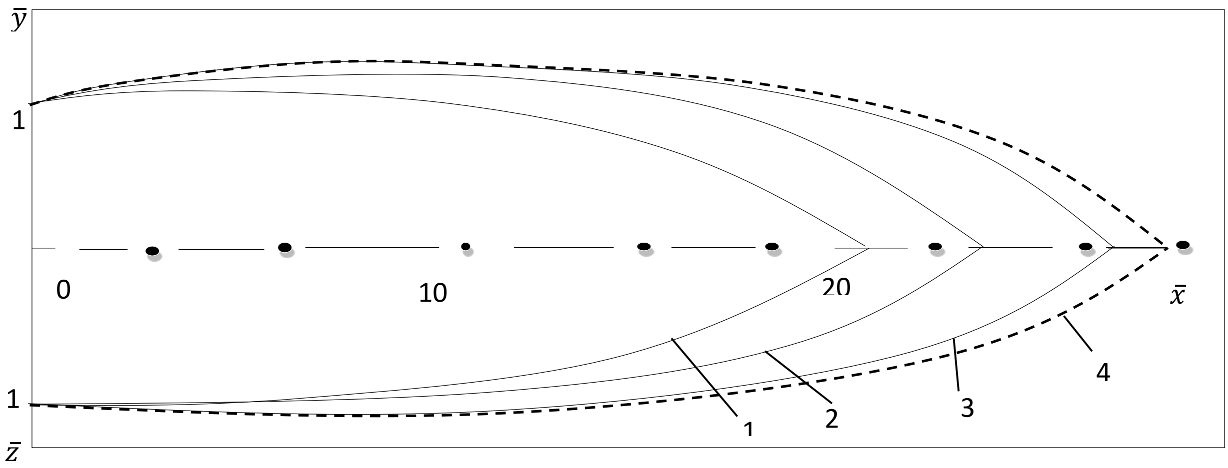


Fig. 1. Diffusion torch shapes: 1- $\mu_\tau=0$, $\alpha= 0.65$; $\beta = 0.2 - \mu_\tau = 0, \alpha = 0.65;$ $\beta = 0; 3 - \mu_\tau = 0, \alpha = 0, \beta = 0; 4 - \mu_\tau = 0, \alpha = 0, \beta = 0.4$

In fig. 1 shows comparisons of the shape of the diffusion plume at μ_τ ≠ 0, α = 0.65 (form 1); μ_τ = 0, α = 0.65 (form 2); μ_τ = 0, α = 0 (form 3); μ_τ = 0, α = 0 taking into account pressure (form 4). From a comparison of the shape of the flares, it follows that, taking into account the variability and constancy of pressure, it shows that the length of the flare in the first variant is higher, but does not significantly affect the configuration of the flare. In these variants, the flame length $L_ф$ / 2b is in the interval (24, 25). It should be noted that the torch length obtained in the framework of the equivalent problem of the theory of heat conduction is approximately $L_ф$ /2b = 27.

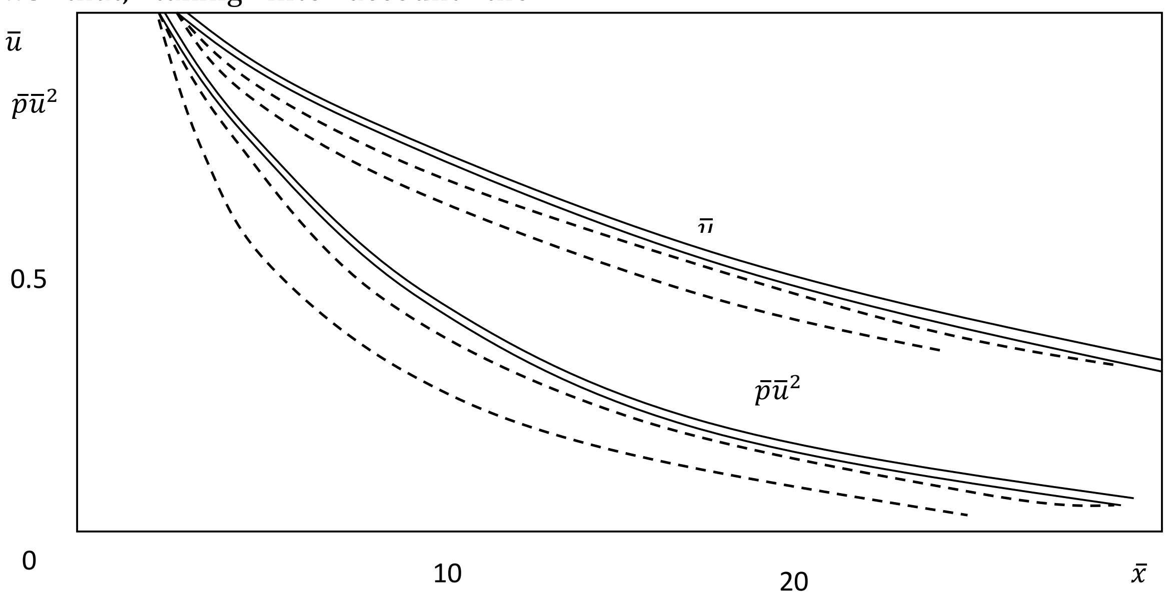
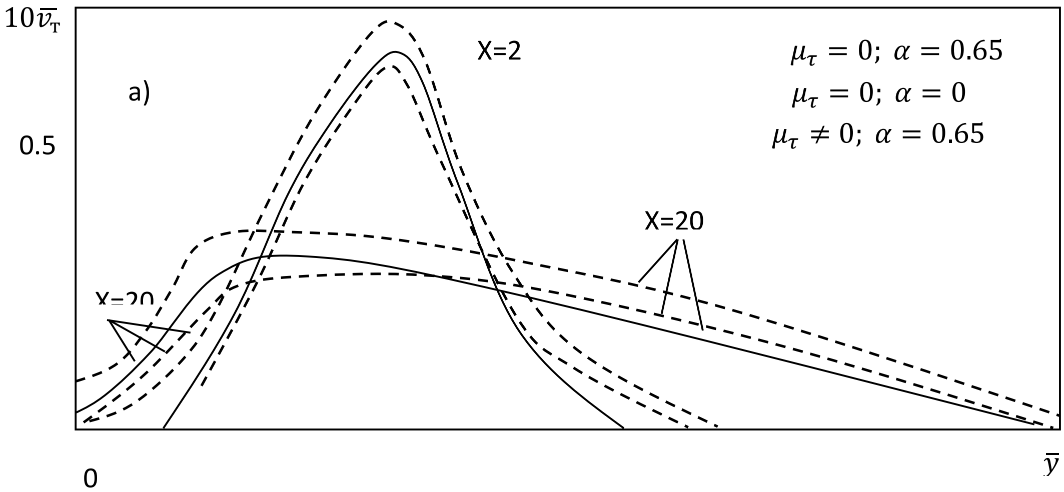


Fig. 2. Axial variation of the longitudinal velocity and pulse flow.----- T_2=700 K; --------T_2=900 K; ------- T_2=1200 K; -------T_2=500 K, T_2=1200 K.

Figure 2 shows the axial variation of the longitudinal velocity and pulse flux along the axis of the submerged diffusion plume at different initial values of the temperature of the combustible jet and oxidizer. Judging by the axial change in these parameters, we can say that their behavior correctly reflects the physics of the phenomenon, i.e. an increase in the initial temperature value leads to a slow decrease in the axial velocity of the pulse flow. At low temperatures of the combustible jet (T2 <900 K), the temperature at the flame front does not exceed 1750 K.

From the profiles of the kinematic coefficient of turbulent viscosity, given in different sections of the jet along the axes OY and OZ (Fig. 3), it can be seen that its maximum value is observed in the flame front, where the temperature has a maximum, and this, in turn, leads to its increase. In the variants μ_τ = 0 and a = 0, where the jet core exists, the value of the kinematic coefficient of viscosity is zero, and with distance from the nozzle exit, its maximum value moves to the jet axis and the change along the OY and OZ axes is gradually smoothed out.

For the development of a turbulent flame, not only the speed, density, concentration of fuel and oxidizer, their temperature also plays a significant role. An increase in the fuel temperature from 700 K to 1200 K leads to an increase in the length of the diffusion flame from LF / 2b = 24 to 26.5, at an oxidizer temperature of 300 K, and a more heated oxidizer (T1 = 500 K, T2 = 1200 K) dimensionless flame length reaches 27.5



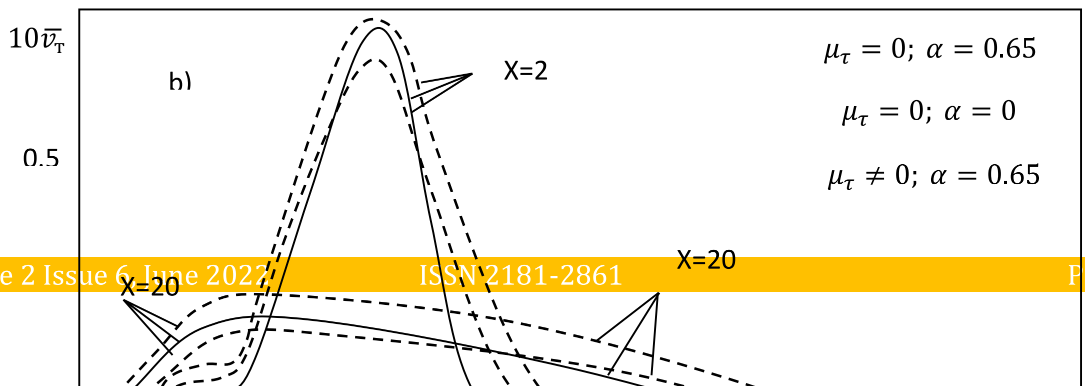


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Fig. 3. Change in kinematic viscosity for different algebraic models of the turbulence coefficient: a) - along the y-axis; b) - along the z-axis.

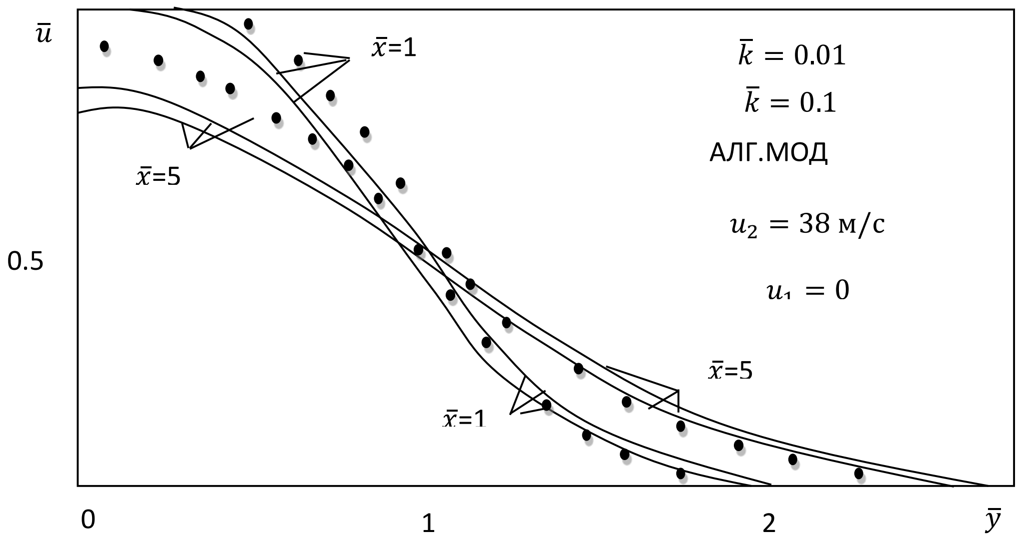

Fig. 4. Comparison of results in the framework of the algebraic and "k-ε" turbulence models.

Figure 4 shows a comparison of the longitudinal velocity profiles along the OY axis in different sections in the longitudinal direction; within the framework of the algebraic and "k-ε" turbulence model. Slightly different results were obtained with the initial values of the kinetic energy of turbulence equal to 1% of the initial velocity of the modified empirical constants "k-ε" of the turbulence model C1=1.3, C2=1.5 instead of C1=1.4, C2=1.92 [16, 17,18].

The pressure variability noticeably affects the velocity and temperature profiles in the initial sections of the jet, and with distance from the nozzle exit, the effect of pressure can be considered insignificant, so the results obtained assert that in free jets the role of the pressure gradient on the jet and flame parameters is insignificant. The increase in the displacement boundary in the XOY and XOZ planes in the initial sections is different in all calculations, and with a distance from the cut by 4-5 calibers, the shape of the jet and the plume becomes round for a nozzle with a square cross section.

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