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# On one efficient method for calculating three-dimensional turbulent jets of reacting gases

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# On one Efficient Method for Calculating Three-Dimensional Turbulent Jets of Reacting Gases.

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**Abstract.** This paper presents a method and algorithm for calculating the outflow of a multicomponent chemically reacting gas mixture flowing out of a rectangular nozzle with different aspect ratios and propagating into a cocurrent (flooded) flow. To describe the turbulent flow, the three-dimensional parabolic system of Navier-Stokes equations for multicomponent chemically reacting gases is used. Justified initial and boundary conditions are given. The system of equations is given after non-dimensionalization of spatial coordinates and physical parameters, as well as with the help of mathematical transformations, allowing the inlet section of the nozzle to be reduced to a unit square. To calculate the turbulent viscosity, a modified algebraic turbulence model is used that takes into account temperature inhomogeneity and velocity effects in spatial coordinates. For the numerical integration of the system of equations, a two-layer ten -point implicit finite-difference scheme was used. The continuity equation is used to calculate the mass imbalance in each computational grid. The calculation algorithm and the method for determining the boundary of jet displacement are given in detail. A number of numerical experiments have been carried out to refine the empirical Karman constant included in the turbulence moduli. Poisson's difference equation, relative to the potential function for calculating the correction for three velocities at each point in space, is solved by introducing reasonable assumptions, allowing to have a tridiagonal system of equations. This allows efficient computation. The reliability of the results was verified by comparing the numerical results with the experimental works of other authors.



## INTRODUCTION

At present and for many years to come, a significant part of the energy used in the world is produced by burning natural gases in a turbulent jet stream. This method of obtaining energy remains predominant, especially in transport, internal combustion engines, furnaces, heating installations and other branches of technology. Therefore, the study of turbulent combustion of reacting jets is of considerable practical interest.

A significant number of works are devoted to the study of the combustion process in a turbulent flow [1 – 9, 32,33], reflect the leading position of combustion, and remain the basis for further deepening and development of the theory and mechanism of combustion, flame propagation, and is also a practical guide for workers dealing with combustion processes.

Numerous studies devoted to the combustion of reacting turbulent flows are experimental or numerical - theoretic based on parabolized two-dimensional Navier-Stokes equations [9,31].

Three-dimensional turbulent boundary layers and jet streams have become the subject of numerous experimental and computational-theoretical studies in the last decade.[10].

The study of turbulent jets flowing from nozzles of rectangular cross section has been carried out by various authors for about ninety years.

A number of detailed experiments have been carried out and attempts have been made to theoretically and numerically calculate the process, the three-dimensional outflow of air flowing out of a rectangular nozzle[11 – 23].

To describe the combustion process, various models are adopted based on the law of mass action, one of the simple models is diffusion combustion [5], where expressions for engineering calculations of a turbulent diffusion flame flowing out of a rectangular nozzle are derived.

A complete picture of the flow of three-dimensional turbulent jets of reacting gases flowing out of a rectangular nozzle can be obtained by describing this process by mathematically modeling the generally accepted system of coupled nonlinear partial differential equations expressing the laws of conservation of mass, momentum, energy, and matter, using efficient calculation methods involving powerful modern computing machines[24 – 30].

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## FORMULATION OF THE PROBLEM

The aim of this work is to model, develop an effective method for numerical solution and study of three-dimensional turbulent jets of reacting gases flowing out of a rectangular nozzle with different aspect ratios and propagating in a cocurrent (flooded) oxidizer flow during diffusion combustion.

Let us assume that the origin of the Cartesian coordinate system is in the center of the initial section of the main (combustible) jet, the axis $x$is directed along the jet, and the axis $y$ и $z$ is parallel to the sides of the nozzle, respectively, with the size of the sides $2a$ и $2b$,and the properties of the central symmetry of the flow about the axis $x$are used so that it allows us to consider only one quarter of the rectangle (square) of the jet, two boundaries of the integration region are formed by symmetry planes.

The flow under consideration can be represented in physical coordinates in the following form[25 − 28,30].

Continuity equation for a mixture of gases

$$\frac{\partial \rho u}{\partial x}+\frac{\partial \rho \vartheta}{\partial y}+\frac{\partial \rho \omega}{\partial z}=0\,. \tag{1}$$

Equation of motion along the coordinate $x$

$$\rho u\frac{\partial u}{\partial x}+\rho \vartheta \frac{\partial u}{\partial y}+\rho \omega \frac{\partial u}{\partial z}=-\frac{\partial P}{\partial x}+\frac{\partial}{\partial y}\left(\mu\frac{\partial u}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mu\frac{\partial u}{\partial z}\right). \tag{2}$$

Equation of motion along the coordinate $y$

$$\rho u\frac{\partial \vartheta}{\partial x}+\rho \vartheta \frac{\partial \vartheta}{\partial y}+\rho \omega \frac{\partial \vartheta}{\partial z}==-\frac{\partial P}{\partial y}+\frac{4}{3}\frac{\partial}{\partial y}\left(\mu\frac{\partial \vartheta}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mu\frac{\partial \vartheta}{\partial z}\right)-\frac{2}{3}\frac{\partial}{\partial y}\left(\mu\frac{\partial \omega}{\partial z}\right)+\frac{\partial}{\partial z}\left(\mu\frac{\partial \omega}{\partial y}\right). \tag{3}$$

Equation of motion along the coordinate $z$

$$\rho u\frac{\partial \omega}{\partial x}+\rho \vartheta \frac{\partial \omega}{\partial y}+\rho \omega \frac{\partial \omega}{\partial z}=-\frac{\partial P}{\partial z}+\frac{4}{3}\frac{\partial}{\partial z}\left(\mu\frac{\partial \omega}{\partial z}\right)+\frac{\partial}{\partial y}\left(\mu\frac{\partial \omega}{\partial y}\right)+\frac{\partial}{\partial y}\left(\mu\frac{\partial \vartheta}{\partial z}\right)-\frac{2}{3}\frac{\partial}{\partial z}\left(\mu\frac{\partial \vartheta}{\partial y}\right). \tag{4}$$

Energy transfer equation (total enthalpy)

$$\rho u\frac{\partial H}{\partial x}+\rho \vartheta \frac{\partial H}{\partial y}+\rho \omega \frac{\partial H}{\partial z}=\frac{1}{Pr}\frac{\partial}{\partial y}\left(\mu\frac{\partial H}{\partial y}\right)+\frac{1}{Pr}\frac{\partial}{\partial z}\left(\mu\frac{\partial H}{\partial z}\right)+Q_{DIS}\,, \tag{5}$$

where $Q_{DIS}=\left(1-\frac{1}{Pr_T}\right)\left[\frac{\partial}{\partial y}\left(\mu u\frac{\partial u}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mu u\frac{\partial u}{\partial z}\right)+\frac{\partial}{\partial z}\left(\mu\vartheta\frac{\partial \vartheta}{\partial y}\right)\right]+\frac{\partial}{\partial y}\left(\mu\omega\frac{\partial \omega}{\partial y}\right)+\left(\frac{4}{3}-\frac{1}{Pr_T}\right)\left[\frac{\partial}{\partial y}\left(\mu\vartheta\frac{\partial \vartheta}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mu\omega\frac{\partial \omega}{\partial z}\right)\right]-\frac{\partial}{\partial y}\left(\frac{2}{3}\mu\vartheta\frac{\partial \omega}{\partial z}\right)+\frac{\partial}{\partial z}\left(\mu\vartheta\frac{\partial \omega}{\partial y}\right)+\frac{\partial}{\partial y}\left(\mu\omega\frac{\partial \vartheta}{\partial z}\right)-\frac{\partial}{\partial z}\left(\frac{2}{3}\mu\omega\frac{\partial \vartheta}{\partial y}\right)$.

Concentration equation of *the i-th* component

$$\rho u\frac{\partial C_i}{\partial x}+\rho \vartheta \frac{\partial C_i}{\partial y}+\rho \omega \frac{\partial C_i}{\partial z}=\frac{1}{Sc_T}\frac{\partial}{\partial y}\left(\mu\frac{\partial C_i}{\partial y}\right)+\frac{1}{Sc_T}\frac{\partial}{\partial z}\left(\mu\frac{\partial C_i}{\partial z}\right)+\dot{\omega}_i\,. \tag{6}$$

The equation of state of the gas mixture

$$P=\rho TR\sum_{i=1}^{N_k}\frac{C_i}{m_i}\quad. \tag{7}$$

Here the total enthalpy *H* is expressed by the equality

$$H=C_PT+\frac{u^2+\vartheta^2+\omega^2}{2}+\sum_{i=1}^{N_K}C_ih_i^*\,. \tag{8}$$

Here, $u,\vartheta,\omega$ −respectively, the velocity along the axis is the $ox, oy, oz$; $\rho, P, T$ −density, pressure and temperature of the mixture, $Pr_T, Sc_T$ −the turbulent Prandt and Schmidt numbers;$R$ − universal gas constant; $\mu$ −coefficient of effective turbulent viscosity; $H$ is the total enthalpy, $C_P$ −heat capacity of the mixture at constant pressure; $C_i, m_i, h_i^*$ −respectively concentration, molecular weight, heat of formation of the $i$ − ойcomponent.

To close the system of equations ( $1-8$), it is necessary to set expressions for the coefficient of effective turbulent viscosity $\mu$and the rate of formation of the -th component $\dot{\omega}_i$ . A modified semi-empirical model for the effective viscosity coefficient is used, which has the form

$$\mu=\mu_e+æ\rho\left(f^2(y)+f^2(z)\right)\sqrt{\left(\frac{\partial u}{\partial y}\right)^2+\left(\frac{\partial u}{\partial z}\right)^2+\left(\frac{\partial \omega}{\partial y}\right)^2}\cdot\left(\frac{T}{T_2}\right)^{\alpha} \tag{9}$$

where æ and α are empirical constants.

## INITIAL AND BOUNDARY CONDITIONS

The system of differential equations (1 −6) with relations (7 −9) completely determines the phenomena that occur when a jet of reacting gas flows out of a rectangular nozzle and propagates in a cocurrent (flooded) air flow, if the initial and boundary conditions are attached to this system of equations, which determine the unique solution of the stated problem, i.e. characteristic of the free jet problem.
The boundary conditions for the problem under consideration, taking into account the above assumptions, will take the following form:

I. $x = 0$: 1)$0 \le y \le a,\ 0 \le z \le b; u = u_2, \vartheta = 0, \omega = 0, H = H_2,$

$$P = P_2, C_i = (C_i)_2, i = \overline{1, N_k}\,. \tag{10}$$

2) $a < y < y_{+\infty}, b < z < z_{+\infty}; u = u_1, \vartheta = 0, \omega = 0, H = H_1,$

$P = P_1, C_i = (C_i)_1, i = \overline{1, N_k}$ .

II. $x > 0$: 1) $z = 0, 0 < y < y_{+\infty}$;

$$\frac{\partial u}{\partial z} = 0, \frac{\partial \vartheta}{\partial z} = 0, \omega = 0, \frac{\partial H}{\partial z} = 0, \frac{\partial C_i}{\partial z} = 0, , i = \overline{1, N_k}\ . \tag{11}$$

2)$y = 0, 0 < z < z_{+\infty}$; $\frac{\partial u}{\partial y} = 0, \vartheta = 0, \frac{\partial \omega}{\partial y} = 0, \frac{\partial H}{\partial y} = 0, \frac{\partial C_i}{\partial y} = 0, i = \overline{1, N_k}$

3) $z = 0,\ y = 0$; $\frac{\partial u}{\partial y} = \frac{\partial u}{\partial z} = \frac{\partial H}{\partial y} = \frac{\partial H}{\partial z} = \vartheta = \omega = 0$

4) $z \to z_{+\infty}, y \to y_{+\infty}\ u = u_1, \vartheta = 0, \omega = 0, H = H_1, P = P_1, C_i = (C_i)_1$

Here index 2 means that the value refers to the parameter of the main jet, 1(st) jet.

## TRANSFORMATION OF THE SYSTEM OF EQUATIONS

The use of a dimensionless form of writing the initial equations and boundary conditions can significantly reduce the degree of specification of the problem being solved. On the other hand, which is important from the point of view of the rational organization of calculations, it must be taken into account that with a reasonable and justified choice of scales, the use of a dimensionless form makes it possible to bring all variables to a single scale, which significantly increases the accuracy of calculations on a computer carried out with a finite number of significant digits. The relationship between dimensional and dimensionless quantities has the form:

$$\overline{x} = \frac{x}{b}, \overline{y} = \frac{y}{b}, \overline{z} = \frac{z}{b}, \overline{u} = \frac{u}{u_2}, \vartheta = \frac{\vartheta}{u_2}, \overline{\omega} = \frac{\omega}{u_2}, \overline{\rho} = \frac{\rho}{\rho_2}, \overline{T} = \frac{T}{u_2^2/\left(R/m_1\right)},$$

$$\overline{P} = \frac{P}{\rho_2 u_2^2}, \overline{H} = \frac{H}{u_2^2}, \mu = \frac{\mu}{\rho_2 u_2 b}, \overline{C}_P = \frac{C_P}{R/m_1}, \overline{h_i} = h_i^* \Big/ u_2^2, \overline{\dot{\omega}} = \overline{\dot{\omega}_\iota}/(\rho_2 u_2/b)$$

For the convenience of numerical implementation, we transform the outlet section of the nozzle into a square one using the analytical transformation

$$y = \overline{y}/L \tag{12}$$

where $L = a/b$, $y$ −is assumed to be dimensionless below.

In this work, we use a model of diffusion combustion of non-displaced gases, that the reaction proceeds in the zone of contact between the fuel and the oxidizer.

From the point of view of mathematical calculation, we consider a four-component mixture of gases in the displacement zone, consisting of oxygen $O_2$ - index “1”, a mixture of propane-butane ( $C_3H_8 + C_4H_{10}$ ) - “2”, combustion products $CO_2 + 9\,H_2O$ - “3”, inert gas $N_2$ - “4”.
Using the conservative Schwab-Zeldovich function [1,9,31]with respect to excess concentrations

$$\tilde{\tilde{C}} = \frac{\tilde{C}_i - \left(\tilde{C}_i\right)_1}{\left(\tilde{C}_i\right)_2 - \left(\tilde{C}_i\right)}\ , \qquad i = \overline{1 \div 3} \tag{13}$$

does not change the form of the equation

$$\rho u \frac{\partial \tilde{C}_i}{\partial x} + \rho \vartheta \frac{1}{L} \frac{\partial \tilde{C}_i}{\partial y} + \rho \omega \frac{\partial \tilde{C}_i}{\partial z} = \frac{1}{Sc_T} \frac{1}{L^2} \frac{\partial}{\partial y}\left(\mu \frac{\partial \tilde{C}_i}{\partial y}\right) + \frac{1}{Sc_T} \frac{\partial}{\partial z}\left(\mu \frac{\partial \tilde{C}_i}{\partial z}\right) \tag{14}$$

where

$$\tilde{C}_i = C_i \nu_3 m_3 + C_3 \nu_i m_i \tag{15}$$

and get

$$\rho u \frac{\partial \tilde{\tilde{C}}}{\partial x} + \rho \vartheta \frac{1}{L} \frac{\partial \tilde{\tilde{C}}}{\partial y} + \rho \omega \frac{\partial \tilde{\tilde{C}}}{\partial z} = \frac{1}{Sc_T} \frac{1}{L^2} \frac{\partial}{\partial y} \left( \mu \frac{\partial \tilde{\tilde{C}}}{\partial y} \right) + \frac{1}{Sc_T} \frac{\partial}{\partial z} \left( \mu \frac{\partial \tilde{\tilde{C}}}{\partial z} \right) \tag{16}$$

In equality (15) $\nu_i$ are stoichiometric coefficients $i$(th) components. Function $\tilde{C}$takes the value 1 in the fuel nozzle exit, and 0 in the oxidizer zone (here the second indices indicate that this value belongs to the air nozzle exit -1 or fuel -2). The introduction of function (13) makes it possible to release the axis of the source term $\dot{\omega}$in the diffusion equation (6) and reduces the number of diffusion equations to one for a four-component mixture (16).

## SOLUTION METHOD AND CALCULATION ALGORITHM

When calculating three-dimensional free jet flows, the pressure gradient in the longitudinal direction can be neglected. Such a situation arises when a subsonic free jet flows through a rectangular nozzle into a medium that is either at rest or moves in the direction of the nozzle axis. The shape of such a jet in cross section gradually changes in the longitudinal direction and, finally, becomes round. For such flows, it is reasonable to assume that the pressure gradient in the longitudinal plane and its small changes in the transverse plane are neglected, which sometimes makes it possible to carry out calculations without taking pressure into account.

For numerical integration of the system of equations ( $1-8,16$) with initial and boundary conditions ($10 \div 11$), we use a two-layer ten-point implicit finite-difference scheme. Figure 1 shows the scheme and grid designations. The area under consideration is covered with a grid $x = i\Delta x, y = j\Delta y, z = k\Delta z$. In this case, the indices $i, j, k$will denote the numbers of nodes along the coordinate axes $x, y, z$. Finite-difference analogues of individual terms of equations ($1-5,16$) are written with an accuracy of $O(\Delta x, \Delta y^2, \Delta z^2)$.

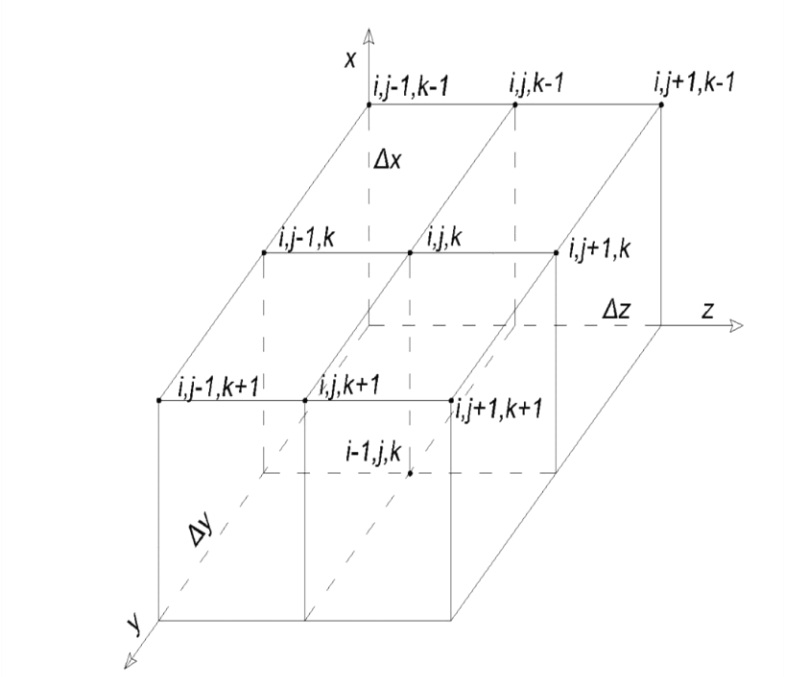


**Figure 1.** Finite difference scheme and grid notation.

Difference analogues of terms $A\frac{\partial F}{\partial z}$ , $\frac{\partial}{\partial z}\left(A\frac{\partial F}{\partial z}\right)$, $\frac{\partial}{\partial y}\left(A\frac{\partial F}{\partial z}\right)$, $\frac{\partial}{\partial z}\left(A\frac{\partial F}{\partial y}\right)$

contain unknowns and in cross section $(\mathrm{k}+1)$, i. e. along the axis $z$, and this, in turn, does not allow using simpler solution approaches. As explicit values ( $A$ and $F$ )$A_{i,j,k+1}^{(S)}$ и $F_{i,j,k+1}^{(S+1)}$ for jet streams, one can take the values of the co -current (flooded) flow, and this allows using a two-layer six -point difference scheme of the Crank-Nicolson type in each fixed plane along the [34]*x axis* . The results of numerical studies have shown that, if expressed $F_{i,j,k+1}^{(S+1)}$ as

$$F_{i,j,\mathrm{k}+1}^{(S+1)} = F_{i,j,\mathrm{k}+1}^{(S)} \qquad \left(or\ F_{i,j,\mathrm{k}+1}^{(S+1)} = F_{\mathrm{BH}}\right) \tag{17}$$

then this does not affect the convergence and the reliability of the results (the $F_{\mathrm{BH}}$ −external value of the parameters, the parameters of the cocurrent flow)

The use of finite-difference analogues of differentials makes it possible to write the equations of momentum (2 −4), energy (15), concentration (16) taking into account the boundary conditions

$$\frac{\partial F}{\partial y} = 0, \left(F = u, \vartheta, \omega, H, \tilde{\tilde{C}}\right) \tag{18}$$

$$F = F_{\mathrm{BH}} \tag{19}$$

into a system of finite difference equations as follows:

$$\begin{cases} B_{i,1,\mathrm{k}}^{(S)}\ F_{i,1,\mathrm{k}}^{(S+1)} + C_{i,1,\mathrm{k}}^{(S)}\ F_{i,1,\mathrm{k}}^{(S+1)} = E_{i,1,\mathrm{k}}^{(S)}\ , j = 1 \\ A_{i,j,k}^{(S)}\ F_{i,j-1,\mathrm{k}}^{(S+1)} + B_{i,j,\mathrm{k}}^{(S)}\ F_{i,j,\mathrm{k}}^{(S+1)} + C_{i,j,\mathrm{k}}^{(S)}\ F_{i,j+1,\mathrm{k}}^{(S+1)} = E_{i,j,\mathrm{k}}^{(S)}\ , j = \overline{2, Ny-1} \\ F_{Ny}^{(S+1)} = F_{\mathrm{BH}}\ . \end{cases} \text{ (twenty)}$$

Here$A_{i,j,\mathrm{к}}^{(S)}$ , $B_{i,j,\mathrm{к}}^{(S)}$ , $C_{i,j,\mathrm{к}}^{(S)}$ , $E_{i,j,\mathrm{к}}^{(S)}$ - non-linear coefficients, which are determined at ( $S$ + 1)th stage of iteration by known values of unknown variables $u_{ijk}^{(S)}, \vartheta_{ijk}^{(S)}, \omega_{ijk}^{(S)}, \rho_{ijk}^{(S)}, P_{ijk}^{(S)}, H_{ijk}^{(S)}, \tilde{\tilde{C}}_{ijk}^{(S)}$, here $(S) -$ iteration.

The coefficients of the first equation (20), $B_{i,1,\mathrm{k}}^{(S)}$ , $\mathrm{C}_{i,1,k}^{(S)}$ and $\mathrm{E}_{i,1,\mathrm{k}}^{(S)}$ are determined from the boundary conditions for F. For example, if a condition like (19) is used, then from the difference analogue we find (for $j$ =1)

$$C_{i,1,\mathrm{к}}^{(S)} = -1, \quad B_{i,1,\mathrm{к}}^{(S)} = 1, \qquad E_{i,1,\mathrm{к}}^{(S)} = 0\ , \tag{21}$$

here $j$ =1 means the beginning of the calculated point along the *y axis.*

The system of equations (20) with a three diagonal matrix is reduced to the upper triangular form by changing the coefficients according to the formula [34].

$$B_{i,j,\mathrm{к}}^{(S)} = B_{i,j,\mathrm{к}}^{(S)} - \frac{A_{i,j,\mathrm{к}}^{(S)}}{B_{i,j-1,\mathrm{к}}^{(S)}} C_{i,j-1,\mathrm{к}}^{(S)}\ , j = \overline{2, Ny-1} \tag{22}$$

a $E_{i,j,\mathrm{к}}^{(S)}$ , as

$$E_{i,j,\mathrm{к}}^{(S)} = E_{i,j,\mathrm{к}}^{(S)} - \frac{A_{i,j,\mathrm{к}}^{(S)}}{B_{i,j-1,\mathrm{к}}^{(S)}} E_{i,j-1,\mathrm{к}}^{(S)}\ ,\ j = \overline{2, Ny-1} \tag{23}$$

After that, starting from the known value $F_{Ny}^{(S+1)}$, the reverse substitution of values is carried out to calculate the unknowns $F_{ijk}^{(S+1)}$by the formula

$$F_{ijk}^{(S+1)} = \left(E_{i,j,\mathrm{к}}^{(S)} - C_{i,1,\mathrm{к}}^{(S)}\ F_{i,j+1,k}^{(S+1)}\right)/B_{i,j,\mathrm{к}}^{(S)}\ ,\quad j = \overline{2, Ny-1} \tag{23}$$

The type of the equation of momentum, energy and concentration (2-5,16) is completely parabolic [35] and it is possible to obtain a solution using the marching procedure, respectively, by the direction of the axis $x, y, z$ to define $u, \vartheta, \omega, H, \tilde{\tilde{C}}$.

Obtained preliminary solutions $u, \vartheta, \omega$in the plane of the cross section $x$ usually do not satisfy the continuity equation [25,26], written in difference form. Therefore, supposedly, the extra continuity equation (1) is used to calculate the mass imbalance at each calculated grid point ( $i, j, k$).

The solution found $u, \vartheta, \omega$in the iteration (S +1) is expressed as calculated $(u_P, \vartheta_P, \omega_P)$and plus correction $(u_C, \vartheta_C, \omega_C)$in the form

$$u = u_C + u_P, \quad \vartheta = \vartheta_C + \vartheta_P, \qquad \omega = \omega_C + \omega_P \tag{24}$$

The question is how to determine in each ( $i, j, k$) space $u_C, \vartheta_C, \omega_C$ ? The corrected velocities must satisfy the continuity equation (1), i.e.

$$\frac{\partial \rho(u_P + u_C)}{\partial x} + \frac{1}{L}\frac{\partial \rho(\vartheta_P + \vartheta_C)}{\partial y} + \frac{\partial \rho(\omega_P + \omega_C)}{\partial z} = 0. \quad (25)$$

We transform the last equation in the form

$$\frac{\partial \rho u_C}{\partial x} + \frac{1}{L}\frac{\partial \rho \vartheta_C}{\partial y} + \frac{\partial \rho \omega_C}{\partial z} = -\left(\frac{\partial \rho u_P}{\partial x} + \frac{1}{L}\frac{\partial \rho \vartheta_P}{\partial y} + \frac{\partial \rho \omega_P}{\partial z}\right) = Q_p\,. \quad (26)$$

Let us define the potential f:

$$\rho u_C = \frac{\partial \phi}{\partial x}, \rho \vartheta_C = \frac{\partial \phi}{\partial y}\,, \rho \omega_C = \frac{\partial \phi}{\partial z}, \quad (27)$$

then from (26) we obtain the Poisson equation

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{L\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} = Q_P. \quad (28)$$

The desired corrections to the velocity (27) can be calculated from the distribution φ obtained from the solution of equation (28) in the transverse plane.

The corresponding difference equation (28) has the form

$$\frac{\phi_{i+1,j,k} - 2\phi_{i,j,k} + \phi_{i-1,j,k}}{\Delta x^2} + \frac{\phi_{i,j+1,k} - 2\phi_{i,j,k} + \phi_{i,j-1,k}}{L\Delta y^2} + \frac{\phi_{i,j,k+1} - 2\phi_{i,j,k} + \phi_{i,j,k-1}}{\Delta z^2} = (Q_P)_{i,j,k}\,. \quad (29)$$

Such an algebraic equation can be written for the potential Øat each point of the grid across the flow in the plane along ($i$) and thus has a tridiagonal system of equations, provided that the values are known

$$\phi_{i-1,j,k}\ ,\quad \phi_{i+1,j,k}\ ,\ \phi_{i,j,k+1}\ ,\ \phi_{i,j,k-1}\,.$$

Equation (29) can be solved under the following reasonable assumptions:

1) $\phi_{i-1,j,k} = 0, \phi_{i,j,k-1} = 0$ - mean that the corrections to the velocity are equal to zero in the plane ( $i - 1$) and in the section (k-1), in which the conservation of mass is already ensured.
2) $\phi_{i+1,j,k} = 0\,, \phi_{i,j,k+1} = 0$ - mean that the corrections to the velocity are equal to zero both in the plane ( $i +$ 1) and in the section (k +1), when their convergence in this plane and in the section (k + 1) is obtained, respectively. These assumptions allow us to reduce the system of algebraic equations (29) to the solution of a tridiagonal system with respect to φ :

$$\frac{1}{\mathrm{L}\Delta y^2}\phi_{i,j-1,k} + 2\left(-\frac{1}{\Delta x^2} - \frac{1}{\mathrm{L}\Delta y^2} - \frac{1}{\Delta z^2}\right)\phi_{i,j,k} + \frac{1}{\mathrm{L}\Delta y^2}\phi_{i,j+1,k} = (Q_P)_{i,j,k}\,. \quad (30)$$

The boundary conditions necessary for solving the system of equations (30) are chosen so that they are consistent with the given boundary conditions for the velocity (11).

As can be seen from the boundary condition (11), if the velocities of the external flow are known in advance, then φ will be equal to zero at this boundary, i.e.

$$\phi_{i,Ny+1,k} = 0\,. \quad (31)$$

On the plane of symmetry at $y = 0, 0 < z < z_{+\infty}$, in order for condition (11) item 2) to be satisfied, the condition

$$\phi_{i,1,k} = \phi_{i,2,k} \quad (32)$$

Now, having the lower (32) and upper (31) boundary conditions, with the help of a scalar sweep [34] over all $j$ ($j = \overline{1, Ny}$) we find $\phi_{i,j,k}$. Once $\phi_{i,j,k}$ found, we determine the corrections to the velocity using difference approximations of expressions (27), taking into account assumption 1, namely:

$$\begin{cases} (u_C)_{ijk} = \dfrac{\phi_{ijk}}{\Delta x\ \rho_{ijk}^{(S)}}, (\omega_C)_{ijk=} \dfrac{\phi_{ijk}}{\Delta z\ \rho_{ijk}^{(S)}}, (\vartheta_C)_{ijk} = \dfrac{\phi_{i,j+1,k} - \phi_{i,j-1,k}}{2\ \Delta y\ \rho_{ijk}^{(S)}}. \end{cases} \quad (33)$$

$$\begin{cases} (u)^{(s+1)}{}_{ijk} = \left(u_p\right)_{ijk} + \dfrac{\phi_{ijk}}{\Delta x\ \rho_{ijk}^{(S)}},\ (\omega_C)^{(s+1)}{}_{ijk} = \left(\omega_p\right)_{ijk} + \dfrac{\phi_{ijk}}{\Delta z\ \rho_{ijk}^{(S)}}, \\ (\vartheta)^{(s+1)}{}_{ijk} = \left(\vartheta_p\right)_{ijk} + \dfrac{\phi_{i,j+1,k} - \phi_{i,j-1,k}}{2\ \Delta y\ \rho_{ijk}^{(S)}}. \end{cases} \quad (34)$$

Now the corrected velocities (34) satisfy the continuity equation at each point of the section ( $k$) in the plane ( $i$), but do not exactly satisfy the equation of motion and other equations of the system (2 $-5,16$) until convergence is achieved.

The iteration for finding a solution to the system of equations (4 $-4; 5-9, 16$) for a fixed plane ( $i$) with a section ( k ) at $j= \overline{1, Ny}$ is repeated until the convergence condition is satisfied

$$\left|F_{i,j,k}^{(s+1)} - F_{i,j,k}^{(s)}\right| \le \delta_F^{(1)} \tag{35}$$

Where $F$ can be the value of the unknowns $u, \vartheta, \omega$ and H, $\tilde{\tilde{c}}$; $\delta_F^{(1)}$- a small number characterizing the accuracy of the calculation.

## LET US FORMULATE A DETAILED CALCULATION ALGORITHM

1) On each computational plane $yOz$ along the axis direction, the $Ox$ values of the unknowns from the previous plane are initially set as the first approximations of the unknowns ( S ) - iteration (index $i$=1 corresponds to the input conditions (10));

2) The difference equation of motion along the axis is solved $x$, is found $\left(u_p\right)_{ijk}$(on each new calculation plane along the axis of the $x$ solution of the equation system begins with k=2, and k=1 corresponds to the plane of symmetry);

3) The difference equation of motion along the axis is solved $y$and the$\left(\vartheta_p\right)_{ijk}$ using value $\left(u_p\right)_{ijk}$;

4) The difference equation of motion along the axis is solved $z$and the$\left(\omega_p\right)_{ijk}$ using the value $\left(u_p\right)_{ijk}$ and $\left(\vartheta_p\right)_{ijk}$;

5) The system of equations (30) is solved and the corrected speeds are calculated using formula (34);

6) The corrected values of velocity (34) solve the equations of energy and concentration, respectively,$H_{i,j,k}^{(s+1)}$ , $\tilde{\tilde{C}}_{i,j,k}^{(s+1)}$

7) The values of individual components are calculated $C_i$[2,31]. The condition $\tilde{\tilde{C}} > \tilde{\tilde{C}}_\Phi$corresponds to the fuel region, $0 \le L(y,z) < L_\Phi(y,z)$, the concentrations of the components $C_{i,j,k}^{(s+1)}$ are defined as

$\left\{C_1 = 0\,, C_2 = \tilde{\tilde{C}}((C_2)_2 + (C_1)_1 A) - A(C_1)_1, C_3 = (C_1)_1 A\left(1 - \tilde{\tilde{C}}\right)\right.$,where $A = \nu_3 m_3/(\nu_1 m_1)$

and for the oxidizer zone, where the condition $\tilde{\tilde{C}} < \tilde{\tilde{C}}_\Phi$, $(L(y,z) > L_\Phi(y,z))$;

$\left\{C_2 = 0\,, C_1 = ((C_1)_1 + B(C_2)_2)\tilde{\tilde{C}},\ C_3 = B(C_2)_2\tilde{\tilde{C}}\right.$, where $B = \nu_3 m_3/(\nu_2 m_2)$.

The index ϕ- indicates the values at the flame front, $L_\Phi$- the line of the torch. For an inert gas $N_2$, its distribution relative to the excess concentration and the boundary conditions will be the same as for $\tilde{\tilde{c}}$, therefore

$$C_4 = (C_4)_1 + ((C_4)_1 - (C_4)_2)\tilde{\tilde{C}}.$$

8) The temperature is calculated $T_{i,j,k}^{(s+1)}$from relation (8), and then the density $\rho_{i,j,k}^{(s+1)}$from the equation of state (7);

9) The effective turbulent viscosity is calculated $\hat{\mu}_{i,j,k}^{(s+1)}$according to the formula (9), while the values $b(y)$and $b(z)$are defined as $b(y) = L \cdot NY\Delta y\,, b(z) = NZ\Delta z$ . $(NY, NZ -$ number of points along the axis $Y$ and $Z)$.

10) The convergence of the iteration by condition (35) is checked. If this condition is not met, then the solution is averaged,

$$F_{i,j,k}^{(s)} = \left(F_{i,j,k}^{(s)} + F_{i,j,k}^{(s+1)}\right)/2\ , \quad (F = u, \vartheta, \omega, H)$$

and these decisions are taken as the values of the previous iteration, i.e. ( S )-th and the calculation process is repeated from the 2nd step.

Otherwise, the condition is checked

$$\max_k \left|F_{i,j,k}^{(s+1)} - F_{BH}\right| > \delta_F^{(2)} \tag{36}$$

$\delta_F^{(2)}$- a small positive number characterizing the accuracy of convergence. If condition (36) is satisfied, then the number of calculated points along the axis $y$is increased by one calculated point according to the recursive relation

$$Ny = Ny + 1 \tag{37}$$

and again the calculations continue from the 2nd step.

If condition (36) is not satisfied, then it is considered that the solutions of the system of equations on the plane ( $i$) in the section (k) are found.

Condition (37) characterizes the growth of the computational domain, i.e. jet boundary $y$propagation along the axis :

11) The condition of growing the computational domain along the axis is checked $OZ$.

$$\max_j \left|F_{i,j,k}^{(s+1)} - F_{BH}\right| > \delta_F^{(3)} \quad (38)$$

где $\delta_F^{(3)}$ is a small positive number.

If condition (38) is met, then the number of calculated points along the Z axis is increased by one calculated point according to the recursive relation $Nz = Nz + 1$.

(the value (k) increases by one), then we go to the section (k + 1) and again the calculation continues from the 2nd step.

If condition (38) is not satisfied, then the solution on the plane ( $i$) has been found and it is necessary to move to the next plane along the longitudinal coordinate $x$ . Having performed, $F_{i,j,k}^{(S)} = F_{i,j,k}^{(S+1)}$( F - unknown unknowns) the calculation process is repeated from the 2nd stage.

## NUMERICAL RESULTS

The first step was to check the reliability of the developed methodology. Considered is a free air jet flowing from a rectangular nozzle borrowed from [17], which is the ratio of the lengths of the sides (2:1) and (3:1), from the speed of the main flow $u_2$=38 m / s, and satellite $u_1$ =0, temperature $T_1$=$T_2$=300 K.

On fig. Figure 2 shows a comparison of the experimental and calculated data on the distribution of the momentum flux density in the jet cross sections (x=2), which confirms the validity of the

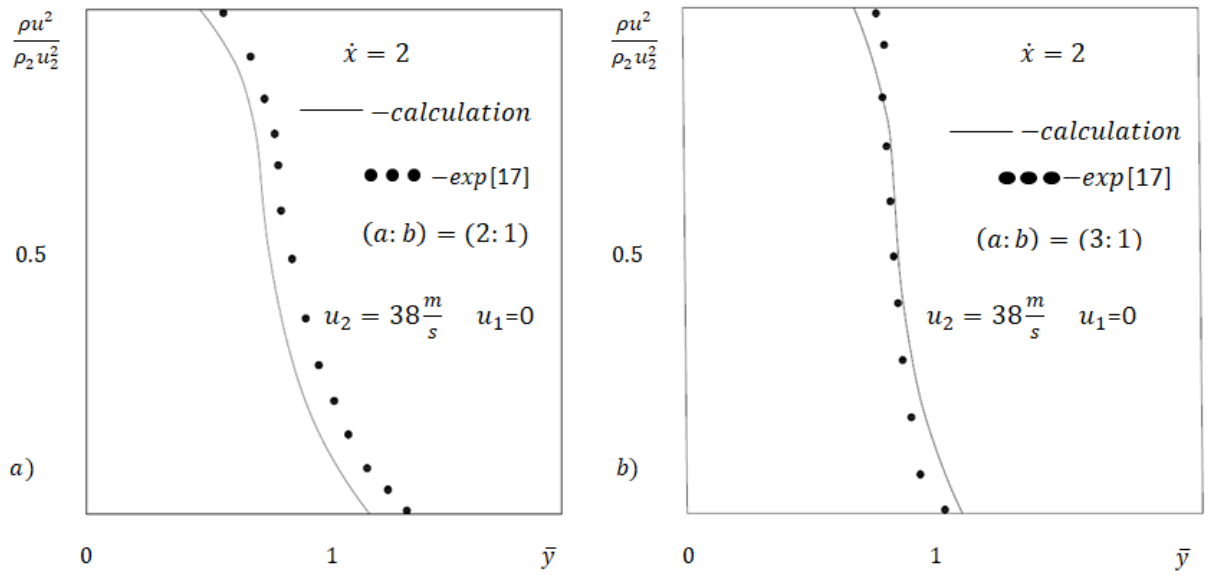


**Figure 2.** Comparison of experimental and calculated data on the distribution of the momentum flux density in the cross sections of the jet flowing from the nozzle by the aspect ratio a) (2:1); b) (3:1).

numerical results obtained by sufficient agreement of the results. These results were obtained with empirical constants æ =0.01, α=0.5 and Pr =0.7.

As an example, the combustion of a mixture of propane-butane in air was calculated, where the options for the initial values of the parameters were taken from [5,9].

I. Oxidizer zone.
$T_1$= 300K; $u_1$= 0;
$(C_1)_1 = 0{,}232$; $(C_2)_1 = 0$;
$(C_3)_1 = 0$; $(C_4)_1 = 0{,}768$;

II. Fuel zone:
$T_2$= 1200K; $u_2$= 61 $m/s$;
$(C_1)_2 = 0$; $(C_2)_2 = 0{,}12$;
$(C_3)_2 = 0$; $(C_4)_2 = 0{,}88$;

$Pr_T = Sc_T = 0.65; P_1 = P_2 = 1$ атм; $(a:b) = (1:1)$.
The heat of formation of the oxidizer, reaction product and inert gas is taken equal to zero $h_1^* = h_3^* = h_4^*$= 0, and the fuel $h_2^*$ =11490 kcal/kg [9].

The main numerical results of the calculations are given in the form of graphs in Fig. 2(a,b), 3(a,b). So, Fig. 3(a,b) shows the shape of the torch at different temperatures of the oxidizer $T_1 = 300$K, $T_1$ =500K. These results show that a decrease in the value of the empirical constant æin expression (9) leads to an increase in the length of the torch, and an increase value æleads to a decrease in its length. In addition, the width of the torch also narrows. The results are shown in fig. 3(a, b) also confirm what was found in the experimental study [5].

When using an algebraic model for the turbulent viscosity coefficient (9) for multicomponent chemical reactions, it is necessary to choose an empirical constant æso that the results obtained correspond to the experimental (real) data.

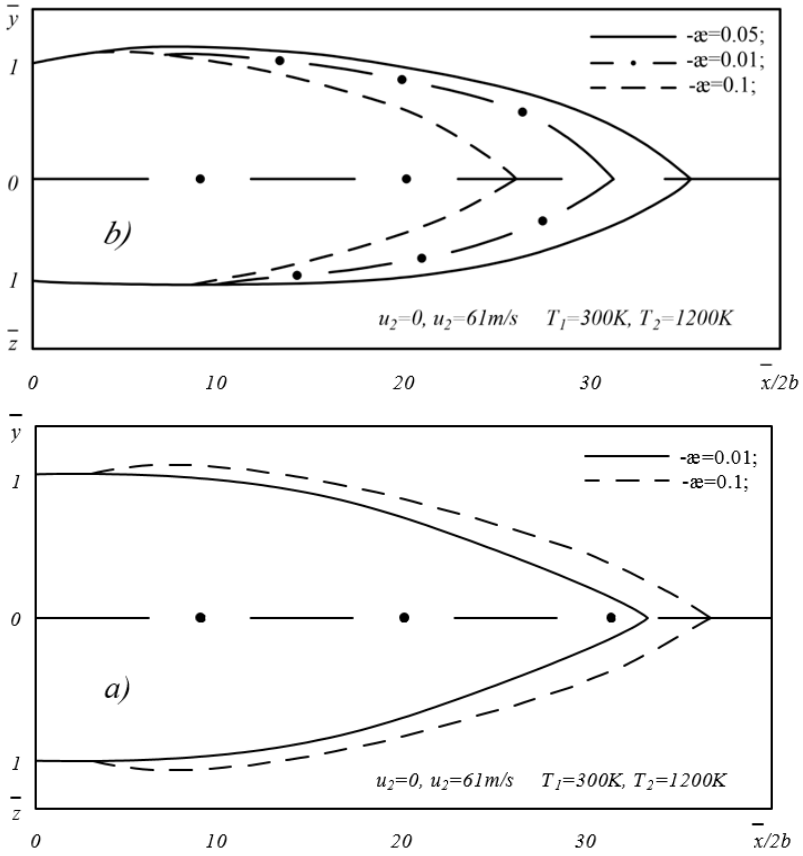


**Figure 3.** Flame configuration at various values

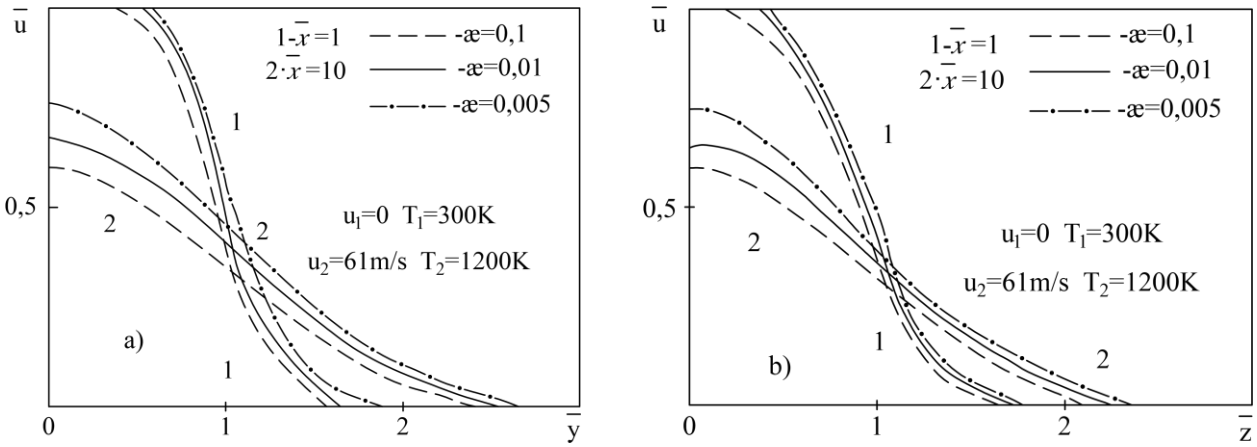


**Figure 4.** Distribution of the longitudinal velocity in different cross sections of the jet; a) long the y axis; b) along the z

With an unreasonable value æ, numerically it is possible to obtain an overestimated length of the torch. For example, the dimensionless length equal is $L_ф = 30$ obtained at a value of $æ = 0{,}005$,and also at $æ = 0{,}01$,but at a higher temperature of the oxidizer.

Comparison of the estimated length of the flame obtained by us and the approximate formula obtained in the framework of the method of the equivalent problem of the theory of heat conduction [5] are consistent at $æ = 0{,}01$, where the length of the flame is $L_ф = 27$.

Figure 4(a,b) shows the longitudinal velocity profiles in different sections of the jet along the y and z axes . It can be seen that at small values of æ, the jet core along the longitudinal axis is noticeably preserved. Comparison of the velocity profiles along the y (Fig. 4(a)) and z (Fig. 4(b)) axes and the flame shape (Fig. 3) shows that in three-dimensional jets and flame, as the distance from the nozzle mouth increases, the flow, accompanied by the transformation of three-dimensional motion into two-dimensional.

The presented method and algorithm of calculation makes it possible to study the effect of the initial parameters of the combustible gas and oxidizer on the parameters of diffusion combustion.

## CONCLUSION

An effective calculation method and algorithm are presented, as well as some numerical results of the study of three-dimensional turbulent jets of reacting gases flowing out of a rectangular nozzle with a finite aspect ratio. For the proposed algebraic model of turbulence, taking into account the three-dimensionality and temperature inhomogeneity of the jet, the empirical constants included in the models for diffusion combustion are numerically refined. Numerically revealed that a decrease in the value of the empirical constant æ (Karman) in the turbulence model leads to an elongation of the flame length, and an increase leads to a decrease in its length. In addition, the width of the torch also narrows. The results show that in three-dimensional jets and flames, as they move away from the mouth of a rectangular nozzle, the flow is restructured, accompanied by the transformation of three-dimensional motion into two-dimensional.

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