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Mathematical Modeling of an Axially Symmetric Turbulent Jet of Gas Mixture During Combustion

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Abstract. This article examines the mixing of propane-butane gases and the formation of a new type of fuel, its diffusion in the free air stream, and its chemical reaction and combustion. to model this process, the equations for reacting gases using Mises coordinates were selected. In this case, the processes created by the interaction and combustion of gases form a turbulent flow. Therefore, the equations of the turbulent boundary layer were made dimensionless and solved based on these equations. The concentration equations for reacting gases are 5. For each of these, it is possible to determine the composition of each gas by solving nonlinear differential equations. In this work, these 5 concentration equations are reduced to 1 nonlinear differential equation. For this, the Schwab-Zeldovich function was used. When solving the equations, 1st-order accuracy was used for the longitudinal coordinate and 2nd-order accuracy for the transverse coordinate. A four-point finite difference scheme was used to approximate the equations. Ensuring complete combustion of gases in gas burners leads to high efficiency and economic savings.
Keywords: combustion, concentration equations, nonlinear differential equations, Mises coordinates, propane-butane gases, Schwab-Zeldovich function, turbulents.

INTRODUCTION

The issues of reaction and combustion of various types of gases were also studied in works [1-7]. In these works, the combustion of methane gas in different modes was considered, and k-e, k-w models were used to determine turbulence.

In [8], a method was proposed for solving problems with discontinuous coefficients based on the application of an exact analytical solution of the equation in a discrete step, taking into account the quadratic characteristic equation of the original parabolic equation. The finite difference equations they constructed for internal and boundary nodes have the usual form for sweeps with frozen coefficients. By the example of the Dirichlet problem for the equation $\frac{\partial u}{\partial x}-\frac{1}{\mathrm{Re}}\frac{\partial^2 u}{\partial x^2}=\sin \pi x$ the advantages of the proposed method are shown. The problem solution for $\mathrm{Re}\to\infty$, when one- and two-sided boundary layers are formed.

The reaction and combustion of gases have been studied in many works. In this, the reaction of methane, propane and other gases with oxygen in the air as the main gases has been studied theoretically [6-15]. The reaction and combustion of gases have been studied in many works. In this, the reaction of methane, propane and other gases with oxygen in the air as the main gases has been studied theoretically. It is impossible to determine these studies experimentally or it requires great difficulties and large funds. Although these combustion issues have been studied for several years, these issues have not yet found their solution. Therefore, in this research work, the issue of the combustion of mixtures of propane and butane gases by reacting with oxygen in the air was considered using modern turbulent models. This model is available in modern package programs, and the authors obtained results for these issues using these models. The reliability of turbulent models is based on the complete representation of the physics of the process.]. It is impossible to determine these studies experimentally or it requires great difficulties and large

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$$\begin{cases} \rho u\frac{\partial k}{\partial x}+\rho\vartheta\frac{\partial k}{\partial r}=\frac{1}{r}\frac{\partial}{\partial r}\left(\rho r\nu_t\frac{\partial k}{\partial r}\right)+G_k-\rho\varepsilon, \\ \rho u\frac{\partial \varepsilon}{\partial x}+\rho\vartheta\frac{\partial \varepsilon}{\partial r}=\frac{1}{1.3r}\frac{\partial}{\partial r}\left(\rho r\nu_t\frac{\partial \varepsilon}{\partial r}\right)+1.44f_1\frac{\varepsilon}{k}G_k-1.92\rho f_2\frac{\varepsilon^2}{k}. \end{cases} \tag{1}$$

$$\nu_t=\frac{c_\mu f_\mu k^2}{\varepsilon},\quad R_R=\frac{\sqrt{k}\,r}{\nu},\quad f_1=1+\left(\frac{A_1}{f_\mu}\right)^3,\quad f_2=1-e^{-R_t^2},\quad R_t=\frac{k^2}{\nu\varepsilon} \tag{2}$$

$$f_\mu=\left(1-e^{-A_\mu R_R}\right)^2\left(1+\frac{A_t}{R_t}\right),\quad \mathrm{G}_k=4\rho\nu_t\left(\frac{\partial u}{\partial r}\right)^2 \tag{3}$$

$$c_\mu=0.09,\quad \delta_k=1, A_1=0.05,\quad A_\mu=0.0165$$

A combustible gas mixture enters through a nozzle with a diameter of 2a and reacts with the oxygen contained in the air. In this case, it was assumed that the combustible gas does not pass into the air zone, and the air does not pass into the fuel zone. The combustion processes were studied assuming that these mixtures retain their properties. In this case, all parameters such as fuel temperature and velocity were taken as component 1. The values of oxygen contained in the air are given by component 2.

THE MATHEMATICAL MODEL OF THE PROBLEM

The form of the system of equations was obtained as follows (2). In this case, the equations were used in a simplified form, assuming that *Le=1*. Prantl and Schmid numbers are equal to each other, i.e. equal to 0.72.

$$\begin{cases} \rho u\frac{\partial u}{\partial x}+\rho v\frac{\partial u}{\partial r}=-\frac{dp}{dx}+\frac{1}{r}\frac{\partial}{\partial r}\left(\rho\nu_t r\frac{\partial u}{\partial r}\right), \\ \frac{\partial(\rho ur)}{\partial x}+\frac{\partial(\rho\vartheta r)}{\partial r}=0, \\ \rho u\frac{\partial H}{\partial x}+\rho v\frac{\partial H}{\partial r}=\frac{1}{\Pr r}\frac{\partial}{\partial r}\left(\rho\nu_t r\frac{\partial}{\partial r}\left(H-(1-\Pr)\frac{u^2}{2}\right)\right), \\ \rho u\frac{\partial c_k}{\partial x}+\rho v\frac{\partial c_k}{\partial r}=\frac{1}{\mathrm{Sc}\, r}\frac{\partial}{\partial r}\left(\rho\nu_t r\frac{\partial c_k}{\partial r}\right)+\omega_k,\quad (k=1..N); \end{cases} \tag{4}$$

The equation of state was obtained as follows.

$$p=\rho R_0 T/m \tag{5}$$

$$H=c_pT+\frac{U^2}{2}+\sum_{k=1}^{N}c_k h_k^* \tag{6}$$

where $c_p=\sum_{k=1}^{N}c_{pk}c_k a$ and c_{pk} – the heat capacity of the gas mixture and $k-$ component at constant pressure $\left(Dj\ kg^{-1}\ K^{-1}\right)$; $U^2/2=\left(u^2+v^2\right)/2$ – kinetic energy of a gas mixture of unit mass in the approximation of the theory of a boundary layer; h_k^* –calorific value of the k-st component $\left(Dj\ kg^{-1}\right)$.

The boundary conditions of the problem for the input section $x=0$ are set in the following form:

$$\text{at } 0 \le r \le a: \; u(0,r)=u_2, \;\; T(0,r)=T_2, \;\; c_k(0,r)=\left(c_k\right)_2;$$

$$\text{at } a \le r \le r_\infty: \; u(0,r)=u_1, \;\; T(0,r)=T_1, \;\; c_k(0,r)=\left(c_k\right)_1.$$

At $x>0$ no leakage conditions are set on the axis of the jet:

$\frac{\partial u(x,0)}{\partial r}=0, \;\; \frac{\partial T(x,0)}{\partial r}=0, \;\; \frac{\partial c_k(x,0)}{\partial r}=0, \;\; \vartheta(x,0)=0$ a at the jet boundary $r=b(x)$ – according to the indicators of the satellite flow: $u(0,r)=u_1, \;\; T(0,r)=T_1, \;\; c_k(0,r)=\left(c_k\right)_1$ The boundary conditions for the total enthalpy are determined according to formula (4).

A WAY TO BRING THE EQUATIONS OF CONSERVATION OF COMPONENTS TO A SINGLE EQUATION

The problem of the distribution and combustion of a mixture of propane-butane mixture in a satellite air stream is considered. We believe that in a combustible mixture propane and butane have equal concentrations. In this case, the stoichiometric equation of the process can be written as

$$v_2 A + v_1 O_2 \rightarrow v_3 CO_2 + v_4 H_2 O + h_2^*,$$

where are the stoichiometric coefficients $\nu_1 = 5.75, \; \nu_2 = 1, \; \nu_3 = 3.5, \; \nu_4 = 4.0$, include oxygen, fuel, carbon monoxide and water vapor, $h_2^* = 45000$ *kdj/kg*.

$$L(c_k) = \omega_k, \qquad k = 1..5 \tag{7}$$

Where $L(c_k) = \rho u \frac{\partial c_k}{\partial x} + \rho \vartheta \frac{\partial c_k}{\partial r} - \frac{1}{Sc\, r} \frac{\partial}{\partial r}\left(\rho \nu_t r \frac{\partial c_k}{\partial r}\right)$ – The concentration of each of the 5 components involved in the reaction is found using this formula. The nitrogen gas involved in the mixture is taken unchanged. This rule was used for each component.

$$\begin{aligned} &\omega_3 \nu_k m_k + \omega_k \nu_3 m_3 = 0 \;\; \text{at} \;\; k=1,2; \\ &\omega_3 \nu_k m_k - \omega_k \nu_3 m_3 = 0 \;\; \text{at} \;\; k=4; \end{aligned} \tag{8}$$

where did $\omega_1, \; \omega_2 \le 0, \; \omega_3, \; \omega_4 \ge 0$.

The above dependences indicate the way by which one can get rid of the rates of a chemical reaction in the equations of conservation of components (5). If we introduce the Schwab-Zeldovich functions according to (6),

$$\tilde{C}_k = \begin{cases} c_3 \nu_k m_k + c_k \nu_3 m_3 = 0 \;\; \text{at} \;\; k=1,2; \\ c_3 \nu_k m_k - c_k \nu_3 m_3 = 0 \;\; \text{at} \;\; k=4, \end{cases} \tag{9}$$

then the component conservation equations for k=1,2 end 4 acquire a sourceless appearance

$$L(\tilde{C}_k) = 0 \tag{10}$$

The equation for the concentration of inert gas, since $\omega_5 = 0$, also has a similar appearance $L(c_5) = 0$.

When accounting for dependencies

$$\left(c_2\right)_2 + \left(c_3\right)_2 + \left(c_4\right)_2 + \left(c_5\right)_2 = 1, \tag{11}$$

$$\left(c_1\right)_1 + \left(c_3\right)_1 + \left(c_4\right)_1 + \left(c_5\right)_1 = 1 \tag{12}$$

The mass balance law for all mixtures is as follows:

$$\nu_1 m_1 + \nu_2 m_2 = \nu_3 m_3 + \nu_4 m_4 \tag{13}$$

the summation of the concentrations in each of the zones is equal to unity, although the mass concentrations of the components depend on the variable $\approx\!C$. The concentration can be found by solving a single nonlinear differential equation common to all components, for which the Schwab-Zelidovich function was introduced.

$$\overset{\approx}{C}(0,y)=\begin{cases}1 \ \ at \ \ 0\le y\le a,\\ 0 \ \ at \ \ y>a,\end{cases} \quad \frac{\partial \overset{\approx}{C}(x,0)}{\partial x}=0 \quad \text{and} \quad \overset{\approx}{C}\left(x, y_\infty\right)\to 0. \tag{14}$$

To solve the problem, we passed to dimensionless coordinates using characteristic quantities a, u_2, H_2, ρ_2:

$$\bar{x}=\frac{x}{a},\ \ \bar{r}=\frac{r}{a},\ \ \bar{u}=\frac{u}{u_2},\ \ \bar{\vartheta}=\frac{\vartheta}{u_2},\ \ \bar{\varepsilon}=\frac{\varepsilon}{au_2}, \tag{15}$$

$$\bar{H}=\frac{H}{H_2},\ \ \bar{\rho}=\frac{\rho}{\rho_2},\ \ \bar{T}=\frac{T}{T_2},\ \ \bar{p}=\frac{p}{\rho_2 u_2^2},\ \ \bar{h}_2^*=\frac{h_2^*}{H_2}. \tag{16}$$

Then the equations take the

$$\begin{cases}\rho u\dfrac{\partial u}{\partial x}+\rho v\dfrac{\partial u}{\partial r}=-\dfrac{dp}{dx}+\dfrac{1}{r}\dfrac{\partial}{\partial r}\left(\rho v_t r\dfrac{\partial u}{\partial r}\right),\\ \dfrac{\partial(\rho ur)}{\partial x}+\dfrac{\partial(\rho\vartheta r)}{\partial r}=0,\\ \rho u\dfrac{\partial H}{\partial x}+\rho v\dfrac{\partial H}{\partial r}=\dfrac{1}{\Pr r}\dfrac{\partial}{\partial r}\left(\rho v_t r\dfrac{\partial}{\partial r}\left(H-(1-\Pr)\dfrac{\gamma-1}{2}M_2^2u^2\right)\right),\\ \rho u\dfrac{\partial \overset{\approx}{C}}{\partial x}+\rho v\dfrac{\partial \overset{\approx}{C}}{\partial r}=\dfrac{1}{\mathrm{Sc}\, r}\dfrac{\partial}{\partial r}\left(\rho v_t r\dfrac{\partial \overset{\approx}{C}}{\partial r}\right).\end{cases} \tag{17}$$

To solve this system of equations, we can introduce Mises substitutions to make the sphere a regular rectangle:

$$\rho ur=\psi\frac{\partial\psi}{\partial r},\ \ \rho\vartheta r=-\psi\frac{\partial\psi}{\partial x}. \tag{18}$$

The resulting integral was taken to be equal to $\dfrac{r^2}{2}=\int_0^{\psi}\dfrac{\psi d\psi}{\rho u}$.

In the remaining equations of the system, the transition from coordinates (x, r) to coordinates (ξ, ψ) is carried out according to the formulas:

$$\begin{aligned}\frac{\partial}{\partial x}&=\frac{\partial}{\partial\xi}+\frac{\partial\psi}{\partial x}\frac{\partial}{\partial\psi}=\frac{\partial}{\partial\xi}-\frac{r}{\psi}\rho\vartheta\frac{\partial}{\partial\psi},\\ \frac{\partial}{\partial r}&=\frac{\partial\psi}{\partial r}\frac{\partial}{\partial\psi}=\frac{r}{\psi}\rho u\frac{\partial}{\partial\psi}.\end{aligned} \tag{19}$$

Having reduced both sides of the equations by ρu and applying the transition formula to the coordinate r in the form $r^2=2\int_0^{\psi}\dfrac{\psi d\psi}{\rho u}$, we obtain the system of equations:

$$\begin{cases}\dfrac{\partial u}{\partial\xi}=\dfrac{1}{\psi}\dfrac{\partial}{\partial\psi}\left[\dfrac{\rho^2\varepsilon u}{\psi}\left(2\int_0^{\psi}\dfrac{\psi d\psi}{\rho u}\right)\dfrac{\partial u}{\partial\psi}\right],\\ \dfrac{\partial H}{\partial\xi}=\dfrac{1}{\Pr\psi}\dfrac{\partial}{\partial\psi}\left[\dfrac{\rho^2\varepsilon u}{\psi}\left(2\int_0^{\psi}\dfrac{\psi d\psi}{\rho u}\right)+\dfrac{\partial}{\partial\psi}\left(H-f\,u^2\right)\right],\\ \dfrac{\partial \overset{\approx}{C}}{\partial\xi}=\dfrac{1}{\mathrm{Sc}\,\psi}\dfrac{\partial}{\partial\psi}\left[\dfrac{\rho^2\varepsilon u}{\psi}\left(2\int_0^{\psi}\dfrac{\psi d\psi}{\rho u}\right)\dfrac{\partial \overset{\approx}{C}}{\partial\psi}\right].\end{cases} \tag{20}$$

Hereinafter $f = (1-\Pr)\frac{\gamma-1}{2}M_2^2$.

SOLUTION METHOD

The finite-difference representation of differential equations is feasible with respect to the dimensionless equation of total enthalpy:

$$\frac{\partial H}{\partial \xi} = \frac{1}{\psi}\frac{\partial}{\partial \psi}\left[\frac{\rho^2 \nu_t u}{\psi}\left(2\int_0^{\psi}\frac{\psi d\psi}{\rho u}\right)\frac{\partial}{\partial \psi}\left(H - f u^2\right)\right]. \tag{21}$$

$$2\int_0^{\psi}\frac{\psi d\psi}{\rho u} \approx 2\left(\frac{0}{(\rho u)_{\psi=0}} + \frac{h}{(\rho u)_{\psi=h}}\right)\frac{h}{2} = \frac{\psi^2}{(\rho u)_{\psi=0}} \tag{22}$$

Then the components of the right side of the equations can be represented as:

$$\begin{aligned}\frac{1}{\psi}\frac{\partial}{\partial \psi}\left(\frac{\rho^2 \nu_t u}{\psi}\frac{\psi^2}{(\rho u)_{\psi=0}}\frac{\partial}{\partial \psi}\right) &\approx \frac{1}{\psi}\frac{\partial}{\partial \psi}\left(\rho \nu_t \psi \frac{\partial}{\partial \psi}\right) = \\ &= \frac{\partial \rho \nu_t}{\partial \psi}\frac{\partial}{\partial \psi} + \frac{1}{\psi}\rho \nu_t \frac{\partial}{\partial \psi} + \rho \nu_t \frac{\partial^2}{\partial \psi^2} \approx 2\rho \nu_t \frac{\partial^2}{\partial \psi^2}.\end{aligned} \tag{23}$$

$$\left.\frac{\partial H}{\partial \xi}\right|_{\psi=0} = \frac{2}{\Pr}\rho \nu_t \frac{\partial^2}{\partial \psi^2}\left(H - f u^2\right)\Big|_{\psi=0} \tag{24}$$

$$\begin{aligned}\frac{H_{i,0}^{s} - H_{i-1,0}}{h_{\xi}} &= \frac{2\rho_{i,0}^{s-1}\nu_{ti}^{s-1}}{\Pr h_{\psi}^2}\left[H_{i,1}^{s} - 2H_{i,0}^{s} + H_{i,-1}^{s} - f\left(\left(u^2\right)_{i,1}^{s-1} - 2\left(u^2\right)_{i,0}^{s-1} + \left(u^2\right)_{i,-1}^{s-1}\right)\right] = \\ &= \frac{4\rho_{i,0}^{s-1}\nu_{ti}^{s-1}}{\Pr h_{\psi}^2}\left[H_{i,1}^{s} - H_{i,0}^{s} - f\left(\left(u^2\right)_{i,1}^{s-1} - \left(u^2\right)_{i,0}^{s-1}\right)\right].\end{aligned} \tag{25}$$

THE RESULTS OF A COMPUTATIONAL EXPERIMENT AND THEIR ANALYSIS

Based on the proposed model of diffusion combustion, a program was compiled where, based on the mass concentrations of the components of the combustible mixture and air, the stoichiometric equation of combustion of the propane-butane mixture in oxygen, the molar masses, specific heat at constant pressure and the calorific value of the combustible component, the necessary parameters of the components, velocity fields and temperature. The concentration of air was set in the form $(c_1)_1 = 0.232$, $(c_5)_1 = 0.768$. The composition of the combustible mixture included propanobutane mixture and nitrogen. The main flow rate was 60 m/s $M_2 \approx 0$, a satellite stream – 18.3 m/s. Air temperature - $T_1 = 297\,K$, a combustible mixture and the combustible mixture – $T_2 = 600\,K$.

The step of numerica x integration was equal to 1 0.001, for ψ - 0.02. When moving to a dimensionless coordinate, the data was presented with a constant step of 0.02.

Separate calculation results are given in the form of graphs in Fig.4.

In Fig.4 shows the concentration of reagents and combustion products obtained with $(c_2)_2 = 0.120$ in various sections. In this case, the value of the place of the front is determined from the equality $C^* = 0.349348$. The temperature at the flame front was 2144.93 K.

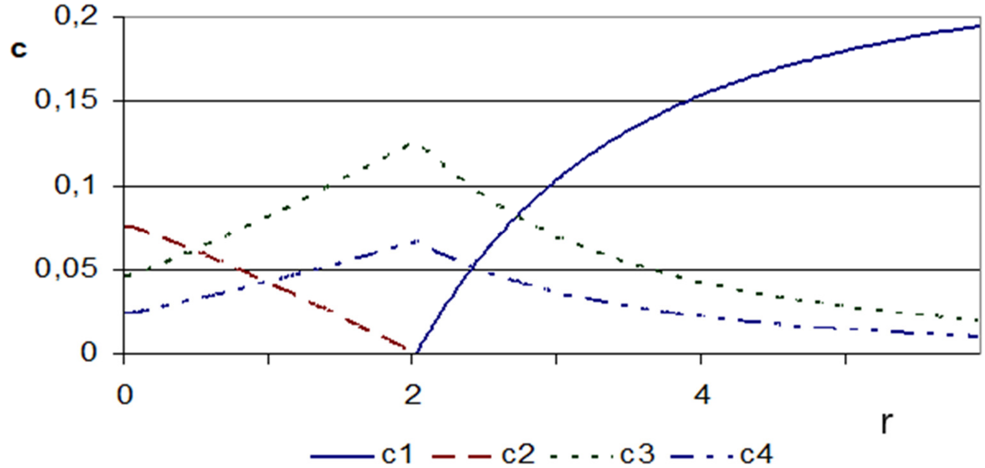

FIGURE 1. Mass concentration curves of reagents and products burning at $\overline{x} = 8,16,\ 24.(c_2)_2 = 0.120$.

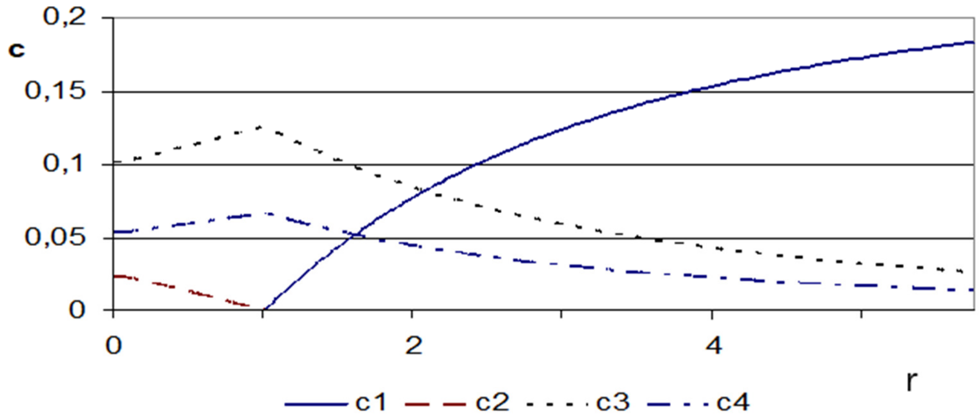

FIGURE 2. Mass concentration curves of reagents and products burning at $\overline{x} = 8,16,\ 24.(c_2)_2 = 0.120$.

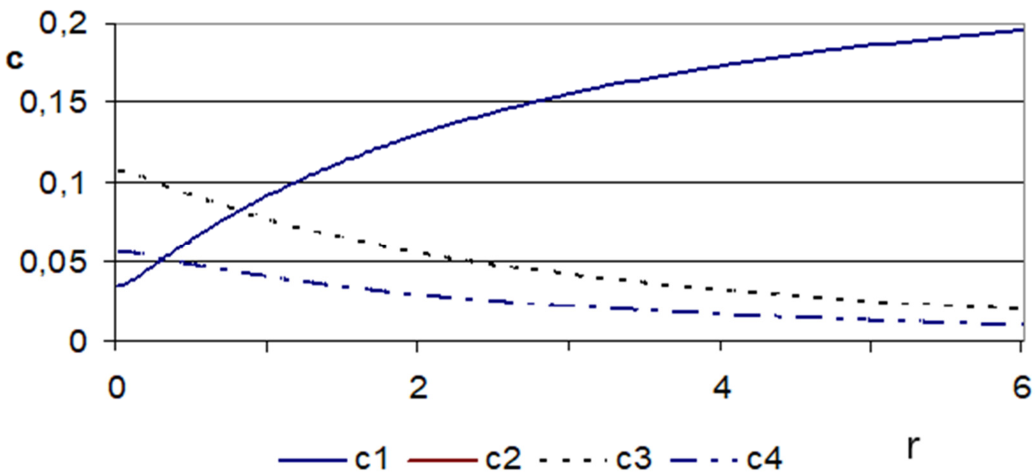

FIGURE 3. Mass concentration curves of reagents and ducts burning at $\overline{x} = 8,16,\ 24.(c_2)_2 = 0.120$.

The following Figurers shows the impulse curves in different sections of the jet. It is noticeable that at the flame front this indicator has the smallest value.

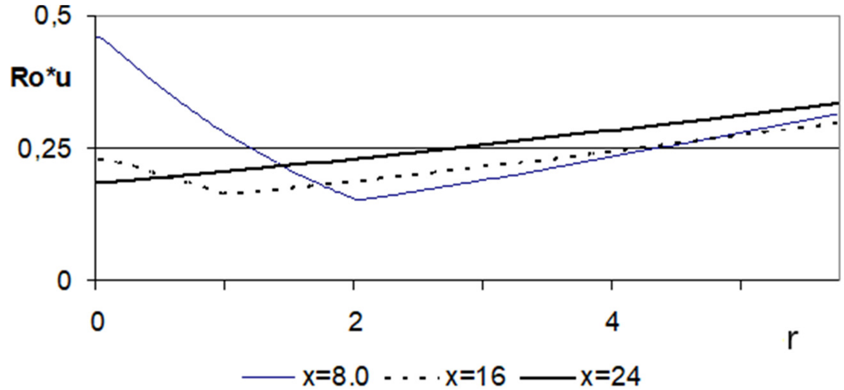

FIGURE 4. Impulse curves in various sections, received at $(c_2)_2 = 0.120$.

Typical changes in the dimensionless temperature in the middle and in the final part of the flame front, as well as after the flame front, are shown in Fig.6.

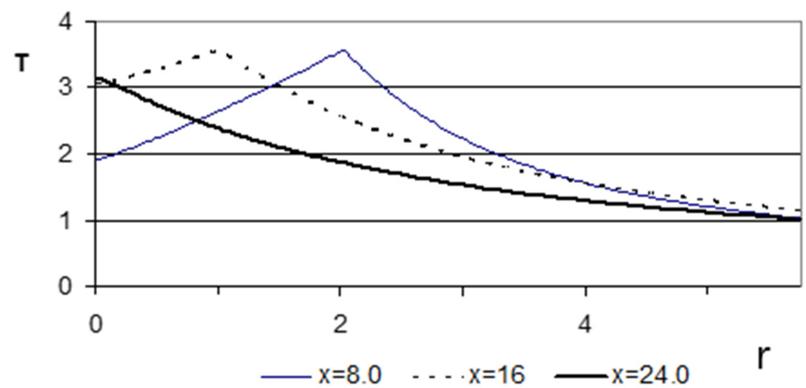

FIGURE 5. Change in dimensionless temperature in sections $\overline{x} = 8.0$, 16.0 and 24.0, received at $(c_2)_2 = 0.120$

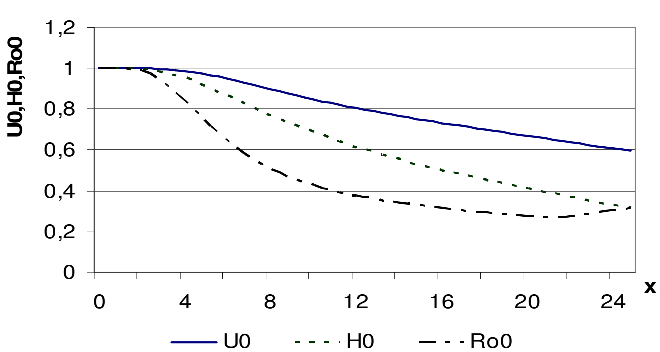

FIGURE 6. Changes in axial values of dimensionless longitudinal velocity, total enthalpy, and density of the gas mixture at $(c_2)_2 = 0.120$

The calculations were carried out for the values of the initial fuel concentration $(c_2)_2 = 0.120$, 0.25, 0.40 and 1.00, The shapes of the flame fronts of the first of these three options are shown in Fig.8. For these four calculation options, the end of the flame front corresponded to a dimensionless longitudinal coordinate 21.428, 47.418, 80.892 and 281.150.

With an increase in the concentration of fuel in the composition of the mixture of the main stream, expansion and elongation of the flame front are observed.

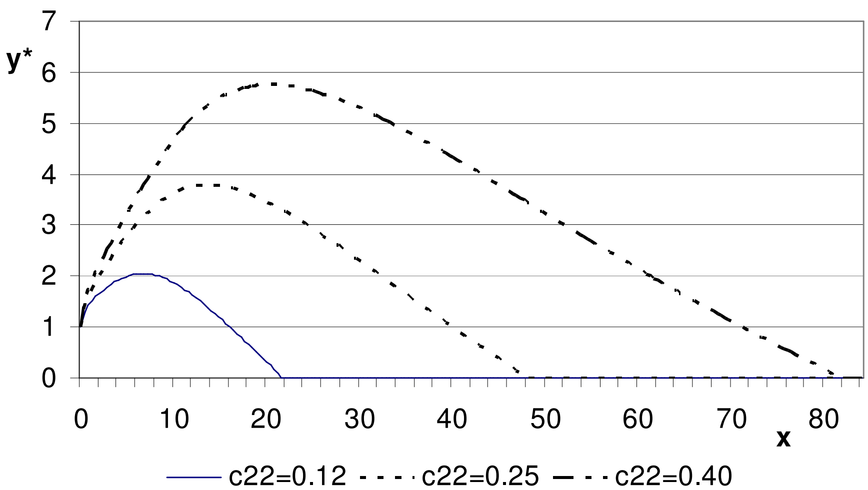

FIGURE 7. Forms of flame fronts at $(c_2)_2 = 0.120$, 0.25 and 0.40

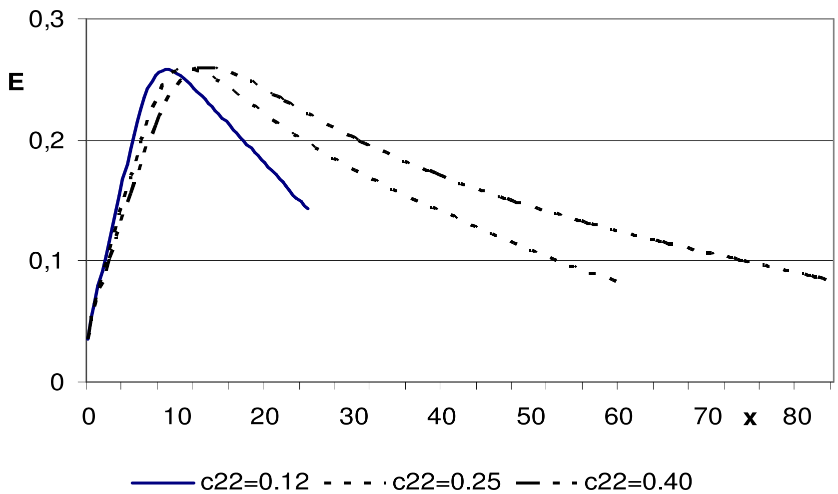

FIGURE 8. Change in the value of the turbulence coefficient along the jet at $(c_2)_2 = 0.120$, 0.25 and 0.40

In Fig.8 shows the directional changes in the turbulent exchange coefficient according to the new L. Prandtl modification. As can be seen from the graphs, their maximum values remain almost the same. Similar calculations were also performed at the inlet temperature of the combustible mixture $T_2 = 1210\,K$, when the temperature at the flame front will be higher than in previous versions, and the flame front will be shorter.

CONCLUSION

The combustion parameters formed during the reaction and combustion of fuel mixtures with different concentrations were determined. In this case, the problem was solved numerically, assuming that the fuel does not mix with the air, and the air does not mix with the fuel. In this case, results were obtained using Prantl's algebraic model and the modern k-e model in determining turbulence. In order to fully represent the combustion processes, the Arrhenius model of the combustion model was used with 2nd order accuracy, and the flame length, generated energy, and velocity changes were determined.

Using the Schwab Zeldovich function to determine the concentration in the combustion process reduced the program's running time by 2 times and reduced the number of equations from 5 to 1. When the results were analyzed, it was determined by comparing the results obtained using this function that each equation produced values that were very close to the results obtained by solving it. These obtained results allow to define new variants of modern gas-burning stoves.

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