14th International Conference on

APPLICATION of INFORMATION and COMMUNICATION TECHNOLOGIES

07-09 October 2020

Numerical algorithm for modeling turbulence in a jet with diffusion combustion

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Annotation. The paper proposes a method for calculating the diffusion combustion of a propane-butane mixture in a turbulent jet using the "k-e" model of turbulence. For mathematical modeling of the combustion object, the equations of the theory of the boundary layer are used. The equations for the components of the gas mixture are reduced to one using the Schwab-Zeldovich function.. The formulated system of partial differential equations with boundary conditions is solved numerically and its algorithm is implemented using the DELPHI graphical environment.

Keywords: modeling, turbulent jet, gas mixture, diffusion combustion, Schwab-Zeldovich function, total enthalpy, finite differences, computational experiment.

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Introduction

A comprehensive study of turbulent combustion processes is a very urgent problem of fluid mechanics and heat transfer, since they are often found in many practical problems, for example, energy, mechanical engineering, industrial plants, etc., which are associated with efficient (rational) use of energy resources, the relevance of which is reflected in decrees and resolutions of the leadership of our republic [1].

Combustion is still the main source of energy in the world and will remain so in the foreseeable future. In 2010, approximately 90% of all energy produced by mankind on Earth was produced by burning fossil fuels or biofuels [2], and, according to forecasts by the Department of Energy Research and Development (USA), this share will not fall below 80% until 2040 with a simultaneous increase energy consumption by 56% between 2010 and 2040 [3]. The global problems of modern civilization, such as the depletion of non-renewable energy resources, environmental pollution and global warming are associated with it.

The main raw material for combustion is natural gas. Over the past decades, the role and importance of natural gas in the energy balance of the world economy has been constantly growing, due to both its high efficiency as an energy resource and raw material for industry, and environmental friendliness increased in comparison with oil and coal.

Based on these considerations, modeling the combustion process in turbulent flows to find the optimal conditions is the main task in fluid mechanics.

There are several problems in modeling the combustion process. One of them is a combustion model. Often used the combustion model of a premixed mixture [4,5,6], as well as diffusion /7/. Based on practical conditions, one or another combustion model is used.

Another problem is this turbulence model [8,9,10,11], as well as the solution method [12,13,14]. Significant progress has recently been made to simulate the nature of turbulence; differential models of turbulence, as well as numerical methods of solution have appeared. The literature proposes ever new approaches to solving these problems.

[7] presents a Computational Fluid Dynamics (CFD) study of the non-premixed combustion of natural gas with air in an axisymmetric cylindrical chamber, focusing on the contribution of the chemical reaction modeling on the temperature and the chemical species concentration fields. Simulations are based on the solution of mass, momentum, energy and chemical species conservation equations. Turbulence is modeled by the standard k-ε model.

In [8] principles of mathematical models as tools in engineering and science are discussed in relation to turbulent combustion modeling. A model is presented for the rate of combustion which takes into account the intermittent appearance of reacting species in turbulent flames. Special attention is given to soot formation and combustion in turbulent flames. ll predictions in the present paper have been made by modeling turbulence by the k-∈ model.

An analysis of several other literatures shows [5,6,8,10] that in these studies the main attention is paid to modeling diffusion combustion of mixed gases, where as the feedstock is used methane. Not used graphic means of the algorithmic language. In this work, a computer simulation technique and a numerical solution for the combustion of a propane-butane mixture in a free turbulent jet using graphic means of an algorithmic language are proposed.

Formulation of the problem.

Consider the flow of combustible gas flowing from a circular nozzle of radius a and propagating in a tangled (flooded) oxidizer stream. A schematic picture of the flow is given in [11]

The profiles of velocity, total enthalpy, and concentration of components at the nozzle exit are defined as homogeneous and stepwise, and we consider the pressure to be static, i.e.

$$P_1 = P_2 = P_{atm} = const$$

Suppose that the process occurs in the diffusion combustion mode, i.e. combustion occurs in the mixing zone of the "fuel" and the "oxidizing agent," called the flame zone. Usually, this zone is approximated by the flame front (the rate of the chemical reaction is infinite). In this case, the flow of reagents at the flame front should be in a stoichiometric ratio [13].

The system of differential equations describing this physical process in the approximation of the theory of turbulent boundary layer has the form [5,6,11,14]:

$$\left.\begin{aligned}
&\frac{\partial(\rho u)}{\partial x} + \frac{1}{y}\frac{\partial(\rho \vartheta y)}{\partial y} = 0,\\
&\rho u \frac{\partial u}{\partial x} + \rho \vartheta \frac{\partial u}{\partial y} = \frac{1}{y}\frac{\partial}{\partial y}(\rho y \nu_T \frac{\partial u}{\partial y}),\\
&\rho u \frac{\partial H}{\partial x} + \rho \vartheta \frac{\partial H}{\partial y} = \frac{1}{y}\frac{1}{P_r}\frac{\partial}{\partial y}\left(\rho y \nu_T \frac{\partial H}{\partial y}\right) + \left(1 - \frac{1}{P_r}\right) *\\
&\frac{1}{y}\frac{\partial}{\partial y}\left[\rho y \nu_T \frac{\partial}{\partial y}\left(\frac{u^2}{2}\right)\right]\\
&\rho u \frac{\partial \overset{\approx}{c}}{\partial x} + \rho \vartheta \frac{\partial \overset{\approx}{c}}{\partial y} = \frac{1}{y}\frac{1}{sc}\frac{\partial}{\partial y}\left(\rho y \nu_T \frac{\partial \overset{\approx}{c}}{\partial y}\right)
\end{aligned}\right\} \quad (1)$$

The system of differential equations (1) is supplemented by algebraic equations of enthalpy and state of the gas mixture, respectively:

$$H = C_p T + \frac{u^2}{2} + \sum C_i h_i \quad (2), \qquad P = \frac{R_0 T \rho}{m} \quad (3), \qquad \text{где} \qquad m = \left(\sum_{i=1}^{n} \frac{C_i}{m_i}\right) \quad (4)$$

All notation in (1-4) is generally accepted (see [5]).

To close the system of differential equations (1), taking into account (2-4), the turbulence coefficient "" of the turbulence model [7,8] is used with respect to the turbulent viscosity coefficient [7,8]:

$$\left.\begin{aligned}\rho u\frac{\partial k}{\partial x}+\rho\vartheta\frac{\partial k}{\partial y}&=\frac{1}{y}\frac{\partial}{\partial y}\left[\frac{\rho y\nu_T}{P_{r_k}}\frac{\partial k}{\partial y}\right]+\rho\nu_T\left(\frac{\partial u}{\partial y}\right)^2-\rho\varepsilon\\ \rho u\frac{\partial \varepsilon}{\partial x}+\rho\vartheta\frac{\partial \varepsilon}{\partial y}&=\frac{1}{y}\frac{\partial}{\partial y}\left[\frac{\rho y\nu_T}{P_{r_\varepsilon}}\frac{\partial \varepsilon}{\partial y}\right]+C_1\frac{\varepsilon}{k}\rho\nu_T\left(\frac{\partial u}{\partial y}\right)^2-C_2\frac{\rho\varepsilon^2}{k}\end{aligned}\right\} \quad (5)$$

The relationship between the kinetic energy of turbulence « k » и and its dissipation rate « ε » will be written in the following form [7,8]:

$$\nu_T=C_\nu\frac{k^2}{\varepsilon} \quad (6)$$

The boundary conditions under which the system of differential equations (1) is solved taking into account (2-5) has the form;

$$\left.\begin{aligned}x=0:&\begin{cases}u=u_2, H=H_2, \overset{\approx}{C}=1,\ \mathrm{K}=\mathrm{K}_2,\ \varepsilon=\varepsilon_2, v=0 \quad \text{при} \quad 0\le y\le a\\ u=u_1, H=H_1, \overset{\approx}{C}=0,\ \mathrm{K}=\mathrm{K}_1,\ \varepsilon=\varepsilon_1,\ v=0 \ \text{при} \quad a<y\le\infty\end{cases}\\ x>0:&\begin{cases}\dfrac{du}{dy}=v=\dfrac{dH}{dy}=\dfrac{d\overset{''}{C}}{dy}=\dfrac{dK}{dy}=\dfrac{d\varepsilon}{dy}=0, \quad \text{при} \ \ \mathrm{y}=0\\ \mathrm{u}\to\mathrm{u}_1,\ v\to 0,\ \mathrm{H}\to\mathrm{H}_1,\ \overset{''}{\mathrm{C}}\to 0, K\to K_1,\ \varepsilon\to\varepsilon_1 \quad \text{при} \quad y\to y_\infty\end{cases}\end{aligned}\right\} \quad (7)$$

Main part

The system of differential equations (1) with allowance for (2–7) was solved numerically using a two-layer, implicit finite-difference scheme and the iteration method with iterations [15,16].

When numerically solving the system of equations of the boundary layer together with the equations of the "k-ε" model of turbulence, additional difficulties arise due to the significant non-linearity of the equations of this model. The literature does not describe methods for numerically solving the boundary layer equations in conjunction with the equations of the "k-ε" turbulence model. In this regard, we used the following iterative solution scheme. The system of equations of motion, energy, and diffusion is solved in conjunction with the equations of the "k-ε" turbulence model. The final criterion for exiting the iterative cycle was the condition

$$\Delta\Phi=max\left\{\frac{\left|\Phi_i^{(l)}-\Phi_i^{(l-1)}\right|}{\Phi_{max}^{(l)}}\right\}\le\varepsilon_1$$

where 1≤i≤n is the point number in the direction of the flow axis;

n is the number of design nodes; l is the iteration number; ε_1 - specified accuracy of convergence; Φ - any of the quantities $(u,)\bar{}\,v\bar{}$, $\rho\bar{}$, $\varepsilon\bar{}$, $(\nu\_t)\bar{}$.

Combustion of a propane-butane mixture in air was calculated using the initial data taken from / 11 /.

In numerical calculations, the empirical constants of the turbulence model were borrowed from [6] with some refinements and used in the following form:

$$C_\nu=0{,}09; C_1=1{,}45;\ C_2=1{,}96;\quad Pr_k=1;\quad Pr_\varepsilon=1{,}3$$

To test the numerical results, we compared the dynamic pressure and temperature profiles with the experimental and theoretical data of [11].

The main calculation results are given in the form of graphs in Figs. 1-3.

Figure 1 shows the axial changes in the kinetic energy of turbulence at different initial values of the fuel concentration. It is seen that with an increase in the initial value of the fuel

concentration, the axial value of the kinetic energy of turbulence begins to increase, and also mixes slightly towards the nozzle exit. This can be explained by the fact that with an increase in the initial value of the fuel concentration, the axial temperature values begin to increase faster, which leads to a decrease in density, as well as an increase in the velocity gradients.

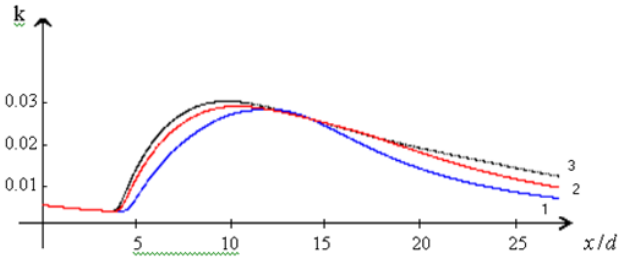

Fig. 1. Axial changes in the kinetic energy of turbulence at various initial values of the fuel concentration equal to: 1- $(C_2)_2$= 0,055; 2- $(C_2)_2$=0,085; 3- $(C_2)_2$= 0,12.

Figure 2 shows the axial changes in the kinematic coefficient of turbulent viscosity. Their maxima are in the region of maximum temperatures and do not have such a pronounced maximum as the kinetic energy of turbulence. The coefficient of turbulent viscosity remains close to the maximum values where there are high temperatures

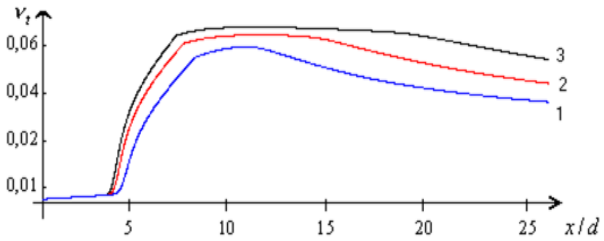

Fig. 2. axial changes in the kinematic coefficient of turbulent viscosity are given. 1-$(C_2)_2$=0,055; 2-$(C_2)_2$=0,085; 3-$(C_2)_2$=0,12.

This can be observed from Fig. 3, where the axial values of turbulence, temperature, and turbulent viscosity calculated at an initial fuel concentration of 0.055 are shown in one figure.

This flow pattern is observed in the calculations obtained by other initial values of the fuel concentration.

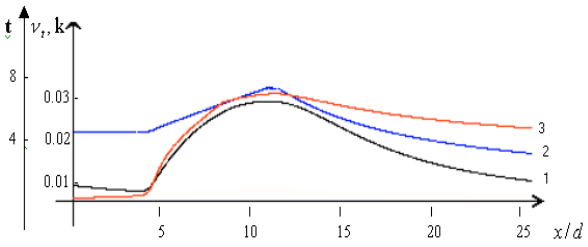

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Fig. 3. Axial changes in the kinetic energy of turbulence (1), temperature (2) and turbulent viscosity (3) at an initial fuel concentration of 0.085.

Conclusion

Thus, we can conclude that an increase in the initial value of the fuel concentration leads to an extension of the zone of maximum values of the kinematic coefficient of turbulent viscosity and, thereby, to an increase in the range of the torch, which are inherent in the combustion of reacting systems. The maximum temperature is reached following the development of turbulence.

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