COMPARISON OF DIFFERENT METHODS
OF MODELING TURBULENT COMBUSTION
IN A BOUNDARY LAYER

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Three methods of modeling a chemical reaction in the combustion of ethanol injected into the boundary layer through a porous plate are compared. In calculations of the average velocity and temperature and also heat-transfer coefficients, simple models of combustion are shown to be close in accuracy to a model that takes into complete account the kinetics of all reactions occurring during combustion. Simple models fail to determine the composition of reaction products, and it is necessary to take into account the formation rate of each substance entrained in combustion.

In modeling turbulent, chemically reacting flows, an important problem, along with that of taking into account the effect of turbulence on combustion, is a complete estimation of the mechanism of chemical reactions. In some studies, the fuel combustion velocity is assumed to be infinite, and the composition of combustion products is given from a single-stage global reaction, the fuel combustion being confined only to the diffusion of fuel and oxidizer [1]. In other studies, one-stage reactions of fuel oxidation are given with consideration for the combustion velocity and with a preassigned product composition in complete fuel combustion [2]. Sometimes, a one-stage reaction is only used to determine from it the amount of combustion products, whereas their composition is calculated from the condition of chemical equilibrium [3].

However, in all these cases, the heat effect and the reaction rate can be overestimated, because in fact some substances have no time to react because of low reaction rates. Therefore, sometimes, although some models of turbulent combustion, for example, that of dissipation of turbulent eddies [4], take into account the real physical processes of mixing of reactants, they can decrease reaction rates overestimated artificially due to a simplified reaction mechanism.

In the present work, we compare three methods of modeling chemical reactions in a turbulent boundary layer on a plate with a reactant (ethanol) injected into the flow through a porous wall. The influence of the kinetics of multistage reactions on the combustion temperature and on the composition of the products formed upon ethanol combustion in air was studied. The results are compared with those obtained using the above simplified models [1, 3]. A modified $k - \varepsilon$-turbulence model intended for the calculation of flows with small Reynolds numbers is used. In this model the entire flow field including the region with large temperature, density, and concentration gradients is described by differential equations [5].

The use of the eddy dissipation model of [2, 6] at low turbulence intensities has led to flame extinction, and, hence, it was not used in the calculations. It should be noted that the eddy dissipation model excludes combustion when the flow becomes laminar, because, in this case, the reaction rates tend to zero.

A system of partial differential equations that describes turbulent flow on a solid surface can be represented in the Cartesian coordinates in generalized form [3] as

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TABLE 1

Φ	Γ_Φ	S_Φ
u	μ_{eff}	0
k	μ_{eff}/σ_k	$G_k - \rho\varepsilon - 2\mu(\partial k^{1/2}/\partial y)^2$
ε	$\mu_{eff}/\sigma_\varepsilon$	$(\varepsilon/k)(C_1 G_k - C_2 f_2 \rho\varepsilon) + 2\nu\mu_t(\partial^2 u/\partial y^2)^2$
h	μ_{eff}/σ_h	0
f	μ_{eff}/σ_f	0
m_{fu}	μ_{eff}/σ_{fu}	$A[\rho\sigma]_{fu}^{0.15}[\rho\sigma]_{ox}^{1.6}\exp\left(-15100/T\right)$
m_i	μ_{eff}/σ_i	$M_i \sum\limits_{j=1}(\alpha''_{ij} - \alpha'_{ij})(R_j - R_{-j})$

$$\frac{\partial(\rho u\Phi)}{\partial x} + \frac{\partial(\rho v\Phi)}{\partial y} = \frac{\partial}{\partial y}\left(\Gamma_\Phi \frac{\partial\Phi}{\partial y}\right) + S_\Phi. \tag{1}$$

Here Φ is any variable determined in the calculation: u is the velocity component, k is the kinetic energy of turbulence and ε is the dissipation rate of turbulence, h is the mixture enthalpy, f is a conservative scalar quantity for describing the combustion process (it is defined below), and m_{fu} and m_i are the mass fractions of unburnt fuel and nitrogen oxides, respectively. The values of Γ_Φ and S_Φ are listed in Table 1 for the following equations: $\mu_t = \rho C_\mu f_\mu(k^2/\varepsilon)$, $\mu_{eff} = \mu_t + \mu$, $C_1 = 1.44$, $C_2 = 1.92$, $C_\mu = 0.09$, $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.3$, $\sigma_h = \sigma_f = \sigma_{fu} = 0.9$, $G_k = \mu_t(\partial u/\partial y)^2$, $A = 1.3 \cdot 10^9$, $f_2 = 1.0 - 0.3\exp(-R_t^2)$, $f_\mu = \exp(-2,5/(1 + R_t/50))$, and $R_t = \rho k^2/\mu\varepsilon$. Here and in Table 1, R_j and R_{-j} are the rates of the direct and reverse reactions j; α'_{ij} and α''_{ij} are the stoichiometric coefficients of substance i in reaction j on the sides of the reagents and products, respectively.

The values of the global-reaction rate and methods of calculating the chemical-component concentrations were different in the three methods of modeling. In model No. 1, the fuel combustion velocity is assumed to be infinite, and combustion was given by a single global reaction. Therefore, to determine the composition of all the substances it is sufficient to calculate the scalar f without using Eqs. (1) for the combustion-product and fuel concentration. Model No. 2 takes into account the fuel-combustion rate with an equilibrium composition of combustion products [3]. Here Eq. (1) for m_i is not used, and the product composition is found from their total concentration and temperature. The expression for the global ethanol oxidation reaction rate is as that in [7]. The full system of equations taking into account the fuel-combustion velocity and the formation rates of combustion products corresponds to model No. 3.

System (1) is supplemented by the Clapeyron equation. In this case, the chemical transformations influence hydrodynamic characteristics via density and viscosity changes.

The difference scheme of system (1) was obtained by the method of control volumes and solved using the SIMPLE procedure of [8]. The calculation domain was a rectangle whose lower side was formed by a porous plate through which ethanol was injected and a uniform air flow was supplied through the left-side boundary. The upper and right-hand sides of the rectangle were open and in contact with atmospheric air. At the inlet of the calculation domain the air-flow rate and the initial uniform profile of kinetic turbulence energy were specified, and the dissipation rate was determined from the relationship $\varepsilon = C_\mu k^{3/2}/0.03L$, where L is the linear scale (inlet-channel height). At the outlet of the calculation domain and on the upper boundary, the gradients of all the parameters were considered equal to zero. The transverse velocity component was calculated from a continuity equation.

On the adiabatic porous wall, the boundary conditions were specified as follows:

$$u = 0, \quad k = 0, \quad \varepsilon = 0, \quad \Phi = \Phi^0 + \frac{1}{(\rho v)_w}\left(\Gamma_\Phi \frac{\partial\Phi}{\partial y}\right)_w, \quad \Phi = h, m_{fu}, f.$$
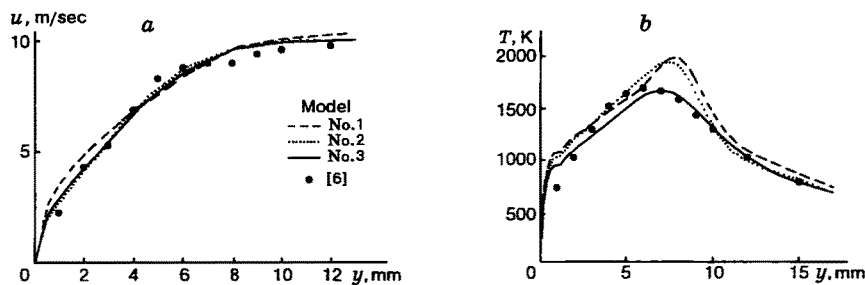
Fig. 1. Profiles of rate (a) and temperature (b) in the section $x = 0.16$ m.

The values of $(\rho v)_w$, T_w, and m^0_{fu} are the same as in experiments, the superscript 0 refers to the value of the fuel fed to the porous plate, and the subscript w, to the values on the wall.

The combustion is calculated using the model of a single-stage reaction between fuel and oxidizer:

$$1 \text{ kg of fuel } + s \text{ kg of oxidant } = (1 + s) \text{ kg of reaction products}, \qquad (2)$$

where the fuel is ethanol (C_2H_5OH) and the oxidizer is oxygen. For model No. 1, the reaction products are CO and CO_2, and for models No. 1 and No. 2, a mixture of the components CO, CO_2, H_2O, O, H, H_2, OH, and HO_2. The total composition of the mixture upon ethanol combustion, under the assumption that the diffusion coefficients of all the components are equal, is simplified by solution of the equation for the normalized passive scalar f in the Shvab–Zel'dovich form [6] determined as follows:

$$f = \frac{m_{fu} - (m_{ox}/s) - \xi_{ox}}{\xi_{fu} - \xi_{ox}},$$

where $\xi_{ox} = -(m_{ox})_{in}/s$ and $\xi_{fu} = (m_{fu})_{in}$. Here the subscript in indicates the mass fractions of oxygen at $x = 0$ and of fuel on the porous surface.

The equilibrium concentrations of the reaction products are unambiguously determined by the total enthalpy of the products h_{pr}, the total reaction product concentration obtained with allowance for the global reaction, and by the pressure [3]. Under kinetic conditions, the product concentrations also depend on one more variable: the time of chemical reaction. If in calculation of the product concentrations the above substances are assumed to be in chemical equilibrium at the temperature determined by the heat effect of reaction (2) (model No. 2), their concentrations can be determined from the minimum Gibbs free energy condition. To save computer time and memory, it will suffice to predetermine the mass fraction of a particular chemical component for several values of h_{pr} over the entire range of enthalpy variation, and to calculate the mass fractions of combustion products by interpolation using the corresponding polynomial coefficients [3].

In taking into account the kinetics of formation of chemical components, in addition to the equilibrium interpolation polynomials in the temperature and combustion-product concentration, polynomials in the reaction time were also constructed (model No. 3).

Table 2 lists the kinetic mechanism and the reaction-rate constants expressed in the Arrhenius form: $k = A T^B \exp(-T_a/T)$.

Figure 1 shows the velocity and temperature profiles in the cross section $x = 160$ mm (calculated by model Nos. 1–3) in comparison with the experimental data of [9, 10]. In the experiments, the length of the plate was 700 mm, and the velocity of the external flow was 10 m/sec. It can be seen that in all cases the velocity distributions are close, although model Nos. 2 and 3 are in somewhat better agreement with the experiment. In the calculations by model Nos. 1 and 2, the maximum temperature is ~15% lower than its experimental value, but, on the whole, the agreement with experiment is satisfactory.

Figure 2 shows the distribution of the Stanton number St along the plate as compared with the experiment in [9]. The number St was determined in the calculations and experiment on the assumption that

TABLE 2

Reaction	k [m, mole, sec]			
	$\log A$	B	T_a	Da_k
$CO+OH \rightarrow CO_2+H$	6.602	0.5	0.0	3500
$CO_2+M \rightarrow CO+O+M$	12.0	0.0	50353.0	4.6
$H+OH \rightarrow H_2+O$	6.903	1.0	3525.0	10
$H_2O+M \rightarrow OH+H+M$	12.477	0.0	52870.0	3
$H+HO_2 \rightarrow OH+OH$	11.398	0.0	957.0	1800
$OH+H_2 \rightarrow H+H_2O$	10.398	0.0	2618.0	4000
$H+O+M \rightarrow OH+M$	9.903	0.0	0.0	0.3
$OH+O \rightarrow H+O_2$	10.398	0.0	0.0	14
$H+O_2+M \rightarrow HO_2+M$	9.176	0.0	503.5	260
$OH+OH \rightarrow H_2O+O$	9.778	0.0	503.5	300

the entire heat that comes to the wall goes to ethanol evaporation:

$$\mathrm{St} = \frac{(\rho v)_w r}{(\rho u)_\infty (h_\infty - h_w)}.$$

Here r is the alcohol-evaporation heat, and the subscript ∞ refers to the values in the external flow. The Reynolds number is $\mathrm{Re}_x = \rho_\infty u_\infty x / \mu_\infty$.

Calculations by different models suggest that the average flow parameters can be calculated with high accuracy under the assumption of an infinite reaction rate. In this case, the convective-transfer characteristics, the temperature level, and the heat-release coefficients are close to the experimental ones, although model Nos. 1 and 2 overestimate flow temperatures by $\sim 15\%$. The difference between the calculation results for the reaction-product composition is shown in Fig. 3. It can be seen that model Nos. 1 and 2 overestimate the CO_2 concentration by 40% as compared with experiment. In model No. 1, CO concentrations are not calculated, and model No. 2 considerably underestimates the CO fraction, while allowance for the kinetics yields a more realistic picture of the reaction-product composition. Obviously, the times of formation of the above components in chemical reactions are comparable with the characteristic time of impulse and mass transfer for a given region.

The characteristic times of chemical transformations can be determined directly from the Arrhenius-type expression. The characteristic time of chemical reaction 2 is determined from the reaction temperature, the mass concentrations of reactants, and also the mixture density in a given region, as in [6]:

$$\tau_c = [m_{fu} m_{ox} \rho A T_c^B \exp(-T_a/T_c)]^{-1}$$

and compared with characteristic hydrodynamic times. Here T_c is the reaction temperature, and T_a is a constant. The dimensionless parameters of this type are called Damköhler numbers Da. There are many variants of Damköhler numbers. For instance, a classification for the flow of nonpremixed reactants depending on the number $\mathrm{Da} = l_0/(U_0 \tau_c)$, where l_0 and U_0 are certain characteristic scales of length and rate, was proposed in [6]. For the global reaction in the flow under discussion, $\mathrm{Da} \approx 10$; for the intermediate reactions $\mathrm{Da}_k = 0.3-4000$. Therefore, for reactions with small Damköhler numbers (≈ 1), use of a chemical equilibrium model leads to great errors of the product compositions in these reactions.

Thus, in modeling chemical processes in flows of the boundary-layer type for the given range of Da numbers it is necessary to solve a mass balance equation for the mixture's chemical components with allowance
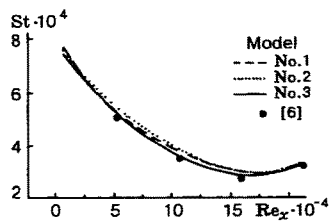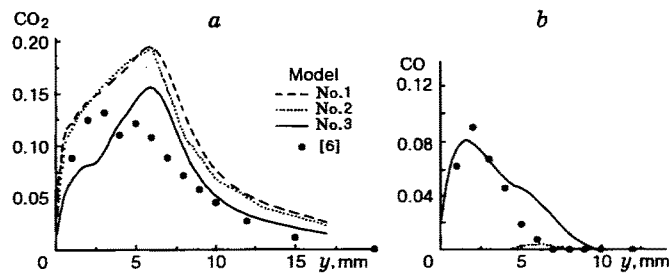
Fig. 2

Fig. 3

Fig. 2. Distribution of heat-release coefficient along the plate.

Fig. 3. Profiles of mass concentrations of CO_2 (a) and CO (b) in the section $x = 0.16$ m.

for chemical kinetics.

From the results obtained, we can draw the conclusion that simple models with an infinite fuel combustion rate and a single global reaction and also models with a finite reaction rate and an equilibrium composition of combustion products yield satisfactory results in calculations of the heat-release coefficient and the velocity and temperature profiles in the boundary layer. However, in determination of the combustion-product composition, the kinetics of combustion-product formation should be taken into account.

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