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MATHEMATICAL MODELING OF TURBULENT COMBUSTION OF HYDROGEN IN A BOUNDARY LAYER

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Turbulent flow in a boundary layer with injection of hydrogen through a permeable plate into an external air flow is modeled. To calculate turbulence characteristics the Lam–Bremhorst modification of the k–ε model is employed. Calculations are made both with and without account for the non-unity of the Lewis number. In determining the concentrations of the intermediate and end combustion products and the temperature the assumption of chemical equilibrium is made. The obtained distribution of turbulent pulsations allows the conclusion of flow laminarization under combustion conditions to be made.

Introduction. A considerable number of theoretical [1-3] and experimental [4-8] works are devoted to the problem of combustion in a turbulent layer. In many of them a modified $k-\varepsilon$ model is used to predict combustion in turbulent flows, and a global reaction with a finite rate is used to calculate its chemical part [1, 3]. In [9] the authors note, by the way, that in modeling turbulent combustion of ethanol in a boundary layer use of the kinetic mechanism exerts a considerable influence on the distribution of the concentration of the chemical components and the temperature of the flame front.

In addition to simplifications of the chemical processes, in calculations of turbulent flows in some cases molecular heat conduction and molecular diffusion are neglected compared to turbulent transfer [10] or the assumption $\mathrm{Pr} = \mathrm{Sc} = 1$ is adopted. Even for calculation of laminar flows with heat and mass transfer the assumption $\mathrm{Pr} = \mathrm{Sc} = 1$ is made in some problems, e.g., in [2] in the calculation of a flow under combustion conditions. Calculations in a simplified mathematical statement require less time and in many cases lead to satisfactory agreement with experimental data. On the other hand, in multicomponent media the diffusion coefficients of individual components can differ from each other by severalfold (by comparison, the Schmidt numbers in dilute mixtures of hydrogen and ethanol with air are 0.2 and 1.3, respectively). The Prandtl number, though being weakly related to the temperature, can depend on the composition (for a hydrogen–air mixture with different hydrogen concentrations the Prandtl number varies from 0.7 to 0.45) [11]. As a result, the Lewis numbers $\mathrm{Le} = \mathrm{Pr}/\mathrm{Sc}$ of individual components of a mixture can differ from unity by severalfold.

The non-unity of the Lewis number can exert a considerable influence on calculation results. For instance, in [12, 13] in the calculation of combustion a strong influence of the Lewis number on the flame temperature is noticed. In boundary layers with injection or evaporation of a reagent from a plate the processes in the viscous sublayer, where molecular diffusion and heat conduction are of importance, play a crucial role. Therefore the assumption $\mathrm{Le} = 1$ made for prediction of the flow with combustion of hydrogen can lead to erroneous results.

Furthermore, it is of interest to investigate the mutual influence of turbulence and combustion. In experimental works in measuring turbulent pulsations it is observed that in combustion of different fuels the relative value of turbulent pulsations decreases [4, 7] over some initial section [4]. Flow laminarization and subsequent turbulization are also a matter of concern in the present work.

Mathematical Statement of the Problem and Method of Solution. In this work we use a $k-\varepsilon$ turbulence model with allowance for laminarization effects [14]. The choice of this modification of the widely adopted $k-\varepsilon$ model has been motivated by the fact that on a flat plate it produces more satisfactory results for turbulence

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TABLE 1. Diffusion Coefficients and Source Terms in Eq. (1)

Φ	Γ_Φ	S_Φ
1	0	0
u	$\mu + \mu_t$	0
k	$\mu + \mu_t/\sigma_k$	$G_k = \rho\varepsilon$
ε	$\mu + \mu_t/\sigma_\varepsilon$	$(\varepsilon/k)(C_{1\varepsilon} f_1 G_k - C_{2\varepsilon} f_2 \rho\varepsilon)$
h	$\mu/\mathrm{Pr} + \mu_t/\mathrm{Pr}_t$	$(\partial/\partial y)(\mu/\mathrm{Pr}) \sum_{i=1}^{N} (\mathrm{Pr}/\mathrm{Sc}_i - 1) h_i (\partial c_i/\partial y)$
c_i	$\mu/\mathrm{Sc}_i + \mu_t/\mathrm{Sc}_t$	$M_i \sum_{j=1}^{N_i} (\alpha''_{ij} - \alpha'_{ij})(R_j - R_{-j})$

TABLE 2. System of Reactions

Reaction	Direct-reaction rate		
	A, mole/(m·sec)	B	E_a, cal/mole
$H_2 + O_2 \rightarrow OH + OH$	1.7*E*13	0.0	47,780
$H_2 + OH \rightarrow H_2O + H$	2.2*E*13	0.0	5146.0
$H + O_2 \rightarrow OH + O$	5.13*E*16	−0.82	16,510.0
$O + H_2 \rightarrow OH + O$	1.8*E*10	1.0	8900.0
$H + O_2 + M \rightarrow HO_2 + M$	1,65*E*15	0.0	−1000.0
$OH + HO_2 \rightarrow O_2 + H_2O$	5.0*E*13	0.0	1000.0
$H + HO_2 \rightarrow OH + OH$	2.5*E*14	0.0	1900.0
$O + HO_2 \rightarrow O_2 + OH$	5.0*E*13	0.0	1000.0
$OH + OH \rightarrow O + H_2O$	6.3*E*12	0.0	1100.0
$H_2 + M \rightarrow H + H + M$	2.2*E*14	0.0	96,000.0
$O_2 + M \rightarrow O + O + M$	5.1*E*15	0.0	115,000.0
$H + OH + M \rightarrow H_2O + M$	1.4*E*23	−2.0	0.0
$H + HO_2 \rightarrow H_2 + O_2$	2.5*E*13	0.0	700

characteristics [15] as compared to other modifications. The equation for each variable, namely, the longitudinal velocity u, the enthalpy of the mixture h, and the mass concentrations of the components c_i, and for the turbulence quantities, namely, the kinetic energy of turbulence k and its dissipation rate ε, can be represented in the generalized form

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

Table 1 gives the quantities of Φ, the diffusion coefficients Γ_Φ, and the source terms S_Φ, where

$$\mu_t = \rho C_\mu f_\mu \frac{k^2}{\varepsilon}, \quad C_1 = 1.44, \quad C_2 = 1.92, \quad C_\mu = 0.09, \quad \sigma_k = 1.0, \quad \sigma_\varepsilon = 1.3,$$

$$\mathrm{Pr}_t = \mathrm{Sc}_t = 0.9, \quad G_k = \mu_t \left(\frac{\partial u}{\partial y}\right)^2, \quad f_1 = 1 + (0.05/f_\mu)^3,$$

$$f_2 = 1 - \exp(-R_t^2), \quad f_\mu = (1 - \exp(-0.0165R_y))^2 (1 + 20.5/R_t),$$

$$R_t = k^2/\nu\varepsilon, \quad R_y = \sqrt{k}\, y/\nu .$$

The rate R_j of direct reaction j is expressed in the form

$$R_j = k_j(T) \left(\frac{\rho}{M}\right)^{\overline{\alpha}_j} \prod_{i=1}^{N} \left(\rho \frac{c_i}{M_i}\right)^{\alpha'_{ij}} .$$

The rate of the reverse reaction is of a similar form. In this expression k_j, i.e., the reaction rate constant, is represented in the modified Arrhenius form

$$k_j = AT^B \exp\left(-\frac{E_a}{RT}\right) . \tag{2}$$

The constants entering Eq. (2) are determined in Table 2.

In using the equilibrium approximation to calculate the combustion process, we employed the efficient method of calculation of the equilibrium mixture composition of [16], which is independent of the choice of the system of elementary reactions. The method is based on the principle of minimization of the Gibbs free energy and allows calculation of the concentration of the equilibrium products of combustion of hydrocarbons in air.

System of equations (1) is supplemented with the equation of state of an ideal gas

$$\rho = \frac{P}{RT \sum\limits_{i=1}^{N} c_i/M_i} , \tag{3}$$

where M_i is the molecular weight of the i-th component, and with auxiliary thermodynamic expressions relating the enthalpy of each component to the temperature:

$$h = \sum_{i=1}^{N} h_i c_i , \quad h_i = \int_{T_0}^{T} c_{pi}(T)\, dT + h_{0i} ,$$

h_{0i} is the enthalpy of formation of the i-th component at the temperature T_0.

The viscosity of the multicomponent mixture was determined using the Wilke formula [17], widely adopted in practical calculations. The Schmidt numbers of individual components in the multicomponent mixture were determined as follows: $\mathrm{Sc}_i = \mu/\rho D_i$, where D_i is the effective diffusion coefficient, calculated by mean of the formula $D_i = (1/M - c_i/M_i)/\sum\limits_{k \neq i}^{N} (c_k/M_k D_{ki})$, where D_{ki} are the binary diffusion coefficients [17].

To take into account the Prandtl number $\mathrm{Pr} = c_p\mu/\lambda$ as a function of the mixture composition, the thermal conductivity of the mixture λ was calculated by means of the Mason and Saxena formula [17]. The boundary conditions were as follows. At $x = 0$ at the entrance to the calculation region the temperature, velocity, and composition of the external flow were specified. The calculations were made for air at a temperature of 300 K. All the calculations were carried out at Reynolds numbers ranging from $1 \cdot 10^3$ to $1 \cdot 10^5$, plotted on the longitudinal coordinate. For the injected substance, its temperature and composition prior to its supply to the porous wall were specified. At $y = 0$ on the plate the mass flow rate was prescribed proceeding from the condition $J_w = (\rho v)_w = 0.01(\rho u)_0$, which corresponded to the experimental conditions in [4]. The enthalpy and the temperature were calculated from the condition of heat balance on the plate $h_w = q_w/(\rho v)_w + h'$; where h' is the enthalpy of the supplied gas, h_w is the enthalpy of the gas on the wall. The mass concentration of each component of the mixture was determined from the condition of substance balance on the wall $c_{iw} = c'_i + (\mu/J_w \mathrm{Sc}_i)(\partial c_i/\partial y)_w$.

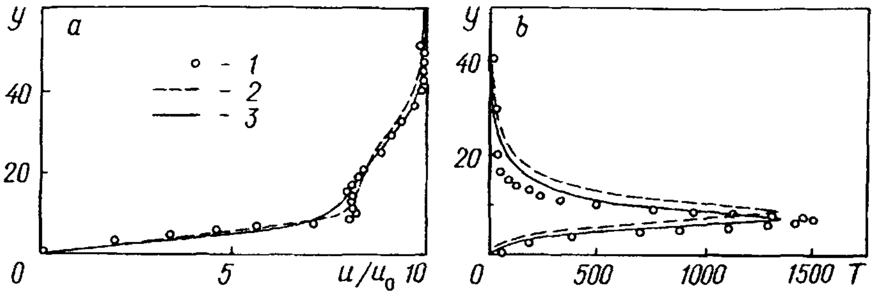
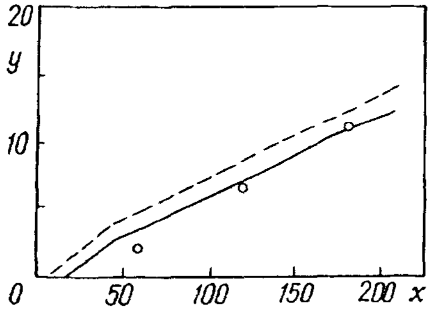


Fig. 1. Velocity (a) and temperature (b) profiles in the 120-mm cross section: 1) experiment; 2) calculation, Le = 1; 3) calculation, Le ≠ 1. y, mm; T, °C.



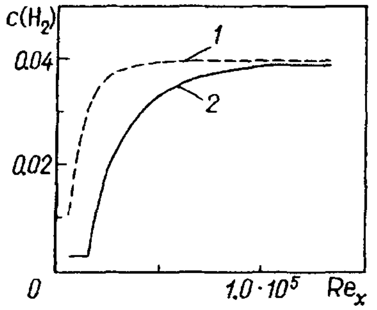


Fig. 2. Flame front position along the plate. The notation is the same as in Fig. 1. x, mm.

Fig. 3. Mass concentrations of hydrogen over the plate: 1) Le = 1; 2) Le ≠ 1.

The system of equations was solved by the method of reference volume [18]. In the nonuniform grid network the number of nodes in the x and y directions was 44 each. It should be noted that when a 22 × 22 grid was used, the results differed insignificantly.

Results and Discussion. We investigated combustion with injection of gaseous fuel (hydrogen) into an air flow. Calculation results were compared with the experimental data [4] and were determined for conditions similar to the experimental: $u_0 = 10$ m/sec, Tu = 1%. In the experiment, use was made of the long initial section (1 m) of an impermeable plate, and therefore the dynamic boundary layer was considerably thicker than the thermal one. Calculations were made using four models:

a) Le = Pr = Sc = 1, chemical equilibrium;

b) the Prandtl and Schmidt numbers vary with the temperature and the composition, i.e., Le ≠ 1, chemical equilibrium;

c) Le = Pr = Sc = 1, the kinetic mechanism of oxidation of hydrogen;

d) Le ≠ 1, the kinetic mechanism of oxidation of hydrogen.

The kinetic mechanism used is shown in Table 2, it involves 26 reactions (the table provides the direct reactions) and is similar to that described in [13]. Eight different chemical components, namely, H_2, O_2, H, O, OH, H_2O, HO_2, and N_2, are considered. It should be noted that the flame front lies in the region of flow velocities 2–7 m/sec, the characteristic rates of the chemical transformations in this case are comparable to or higher than the characteristic hydrodynamic velocity, and therefore use of the kinetic mechanism does not cause marked changes in the results calculated for the velocity, temperature, or concentrations of the reagents or the final products of combustion of hydrogen. Differences are observed only in the concentrations of such intermediate products as OH, HO_2, H, and O, being present in small amounts. The same findings are observed by the authors of [13], who investigated combustion using the single-step and multistep mechanisms of oxidation of hydrogen. Therefore, below, a comparison is made of the results calculated by models a) and b).

The calculations revealed that all the models give satisfactory results for the velocity field. Figure 1a shows velocity profiles for the 120-mm cross section. The temperature profiles (Fig. 1b) differ in both position and the

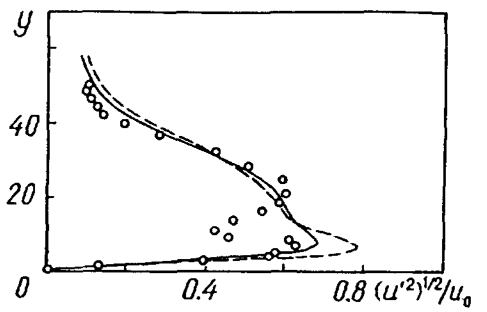


Fig. 4. Profiles of the relative pulsations of the longitudinal velocity in the 120-mm section. The notation is the same as in Fig. 1.

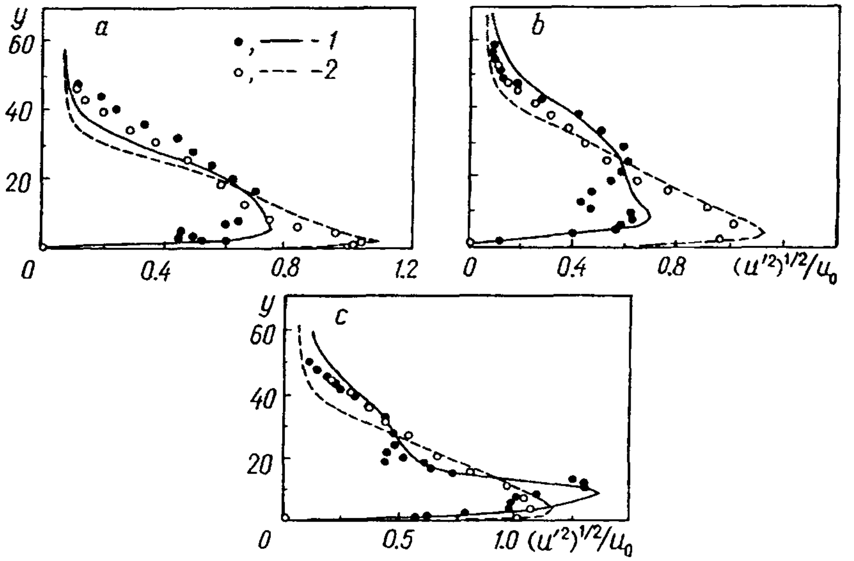


Fig. 5. Profiles of the relative pulsations of the longitudinal velocity in the cross sections of 60 (a), 120 (b), and 180 mm (c) in comparison with the isothermal flow (points, experiment; curves, calculation): 1) combustion, 2) no combustion.

value of the maximum, i.e., the flame front, in the cases $Le = 1$ and $Le \neq 1$. As was noted, use of the kinetic mechanism does not exert a pronounced influence on the temperature field.

Figure 2 shows flame front positions calculated by models a) and b) as compared to experimental data. It is seen that the model allowing for variation of the Prandtl and Schmidt numbers with the temperature and the composition gives a more correct prediction of the flame front position, while use of the assumption $Le = 1$ leads to a constant displacement of the flame front from the wall.

The hydrogen concentrations on the wall are also different for the two models (Fig. 3). The concentrations calculated by model b) show a slower increase as compared to model a), and on the initial section they differ by almost a factor of two.

Figure 4 provides profiles of the relative pulsations of the longitudinal velocity in the 120-mm cross section. As is seen, both models (a and b) give an adequate description of the distribution of the turbulence characteristics.

In Fig. 5 the change in the level of turbulent pulsations along the plate is shown in three cross sections and is compared to the isothermal flow. Comparison of the results of calculation of turbulent pulsations in the isothermal flow with the experimental data of [4] revealed their agreement. At first, combustion causes laminarization in the boundary layer, and then the turbulent pulsations undergo considerable enhancement. As seen in Fig. 5c, the turbulent pulsations in the flame zone in the last cross section even exceed those in the case of the isothermal flow. An increase in the coefficient of friction on the plate and in the heat-transfer coefficients can be related to an increase in the level of turbulence.

Conclusion. The investigations performed allow some conclusions to be made about special features of modeling combustion of hydrogen in a turbulent boundary layer and special features of the combustion process itself. Use of the kinetic mechanism does not exert an influence on the results, and the combustion can be considered to be a chemically equilibrium process. But molecular diffusion and heat conduction should not be neglected, since account for $\mathrm{Le} \neq 1$ leads to better agreement with experimental data on the flame front position. Combustion in the boundary layer causes laminarization on the initial section, and then turbulization of the flow proceeds.

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NOTATION

c, mass concentration; c_p, heat capacity; E_a, activation energy, a constant; h, enthalpy; J, mass flow; M, molecular weight of the mixture; N, number of components in the mixture; N_r, number of reactions; Pr, Prandtl number; q, heat flux; R, universal gas constant; R_t, turbulent Reynolds number; R_j and R_{-j}, rates of the direct and reverse reactions; Sc, Schmidt number; S_Φ, source term; T, temperature; Tu, degree of turbulence; u, v, velocity components; x, y, coordinates; α'_{ij}, α''_{ij}, stoichiometric coefficients of substance i in reaction j as regards the reagents and the products, respectively; $\overline{\alpha}_j$, stoichiometric coefficient of the third body in reaction j, equal to 0 or 1; Γ_Φ, diffusion coefficient; Φ, generalized variable; μ, μ_t, molecular and turbulent viscosity, respectively. Subscripts: w, on the wall, 0, in the external flow; i, an individual chemical component; t, turbulent.

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