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Heat and mass transfer in a multi-component chemically reactive gas above a liquid fuel layer

N. N. SMIRNOV
Moscow State University, 117234, Moscow, U.S.S.R.

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Abstract—The flow of a chemically reactive gas mixture above a thermally destructing surface of liquid fuel is studied. The burning of a quiescent fuel in the flow of an oxidant and the boundary layer with chemical reactions behind a shock wave sliding over the fuel layer are considered. The solution has been obtained with allowance for the motion induced in the liquid layer on its interaction with the gas flow and with allowance for the change in the thermophysical properties of the gas depending on its composition. The distributions of the parameters (velocities, temperatures, concentrations) in liquid and gas phases have been found. The mass flow rate of the fuel surface burnoff has been determined.

THE PROBLEMS of boundary layers with chemical reactions in the course of liquid fuel burning in an oxidant gas flow turn up in investigations of various processes, for example: burning of fuel in hybrid engines; interaction of hypersonic flying vehicles with the atmosphere; exo- and endothermic reactions in chemical engineering; spreading of flame over the fuel surface, the origination of explosions and the propagation of detonation in unmixed two-phase systems of the gas-film type. For all of the above processes it is necessary to calculate the heat and mass transfer between a chemically reacting gas boundary layer and a reacting, melting, subliming, or otherwise destructing, surface. The methods of investigations in this field are very complicated, because the motion of a gas is governed not only by force and temperature fields but also by chemical processes depending in turn on velocity and temperature fields. This requires a conjugate solution of dynamic, thermal and diffusional problems with allowance for the equations of chemical kinetics, multi-component diffusion and variability of thermophysical properties of a medium with distributed parameters. The picture of the process is more involved because of the thermochemical destruction of the surface when some of the vapours of fuel substances, comprising the surface material, diffuses into a boundary layer and reacts chemically with the external flow.

In connection with the demands of practice, a considerable amount of research has been carried out, especially in the past 15–20 years, to investigate the dynamics of a gas of variable composition in the course of its interaction with thermally destructing surfaces [1–7]. The analysis of this trend in the researches allows one to identify two types of problems. First, these are the problems with a stationary zone of chemical reaction stabilized in an oxidant flow over a fuel layer [1–3, 5, 6, 10, 11]. Here tangential displacements in the fuel layer tend to zero as the depth of the layer increases. Second, these are the problems of combustion in a boundary layer behind a shock wave sliding over the fuel surface [4, 7–9]. Such problems arise when the development and propagation of detonation in unmixed heterogeneous gas-film type systems are studied [12–14]. One of the main parameters governing the propagation of detonation in heterogeneous systems is the rate of fuel mass supply to the boundary layer, since it is this rate that is responsible for energy release in the reaction zone [15]. The possible mechanisms for the mixture formation are: the diffusion of fuel having evaporated from the surface [7–9, 13], when the fuel layer preserves its stability, and the sweeping of drops or particles, when the stability of the interface is disturbed [16]. In the case of the latter mechanism it is especially important to know velocity distribution in a liquid layer behind a shock wave up to the moment of wave formation and beginning of sweeping. The velocity field in a liquid depends on the boundary-layer parameters of a gas with regard for evaporation and burning and, as is noted in ref. [16], it allows one to determine the mass of fluid being swept from the surface in the form of fine droplets or particles.

Although a considerable experimental information bearing on surface burning of both solid [5, 17] and liquid fuels with different thermophysical properties [6, 7, 12] has been accumulated up to date, almost all of the pertinent theoretical investigations ignore the motion taking place in the fuel layer [2, 4, 7–11]. To the author's knowledge, there is only one work [17] where an attempt has been made to approximately allow for the motion of the surface melt of material on a body in a hypersonic flow.

The present work investigates the burning of the flat surface of liquid fuel in an oxidant flow in the absence of an axial pressure gradient. The problem is solved within the framework of the assumptions of the laminar boundary-layer theory. Near the fuel surface in the gas, the boundary layer develops in the interior of which there proceed chemical reactions between the fuel vapours and the oxidant. Since these are exothermic reactions, energy is given up by the boundary layer in the gas. The heat from the heated gas transfers to the

NOMENCLATURE

B	non-dimensional parameter of mass transfer
c_p	specific heat at constant pressure
Δc_p	change of mean specific heat in mixture as a result of chemical reaction
D	diffusion coefficient
$g(\eta)$, $f(\eta)$, $i(\eta)$, $r(\eta)$	non-dimensional functions of self-similar variables
g_{iw}	rate of ith component production of the surface as a result of heterogeneous reaction
H	total specific enthalpy of mixture
ΔH	specific heat of chemical reaction at absolute zero
h_i	specific enthalpy of ith component
h_i^0	specific enthalpy of ith component formation
h_{iL}	specific heat of phase transition
$K_p(T)$	equilibrium constant
m_i	molecular mass of ith component
P	pressure
Pr	Prandtl number
$Q_p(T)$	specific heat of chemical reaction at temperature T
R	universal gas constant
Re_x	Reynolds number
T	temperature
u, v	velocity components along axes x and y
We	Weber number
Y_i	ith component mass concentration.

Greek symbols

β, w, ζ, z, η	novel dependent and independent variables
δ	boundary-layer thickness
λ	thermal conductivity
μ	dynamic viscosity
ν_i', ν_i''	stoichiometric coefficients of ith component before and after reaction
σ	surface tension factor
τ	flow shear on surface
Φ_i	stoichiometric relationship
Ψ	stream function
ω_i	rate of ith component production as a result of chemical reaction.

Vectors

$\mathbf{J}_i$	ith component diffusion flux vector
$\mathbf{n}$	vector of normal to phase interface
$\mathbf{q}$	heat flux vector
$\mathbf{P}_n$	density of surface forces
$\mathbf{V}$	velocity vector
$\boldsymbol{\sigma}$	vector of tangent to phase interface.

Subscripts

e	parameters of external flow in gas phase
f	parameters of liquid phase
i	number of a component
w	parameters on phase interface
∞	parameters on external flow in liquid phase.

fuel layer which, having evaporated, gains access, as a result of diffusion, to the boundary layer, where it enters into reaction with the oxidant. As a result of continuous inflow of heat from the gas phase, the fuel becomes warmed up and a temperature boundary layer develops near the phase interface in the liquid. The frictional force originating on the surface due to the presence of velocity gradient involves the liquid particles into motion. Because of a high friction coefficient the interphase interaction induced changes of velocity in the liquid are essentially smaller than in the gas, and they take place only in a narrow zone close to the surface. Thus, beside the temperature boundary layer, there is also a velocity boundary layer in the liquid fuel.

In this case the ratio of the boundary-layer thickness in the gas (δ) and in the liquid (δ_f) is determined by the relationship between the Reynolds numbers

$$\frac{\delta}{\delta_f} = \sqrt{\frac{Re_x^f}{Re_x}} = \sqrt{\frac{\rho_f}{\rho_e}\cdot\frac{u_w}{u_e}\cdot\frac{\mu_e}{\mu_f}},$$

where ρ, μ and u are the density, dynamic viscosity and velocity of the medium.

The solution, having been constructed in such a way, remains valid until on the liquid surface disturbances start to develop, comparable in value with the boundary-layer thickness, as well as the sweeping of drops or particles by the gas flow [16, 21]. Thus, the sought-after solution may be used for the determination of interphase heat and mass transfer so long as the Weber number, characterising the relationship between the dynamic head in a gas phase and the effects of surface tension on the phase interface, is below the critical value [21]

$$We = \frac{\rho u_w^2 x}{\sigma} < We_*$$

where σ is the surface tension coefficient.

With a further increase of the Weber number, the phase interface becomes wavy and mass transfer takes place not only by evaporation but as a result of the sweeping of liquid particles from wave crests [16].

In solving the problem it will be assumed that in the course of chemical transformations the reagents in the reaction zone are interrelated as

$$\sum_{i=1}^{N} m_i \nu_i' = \sum_{i=1}^{N} m_i \nu_i'' \tag{1}$$

where ν_i', ν_i'' are the stoichiometric coefficients of the ith component before and after reaction and m_i is the ith component molecular mass ($i = 1$ is an oxidant, $i = N$ is fuel, $i = 2$ is an inert component: $\nu_2' = \nu_2''$; $i = 3, \ldots,$ $N-1$ are the reaction products). The specific heats at constant pressure for the components will be considered constant ($c_{pi} = \text{const.}$). Then the mean heat capacity of the mixture $\hat{c}_p$ will depend on the concentrations of the components Y_i:

$$\hat{c}_p = \sum_{i=1}^{N} c_{pi} Y_i. \tag{2}$$

Let the rectangular coordinate systems (x, y) and $(\tilde{x}, \tilde{y})$ be chosen so that the axis x would be coincident with the phase interface and would be aligned with the oxidant flow, while the axis y and $\tilde{y}$ in the gas and liquid, respectively, would be aligned against the interface. The coordinate origin coincides with the start of the boundary layer. In the case of combustion behind a moving shock wave the coordinate system moves with the shock wave velocity (see Fig. 1).

In the derivation of equations, the effects of mass forces, thermal diffusion and difusional pressure gradients will be neglected; the coefficients of binary diffusion for different components will be considered identical ($D_{ij} = D_{kl} = D$). Then, the equations of a boundary layer in a gas, provided that the Prandtl and Schmidt numbers are equal to unity, are [8, 11]:

$$\frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = 0,$$

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} = \frac{\partial}{\partial y} \mu \frac{\partial u}{\partial y},$$

$$\rho u \frac{\partial Y_i}{\partial x} + \rho v \frac{\partial Y_i}{\partial y} = \frac{\partial}{\partial y} \mu \frac{\partial Y_i}{\partial y} + \omega_i; \quad i = 1, \ldots, N, \tag{3}$$

$$\rho u \frac{\partial H}{\partial x} + \rho v \frac{\partial H}{\partial y} = \frac{\partial}{\partial y} \mu \frac{\partial H}{\partial y},$$

$$p = \rho R T \sum_{i=1}^{N} Y_i / m_i$$

where

$$H = \sum_{i=1}^{N} Y_i (c_{pi} T + h_i^0) + \frac{u^2}{2}$$

is the total specific enthalpy of the mixture and

$$h_i = c_{pi} T + h_i^0$$

is the ith component specific enthalpy.

The equations for a boundary layer in an incompressible one-component liquid at constant heat capacity c_f, viscosity μ_f and thermal conductivity λ_f are of the form:

$$\frac{\partial \tilde{u}}{\partial x} + \frac{\partial \tilde{v}}{\partial \tilde{y}} = 0,$$

$$\tilde{u} \frac{\partial \tilde{u}}{\partial x} + \tilde{v} \frac{\partial \tilde{u}}{\partial \tilde{y}} = (\mu/\rho)_f \frac{\partial^2 \tilde{u}}{\partial \tilde{y}^2}, \tag{4}$$

$$\tilde{u} \frac{\partial c_f T}{\partial x} + \tilde{v} \frac{\partial c_f T}{\partial \tilde{y}} = (\lambda/\rho)_f \frac{\partial^2 T}{\partial \tilde{y}^2} + (\mu/\rho)_f \left(\frac{\partial \tilde{u}}{\partial \tilde{y}} \right)^2.$$

For the joining together of the solutions of the systems obtained the laws of mass, momentum and energy conservation at the phase interface and the thermodynamic condition of phase transition are used. All the conditions are written in terms of the coordinate system whose origin is located in the zone of discontinuity. The structure of the latter is assumed to be stationary.

(1) Total mass flux conservation condition

$$(\rho \mathbf{V})_{fw} \cdot \mathbf{n} = (\rho \mathbf{V})_w \cdot \mathbf{n} = (\rho v_n)_w \tag{5}$$

where the vector $\mathbf{n}$ is aligned with the y axis.

(2) No-slip condition

$$\mathbf{V}_{fw} \cdot \boldsymbol{\sigma} = \mathbf{V}_w \cdot \boldsymbol{\sigma}, \tag{6}$$

where $\boldsymbol{\sigma}$ is the tangent vector.

(3) Condition of variation in the mass flow of each of the components

$$(\rho v_n)_w (Y_{iw} - Y_{iwf}) + (\mathbf{J}_{iw} - \mathbf{J}_{iwf}) \cdot \mathbf{n} = g_{iw}, \tag{7}$$

where g_{iw} is the ith component production at the phase interface as a result of a heterogeneous reaction; $\mathbf{J}_i$ is the ith component diffusion flux vector:

$$\mathbf{J}_i = -\rho D \operatorname{grad} Y_i. \tag{8}$$

(4) Total momentum flow conservation condition

$$(\mathbf{P}_n)_{fw} + (\rho v_n)_w \mathbf{V}_{fw} = (\mathbf{P}_n)_w + (\rho v_n)_w \mathbf{V}_w \tag{9}$$

where $\mathbf{P}_n$ is the density of the surface forces on the surface with the normal $\mathbf{n}$. Projecting condition (9) on the normal and tangent and using condition (2) yield the relationships:

$$p_{fw} + (\rho v_n)_w v_f = p_w + (\rho v_n)_w v, \tag{9a}$$

$$(\mathbf{P}_n)_{fw} \cdot \boldsymbol{\sigma} = (\mathbf{P}_n)_w \cdot \boldsymbol{\sigma} = \tau_w. \tag{9b}$$

(5) Total energy flux concentration condition

$$\mathbf{q}_w \cdot \mathbf{n} - \mathbf{q}_{fw} \cdot \mathbf{n} = (\rho v_n)_w \sum_{i=1}^{N} (Y_{iwf} h_{iwf} - Y_{iw} h_{iw})$$

$$+ (V_{fw}^2 - V_w^2)/2 + \sum_{i=1}^{N} (\mathbf{J}_{iwf} h_{iwf} - \mathbf{J}_{iw} h_{iw}) \cdot \mathbf{n} \tag{10}$$

where $\mathbf{q} = -\sum_{i=1}^{N} \lambda_i \operatorname{grad} T$ is the heat flux vector.

(6) ith component phase transition condition [8]

$$\frac{\mathrm{d}p_{iw}}{\mathrm{d}T_w} = \frac{h_{iL}}{T_w(\rho_w^{-1} - \rho_{fw}^{-1})}; \quad p_{iw}(T_{ke}) = p_e \tag{11}$$

where T_{ke} is the phase transition temperature at the pressure p_e.

Thus, the boundary conditions of the systems of

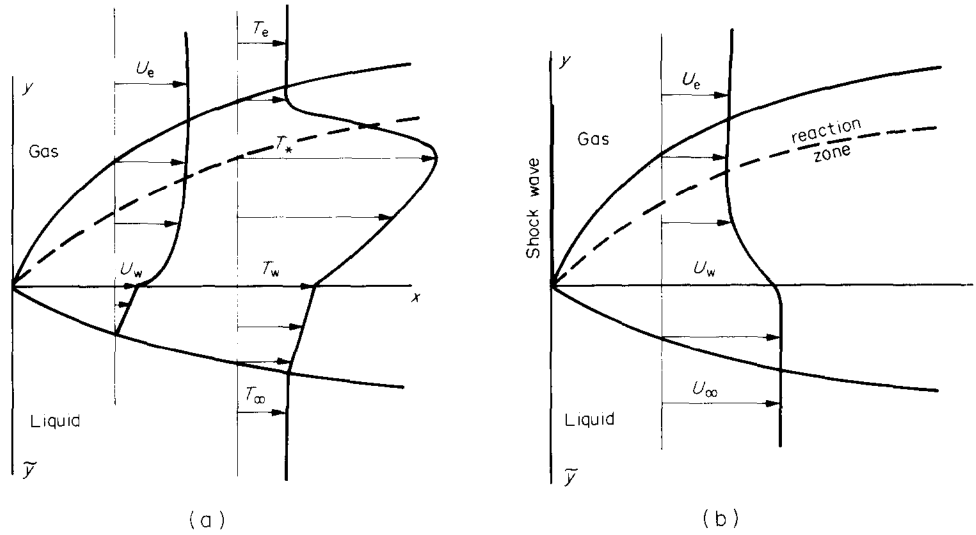

FIG. 1. Velocity and temperature profiles for the case of combustion of a liquid fuel in an oxidant flow (a) and behind a moving shock wave (b).

equations (3) and (4) are presented by three groups of conditions [9, 10]:

I. The conditions on the outer edge of a boundary layer in a gas ($y \to +\infty$)

$$T = T_e; \quad p = p_e; \quad u = u_e; \quad Y_1 = Y_{1e}; \quad Y_{1e} + Y_{2e} = 1.$$

II. The conditions on the edge of a boundary layer in a liquid ($\tilde{y} \to +\infty$)

$$\tilde{T} = T_\infty; \quad \tilde{u} = u_\infty.$$

III. The balance relations at the phase interface ($y = 0$; $x > 0$), which can be derived from the boundary conditions (5)–(11), provided that: the fuel is one-component ($Y_{Nfw} = 1$), the heterogeneous reactions are absent ($g_{iw} = 0$), the squares of the velocity components on the axis y (v_{fw}^2, v_w^2) may be neglected, the pressure drop at the phase transition surface, equation (9a), is also negligibly small [11]

$$\begin{gathered}
(\rho v)_w = -(\rho\tilde{v})_{fw}; \quad u = \tilde{u} = u_w; \\
\tau_w = -\tau_{fw}, \quad \left(\tau = -\mu\frac{\partial u}{\partial y}\right); \\
(\rho v)_w(Y_{iw} - Y_{iwf}) - (\rho D)_w\left(\frac{\partial Y_i}{\partial y}\right)_w = 0; \\
\lambda_f\left(\frac{\partial \tilde{T}}{\partial \tilde{y}}\right)_{fw} = -\lambda\left(\frac{\partial T}{\partial y}\right)_w + (\rho v)_w h_L.
\end{gathered} \tag{12}$$

The integration of equation (11) and the assumption of linear temperature dependence of h_L [9] will give

$$\frac{p_e}{p_{Nw}} = \left(\frac{T_{ke}}{T_w}\right)^{\Delta c_p m_N/R} \exp\left[\frac{\Delta c_p m_N T_{kp}}{R}\left(\frac{1}{T_{ke}} - \frac{1}{T_w}\right)\right] \tag{13}$$

$$p_{Nw} = Y_{Nw} p_e \frac{m_w}{m_N}; \quad \frac{1}{m_w} = \sum_{i=1}^{N} \frac{Y_{iw}}{m_i};$$

$$\Delta c_p = c_f - c_{pN}.$$

Note that the velocity, u_w, and temperature, T_w, of the phase interface are unknown and are to be determined in the process of solution.

For the chemical reaction of type (1) the following relation will hold [17, 18]:

$$\frac{\omega_i}{m_i(v_i'' - v_i')} = \frac{\omega_j}{m_j(v_j'' - v_j')} = \omega. \tag{14}$$

The reaction rate ω in the absence of equilibrium chemical composition is determined by the formula [18, 19], which for non-premixed systems will have the form

$$\omega = kT^{\phi} \prod_{i=1}^{N} P_i^{v_i'}\left[K_p(T) - \prod_{i=1}^{N} P_i^{v_i'' - v_i'}\right] \times \left(\frac{\partial Y_i}{\partial y}\right)^{\operatorname{sign} v_i'} = \omega_0 \prod_{i=1}^{N}\left(\frac{\partial Y_i}{\partial y}\right)^{\operatorname{sign} v_i'}, \tag{15}$$

where $K_p(T)$ is the equilibrium constant

$$K_p(T) = JT^{m_1(v_1'' - v_1')\Delta c_p/R} \exp\left[-\frac{m_N(v_N' - v_N'')\Delta H}{RT}\right];$$

$$\Delta H = \frac{\sum_{i=1}^{N} h_i^0 m_i(v_i'' - v_i')}{m_N(v_N'' - v_N')}$$

is the specific heat of reaction at the absolute zero; and

$$\Delta c_p = \frac{\sum_{i=1}^{N} c_{pi} m_i(v_i'' - v_i')}{m_1(v_1'' - v_1')}$$

is a change in the mean specific heat of the mixture as a result of chemical reaction.

In order to obtain an equation to describe a change in the mean specific heat of the mixture $\bar{c}_p$, equation (2), the third equation of system (3) will be multiplied by c_{pi} with a subsequent summation over the components:

$$\rho u \frac{\partial \hat{c}_p}{\partial x} + \rho v \frac{\partial \hat{c}_p}{\partial y} = \frac{\partial}{\partial y} \mu \frac{\partial \hat{c}_p}{\partial y} + \omega \Delta c_p m_1 (v_1'' - v_1'). \tag{16}$$

The energy equation of system (4) will be transformed by introducing the full specific enthalpy $H_f = c_f T + \tilde{u}^2/2$ and designating $Pr_f = \mu_f c_f / \lambda_f$

$$\tilde{u} \frac{\partial H_f}{\partial x} + \tilde{v} \frac{\partial H_f}{\partial y} = \frac{\mu_f}{\rho_f} \frac{1}{Pr_f} \left[\frac{\partial^2 H_f}{\partial \tilde{y}^2} + (Pr_f - 1) \frac{\partial}{\partial \tilde{y}} \tilde{u} \frac{\partial \tilde{u}}{\partial \tilde{y}} \right]. \tag{17}$$

The system of equations (3) and (16) admits the first integrals [10]:

$$\beta_j = (\beta_{je} - \beta_{jw}) \frac{u - u_w}{u_e - u_w} + \beta_{jw};$$

$$j = 2, \ldots, N, H, c, \tag{18}$$

$$\beta_H = \frac{\hat{c}_p T + u^2/2}{m_N (v_N' - v_N'') \Delta H} - \frac{Y_1}{m_1 (v_1'' - v_1')},$$

$$\beta_c = \frac{\hat{c}_p}{m_1 (v_1'' - v_1') \Delta c_p} - \frac{Y_1}{m_1 (v_1'' - v_1')},$$

$$\beta_i = \frac{Y_i}{m_i (v_i'' - v_i')} - \frac{Y_1}{m_1 (v_1'' - v_1')}, \quad i = 2, \ldots, N,$$

whose presence allows the reduction of the solution of system (3) and (16) to the solution of three equations. It is seen from equation (17) that system (4) admits the Crocco integral only in the case of $Pr_f = 1$. For liquid fuels $Pr_f > 1$, and the system of equations (4) and (16) should be solved in full. New similarity variables will now be used in a manner similar to that given in ref. [11] for the case of diffusional combustion and in ref. [8] for the case of combustion behind a shock wave sliding over a fuel layer. For this, the following independent variables will be introduced

$$\zeta = \rho \mu x; \quad \tilde{\zeta} = \rho_f \mu_f x;$$

$$z = \int_0^y \rho \, dy; \quad \tilde{z} = \rho_f \tilde{y},$$

as well as the dependent variables

$$\tilde{w} = \tilde{v}/\mu_f; \quad w = \frac{1}{\rho \mu} \left(\rho v + u \frac{\partial z}{\partial x} \right),$$

and stream functions Ψ and Ψ_f:

$$u = u_w + \frac{\partial \Psi}{\partial z}; \quad w = -\frac{\partial \Psi}{\partial \zeta};$$

$$\tilde{u} = u_w + \frac{\partial \Psi_f}{\partial \tilde{z}}; \quad w = -\frac{\partial \Psi_f}{\partial \tilde{\zeta}}.$$

Then, the first equations of systems (3) and (4) are satisfied identically, while the remaining equations, after the transition to the similarity variables

$$\eta = z \sqrt{\frac{|u_e - u_w|}{2\zeta}};$$

$$\Psi = \sqrt{2\zeta |u_e - u_w|} g(\eta) \text{ sign } (u_e - u_w);$$

$$\tilde{\eta} = \tilde{z} \sqrt{\frac{|u_\infty - u_w|}{2\tilde{\zeta}}};$$

$$\Psi_f = \sqrt{2\tilde{\zeta} |u_\infty - u_w|} f(\tilde{\eta}) \text{ sign } (u_\infty - u_w);$$

$$i(\eta) = \frac{Y_1 - Y_{1w}}{Y_{1e} - Y_{1w}}; \quad r(\tilde{\eta}) = \frac{H_f - H_{fw}}{H_{f\infty} - H_{fw}},$$

are reduced to the ordinary differential equations

$$g'''(\eta) \text{ sign } (u_e - u_w) + g''(\eta) \left[g(\eta) + \eta \frac{u_w}{u_e - u_w} \right] = 0, \tag{19}$$

$$i''(\eta) \text{ sign } (u_e - u_w) + i'(\eta) \left[g(\eta) + \eta \frac{u_w}{u_e - u_w} \right]$$

$$+ m_1 (v_1'' - v_1') \frac{\omega_0}{\mu} i'(\eta) [A_1 i'(\eta) + A_2 g''(\eta)] = 0, \tag{20}$$

$$A_1 = (Y_{1e} - Y_{1w}) \Phi_N;$$

$$A_2 = Y_{Ne} - Y_{Nw} - (Y_{1e} - Y_{1w}) \Phi_N,$$

$$f'''(\tilde{\eta}) \text{ sign } (u_\infty - u_w)$$

$$+ f''(\tilde{\eta}) \left[f(\tilde{\eta}) + \tilde{\eta} \frac{u_w}{u_\infty - u_w} \right] = 0, \tag{21}$$

$$r''(\tilde{\eta}) \text{ sign } (u_\infty - u_w) + r'(\tilde{\eta}) \left[f(\tilde{\eta}) + \tilde{\eta} \frac{u_w}{u_\infty - u_w} \right] Pr_f$$

$$+ (Pr_f - 1) \text{ sign } (u_\infty - u_w) \frac{1}{H_{f\infty} - H_{fw}}$$

$$\times \{ u_w (u_\infty - u_w) f'''(\tilde{\eta}) + (u_\infty - u_w)^2$$

$$\times [f''^2(\tilde{\eta}) + f'(\tilde{\eta}) f'''(\tilde{\eta})] \} = 0. \tag{22}$$

When the first integrals of the gas boundary layer equations (18) and the balance relations at the phase interface, (12), (13), on having substituted into them the friction functions τ_w, τ_{wf}, mass flow rate $(\rho v)_w$ and heat fluxes $\mathbf{q}_w$, $\mathbf{q}_{wf}$, one obtains in the new similarity variables, the boundary conditions of system (19)–(22):

$$g'(0) = 0; \quad f'(0) = 0; \quad r(0) = 0; \quad i(0) = 0;$$

$$g'(\infty) = 1; \quad f'(\infty) = 1; \quad r(\infty) = 1; \quad i(\infty) = 1;$$

$$g(0) = -\text{sign}(u_e - u_w) B g''(0);$$

$$-g(0) Y_{1w} \text{sign}(u_e - u_w) = (Y_{1e} - Y_{1w}) i'(0); \tag{23}$$

$$g''(0) = f''(0)\sqrt{\frac{\rho_f\mu_f}{\rho\mu}}\left(\frac{u_\infty - u_w}{u_w - u_e}\right)^{3/2};$$

$$g(0) = -f(0)\sqrt{\frac{\rho_f\mu_f}{\rho\mu}}\left(\frac{u_\infty - u_w}{u_w - u_e}\right)^{1/2};$$

$$\begin{aligned}\frac{r'(0)}{f''(0)}c_f(T_w - T_\infty) &= Pr_f\frac{u_w - u_\infty}{u_e - u_w}\\ &\times[\hat{c}_{pe}(T_e - T_w) + Y_{1e}Q_p(T_w) - Bh_L]\\ &+\tfrac{1}{2}(u_w - u_\infty)\left[Pr_f(u_e - u_w) + 2u_w - \frac{r'(0)}{f''(0)}(u_w - u_\infty)\right];\end{aligned} \tag{24}$$

$$\begin{aligned}B = \Bigg[&(Y_{1w}\Phi_N + Y_{Ne} - Y_{1e}\Phi_N)\left(1 - \frac{p_e}{p_{Nw}}\right)\\ &+ \sum_{i=1}^{N-1}\frac{m_N}{m_i}(Y_{1w}\Phi_i + Y_{ie} - Y_{1e}\Phi_i)\Bigg]\Bigg/\Bigg[\frac{p_e}{p_{Nw}}(1 + Y_{1w}\Phi_N)\\ &- \left(1 + Y_{1w}\sum_{i=1}^{N}\frac{m_N}{m_i}\Phi_i\right)\Bigg]\end{aligned} \tag{25}$$

where

$$B = \frac{(\rho v)_w(u_w - u_e)}{\tau_w}$$

is the dimensionless parameter of mass transfer;

$$Q_p(T) = \Delta c_p T + \Phi_N \Delta H$$

is the specific heat of reaction at the temperature T; and

$$\Phi_i = \frac{m_i(v_i'' - v_i')}{m_1(v_1'' - v_1')}$$

is the stoichiometric relation.

The system of equations (19)–(22) with boundary conditions (23)–(25) and (13) forms a closed system of differential and transcendental equations in the unknown functions $g(\eta), f(\eta), r(\eta), i(\eta)$ and parameters Y_{1w}, T_w, u_w, B. In this case, the unknown functions $Y_i(\eta)$, $T(\eta)$, $\hat{c}_p(\eta)$, which enter into equation (20), are determined by the relations

$$\begin{aligned}T(\eta) &= \frac{\hat{c}_{pw}}{\hat{c}_p(\eta)}T_w - i(\eta)\frac{(Y_{1e} - Y_{1w})\Phi_N\Delta H}{\hat{c}_p(\eta)}\\ &- \frac{1}{2\hat{c}_p(\eta)}[u_w + (u_e - u_w)g'(\eta)]^2\\ &+ \frac{u_w^2}{2\hat{c}_p(\eta)} + \frac{g'(\eta)}{\hat{c}_p(\eta)}\Bigg[\hat{c}_{pe}(T_e - T_w)\\ &+ \frac{u_e^2 - u_w^2}{2} + (Y_{1e} - Y_{1w})Q_p(T_w)\Bigg];\\ Y_i(\eta) &= (Y_{1e} - Y_{1w})\Phi_i i(\eta) + g'(\eta)\\ &\times[Y_{ie} - Y_{iw} - (Y_{1e} - Y_{1w})\Phi_i] + Y_{iw},\\ i &= 2, \ldots, N;\\ \hat{c}_p(\eta) &= [1 - g'(\eta)]c_{pw} + g'(\eta)\hat{c}_{pe} + \sum_{i=1}^{N}c_{pi}\Phi_i\\ &\times[(Y_{1e} - Y_{1w})i(\eta) + Y_{1w} - g'(\eta)Y_{1e}]\end{aligned} \tag{26}$$

where the surface concentration Y_{iw} $(i = 2, \ldots, N)$ can be found from equations (18) and (12)

$$Y_{iw} = Y_{1w}\Phi_i + \frac{BY_{iwf} + Y_{ie} - Y_{1e}\Phi_i}{1 + B}.$$

The attempts to integrate the boundary-layer equations with combustion behind a shock wave [only one equation (19)] have been made in ref. [7]. However, having formulated the boundary conditions incompletely, the author failed to obtain a unique solution: for each value of the shock wave velocity there are several types of solutions.

As an example, in present work, calculations were made for the combustion of ethyl alcohol in air flow at $u_e \sim 1\ \mathrm{ms^{-1}}$. The choice of this specific example allows a comparison with the experimental data of refs. [3, 6]. The calculations were conducted for a model reaction

$$C_2H_5OH + 3O_2 \xrightarrow{\omega} 2CO_2 + 3H_2O.$$

The reaction rate ω_0 was assigned by the formula

$$\omega_0 = kT^{\Psi}p_e^4\left(\frac{m}{m_1}Y_1\right)^3\left(\frac{m}{m_N}Y_N\right)\exp(-15000/T),$$

$$\text{where}\quad k = 10^{-15},\quad \Psi = 2.5.$$

In writing equations (19)–(22) and boundary conditions (23) for this problem, it will be taken into account that sign $(u_e - u_w) = 1$; sign $(u_\infty - u_w) = -1$; $u_\infty = 0$. The estimates show that in the case of combustion of this kind of heterogeneous systems the following conditions are satisfied for subsonic regimes of flow

$$u_w^2;\ u_e^2 \ll c_f(T_w - T_\infty),$$

thus allowing the simplification of equations and boundary conditions for the given class of problems. Thus, equation (22) will have the form

$$r''(\tilde{\eta}) - Pr_f\, r'(\tilde{\eta})\,[f(\tilde{\eta}) + \tilde{n}] = 0, \tag{22'}$$

and boundary condition (24) can be rewritten as

$$\begin{aligned}\frac{r'(0)}{f''(0)}c_f(T_w - T_\infty) &= Pr_f\frac{u_w}{u_e - u_w}\\ &\times[\hat{c}_{pe}(T_e - T_w) + Y_{1e}Q_p(T_w) - Bh_L].\end{aligned} \tag{24'}$$

The results of numerical integration of system (19)–(22′) with boundary conditions (23), (24′), (25) are given in Fig. 2. The values of the unknown parameters obtained as a result of the joint solution of differential and transcendental equations are displayed in tabular form. Figure 3 presents concentration and temperature profiles calculated by formula (26) with solution of system (19)–(22′) being known (Fig. 2). The dash-dotted curves show the results of experimental measurements of concentration profiles (according to ref. [3]) and temperature profiles (according to ref. [6]). As is seen from Table 1, oxygen concentration near the fuel surface is very small ($Y_{1w} \sim 0.3\text{–}1.0 \times 10^{-3}$), which coincides with the results of ref. [20].

It is seen from Figs. 2 and 3 that there is a narrow zone in the flow with very rapidly changing parameters

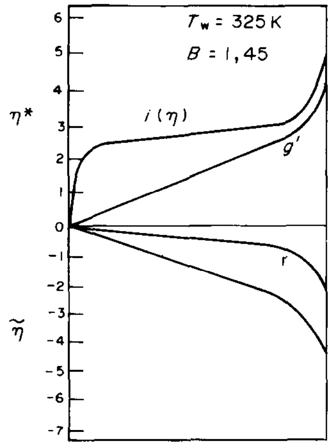

FIG. 2. Results of numerical integration of equations in gas and liquid.

making numerical calculations difficult. The presence of the zone of large concentration gradients testifies to the fact that chemical reaction has a strong effect not on the whole flow but on a narrow zone which may be taken for the surface of a diffusional flame. The comparison of the present calculations with those made within the framework of flame surface hypothesis (see ref. [11]) shows that this hypothesis allows one to describe, with a sufficient accuracy, the diffusional combustion and to substantially simplify the calculations. Therefore, the diffusional model seems to be adequate for the determination of the macroscopic characteristics of flame. The internal structure of the flame and the values of the parameters in the immediate vicinity of the flame surface should be found from the solution of the complete system of equations (19)–(22).

In order to simplify the calculations of macroscopic characteristics, the diffusional flame surface will be introduced which divides the boundary layer into two regions. In the region above the flame surface (superscript +), fuel vapours are absent ($Y_N^+ = 0$), but there are an oxidant and reaction products; in the region below the flame surface (superscript −) an oxidant is absent ($Y_1^- = 0$), but there are fuel vapours and reaction products [20]. The fuel, arriving by diffusion at the flame surface, combines with the oxidant and immediately enters into reaction. The rate of reaction product formation is governed by the rate of reagent supply to the flame surface as a result of diffusion.

Additional restrictions placed in this work on the distribution of the concentrations in the boundary layer ($Y_N^+ \equiv 0$; $Y_1^- \equiv 0$ and, consequently, $Y_{1\mathrm{w}} = 0$) make it possible to eliminate equation (20) and corresponding boundary conditions from the system. The resulting system of equations (19), (21), (22′) for the given problem of ethyl alcohol combustion in an oxidant flow is of the form:

$$g'''(\eta)+g''(\eta)\left[g(\eta)+\eta\frac{u_\mathrm{w}}{u_\mathrm{e}-u_\mathrm{w}}\right]=0,$$
$$f'''(\tilde{\eta})-f''(\tilde{\eta})\,[f(\tilde{\eta})-\tilde{\eta}]=0, \qquad (27)$$
$$r''(\tilde{\eta})-Pr_\mathrm{f}\,r'(\tilde{\eta})\,[f(\tilde{\eta})-\tilde{\eta}]=0$$

with the boundary conditions

$$g'(0)=0;\quad f'(0)=0;\quad r(0)=0;$$
$$g'(\infty)=1;\quad f'(\infty)=1;\quad r(\infty)=1;$$
$$g''(0)=f''(0)\sqrt{\frac{(\rho\mu)_\mathrm{f}}{\rho\mu}}\left(\frac{u_\mathrm{w}}{u_\mathrm{e}-u_\mathrm{w}}\right)^{3/2};$$
$$g(0)=-f(0)\sqrt{\frac{(\rho\mu)_\mathrm{f}}{\rho\mu}}\left(\frac{u_\mathrm{w}}{u_\mathrm{e}-u_\mathrm{w}}\right)^{1/2};$$
$$g(0)=-Bg''(0); \qquad (28)$$
$$\frac{r'(0)}{f''(0)}c_\mathrm{f}(T_\mathrm{w}-T_\infty)=Pr_\mathrm{f}\frac{u_\mathrm{w}}{u_\mathrm{e}-u_\mathrm{w}}$$
$$\times\,[\hat{c}_{\mathrm{pe}}(T_\mathrm{e}-T_\mathrm{w})+Y_{1\mathrm{e}}Q_\mathrm{p}(T_\mathrm{w})-Bh_1];$$
$$B=Y_{1\mathrm{e}}\Phi_N+\sum_{i=1}^{N-1}\frac{m_N}{m_i}(Y_{i\mathrm{e}}-Y_{1\mathrm{e}}\Phi_i)\left(\frac{p_\mathrm{e}}{p_{N\mathrm{w}}}-1\right)^{-1}.$$

Conditions (28) are supplemented by relation (13) for the determination of the partial pressure of fuel vapour ($p_{N\mathrm{w}}$) at the surface.

In the case when the Prandtl number in liquid is close to unity ($Pr_\mathrm{f} \sim 1$), the availability of the first integral of liquid boundary-layer equations

$$H_\mathrm{f}=(H_{\mathrm{f}\infty}-H_{\mathrm{fw}})\frac{u_\mathrm{w}-\tilde{u}}{u_\mathrm{w}}+H_{\mathrm{fw}} \qquad (29)$$

allows one to solve only the first two equations of system (27). In a general case ($Pr_\mathrm{f} \neq 1$), system (27) with boundary conditions (28) makes it possible to find the unknown functions $g(\eta), f(\tilde{\eta}), r(\tilde{\eta})$ and the values of the unknown parameters T_w, u_w, B. In this case the profiles of concentrations (Y_i), velocities ($u, \tilde{u}$), and temperatures (T) above and below the flame surface in a gas and in a fuel layer are determined from the first integrals of

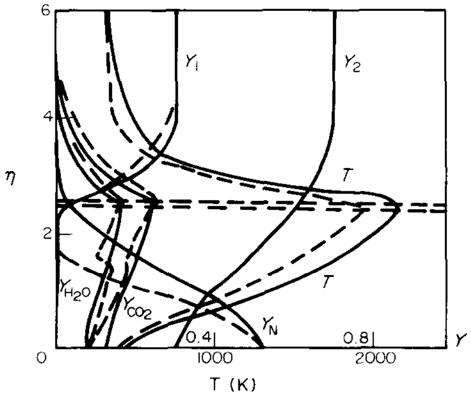

FIG. 3. Concentration and temperature profiles in a gas phase for the case of combustion of ethanol in an air flow (Y_1, oxidant O_2; Y_2, inert component N_2; Y_N, fuel C_2H_5OH).

Table 1. Parameters of the surface combustion of C_2H_5OH in the flow of air ($Y_{1e} = 0.3$) and pure oxygen ($Y_{1e} = 1.0$)

Y_{1e}	u_e (ms^{-1})	T_e (K)	T_∞ (K)	Y_{Nw}	T_w (K)	B	Y_{1w}	$g''(0)$	$f''(0)$	$r'(0)$	$i'(0)$	$\frac{u_w}{u_e - u_w}$
0.3	1	300	300	0.53	325	1.45	0.36×10^{-3}	0.250	0.610	2.153	4.4×10^{-4}	0.033
1.0	1	300	300	0.72	342	4.55	1.0×10^{-3}	0.126	0.592	2.063	6.0×10^{-4}	0.022

equation (14) and from the conditions $Y_1^- \equiv 0$, $Y_N^+ \equiv 0$:

$$\begin{aligned}
u &= (u_e - u_w)g'(\eta) + u_w; \\
\tilde{u} &= (u_\infty - u_w)f'(\tilde{\eta}) + u_w; \quad Y_N^+ = 0; \\
Y_N^- &= \frac{1}{1+B}[B - Y_{1e}\Phi_N - Bg'(\eta)(1 + Y_{1e}\Phi_N)]; \\
Y_1^- &= 0; \\
Y_1^+ &= \frac{1}{(1+B)\Phi_N}\{Y_{1e}\Phi_N[1 + Bg'(\eta)] \\
&\quad - B[1 - g'(\eta)]\}; \\
Y_i^- &= \frac{-\Phi_i Y_{1e}}{1+B}[1 + Bg'(\eta)]; \\
Y_i^+ &= \frac{-\Phi_i B}{(1+B)\Phi_N}[1 - g'(\eta)], \quad (i = 3, \ldots, N-1) \\
Y_2^\pm &= Y_{2e}\frac{1 + Bg'(\eta)}{1+B}; \\
\hat{c}_p^- &= [1 - g'(\eta)]\hat{c}_{pw} + g'(\eta)(\hat{c}_{pe} - Y_{1e}\Delta C_p); \\
\hat{c}_p^+ &= [1 - g'(\eta)]\hat{c}_{pw} + g'(\eta)\hat{c}_{pe} \\
&\quad + \Delta c_p \frac{Y_{1e}\Phi_N - B}{(1+B)\Phi_N}[1 - g'(\eta)]; \\
T- &= T_w \frac{\hat{c}_{pw}}{\hat{c}_p^-} + g'(\eta)(T_e - T_w)\frac{\hat{c}_{pe}}{\hat{c}_p^-} \\
&\quad + \frac{(u_e - u_w)^2}{2\hat{c}_p^-}[g'(\eta) - g'^2(\eta)] \\
&\quad + \frac{g'(\eta)Y_{1e}Q_{pw}}{\hat{c}_p^-}; \\
T^+ &= T_w \frac{\hat{c}_{pw}}{\hat{c}_p^+} + g'(\eta)(T_e - T_w)\frac{\hat{c}_{pe}}{\hat{c}_p^+} \\
&\quad + \frac{(u_e - u_w)^2}{2\hat{c}_p^+}[g'(\eta) - g'^2(\eta)] \\
&\quad + [1 - g'(\eta)]\frac{B - Y_{1e}\Phi_N}{1+B}\frac{\Delta H}{\hat{c}_p^+} \\
&\quad + g'(\eta)T_w \frac{\Delta c_p Y_{1e}}{\hat{c}_p^+}; \\
\tilde{T} &= T_w + r(\tilde{\eta})(T_\infty - T_w) + \frac{u_\infty^2 - u_w^2}{2c_f}r(\tilde{\eta}) \\
&\quad + \frac{f'(\tilde{\eta})}{c_f}(u_w - u_\infty)u_w - \frac{f'^2(\tilde{\eta})}{2c_f} \\
&\quad \times (u_\infty - u_w)^2.
\end{aligned} \tag{30}$$

In order to find the position of the flame surface in the boundary layer, use will be made of the property specifying the absence of fuel above, and absence of oxidant below, the flame surface. Then, the function β_N above and below the fuel surface has respectively the form

$$\beta_N^+ = \frac{-Y_1}{m_1(v_1'' - v_1')}; \quad \beta_N^- = \frac{Y_N}{m_N(v_N'' - v_N')}. \tag{31}$$

Since the differences between the stoichiometric coefficients for a fuel and oxidant $(v_N'' - v_N')$ and $(v_1'' - v_1')$ have the same sign, it can be seen from equation (31) that the function β_N changes its sign on transition through the flame surface. It follows from the continuity of the function β_N that at the flame surface ($\eta = \eta_*$) it is equal to zero:

$$\beta_N(\eta_*) = 0. \tag{32}$$

The use of equation (18) and relations at the phase interface makes it possible to obtain from equation (32) the condition for the determination of the flame surface [8, 11]

$$\begin{aligned}
g'_*(\eta_*) &= \frac{u^* - u_w}{u_e - u_w} = \frac{-\beta_{Nw}}{\beta_{Ne} - \beta_{Nw}} \\
&= \frac{Y_{Nw}}{Y_{Nw} + Y_{1e}\Phi_N} = \frac{B - Y_{1e}\Phi_N}{B(1 + Y_{1e}\Phi_N)},
\end{aligned}$$

from where the function $g'(\eta)$ known, it is not difficult to obtain the value of η_*.

Figure 4 presents the results of numerical integration of system (27) for the case when the liquid Prandtl number $Pr_f = 10$, which corresponded to the experimental conditions [6]. As is seen, a change in the oxidant concentration in the external flow Y_{1e} exerts a strong influence on the solution in a gas ($\eta > 0$) and practically has no effect on the solution in a liquid ($\tilde{\eta} > 0$).

For comparative purposes, the calculation for the case of $Pr_f = 1$ was made. In this case, the presence of the first integral in equation (29) substantially simplifies the procedure and reduces the time required for computations. The results have shown that for the problems investigated a change in the liquid Prandtl number from 1 to 10 has actually no effect on the basic parameters of the problem.

The distribution of concentration components above and below the flame surface, equation (30), is presented in Fig. 5 (Y_2 is the concentration of inert component N_2 (nitrogen), Y_3 is the concentration of CO_2, Y_4, of H_2O). The dash-dotted curves show

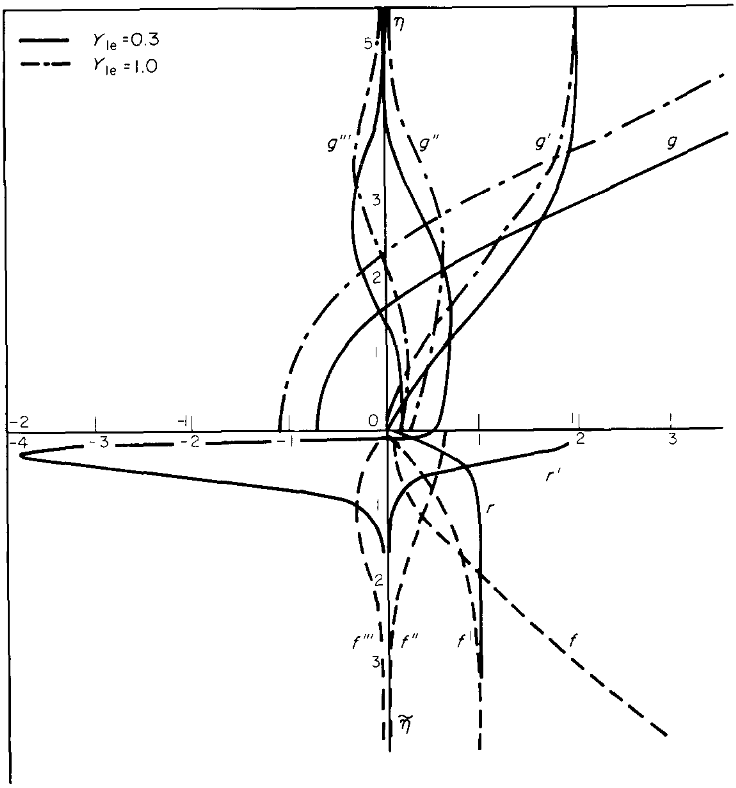

FIG. 4. Results of numerical integration of equations in gas and liquid based on the diffusional model of combustion (liquid Prandtl number $Pr_f = 10$).

variation of concentrations in accordance with the experimental data [3]. The comparison of the results of calculations on the basis of the diffusional model (Fig. 5) and kinetic model (Fig. 3) shows that the differences are insignificant and are basically concentrated near the flame surface. The discrepancy between the theoretical and experimental profiles of fuel concentration and the presence of carbon monoxide (CO) in reaction products [3] show that for a more accurate description of the reaction zone structure it is necessary to introduce additional stages of chemical reaction with their specific rates ω^k.

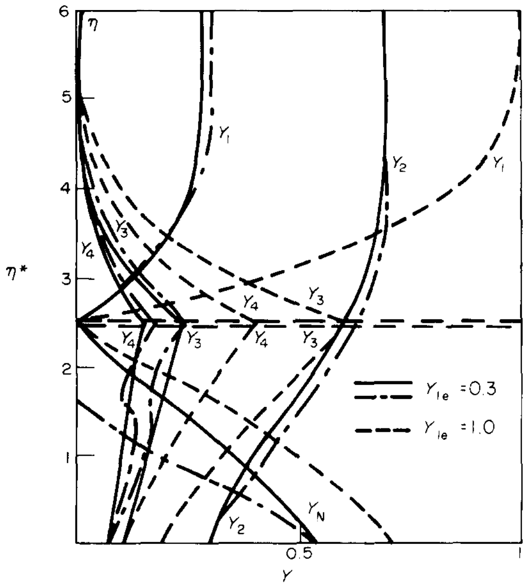

FIG. 5. Concentration profiles determined from the diffusional model for the combustion of ethyl alcohol in air ($Y_{1e} = 0.3$) and pure oxygen ($Y_{1e} = 1.0$): $Y_1 = O_2$; $Y_2 = N_2$; $Y_3 = CO_2$; $Y_4 = H_2O$; $Y_N = C_2H_5OH$.

Thus, in the present work the heat/mass transfer and combustion in an oxidant flow above a liquid fuel layer has been studied. The parameters of heat and mass transfer, the profiles of concentrations, velocities, and temperatures in a gas and liquid have been found. It is shown that for a wide class of problems the use of the diffusional model is possible, which allows substantial simplification of calculations.

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TRANSFERT DE CHALEUR ET DE MASSE DANS UN MELANGE GAZEUX EN REACTION CHIMIQUE AU-DESSUS D'UNE COUCHE LIQUIDE COMBUSTIBLE

Résumé—On étudie l'écoulement d'un mélange en réaction chimique au-dessus d'une surface de liquide combustible qui se détruit thermiquement. On considère la combustion du fioul dans l'écoulement d'un oxydant et la couche limite réactive derrière une onde de choc qui glisse sur la couche de fioul. La solution est obtenue en tenant compte du mouvement induit dans la couche liquide et de son interaction avec l'écoulement gazeux et aussi du changement des propriétés thermophysiques du gaz en fonction de sa composition. Les distributions des paramètres (vitesse, température, concentrations) sont obtenues pour les phases gazeuse et liquide. On détermine le débit masse de consommation surfacique du liquide.

WÄRME- UND STOFFTRANSPORT IN EINEM CHEMISCH REAKTIVEN MEHRKOMPONENTEN-GAS ÜBER EINER FLÜSSIGEN TREIBSTOFFSCHICHT

Zusammenfassung—Die Strömung einer chemisch reaktiven Gasmischung über einer brennenden Oberfläche von flüssigem Treibstoff wird untersucht. Das Verbrennen von unbewegtem Treibstoff in der Strömung eines Oxidanten und die Grenzschicht mit chemischen Reaktionen hinter einer über die Fluidschicht gleitenden Stoßwelle werden betrachtet. Die gewonnene Lösung läßt zu, daß die Gasströmung in der Flüssigkeitsschicht Bewegung induziert und daß sich die thermophysikalischen Stoffwerte des Gases je nach seiner Zusammensetzung ändern. Die Verteilungen von Geschwindigkeit, Temperatur und Konzentration in der Flüssig- und Gasphase und der Massenstrom der Verbrennungsprodukte wurden ermittelt.

ТЕПЛО- И МАССОПЕРЕНОС В МНОГОКОМПОНЕНТНОМ ХИМИЧЕСКИ РЕАГИРУЮЩЕМ ГАЗЕ НАД СЛОЕМ ЖИДКОГО ГОРЮЧЕГО

Аннотация—В работе исследовано течение химически реагирующей смеси газа над термически разрушающейся поверхностью жидкого горючего. При этом рассмотрено горение покоящегося топлива в потоке окислителя и пограничный слой с химическими реакциями за ударной волной, скользящей над слоем топлива. Решение получено с учетом движения, индуцируемого в слое жидкости при взаимодействии с потоком газа, и с учетом изменения теплофизических свойств газа в зависимости от состава. Найдены распределения параметров (скоростей, температур, концентраций) в жидкой и газообразной фазах. Определена массовая скорость выгорания поверхности топлива.