Reports of the Academy of Sciences of the USSR

1964

SovietRxiv

Abstract

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Reports of the Academy of Sciences of the USSR

1964. Volume 156, No. 4

HYDROMECHANICS

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ON THE THEORY OF A LAMINAR MULTICOMPONENT BOUNDARY LAYER ON A CHEMICALLY ACTIVE SURFACE

(Presented by Academician L. I. Sedov, 9 III 1964)

In the present note, by using the definitions of effective diffusion coefficients introduced in ([1]), a solution is given of the equations of a laminar multicomponent boundary layer in the neighborhood of a critical point (line) on the burning surface of a body of complex composition.

I. The problem of heterogeneous combustion of a material of complex composition in a steady gas flow in the neighborhood of a critical point (line) reduces to solving the following system of equations ([2]):

$$(l\varphi'')' + n\varphi\varphi'' = \varphi'^2 - \frac{\rho_e}{\rho}, \qquad (lS_i^{-1}c_i')' + n\varphi c_i' = 0 \quad (i = 1, \dots, N); \quad (1)$$

$$\left\{ l\sigma^{-1}\left[h' + \sum_{k=1}^{N}(L_k - 1)h_k c_k'\right]\right\}' + n\varphi h' = 0, \qquad l = \frac{\mu\rho}{\mu_0\rho_0},$$

$$S_i = \frac{\mu}{\rho D_i}, \qquad \sigma = \frac{\mu c_p}{\lambda}, \qquad L_i = \frac{\sigma}{S_i}$$

or

$$\left[l\sigma^{-1}(c_pT')\right]' + \sum_{k=1}^{N}\frac{l}{S_k}c_{pk}c_k'T' + n\varphi c_pT' = 0$$

with boundary conditions:

1) at the outer edge of the boundary layer

$$\varphi'(\infty) = 1, \qquad h(\infty) = h_e, \qquad c_i(\infty) = c_{ie}; \tag{2}$$

2) at the combustion front

$$(c_l^* - c_l^{*(1)})\, n\varphi(0) + \sum_{k=1}^{N} \frac{m_{lk}}{S_{k0}} c_k'(0) = 0, \qquad c_l^* = \sum_{k=1}^{N} m_{lk} c_k \quad (l = 1, \dots, p); \tag{3}$$

$$n\varphi(0)\,[h(0) - h^{(1)} + \Delta h^{(1)}] + \frac{1}{\sigma_0}\left[h'(0) + \sum_{k=1}^{N} (L_{k0} - 1) h_{k0} c_k'(0)\right] + \frac{q_r - \varepsilon\sigma_r T_0^4}{\sqrt{\beta\mu_0\rho_0}} = 0; \tag{4}$$

$$\varphi'(0) = 0, \qquad K_r(T) = \frac{p_1^{\nu_{1r}} p_2^{\nu_{2r}} \dots}{p_1^{\nu_{1r}'} p_2^{\nu_{2r}'} \dots} \quad (r = 1, \dots, N - p). \tag{5}$$

Here the subscript 0 refers to the values of the parameters at the combustion front, the subscript e to the values at the outer edge of the boundary layer; $n = 1$ corresponds to the plane case, $n = 2$ to the axisymmetric case; $\varphi(\eta)$ is the unknown function related to the stream function $\psi(x, y)$ by the relation

$$\psi(x, y) = \sqrt{\beta\mu_0\rho_0}\, \frac{x^2}{2}\, n\varphi(\eta),$$

where β is the velocity gradient of the inviscid flow in the neighborhood of the critical point (line); x, y are coordinates associated with the combustion front and directed along and normal to the combustion surface;

$$\eta = \left(\frac{\beta}{\mu_0\rho_0}\right)^{1/2} \int_0^y \rho\, dy;$$

D_i is the effective diffusion coefficient defined in ([1]); c_l^* is the concentration of element l;

p is the number of elements; m_{lk} is the mass fraction of element l in component k; q_r is the specific radiative flux from the shock wave to the combustion front; $\varepsilon\sigma_r T_0^4$ is the radiative flux from the front; $K_r(T)$ is the equilibrium constant of the r-th reaction at the combustion front; N is the number of components in the boundary layer; the remaining notation is standard. In the absence of reactions on the surface, instead of relations (3) one should impose the conditions of conservation of the mass of the individual components

$$(c_{i0} - c_i^{(1)})\, n\varphi(0) + S_{i0}^{-1} c_i'(0) = 0 \quad (i = 1, \dots, N), \tag{6}$$

where $c_i^{(1)}$ is the concentration of the i-th component at the blowing front on the condensed-phase side. Equation (4) expresses the law of conservation of energy at the combustion front. After solving problem (1)–(5), the mass burning rate $\rho_1 D$ will be determined from formula (2)

$$\rho_1 D = \sqrt{\beta\mu_e\rho_e}\,\frac{n\varphi(0)}{l_e^{1/2}}, \qquad l_e = \frac{\mu_e\rho_e}{\mu_0\rho_0}. \tag{7}$$

II. Let us give an approximate solution of the problem posed above without restrictions on the number of components in the mixture, based on the numerical solution of system (1) for homogeneous and binary boundary layers and on asymptotic integration of the diffusion equations at large generalized Schmidt numbers S_{i0}. As was shown in [1], for moderate blowing–$n\varphi(0) = 0.2$–0.6 and $0.30 < S_{i0} < 3$, the ratios of the mass-transfer coefficients are equal to

$$\frac{c_i'(0)}{c_{ie}-c_{i0}} = -\frac{S_{i0}}{\omega(\infty, S_i)}, \qquad \omega(\infty, S_i) = \int_0^\infty \frac{S_i}{l}\exp\left(-n\int_0^\lambda \varphi\frac{S_i}{l}\,dt\right)d\lambda; \tag{8}$$

$$\frac{c_i'(0)}{c_j'(0)}\,\frac{c_{je}-c_{j0}}{c_{ie}-c_{i0}} = 1. \tag{9}$$

If the heat capacities of the blown-in components are close to the heat capacities of the components of dissociated air, then the heat-influx equation (1), written in terms of temperature, contains no term with a sum and, similarly to the diffusion equations, one can immediately write a generalized analogy between heat and mass transfer. For example, for moderate blowing, instead of (9) we have

$$\frac{c_i'(0)}{h^{*\prime}(0)} = \frac{c_{ie}-c_{i0}}{h_e^*-h_0^*}, \qquad h^* = c_pT', \tag{10}$$

where

$$h_e^* - h_0^* = \sum_{k=1}^{N} c_{ke}(h_{ke}-h_{k0})$$

is the enthalpy drop in the boundary layer due to cooling of the mixture with composition c_{ke} from temperature T_e to temperature T_0 in the absence of chemical transformations. The solution of the heat-influx equation (1) under blowing of an arbitrary number of components with different heat capacities, i.e., when the boundary conditions (6) are satisfied, can be obtained by the method of integral relations. Indeed, as follows from the numerical solutions [3], the velocity, temperature, and concentration profiles in a frozen multicomponent boundary layer are close to linear. Then, approximating these profiles by straight lines over the corresponding boundary-layer thicknesses, we obtain, by the method of integral relations, analogously to how this was done in [4] for a binary mixture, the following expression for the heat-transfer coefficient:

$$\theta'(0) = \theta_0'(0) + \sigma_0 n \varphi(0) k, \qquad k = (1 - \tfrac{1}{3}\sigma_0^{-2/3}) k',$$

$$k' = 1 + \sum_{i=0}^{N} \left(\frac{c_{pi}}{c_{pe}} - 1 \right) (c_i^{(1)} - c_{ie})\, a_i(S_{i0}, \sigma_0), \tag{11}$$

$$\theta'(0) = \frac{h^{*\prime}(0)}{h_e^* - h_0^*}, \qquad a_i(S_i, \sigma) = \frac{\sigma_0^{1/3}}{2 S_{i0}^{1/3} (1 - \frac{1}{3}\sigma_0^{-2/3})},$$

where $\theta_0'(0)$ is the value of the function $\theta'(0)$ for zero blowing, and this value can be taken from the numerical solutions ([5])

$$\theta_0'(0) = 0.570(1 + 0.34n)\sigma_0^{0.4} l_e^{0.44 - 0.04n}. \tag{12}$$

Formula (11), for the case of a homogeneous boundary layer, for example for $-\varphi(0) = 0.5$ and $\sigma_0 = 0.7$, gives

$$\theta'(0) = \theta_0'(0) - 0.202\ (0.210) \quad (n = 1), \qquad \theta'(0) = \theta_0'(0) - 0.404\ (0.387) \quad (n = 2),$$

where the numbers given in parentheses are those obtained from the numerical solution. In the case of combustion at the surface, i.e., when the conditions of conservation of the chemical elements (3) at the front must be satisfied, one can also obtain, by the method of integral relations, an expression for $\theta'(0)$ analogous to (11). However, in view of its complexity we shall not give it, but in this case, for the quantity k', we shall use the simpler expression ([6]) $k' = (29/m_0)^{0.25}$, obtained for a binary boundary layer, where m_0 is the mean molecular weight at the wall.

From (11), putting $c_{pi} = c_{pe}$, one can obtain expressions for the mass-transfer coefficients in the form

$$z_i'(0) = \frac{c_i'(0)}{c_{ie} - c_{i0}} = \frac{S_{i0}}{\omega(\infty, S_i)} = z_{i0}'(0) + n\varphi(0) \left(1 - \frac{1}{3} S_{i0}^{-2/3} \right) S_{i0}, \tag{13}$$

where $z_{i0}'(0)$ is calculated from formula (12) with σ_0 replaced by S_{i0}. Using equation (9), the conditions (3) can be rewritten in the form

$$-\xi = \sum_{k=1}^{N} m_{lk} \frac{c_{k0} - c_{ke}}{c_{l0}^{*} - c_{l}^{*(1)}} \frac{D_{k0}}{D_{m0}} \quad (l = 1, \dots, p-1), \qquad \xi = -n\varphi(0)\,\omega(S_m), \quad (14)$$

where the index m refers to some component of the mixture; the auxiliary parameter ξ is related to the blowing parameter $n\varphi(0)$, by virtue of (13), by the relation

$$-\frac{n\varphi(0)}{(1+0.34n)l_e^{1/2}} = \frac{0.570}{S_{i0}^{0.6} l_e^{0.06+0.04n}} \frac{\xi}{1+\left(1-\frac{1}{3}S_{i0}^{-2/3}\right)\xi}. \qquad (15)$$

Assume that the following reactions occur at the combustion front:

$$2\mathrm{O} \rightleftarrows \mathrm{O}_2, \qquad 2\mathrm{N} \rightleftarrows \mathrm{N}_2, \qquad \mathrm{O}+\mathrm{N} \rightleftarrows \mathrm{NO}, \qquad \mathrm{C(g)} + \tfrac{1}{2}\mathrm{O}_2 \rightleftarrows \mathrm{CO}, \qquad (16)$$

$$\mathrm{C(g)} + \tfrac{1}{2}\mathrm{N}_2 \rightleftarrows \mathrm{CN}, \qquad \mathrm{C(g)} + \tfrac{1}{2}\mathrm{H}_2 + \tfrac{1}{2}\mathrm{N}_2 \rightleftarrows \mathrm{HCN}, \qquad \mathrm{C(g)} + \mathrm{O}_2 = \mathrm{CO}_2.$$

Then relation (4) may be represented in the following form, if one uses expressions (9), (10), (11), (12):

$$-\frac{n\varphi(0)}{l_e^{1/2}(1+0.34n)} = \frac{0.570}{\sigma_0^{0.6} l_e^{0.06+0.04n}} \frac{X + r_e - r_0 T_0^4}{\Delta + kX}, \qquad (17)$$

where

$$X = h_e - h_0 + (L_a - 1)h_d + (L_i)_0(1+\xi)\,[7029(c_{\mathrm{CO}})_0 + 3138(c_{\mathrm{CN}})_0 +$$

$$+5130(c_{\mathrm{HCN}})_0 + 5991(c_{\mathrm{CO2}})_0 \left(\frac{D_{\mathrm{CO2}}}{D_i} + \xi\right)(1+\xi)^{-1}\Big]; \qquad (18)$$

$$L_a = (L_i)_0 \left(\frac{D_a}{D_i}\right)_0, \qquad (L_i)_0 = \left(\frac{\sigma}{S_i}\right)_0 \quad (i = \mathrm{CO},\ \mathrm{CN},\ \mathrm{HCN});$$

$$r_e = \frac{q_r \sigma_0^{0.6} l_e^{0.06+0.04n}}{0.570(1+0.34n)\sqrt{\beta\mu_e\rho_e}}, \qquad r_0 = \frac{\varepsilon\sigma_r \sigma_0^{0.6} l_e^{0.06+0.04n}}{0.570(1+0.34n)\sqrt{\beta\mu_e\rho_e}};$$

h_d is the energy of dissociation per unit mass of air; Δ is the latent heat of vaporization and decomposition of the material; the numbers in square brackets in expression (18) denote the heats of formation of 1 g of the corresponding component in the reactions (16).

Equations (14), (15), (17), together with the equilibrium conditions at the combustion front, form a closed system for determining the composition, the temperature at the combustion front, and the parameter $n\varphi(0)l_e^{-1/2}$. For each specific material, with the aid of this system one can construct a nomogram of destruction. Indeed, using equations (14), (15) and the equilibrium conditions at the front, one can construct a series (depending on the stagnation pressure p_e) of curves for the parameter $n\varphi(0)l_e^{-1/2}(1+0.34n)^{-1}$, considered as a function of the temperature at the front T_0. The intersection of these curves with the graph of the function (17) of T_0, depending on the stagnation enthalpy h_e and the parameters r_e and r_0, will immediately give the temperature at the combustion front T_0 and the blowing parameter $n\varphi(0)l_e^{-1/2}(1+0.34n)^{-1}$. The mass rate of removal is then determined from formula (7).

III. Let us consider, as an example, the equilibrium combustion of graphite in dissociated air. In this case the above system of equations takes the following form (for simplicity we set $c_{CO_2} = 0$):

$$-\xi = \frac{{}^3/_7 c_{CO} + {}^6/_{13} c_{CN}}{{}^3/_7 c_{CO} + {}^6/_{13} c_{CN} - 1} = \frac{{}^4/_7 c_{CO} - \dfrac{D_{O_2}}{D_i}(c_{O_2})_e - (c_O)_e \dfrac{D_O}{D_i}}{{}^4/_7 c_{CO}}; \tag{19}$$

$$\sum_{k=1}^{N} c_k = 1, \qquad \frac{c_{CN}}{\sqrt{c_{N_2}}} = \frac{13}{\sqrt{7}} \frac{1}{\sqrt{pm}} e^{5.0468 - 19041/T}, \tag{20}$$

which, together with (17), where one should put $\Delta = 14132 + h_0^{(1)} - h_{-\infty}^{(1)}$, and with the expressions for the effective diffusion coefficients [1]

$$D_a = D_{ia}, \qquad D_{O_2} = D_{ij}, \qquad D_i = D_{ij}(1 + 0.63 c_{ae}) \quad (i, j = \mathrm{CO}, \mathrm{CN}) \tag{21}$$

forms a closed system for determining at the combustion front the quantities: c_{CO}, c_{CN}, c_{N_2}, T_0, and ξ. After this the mass rate of combustion is determined from formulas (7) and (15).

If the formation of cyanogen is neglected (low temperatures at the combustion front and sufficiently high pressures), then for the mass rate of combustion, with the aid of expressions (7), (15), and (19), a finite formula for the combustion rate can be obtained:

$$\frac{-\rho_1 D}{(1 + 0.34n)\sqrt{\beta u_e \rho_e}} = \frac{0.570}{S_{i0}^{0.6}} \frac{b}{{}^4/_3 + \left(1 - {}^1/_3 S_{i0}^{-2/3}\right) b}, \tag{22}$$

$$b = \frac{0.231 + 0.63c_{ae}}{1 + 0.63c_{ae}}, \qquad S_{i0} = \frac{0.775}{1 + 0.63c_{ae}},$$

from which it follows that even this simplest case cannot be described by the model of a binary boundary layer, since the effective diffusion coefficient for the combustion products CO and CN changes by 60% depending on the degree of dissociation of the air at the outer boundary of the boundary layer. For more complex materials, for example textolite, it is necessary to introduce at least 5 substantially different effective diffusion coefficients: D_i ($i = \mathrm{CO}, \mathrm{CN}, \mathrm{HCN}$), D_{H_2}, D_{CO_2}, D_a, D_{O_2}, in order to obtain sufficiently accurate values of the concentrations, the temperature at the combustion front, and the mass rate of removal.

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Received
8 III 1964

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Note: Figure translations are in progress. See original paper for figures.