DISTRIBUTION OF THE TRANSFER PARAMETERS DURING A REACTION BETWEEN THE MATERIAL OF A BODY SURFACE AND AN INJECTED SUBSTANCE WITH A BOUNDARY LAYER

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Described are the distributions of the Prandtl number, the Schmidt number, the Lewis number, the temperature, the enthalpy, the concentration, the diffusion currents, and the shear stresses across the height of a boundary layer with multicomponent diffusion.

When studying a reactive boundary layer, one considers either the reaction of the injected substance filtering through the porous wall with the gas in the outer stream, or the breakdown of the surface material of the body without injection [1].

The subsequent analysis here will take into account both these phenomena, i.e., the reaction of a carbon wall with hydrogen injected through it and an oxidizer in the outer laminar stream at infinite rates of both the heterogeneous and the homogeneous reaction:

$$2C + O_2 = 2CO, \tag{a}$$

$$2H_2 + O_2 = 2H_2O$$
, (b)

which occur within an infinitesimally thin zone at the wall surface.

The differential equations of transfer in a reacting transient boundary layer (during laminar flow) and the constraint equations have been transformed in [1] into the following self-adjoint form:

$$2\omega\omega'' + \rho\mu\mu = 0; \quad (\omega j_i)' + \omega'C_i = 0, \quad i = 1, 2, 3;$$

$$\left\{\omega \left[-H'/\Pr - (1 - \Pr^{-1}) u_{\infty}^2 \tilde{u} + \sum_i h_i (C_i/\Pr + \bar{j}_i)\right]\right\}' + \omega'H' = 0, \quad i = 1, 2, 3, 4. \quad (1)$$

$$\omega (1) = 0; \quad \omega' (0) = B^*/2; \quad C_1 (1) = C_{1\infty};$$

$$C_i (1) = 0, \quad i = 2, 3; \quad 2r_{\text{UI}} \bar{J}_3 = \bar{J}_H;$$

$$2r_{\text{II}} \bar{J}_2 = \bar{J}_C; \quad -2\bar{j}_1 \omega (0) = r^{-1} \bar{J}_C + r_1^{-1} \bar{J}_H;$$

$$2\omega' (0) Q (T_{\Pi}) = AT_{e} c_{P\Sigma e} \left[M(n) - M(1)\right] - 2\omega (0) \left(H' - \sum_i h_i C_i'\right) \Pr(0), \quad i = 1, 2, 3, 4, \quad (2)$$

where

 $\overline{j_i} = -C'_i/\mathrm{Sc}_i, \quad \overline{J}_i = \overline{J}_i \omega(0) + \omega'(0) C_i(0).$

The prime sign following a symbol in (1)-(2) and in subsequent expressions denotes a derivative with respect to \tilde{u} ($\tilde{u} = u/u_{\infty}$). The other designations are the same as in [1].

The composite system of nonlinear differential equations and constraints (1)-(2) describing the boundary layer at a porous wall with a chemical reaction between H₂, C, and oxygen O₂ of the outer stream as well as with a displacement of the wetted body surface due to reactions (a) and (b) will simplify appreciably

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• 1974 Consultants Bureau, a division of Plenum Publishing Corporation, 227 West 17th Street, New York, N. Y. 10011. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, microfilming, recording or otherwise, without written permission of the publisher. A copy of this article is available from the publisher for \$15.00. when $Pr = Sc_i = 1$ and $\tilde{\mu}\tilde{\rho} = 1$. The solution for this case is given in [1]. †

Problem (1)-(2) consisting of five second-order differential equations with 10 constraints, together with the system of N-1 relations between transforms of diffusion currents $\overline{j_i}$ ($\overline{j_i} = -C_i'/Sc_i$, i = 1, 2, 3) and derivatives C_i'

$$\frac{\mu}{\rho} \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} \begin{vmatrix} \overline{j}_1 \\ \overline{j}_2 \\ \overline{j}_3 \end{vmatrix} = \begin{vmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{vmatrix} \begin{vmatrix} C_1 \\ C_2 \\ C_3 \end{vmatrix},$$
(3)

obtained from expressions (33) in [1] with

$$\sum_{i} \overline{i}_{i} = 0, \qquad \sum_{i} C_{i} = 1, \quad i = 1, 2, 3, 4,$$
(4)

where

$$\begin{split} a_{11} &= C_1^{-1} \left[(1-C_3)/m_4 D_{14} + C_3/m_3 D_{13} \right], \quad a_{12} = a_{32} = b_{12} = b_{32} = 0, \\ a_{13} &= -(1/m_3 D_{13} + 1/m_4 D_{14}), \quad a_{21} = -(1/m_1 D_{21} + 1/m_4 D_{24}), \\ a_{31} &= -(1/m_1 D_{31} + 1/m_4 D_{34}), \quad a_{33} = C_3^{-1} [C_1/m_1 D_{31} + (1-C_1)/m_4 D_{34}], \\ b_{11} &= -C_1^{-1} [C_3/m_3 + (1-C_3)/m_4], \\ b_{13} &= b_{23} = (1/m_3 - 1/m_4), \quad b_{21} = b_{31} = (1/m_1 - 1/m_4), \\ b_{22} &= -C_2^{-1} [C_1/m_1 + C_3/m_3 + (1-C_1 - C_3)/m_4], \\ b_{33} &= C_3^{-1} [C_1/m_1 + (1-C_1)/m_4], \end{split}$$

and also together with the equations for determining the thermophysical properties of individual gas components $(\mu_i, \lambda_i, c_{Pi})$ as well as of their mixtures (u, λ, c_P) as functions of temperature T and concentration $C_{i\ddagger}$) was solved by numerical integration on a Minsk-22 computer with the following step $S(\tilde{u})$ of the independent variable $u: S(\tilde{u}) = 0.05$ for $0 \le \tilde{u} \le 0.9$ and $S(\tilde{u}) = 0.03$ for $0.9 \le \tilde{u} \le 0.99$. The constraint problem (1)-(2) was reduced to a Cauchy problem by specifying the boundary conditions only at the wall surface at $\tilde{u} = 0$.

With quantities $C_{i\infty}$ (i = 1, 2, 3) and T_{∞} given in (2) as well as with parameters u_{∞} and B, the constraints for $\overline{j_i}(0)$ (i = 1, 2, 3), H(0), $\omega(0)$, and $\omega'(0)$ were found from relations (2), whereupon the constraint problem (1)-(2) was solved with (3) as well as the temperature-dependence and the concentration-dependence of the thermophysical properties taken into account. With parameters thus specified, the Cauchy problem becomes completely determinate. It is solved by the Runge-Kutta method. At the outer edge of the boundary layer, at the point $\tilde{u} = 1$, which is a singular point, the finite values of the sought parameters $\omega(1)$, $\overline{j_1}(1)$, $C_2(1)$, and $C_3(1)$ will be functions of the given approximations to the unknown quantities. For example,

$$\Phi\left[\omega(0), \ \overline{j_1}(0), \ C_2(0), \ C_3(0)\right] = |\Delta\omega(1)|^2 + |\Delta\overline{j_1}(1)|^2 + |\Delta C_2(1)|^2 + |\Delta C_3(1)|^2,$$

where Δ denotes the difference between following and preceding values of respective parameters at point $\tilde{u} = 1$. When $\Phi \rightarrow 0$, the unknown quantities ω , j_i , and C_i become determinate. (The minimum of function Φ is determined by the gradient method [3].) The constraints (2) at $\tilde{u} = 1$ will also be satisfied within the appropriate accuracy, i.e., the solution to the Cauchy problem with initial values determined in this manner does, evidently, coincide with the solution to the original constraint problem. The results of numerical integration have been tabulated for various values of the injection number B, flow velocities u_{∞} , and temperatures T_{∞} , with the variation of thermophysical properties across the boundary layer taken into account (Figs. 1-4, Tables 1-2). Numerical results have also been obtained for $\Pr = Sc_i = 1$ and $\mu\rho = const$ (the curves in Figs. 1-3 and the values in Tables 1-2 correspond to $u_{\infty} = 15 \text{ m/sec}$).

According to the curves in Figs. 1-2, the normalized diffusion currents j_i as well as the Schmidt numbers Sc_i and the Lewis numbers Le_i vary appreciably within the $0.8 \le \tilde{u} \le 1$ zone adjacent to the outer edge of the boundary layer. Within the $\tilde{u} < 0.8$ zone all these quantities vary negligibly little. The largest variation across the boundary layer is characteristic of the numbers Le_i and Sc_i . Thus, while $Le_i = 0.835$,

 $[\]overline{\dagger \text{In } ([1])}$, p. 66) $u_0^{-1/2} = B^*/2$ should be corrected to $\tan \gamma u_0^{-1/2} = B^*/2$. $\ddagger \text{ This is relation } (34) \text{ in } [1].$



Fig. 1. Variation of numbers Pr, Sc_i, Le_i, and of C_i, j_i across the height \tilde{u} of a boundary layer, at various surface temperatures T_S of the porous wall and at various values of the injection number B: a, b) T_S = 1300°K, P = 0.2, B = 75; c, d) T_S = 2000°K, P = 0.2, B = 30; e, f) T_S = 2000°K, P = 0.2, B = 78.7; in f) the solid lines correspond to Pr \neq Sc_i \neq 1 and the dashed lines correspond to Pr = Sc_i = 1.

Fig. 2. Numbers Pr, Sc_i, Le_i, and C_i, $\overline{j_i}$ as functions of \tilde{u} , at various porosities P: a, b) T_S = 2500°K, P = 0.4, B = 25; c, d) T_S = 2500°K, P = 0.2, B = 25; in b) the solid lines correspond to Pr \neq Sc_i \neq 1 and the dashed lines correspond to Pr = Sc_i = 1.

 $Le_2 = 0.826$, $Le_3 = 1.136$, and $Le_4 = 1.058$ at $\tilde{u} = 0$ (Fig. 1a), for example, $Le_1 = 1.175$, $Le_2 = 1.139$, $Le_3 = 1.139$, $Le_$ = 2.261, and Le₄ = 1.963 at \tilde{u} = 0.99 \approx 1. The numbers Sc₃ and Sc₄ are at \tilde{u} = 0 approximately twice as high as at \tilde{u} = 1, the ratios are $Sc_i(0)/Sc_i(1) \approx 1.45$ and $\overline{j_i}(0)/\overline{j_i}(1) \approx 0.7$ for i = 1, 2 (Fig. 1b) but $\overline{j_i}(0)/\overline{j_i}(1) \approx 0.5$ for i = 3, 4. It is to be noted that the Prandtl number (Fig. 1a) varies only slightly (and almost linearly) across the boundary layer (thus, Pr = 0.783 and Pr = 0.756 at $\tilde{u} = 0$ and $\tilde{u} = 1$, respectively). Similar variations in parameters Pr, $\overline{j_i}$, Sc_i , and Le_i (i = 1, 2, 3, 4) are noted also in other cases (Figs. 1-2), with the relation $C_i = C_i(\tilde{u}), 0 \le \tilde{u} \le 1$ for the concentration being almost linear. The absolute values of $\overline{j_i}$ and C_i are very different when $Pr \neq Sc_i \neq 1$ and when $Pr = Sc_i = 1$. According to Figs. 1-2, $Pr = Sc_i = 1$ does not correspond to actual physical conditions. In many cases one may assume, however, that Pr = const across the boundary layer. As the injection of hydrogen (the B number) through the porous wall is increased, $C_3(0)$ and $\overline{j_3}$ increase inasmuch as the entire injected hydrogen H₂ converts into water H₂O according to reaction (b), while $C_2(0)$ and $\overline{j_2}$ decrease, but $C_4(0)$ and $\overline{j_4}$ change insignificantly inasmuch as nitrogen N_2 is in this case an inert substance. The concentrations $C_1(\tilde{u})$ and the normalized currents $\overline{j_1}(u)$ remain invariable as the injection number B is increased (Figs. 1-2), because the entire oxygen O_2 (at a given concentration $C_{1\infty}$) is taken up stoichiometrically in reactions (a) and (b). Numbers Pr and Sc_i (i = 1, 2, 3, 4), which are functions of the thermophysical properties u, \overline{c}_{P} , λ , ρ , and D_{i} determined from the composite system of relations



Fig. 3. Parameters ω and ω' , enthalpy H, and temperature T as functions of \tilde{u} , at various surface temperatures T_S and various values of the injection number B: a, b) P = 0.2, $T_S = 1300^\circ$ K; c, d) P = 0.2 and $T_S = 2000^\circ$ K; e, f) P = 0.2 and $T_S = 2500^\circ$ K. The solid lines correspond to $Pr \neq 1$ and the dashed lines correspond to $Pr = Sc_i = 1$.

TABLE 1. Variation of Parameters ω , ω' , H (kcal/kg), and T ([°]K) across the Height of a Boundary Layer, at P = 0.4

 ~]	Pr≠Sc _i ≠1				$Pr=Sc_i=1$					
u	. ω • 103	ω· · 10 ^a	H	T	@-10 ³	ω' - 103	H	T		
0,00 0,10 0,20 0,30 0,40 0,50 0,60 0,70 0,80 0,90 0,90 0,99 0,99 1,00	186 190 193 194 192 185 172 152 152 152 152 122 78 39 13 0	$\begin{array}{r} 44\\ 39\\ -22\\ -5\\ -43\\ -94\\ -159\\ -245\\ -362\\ -548\\ -763\\ -1029\\ -\infty\end{array}$	$\begin{array}{c} 685\\ 657\\ 628\\ 600\\ 572\\ 544\\ 516\\ 487\\ 458\\ 426\\ 405\\ 392\\ 390 \end{array}$	2500 2431 2361 2290 2218 2145 2069 1991 1908 1817 1755 1716 1702	$\begin{array}{c} 250\\ 261\\ 271\\ 276\\ 277\\ 270\\ 254\\ 226\\ 182\\ 116\\ 58\\ 18\\ 0\\ \end{array}$	$ \begin{array}{c} 118 \\ 108 \\ 80 \\ 34 \\ - 29 \\ - 111 \\ - 216 \\ - 351 \\ - 535 \\ - 822 \\ -2251 \\ - 1568 \\ -\infty \end{array} $	705	2500 2462 2422 2381 2298 2255 2210 2165 2118 2089 2075 2070		
				1	1	1	2			

(33) and (34) in [1], vary in our cases (Figs. 1-2) as follows as the B number is increased: the Pr number remains almost unchanged, the Sc_i (i = 1, 2, 4) numbers decrease, the Sc₃ number increases slightly. Considering that $Pr(\tilde{u}) \approx \text{const}$ within $0 \leq \tilde{u} \leq 1$, an increase or decrease in an Sc_i number causes the Le_i number (Le_i = Pr/Sc_i) to change in the opposite sense. It is to be noted that in the vicinity of point $\tilde{u} = 1$, which is singular, the error of numerical integration is maximum and, consequently, the largest deviation of calculated from exact values of parameters is possible here.

A comparison of Fig. 1a, b with Fig. 1e, f and Fig. 1c, d with Fig. 2c, d shows that, as the surface temperature T_s rises, the $Sc_i(0)$ numbers increase while the $Sc_i(1)$ numbers decrease. The concentrations C_i are almost the same but the normalized currents $\overline{j_i}$ differ appreciably at both surface temperatures as $\tilde{u} \rightarrow 1$. When the porosity is increased from 0.2 (Fig. 2c, d) to 0.4 (Fig. 2a, b), Sc_3 and Sc_4 decrease (Le₃ and Le₄ increase correspondingly). All other parameters remain approximately the same.

Variations of $\omega (\omega = \mu d\bar{u}/d\eta)$ and $\omega' (\omega' = d\omega/d\bar{u})$ as well as of enthalpy H (kcal/kg) and temperature (°K) across the boundary layer are shown in Fig. 3. In Table 1 these parameters are listed for P = 0.4, B = 30, and T_s = 2500°K. For the absolute values of B, T_s, and P considered here, a change of B, rather than of T_s or P, causes the most appreciable change in ω and ω' . Since ω and ω' are functions of the $\mu\rho$ factor in the first of Eqs. (1), hence we have for P = 0.2 (Fig. 3c) or for P = 0.4 (Table 1) with B = 30:

$$\omega'|_{P=0,2} < \omega'|_{P=0,4}, \quad \omega|_{P=0,2} > \omega|_{P=0,4}.$$





TABLE 2. Variation of the Friction Coefficient c_f and the Thermal Flux q_s (kcal/m²·sec) along the Porous Wall (x-Coordinate), at $T_c = 2000^{\circ}$ K, $u_{cc} = 15$ m/sec, B = 78.7

x, t	em	1	3 {	6	10	15	20 }	30	50
			Pr ≠Sc _i =	⊭1					
cf • 105	P=0,2 P=0,3 P=0,35	1533 1496 1475	885 864 852	626 611 602	485 473 466	396 386 381	343 335 330	280 273 269	217 212 209
q _s .10³	P=0,2 P=0,3 P=0,35	5131 5609 5853	2962 3238 3379	2095 2290 2390	1622 1774 1851	1325 1449 1511	1147 1254 1309	937 1024 1069	726 793 828
			Pr=Sci=	=1					
c _f • 10 ⁵	P=0,2 P=0,3	$\begin{array}{c} 2489\\ 2426 \end{array}$	1437 1400	1016 990	787 767	643 626	557 542	454 443	352 343
$q_{\rm S} \cdot 10^3$	P=0,2 P=0,3	4318 4785	2493 2763	1763 1954	1365 1513	1115 1236	965 1070	788 847	611 677

Furthermore, if H(0) and T(0) are, respectively, the same at P = 0.2 and at P = 0.4, then

$$T(1)|_{P=0.2} > T(1)|_{P=0.4}, \quad H(1)|_{P=0.2} > H(1)|_{P=0.4},$$
(5)

because, as the porosity of the graphite wall decreases, both the hydrogen current component \overline{j}_H and T(1) (or H(1)) increase, inasmuch as the heat of the exothermal reaction (b) is higher than that of reaction (a); in other words, the given temperatures T_S ($T_S = T(0)$) is reached at a lower ambient temperature T_{∞} ($T_{\infty} = T(1)$) when P = 0.4 than when P = 0.2. The increase in ω and ω' when $Pr = Sc_i = \tilde{\mu}\tilde{\rho} = 1$, as compared to their increase when $Pr \neq Sc_i \neq 1$, is related to the specifics of the first equation in system (1), where the largest values of ω and ω' correspond to the conditions $\tilde{\mu}\tilde{\rho} \rightarrow 1$ and $Pr = Sc_i = 1$ (Fig. 3, Table 1).

As temperature T_s rises (Fig. 4a, b), the local values of the friction coefficient c_f and of the thermal flux q_s defined as

$$c_{j} = \frac{2\omega(0)}{\sqrt{\operatorname{Re}_{x}}}, \quad q_{s} = \left[\frac{\lambda(0)}{\mu(0)}\omega(0) \frac{\rho_{\infty}u_{\infty}}{\sqrt{\operatorname{Re}_{x}}}\right]T'(0)$$
(6)

increase, with $\omega(0) = u_0^{-3/2}$ when $\Pr = Sc_i = 1$. Such an increase in c_f and q_s is due to a net change not only in the thermophysical properties in (6) but also in T'(0) and $\omega(0)$. The decrease in c_f and the increase in q_s with increasing u_{∞} (Fig. 4c, d) is explained in the light of relations (6), where $c_f \sim u_{\infty}^{-1/2}$ and $q_s \sim u_1^{1/2}$. A higher porosity of the graphite wall (Table 2), too, will reduce c_f and raise q_s because, as has been mentioned earlier, a higher P allows the temperature T_{∞} necessary for reaching the given temperature T_s to be lower and thus makes for a higher Reynolds number Re_x but a lower $\omega(0)$ and thus for a lower c_f and a higher q_s , the latter depending mainly on the temperature difference $\Delta T = T_s - T_{\infty}$ ($q_s \sim \Delta T$).

According to Fig. 4 and Table 2, c_f is higher and q_s is lower when $Pr = Sc_i = 1$ than when $Pr \neq Sc_i \neq 1$. The inequality

$$|c_f|_{\Pr=\operatorname{Sc}_i=1} > c_f|_{\Pr\neq\operatorname{Sc}_i\neq1}$$

is in the former case explained by an increase in $\omega(0)$ and a decrease in Re_X , but in the latter case q_S increases because the derivative T'(0) (T' = dT/du) is larger regardless of the decrease in $\omega(0)$ and the increase in Re_X in (6). Thus, in the first case and in the second case the factor inside the square brackets and T'(0) in (6) are equal to $133 \cdot 10^{-5}$, 532 and $119 \cdot 10^{-5}$, 290, respectively (T_S = 2500°K, B = 25, P = 0.2, x = 1 mm, u_{so} = 15 m/sec). The stream temperature T_{so} is 2180°K for the first case and 1910°K for the second case. In this way, according to Figs. 1-4 and Tables 1-2, the assumption Pr = Sc_i = 1 leads in our case to large deviations values from exact values.

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