

MULTICOMPONENT DIFFUSION AND HEAT EXCHANGE  
DURING THE FLOW OF AN IONIZED GAS IN CHEMICAL  
EQUILIBRIUM ABOUT A BODY

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In the present paper, we investigate the flow of a multicomponent, partially ionized gas mixture in the boundary layer around an impermeable surface; the state in the boundary layer being one of chemical equilibrium. As an example, the flow of partially ionized air about a sphere is considered. The chemical composition at every point of the boundary layer with running values of the pressure, temperature, and concentrations of the chemical elements was found by Newton's method, parallel with the integration of the fundamental system of nonself-similar differential equations by the curve-fitting method. Also discussed is another method of finding the composition, which is more economical from the point of view of expenditure of machine time. It is found that the dimensionless heat flux to the wall at the front critical point of the sphere can be 26% larger for constant concentrations of the chemical elements than it is for variable concentrations.

This paper is a continuation of [1], in which, for the case of flows of ionized mixtures without external electromagnetic fields, the fundamental Navier-Stokes and Prandtl system of equations is reduced to a form that is similar to the corresponding system for a chemically reacting mixture of neutral components by neglect of the electric field generated because of the separation of charges of components having different diffusion properties. In [1] it was shown that when the number of chemical elements in the ionized mixture is greater than 2, the chemical composition at each point of the flow depends not only on the pressure and temperature, but also on the concentrations of the chemical elements as new independent parameters. This circumstance leads to the appearance of additional terms in the energy equation that are proportional to the concentration gradients of the chemical elements.

In the present paper the system of equations for a partially ionized boundary layer in chemical equilibrium is integrated numerically by the curve-fitting method [2]. Profiles of the concentrations of components in the boundary layer with constant and variable concentrations of the chemical elements are compared for the case of flow of partially ionized air about a sphere. It is noticed that, in contrast to the case of dissociated air, when the concentration of the chemical element oxygen at the wall can be larger than it is on the external boundary of the boundary layer, in the case of partially ionized air an excess concentration of the chemical element nitrogen forms on the surface of the body. This is explained by the fact that, under the conditions considered, a larger percent of atoms of nitrogen than of oxygen are ionized at the external boundary of the boundary layer.

For the critical point of the body, approximate formulas are obtained for the dependence of the dimensionless heat flux on the drop in enthalpy and the parameter  $l/\sigma_{ef}$  across the boundary layer. (Here,  $\sigma_{ef}$  is the effective Prandtl number,  $l = \mu\rho/\mu_w\rho_w$ ,  $\mu$  is the viscosity of the mixture,  $\rho$  is the density of the mixture, and the index  $w$  denotes the surface of the body.)

In the case of ionization, the dimensionless heat flux in a chilled boundary layer can be 1.4 times larger than it is in an equilibrium boundary layer. With an accuracy of 5-10% the ratio of the heat fluxes

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at the lateral surface and at the critical point of a sphere up to an angle of  $80^\circ$  was found to be equal to the ratio of these quantities calculated in [3] for dissociated air on the basis of the hypothesis of local similitude, and other simplifying assumptions. This is explained by the mutual compensation of certain terms entering into this ratio. For angles greater than  $85^\circ$  the deviation in the ratio of heat fluxes from that found in [3] amounts to 25-30%.

1. The system of equations for a multicomponent partially ionized boundary layer in chemical equilibrium in the absence of external electromagnetic fields and energy transfer by radiation [1], written in terms of A. A. Dorodnitsyn's variables ( $\xi, \eta$ ) in Liz's form for the unknowns  $f, \theta, z_i^*$  ( $i = 1, \dots, N_e - 2$ )

$$\begin{aligned} \xi &= \int_0^x \mu_e \rho_e u_e r^{2\nu} dx, \quad \eta = u_e r^\nu \left( \frac{l_e}{2\xi} \right)^{1/2} \int_0^\eta \rho dy, \quad l = \frac{\mu \rho}{\mu_w \rho_w} \\ u &= u_e f \eta', \quad \rho v = r^{-\nu} \left[ (2\xi l_e)^{-1/2} \varphi \xi_{x'} + \left( \frac{2\xi}{l_e} \right)^{1/2} \eta_{x'} f \eta' \right] \\ \varphi &= f \left[ 1 - (\ln l_e) \xi' \right] + 2\xi f \xi', \quad \theta = \frac{T - T_w}{T_e - T_w}, \quad z_i^* = \frac{c_i^* - c_{iw}^*}{c_{ie}^* - c_{iw}^*} \end{aligned}$$

reduces to a form that is convenient for numerical integration by the scheme proposed in [2].

Here  $\mu, \rho, u, v$ , and  $r$  are, respectively, the viscosity of the mixture, the density, the projections of the mass-averaged velocity onto the tangent and the normal to the surface, and the distance from the axis of symmetry of the body;  $\nu = 0$  or  $1$ , respectively, for flow about a plane contour or about an axisymmetric body;  $T$  is the temperature,  $c_i^*$  is the concentration of the  $i$ -th chemical element,  $N_e$  is the number of chemical elements, the index  $e$  refers to quantities on the external boundary of the boundary layer,  $w$  to quantities on the body, and here, and throughout what follows a prime denotes a derivative with respect to the variable in the subscript.

This system of differential equations (for the momentum of the mixture, heat influx,  $N_e$  equations for the diffusion of the chemical elements), and the Stefan-Maxwell relations for a partially ionized gas are closed by algebraic conditions for chemical equilibrium and the conditions for the absence of a current and for quasineutrality. The boundary conditions on the nonpermeable surface are the following: the adhesion condition for the velocity components and conditions for the conservation of the chemical elements at a prescribed temperature of the body. At the external boundary layer the boundary conditions ( $u_e, T_e$ ) are found by solving a system of ordinary differential equations along a jet flow for a given pressure distribution, taken from known numerical solutions of the nonviscous problem. (In Section 3 the pressure distribution for a sphere was approximated by the data of [4].) The concentrations  $c_{je}^*$  ( $j = 1, \dots, N_e - 2$ ) of the chemical elements are constant along the external boundary of the boundary layer and are equal to their values  $c_{j\infty}^*$  in the oncoming stream.

For the determination of the chemical composition, it is necessary, parallel with the integration of the fundamental system of differential equations, to solve the following system of algebraic equations (with prescribed running values of the pressure  $p$ , the temperature  $T$ , and the concentrations of the chemical elements  $c_i^*$  ( $i = 1, \dots, N_e - 2$ ))

$$\sum_{i=1}^N \left( A_{ij} - \frac{m_i}{m_j} c_j^* \right) K_{pi} p^{v_i} \prod_{k=1}^{N_e} \exp(A_{ik} v_k) = 0 \quad (j = 1, \dots, N_e - 1)$$

$$\sum_{i=1}^N K_{i1} p^{v_i} \prod_{k=1}^{N_e} \exp(A_{ik} v_k) = 1, \quad v_i = \sum_{j=1}^{N_e} A_{ij} - 1, \quad v_i = \ln x_i \quad (1.1)$$

$$v_j = \sum_{k=1}^{N_e} A_{ik} v_k + \ln K_{pi} + v_i \ln p \quad (i = 1, \dots, N) \quad (1.2)$$

Here  $m_i$  and  $x_i$  are, respectively, the molecular weight and the molar concentration of the  $i$ -th component,  $A_{ik}$  is the stoichiometric coefficient in the reaction for the formation of a component with the chemical symbol  $E_i$  from the elements

$$E_i = \sum_{k=1}^{N_e} A_{ik} E_k - Q_i^*(T) \quad (i > N_e) \quad (1.3)$$

$$E_i \equiv E_i, \quad A_{ik} \equiv 1, \quad K_{pi} \equiv 1, \quad Q_i^*(T) \equiv 0 \quad (i \leq N_e)$$

The quantities  $Q_i^*$  and  $K_{pi}$  are the molar heat and the equilibrium constant of this reaction, respectively.

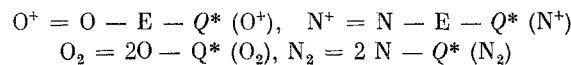
The system (1.1), (1.2) is suitable for solution by Newton's method, since one can first find all the  $v_j$  for  $j \leq N_e$ , from (1.1), and then, the remaining  $v_j$  ( $j > N_e$ ) from (1.2). For the corrections  $\Delta v_j$  ( $j \leq N_e$ ) during solution of the system of equations, one is obliged to determine an inverse matrix of order  $N_e$ . (Recall that usually the number of elements in a concrete problem is far less than the number of components.)

If relations (1.1) are differentiated with respect to  $\eta$ , and the resulting system is then solved for  $(v_i)_{\eta}'$ , we obtain a system of equations of the form

$$(v_i)_{\eta}' = \sum_{j=1}^{N_e-2} E_{ij} (c_j^*)_{\eta}' + E_{iN_e-2} T_{\eta}' \quad (i = 1, \dots, N_e) \quad (1.4)$$

where  $E_{ij}$  is a known function of  $p$ ,  $T$ , and  $v_j$ . Then, with prescribed  $(c_j^*)_{\eta}'$ ,  $c_j^*$ ,  $T$ ,  $T_{\eta}'$ , and  $p$ , we have a Cauchy problem for the determination of  $v_i$  ( $i \leq N_e$ ), and the remaining  $v_i$  ( $i > N_e$ ) are determined at each point from (1.2), it being supposed that the composition has been found at some point or another (for instance, by Newton's method). Thus, the system (1.4), (1.2) is sufficiently adjoined to the fundamental system of differential equations, solved by the curve-fitting method. In comparison with Newton's method this method can give a saving in machine time, since in Newton's method several iterations must be carried out at each point in order to obtain the required accuracy.

2. As an example, the fundamental boundary problem described above was solved in the special case of flow of partially ionized air about a sphere with no mass transfer through the surface. The range of temperature variation at the critical point on the external boundary of the boundary layer was from 10,000 to 16,000°K at stagnation pressures of from  $10^{-2}$  to 100 atm. Wall temperatures of 2000 and 3000°K were assumed. For the elements, O, E, (electrons), and N were considered, the following system of reactions being taken into account:



Heat capacities of the components were approximated by polynomials in  $T$  according to the data of [5], after which the equilibrium constants and reaction heats were expressed in terms of the coefficients of these polynomials and the equilibrium constants and reaction heats at some fixed temperature. The collision cross sections for the pairs neutral particle-neutral particle and neutral particle-charged particle were approximated as power functions of the temperature according to the data of [6, 7], and the charge transfer cross section, according to the data of [8]. The collision cross sections for the pairs charged particle-charged particle were taken as Coulomb cross sections. The coefficients of viscosity and heat conductivity of individual components and of mixtures, and also binary diffusion coefficients were calculated on the basis of formulas in [9].

Figure 1 shows profiles of molar concentrations (1:  $x(O)$ , 2:  $x(E)$ , 3:  $x(N)$ , 4:  $10 x(O^+)$ , 5:  $x(N^+)$ , 6:  $x(O_2)$ , 7:  $x(N_2)$ ) and the concentration  $c^*(O)$  of the chemical element O across the boundary layer at the critical point of the sphere for a stagnation temperature 14,000°K, wall temperature 3000°K, and stagnation pressure 1 atm; the dashed curves denoting profiles of corresponding concentrations under the assumption that  $c^*(O) = \text{const} = 0.231$  across the boundary layer. As can be seen from Fig. 1, in the boundary layer  $c^*(O)$  has a maximum 0.255, and a minimum 0.17, the concentration of the chemical element oxygen taking a value  $0.221 < 0.231$  on the wall. This is explained by the fact that under the external conditions under consideration, a greater percent of nitrogen atoms are ionized than atoms of oxygen, and this leads to an accumulation of the chemical element nitrogen on the surface of the body, so that the mobility of the ions is approximately twice that of the atoms. We recall that in the case of dissociation of air an excess of the element oxygen builds up on a wall [10-12]. It is necessary to take account of the phenomenon of separation of the elements in calculating the rate of disintegration of the body, because, in accord with the laws of conservation of the chemical elements at the wall, the magnitude of the gas blast through the surface is governed by

TABLE 1

$T_e$	$T_w$	2000		3000	
		$x$	$c_h$	$x$	$c_h$
10 000	$10^{-2}$	0.0815	0.326	0.188	0.34
	1	0.291	0.394	0.584	0.384
12 000	$10^{-2}$	0.045	0.223	0.102	0.218
	1	0.142	0.366	0.283	0.372
	10	0.309	0.409	0.465	0.402
	100	0.502	0.417	0.62	0.436
14 000	$10^{-2}$	0.07	0.186	0.156	0.21
	1	0.0745	0.294	0.1475	0.31
	10	0.195	0.381	0.284	0.388
	100	0.377	0.4025	0.464	0.415
16 000	$10^{-2}$	0.0783	0.188	0.173	0.1995
	1	0.0573	0.249	0.106	0.257
	10	0.125	0.339	0.182	0.33

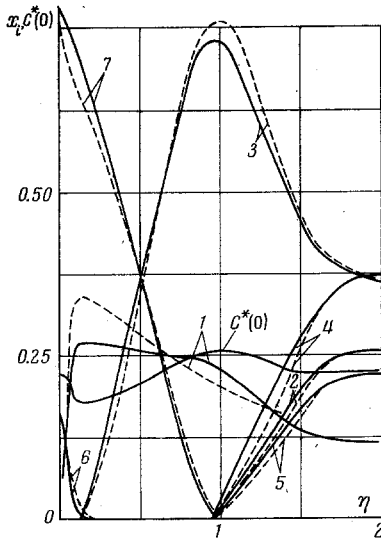


Fig. 1

a dependence on the quantity  $c_{iw}^*$ . This effect can also be important in taking account of radiation, since a change in even small concentrations by a few times can result in a substantial change in the absorption coefficients. The influence of separation of the elements on the heat flux is discussed below. By solving the fundamental boundary problem, one finds the heat flux  $(J_Q)_w$  to the wall according to the formula

$$\begin{aligned} (-J_Q)_w &= [(\nu + 1) \mu_w \rho_w \beta^*]^{1/2} \left[ \frac{c_p}{\sigma} (T_e - T_w) \theta_n' + \sum_{i=1}^N Q_i X_i \right]_w \\ &= [(\nu + 1) \mu_w \rho_w \beta^*]^{1/2} (T_e - T_w) \left[ \frac{\theta_n' \lambda_{ef}}{\mu} \right]_w, \quad \beta^* = \frac{u_e (\ln \xi)_{x'}}{2(\nu + 1)} \end{aligned} \quad (2.1)$$

$$J_i = \mu_w \rho_w u_e r^\nu \left[ \frac{l_e}{2\xi} \right]^{1/2} X_i, \quad \sigma = \frac{\mu c_p}{\lambda}, \quad Q_i^* = m_i Q_i, \quad \lambda_{ef} = \lambda + \lambda_r$$

Here  $\lambda$ ,  $\lambda_{ef}$ ,  $\lambda_r$ ,  $c_p$ , and  $J_i$  are, respectively, the heat conductivity, the effective heat conductivity [1], the heat conductivity due to chemical reactions [1], the heat capacity of the mixture, and the diffusion flux of the  $i$ -th component.

Results of calculation of the heat flux at the critical point of the sphere, given in Table 1, were approximated in the form

$$c_h = (0.772 - 2.9\chi^{-0.49} \frac{h_w}{h_e}) \chi^{0.235}, \quad 2000^\circ\text{K} \leq T_w \leq 3000^\circ\text{K} \quad (2.2)$$

$$c_h = \frac{\sigma_w (-J_Q)_w}{(\beta^* \mu_w \rho_w)^{0.5} (h_e - h_w)}, \quad \chi = \left( \frac{l}{\sigma_{ef}} \right)_e (\sigma_{ef})_w, \quad \sigma_{ef} = \frac{\mu c_p^{ef}}{\lambda_{ef}}, \quad c_p^{ef} = c_{pr} + c_p$$

where  $h$  denotes the total enthalpy and  $c_p$  is the heat capacity due to the course of the reaction (determined in [1]).

As a check on the influence of the separation of elements on the magnitude of the dimensionless heat flux  $c_h$  calculations at a constant value 0.231 for  $c^*(0)$  were carried out. At a wall temperature of 2000°K and a pressure of 1 atm the magnitude of  $c_h$  at constant  $c^*(0)$  was found to be 5-10% greater than the actual value, and at a wall temperature of 3000°K and a pressure of  $10^{-2}$  atm the excess amounted to 7, 26, 15, and 14%, respectively, for stagnation temperatures 10,000, 12,000, 14,000, and 16,000°K. A comparison was also made of the magnitude of  $c_h$  for an equilibrium (present paper) and a chilled [13] boundary layer. In contrast to a dissociated boundary layer around an ideally catalytic wall, where the difference in heat fluxes in the chilled and equilibrium cases is insignificant, with ionization, the  $c_h$  for a chilled boundary layer can exceed that for an equilibrium boundary layer by more than 40%. Thus, at  $T_w = 3000^\circ\text{K}$ ,  $p = 10^{-2}$  atm, the ratio of the dimensionless heat fluxes, calculated in the present paper, and in [13], amounted to 0.865, 0.596, 0.544, and 0.545, respectively, for  $T_e = 10,000, 12,000, 14,000,$  and  $16,000^\circ\text{K}$ . This difference

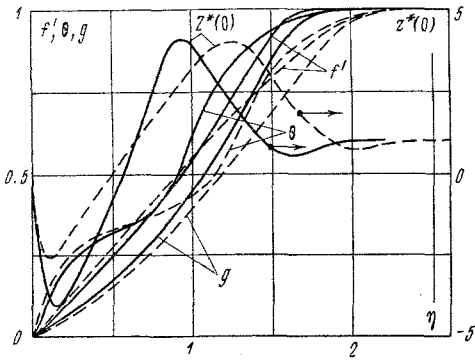


Fig. 2

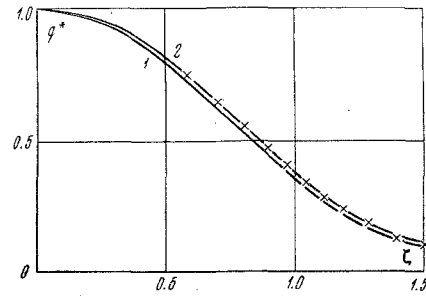


Fig. 3

is explained by the fact that in an equilibrium boundary layer a layer of atoms and molecules is formed at the surface of the body, which inhibits the penetration of charged particles to the wall, and their recombination on it, whereas in a chilled boundary layer the flux of charged particles to the wall can be considerable.

For sufficiently low wall temperatures, results of calculations of the convective heat flux at the critical point, obtained in the present paper, agree within an accuracy of 5-10% with the results of [7], which apply to an equilibrium boundary layer. This can be explained by the decrease in the influence of the separation of chemical elements on the magnitude of  $ch$  when the wall temperature is diminished ( $T_w \leq 2000^\circ\text{K}$ ).

The deviation in the magnitude of the convective heat flux found in the present work from the experimental data of [14] also amounted to 5-10%.

Let us turn to results of the calculation of the flow about the lateral surface of the sphere.

3. Figure 2 shows the profiles

$$f_{\eta}' = \frac{u}{u_e}, \quad \theta = \frac{T - T_w}{T_e - T_w}, \quad g = \frac{H - H_w}{H_e - H_w}, \quad H = \sum_{k=1}^{N_e} c_k \infty h_k - \sum_{k=1}^N c_k Q_k + \frac{u^2}{2} \quad (3.1)$$

and the dimensionless concentration of the chemical element oxygen O

$$z^*(O) = [c^*(O) - c_w^*(O)] / [c_e^*(O) - c_w(O)]$$

for flows about a sphere corresponding to a stagnation temperature of  $14,000^\circ\text{K}$ , a stagnation pressure of 1 atm, and a wall temperature of  $3,000^\circ\text{K}$ , the dashed curves indicating profiles with

$$\zeta = x / R = 1.475$$

while the solid curves correspond to  $\zeta = 0$ .

The ratio of the heat fluxes to the wall at a given point and at the critical point (index  $s$ ) can be represented in the form (we omit the index  $w$ )

$$q^* = \frac{J_q(x)}{J_q(0)} = \left( \frac{\beta^* \mu_{ws} \rho_w}{\beta_s^* \mu_{ws} \rho_{ws}} \right)^{0.5} \frac{\sigma_s^*}{\sigma^*} \frac{g_{\eta}'}{(g_{\eta}')_s},$$

$$\sigma^* = \frac{\mu (c_p^{**})_{ef}}{\lambda_{ef}} \quad (3.2)$$

where the quantity  $(c_p^{**})_{ef}$  has been defined in [1].

Figure 3 shows the distribution of  $q^*$  along the surface of the sphere, curve 1 corresponding to the conditions  $(T_s)_e = 14,000^\circ\text{K}$ ,  $p = 1$  atm, and  $T_w = 3,000^\circ\text{K}$ , the crosses corresponding to a surface temperature of  $2,000^\circ\text{K}$ , while curve 2 was obtained through calculation by an equation in [3], in which the distribution of the heat flux along the surface for the case of flow about a body of dissociated air was found on the basis of the hypothesis of local similitude under the assumption that the Lewis numbers of all the components are the same and equal to unity. Results of calculations of a nonself-similar problem that were made in that paper show that the ratios  $\sigma_s^*/\sigma^*$  and  $g_{\eta}'/(g_{\eta}')_s$ , entering into Eq. (3.2) and calculated from

the complete system of equations compensate each other in such a way that within an accuracy up to 5-10%, their product is equal to the ratio  $g_\eta'/(g_\eta')_S$ ,\* found and approximated in [3], where the simplifications mentioned above were made. For  $\xi > 1.45$  the hypothesis of local similitude ceases to be valid and the deviation in the results of the present paper and of [3] exceed 20%.

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\* As in Russian original - Publisher.