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ON THERMAL-DIFFUSION EFFECTS IN CHEMICALLY FROZEN MULTICOMPONENT BOUNDARY LAYER WITH SURFACE CATALYTIC RECOMBINATION BEHIND A STRONG MOVING SHOCK

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Abstract – Surface catalytic recombination of dissociated atoms in a chemically frozen multicomponent laminar boundary layer behind a strong, moving shock is analyzed. Chung's problem is generalized here to include the effects of thermal-diffusion, diffusion-thermo and multicomponent diffusion. Thermodynamically-coupled species conservation equation is solved, employing our decoupling transformation. New solutions, including the transport cross-coupling effects, are obtained for surface distribution of atoms when the temperature and the atom concentration vary arbitrarily in the inviscid, dissociating gas stream and the surface has an arbitrary but uniform catalycity. Thermal-diffusion effects on surface concentration distribution of dissociated oxygen and of dissociated nitrogen are presented for various temperature gradients across the boundary layer. The present results indicate that thermal-diffusion effects may cause significant changes in surface concentration distribution for large temperature gradients and therefore cannot be neglected in such problems.

NOMENCLATURE

a_m,	series expansion coefficients for the total enthalpy at the boundary layer edge;
b_{im},	series expansion coefficients for the concentration of *i*th species at the boundary layer edge;
b_{ij},	elements of the inverse modal matrix, given in the Appendix;
B_{jm},	series expansion coefficients of the ζ_j field at the boundary layer edge;
c_i,	$=\rho_i/\rho$, mass fraction of species i;
C,	$=\rho\mu/\rho_e\mu_e$, normalized density–viscosity product;
c_{pi},	specific heat of species i;
c_{pf},	$\Sigma_i^n c_i c_{pi}$, specific heat at constant pressure;
D_{ij},	multicomponent coefficient of diffusion of species i due to concentration gradient of species j;
D_{iT},	multicomponent thermal diffusion coefficient of species i;
D_{Ti},	multicomponent coefficient of diffusion-thermo due to concentration gradient of species i;
$\bar{f}(\bar{y})$,	dimensionless stream function;
h,	enthalpy;
$h^{(0)}$,	enthalpy of formation;
I,	$=h+\frac{1}{2}u^2$, total enthalpy;
$\mathbf{J}_{i_y}$,	mass flux of species i, in the y direction;
$\mathbf{J}_{q_y}$,	energy flux in the y direction;
k,	coefficient of thermal conductivity;
K_{iw},	surface recombination specific rate coefficient;
$\mathbf{M}$,	modal matrix defined in the Appendix;
n,	number of species;
p,	static pressure;
Pr,	Prandtl number;
$\tilde{Pr}_i$,	equivalent "Prandtl–Schmidt" numbers;
Sc,	Schmidt number;
t,	time;
T,	static absolute temperature;
u,	velocity component parallel to surface;
u_s,	shock velocity;
v,	velocity component normal to surface;
x,	coordinate along the surface;
y,	coordinate normal to surface;
$\bar{y}$,	transformed coordinate;
z_j,	transformed dimensionless coordinate, for ζ_j field.

Greek symbols

α_{ij}, β_j,	coupling coefficients;
γ_i, γ_{ji},	coupling coefficients;
ζ_j,	transformed "total enthalpy-concentration field";
η_j,	transformed coordinate for ζ_j field;
$\mathbf{\Lambda}$,	diagonal matrix with elements λ_i, defined in the Appendix;
λ_i,	eigenvalues of the matrix $\mathbf{\Omega}$;
μ,	viscosity;
ρ,	density;
ψ,	stream function;
$\mathbf{\Omega}$,	transport coefficient matrix;

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ω_{ij},	elements of the transport coefficient matrix $\mathbf{\Omega}$.

Superscripts

$*$,	dimensionless variable.

Subscripts

e,	boundary-layer edge;
i,	species i;
w,	surface $y = 0$ or $\eta = 0$;
∞,	free-stream.

1. INTRODUCTION

RECOMBINATION of dissociated gas in boundary-layer flows, induced by a strong shock wave advancing into a stationary fluid bounded by a wall, is of importance in chemical diagnostics of shock tubes and in investigation of explosion process and detonation waves. One of the most important current applications of surface recombination theories arises from the fact that the heat-transfer measurements on the surfaces of known catalycities, can be interpreted with those theories to determine the free stream atom concentration in high temperature laboratory facilities. The detailed discussion of the techniques and some of the measurements are given in the literature [1–3]. Most accurate diagnostics are possible when the gas-phase recombination is frozen.

The general theory for the boundary layer behind a moving shock has been extensively developed by Mirels [4, 5] and by Chung [6]. Chung [1] also composed a comprehensive review of chemically reacting nonequilibrium boundary layers including recombination problems. The particular problem analyzed by Chung [6] was concerned with strong, moving shock waves which produce substantial amounts of dissociation behind them. The gas which is set to motion by the shock, forms a boundary layer along the wall. The dissociated atoms diffuse through the boundary layer and recombine on the catalytic cold solid surface. The surface was considered to be of an arbitrary, constant, finite catalycity rate and the recombination process in the boundary layer itself was assumed frozen. The streamwise distribution of atom concentration in the inviscid flow behind the shock was considered to be given as an arbitrarily continuous function of the distance from the shock. However, the cross-coupling effects of transport phenomena, i.e. thermal-diffusion, diffusion-thermo and multicomponent diffusion effects have been omitted in Chung's analysis.

These thermodynamic coupling effects may, under certain operating conditions [7–10], cause appreciable changes in the values of heat and mass fluxes and cannot be neglected on an *a priori* basis, i.e. before estimating the expected results under the expected operating conditions. For instance, the experimental results of Tewfik *et al.* [7] show that the heat flux due to thermodynamic coupling is of the same order of magnitude (or even exceeds) the familiar Fourier heat flux and may be in the opposite direction. Inger [8] recently analyzed the effects of thermal-diffusion on oxygen distributions near intense fires and using a simple theoretical model he showed that these effects may cause local "over-shoots" relative to ambient conditions. Another comprehensive theoretical and experimental investigation of flame structure and flame reaction kinetics carried out by Dixon-Lewis *et al.* [9, 10] show that thermal-diffusion flux, for example hydrogen flux in a rich hydrogen + nitrogen + oxygen flame, may be of the same order of magnitude [9] or even exceeds [10] the ordinary diffusional flux.

Thermal-diffusion flux may be not only of the same order of magnitude but also in the opposite direction to the ordinary diffusional flux, (for example nitrogen flux in the above mentioned case [9]).

On the other hand, there are cases in which these coupling effects are negligible. For instance, Weihs and Gal-Or [11] analyzed the relaxation regions behind a moving shock of dissociated oxygen and of dissociated carbon-dioxide including thermodynamic coupling effects and showed that the contribution of these effects is small in the gas medium behind the shock. However, the boundary layer along the solid wall was not included in their analysis. In such boundary-layer problems the temperature of the gas medium behind the shock is raised very markedly relative to surface temperature. These steep temperature gradients across the boundary layer may cause (due to thermal-diffusion) significant changes in the flux values of dissociated atoms which diffuse through the boundary layer to recombine on the surface, as indicated in the present work. In addition, due to dissociation process caused by the moving shock wave and due to surface recombination, concentration gradients and diffusion fluxes may affect surface heat flux (diffusion-thermo phenomena). Hence, it becomes necessary to include these transport-coupling effects in the analysis of such boundary-layer problems. It is the purpose of this paper to present such an analysis.

2. GOVERNING EQUATIONS AND BOUNDARY CONDITIONS

A strong shock wave moving along a solid wall is considered. Unsteady coordinate system fixed to the wall is used (see Fig. 1), with an arbitrary origin, $x = 0$, where $t = 0$ denotes the time that the shock passes this origin. The boundary-layer equations are valid for the region behind the shock, i.e. $x \leq u_s t$, where u_s is the shock velocity. We consider here a laminar multicomponent compressible boundary layer which is induced by the strong shock wave advancing into the stationary fluid bounded by the wall. The boundary-layer equations are as follows:

continuity:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = 0 \qquad (1)$$

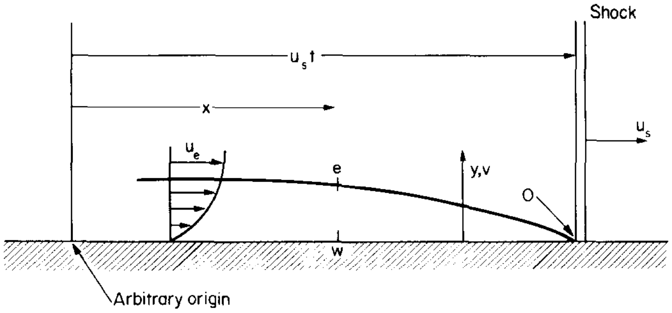

FIG. 1. Coordinate system for moving shock and boundary layer.

species:

$$\rho\frac{\partial c_i}{\partial t} + \rho u\frac{\partial c_i}{\partial x} + \rho v\frac{\partial c_i}{\partial y} = -\frac{\partial}{\partial y}(\mathbf{J}_{i_y}) \qquad (2)$$

$$i = 1,2,\ldots(n-1)$$

energy:

$$\rho\frac{\partial h}{\partial t} + \rho u\frac{\partial h}{\partial x} + \rho v\frac{\partial h}{\partial y} = -\frac{\partial}{\partial y}(\mathbf{J}_{q_y}) + \mu\left(\frac{\partial u}{\partial y}\right)^2 \qquad (3)$$

momentum:

$$\rho\frac{\partial u}{\partial t} + \rho u\frac{\partial u}{\partial x} + \rho v\frac{\partial u}{\partial y} = -\frac{\partial}{\partial y}\left(-\mu\frac{\partial u}{\partial y}\right) \qquad (4)$$

where the thermodynamically coupled multicomponent diffusion and energy fluxes, respectively are [15]

$$\mathbf{J}_{i_y} = -\sum_{j=1}^{n-1} D_{ij}\frac{\partial c_j}{\partial y} - D_{iT}\frac{\partial T}{\partial y} \qquad (5)$$

$$\mathbf{J}_{q_y} = -k\frac{\partial T}{\partial y} - \sum_{i=1}^{n-1} D_{Ti}\frac{\partial c_i}{\partial y} + \sum_{i=1}^{n-1} h_i J_{i_y}. \qquad (6)$$

Here the effects of thermal-diffusion, diffusion-thermo and multicomponent diffusion are considered.

Following Chung [6], the pressure and the streamwise velocity are assumed to be constant along the boundary-layer edge, as it is seen from equations (2) and (3). The pressure and inviscid velocity behind the shock, in practice, vary with the dissociative relaxation of the gas. However, the present study is concerned only with strong shocks which produce a significant amount of dissociation, for such strong shocks the variation of u_e and of the pressure can be neglected [6]. Other effects, such as variation of the concentration and the temperature along the boundary-layer edge, due to dissociation, will be considered here. As to the recombination process, it will be assumed that recombination takes place only on the solid surface, within the boundary layer, recombination will be taken as negligible [6]. (The existence of such flow regime was investigated also by Inger [12].)

The boundary conditions for the continuity, momentum and energy equations are: at $y = 0, u = 0, v = 0, h = h_w$, and at $y = \infty: u = u_e =$ constant, $h = h_e(x,t)$, where the subscripts w and e refer to the wall and edge of the boundary layer, respectively, and the enthalpy h is given by

$$h = \sum_i c_i\left[\int_0^T c_{pi}\,\mathrm{d}T + h_i^{(0)}\right].$$

For the species equations (2) the boundary conditions at the wall are much more complicated, since they are coupled, through thermal-diffusion and multicomponent-diffusion terms with the solutions of both, the species and energy equations. At $y = 0$ species boundary condition is

$$D_{ii}\left(\frac{\partial c_i}{\partial y}\right)_w + \sum_{\substack{j=1\\ j\neq i}}^{n-1} D_{ij}\left(\frac{\partial c_j}{\partial y}\right)_w + D_{iT}\left(\frac{\partial T}{\partial y}\right)_w = \rho_w K_{iw} c_{iw} \qquad (7)$$

and at $y = \infty$

$$c_i = c_{ie}(x,t). \qquad (8)$$

The RHS of equation (7) represents the rate of recombination of atoms on the cold wall. Assuming that the dissociative gas is diatomic, the recombination is usually a first-order chemical reaction [13, 14]. The rate of diffusion of atoms to the wall is equal to the rate at which the atoms recombine at the wall. Taking into account thermodynamic coupling contributions, the diffusion flux of ith species is not only due to its concentration gradient but also due to the temperature gradient (thermal-diffusion effect) and due to the concentration gradients of all other components present (multicomponent diffusion).

3. TRANSFORMATION OF GOVERNING EQUATIONS AND SOLUTION PROCEDURE

The solution of the field-equation set, equations (1)–(4), is difficult since it is mutually coupled. Furthermore, the species boundary condition, equation (7) is coupled to the solutions of both the species and energy equations through the species and temperature gradients at the wall.

To overcome these difficulties we first employ the general transformation presented in [15], in which the energy and species equations are decoupled and transformed into a widely useful energy-species equation. Thus, the energy and species equations (equation (3) and equation (2), $i = 1, 2 \ldots (n-1)$], are replaced by the energy-species equation

$$\rho \frac{\partial \zeta_j}{\partial t} + \rho u \frac{\partial}{\partial s} \zeta_j + \rho v \frac{\partial}{\partial y} \zeta_j = -\frac{\partial}{\partial y}\left[-\frac{\mu}{\tilde{P}r_j} \times \frac{\partial}{\partial y}\zeta_j - \frac{\mu}{\tilde{P}r_j}(\tilde{P}r_j - 1)\frac{\partial}{\partial y}\left(\frac{1}{2}u^2\right)^*\right] \quad (9)$$

where ζ_j is the transformed total enthalpy-concentration field defined by [15]

$$\zeta_j = \sum_{i=1}^{n-1} \alpha_{ji} c_i + \beta_j I^*. \quad (10)$$

Here, I is the total enthalpy

$$I = h + \frac{1}{2}u^2 \quad (11)$$

and α_{ji}, β_j are coefficients resulting from the diagonalization of the phenomenological coefficients matrix, and $\tilde{P}r_j$ is the equivalent Prandtl–Schmidt number in terms of eigenvalues of this matrix. (The asterisk denotes dimensionless values normalized by h_∞, the free-stream enthalpy.) In addition,

$$c_i = \sum_{j=1}^{n} \gamma_{ij} \zeta_j, \quad (12)$$

$$I^* = \sum_{j=1}^{n} \gamma_j \zeta_j, \quad (13)$$

where γ_{ij} and γ_j are defined in [15]. Thus, following the solutions of the transformed field ζ_j, one can arrive back at the physical fields c_i and I.

Next, the wall boundary conditions are to be expressed in terms of the ζ_j field. For that purpose, we first note that the coupled diffusion flux is obtained in transformed form by multiplying equation (9) by γ_{ij} and then summing over all n. Then, examining the nature of equation (12) we express the flux $J_{iy}(c_i, T)$ as $J_{iy}(\zeta_j)$. The latter obeys the conservation form equation

$$\rho \frac{\partial c_i}{\partial t} + \rho u \frac{\partial c_i}{\partial s} + \rho v \frac{\partial c_i}{\partial y} = -\frac{\partial}{\partial y}[J_{iy}(\zeta_j)], \quad (14)$$

where

$$J_{i_y}(c_i, T) \equiv J_{i_y}(\zeta_j) = -\left[\sum_{j=1}^{n} \gamma_{ij} \frac{\mu}{\tilde{P}r_j} \frac{\partial}{\partial y}\zeta_j + \sum_{j=1}^{n} \gamma_{ij} \frac{\mu}{\tilde{P}r_j}(\tilde{P}r_j - 1)\frac{\partial(\frac{1}{2}u^2)^*}{\partial y}\right]. \quad (15)$$

Hence, the diffusion flux of species i at the wall ($u = 0$) becomes

$$J_{iw} = -\left(\sum_{j=1}^{n} \gamma_{ij} \frac{\mu}{\tilde{P}r_j} \frac{\partial}{\partial y}\zeta_j\right)_w, \quad (16)$$

and by employing equations (5), (16) and (12), the species boundary conditions at the wall, equation (7), takes the form

$$\sum_{j=1}^{n} \gamma_{ij} \frac{\mu}{\tilde{P}r_j}\left(\frac{\partial \zeta_j}{\partial y}\right)_w = \rho_w K_{iw} \sum_{j=1}^{n} \gamma_{ij} \zeta_j. \quad (17)$$

This boundary condition will be satisfied here for each ζ_j, as follows

$$\frac{\mu}{\tilde{P}r_j}\left(\frac{\partial \zeta_j}{\partial y}\right)_w = \rho_w K_{iw} \zeta_j. \quad (18)$$

As to the remaining continuity and momentum equations, we follow Chung's [6] approach, and define a stream function ψ, as

$$\rho u = \rho_{e0}\left(\frac{\partial \psi}{\partial y}\right) \quad (19)$$

$$\rho v = -\rho_{e0}\left(\frac{\partial \psi}{\partial x} + \frac{\partial}{\partial t}\int_0^y \frac{\rho}{\rho_{e0}}\,\mathrm{d}y\right). \quad (20)$$

Then, in terms of the variable

$$\bar{y} = \left(\int_0^y \frac{\rho}{\rho_{e0}}\,\mathrm{d}y\right)\left[2C\frac{\mu_{e0}}{\rho_{e0}u_s}(u_s t - x)\right]^{-1/2} \quad (21)$$

a dimensionless stream function is introduced as [6]

$$\bar{f}(\bar{y}) = \psi(x, y, t)\left[2C\frac{\mu_{e0}}{\rho_{e0}}\frac{u_e^2}{u_s}(u_s t - x)\right]^{-1/2} \quad (22)$$

Hence, the momentum conservation equation becomes

$$\bar{f}''' + \left(\bar{y} - \frac{u_e}{u_s}\bar{f}\right)\bar{f}'' = 0 \quad (23)$$

subject to the following boundary conditions:

at $\bar{y} = 0$ $\bar{f} = \bar{f}' = 0$, and at $\bar{y} = \infty$ $\bar{f}' = 1$,

where the primes denote differentiation with respect to $\bar{y}$.

Now, to enable comparison with Chung's [6] results and to allow the new coupled solutions of the present study to be obtained in terms of Chung's solutions, we define here for each field ζ_j, the following dimensionless independent variables

$$\eta_j = \left(\frac{Pr_j}{Sc}\right)^{1/2}\bar{y} \quad (24)$$

$$z_j = \tilde{P}r_j(\rho_w K_{iw})(u_s t - x)^{1/2}\left(\frac{1}{2}C\rho_{e0}\mu_{e0}u_s\right)^{-1/2}. \quad (25)$$

Then, the energy-species equations finally becomes

$$\frac{1}{Sc}\frac{\partial^2 \zeta_j}{\partial \eta_j^2} + \left[\eta_j - \left(\frac{u_e}{u_s}\right)\left(\frac{Sc}{\tilde{P}r_j}\right)^{1/2} f(\eta_j)\right] = z_j\left[1 - \left(\frac{u_e}{u_s}\right)\left(\frac{Sc}{\tilde{P}r_j}\right)^{1/2}\frac{\partial f(\eta_j)}{\partial \eta_j}\right]\frac{\partial \zeta_j}{\partial z_j} \quad (26)$$

and according to equation (18) the wall boundary condition is

$$\text{at} \quad \eta_j = 0, \quad \frac{\partial \zeta_j}{\partial \eta_j} = z_j \zeta_j. \tag{27}$$

In addition, at the outer edge of the boundary layer,

$$\text{at} \quad \eta_j = \infty, \quad \zeta_j = \zeta_{je} = \sum_{m=0}^{\infty} B_{jm} z_j^m. \tag{28}$$

Here, the total enthalpy and the concentration of species distributions along the boundary-layer edge are expressed by the following series of z_j, respectively

$$I = I_e = \sum_{m=0}^{\infty} a_m z_j^m \tag{29}$$

and

$$c_i = c_{ie} = \sum_{m=0}^{\infty} b_{im} z_j^m \tag{30}$$

where, according to equation (10)

$$B_{jm} = \sum_{i=1}^{n} \alpha_{ji} b_{im} + \beta_j a_m. \tag{31}$$

Thus, the multicomponent, thermodynamically-coupled conservation equations and boundary conditions were recast here by means of the transformed field ζ_j to a mathematical form which is similar to Chung's equation form. Hence, solutions for ζ_{iw} are obtained here adopting Chung's method [6]. Then, to arrive back at the physical field, we use here equation (12), i.e. solutions for the surface atom concentration c_{iw} are carried out through the solutions of the transformed field ζ_{jw}, according to the following equation

$$c_{iw} = \sum_{j=1}^{n} \gamma_{ij} \zeta_{jw}. \tag{32}$$

4. RESULTS AND DISCUSSION

To enable comparison with Chung's [6] results, the same given sample of the boundary-layer edge concentration distribution is considered here as

$$c_e = 0.9998\,z - 0.6665\,z^2 + 0.1481\,z^3 \tag{33}$$

although the present solution is valid for any arbitrary variation of c_e (and T_e).

The surface atom concentration is calculated here using equation (32) for dissociated oxygen and for dissociated nitrogen for various temperature gradients across the boundary layer, where the normalized total enthalpy distribution $I/I_{\max}$, along the boundary-layer edge, is described here using the same coefficients that appear in equation (33).

The procedure by which the coupling coefficients can be determined for multicomponent mixtures is described in detail in [15]. However, the particular formulations for the cases that are illustrated in the present study, namely binary mixtures of atoms and homonuclear diatomic molecules, are given in the Appendix.

The surface atom distribution, for variable temperature and concentrations at the boundary layer edge, is presented in Fig. 2 for dissociated oxygen and for dissociated nitrogen. When thermodynamic coupling contributions are omitted from the present solution, the results reduce to Chung's [6] known solution. The effect of temperature gradient at a certain station (z = 1.4) is also presented (Fig. 3). The present results indicate that thermodynamic coupling effects, especially the thermal-diffusion effect, may cause significant changes in surface concentrations for large temperature gradients across the boundary layer. These effects cannot therefore be neglected in such problems as those encountered with strong moving shocks explosion processes and detonation waves.

It is also shown that thermal-diffusion has a greater effect upon the lighter gas (nitrogen in the present case), as seen by comparison with Chung's uncoupled solution.

In conclusion, a general analysis of thermodynamic coupling effects in boundary layer flows behind a strong moving shock has been presented. It was demonstrated how surface atom concentrations depend on temperature gradients across the boundary layer and on the molecular weight of the dissociated gas.

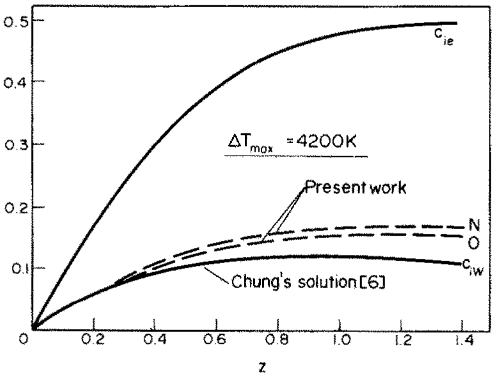

FIG. 2. Surface atom distribution (for variable temperature and concentrations at the boundary layer edge, N—nitrogen, O—oxygen).

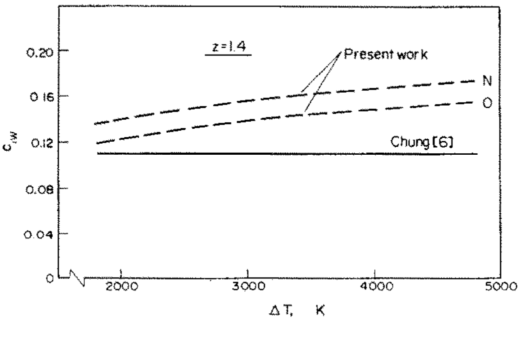

FIG. 3. Effect of temperature differential on surface atom concentration for z = 1.4 (N—nitrogen, O—oxygen).

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APPENDIX

The explicit particular formulations for the various coupling coefficients of binary mixtures of atoms and homonuclear diatomic molecules are given.

The transport coefficient matrix **Ω**, which is given in [15] for multi-component mixtures, reduces in the case of binary mixtures to the following form

$$\mathbf{\Omega} = \begin{pmatrix} \omega_{1,1} & \omega_{1,2} & \omega_{1,3} \\ \omega_{2,1} & \omega_{2,2} & \omega_{2,3} \\ 0 & 0 & 1 \end{pmatrix}, \tag{A.1}$$

where the elements of this matrix are given by

$$\omega_{1,1} = \frac{1}{\mu}\left[D_{1,2} - \frac{D_{1,T}}{c_{pf}}(h_1 - h_2)\right]; \tag{A.2}$$

$$\omega_{1,2} = \frac{1}{\mu}\left(\frac{D_{1,T}}{c_{pf}} h_x\right); \tag{A.3}$$

$$\omega_{1,3} = -\omega_{1,2}; \tag{A.4}$$

$$\omega_{2,1} = \frac{k+(h_1-h_2)D_{1,T}}{\mu c_{pf}}\left[\frac{\left(D_{1,2} + \dfrac{D_{T,1}}{(h_1-h_2)}\right)c_{pf}}{k+(h_1-h_2)D_{1,T}} - 1\right]\frac{(h_1-h_2)}{h_x}; \tag{A.5}$$

$$\omega_{2,2} = \frac{k + (h_1 - h_2)D_{1,T}}{\mu c_{pf}}; \tag{A.6}$$

$$\omega_{2,3} = 1 - \frac{k + (h_1 - h_2)D_{1,T}}{\mu c_{pf}}. \tag{A.7}$$

The transport coefficients are calculated according to the molecular theory of gases: $D_{1,2}$ is evaluated on the basis of the Lennard–Jones model [16] and for the thermal diffusion ratio the modified hard-sphere model is used [17]. The subscripts 1 and 2 refer to the atoms and to the homonuclear diatomic molecules, respectively.

The procedure by which the equivalent Prandtl–Schmidt numbers and the coefficients α_{ji}, β_i, γ_{ij} and γ_i are determined is described in detail in [15]. However, the explicit particular formulations for the present studied cases, are determined as follows:

Let **Λ** be the diagonal matrix with elements λ_1, λ_2 and a unity, which are the eigenvalues of the matrix **Ω**. **Λ** may be expressed as [15]

$$\mathbf{\Lambda} = \mathbf{M}^{-1}\mathbf{\Omega}\mathbf{M}, \tag{A.8}$$

where **M** is the model matrix, and $\mathbf{M}^{-1}$ is the inverse model matrix with elements b_{ij} (see [15])

$$\mathbf{M}^{-1} = \begin{pmatrix} b_{1,1} & b_{1,2} & b_{1,3} \\ b_{2,1} & b_{2,2} & b_{2,3} \\ 0 & 0 & b_{3,3} \end{pmatrix}. \tag{A.9}$$

Thus, the equivalent Prandtl–Schmidt numbers are defined by means of the eigenvalues of the coefficient matrix **Ω**, as

$$\tilde{P}r_1 = \frac{1}{\lambda_1} \qquad \tilde{P}r_2 = \frac{1}{\lambda_2}. \tag{A.10}$$

The coefficients α_{ji} and β_i are defined by means of the elements of the inverse modal matrix $\mathbf{M}^{-1}$

$$\alpha_{1,1} = \frac{b_{1,1}}{-b_{1,3}}; \quad \alpha_{2,1} = \frac{b_{2,1}}{-b_{2,3}}; \qquad \beta_1 = \frac{b_{1,2}}{-b_{1,3}}; \quad \beta_2 = \frac{b_{2,2}}{-b_{2,3}}; \tag{A.11}$$

and the coefficients γ_i and $\gamma_{i,j}$ are given by

$$\gamma_1 = \frac{-\alpha_{2,1}}{\alpha_{1,1}\beta_2 - \alpha_{2,1}\beta_1}; \quad \gamma_2 = \frac{\alpha_{1,1}}{\alpha_{1,1}\beta_2 - \alpha_{2,1}\beta_1}; \qquad \gamma_{1,1} = \frac{\beta_2}{\alpha_{1,1}\beta_2 - \alpha_{2,1}\beta_1}; \quad \gamma_{1,2} = \frac{-\beta_1}{\alpha_{1,1}\beta_2 - \alpha_{2,1}\beta_1}. \tag{A.12}$$

LES EFFETS DE LA DIFFUSION THERMIQUE DANS UNE COUCHE LIMITE A PLUSIEURS COMPOSANTS, CHIMIQUEMENT GELEE, AVEC UNE RECOMBINAISON SUR UNE SURFACE CATALYTIQUE, DERRIERE UN CHOC INTENSE ET MOBILE

Résumé — On analyse une recombinaison catalytique sur surface d'atomes dissociés dans une couche limite laminaire à plusieurs composants, chimiquement gelée, derrière un choc intense en déplacement. Le problème de Chung est généralisé pour inclure les effets de la thermodiffusion. On résout l'équation de conservation des espèces thermodynamiquement couplées, en employant une transformation de découplage. De nouvelles solutions qui incluent les effets de transport simultanés sont obtenues pour la distribution superficielle des atomes quand la température et la concentration atomique varie arbitrairement dans le gaz sans viscosité, et la surface a une propriété quelconque mais uniforme de catalyse. Les effets de thermodiffusion sur la distribution superficielle de concentration d'oxygène dissocié et d'azote dissocié sont présentés pour plusieurs gradients de température à la traversée de la couche limite. Les résultats indiquent que les effets de thermodiffusion peuvent provoquer des modifications sensibles de la distribution superficielle de concentration pour de forts gradients de température et ne doivent pas être négligés dans de tels problèmes.

ÜBER THERMISCHE DIFFUSIONSEFFEKTE IN EINER CHEMISCH EINGEFRORENEN, AUS MEHREREN KOMPONENTEN BESTEHENDEN GRENZSCHICHT MIT KATALYTISCHER REKOMBINATION AN DER OBERFLÄCHE HINTER EINER STARKEN DURCHLAUFENDEN STOSSWELLE

Zusammenfassung — Es wird die katalytische Oberflächenrekombination von dissoziierten Atomen in einer chemisch eingefrorenen, aus mehreren Komponenten bestehenden laminaren Grenzschicht hinter einer starken durchlaufenden Stoßwelle untersucht. Das Problem von Chung wird hier dahingehend verallgemeinert, daß die Effekte der Thermodiffusion und der Mehrkomponenten-Diffusion mitberücksichtigt werden. Die thermodynamisch gekoppelte Massenerhaltungsgleichung wird gelöst, indem unsere Entkopplungs-Transformation angewendet wird. Neue Lösungen, die die Querkopplungseffekte des Transports beinhalten, werden für die Oberflächenverteilung der Atome erhalten, wenn die Temperatur und die Atomkonzentration willkürlich in dem nicht-viskosen, dissoziierenden Gasstrom variieren und die Oberfläche eine willkürliche aber gleichförmige katalytische Wirksamkeit besitzt. Thermodiffusionseinflüsse auf die Oberflächenkonzentrationsverteilung von dissoziiertem Sauerstoff und dissoziiertem Stickstoff werden für verschiedene Temperaturgradienten in der Grenzschicht angegeben. Die vorliegenden Ergebnisse zeigen, daß Thermodiffusionseffekte signifikante Änderungen in der Oberflächenkonzentrations-Verteilung bei großen Temperaturgradienten verursachen und deshalb bei solchen Problemen nicht vernachlässigt werden dürfen.

О ТЕРМОДИФФУЗИОННЫХ ЭФФЕКТАХ В ХИМИЧЕСКИ ЗАМОРОЖЕННОМ МНОГОКОМПОНЕНТНОМ ПОГРАНИЧНОМ СЛОЕ ПРИ НАЛИЧИИ КАТАЛИТИЧЕСКОЙ РЕКОМБИНАЦИИ НА ПОВЕРХНОСТИ ЗА ПЕРЕМЕЩАЮЩИМСЯ СИЛЬНЫМ СКАЧКОМ УПЛОТНЕНИЯ

Аннотация — Анализируется поверхностная каталитическая рекомбинация диссоциированных атомов в химически замороженном многокомпонентном ламинарном пограничном слое за сильным перемещающимся скачком уплотнения. Уравнение сохранения термодинамически связанных компонентов решается нашим методом несвязанных преобразований. Новые решения, включающие перекрестные эффекты переноса, получены для распределения атомов по поверхности, когда температура и концентрация атомов изменяются произвольно в потоке невязкого диссоциирующего газа, а поверхность имеет произвольную, но однородную каталитическую способность. Показано влияние термической диффузии на распределение по поверхности концентрации диссоциированного кислорода и диссоциированного азота при различных градиентах температуры поперек пограничного слоя. Полученные результаты свидетельствуют о том, что термодиффузионные эффекты могут вызывать значительные изменения в распределении концентрации по поверхности при больших градиентах температуры, а поэтому должны учитываться в задачах такого типа.