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Natural convection due to horizontal temperature and concentration gradients—2. Species interdiffusion, Soret and Dufour effects

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Abstract—This study examines the influence of species interdiffusion, Soret and Dufour effects on the natural convection heat and mass transfer in a cavity due to combined temperature and concentration gradients. Results from numerical computations indicate that species interdiffusion reduces the overall heat transfer, but increases the mass transfer through the cavity for $h_A/h_B < 1$ and reduces the mass transfer for $h_A/h_B > 1$. Furthermore, contributions to the total mass flux through the cavity due to Soret diffusion can be as much as 10–15%. Similarly, energy transfer due to Dufour effects can be appreciable compared to heat conduction.

INTRODUCTION

THE CONSERVATION equations which describe the transport of energy and mass in fluid systems are well developed [1–4]. The energy flux includes contributions due to a temperature gradient (Fourier heat conduction), concentration gradient (Dufour diffusion) and a term which accounts for the energy transport as a result of each species having different enthalpies (species interdiffusion). The mass flux consists of terms due to a concentration gradient (Fickian diffusion), temperature gradient (Soret diffusion), pressure gradient (pressure diffusion) and a term which accounts for external forces affecting each species by a different magnitude.

The Soret mass flux and Dufour energy flux become significant when the thermal diffusion factor and the temperature and concentration gradients are large. The thermal diffusion factor increases as the ratio of molecular weights and ratio of the diameters of the molecules increases. Furthermore, the thermal diffusion factor depends on the molecular force interaction between like and unlike molecules [3]. If the molecular weight (mass) difference between species A and B is large and positive, the thermal diffusion factor is positive for all compositions. Hence, the heavier molecules (species A) migrate to the cold region. If the molecular weights are equal, then the larger diameter molecules concentrate in the colder region [3]. Species interdiffusion becomes appreciable as the difference between the specific heats of species A and B becomes large.

Typically, the energy transport is described adequately by Fourier diffusion and the mass transport by Fickian diffusion alone. Otherwise, several investigators [5–8] have shown both analytically and experimentally that both Soret and Dufour effects can be important contributions to the total mass and energy transfer, respectively. More recently, Rosner [9] has stressed that Soret diffusion is significant in several important engineering applications. Similarly, Atimtay and Gill [10] have shown Soret and Dufour diffusion to be appreciable for convection on a rotating disc. An error as high as 30% for the wall mass flux is introduced when the Soret effect is not accounted for. Of particular interest, crystal growth from the vapor is sometimes carried out under conditions conducive to appreciable species interdiffusion and Soret and Dufour effects. As greater demands are made for tighter control of industrial processes, species interdiffusion and second-order effects such as Soret and Dufour diffusion must be considered. Because of the limited number of studies available, the knowledge concerning the influence of these effects on the heat and mass transfer and fluid flow is incomplete.

ANALYSIS

Model equations

The system under consideration is described in a companion paper [11]. The governing conservation equations are identical except for the energy and species equations which are discussed below. By considering the thermodynamics of irreversible processes, it can be shown that the energy and mass fluxes are dependent on both concentration and temperature gradients [2]. Accounting for species interdiffusion and Soret and Dufour effects, the heat and species fluxes [3, 4] are, respectively

$$\mathbf{q} = -k\nabla T + \alpha_d RT \frac{M^2}{M_A M_B} \mathbf{j}_A + (h_A \mathbf{j}_A + h_B \mathbf{j}_B) \quad (1)$$

NOMENCLATURE

A_ξ	L/H
c_p	specific heat at constant pressure of binary mixture
c_p^*	specific heat ratio, c_p/c_{pr}
C_T	$T_C/(T_H - T_C)$
C_w	$\omega_C/(\omega_H - \omega_C)$
C_{wv}	$(1 - \omega_C)/(\omega_H - \omega_C)$
D_{AB}	binary mass diffusion coefficient
D_{AB}^*	binary mass diffusion coefficient ratio, D_{AB}/D_{ABr}
Gr	Grashof number, $g\beta_T(T_H - T_C)H^3/\nu_r^2$
h	enthalpy or heat transfer convection coefficient
h_m	mass transfer convection coefficient
H	test cavity height
$\mathbf{j}$	mass flux vector
$\mathbf{J}$	dimensionless mass flux vector, $\mathbf{j}H/\rho_r D_{ABr}(\omega_H - \omega_C)$
$\bar{J}$	average mass flux
J_d	mass flux due to diffusion (relative to the mixture velocity)
J_S	mass flux due to Soret effects
k	thermal conductivity of binary mixture
k^*	thermal conductivity ratio, k/k_r
K	constant in energy equation, $\Delta\omega_A c_{pr} \Delta T/(h_H - h_C)$
L	test cavity length
Le	Lewis number, α_r/D_{ABr}
M	molecular weight
M^*	molecular weight ratio, M_A/M_B
N^*	buoyancy parameter, $(\rho_C - \rho_H)/[\rho_r \beta_T (T_H - T_C)]$
Nu	Nusselt number
$\overline{Nu}$	average Nusselt number
Nu^+	Nusselt number including Dufour effects
Nu^*	Nusselt number including species interdiffusion
Pr	Prandtl number, ν_r/α_r
q	heat flux
$\mathbf{q}$	heat flux vector
Q	dimensionless heat flux, $qH/k_r\Delta T$
$\bar{Q}$	average heat flux
Q_a	advected energy flux
Q_d	energy flux due to diffusion
Q_{Du}	energy flux due to Dufour effect
Q_I	energy flux due to species interdiffusion
R	universal gas constant
Ra	Rayleigh number, $Gr\ Pr$
Sc	Schmidt number, ν_r/D_{ABr}
Sh	Sherwood number
$\overline{Sh}$	average Sherwood number
Sh^+	Sherwood number including Soret effect
T	temperature
ΔT	temperature difference across the cavity, $T_H - T_C$
u, w	dimensionless velocity in the ξ-direction (U/U_r) and ζ-direction (W/U_r), respectively
U_r	reference velocity, $(\nu/H)\ Gr^{0.5}$
x, z	Cartesian coordinate directed along the length and height of the test cell, respectively.

Greek symbols

α	thermal diffusivity, $k/\rho c_p$
α_d	thermal diffusion factor
β_C	solutal coefficient of volumetric expansion
β_T	thermal coefficient of volumetric expansion
ζ, ξ	dimensionless $z(z/H)$ and $x(x/H)$ direction, respectively
θ	dimensionless temperature, $(T - T_C)/(T_H - T_C)$
ι	dimensionless enthalpy, $(h - h_C)/(h_H - h_C)$
μ	dynamic viscosity of binary mixture
μ^*	dynamic viscosity ratio, μ/μ_r
ν	kinematic viscosity of binary mixture, μ/ρ
ρ	density of binary mixture
ρ^*	density ratio, ρ/ρ_r
ϕ	normalized mass fraction, $(\omega_A - \omega_C)/(\omega_H - \omega_C)$
ω	mass fraction
ω_H, ω_C	mass fraction of species A at the hot wall and at the cold wall, respectively
$\Delta\omega_A$	concentration difference across the cavity, $\omega_H - \omega_C$.

Subscripts

A	species A
B	species B
C	cold wall
H	hot wall
r	reference value, evaluated at $(T_H + T_C)/2$ and $(\omega_H + \omega_C)/2$
w	wall
ζ	in the ζ-direction
ξ	in the ξ-direction.

$$\mathbf{j}_A = -\rho D_{AB}[\nabla\omega_A + \alpha_d\omega_A(1 - \omega_A)\nabla \ln T] \quad (2)$$

where α_d is the thermal diffusion factor (dimensionless). The flux of species B in equation (1) can be eliminated because $\mathbf{j}_B = -\mathbf{j}_A$. The second and third terms on the right-hand side of equation (1) are the contributions to the energy flux due to a concentration gradient (Dufour effect) and to the interdiffusion of species (energy transfer because the species have different enthalpies). The second term on the right-hand side of equation (2) is the mass flux due to a temperature gradient (Soret effect). Using equations (1) and (2), the dimensionless conservation equations for energy and species are, respectively:

energy

$$\begin{aligned}
&\frac{\partial}{\partial \xi}(\rho^* u \imath)+\frac{\partial}{\partial \zeta}(\rho^* w \imath)\\
&=\frac{1}{Pr\sqrt{(Gr)}}\left[\frac{\partial}{\partial \xi}\left(\frac{k^*}{c_p^*}\frac{\partial \imath}{\partial \xi}\right)+\frac{\partial}{\partial \zeta}\left(\frac{k^*}{c_p^*}\frac{\delta \imath}{\partial \zeta}\right)\right]\\
&\quad-\frac{K}{Sc\sqrt{(Gr)}}\left[\frac{\partial}{\partial \xi}\left\{\left[\frac{R}{M_A M_B c_{pr}}[\alpha_d M^2(\theta+C_T)]\right.\right.\right.\\
&\quad\left.\left.+\frac{h_A-h_B}{c_{pr}(T_H-T_C)}\right]J_{A\xi}\right\}\\
&\quad+\frac{\partial}{\partial \zeta}\left\{\left[\frac{R}{M_A M_B c_{pr}}[\alpha_d M^2(\theta+C_T)]\right.\right.\\
&\quad\left.\left.\left.+\frac{h_A-h_B}{c_{pr}(T_H-T_C)}\right]J_{A\zeta}\right\}\right];
\end{aligned}\tag{3}$$

species A

$$\begin{aligned}
&\frac{\partial}{\partial \xi}(\rho^* u \phi)+\frac{\partial}{\partial \zeta}(\rho^* w \phi)\\
&=\frac{1}{Sc\sqrt{(Gr)}}\left[\frac{\partial}{\partial \xi}\left(\rho^* D_{AB}^*\frac{\partial \phi}{\partial \xi}\right)\right.\\
&\quad\left.+\frac{\partial}{\partial \zeta}\left(\rho^* D_{AB}^*\frac{\partial \phi}{\partial \zeta}\right)\right]+\frac{\omega_H-\omega_C}{Sc\sqrt{(Gr)}}\left\{\frac{\partial}{\partial \xi}\left[\rho^* D_{AB}^*\alpha_d(\phi\right.\right.\\
&\quad\left.+C_w)(C_{wv}-\phi)\frac{1}{\theta+C_T}\frac{\partial \theta}{\partial \xi}\right]+\frac{\partial}{\partial \zeta}\left[\rho^* D_{AB}^*\alpha_d(\phi\right.\\
&\quad\left.\left.+C_w)(C_{wv}-\phi)\frac{1}{\theta+C_T}\frac{\partial \theta}{\partial \zeta}\right]\right\}.
\end{aligned}\tag{4}$$

Further details can be found elsewhere [12].

The enthalpy at the wall is constant, because the temperature and concentration at the wall are constant ($x = 0$ and L)

$$\imath(0,\zeta)=1, \quad \imath(A_\xi,\zeta)=0. \tag{5}$$

At $z = 0$ and H, no energy is transferred (adiabatic wall), and the energy transfer due to diffusion is equal to that due to Dufour and species interdiffusion effects (equation (1)). Since the mass flux is zero at the impermeable top and bottom wall, the boundary condition on enthalpy is

$$\frac{\partial \imath}{\partial \zeta}=0 \quad \text{at } \zeta=0 \text{ and } 1. \tag{6}$$

Concentrations of species A are specified at the hot and cold walls

$$\phi(0,\zeta)=1, \quad \phi(A_\xi,\zeta)=0. \tag{7}$$

Impermeable walls at $z = 0$ and H specify no mass transfer at the boundaries. Therefore, mass transfer due to diffusion is counterbalanced by that due to Soret effects (equation (2)). Since the walls are adiabatic, the temperature gradient is zero (equation (6)) and the concentration boundary condition becomes

$$\frac{\partial \phi}{\partial \zeta}=0 \quad \text{at } \zeta=0 \text{ and } 1. \tag{8}$$

The velocity boundary conditions in terms of dimensionless variables are

$$\begin{aligned}
w(0,\zeta)=w(A_\xi,\zeta)=u(\xi,0)&=w(\xi,0)\\
&=u(\xi,1)=w(\xi,1)=0.
\end{aligned}\tag{9}$$

At the endwalls where heat and mass are transported, the boundary conditions are

$$u(0,\zeta)=\frac{1}{C_{wv}-1}\frac{1}{\rho^*\,Sc\,Gr^{1/2}}J_{A\xi}|_{\xi=0} \tag{10}$$

$$u(A_\xi,\zeta)=\frac{1}{C_{wv}}\frac{1}{\rho^*\,Sc\,Gr^{1/2}}J_{A\xi}|_{\xi=A_\xi} \tag{11}$$

where J_A includes Soret diffusion (equation (2)) and is not known a priori.

Dimensionless transport parameters

In addition to the transport parameters defined in the companion paper [11], the following parameters are defined. If the Dufour effect is considered, the energy flux at the wall is increased if the thermal diffusion factor and Q_d are positive. With the Dufour effect accounted for, the Nusselt number becomes

$$\begin{aligned}
Nu^+ &= -\frac{k^*}{c_p}\frac{h_H-h_C}{T_H-T_C}\frac{\partial \imath}{\partial \xi}\bigg|_{\text{wall}}\\
&\quad+Pr\,Gr^{0.5}\rho^* u\frac{h_A}{c_{pr}(T_H-T_C)}\\
&\quad+\frac{\omega_H-\omega_C}{Le}\left\{\frac{R}{c_{pr}}\frac{M^2}{M_A M_B}\alpha_d(\theta+C_T)J_{A\xi}\right\}
\end{aligned}\tag{12}$$

or $Nu^+ = (Q_d+Q_a+Q_{Du})$ where Q_{Du} is the dimensionless energy flux due to the Dufour effect. If species interdiffusion is considered (and the Dufour effect is neglected), the energy transfer at the wall becomes

$$\begin{aligned}
Nu^* &= -\frac{k^*}{c_p}\frac{h_H-h_C}{T_H-T_C}\frac{\partial \imath}{\partial \xi}\bigg|_{\text{wall}}\\
&\quad+Pr\,Gr^{0.5}\rho^* u\frac{h_A}{c_{pr}(T_H-T_C)}\\
&\quad+\frac{\omega_H-\omega_C}{Le}\left\{\frac{h_A-h_B}{c_{pr}\Delta T}\right\}J_{A\xi}
\end{aligned}\tag{13}$$

or $Nu^* = (Q_d+Q_a+Q_I)$ where Q_I is the dimensionless energy flux due to species interdiffusion. Species interdiffusion occurs at the hot and cold walls even though the mass flux of species B is zero ($n_B = 0$), because J_B is nonzero ($\rho_B U_B = n_B = \omega_B(n_B+n_A)+J_B$ or $J_B = -\omega_B n_A$). With the Soret effect accounted for, the Sherwood number is defined as

$$Sh^{+} = -\rho^* D^*_{\mathrm{AB}} \left\{ \left.\frac{\partial \phi}{\partial \xi}\right|_{\mathrm{wall}} + \alpha_{\mathrm{d}}(\omega_{\mathrm{H}} - \omega_{\mathrm{C}})(\phi + C_{\mathrm{w}})(C_{\mathrm{wv}} - \phi)\frac{1}{\theta + C_{\mathrm{T}}} \left.\frac{\partial \theta}{\partial \xi}\right|_{\mathrm{wall}} \cdot \right\} \tag{14}$$

or $Sh^{+} = (J_{\mathrm{d}} + J_{\mathrm{S}})$ where J_{S} is the dimensionless mass flux due to the Soret effect. The dimensionless mass flux J_d is equivalent to *Sh*, and is used to clarify the distinction between *Sh* and Sh^{+}.

RESULTS AND DISCUSSION

Influence of species interdiffusion

Interdiffusion accounts for energy transfer because the species have different enthalpies. Therefore, species interdiffusion becomes more significant as the difference in enthalpies of the species or the diffusive mass flux increases. To investigate the effect of species interdiffusion on the heat and mass tansfer, the specific heat of species B was varied only. The remaining parameters are $Gr = 1 \times 10^5$, $Pr = Sc = 1.0$, $N^* = -1.209$, $M^* = 5$, $\Delta\omega_{\mathrm{A}} = 0.3$, $\omega_{C} = 0.0$, $\Delta T = 37.7$ K, $T_{C} = 283.15$ K and $\alpha_{\mathrm{d}} = 0$ (Soret and Dufour effects are neglected). Note, since $\Delta\omega_{\mathrm{A}} = 0.3$ and $\omega_{\mathrm{C}} = 0$, the mixture is largely composed of species B and some of the following trends are particular to this situation. The average values of the mass flux, Nusselt number, advective energy flux, diffusive energy flux, energy flux due to species interdiffusion and the Sherwood number at the hot and cold walls are given in Table 1 (nt and wnt denote simulations which account for and which neglect species interdiffusion, respectively). To reiterate, the advection in and out of the cavity refers to the enthalpy of species A only (not the mixture enthalpy, since species B is noncondensable). This distinction becomes significant as $c_{p\mathrm{A}}/c_{p\mathrm{B}}$ differs from unity (species interdiffusion exhibits the same trend). The thermophysical properties of species A are represented by those of ethanol and of species B by nitrogen except for the specific heat which is varied for each case [13–17] (for both nt and wnt: case 1, nitrogen, $c_{p\mathrm{B}} = 1041$ J kg^{-1} K^{-1}; case 2, argon, $c_{p\mathrm{B}} = 521$ J kg^{-1} K^{-1}; case 3, arbitrarily chosen to be half of $c_{p\mathrm{B}}$ for helium, $c_{p\mathrm{B}} = 2597$ J kg^{-1} K^{-1}; case 4, helium, $c_{p\mathrm{B}} = 5193$ J kg^{-1} K^{-1}).

Case 1nt is the same as case 1wnt except species interdiffusion is accounted for in the model equations. Since $h_{\mathrm{A}}/h_{\mathrm{B}}$ is approximately one, the heat and mass transfer changes little as expected. Consider the one-dimensional transport situation which examines diffusion and species interdiffusion energy transfer only

$$\frac{\partial}{\partial x}\left[-\frac{k}{c_p}\frac{\partial h}{\partial x} + (h_{\mathrm{A}} - h_{\mathrm{B}})J_{\mathrm{A}x}\right] = 0. \tag{15}$$

Integration of this equation with respect to x yields

$$-\frac{k}{c_p}\frac{\partial h}{\partial x} = \mathrm{constant} - (h_{\mathrm{A}} - h_{\mathrm{B}})J_{\mathrm{A}x} \tag{16}$$

or

$$Q_{\mathrm{d,nt}} = Q_{\mathrm{d,wnt}} - Q_{\mathrm{I,nt}} \tag{17}$$

where the constant of integration is the diffusive

Table 1. Summary of the average mass flux, Nusselt number, energy flux due to advection, diffusion and species interdiffusion and Sherwood number at the hot and cold walls for natural convection in binary gases (nt denotes cases where species interdiffusion is accounted for and wnt where species interdiffusion is neglected in the analysis: case 1, $h_{\mathrm{A}}/h_{\mathrm{B}} = 1.08$, case 2, $h_{\mathrm{A}}/h_{\mathrm{B}} = 2.16$; case 3, $h_{\mathrm{A}}/h_{\mathrm{B}} = 0.44$; case 4, $h_{\mathrm{A}}/h_{\mathrm{B}} = 0.22$)

Case	$\overline{\rho^* u} \times 10^3$	$\overline{Nu^*}$	$\overline{Q}_{\mathrm{a}}$	$\overline{Q}_{\mathrm{d}}$	$\overline{Q}_{\mathrm{I}}$	$\overline{Sh}$
			Hot wall			
1wnt	5.61	18.58	15.12	3.46		4.14
1nt	5.53	18.73	14.91	3.01	0.81	4.08
2wnt	5.52	25.06	24.48	0.58		4.07
2nt	3.42	16.96	15.19	−3.94	5.72	2.53
3wnt	5.59	12.56	6.94	5.62		4.13
3nt	6.22	9.00	7.72	8.30	−7.03	4.59
4wnt	5.59	10.07	3.65	6.42		4.13
4nt	6.42	4.02	4.19	10.39	−10.56	4.74
			Cold wall			
1wnt	5.53	18.57	12.42	6.15		5.83
1nt	5.51	18.76	12.38	6.10	0.27	5.81
2wnt	5.58	25.14	20.58	4.57		5.88
2nt	3.42	16.85	12.62	−2.22	6.45	3.61
3wnt	5.61	13.02	5.80	7.21		5.92
3nt	6.24	9.48	6.45	12.29	−9.27	6.57
4wnt	5.61	10.63	3.05	7.57		5.91
4nt	6.43	4.63	3.50	14.67	−13.54	6.78

energy flux without accounting for species interdiffusion. For case 1nt, $Q_{\mathrm{d,wnt}}$ and $Q_{\mathrm{I,nt}}$ are both positive which results in $Q_{\mathrm{d,nt}} < Q_{\mathrm{d,wnt}}$. This trend is evident in Table 1 where Q_{d} for case 1nt is smaller than Q_{d} for case 1wnt (Q_{d} decreased less at the cold wall where the interdiffusion contribution is smaller).

Some general trends are noted from Table 1. When species interdiffusion is not included (cases denoted by wnt), changing $c_{p\mathrm{B}}$ results in an appreciable variation of $\overline{Q}_{\mathrm{A}}$ and $\overline{Q}_{\mathrm{d}}$ only (i.e. enthalpy or temperature field is affected). Advection at the wall is enhanced as $c_{p\mathrm{B}}$ is reduced (Fig. 1), because the enthalpy of the fluid leaving the cavity is greater compared to the mixture enthalpy (or specific heat). Furthermore, $\overline{Q}_{\mathrm{d}}$ is decreased as $c_{p\mathrm{B}}$ is reduced (Fig. 2).

When the effect of species interdiffusion is accounted for in the analysis (cases denoted by nt), $\overline{Q}_{\mathrm{a}}$, $\overline{Q}_{\mathrm{d}}$ and $\overline{Sh}$ (Figs. 1–3, respectively) are changed appreciably with variations of $c_{p\mathrm{B}}$ (i.e. enthalpy and concentration fields are affected). Since the temperature field is significantly altered when species interdiffusion is accounted for, the variation in thermophysical properties is also changed which affects both the velocity and concentration fields (Figs. 4–7). If $c_{p\mathrm{B}}$ is reduced, $\overline{Sh}$ is decreased. Similar trends for $\overline{Q}_{\mathrm{d}}$ for cases without species interdiffusion are noted for cases with species interdiffusion. However, the variation of $\overline{Q}_{\mathrm{a}}$ owing to decreasing $c_{p\mathrm{B}}$ with interdiffusion included is quite different from that when interdiffusion is not included (Fig. 2). The advected energy increases only slightly when $c_{p\mathrm{B}}$ is decreased because of the offsetting effects of a decreasing $c_{p\mathrm{B}}$ and decreasing mass flux (concentration gradient at the wall is decreased). The variation of $\overline{Q}_{\mathrm{a}}$ directly affects $\overline{Nu^*}$ which results in $\overline{Nu^*}$ decreasing when $c_{p\mathrm{B}}$ is decreased. These results must be viewed with prudence due to the limited number of cases presented.

Effect of decreasing h_{B}. If $c_{p\mathrm{B}}$ is decreased (case 2wnt), the variation in c_p^* is increased, and the mixture enthalpy decreases (compared to case 1wnt). This decreases the diffusive energy flux and slightly increases the advective flux at the hot and cold walls. The larger variation in c_p^* results in a greater difference between the diffusive energy flux at the hot and cold wall for case 2wnt as compared to case 1wnt. For case 2nt, the species interdiffusion opposes the diffusive energy transfer. The advective contributions to the energy balance are smaller (circulation is weaker, Fig. 4(b)), resulting in an enthalpy field influenced more by diffusion effects (Fig. 5(b)). If the enthalpy field is due to diffusion only, the enthalpy isolines would be approximately linear and parallel to the hot and cold walls. The enthalpy field affects the velocity field (Fig. 4(b)) which, in turn, influences the concentration distribution (Fig. 6(b)) in the cavity. The velocity, enthalpy and concentration fields are intimately coupled through the thermophysical properties and buoyancy term. From Table 1, $Q_{\mathrm{d,wnt}}$ and $Q_{\mathrm{I,nt}}$ are positive, but $Q_{\mathrm{I,nt}} > Q_{\mathrm{d,wnt}}$ resulting in $Q_{\mathrm{d,nt}} < 0$.

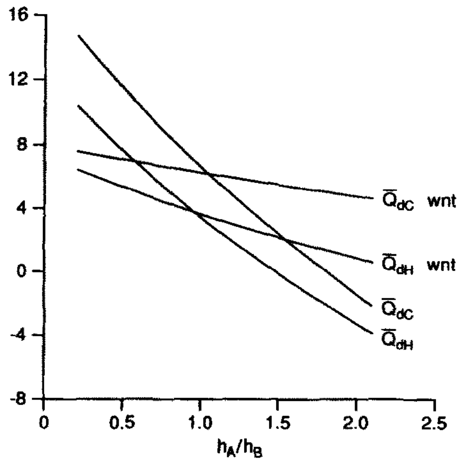


FIG. 2. Variation of the average energy flux due to diffusion with $h_{\mathrm{A}}/h_{\mathrm{B}}$.

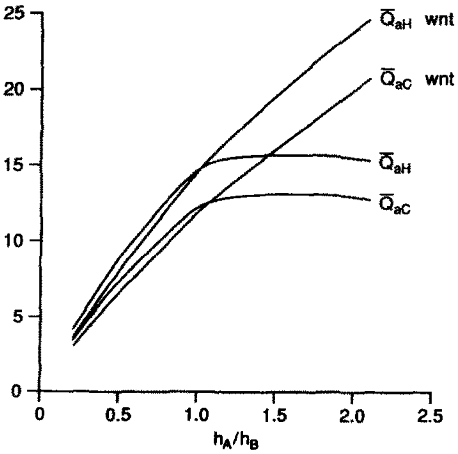


FIG. 1. Variation of the average energy flux due to advection with $h_{\mathrm{A}}/h_{\mathrm{B}}$.

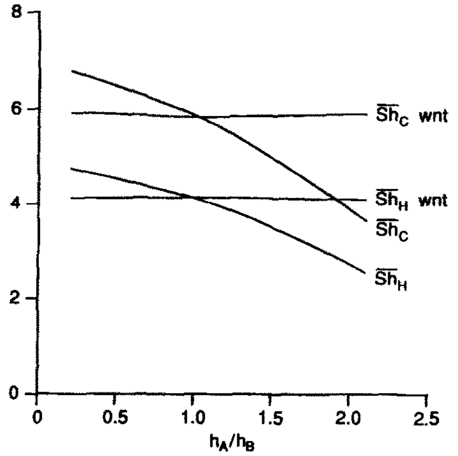


FIG. 3. Variation of the average Sherwood number with $h_{\mathrm{A}}/h_{\mathrm{B}}$.

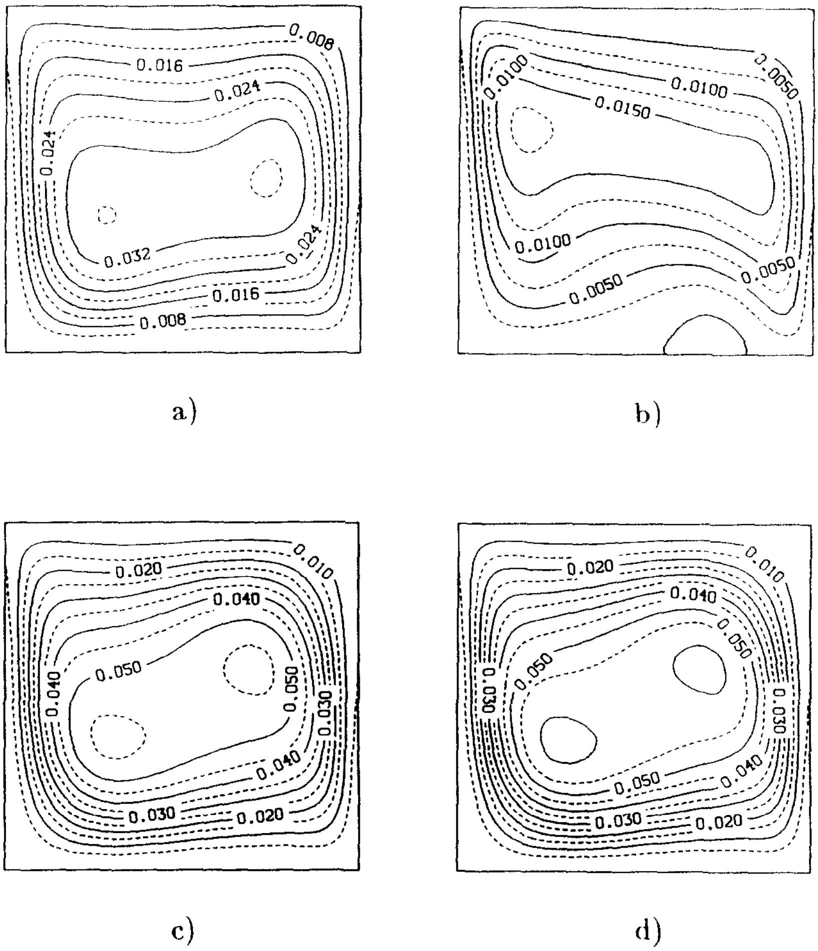


FIG. 4. Streamlines for natural convection in binary gases with species interdiffusion accounted for: (a) $h_A/h_B = 1.08$ (case 1nt), (b) $h_A/h_B = 2.16$ (case 2nt), (c) $h_A/h_B = 0.44$ (case 3nt) and (d) $h_A/h_B = 0.22$ (case 4nt).

Again, the diffusive energy flux (case 2nt) decreased further at the cold wall than at the hot wall (as compared to case 2wnt), since the interdiffusion flux at the cold wall is greater.

Because the enthalpy of species A (entering and leaving the cavity) is greater than the enthalpy of species B, the energy content of the fluid entering and leaving the cavity is much greater than the mixture enthalpy of the binary fluid. Correspondingly, the temperature of the fluid near the hot wall is greater than the hot wall temperature (Fig. 7(b)). Similarly, the temperature of the fluid adjacent to the cold wall is less than the cold wall temperature. Hence, the diffusive energy flux is in the negative ξ-direction (out at the hot wall and in at the cold wall), but the total energy transfer across the cavity is positive from the hot to the cold wall. The distribution of the Nusselt number, energy flux due to advection, diffusion and species interdiffusion and Sherwood number are given in Fig. 8.

Effect of increasing h_B. If c_{pB} is increased (cases 3wnt and 4wnt), the variation of c_p^* is reversed ($c_{pC} > c_{pH}$). This increases and decreases the diffusive energy flux at the hot and cold wall, respectively, resulting in a smaller difference between Q_{dH} and Q_{dC}. The magnitude of the diffusive energy flux increased (as compared to case 1wnt) since the mixture enthalpy increased. Also, because the mixture enthalpy increased, the advective flux at the hot and cold walls is decreased. When species interdiffusion is accounted for (cases 3nt and 4nt), the diffusive energy flux is increased because $Q_{d,wnt}$ is positive and $Q_{I,nt}$ is negative. Hence, $Q_{d,nt} > Q_{d,wnt}$. The convection in the cavity increases due to the altered density field (buoyancy force) since the range of the thermophysical properties is unchanged. This increases the concentration gradients at the hot and cold walls and correspondingly the mass flux at the vertical walls. In turn, this increases the advective flux at the walls. Overall, the total energy flux is decreased because the diffusion energy and species interdiffusion oppose each other. The variation of the Nusselt number,

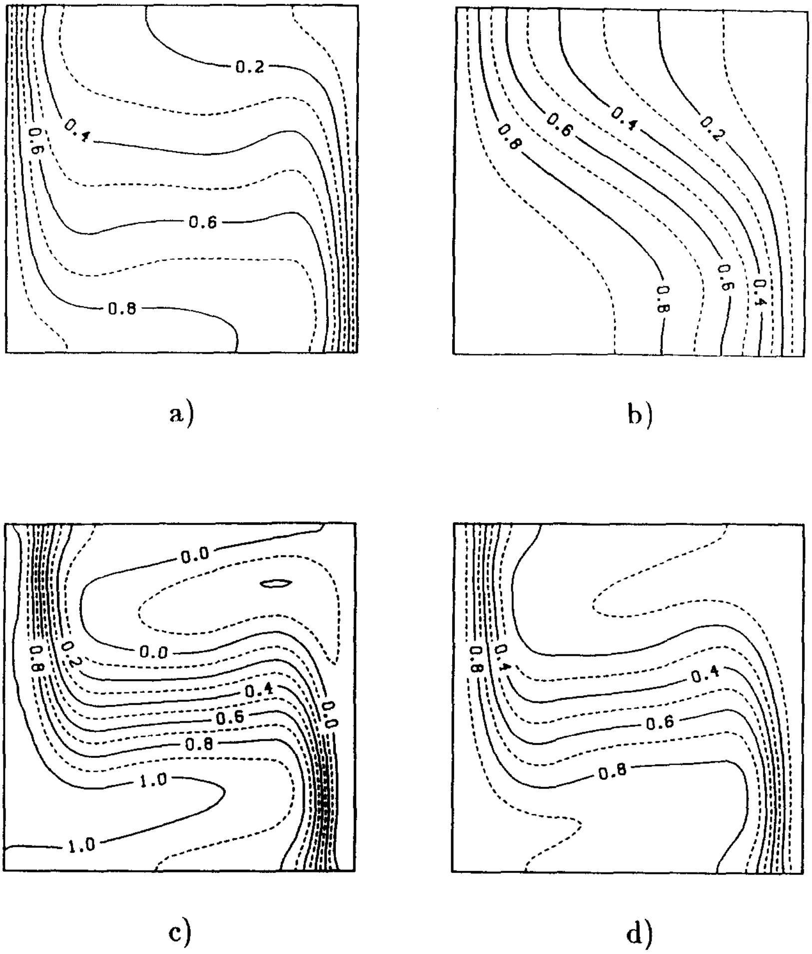


Fig. 5. Isolines of the mixture enthalpy for natural convection in binary gases with interdiffusion accounted for: (a) $h_A/h_B = 1.08$ (case 1nt), (b) $h_A/h_B = 2.16$ (case 2nt), (c) $h_A/h_B = 0.44$ (case 3nt) and (d) $h_A/h_B = 0.22$ (case 4nt).

energy fluxes due to advection, diffusion and species interdiffusion and the Sherwood number for case 3nt are given in Fig. 9.

Soret and Dufour effects

Since the Soret and Dufour effects are diffusive processes, the Grashof number was decreased to 1×10^3 to reduce the influence of natural convection (decrease the advective flux relative to the diffusive flux). Furthermore, the Soret effect is small when the mass fraction of either component is small or when C_T is large (ΔT is small). The base case for investigating Soret and Dufour effects is given by case 1sd (where sd denotes that Soret and Dufour effects are considered) in Table 2. The thermophysical properties of species A and B are represented by those of ethanol and nitrogen, respectively [13–17].

From a review of the literature [3, 18, 19], the absolute value of the thermal diffusion factor (α_d) ranges approximately between 0 and 1 for gases. The thermal diffusion factor varies with temperature and concentration, but is taken as a constant. The variation with temperature would be small over the temperature difference considered, and the variation with concentration is small (the significance of the variation of composition for the Soret mass flux is apparent from the term $\omega_A\omega_B$). Also, no experimental data are available for these binary systems, and the accuracy of the first-order predictions is not sufficiently reliable to justify the effort. The variable thermophysical property formulation is retained. Again, the advected energy at the hot and cold walls pertains to the enthalpy of species A only since species B is noncondensable.

In general, for the range of parameters investigated, Soret and Dufour effects have little influence on the velocity, enthalpy, concentration and temperature fields in the core of the cavity. If the Soret and Dufour effects are constant throughout the cavity, the enthalpy and concentration fields would not be altered. Mathematically, from equation (4) for example, if the Soret mass flux is constant, the derivative of a constant is zero and the differential equation is unchanged from the formulation where Soret mass

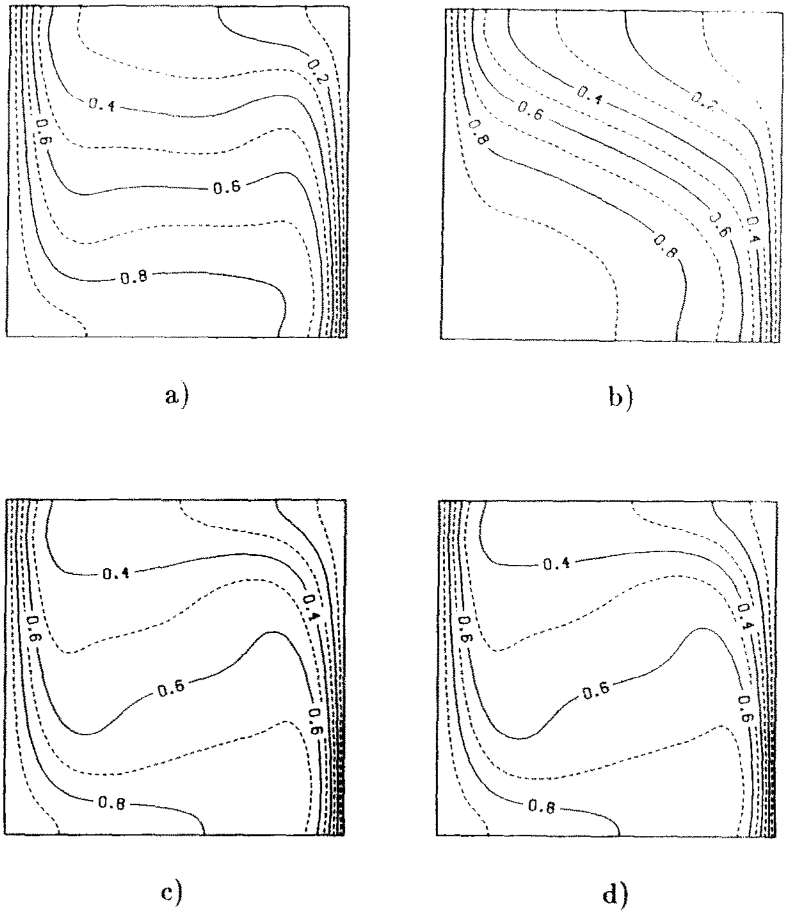
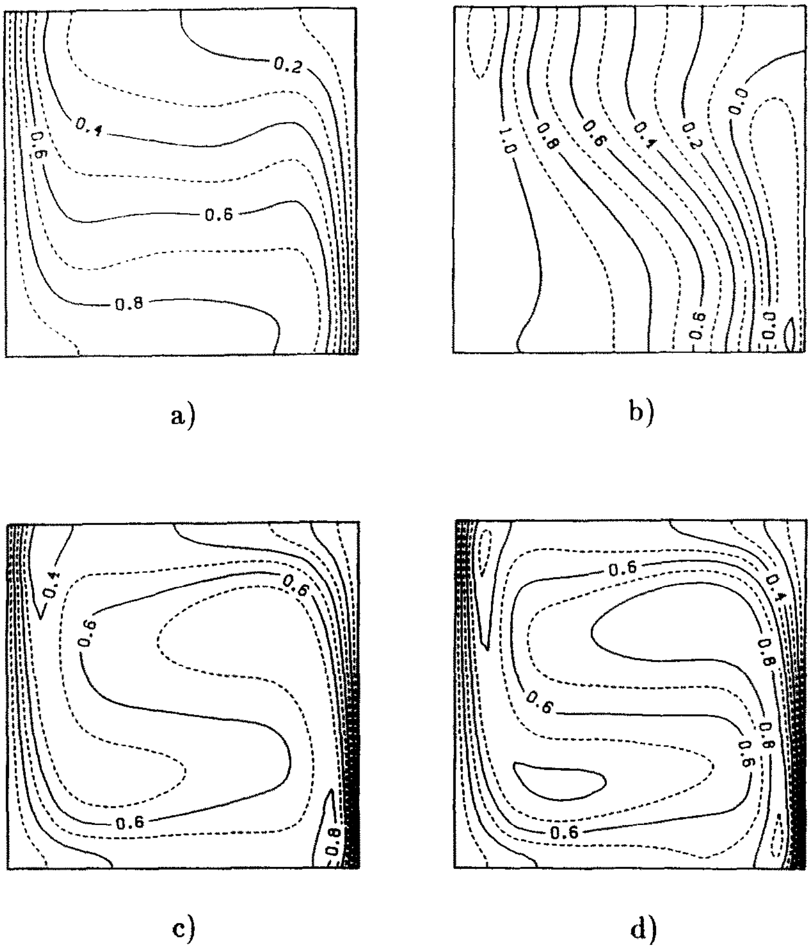


FIG. 6. Isolines of the concentration for natural convection in binary gases with interdiffusion accounted for: (a) $h_A/h_B = 1.08$ (case 1nt), (b) $h_A/h_B = 2.16$ (case 2nt), (c) $h_A/h_B = 0.44$ (case 3nt) and (d) $h_A/h_B = 0.22$ (case 4nt).

diffusion is not considered. Furthermore, the Soret and Dufour effects are greatest where the mass and temperature gradients are largest (i.e. at the hot and cold walls). Therefore, few plots of the streamlines or enthalpy, concentration and temperature isolines are presented.

Separate and combined influence of the Soret and Dufour effects. The base case 1sd is for $\alpha_d = 0$. The streamlines and isolines of enthalpy, concentration and temperature are shown in Fig. 10 to illustrate the variation of these dependent variables. Note that a larger fraction of the flow in the cavity is from the hot to the cold wall, and, correspondingly the recirculation cell is smaller. This is due to the weaker natural convection circulation ($Gr = 1 \times 10^3$) in the cavity. If natural convection is absent ($N^* = 0$), the mass flow is from the hot to the cold wall with no recirculation. For $N^* = 0$, the streamlines would be approximately parallel to the horizontal connecting walls of the cavity, but not straight lines due to the no slip velocity boundary condition at the horizontal walls. If the Soret effect is accounted for (case 2sd), the mass flux at the walls is increased (Tables 3 and 4). The Soret mass flux is approximately the same at both walls, and therefore is a smaller fraction of the total mass flux at the cold wall because $J_{dC} > J_{dH}$. Since the mass flux is increased, the blowing and suction effects on the boundary layer at the hot and cold walls are increased. Hence, the diffusive energy flux decreases and increases slightly at the hot and cold walls, respectively. Similarly, accounting for the Dufour effect (case 3sd) increases the energy flux at the walls. Inclusion of both phenomena results in approximately the combined effect of each separately.

Effects of the thermal diffusion factor. If the thermal diffusion factor is negative, the Soret and Dufour effects oppose the mass and energy flux due to diffusion, respectively. In case 5sd, $\alpha_d = -1$. Since the mass flux decreases, the diffusive energy flux increases at the hot and cold wall, respectively, due to the reduced suction and blowing (as compared to case 1sd). Reducing α_d to 0.5, decreases the Soret mass and Dufour energy fluxes to approximately half the value of J_S and Q_{Du} for case 4sd ($\alpha_d = 1$). Correspondingly, the advective energy and mass fluxes increased only half as much as case 4sd over the base case. Since the



a) b) c) d)

FIG. 7. Isotherms for natural convection in binary gases with interdiffusion accounted for: (a) $h_A/h_B = 1.08$ (case 1nt), (b) $h_A/h_B = 2.16$ (case 2nt), (c) $h_A/h_B = 0.44$ (case 3nt) and (d) $h_A/h_B = 0.22$ (case 4nt).

Soret and Dufour effects influence only slightly the concentration and temperature fields, this linear variation in J_S and Q_{Du} is expected.

Results for an increased Grashof number. Increasing the Grashof number increases the mass and enthalpy gradients at the hot and cold walls. Correspondingly, the Soret mass and Dufour energy flux are increased but remain about the same fraction of the total mass and energy flux, respectively (case 7sd, $Gr = 1 \times 10^4$). Cases 8sd and 9sd are for the same parameters ($Gr = 1 \times 10^5$) but $\alpha_d = 0$ and 1, respectively. Comparison of the results for these cases shows the Dufour energy and Soret mass fluxes are again about the same fraction of the total energy and mass flux, respectively, as for case 4sd. Therefore, these fluxes should be accounted for in the conservation equations (if an accurate value of the thermal diffusion factor can be determined) to obtain the total energy and mass flux at the walls even at higher Grashof numbers. In particular, the Soret mass flux should be accounted for in the conservation equations if the mass flux at the walls is significant enough to affect the velocity, temperature and concentration gradients at the hot and cold walls.

Influence of the Prandtl and Schmidt numbers. In case 10sd the Prandtl number is reduced to 0.4. This reduces the advection as illustrated mathematically by equation (12). Decreasing the Prandtl number also reduces the Dufour energy flux. Physically, as the Prandtl number decreases, the velocity boundary layer becomes thinner with respect to the thermal boundary layer. Hence, thermal transport processes which depend on the mass flux are reduced (Q_a and Q_{Du}). The diffusion becomes a more significant fraction of the total energy transport as the Prandtl number is reduced. The temperature gradient is increased and decreased at the hot and cold wall, respectively, as can be observed from the increase in J_S and Q_d (over case 4sd) at the hot wall and decrease in J_S and Q_d at the cold wall.

Decreasing the Schmidt number increases the mass flux at the hot and cold walls. This increases the advective contribution and the Dufour energy flux. Also, since the suction at the cold wall and blowing at the

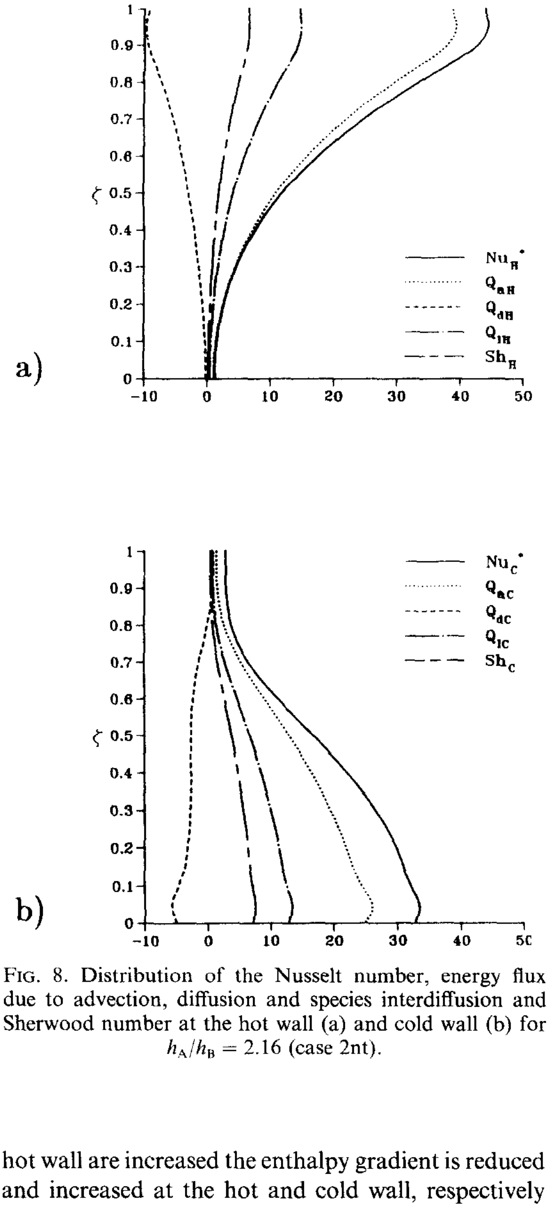


FIG. 8. Distribution of the Nusselt number, energy flux due to advection, diffusion and species interdiffusion and Sherwood number at the hot wall (a) and cold wall (b) for $h_A/h_B = 2.16$ (case 2nt).

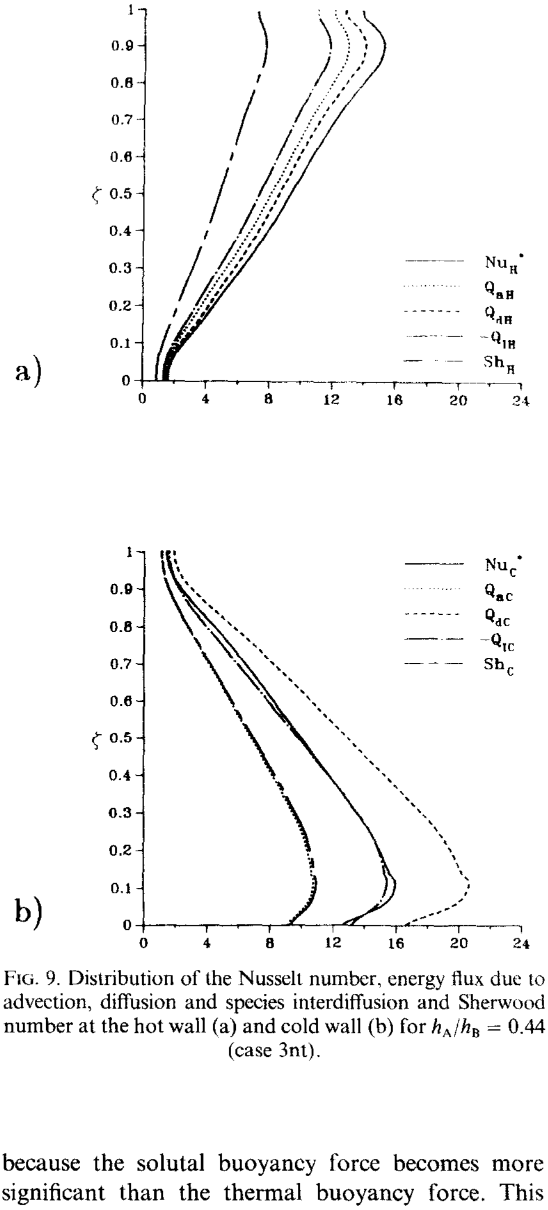


FIG. 9. Distribution of the Nusselt number, energy flux due to advection, diffusion and species interdiffusion and Sherwood number at the hot wall (a) and cold wall (b) for $h_A/h_B = 0.44$ (case 3nt).

hot wall are increased the enthalpy gradient is reduced and increased at the hot and cold wall, respectively (Tables 3 and 4). Correspondingly, the Soret flux is decreased and increased at the hot and cold walls, respectively. The reduced Schmidt number results in a concentration field influenced more by diffusion. Hence with a reduction in the Schmidt number, the diffusive mass flux is increased and decreases at the hot and cold wall, respectively.

Effects of the temperature and concentration difference across the cavity. Case 12sd is for the same concentration difference across the cavity but the cold wall concentration of species A is zero. Correspondingly, the buoyancy parameter is reduced and C_{wv} is increased which reduces the wall mass flux. The particular result of interest is that the Soret mass flux at the cold wall vanishes. As stated earlier, the Soret mass flux is greatest when the mass fraction of either species is neither large nor small.

If the temperature difference across the cavity is decreased, the buoyancy parameter is increased, because the solutal buoyancy force becomes more significant than the thermal buoyancy force. This increases the convection in the cavity resulting in larger concentration and temperature gradients at the walls. Hence, the advective, diffusive and Dufour energy fluxes and diffusive mass flux increase. In particular, the Soret mass flux decreases because the smaller temperature difference across the cavity reduces the temperature gradient.

CONCLUSIONS

From the results presented, species interdiffusion can significantly affect the natural convection heat and mass transfer and fluid flow due to combined temperature and concentration gradients in a cavity. The overall dimensionless heat transfer rate ($\overline{Nu^*}$) is decreased for all values of h_A/h_B when species interdiffusion is accounted for in the analysis. However, the mass flux is decreased as c_{pB} is decreased. Alter-

Table 2. Range of parameters examined in the numerical study which accounted for Soret and Dufour effects

Case	*Gr*	*Pr*	*Sc*	N^*	α_d	Soret	Dufour
1sd[a]	1×10^3	1.0	1.0	−0.864	0		
2sd					1.0	yes	no
3sd					1.0	no	yes
4sd					1.0	yes	yes
5sd					−1.0	yes	yes
6sd					0.5	yes	yes
7sd	1×10^4				1.0	yes	yes
8sd	1×10^5				0		
9sd	1×10^5				1.0	yes	yes
10sd		0.4			1.0	yes	yes
11sd			0.4		1.0	yes	yes
12sd[b]				−0.514	1.0	yes	yes
13sd[c]				−2.577	1.0	yes	yes

[a] $M^* = 5$, $M_B = 20$, $\Delta\omega_A = 0.3$, $\omega_C = 0.2$, $C_{wv} = 2.67$, $C_w = 0.67$, $T_C = 283.15$ K, $\Delta T = 56.6$ K, $C_T = 5$.

[b] $\omega_C = 0$, $C_{wv} = 3.33$, $C_w = 0$.

[c] $\Delta T = 28.3$ K, $C_T = 10.0$.

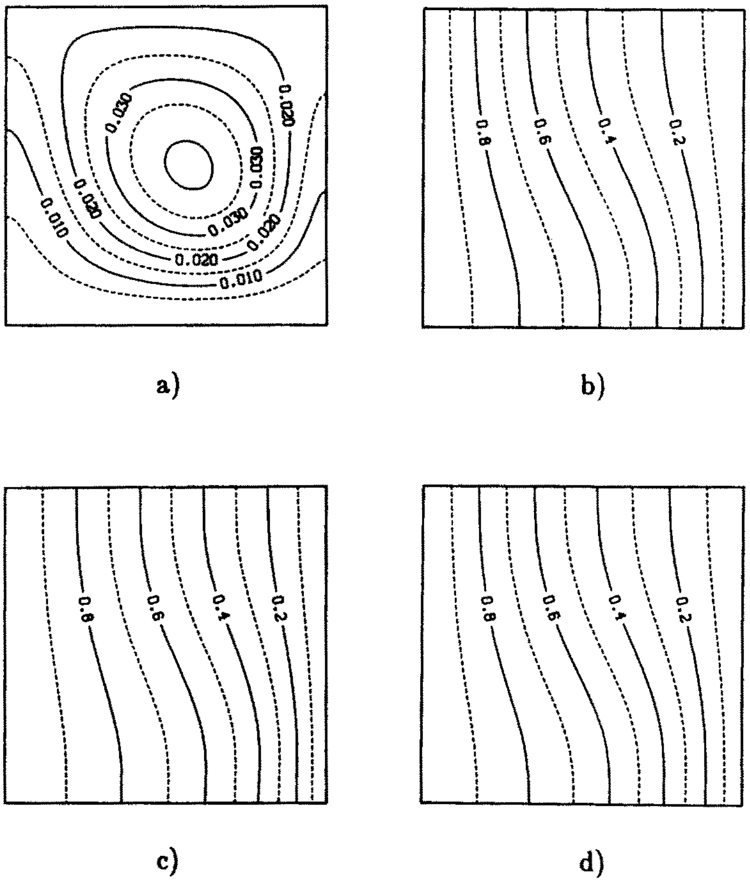


FIG. 10. Streamlines (a), isolines of the enthalpy (b), isolines of the concentration (c) and isotherms (d) for case 4sd ($\alpha_d = 1$, $Gr = 1\times10^3$, $Pr = Sc = 1$, $N^* = -0.864$, $M^* = 5$, $\Delta\omega_A = 0.3$, $\omega_C = 0.2$, $C_{wv} = 2.67$, $\Delta T = 56.6$ K and $C_T = 5$).

Table 3. Summary of the average mass flux, Nusselt number, energy flux due to advection, diffusion and Dufour effects, Sherwood number and mass flux due to diffusion and Soret effects at the hot wall

Case	$\overline{\rho^* u}\times 10^2$	$\overline{Nu}^+$	$\bar{Q}_a$	$\bar{Q}_d$	$\bar{Q}_{Du}$	$\overline{Sh}^+$	$\bar{J}_d$	$\bar{J}_S$
1sd	1.67	3.66	2.94	0.72		0.88	0.88	
2sd	1.88	3.97	3.30	0.67		0.99	0.88	0.11
3sd	1.67	3.82	2.94	0.71	0.18	0.88	0.88	
4sd	1.87	4.15	3.29	0.66	0.20	0.99	0.88	0.11
5sd	1.45	3.19	2.55	0.79	−0.15	0.76	0.89	−0.14
6sd	1.74	3.84	3.07	0.68	0.09	0.92	0.86	0.06
7sd	1.13	7.95	6.29	1.28	0.38	1.90	1.68	0.22
8sd	0.68	15.04	11.99	3.05		3.59	3.59	
9sd	0.74	16.42	13.02	2.62	0.78	3.92	3.48	0.45
10sd	1.87	2.24	1.31	0.85	0.08	0.99	0.84	0.15
11sd	4.37	8.29	7.70	0.13	0.46	0.94	0.92	0.02
12sd	1.27	3.31	2.48	0.67	0.16	0.94	0.85	0.09
13sd	2.27	8.37	7.10	0.83	0.44	1.20	1.12	0.08

Table 4. Summary of the average mass flux, Nusselt number, energy flux due to advection, diffusion and Dufour effects, Sherwood number and mass flux due to diffusion and Soret effects at the cold wall

Case	$\overline{\rho^* u}\times 10^2$	$\overline{Nu}^+$	$\bar{Q}_a$	$\bar{Q}_d$	$\bar{Q}_{Du}$	$\overline{Sh}^+$	$\bar{J}_d$	$\bar{J}_S$
1sd	1.65	3.66	2.22	1.43		1.39	1.39	
2sd	1.84	3.93	2.48	1.45		1.55	1.44	0.11
3sd	1.65	3.80	2.22	1.42	0.17	1.39	1.39	
4sd	1.84	4.11	2.48	1.44	0.18	1.56	1.44	0.11
5sd	1.47	3.25	1.97	1.42	−0.15	1.24	1.35	−0.11
6sd	1.76	3.89	2.37	1.44	0.09	1.48	1.43	0.06
7sd	1.15	8.10	4.88	2.85	0.36	3.06	2.84	0.22
8sd	0.68	15.12	9.17	5.95		5.74	5.74	
9sd	0.73	16.37	9.88	5.75	0.73	6.19	5.74	0.45
10sd	1.84	2.27	0.99	1.21	0.07	1.55	1.46	0.09
11sd	4.45	8.31	5.99	1.87	0.45	1.50	1.36	0.15
12sd	1.28	3.37	1.91	1.31	0.15	1.35	1.35	0.0
13sd	2.24	8.27	6.11	1.71	0.45	1.89	1.83	0.06

natively, Soret and Dufour effects do not appreciably influence the velocity, temperature and concentration fields, but rather only tend to increase the mass and energy flux (if α_d is positive) due to the added contributions. However, if the mass flux at the wall is appreciable, inclusion of the Soret contribution is important since the blowing and suction effect decreases (at the hot wall) and increases (at the cold wall) the velocity, temperature and concentration gradients, respectively.

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CONVECTION NATURELLE DUE A DES GRADIENTS HORIZONTAUX DE TEMPERATURE ET DE CONCENTRATION—2. INTERDIFFUSION DES ESPECES, EFFETS SORET ET DUFOUR

Résumé—On examine l'influence de l'interdiffusion des espèces, des effets Soret et Dufour sur la convection naturelle de chaleur et de masse dans une cavité sous l'action combinée des gradients de chaleur et de masse. Les résultats de calculs numériques indiquent que l'interdiffusion des espèces réduit le transfert global de chaleur mais accroît le transfert de masse à travers la cavité pour $h_A/h_B < 1$ et réduit le transfert de masse pour $h_A/h_B > 1$. Les contributions de la diffusion Soret au transfert total de masse peut atteindre 10 à 15%. De façon semblable, le transfert d'énergie dû à l'effet Dufour peut être appréciable comparé à la conduction thermique.

NATÜRLICHE KONVEKTION AUFGRUND HORIZONTALER TEMPERATUR- UND KONZENTRATIONSUNTERSCHIEDE—2. STOFFDIFFUSION, SORET- UND DUFOUR-EFFEKTE

Zusammenfassung—In der vorliegenden Arbeit wird der Einfluß von Stoffdiffusion, Soret- und Dufour-Effekten auf den Wärme- und Stofftransport durch natürliche Konvektion aufgrund von Konzentrations- und Temperaturunterschieden in einem Hohlraum untersucht. Numerische Berechnungen zeigen, daß die Stoffdiffusion den Wärmetransport beeinträchtigt, den Stofftransport durch den Hohlraum jedoch für $h_A/h_B < 1$ erhöht und für $h_A/h_B > 1$ verringert. Die Soret-Diffusion trägt zum gesamten Stofftransport durch den Hohlraum mit 10–15% bei. In ähnlicher Weise kann der Energietransport durch Dufour-Effekte im Vergleich zur Wärmeleitung erheblich sein.

ЕСТЕСТВЕННАЯ КОНВЕКЦИЯ, ВЫЗВАННАЯ ГОРИЗОНТАЛЬНЫМИ ГРАДИЕНТАМИ ТЕМПЕРАТУРЫ И КОНЦЕНТРАЦИИ—2. ВЗАИМНАЯ ДИФФУЗИЯ ВЕЩЕСТВА, ЭФФЕКТЫ СОРЭ И ДЮФУРА

Аннотация—Исследуется влияние взаимной диффузии вещества, а также эффектов Сорэ и Дюфура на естественноконвективный тепло- и массоперенос в полости, вызванный совместным влиянием градиентов температуры и концентрации. Результаты численных расчетов показывают, что взаимная диффузия вещества уменьшает суммарный теплоперенос, но увеличивает массоперенос через полость при $h_A/h_B < 1$ и снижает его при $h_A/h_B > 1$. Найдено также, что вклад диффузии Сорэ в общий массовый поток через полость может достигать 10–15%. Аналогичным образом перенос энергии, обусловленный эффектами дюфура, может быть соизмерим с теплопроводностью.