Double-diffusive convection affected by conductive and insulating side walls during physical vapor transport of Hg$_2$Br$_2$

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Abstract In last few decades, although thermal and/or solutal buoyancy-driven recirculating flows in a closed ampoule have been intensively studies as a model problem, there exist interesting total molar flux of Hg$_2$Br$_2$ that have been unreported in the literature. It is concluded that the total molar flux of Hg$_2$Br$_2$(A) increases linearly and directly as the temperature difference regions in the range of $10^oC \leq \Delta T \leq 50^o$, $3.5 \times 10^3 \leq Gr_t \leq 4.08 \times 10^3$, $4.94 \times 10^4 \leq Gr_s \leq 6.87 \times 10^4$. For the range of $10 \text{ Torr} \leq P_B \leq 150 \text{ Torr}$, the total molar flux of Hg$_2$Br$_2$(A) decays second order exponentially as the partial pressure of component B (argon as an impurity), $P_B$ increases. From the view point of energy transport, the fewer the partial pressure of component B (argon), $P_B$ is, the more the energy transport is achieved.

Key words Double diffusion, Physical vapor transport, Hg$_2$Br$_2$

1. Introduction

During the past few decades one area of interest in double diffusion has been the study of the physical vapor transport (PVT) processes in a sealed chamber. In recent years, the problems of Cattaneo-Christov double diffusion have been studied for Williamson nanomaterials slip flow subject to porous medium [1], and bi-directional stretched nanofluid flow with Cattaneo-Christov double diffusion [2]. Muhammad et al. [3] addressed Darcy-Forchheimer flow over an exponentially stretching curved surface with Cattaneo-Christov double diffusion. Asha and Sunitha [4] reported thermal radiation and hall effects on peristaltic blood flow with double diffusion in the presence of nanoparticles.

Mercurous halide materials are well known as the most promising materials in applications for acousto-optic materials and signal processing optics, for example, Bragg cells. Singh and his group investigated systematically the growth and characterization and development of large single crystals of Hg$_2$Br$_2$ [5-11]. Many reports of Hg$_2$Br$_2$ could be found in references [12-16]. Kim and his coworkers [17-19] have performed two-dimensional numerical studies of double diffusion convection in the vapor phase during physical vapor crystal growth. Duval [20] published that four flow structure regions appear during the physical vapor transport of mercurous chloride crystal growth.

Our numerical simulations are motivated by the desire to study the influences of hybrid thermal boundary conditions on the convective flow because the final quality of crystal is affected by convection fields. In this paper, the effects of the temperature differences between the source and crystal, the Peclet number, Pe, and the partial pressure of component B (argon as inert gas), $P_B$ on the total molar flux of Hg$_2$Br$_2$ and the maximum magnitudes of velocity vector, $|U|_{\text{max}}$ in the dimensional unit (cm/sec) shall be addressed.

2. Numerical Simulations

Consider steady state thermal and solutal buoyancy driven recirculating flows of Hg$_2$Br$_2$(A)-argon (B) with thermo-physical properties listed in Table 1, in PVT crystal growth enclosure for hybrid thermal boundary conditions with linear temperature profiles, i.e., conductive walls, and insulating walls, shown in Fig. 1, accompanied by a $42 \times 22 \ (x \times y)$ grid system. The detailed assumptions and nomenclature can be found in reference [17]. Also, the dimensionless parameters of Prandtl, Lewis, Peclet, Grashof, concentration, aspect ratio are described in reference [20].

In non-dimensional form, continuity, Navier-Stokes momenta, energy transport, and mass transport are gov-
Bernoulli’s equation (1) to (4) are given as follows:

\[ \nabla^2 \mathbf{V} = 0, \]  
\[ \nabla \cdot \mathbf{V} = -\mathbf{V}^* \cdot \mathbf{p} + \mathbf{P} \nabla^2 \mathbf{I} - \frac{G_r \cdot P \cdot R}{\beta A^t} \left(1 - \frac{\rho}{\rho_A}\right), \]  
\[ \nabla \cdot \mathbf{T} = \mathbf{V}^* \cdot \mathbf{T}, \]  
\[ \nabla \cdot \mathbf{e} \cdot \mathbf{e} = \frac{1}{\operatorname{Le}} \nabla \cdot \mathbf{e} \cdot \mathbf{e}^*. \]  

The boundary conditions corresponding to the above equations (1) to (4) are given as follows:

On the walls

\[ 0 < x^* < 1, \quad y^* = 0 \text{ and } 1: \]
\[ u(x^*, 0) = u(x^*, 1) = v(x^*, 0) = v(x^*, 1) = 0, \]  
\[ \frac{\partial \omega_A^*(x^*, 0)}{\partial y^*} = \frac{\partial \omega_A^*(x^*, 1)}{\partial y^*} = 0, \]  
\[ T^*(x^*, 0) = -\frac{1}{\operatorname{Ar}} x^* + 1 \]
\[ 1 < x^* < 3, \quad y^* = 0 \text{ and } 1: \]
\[ u(x^*, 0) = u(x^*, 1) = v(x^*, 0) = v(x^*, 1) = 0 \]  

On the source \((x^* = 0, \quad 0 < y^* < 1): \)
\[ u(0, y^*) = -\frac{1}{\operatorname{Le} (Cv - 1)} \frac{\partial \omega_A(0, y^*)}{\partial x^*}, \]  
\[ v(0, y^*) = 0, \]  
\[ T^*(0, y^*) = 1, \]  
\[ \omega_A(0, y^*) = 1. \]

On the crystal \((x^* = L/H, \quad 0 < y^* < 1): \)
\[ u(L/H, y^*) = -\frac{1}{\operatorname{Le} (Cv - 1)} \frac{\partial \omega_A(L/H, y^*)}{\partial x^*}, \]  
\[ v(L/H, y^*) = 0, \]  
\[ T^*(L/H, y^*) = 0, \]  
\[ \omega_A(L/H, y^*) = 0. \]

The code verification of one’s results can be found in reference [17], for the Semi-Implicit Method Pressure-Linked Equations Revised (SIMPLER) [21].

3. Results and Discussion

When \(M_A \neq M_B\), the two molecular weights of Hg_Br_2 and argon are different, i.e., \(M_A = 560.988 \text{ g/mol, } M_B = 39.944 \text{ g/mol, }\) solutally buoyancy driven convection is much important compared with thermally buoyancy driven convection, but solutal and/or thermal convection are coupled and the effects of thermal buoyancy convection cannot be neglected during the physical vapor transport of Hg_Br_2 in the vapor phase. Therefore, our interest is restricted on our studies to investigate the relations of the driving force, the temperature difference, \(\Delta T\), the maximum magnitudes of velocity vector, \(|U|_{\max}\) and the Prandtl number for the transport of crystal species.

As shown in Fig. 2, it is clear that the total molar flux of Hg_Br_2(A) increases linearly and directly as the temperature difference in the range of \(10^\circ \text{C} \leq \Delta T \leq 50^\circ \text{C},\)
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\[3.5 \times 10^3 \leq \text{Gr}_t \leq 4.08 \times 10^3, 4.94 \times 10^4 \leq \text{Gr}_s \leq 6.87 \times 10^4,\]

For \(\Delta T = 10^\circ C\), the corresponding thermal (Gr\(_t\)) and solutal (Gr\(_s\)) Grashof number is \(4.08 \times 10^3\) and \(6.87 \times 10^4\), respectively; for \(\Delta T = 50^\circ C\), the corresponding thermal (Gr\(_t\)) and solutal (Gr\(_s\)) Grashof number is \(3.5 \times 10^3\) and \(4.94 \times 10^4\), respectively. With increasing the temperature difference, the corresponding thermal (Gr\(_t\)) and solutal (Gr\(_s\)) Grashof number reversely decrease, which reflected the variations in the density of the mixture of Hg\(_2\)Br\(_2\) and argon. In other words, for \(\Delta T = 10^\circ C\), the kinematic viscosity is \(0.18 \text{ cm}^2/\text{sec}\); for \(\Delta T = 50^\circ C\), the kinematic viscosity is \(0.44 \text{ cm}^2/\text{sec}\). The system considered in Fig. 1 is Ar (aspect ratio, transport length-to-width) = 4, \(T_s\) (source temperature) = 300\(^\circ\)C, \(P_B\) (partial pressure of component B, argon) = 10 Torr, on earth. For \(\Delta T = 10^\circ C\), the thermal diffusivity and binary mass diffusivity is \(0.18\), and \(1.28 \text{ cm}^2/\text{sec}\); for \(\Delta T = 50^\circ C\), the thermal diffusivity and binary mass diffusivity is \(0.45\), and \(1.28 \text{ cm}^2/\text{sec}\). For the range of \(10^\circ C \leq \Delta T \leq 30^\circ C\), the total molar flux of Hg\(_2\)Br\(_2\)(A) increases sharply with increasing the temperature difference, whereas for the range of 30\(^\circ\)C \(\leq \Delta T \leq 50^\circ C\), the total molar flux of Hg\(_2\)Br\(_2\)(A) increases relatively gradually. As mentioned before, this difference is likely be due to the variations in the density of the mixture of Hg\(_2\)Br\(_2\) and argon.

Figure 3 illustrates the effects of Peclet number, Pe on as the temperature difference, \(\Delta T\) in the range of \(10^\circ C \leq \Delta T \leq 50^\circ C\), \(3.5 \times 10^3 \leq \text{Gr}_t \leq 4.08 \times 10^3, 4.94 \times 10^4 \leq \text{Gr}_s \leq 6.87 \times 10^4,\)

6.87 \times 10^4. The Peclet number, Pe increases linearly and directly with the temperature differences. Figure 4 shows the relation of the maximum magnitude of velocity vector, |\(U_{max}\)| and Peclet number, Pe for \(10^\circ C \leq \Delta T \leq 50^\circ C\), aspect ratio = 4, \(T_s = 300^\circ C\), \(P_B = 10\) Torr, on earth. This relation illustrates that the |\(U_{max}\)| increases linearly with the Peclet number, Pe. Note that the Peclet number is
intimately related to the advections across the interfaces at the source and the crystal regions.

Figure 5 shows the profiles of velocity vector, streamline, temperature, mass concentration, based on aspect ratio = 4, $\Delta T = 50^{\circ}C$ ($300^{\circ}C \to 250^{\circ}C$), $P_B = 10$ Torr, Peclet number = 3.65, thermal Grashof number ($Gr_t = 3.5 \times 10^3$), solutal Grashof number ($Gr_s = 4.94 \times 10^4$), Prandtl number = 0.97, Lewis number = 0.35, concentration parameter = 1.02, total pressure = 108 Torr, $|U|_{\text{max}} = 1.87 \text{ cm/sec}$, on earth.

Figure 6 shows the effects of the partial pressure of component B (argon), $P_B$, on the total molar flux of $\text{Hg}_2\text{Br}_2$(A), for $10 \text{ Torr} \leq P_B \leq 150$ Torr, based on aspect ratio = 4, $\Delta T = 50^{\circ}C$, $T_s = 300^{\circ}C$, $P_B = 10$ Torr, $1.8 \times 10^3 \leq Gr_t \leq 2.9 \times 10^3$, $2.6 \times 10^4 \leq Gr_s \leq 4.9 \times 10^4$, on earth. For the range of $10 \text{ Torr} \leq P_B \leq 150$ Torr, the total molar flux of $\text{Hg}_2\text{Br}_2$(A) decays second order exponentially with the partial pressure of component B (argon), $P_B$. Figure 7 shows the influences of the partial pressure of component B (argon), $P_B$, on the Peclet number, $Pe$, for $10 \text{ Torr} \leq P_B \leq 150$ Torr, corresponding to Fig. 6.

Figure 8 shows the profiles of velocity vector, streamline, temperature, mass concentration, based on aspect ratio = 4, $\Delta T = 50^{\circ}C$ ($300^{\circ}C \to 250^{\circ}C$), $P_B = 60$ Torr, $|U|_{\text{max}} = 0.99 \text{ cm/sec}$, on earth. As shown in Fig. 8, one convective roll is present in the vapor phase. In a comparison of Fig. 8(c) temperature with Fig. 5(c) temperature, from the view point of energy transport, the fewer the partial pressure of component B (argon), $P_B$ is, the more...
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Fig. 6. The total molar flux of Hg$_2$Br$_2$ as the partial pressure of component B, $P_B$, based on aspect ratio = 4, $\Delta T = 50^\circ$C, $T_s = 300^\circ$C, $P_a = 10$ Torr, $1.8 \times 10^3 \leq \text{Gr}_t \leq 2.9 \times 10^3$, $2.6 \times 10^4 \leq \text{Gr}_s \leq 4.9 \times 10^4$, on earth.

Fig. 7. The Peclet number, Pe as the partial pressure of component B, $P_B$, $\Delta T$ ($^\circ$C), based on aspect ratio = 4, $T_s = 300^\circ$C, $P_a = 10$ Torr, $3.5 \times 10^3 \leq \text{Gr}_t \leq 4.6 \times 10^3$, $4.9 \times 10^4 \leq \text{Gr}_s \leq 5.6 \times 10^4$, on earth.

Fig. 8. (a) Velocity vector, (b) streamline, (c) temperature, (d) mass concentration profile, based on aspect ratio = 4, $\Delta T = 50^\circ$C ($300^\circ$C $\rightarrow$ $250^\circ$C), $P_a = 60$ Torr, Peclet number = 2.19, thermal Grashof number ($\text{Gr}_t$) = $3.8 \times 10^3$, solutal Grashof number ($\text{Gr}_s$) = $5.07 \times 10^4$, Prandtl number = 0.92, Lewis number = 0.51, concentration parameter = 1.12, total pressure = 158 Torr, $|U|_{\text{max}} = 0.99$ cm/sec, on earth.
the energy transport is achieved.

4. Conclusions

It is concluded that the total molar flux of Hg\textsubscript{2}Br\textsubscript{2}(A) increases linearly and directly as the temperature difference, \(\Delta T\), in the range of 10\(^\circ\)C \(\leq \Delta T \leq 50\(^\circ\)C\), 3.5 \(\times\) 10\(^3\) \(\leq Gr\) \(\leq 4.08 \times 10^3\), 4.94 \(\times\) 10\(^3\) \(\leq Gr\) \(\leq 6.87 \times 10^3\). For the range of 10 Torr \(\leq P_b \leq 150\) Torr, the total molar flux of Hg\textsubscript{2}Br\textsubscript{2}(A) decays second order exponentially with the partial pressure of component B (argon), \(P_b\). From the view point of energy transport, the fewer the partial pressure of component B (argon), \(P_b\) is, the more the energy transport is achieved.

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