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Convective heat and mass transfer affected by aspect ratios for physical vapor transport crystal growth in two dimensional rectangular enclosures

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Abstract Natural convection of a two dimensional laminar steady-state incompressible fluid flow in a rectangular enclosure has been investigated numerically for low aspect ratios with the physical vapor transport crystal growth. Results show that for aspect ratio ($Ar = L/H$) range of $0.1 \leq Ar \leq 1.5$, with the increase in Grashof number by one order of magnitude, the total mass flux is much augmented, and is exponentially decayed with the aspect ratio. Velocity and temperature profiles are presented at the mid-width of the rectangular enclosure. It is found that the effect of Grashof number on mass transfer is less significant when the enclosure is shallow ($Ar = 0.1$) and the influence of aspect ratio is stranger when the enclosure is tall and the Grashof number is high. Therefore, the convective phenomena are greatly affected by the variation of aspect ratios.

Key words Aspect ratio, Convection

1. Introduction

In recent years, numerical simulations of the effects of aspect ratios on natural convection in enclosures have been studied extensively in the views of heat transfer [1-20]. In particular, Wang et al. [1] investigated natural convection with low aspect ratio (Ar) less than 5, Rayleigh (Ra) numbers ranged from 10^5 up to 10^6. They reported the local Nusselt number is affected much by low aspect ratio less than 5, but there is no change for higher aspect ratio of 10. Yigit et al. [3] presented the effects of aspect ratio on natural convection of the Ostwald-Waele model fluids within rectangular enclosures. Choudhary and Subudhi [9] performed a systematic investigation of the turbulent natural convection of Al_2O_3/water nanofluids for aspect ratio range of $0.3 \leq Ar \leq 2.5$, and Rayleigh number range of $10^7 \leq Ra \leq 10^{12}$. Cheong and Sivasankaran [11] investigated to understand the essence of the natural convection flow and heat transfer in inclined rectangular enclosures with sinusoidal temperature profile on the left wall for aspect ratio range of $0.25 \leq Ar \leq 10$, and Rayleigh number range of $10^3 \leq Ra \leq 10^6$. Bouhalleb and Abbassi [12] addressed the natural convection in inclined cavity filled with CuO-water nanofluid for aspect ratio range of $0.1 \leq Ar \leq 0.5$ and Rayleigh number range of $10^4 \leq Ra \leq 10^7$, and found that an anticlockwise rotating sing cell exists for all Rayleigh number, a secondary cell for $Ar = 0.5$ and $Ra = 10^7$. Kurian et al. [20] reported numerical studies on natural convection inside inclined cylinders with a unity aspect ratio, and the flow patterns induced natural convection were three dimensional and sensitive to the inclination angle. Duval [21-24] performed a systematical study for a wide range of convective parameters of Rayleigh number from 1.80×10^{1} up to 5.03×10^7. Moreover, Duval studied numerically the time dependent problems [21-24].

This paper concerns the two dimensional laminar steady-state thermal and solutal convection problems, which arise from the physical vapor transport processes of the mixture of Hg_2Cl_2-I_2 system. As a model sample, we chose a material of Hg_2Cl_2 and consider the physical vapor transport of a mixture of Hg_2Cl_2 vapor and impurity of I_2 in the vapor phase. The wall effects due to the aspect ratio and convection sometimes oppose to each other particularly in certain regimes. Our simulation analyses are motivated by the desire to optimize the enclosure width such that mass transfer is either maximized or minimized as the aspect ratio (Ar) varies. Therefore, the subject of this paper is to study the effect of aspect ratio and Grashof number on convective flow inside the two dimensional enclosure.

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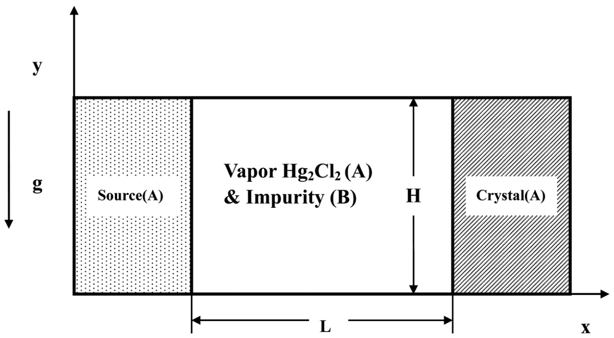

Fig. 1. Schematic description of a two-dimensional Physical Vapor Transport model for a mixture of vapor Hg_2Cl_2 (A) and impurity (B) in a horizontal position with respect to the gravity vector.

2. Numerical Simulation

We consider convective heat and mass flows in the ampoule with a source of and a crystal of material Hg_2Cl_2 with the source temperature T_s and the crystal temperature T_c, with $T_s > T_c$, as shown in Fig. 1. The source material of mercurous chloride (Hg_2Cl_2) is placed with a furnace, the source of mercurous chloride sublimes and is transported as a mixture of Hg_2Cl_2 vapor and impurity of I_2 and is recrystallized into the crystal region. The interfaces are assumed to be flat for simplicity. The finite normal velocities at the interfaces can be expressed by Stefan flow deduced from the one-dimensional diffusion-limited model [25], which would provide the coupling between the fluid dynamics and species calculations. We consider a linear temperature profile which is imposed on the furnace, and assume thermodynamic equilibrium at the interfaces. Continuity, Navier-Stokes momenta, energy transport, and species (diffusion) are governed by [24]:

$$\nabla \cdot \vec{V} = 0, \tag{1}$$

$$\rho \frac{D\vec{V}}{Dt} = -\nabla p + \mu \nabla^2 \vec{V} + \rho \vec{g}, \tag{2}$$

$$\frac{DT}{Dt} = \alpha \nabla^2 T, \tag{3}$$

$$\frac{D\omega_A}{Dt} = D_{AB} \nabla^2 \omega_A. \tag{4}$$

The corresponding boundary conditions are as follow [24]:

On the walls ($0 < x < L$, $y = 0$ and H):

$$u(x,\ 0) = u(x,\ H) = v(x\ 0) = v(x,\ H) = 0, \tag{5}$$

$$\frac{\partial \omega_A(x, 0)}{\partial y} = \frac{\partial \omega_A(x, H)}{\partial y} = 0,$$

$$T(x, 0) = T(x, H) = \frac{T - T_c}{T_s - T_c}.$$

On the source ($x = 0$, $0 < y < H$):

$$u(0, y) = -\frac{D_{AB}}{(1 - \omega_{A, c})} \frac{\partial \omega_A(0, y)}{\partial x}, \tag{6}$$

$$v(0,\ y) = 0,$$
$$T(0,\ y) = T_s,$$
$$\omega_A(0,\ y) = \omega_{As}.$$

On the crystal ($x = L$, $0 < y < H$):

$$u(L, y) = -\frac{D_{AB}}{(1 - \omega_{A, s})} \frac{\partial \omega_A(L, y)}{\partial x}, \tag{7}$$

$$v(L,\ y) = 0,$$
$$T(L,\ y) = T_c,$$
$$\omega_A(L,\ y) = \omega_{Ac}.$$

These coupled conservation equations (1)-(4) are solved subject to the boundary conditions (5)-(7) using a methodology based on the implicit, control volume, finite difference technique SIMPLER (Semi-Implicit Method for Pressure-Linked Equation Revised) [26]. A 23×43 non-uniform grid is employed for the finite-difference mesh in this numerical work. The nodes are closely spaced at the walls. With this set of boundary conditions, Eqs. (5)-(7), the pressure does not need to be explicitly specified at the interface boundaries. However, to accelerate numerical convergence, the total pressure is assumed to be fixed at the one point in the middle of the computational domain. In order to have confidence of the numerical methodology and to ensure that computer program was implemented correctly, checks were made against the results of Markham, Greenwell and Rosenberger [27] for thermal convection PVT in cylindrical vertical ampoules with insulating walls, an aspect ratio of 0.5. Further details can be found elsewhere [28].

3. Results and Discussion

As shown in Fig. 2, the total molar flux exponentially decayed as the aspect ratio increases in the range of $0.1 \le Ar \le 1.5$ for $1.79 \times 10^4 \le Gr \le 1.75 \times 10^6$. For aspect ratio range of $0.1 \le Ar \le 1.5$, the total mass flux is much augmented with the increase in Grashof number (Gr) by one order of magnitude. The dimensionless Grashof number which appears in the natural

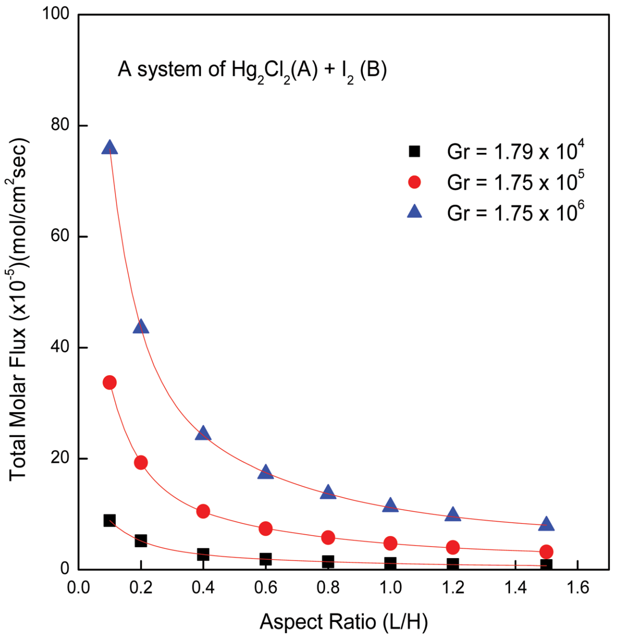

Fig. 2. Effects of aspect ratio (L/H) on the total molar flux of Hg_2Cl_2 for three different Grashof numbers: $Gr = 1.79 \times 10^4$, 1.75×10^5, 1.75×10^6.

convection flow represents a ratio of the buoyancy force to the inertial force. At the aspect ratio of 0.1, the total molar flux is increased by the factor of 8.5 with increasing the Grashof number by two orders of magnitude, from 1.79×10^4 to 1.75×10^6. On the other hand, as the aspect ratio is increased from 0.1 into 1.5, the factor of increase in the total molar flux becomes 10.9 for a same change in the magnitude of Grashof number. It reflects that the total molar flux is much more affected by the variation of aspect ratios than by the Grashof number. For three different Grashof numbers, $Gr = 1.79 \times 10^4$, 1.75×10^5, 1.75×10^6, the total molar flux is sharply decreased with increasing the aspect ratio from 0.1 up to 0.4, in other words, the total molar flux at $Gr = 1.79 \times 10^4$ is reduced by 80 percent; at $Gr = 1.75 \times 10^5$ and 1.75×10^6, it is reduced by 70 percent. There exists gradually a change in the total molar flux since $Ar = 0.4$. Therefore further incremental increase of the aspect ratio are expected to have a weak effect on the convective heat and mass transfer during the physical vapor transport crystal growth of Hg_2Cl_2. The parameters corresponding to $Gr = 1.79 \times 10^4$ are Prandtl number = 1.17, Lewis number = 0.66, Peclet number = 0.49, concentration number = 2.58, $\Delta T = 10^oC$; at $Gr = 1.75 \times 10^5$, Prandtl number = 1.17, Lewis number = 0.67, Peclet number = 1.38, concentration number = 1.33, $\Delta T = 30^oC$; at $Gr = 1.75 \times 10^6$, Prandtl number = 1.17, Lewis number = 0.69,

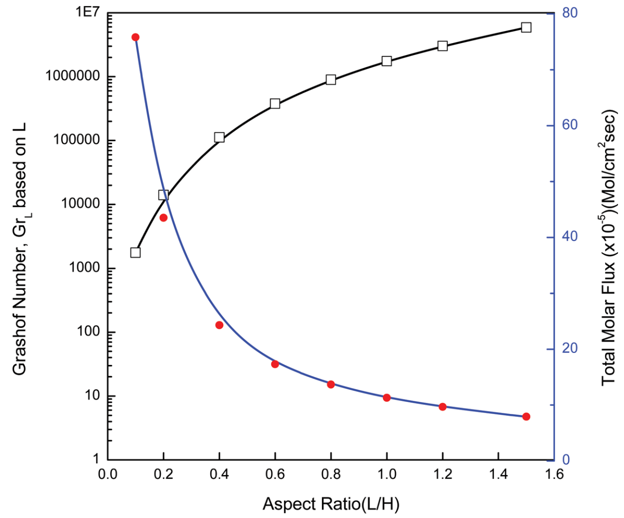

Fig. 3. Grashof number based on L instead of H and total molar flux versus aspect ratio at $Gr = 1.75 \times 10^6$.

Peclet number = 2.52, concentration number = 1.08, $\Delta T = 60^oC$. The Grashof number is based on the width H. ΔT is the temperature difference between the source and crystal region, which is the driving force for the physical vapor transport crystal growth based on the sublimation-condensation mechanism. The variations in the total molar flux and the Grashof number based on L with the aspect ratio are presented in Fig. 3. For the sake of detailed explanation on the effects of aspect ratio, the Grashof number based on the transport length L, Gr_L is used instead of the Grashof number based on the width H, at $Gr = 1.75 \times 10^6$. The aspect ratio was varied through changes to the transport length, with the width of the enclosure kept constant. It can be seen that the Grashof number based on L increases non-linearly with the aspect ratio, indicating the importance of transport length. Increasing the aspect ratio by varying the enclosure length results in an increase of the surface area and leads to the resistance due to the existence of the side walls, and consequently, the decrease of the total molar flux occurs.

Fig. 4 presents the dependence of the horizontal velocity (U) at the mid-width position versus x/H parameterized in aspect ratio (Ar) at $Gr = 1.75 \times 10^6$. To describe the convective flow behaviors, we choose a PVT model at $Gr = 1.75 \times 10^6$. With increasing the aspect ratio, the horizontal velocity exhibits a steep increase for $0.1 \le Ar \le 0.6$ along x/H, and approaches within the range of 1 cm/sec. It is observed that the maximum horizontal velocity at $Ar = 0.6$ is greater than at $Ar = 0.4$, which shows the diametrical opposite of

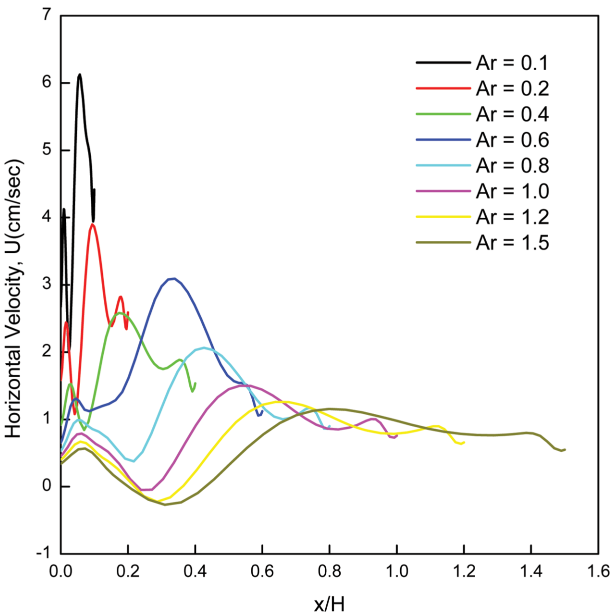

Fig. 4. Horizontal velocity (U) at the mid-width position versus x/H parameterized in aspect ratio (Ar) at Gr = 1.75 × 10^6.

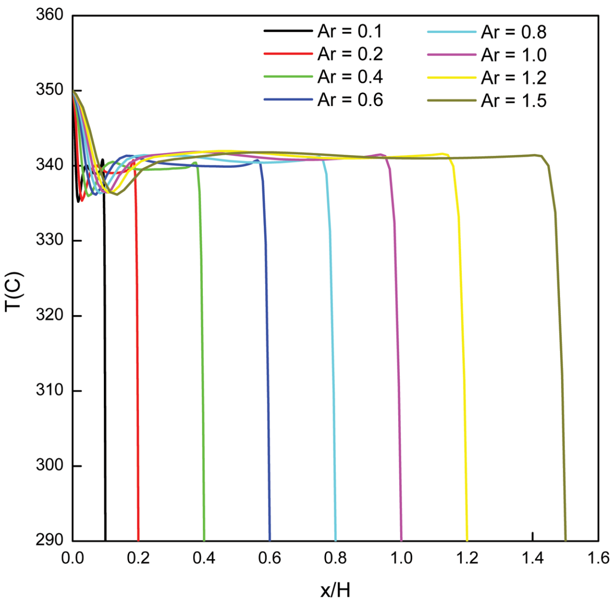

Fig. 5. Temperature (T) at the mid-width position versus x/H parameterized in aspect ratio (Ar) at Gr = 1.75 × 10^6.

the trend which the horizontal velocity decreases with an increase in the aspect ratio along the x/H. Further studies on such an occurrence would remain a problem to be understood in the future. As shown in Fig. 5, the convective flow prompts the temperature profile to look straight and to behave as if it should be one dimensional steady state heat conduction case, which would be shown in Figs. 7 and 8.

The curves of temperature are sharply bend down,

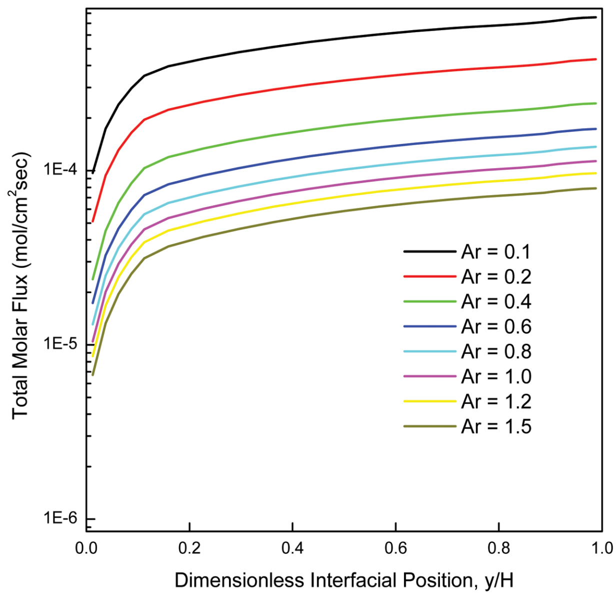

Fig. 6. Effects of aspect ratio on interfacial distribution at Gr = 1.75 × 10^6.

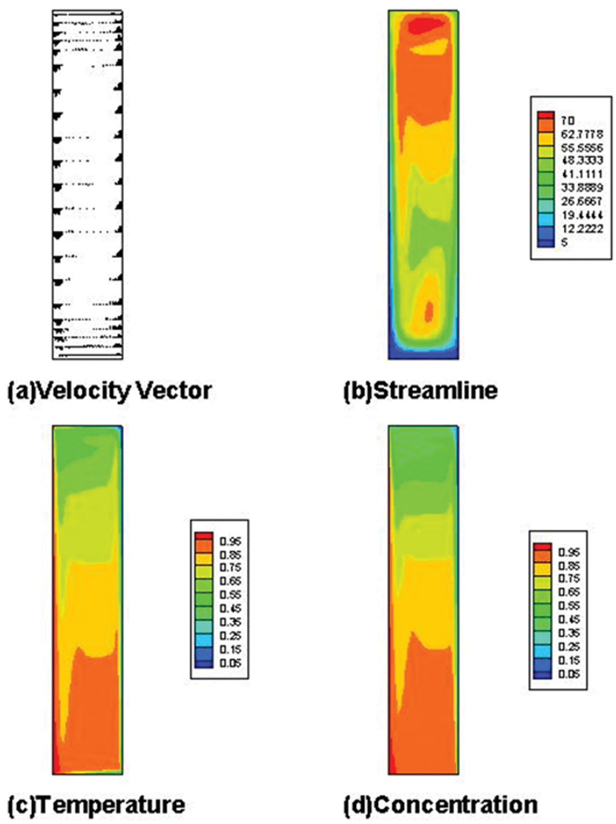

Fig. 7. (a) velocity vector, (b) streamline, (b) temperature, (d) concentration, based on Ar = 0.2, Gr = 1.75 × 10^6, ΔT = 60°C (290°C → 350°C).

i.e. near the crystal region.

Fig. 6 shows the effects of aspect ratio on interfacial distribution at Gr = 1.75 × 10^6. The dimensionless

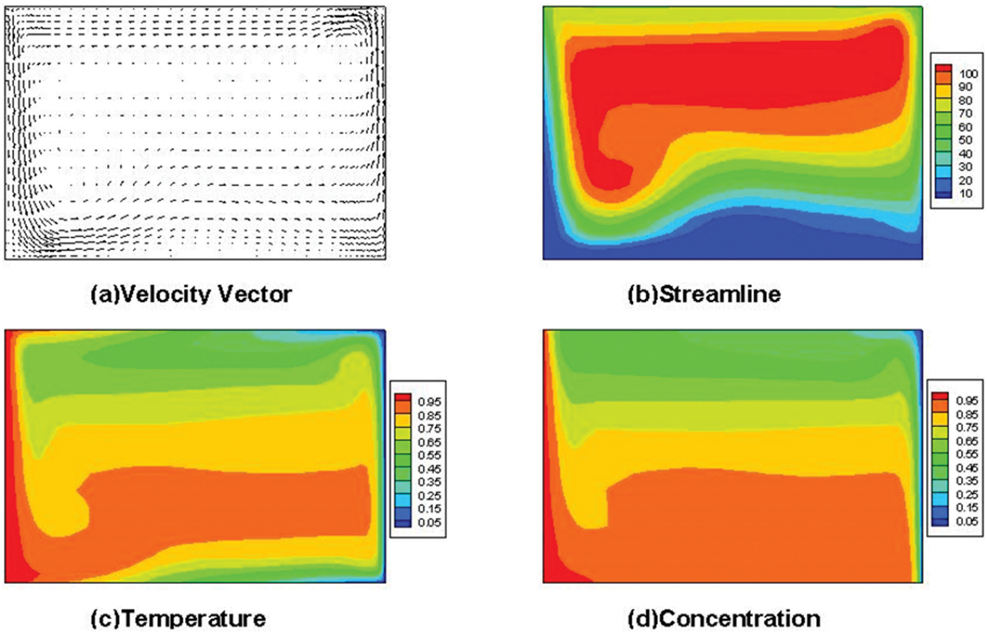

Fig. 8. (a) Velocity vector, (b) streamline, (b) temperature, (d) concentration, based on Ar = 1.5, Gr = 1.75×10^6, $\Delta T = 60^oC$ ($290^oC \rightarrow 350^oC$).

interfacial position, y/H is related to the interface at the flat crystal regions. The total molar flux increases a steep increase near the dimensionless interfacial position of 0.2, which is projected to a convection-dominated system and since y/H = 0. 2, gradually bend up for the aspect ratio range of $0.1 \le Ar \le 1.5$, which reflects the diffusion-dominated system.

Fig. 7 shows the convective structures of velocity field, stream function, temperature and concentration, based on aspect ratio (Ar) = 0.2, width = 5 cm, a linear wall temperature profile between $T_s = 350^oC$ and $T_c = 290^oC$, Gr = 1.75×10^6, $\Delta T = 60^oC$, partial pressure of impurity (I_2) = 50 Torr, Prandtl number = 1.17, Lewis number = 0.69, Peclet number = 2.52, concentration number = 1.08. The (a) velocity field, (b) stream function ($\Delta\psi = 7.77$, $\psi_{max} = 73.9$, $\psi_{min} = 0$), (c) temperature ($\Delta T = 0.1$, $T_{max} = 0.95$, $T_{min} = 0.05$), (d) concentration ($\Delta C = 0.1$, $C_{max} = 0.9$, $C_{min} = 0.1$) are given. It can be observed that the flow fields are asymmetrical and have a single cell at Gr = 1.75×10^6. Fig. 8 shows the convective structures of velocity field, stream function, temperature and concentration, under the same conditions as in Fig. 7 except for the aspect ratio (Ar) = 1.5. There is found to be of little difference between both cases with respect to the convective flow structure. In Fig. 8, the (a) velocity field, (b) stream function ($\Delta\psi = 10$, $\psi_{max} = 108.2$, $\psi_{min} = -1.26$), (c) temperature ($\Delta T = 0.1$, $T_{max} = 0.95$, $T_{min} = 0.05$), (d) concentration ($\Delta C = 0.1$, $C_{max} = 0.95$, $C_{min} = 0.05$) are given. Further studies or extensions on the correlation of the convective flow and the quality of crystals for different aspect ratios can be made in the future.

4. Conclusions

Effects of the aspect ratio (Ar = L/H) on heat and mass transfer characteristics in steady natural convection in rectangular enclosures have been numerically investigated. It is found that the total molar flux exhibits a same trend for the Grashof numbers, $1.79 \times 10^4 \le Gr \le 1.75 \times 10^6$ when the aspect ratio varies from 0.1 to 1.5. This trend is governed by mechanisms of diffusion and convection competition. Future studies may include the extension of the present work to Nusselt numbers in the heat transfer and Sherwood numbers in the mass transfer. The following conclusions can be extracted:

1) For aspect ratio (Ar = L/H) range of $0.1 \le Ar \le 1.5$, with the increase in Grashof number by one order of magnitude, the total mass flux is much augmented, and is exponentially decayed with the aspect ratio.

2) It is found that the effect of Grashof number on mass transfer is less significant when the enclosure is shallow (Ar = 0.1) and the influence of aspect ratio is stranger when the enclosure is tall and the Grashof number is high. Therefore, the convective phenomena are greatly affected by the variation of aspect ratios.

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