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# Double diffusion natural convection in open lid enclosure filled with binary fluids

L.B. Younis [a], A.A. Mohamad [b,*], A.K. Mojtabi [c]

[a] SNC-Lavalin, 605 5th Ave, S.W., Calgary, Alberta T2P 3H5, Canada
[b] Department of Mechanical and Manufacturing Engineering, Schulich School of Engineering, The University of Calgary, Calgary, AB T2N 1N4, Canada
[c] IMFT, UMR 5502 CNRS, Laboratoir de mécanique des fluides, Université Paul Sabatier, 118 route de Narbonne, 31062 Toulouse, France

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**Abstract**

Double diffusion natural convection in an enclosure filled with a liquid and subjected to differential heating and differential species concentration is investigated. Four models were developed to address the hydraulic effect of the upper lid on the rate of heat and mass transfer and on the flow structures. It is found that free surface yields higher rate of heat and mass transfer. Also, there is noticeable difference between the results of two- and three-dimensional results. Hence, the effect of upper lid condition cannot be underestimated. The effect of boundary condition on the rate of heat transfer is more profound for natural convection without double diffusion effects.


*Keywords:* Natural convection; Double diffusion; Free surface

## 1. Introduction

Double diffusive convection has been subject of an intensive research due to its importance in various engineering and geophysical problems. For instance, pollution desperation in lakes and reveres, solute intrusion in sediments in coastal environments, nuclear waste disposals, contaminant transport in ground water, chemical processes and species transport through biological membranes are a few examples to mention. In such process the thermal and concentration buoyancy forces either aid or oppose each other, depending on the type of alloy and process of heating.

The subject of natural convection for single fluid flow and double diffusion has been studied extensively [1–19]. Yet, most work done considers flow inside closed enclosures. In some applications, such as pollution dispersion in lakes, chemical deposition, melting and solidification process, it is more appropriate to model the process of heat and mass transfer in open lid cavities, which is the subject of the present work. The governing equations are elliptical in nature and the boundary conditions effects are very important on the solution of the domain of integrations. Enclosed enclosure imposed shear stress at the boundary, which has a dissipative effect and restricts the fluid particle motion. While, free surface (shear stresses equal to zero) increases the freedom of motion at the boundary, which may change the dynamics of the flow due to the elliptical nature of the problem. Three- and two-dimensional models are developed to investigate the flow structure, heat and mass transfer process in enclosures with free upper surface. Also, the results compared with that of a closed lid enclosure. This step is taken to critically evaluate the effect of upper boundary on the flow structure. The hypothesis is that the Navier–Stokes equation is elliptical in nature and shear at the upper boundary should have significant effect on the flow and on the rate of energy and mass transfer. Complex flow patterns may form due to difference in the rate of heat and mass transfer, competition between thermal and concentration boundary layers development and density reversal in the mixing zone. Complex flow is expected when the thermal/concentration buoyancy force opposes the concentration/thermal buoyancy force. Hence, flow bifurcation is expected and flow may become three-dimensional. Two-dimensional flow patterns may be justified for a certain range of controlling parameters in an enclo-

* Corresponding author.
*E-mail address:* mohamad@ucalgary.ca (A.A. Mohamad).

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sure imposed to thermal and concentration gradients along vertical boundaries. Double diffusive, natural convection in differentially heated enclosures with aiding thermal and concentration gradients were considered in references. Most of the mentioned works were assumed that the flow is two-dimensional. Sezai and Mohamad [19] explored the three-dimensional flow in cubic enclosures filled with a saturated porous medium where the flow was driven by opposing buoyancy forces due to thermal and concentration gradients. Their results revealed that for certain range of controlling parameters (porous thermal Rayleigh ($Ra^*$), Lewis ($Le$) and buoyancy ratio parameters) the flow might become three-dimensional. The flow became three-dimensional for the concentration to thermal buoyancy ratio ($N$) equal to $-0.5$, $Ra^* = 10$ and $Le > 20$. Also, three-dimensional flow pattern is predicted for $N = -0.5$, $Le = 10$ and $Ra^* > 20$. The rate of mass transfer was more sensitive for flow bifurcations from 2-D to 3-D than the rate of heat transfer. When the flow becomes three-dimensional, multiple dipole vortices form in the transverse planes, similar to those created by injection of fluid into stratified medium. On the other hand, the results of Mohamad and Bennacer [20] on doubled diffusion in an enclosure heated differentially and species gradient imposed vertically, cross gradient conditions, showed that the flow is three-dimensional in general, but the difference between results of 2-D and 3-D simulation is not that significant as far as the rate of heat and mass transfer is concerned.

The present study address the effect of upper boundary on the flow structure and on the rate of heat and mass transfer in a cubic cavity filled with binary fluid and imposed to temperature and species gradients horizontally. Three- and two-dimensional models are developed to investigate the flow structure, heat and mass transfer process in enclosures with free upper surface. Also, the results were compared with that of closed enclosure. This step is taken to critically evaluate the effect of upper boundary on the flow structure.

Complex flow patterns may form due to differences in the rate of heat and mass transfer, competition between thermal and concentration boundary layers development and density reversal in the mixing zone. Such a phenomenon is more probable when the thermal/concentration buoyancy force oppose each other and order of magnitude of the opposing forces becomes unity. Hence, flow bifurcation is expected and flow may become three-dimensional. When the flow becomes three-dimensional, multiple dipole vortices form in the transverse planes, similar to those created by injection of fluid into stratified medium. Also, the results indicate that the rates of heat and mass transfer are substantially higher for the open lid enclosure compared with results of closed lid enclosure. This may be explained due the fact that the shear at the upper boundary reduces the fluid parcels velocity, consequently reduces the advected rate of heat and mass transfers.

## 2. Problem definition and governing equations

The problem under consideration is an open lid rectangular cross section enclosure filled with a binary fluid, Fig. 1. The rectangular enclosure of sides $L_x$, $L_y$ and $L_z$. Different

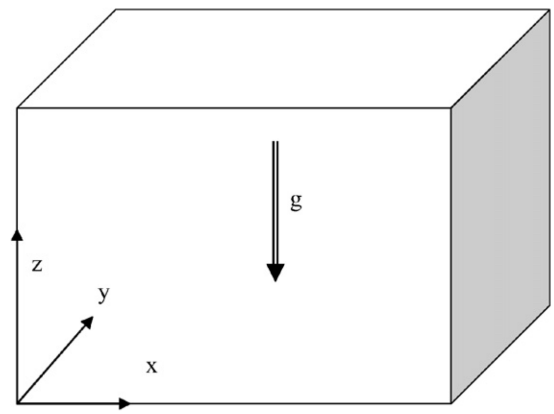

Fig. 1. Schematic of the problem.

temperature and concentrations were imposed between the left ($T_1$, $C_1$) and right vertical walls ($T_2$, $C_2$), where the $C_1 > C_2$ and $T_1 > T_2$. Adiabatic and impermeable boundary conditions were imposed on the remaining boundaries. Except at the upper boundary where the shear stress is assumed to be negligible, i.e., the effect of surface tension is neglected. This assumption can be justified for water–air interface and for thick layer of fluid body, i.e., volume per surface area $\gg 1$. Also, it is assumed that the free surface is non-deformable. Further more, the rate of heat exchange between the fluid in the container and ambient through the free surface is neglected. This assumption is difficult to justify, but for stagnant air the heat transfer coefficient is order of $10\ \mathrm{W\,m^{-2}\,K^{-1}}$, which translates to small value of Biot number, therefore the assumption may be justified. However, for analysis process and to isolate the effect of Biot number, the effect of heat transfer from the upper boundary is assumed to be negligible. Therefore, the upper boundary is assumed to be adiabatic. The flow is assumed to be laminar and steady. The binary fluid of Prandtl number of 10 (aqua solution) was assumed to be Newtonian and incompressible with Boussinesq approximation is valid. The Soret and Dufour effects were assumed to be negligible.

Using the following dimensionless variables: $X = x/L_x$, $Y = y/L_x$, $Z = z/L_x$, $\vec{V} = \vec{v}L_x/\nu$, $P = pL_x^2/\rho\nu^2$, $\Theta = (T - T_2)/(T_1 - T_2)$, $\Phi = (C - C_2)/(C_1 - C_2)$, where $\nu$ is the kinematical viscosity of the fluid and $\vec{v}$ is the velocity vector. The equations governing the conservation of mass, momentum and energy in non-dimensional form can be written as:

*Continuity*:

$$\vec{\nabla}.\vec{V} = 0 \tag{1}$$

*Momentum*:

$$(\vec{V}.\vec{\nabla})\vec{V} = -\vec{\nabla}P + \nabla^2\vec{V} + \frac{Ra}{Pr}(\Theta + N\Phi)\vec{k} \tag{2}$$

*Energy*:

$$\vec{V}.\nabla\Theta = \frac{1}{Pr}\nabla^2\Theta \tag{3}$$

*Species conservation*:

$$\vec{V}.\nabla\Phi = \frac{1}{Le\,Pr}\nabla^2\Phi \tag{4}$$

where $\vec{k}$ is the unit vector in $Z$ direction, $Ra = (g\beta_T \Delta T L^3)/\nu\alpha$ is the thermal Rayleigh number, $Pr = \nu/\alpha$ is the Prandtl number, $N$ is the ratio of the buoyancy forces, $Ra_s/Ra\,Le$, $Ra_s = (g\beta_c \Delta C L^3)/\nu D$ is the solutal Rayleigh number, $Le = \alpha/D$ is the Lewis number, $\alpha$ and $D$ are the thermal and molecular diffusities, respectively. In the limit of vanishing capillary number $Ca = |\gamma|\Delta T \ll 1$ surface deformations cannot occur so that the boundary conditions at the open top surface ($Z = A_z$) are

$$\frac{\partial U}{\partial Z} + Ma\frac{\partial \Theta}{\partial X} = 0 \tag{5a}$$

$$\frac{\partial V}{\partial Z} + Ma\frac{\partial \Theta}{\partial Y} = 0 \tag{5b}$$

$$W = 0 \tag{5c}$$

$$\frac{\partial \Theta}{\partial Z} + Bi\,\Theta = 0 \tag{5d}$$

$$\frac{\partial \Phi}{\partial Z} = 0 \tag{5e}$$

where $Ma = -(\partial\sigma/\partial T)\Delta T L/\mu\alpha$ is the Marangoni number and $Bi = hL_x/k$ is the Biot number with $h$ being the surface heat transfer coefficient. As mentioned before, the effect of $Ma$ and $Bi$ numbers are neglected.

At the rigid walls no-slip and no penetration boundary conditions are imposed for the velocities,

$$U = V = W = 0 \quad \text{on } X = 0, A_x \tag{6a}$$

$$U = V = W = 0 \quad \text{on } Y = 0, A_y \tag{6b}$$

$$U = V = W = 0 \quad \text{on } Z = 0 \tag{6c}$$

Since the side walls are of the cavity are heated at $X = 0$ and cooled at $X = A_x$ and all other walls are adiabatic, we impose

$$\Theta = 1 \quad \text{and} \quad \Phi = 1 \quad \text{on } X = 0 \tag{7a}$$

$$\Theta = 0 \quad \text{and} \quad \Phi = 0 \quad \text{on } X = A_x \tag{7b}$$

$$\partial\Theta/\partial Y = 0 \quad \text{and} \quad \partial\Phi/\partial Y = 0 \quad \text{on } Y = 0, 1 \tag{7c}$$

$$\partial\Theta/\partial Z = 0 \quad \text{and} \quad \partial\Phi/\partial Z = 0 \quad \text{on } Z = 0 \tag{7d}$$

## 3. Method of solution

Eqs. (1)–(7) are discretized using staggered, nonuniform control volumes. Third order accurate numerical scheme, QUICK scheme is used in approximating the advection terms with the flux limiter known as ULTRA-SHARP is used to eliminate the non-physical oscillations inherent in the QUICK scheme. SIMPLEC algorithm [21] is used to couple momentum and continuity equations. The momentum equations are solved by applying one iteration of the strongly implicit procedure (SIP) of [22]. The pressure correction equation is solved iteratively by applying the conjugate gradient (CG) method until the sum of absolute residuals has fallen by a factor of ten. The coefficient matrix resulting from the discretization of the energy equation is non-symmetric and solved iteratively by Bi-CGSTAB method. SSOR preconditioning is used for accelerating the convergence rates of both CG and Bi-CGSTAB methods with full multigrid method [23]. Generally, under relaxation factors of 0.7, 0.7, 0.7, 1.0, 0.9 and 0.9 were applied to $U$, $V$, $W$, $P$, $T$ and $C$, respectively.

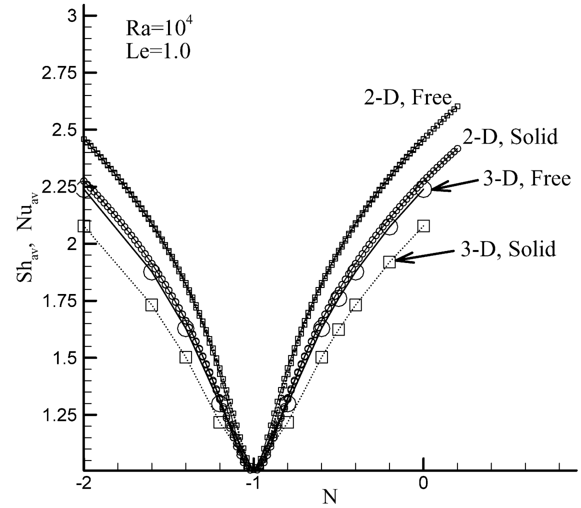


Fig. 2. Comparison between predictions of different models for the rate of heat and mass transfer for $Ra = 10^4$.

$120 \times 120 \times 40$ control volumes are used on the finest level with denser grid clustering near boundaries using the sine function for the grid distribution.

To ensure convergence of the numerical algorithm the following criteria is applied to all dependent variables over the solution domain

$$\frac{\sum |\phi_{ijk}^m - \phi_{ijk}^{m-1}|}{\sum |\phi_{ijk}^m|} \leqslant 10^{-5} \tag{8}$$

where $\phi$ represents a dependent variable $U$, $V$, $W$, $P$ and $T$, the indexes $i$, $j$, $k$ indicate a grid point and the index $m$ the current iteration at the finest grid level.

The method is detailed in the work of Sazai and Mohamad [19]. Also, the code extensively tested for double diffusion problem [19,20].

## 4. Results and discussions

Two- and three-dimensional results are produced for free surface cubic enclosure and are compared with solid lid enclosure. Since the number of controlling parameters is quite few and the main objective of the work is to understand the effect of the upper surface conditions on the dynamics of fluid flow in the enclosure and on the rate of heat and mass transfer. Therefore, some parameters are fixed, such as $Pr$ is set to 10 (aqua solution) and Lewis number is varied within the practical range, i.e., 1, 10 and 50. Also, the results are presented for $Ra$ of $10^4$ and $10^5$, where the flow becomes unstable for high Rayleigh numbers and the flow is mainly controlled by molecular diffusion for low Raleigh numbers. All the results are presented for wide range of $N$ (species buoyancy to thermal buoyancy ratio), $N$ changed from thermal controlled to species buoyancy controlled flows. The following sections discuss, first the average of rates of heat and mass transfer followed by flow structure.

For $Le = 1.0$, thickness of the thermal boundary layer and species concentration boundary layer are the same. Hence, the result must show that $Nu_{av}$ equal to $Sh_{av}$. Also, at $N = -1.0$, the buoyancy force due to the thermal gradient must cancel the

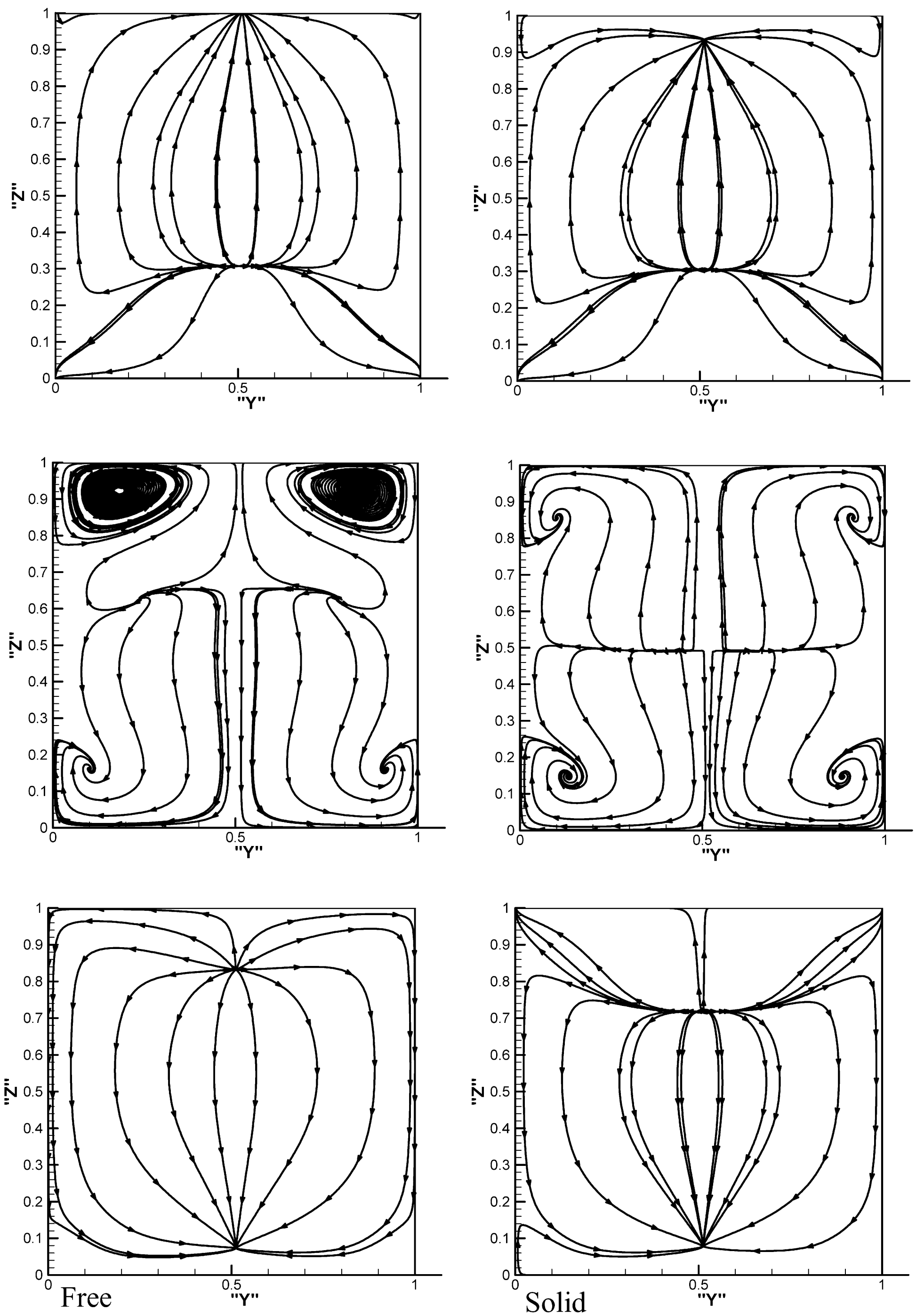


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Fig. 3. Stream trace for $Ra = 10^5$, $Le = 1.0$, $N = 0.0$ for free surface lid and solid surface lid at $X = 0.25$ (top), $X = 0.5$ (middle) and $X = 0.75$ (bottom).

buoyancy force due to the concentration gradient, for opposing case, and Nusselt and Sherwood numbers should equal to unity, conduction condition. The results shown in Fig. 2 testify these facts. The difference in the rate of heat and mass transfer between solid and free surface lids increases for thermally driven flow, $N = 0$. and for species concentration driven flow, $N \leqslant -2.0$. For $N = 0$, the rates of heat are about 2.45, 2.25, 2.25 and 2.07 for 2-D free lid, 2-D solid lid, 3-D free lid and 3-D solid lid, respectively. The results indicate that the flow is three-dimensional because there is a difference in prediction of the rate of heat transfer for 2-D and 3-D models and for same boundary conditions (free or solid). The rate of heat transfer increase for a free surface compared with solid surface are about 9% and about 8%, for 2-D and 3-D predictions, respectively. In general, the rate of heat transfer predicted for 3-D models is less than 2-D models. This can be explained by the fact that the fluid parcels in 3-D model form spiral path as they travel from hot boundary to cold boundary, i.e., more dissipative path. For

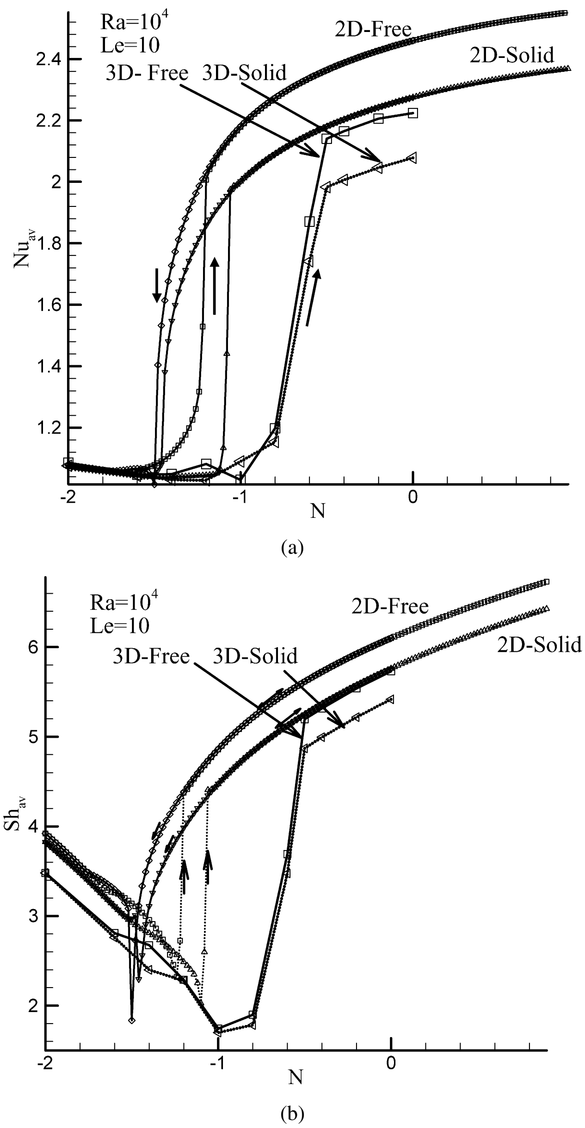


Fig. 4. (a) Average rate of heat transfer as a function of $N$ for $Ra = 10^4$ and $Le = 10$. (b) Average Sherwood number as a function of $N$ for $Ra = 10^4$ and $Le = 10$.

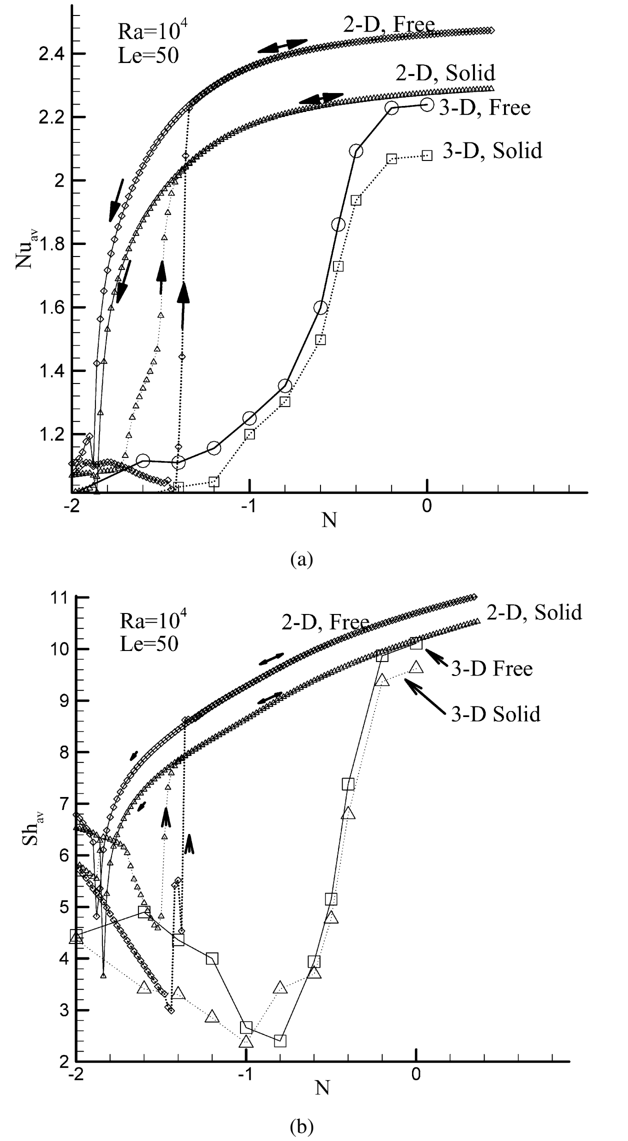


Fig. 5. (a) Nusselt number as a function of $N$ for $Ra = 10^4$ and $Le = 50$. (b) Sherwood number as a function of $N$ for $Ra = 10^4$ and $Le = 50$.

$Ra = 10^5$ the rate of heat transfer predicted for 3-D free surface and 3-D solid lid was about 4.70 and 4.51, respectively. For $Ra = 10^6$, the rate of heat transfer predicted for 3-D free surface and 3-D solid lid was 8.76 and 8.65, respectively.

The difference between flow structures for free and solid boundary is illustrated in Fig. 3 for $Ra = 10^5$ at three different lateral planes ($X = 0.25$, $X = 0.5$ and $X = 0.75$). The difference is not that significant. The strength of the upper vortices at the mid lateral plane for free surface is stronger than that of solid surface. These results indicate that the effect of upper boundary is not that significant at least for the investigated parameters.

For double diffusion problems ($Le > 1$) with opposing conditions, $N$ should be negative and less than one. Also, it is noticed that for $N$ less than $-2$, the flow is mainly controlled by buoyancy induced due to species concentration gradient. In general, a hysteresis is noticed for $N$ order of $-1.0$. For these values of $N$, the flow structure is sensitive to the initial condition. It is possible to obtain different solutions based on the initial condition. Therefore, for a give conditions, the solution is either stared with thermal buoyancy dominated condition and gradually $N$ is decreased after convergence of the solution is insured for a given $N$ value. The solution obtained for a series on $N$ values. Or the solution started with flow controlled by buoyancy induced mainly by species gradient and gradually $N$ value increase after the convergence of the solution is insured for a given $N$ value. It is found that the solution branches depending on the initial condition.

The results for $Ra = 10^4$ and $Le = 10$ is shown in Figs. 4(a) and 4(b). These figures show the average rate of heat and mass transfer, respectively as a function of $N$. The maximum difference in the rate of heat and mass transfer mainly take place for the thermally driven flows. It is possible to obtain different solutions for the range of $N = -1.6$ to $N = -1.0$. In this range of $N$ values the competitions between thermal and species gradients are not stable and the solution depends on the initial conditions.

The transition region is similar to the transient region between laminar and turbulent flow. It should mention that the results converge to a solution but the solution is not unique. Also, the difference between 3-D and 2-D models predictions on the rate of heat and mass transfer is quite significant for the range of $N$ between $-1.6$ and $-0.6$. Figs. 5(a) and 5(b) show the rate of heat transfer and mass transfer for $Ra = 10^4$ and for $Le = 50$, respectively. The trend of prediction is similar to Fig. 4, except that the difference between 2-D and 3-D predictions is significant for wide range of $N$ values (from $-1.6$ to $-0.4$). For the mentioned range of $N$, the prediction of the 3-D model is mainly conduction, $Nu_{\mathrm{av}}$ is order of unity, while 2-D model prediction is mainly convection dominated solution.

## 5. Conclusions

The effect of upper boundary conditions on the flow and rate of heat and mass transfer is addressed in this work, for enclosures filled with a liquid and subjected to differential heating and species concentrations. Four cases were studies, 2-D and 3-D with free surface and with non-permeable, solid surface. The results showed that the difference between four cases become significant for thermally controlled flow. The rate of heat and mass transfer are high for a 2-D enclosure with a free surface. The rate of heat and mass transfer for 3-D with solid surface is the lowest of all the cases. The difference in the rate of heat transfer between the highest and lowest values for different cases can be order of 20% for $N = 0$ (thermally driven flow) and $Ra = 10^4$. Flow and rate of heat and mass transfer become sensitive for initial condition for a range of $N$, depending on the value of the controlling parameter. The strength of upper edge vortices becomes more profound for free surface enclosures.

As a summary the effect of the upper lid conditions is important and cannot be underestimated, especially for thermally driven flows.

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