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Numerical study of fluid stratification in a square cavity due to Thermo-solutal buoyancy forces using velocity - vorticity formulation

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ABSTRACT

Double-diffusive natural convection in a square cavity is numerically analyzed using velocity-vorticity form of Navier-Stokes equations. The governing equations consist of vorticity transport equation, velocity Poisson equations, energy and solutal concentration equations. Galerkin's weighted residual finite element method is employed to solve the coupled governing equations through isoparametric formulation. Numerical predictions of vorticity, velocities, temperature and solutal concentration are computed using an iterative algorithm in order to resolve the coupling between the governing equations. The capability of the velocity-vorticity formulation is demonstrated by a detailed study on the variation of Nusselt and Sherwood numbers for a wide range of the characteristic parameters, $1 \le Le \le 500$, $-25 \le N \le 25$ and $10^3 \le Ra \le 10^6$. Our simulation results show that at high Lewis number, the average Nusselt number decreases and the average Sherwood number increases with increase in buoyancy ratio.

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Introduction

Convective heat and mass transfer by combined thermal and solutal buoyancy forces, called double-diffusive natural convection assumes importance in many applications such as oceanography, food processing, nuclear waste disposal, solar ponds and metal solidification processes etc. In natural convection problems, the fluid momentum transport and convective heat and mass transfer take place solely due to the combined thermal and solutal buoyancy forces. Depending upon the type of application either the thermal buoyancy force or the solutal buoyancy force or the combination of these two will contribute to the resultant convective phenomenon. Buoyancy ratio defined as the ratio of solutal buoyancy force to thermal buoyancy force, is used to indicate the relative importance of these two buoyancy forces. The effect of variation in thermo physical properties of a fluid on the convective heat and mass transfer can be understood by varying the Lewis number. When heat diffusion effect is dominant compared to mass diffusion effect, as observed in problems related to solar ponds, crystal growth and metal solidification, the Lewis number becomes greater than unity. Since double-diffusive convection in a cavity resembles many engineering applications, the study of circulatory flow movement in cavity is considered to be a classical problem to understand the importance of buoyancy ratio and Lewis number on convective heat and mass transfer. Beghein et al. [1] studied aiding and opposing steady-state double diffusive natural convection flows in a square cavity using primitive variable form of Navier-Stokes equations. They obtained Nusselt and Sherwood number correlations for the variation of solutal Rayleigh number and Lewis number.

Experimental and numerical investigations in horizontal and vertical rectangular cavities have been carried out by Wee et al. [2] using $\omega - \psi$ formulation. The rate of heat and moisture

transfer in vertical and horizontal cavities with thermal and solutal gradients acting in the negative vertical coordinate direction was found to be five to nine times that of the horizontal cavity with both the gradients acting in the positive vertical coordinate direction. Lee et al. [3] studied experimentally the various flow patterns in natural convection of a salt-water solution due to the combined horizontal temperature and concentration gradients in rectangular enclosures with aspect ratio of 0.2 and 2.0. They observed smooth variation of temperature at the fluid layer interface contrary to the rapid variation of solutal concentration. Chen and Liu [4] studied numerically double diffusive natural convection due to heated cylinder submerged in a stratified salt solution in a rectangular cavity. Due to the interaction between the upward temperature and downward salinity gradients flow instability was created. Buoyancy ratio and thermal Rayleigh number had great influence on the variations in flow and temperature fields. Bennacer and Gobin [5,6] analyzed flow and heat transfer characteristics in a binary fluid contained in a two-dimensional enclosure with horizontal temperature and concentration gradients and proposed correlations in terms of the influence parameters using scaling law approach. It was observed that at high Lewis numbers, the heat transfer decreases with increasing buoyancy ratios. Weaver and Viskanta [7, 8] examined the effect of thermo-physical properties variation on heat and mass transfer in a cavity due to natural convection driven by combined thermal and solutal buoyancy forces with and without species inter-diffusion Soret and Dufour effects. The thermophysical properties and species inter-diffusion influence the velocity, heat and mass transfer rate but Soret and Dufour effects influence is not appreciable in these fields. Chamkha and Naser [9, 10] used $\omega - \psi$ form to predict the flow characteristics of hydro-magnetic double-diffusive convective flow of a binary gas





mixture in a rectangular enclosure. The effect of magnetic field was found to reduce the overall heat transfer and fluid circulation within the enclosure.

Sundaravadivelu and Kandaswamy [11] found that the average heat and mass transfer rates showed nonlinear dependency on temperature gradient in the cavity and the temperature of maximum density strongly affects both heat and mass transfer in the flow field by giving rise to multi-cellular fluid motions. Double-diffusive convective flow in a rectangular enclosure with a heat source and uniform magnetic field applied in horizontal direction was studied [12] to understand the effect of thermal Rayleigh number, heat generation or absorption coefficient and the Hartmann number. The results indicate that the heat and mass transfer mechanisms and the flow characteristics inside the enclosure depended strongly on the strength of the magnetic field and heat generation or absorption effects. The above results are in good agreement with the results reported in Refs.[9,10]. Sripada and Angirasa [13] studied numerically both aiding and opposing buoyancy flows for a wide range of parameters for an upward facing horizontal surface and explained the mechanisms behind the instabilities in the unsteady flow using $\omega - \psi$ form of momentum equations. For large Schmidt numbers and opposing flows, a shallow stagnant fluid layer is formed near the surface and the fluid is set to move in the upward direction due to the large thermal dispersion effect observed away from the surface. Chamkha and Al-Mudhaf [14] simulated laminar double-diffusive natural convection flow inside an inclined cavity filled with a uniform porous medium. Decreasing the Darcy number was found to reduce the average Nusselt and Sherwood numbers and the fluid circulation within the enclosure. Melting of an ice plate into a homogeneous calcium chloride aqueous solution inside a square cavity was studied experimentally and numerically by Sugawara et al. [15]. Experimental results predicted a monotonic increase of mean melting mass with increase in cavity inclination angle and attains its maximum at θ =180°. But numerical predictions showed this trend to take place in the range of $0^{\circ} < \dot{\theta} < 90^{\circ}$. Al-Amiri et al. [16] simulated double-diffusive natural convection heat transfer in a horizontal annulus subjected to time periodic temperature boundary condition. Their results illustrate that augmentation of heat transfer can be achieved by increasing the thermal forcing amplitude and/or frequency and increase of thermal Rayleigh number. Also a decrease in Lewis number and increase in the buoyancy ratio parameter leads to high heat transfer within the annulus.

In all the above works attention was focused on the variation of one or two characteristic parameters such as buoyancy ratio or Lewis number or Rayleigh number.

In any real problem involving double diffusive convection the effect of all the above three parameters contribute for the resultant heat and mass transfer. Hence a research focusing on the collective variation of Lewis number, Rayleigh number and buoyancy ratio needs to be undertaken. Such an effort requires a large number of simulation trials to compute the variations in the Nusselt and Sherwood numbers. Generally the primary variable form of Navier-Stokes equations has been widely used in convective heat and mass transfer simulation programs. Sometimes in order to capture the vortex dominant flow field, vorticity based momentum equations are used. One such formulation is the vorticity-stream function [9, 10, 16] form of Navier-Stokes equations that have been used with an aim to capture fluid rotation directly and also to avoid the pressure term

which is never computed in a convection problem. The main disadvantages of this formulation are that it cannot be extended to three-dimensional problems and the boundary conditions for vorticity have to be computed using a second order function of stream function. Further the velocity which is the much required dynamic variable in convection problems needs to be computed indirectly using the stream function. In vortex-dominated flows such as the double diffusive convection problems the vorticity advection is a fundamental process that determines the dynamics of the flow and hence the velocity-vorticity description is closer to physical reality. Fasel [17] was the first one to solve the incompressible Navier-Stokes equations in velocity-vorticity form by focusing on the stability analysis of boundary layers using finite difference technique in two dimensions. The main advantages of the velocity-vorticity formulation are that the incompressibility constraint is easily satisfied once the vorticity boundary conditions are enforced at the boundaries accurately and the pressure term is completely eliminated. More details about the advantage of this formulation can be obtained from Reference [18]. This formulation has already been successfully implemented to study convective heat transfer problems. Wong and Baker [19] developed a time-accurate CFD finite element algorithm using the velocity-vorticity form of incompressible Navier-Stokes equations to analyze laminar incompressible flow in three-dimensional square channel, lid-driven cavity and a thermal cavity. Murugesan et al. [20] studied natural convection in a square cavity with a square blockage using velocityvorticity form of Navier-Stokes equations. The governing equations were solved using a global matrix-free finite element method [20] which does not require the formation of global matrices. Lo et al. [21] analyzed natural convection in an inclined cavity using velocity-vorticity equations by employing differential quadrature (DQ) method for the solution of the governing equations.

The present work is an attempt to carry out a detailed numerical study on the variation of Nusselt and Sherwood numbers obtained as a result of wide variations in Lewis number $1 \le Le \le 500$, buoyancy ratio $-25 \le N \le 25$ and Rayleigh number $10^3 \le Ra \le 10^6$. The computational methodology employed to perform a large number of simulations required for the above analysis is demonstrated by applying the velocity-vorticity form of Navier-Stokes equations for double diffusive natural convection in a square cavity. The development of governing equations, finite element procedure and the simulation results obtained are discussed in the following sections.

Mathematical model

The physical model of the problem as shown in Figure 1 is a two-dimensional shallow square cavity filled with Newtonian binary fluid mixture. The fluid motion is assumed to be steady and laminar. The horizontal walls of the cavity are assumed to be adiabatic and impermeable, whereas the vertical walls are maintained at hot and cold temperatures and solutal concentrations in order to generate the fluid motion. The higher temperature and concentration are on the same wall for augmenting fluid flow otherwise it is opposing flow. Assuming Boussinesq approximation small linear variation of density at constant pressure due to temperature and solutal concentration variations can be expressed by $\rho = \rho_0 [1 - \beta_T (T - T_{cold}) -\beta_C(C-C_{cold})]$, where ρ_0 is a characteristic density, and β_T and β_C are volumetric expansion coefficients with temperature and solutal concentration fraction, respectively. Thermal volumetric

expansion coefficient β_T is always positive but β_C may be either positive for augmenting buoyancy forces or negative for opposing buoyancy forces. Also the radiation, Soret and Duffor effects are assumed to be negligible in this study.



Figure 1 Schematic diagram of square cavity Governing equations

The governing equations of the prescribed problem are based on conservation of mass, momentum, energy and solutal concentration. Following are the governing equations expressed in canonical form [22]:

$$\nabla \dot{u} = 0$$
(1)
Momentum equation

$$\frac{\partial \dot{u}}{\partial t} + (\overset{\rho}{u}.\nabla)\overset{\rho}{u} = -\frac{1}{\rho}\nabla p + \upsilon\nabla^{2}\overset{\rho}{u} + g\beta_{T}(T - T_{C})\hat{j} + g\beta_{C}(C - C_{C})\hat{j}$$
(2)

Energy equation

$$\frac{\partial T}{\partial t} + \frac{\rho}{u} (\nabla T) = \alpha \nabla^2 T \tag{3}$$

Solutal concentration equation

$$\frac{\partial C}{\partial t} + \overset{\mathsf{p}}{u} (\nabla C) = D \nabla^2 C \tag{4}$$

where \hat{j} is unit vector in y-direction. The pressure gradient term in the momentum equation (2) can be eliminated by introducing the curl operator on both sides of the equation. The curl of gradient is identically zero and using the vorticity definition ($\omega = \nabla \times u$) and equation (1) the momentum equation (2) becomes

$$\frac{\partial \omega}{\partial t} + \nabla \times \begin{pmatrix} \rho & \rho \\ \omega \times u \end{pmatrix} = \upsilon \nabla^2 \omega + g \beta_T \frac{\partial T}{\partial x} + g \beta_C \frac{\partial C}{\partial x}$$
(5)

Using the vector identity the second term in the L.H.S of equation (5) becomes

$$\nabla \times (\overleftrightarrow{\omega} \times \overleftrightarrow{u}) = (\overleftrightarrow{u} \cdot \nabla) \overleftrightarrow{\omega} - (\overleftrightarrow{\omega} \cdot \nabla) \overleftrightarrow{u}$$
(6)
Substituting (6) in (5), we get

$$\frac{\partial \omega}{\partial t} + \begin{pmatrix} \rho \\ u . \nabla \end{pmatrix} = \begin{pmatrix} \rho \\ \omega . \nabla \end{pmatrix} + v \nabla^2 \omega + g \beta_T \frac{\partial T}{\partial x} + g \beta_C \frac{\partial C}{\partial x}$$
(7)

Equation (7) is called vorticity transport equation and using tensor and vector multiplication the term $(\overset{P}{\omega}.\nabla)\overset{P}{u}$ in equation (7) can be shown to be equal to $(\nabla \overset{P}{u})\overset{P}{\omega}$

then
$$\nabla u = \mathcal{S} + W$$

where **S** is rate of strain tensor and

W is angular rotation

One part of $(\nabla u^{\mathsf{p}}) \overset{\mathsf{p}}{\omega}$ increases the vorticity by stretching the vortex line whereas the remaining part contributes to the angular turning of the vortex line. This aspect of stretching and turning is completely absent in two-dimensional flow. Finally the vorticity transport equation for two-dimensional domain can be rewritten as

$$\frac{\partial \omega}{\partial t} + (\overset{\mathbf{\rho}}{u} \nabla) \omega = \upsilon \nabla^2 \omega + g \beta_T \frac{\partial T}{\partial x} + g \beta_C \frac{\partial C}{\partial x}$$
(8)

In order to obtain solution for vorticity and velocity fields a relationship between velocity and vorticity has to be established. This can be achieved by taking curl of the vorticity definition as $\nabla \times (\nabla \times u) = \nabla \times \omega \qquad (9)$

Using vector identity the LHS of equation (9) becomes $\nabla \times (\nabla \times \overset{O}{u}) = \nabla (\nabla \overset{O}{.u}) - \nabla^2 \overset{O}{u}$

Now after using the incompressibility constraint and vector relationships, the above equation can be rewritten as

$$\nabla^2 \mathcal{U} = -\nabla \times \boldsymbol{\omega} \tag{10}$$

Equation (10) is called velocity Poisson equation which satisfies the kinematic condition.

Equations (8) & (10) are velocity-vorticity form of Navier-Stokes equations and these equations can be represented in dimensionless form using the following scaling factors for double diffusive natural convection problem:

spatial coordinates,
$$X = \frac{x}{H}$$
, $Y = \frac{y}{H}$, velocities,

$$U = \frac{u}{U_0}, V = \frac{v}{U_0}, \text{ vorticity, } \Omega = \frac{\omega H}{U_0}, \text{ time, } \tau = \frac{U_0 \tau}{H},$$

temperature $\theta = \frac{T - T_c}{\Delta T}$, solutal concentration $\Phi = \frac{C - C_c}{\Delta C}$,

where $\Delta T = T_h - T_c$ and $\Delta C = C_h - C_c$. Vorticity transport equation

$$\frac{\partial\Omega}{\partial\tau} + U\frac{\partial\Omega}{\partial X} + V\frac{\partial\Omega}{\partial Y} = \Pr\left(\frac{\partial^2\Omega}{\partial X^2} + \frac{\partial^2\Omega}{\partial Y^2}\right) + Ra\Pr\left(\frac{\partial\theta}{\partial X} + N\frac{\partial\Phi}{\partial X}\right)$$
(11)

Velocity Poisson equations

$$\frac{\partial^2 U}{\partial X^2} + \frac{\partial^2 U}{\partial Y^2} = -\frac{\partial \Omega}{\partial Y}$$
(12)

$$\frac{\partial^2 V}{\partial X^2} + \frac{\partial^2 V}{\partial Y^2} = \frac{\partial \Omega}{\partial X}$$
(13)

Energy equation

$$\frac{\partial\theta}{\partial\tau} + U\frac{\partial\theta}{\partial X} + V\frac{\partial\theta}{\partial Y} = \frac{\partial^2\theta}{\partial X^2} + \frac{\partial^2\theta}{\partial Y^2}$$
(14)

Solutal concentration equation

$$\frac{\partial \Phi}{\partial \tau} + U \frac{\partial \Phi}{\partial X} + V \frac{\partial \Phi}{\partial Y} = \frac{1}{Le} \left(\frac{\partial^2 \Phi}{\partial X^2} + \frac{\partial^2 \Phi}{\partial Y^2} \right)$$
(15)

The various non-dimensional numbers that appear in the above equations are defined as Prandtl number $\Pr_{\mathbf{r}} = \frac{\upsilon}{\alpha}$, Schmidt number $S_{C} = \frac{\upsilon}{D}$ Rayleigh number $Ra_{T} = \frac{g\beta_{T}\nabla TH^{3}}{\alpha \upsilon}$, Lewis number $Le = \frac{Sc}{\Pr}$ and buoyancy ratio $N = \frac{\beta_{C}\Delta C}{\beta_{T}\Delta T}$.

The initial conditions used in the present simulation work are: at $\tau = 0$ the dependent variables are

 $U = V = \Omega = \theta = \Phi = 0. \tag{16}$

The boundary conditions for $\tau > 0$ are summarized as follows:

$$U = V = 0,$$
 $\theta = \Phi = 1,$ $\Omega = \frac{\partial V}{\partial X}$ at $X = 0,$
 $0 \le Y \le 1$

$$U = V = 0,$$
 $\theta = \Phi = 0,$ $\Omega = \frac{\partial V}{\partial X}$ at $X = 1,$

 $0 \le Y \le 1$

$$U = V = 0,$$
 $\frac{\partial \theta}{\partial Y} = \frac{\partial \Phi}{\partial Y} = 0,$ $\Omega = -\frac{\partial U}{\partial Y}$ at $Y = 0,$ $0 < X < 1$

$$U = V = 0, \qquad \frac{\partial \theta}{\partial Y} = \frac{\partial \Phi}{\partial Y} = 0, \qquad \Omega = -\frac{\partial U}{\partial Y} \qquad \text{at}$$
$$Y = 1, \quad 0 < X < 1 \qquad (17)$$

A second order-accurate Taylor series expansion scheme is used to enforce the vorticity boundary conditions on the cavity walls. The heat and mass transfer at the vertical walls under steady state conditions are calculated in terms of average Nusselt number and Sherwood number defined as follows:



Figure 2 (a) Vertical mid plane U-Y plot for mesh sensitivity study at Ra=1x10⁵, Le=1, N=1



Figure 2 (b) Horizontal mid plane X-θ for mesh sensitivity study at Ra=1x10⁵, Le=1, N=1.

Finite element solution procedure

The governing equations (11) - (15) are solved with the initial (Eqn. (16)) and boundary (Eqn. (17)) conditions using Galerkin's weighted residual finite element method [20]. In this method an approximate solution is assumed for the governing equation. Since the assumed solution is only approximate the governing equation with this solution will give rise to a residual. The minimization of this residual in the entire computational domain results in the acceptable solution for the governing equations. The integral or weak forms of the governing equations are written as follows:

Velocity Poisson equations

$$\int N_{i} \left[\frac{\partial^{2} U}{\partial X^{2}} + \frac{\partial^{2} U}{\partial Y^{2}} - \frac{\partial \Omega}{\partial Y} \right] dX dY = 0$$

$$\int N_{i} \left[\frac{\partial^{2} V}{\partial X^{2}} + \frac{\partial^{2} V}{\partial Y^{2}} + \frac{\partial \Omega}{\partial X} \right] dX dY = 0$$
(20)
(21)

Vorticity transport equation

$$\int N_{i} \left[\frac{\partial \Omega}{\partial \tau} + U \frac{\partial \Omega}{\partial X} + V \frac{\partial \Omega}{\partial Y} - \Pr\left(\frac{\partial^{2} \Omega}{\partial X^{2}} + \frac{\partial^{2} \Omega}{\partial Y^{2}} \right) - Ra \Pr\left(N \frac{\partial \Phi}{\partial X} + \frac{\partial \theta}{\partial X} \right) \right] dXdY = 0 \quad (22)$$

Energy equation

$$\int N_i \left[\frac{\partial \theta}{\partial \tau} + U \frac{\partial \theta}{\partial X} + V \frac{\partial \theta}{\partial Y} - \left(\frac{\partial^2 \theta}{\partial X^2} + \frac{\partial^2 \theta}{\partial Y^2} \right) \right] dX dY = 0 \quad (23)$$

Solutal concentration equation

$$\int N_{i} \left[\frac{\partial \Phi}{\partial \tau} + U \frac{\partial \Phi}{\partial X} + V \frac{\partial \Phi}{\partial Y} - \frac{1}{Le} \left(\frac{\partial^{2} \Phi}{\partial X^{2}} + \frac{\partial^{2} \Phi}{\partial Y^{2}} \right) \right] dXdY = 0$$
(24)

The time derivatives are discretized using semi-implicit Crank-Nicolson scheme. In the present work global matrix-free finite element algorithm has been used to obtain the weak form of the governing equations. In this method all the equations are integrated at element level and are stored at element level itself without forming global matrices. The details of this algorithm can be obtained from Ref. [20]. The matrix form of governing equations at element level are written as **Velocity Poisson equations:**

$$\begin{bmatrix} \mathbf{K}_{ijk} \\ \mathbf{U}_{ik} \end{bmatrix} = \begin{bmatrix} \mathbf{T}_{ijk} \\ \mathbf{\Omega}_{ik} \end{bmatrix}$$
(25)
$$\begin{bmatrix} \mathbf{K}_{ijk} \\ \mathbf{V}_{ik} \end{bmatrix} = -\begin{bmatrix} \mathbf{S}_{ijk} \\ \mathbf{\Omega}_{ik} \end{bmatrix}$$
(26)

Vorticity transport equation:

$$\left[\left[C_{\mu}\right] + \Theta\Delta t \Pr[K_{\mu}] + \Theta\Delta t \left[G_{\mu}^{*}\right]\right] \left\{\Omega_{a}^{*i}\right\} = \left[C_{\mu}\right] \left\{\Omega_{a}^{*}\right\} - (1 - \Theta)\Delta t \Pr[K_{\mu}] \left\{\Omega_{a}^{*}\right\} + Ra \Pr \Delta t N[S_{\mu}] \left\{\Phi_{a}^{*}\right\} + Ra \Pr \Delta t N[S_{\mu}] \left\{\Phi_{\mu}^{*}\right\} + Ra \Pr \Delta t N$$

$$Ra \operatorname{Pr} \Delta t \left[S_{ijk} \right] \left\{ \theta_{ik}^{n} \right\} - (1 - \Theta) \Delta t \left[G_{ijk}^{n} \right] \left\{ \Omega_{ik}^{n} \right\}$$
(27)

$$\left\| \begin{bmatrix} C_{ijk} \end{bmatrix} + \Theta \Delta t \begin{bmatrix} K_{ijk} \end{bmatrix} \right\| \left\{ \theta_{ik}^{n+1} \right\} = \begin{bmatrix} C_{ijk} \end{bmatrix} \left\{ \theta_{ik}^{n} \right\} - (1 - \Theta) \Delta t \begin{bmatrix} K_{ijk} \end{bmatrix} \left\{ \theta_{ik}^{n} \right\} - \Delta t \begin{bmatrix} C_{ijk} \end{bmatrix} \left\{ \theta_{ik}^{n} \right\}$$
(28)
Solutal concentration equation

$$\left[\left[C_{\mu}\right] + \Theta \Delta t \left[K_{\mu}\right]\right] \left\{\Phi_{\mu}^{**}\right\} = \left[C_{\mu}\right] \left\{\Phi_{\mu}^{*}\right\} - \frac{(1-\Theta)\Delta t}{Le} \left[K_{\mu}\right] \left\{\Phi_{\mu}^{*}\right\} - \Delta t \left[G_{\mu}^{*}\right] \left\{\Phi_{\mu}^{*}\right\}$$
(29)

where i, j and k are the element, row and column indices respectively and Θ is a weighting factor for time discretization with range, $0 \le \Theta \le 1$ and

$$\left[C_{ijk}\right] = \int_{XY_e} N_j N_k \, dX \, dY$$

$$\begin{bmatrix} K_{ijk} \end{bmatrix} = \int_{XY_e} \left(\frac{\partial N_j}{\partial X} \frac{\partial N_k}{\partial X} + \frac{\partial N_j}{\partial Y} \frac{\partial N_k}{\partial Y} \right) dX dY$$
$$\begin{bmatrix} G_{ijk}^n \end{bmatrix} = \int_{XY_e} N_j \frac{\partial N_k}{\partial X} N_l U_l^n dX dY + \int_{XY_e} N_j \frac{\partial N_k}{\partial Y} N_l V_l^n dX dY$$
$$\begin{bmatrix} S_{ijk} \end{bmatrix} = \int_{XY_e} N_j \frac{\partial N_k}{\partial X} dX dY$$
$$\begin{bmatrix} T_{ijk} \end{bmatrix} = \int_{XY_e} N_j \frac{\partial N_k}{\partial Y} dX dY$$

The computational domain is discretized using 4 node bilinear isoparametric elements. An isoparametric formulation is employed for the solution procedure so that the Gaussian quadrature can be employed for the numerical integration of all the weighted governing equations. The last stage in the finite element formulation is the solution of the global equations to obtain the field variables at all nodes. In the present work, all the computations are carried out by keeping the matrices at element level itself. The matrices are assembled only once at the time of solution of the simultaneous equations by storing only the nonzero entries in a vector form as required by the conjugate gradient iterative method. The steady state is assumed to be reached, when a specified convergence criteria is satisfied for all the primary variables and it is described for any primary variable

 $\Lambda \text{ as } \frac{\left|\Lambda_{q+1}^{n+1}\right| - \left|\Lambda_{q}^{n+1}\right|}{nnode} \le 10^{-4} \text{ where 'nnode' is the total number of}$

grid points in the computational domain, 'n+1' is the time level and 'q' is the iteration number. A time step of 10^{-5} was used through out the computations.



Figure 3(b) Validation results of variation of Nusselt and Sherwood numbers at hot wall at Ra=1x10⁴, Le=1, Pr=0.71, and N=1

0.0

Computational algorithm

The following computational procedure is employed to obtain the solution of the field variables:

(i) Compute the integration of various element level matrices for the governing equations (25) to (29).

(ii) Determine the elements surrounding each boundary node for the velocity field, the temperature and solutal concentration fields based on the specified Dirichlet boundary conditions.

(iii) Start the computations for t=t+ Δt .

(a) Assume initial vorticity field.

(b) Solve the velocity Poisson equations (25) and (26) after enforcing the Dirichlet velocity boundary conditions at element level.

(c) Compute the vorticity boundary values using the velocity field.

(d) Solve the vorticity transport equation (27) after enforcing the Dirichlet vorticity boundary conditions at element level.

(e) Solve the energy equation (28) after enforcing the Dirichlet temperature boundary conditions at element level.

(f) Solve the solutal concentration equation (29) after enforcing the Dirichlet solutal concentration boundary conditions at element level.

(g) Repeat steps (a) to (f) until convergence of velocities, vorticity, temperature and solutal concentration is achieved. (iv) Go to step (iii) for the next time step







Figure 4(b) Concentration variation at horizontal mid-plane at for various Le at Ra=1x104, Pr=1, N=1

Results and discussion

A program in FORTRAN has been developed to obtain solution for the field variables following the computational procedure discussed in the previous section. The main focus of the present research work is to highlight the capability of velocity-vorticity form of Navier-Stokes equations for double

diffusive natural convection problems. Due to wide range of industrial applications of such problems, it is highly essential to study the effect of buoyancy ratio and Rayleigh number on the flow field distributions and heat and mass transfer phenomena. The variation in thermo physical properties of fluids can be studied by including the effect of variation in Lewis number. Numerical simulation results were obtained to understand the heat and mass transport mechanisms in the presence of simultaneous variation of the above three parameters which are characteristics of double diffusive convection problems. For the cases of variation of Lewis number and buoyancy ratio, the following parameters have been assumed: Ra=1.0e04 and Pr=1. The results on flow field, temperature and solutal concentration fields are illustrated in the form of contours and Nusselt and Sherwood numbers distribution. The classical square cavity is considered as a test problem in the present work.

Mesh sensitivity analysis

The accuracy of the numerical algorithm used in the present study is verified with a mesh sensitivity test and the simulated results are compared for double-diffusive convection flow in a square cavity. The square cavity is discretized using three meshes of size 31×31, 41×41 and 51×51 grid points with nonuniform grid spacing, thus providing fine grids near boundary for accurate computation of vorticity values. Simulation results of U-Y along the vertical mid-plane and X-D along the horizontal mid-plane of the cavity are considered for comparison purpose. Figures 2(a) and 2(b) show the U-Y plot and X- \Box plot respectively for three meshes 31×31 , 41×41 and 51×51 at Ra=1.0e05, Le=1 and N=1. As can be seen from the above figures the results of 41×41 and 51×51 meshes almost coincide with each other except a slight variation observed for 31×31 mesh in U-Y plot. In the case of X- \Box plot the results of all the three meshes coincide with each other. These results demonstrate that the present formulation and numerical procedure are not sensitive to the spatial discretization of the computational domain for double diffusive natural convection problem. Based on the mesh sensitivity study the 51×51 mesh was selected for simulating the various cases of double diffusive convection problem discussed in the following sections.







For the purpose of validation, numerical results of Weaver and Viskanta [7] and Beghein et al. [1] are considered. Figure 3(a) shows the comparison of X-V plot obtained by the present work and the results of Weaver and Viskanta [7] at Ra=1.0e05, Le=1 and N=-1.209. The present results show close agreement with the results of the above reference. The comparisons of local Nusselt and Sherwood number variations along the hot wall of a square cavity obtained by the present work and the results of Beghein et al. [1] are shown in Figure 3(b) at Ra=1.0e04, Le=1, and N=1. As can be seen from the above figure the present algorithm is capable of producing the local Nusselt and Sherwood number variations in close agreement with the results of the above reference. Table 1 illustrates the comparison of the average Nusselt number on the hot and cold walls of the square cavity computed for Ra=1.0e05 and Le=1. These results demonstrate excellent agreement between the present work and the results reported in Reference [7].

Effect of Lewis number

Due to the importance of Lewis number in various applications, its variation on heat and mass transfer is studied for a range $1 \le Le \le 500$. Figures 4(a) and 4(b) show the temperature and solutal concentration variations respectively along the horizontal mid-plane of the square cavity at Ra=1.0e04, Pr=1 and N=1. Comparing the above two figures

one can observe that for Le=1, the temperature and concentration variations are similar and they exactly correspond to the case of Ra=1.0e04 for natural convective heat transfer problem. The mass diffusive effect comes into effect only when Le increases above unity. With increase in Lewis number heat diffusion increases compared to mass diffusion, resulting in decrease in temperature gradients near the hot and cold walls of the cavity. A reverse trend is observed for the case of concentration distribution in Figure 4(b), wherein the gradient increases with increase in Lewis number. Figure 5 shows the temperature contours inside the cavity for different values of Lewis number. As observed in Figure 5(a) the temperature gradients for Le=1 show the trends observed in natural convective heat transfer. With increase in Lewis number there is not appreciable variations in the temperature contours as observed in Figure 5. Solutal concentration distributions at various Lewis numbers are depicted in Figure 6. As expected Figure 6(a) replicates the temperature contours for Ra=1.0e04. With increase in Lewis number the gradients near the hot and cold walls increases as noted in Figures 6(b) to 6(e). Hence the convective fluid motion is set inside the cavity and this results in increased convective mass transfer. This will lead to increase in Sherwood number on hot and cold walls as seen from the tabulated values in Table 2. It should be noted that the increase in Sherwood number on the hot wall side is larger than that on the cold wall side, with maximum difference observed at Le=500. These observations also can be supported by the vorticity contours shown in Figure 7 for various Lewis numbers. For Le=1, the vorticity contours exhibit a symmetric flow distribution as noted in Figure 7(a). As Lewis number increases the symmetry of vorticity contours is disturbed and a larger vorticity variation is observed near the hot wall and a smaller vorticity variation is observed near the cold wall. This behavior is due to the combined effect of hot wall temperature and high value of solutal concentration on the left wall of the cavity. Double diffusive convection is always viewed as a superposed mass transfer on natural convective heat transfer phenomenon. Due to the increased circulatory fluid core size on the hot wall side, the concentration gradient also increases with increase in Lewis number as observed in Figures 7(b) to 7(e). These results demonstrate that the present velocity-vorticity formulation has correctly predicted the temperature and concentration variations with variation in Lewis number as expected based on the physics underlying the problem.





Figure 6 Concentration contours for, (a) Le=1, (b) Le=10, (c) Le=50, (d) Le=100, (e) Le=500 at Ra=1x10⁴, Pr=1, N=1

The convective heat and mass transfer inside the cavity can be well represented by plotting the Nusselt and Sherwood numbers variation with Lewis number. Figures 8(a) and 8(b) show the variations of local Nusselt and Sherwood numbers along the hot wall of the cavity respectively for different Lewis numbers. The local Nusselt and Sherwood numbers always start from a value at the lowest point of the hot wall and keep decreasing toward the top most point of the wall for any given value of Lewis number. This is because due to the circulatory fluid movement set up by the buoyancy forces of thermal and solutal concentration gradients steeper temperature and concentration gradients are created at the lowest part of the hot wall compared to the top side of the hot wall. These variations in temperature and solutal concentration gradients also can be verified from Figures 5 and 6. With increase in Lewis number the temperature gradients decrease and hence the local Nusselt number also decreases as observed in Figure 8(a). Since increase in Lewis number results in increased solutal concentration gradients near the hot and cold walls, the local Sherwood number increases as depicted in Figure 8(b). Though local Sherwood variations show almost similar trends for Lewis numbers from 1 to 100, there is a steep increase in its value near the bottom side of the hot wall and a similar drop at the top side of the hot wall at Le=500. This can be explained by looking at the vorticity contour distribution shown in Figure 7(e) for Le=500. It was pointed out earlier that with increase in Lewis number the symmetric fluid circulation observed from Le=1 to 100 gets distorted at Le=500. This fluid distribution near the bottom side of the hot wall results in sharp variation of solutal

concentration gradient and hence an increased value for local Sherwood number.



Figure 7 Vorticity contours for, (a) Le=1, (b) Le=10, (c) Le=50, (d) Le=100, (e) Le=500 at Ra=1x10, Pr=1, N=1 Effect of buoyancy ratio

Flow, temperature and solutal concentration fields are computed for buoyancy ratios 1, 10, 25, -10 and -25 at Ra=1.0e04 and Le=50. Figure 9 shows the stream line distributions in the cavity for the above values of buoyancy

ratios. For positive value of buoyancy ratio thermal and solutal buoyancy forces aid each other whereas for negative value of buoyancy ratio these buoyancy forces oppose each other. As the value of N increases from 1 to 25 the fluid circulation gets intensified due to the aiding nature of the buoyancy forces as observed in Figures 9(a) to 9(c).



Figure 8(a) Variation of local Nusselt number distribution along hot wall side with Le at Ra=1x104, Pr=1, N=1



Figure 8(b) Variation of local Sherwood number distribution along hot wall side with Le at Ra=1x104, Pr=1, N=1

When the value of N becomes negative due to the opposing nature of the buoyancy forces the fluid circulation gets affected as noted in Figures 9(d) and 9(e). The temperature distributions are depicted in Figure 10 for various values of N. When N=1, the temperature contours are similar to those obtained for pure natural convection problem at Ra=1.0e04 as seen from Figure 10(a). As the value of N increases from 1 to 25 temperature gradients are set up inside the cavity due to the convective movement of the fluid medium but the variation is very nominal because of Le=50.



(b)



Figure 9 Stream line pattern for (a) N=1, (b) N=10 (c) N=25, (d) N=-10, (e) N=-25 at Ra=1x10⁴, Le=50, Pr=1

When the buoyancy ratio becomes negative, there is a flow reversal inside the cavity resulting in setting up of reversed temperature gradients as compared to the cases of positive N value as observed in Figures 10(d) and 10(e). Solutal concentration distributions in the cavity are shown in Figure 11 for different values of N.





Figure 10 Temperature contours for (a) N=1, (b) N=10 (c) N=25, (d) N=-10, (e) N=-25 at Ra=1x10⁴, Le=50, Pr=1

Figure 11(a) shows the concentration distribution for N=1 and hence the variation shows only the effect of Lewis number. As the Lewis number is 50, the concentration gradient is not uniform at the centre of the cavity, though sharp gradients are observed near the hot and cold walls. As the buoyancy ratio increases from 1 to 10 and 25 as shown in Figures 11(a) to 11(c), due to the aiding flow the convective mass transfer increases resulting in sharp solutal concentration gradients near the vertical walls. When the buoyancy ratio becomes negative flow reversal takes place due to the opposing nature of the thermal and solutal buoyancy forces. This results in the reversal of the direction of the solutal concentration gradients as seen from Figure 11(d) and 11(e). The distribution of local Nusselt and Sherwood numbers along the hot wall of the cavity for various buoyancy ratios are depicted in Figure 12. The maximum value of local Nusselt number is obtained for N=1 because only for this case the maximum heat transfer is obtained. As the buoyancy ratio increases from 1 to 10 and 25, the convective mass transfer becomes dominant resulting in decrease in the local Nusselt number as observed in Figure 12(a) but this trend is just reversed for the case of local Sherwood number as seen from Figure 12(b), wherein maximum local Sherwood number is obtained for N=25. When the buoyancy ratio becomes negative the same reverse trend is observed between the local Nusselt and Sherwood numbers in which maximum local Nusselt number is obtained for N=-10 whereas the maximum local Sherwood number is obtained for N=-25 as noted in the above figures.



Figure 11 Concentration contours for (a) N=1, (b) N=10 (c) N=25, (d) N=-10, (e) N=-25 at Ra=1x10⁴, Le=50, Pr=1.

After discussing the effect of variations of Lewis number and buoyancy ratio on heat and mass transfer phenomena separately in the previous sections their combined effect is analyzed by plotting the average Nusselt and Sherwood numbers along the hot wall as a function of Le and N. Figure 13(a) shows the variation of Nusselt number with Lewis number for N=1, 10

and 25. At N=1, though the Nusselt number decreases with increase in Lewis number it almost remain constant. With increase in N the maximum Nusselt number observed at Le=1 also increases as seen from Figure 13(a). But there is a sharp decrease in Nusselt number with increase in Lewis number at N=10 and N=25. Because increase in Lewis number results in a mass transfer controlled convection process. The Nusselt number almost becomes equal to unity at Le=100 for N=10 and N=25, indicating at such high value of Lewis number only simple heat diffusion process becomes significant. Similar variations were observed by Gobin and Bennacer [7]. The variation of average Sherwood number along the hot wall of the cavity shows an increasing trend with increase in Lewis number as well as with an increase in the buoyancy ratio as observed in Figure 13(b). This trend is expected because the increase in both the Lewis number and the buoyancy ratio augments the mass transfer in the cavity.



Figure 12(a) Variation of local Nusselt number along hot wall side with N at Ra=1x10⁴, Pr=1, Le=50 of various N



Figure 12(b) Variation of local Sherwood number along hot wall side at Ra=1x10⁴, Pr=1, Le=50 of various N.

Effect of Rayleigh number

Figures 14(a) and 14(b) show the variation of local Nusselt number and Sherwood number along the hot wall of the cavity respectively at N=1, Le=2 and Pr=1 for different values of Rayleigh number. Since the Rayleigh number is based on thermal Grashof number, increase in Rayleigh number results in increased thermal buoyancy force and hence the local Nusselt number increases as observed in Figure 14(a). For the reasons already discussed in section 4.3, the distribution of local Nusselt number decreases from the bottom side of the hot wall towards the top side of the hot wall for all values of Rayleigh number. This variation is observed to be steep for the case of Ra=1.0e06 where maximum convective heat transfer takes place. The variation of local Sherwood number also exhibits a similar trend as noted from Figure 14(b). By comparing Figures 8 and 14 one can conclude that the Nusselt number variation is affected by the Rayleigh number whereas the Sherwood number is affected by the Lewis number.



Figure 13(a) Influence of Lewis number on average Nusselt number of hot wall for various N at Ra=1x10⁴, Pr=1.



Sherwood number of hot wall for various N at $Ra=1x10^4$, Pr=1.

Table 2 shows the average Nusselt and Sherwood numbers on the hot and cold walls of the cavity for variations in Lewis number, buoyancy ratio and Rayleigh number. Maximum value of average Nusselt number is obtained only for N=1 and with increase in buoyancy ratio the Nusselt number decreases as noted in the above table. This is because Le=50 is taken for this case. As far as the variation of average Sherwood number is concerned the maximum value is obtained for maximum value of N. The average Nusselt and Sherwood numbers increase as Rayleigh number is increased. The value of the average Nusselt and Sherwood numbers on the hot wall are almost equal to those values on the cold wall for any given value of buoyancy ratio and Rayleigh number. In any convective heat and mass transfer problems, only when the flow field is computed accurately the temperature and solutal concentration fields can be obtained correctly. In the present numerical procedure the velocityvorticity formulation is capable of predicting the heat and mass transfer phenomena exactly. It should be noted that since the vorticity boundary values are computed using the velocities at the boundary nodes, it is enough to provide boundary conditions only for the velocities, temperature and solutal concentration.



Figure 14(a) Influence of Rayleigh number on local Nusselt number along hot wall side at Le=2, Pr=1, N=1



Figure 14(b) Influence of Rayleigh number on local Sherwood number along hot wall side for Le=2, Pr=1, N=1 Conclusions

Double diffusive natural convection in a square cavity is numerically simulated using velocity-vorticity form of Navier-Stokes equations. A global matrix-free finite element algorithm is employed to solve the governing equations by storing all the matrices at element level itself without forming global matrices. The effect of variations in buoyancy ratio ($-25 \le N \le 25$), Lewis number ($1 \le Le \le 500$) and Rayleigh number ($10^3 \le Ra \le 10^6$) is studied in detail by plotting the flow field, temperature and solutal concentration fields.

A detailed analysis on the variation of Nusselt and Sherwood numbers is also discussed in this work. An increase in the Lewis number results in very little effect in Nusselt number but significantly increases the value of Sherwood number. The vorticity distribution predicted in the present formulation shows a distinct variation in the flow distribution due to the variation in Lewis number. For both aiding and opposing flows the variation in the value of N makes only small changes in the average Nusselt number on both hot and cold walls.

At Le=100 the average Nusselt number approaches unity when N=10 and 25, clearly indicating the diffusion type of heat transfer. When N=1, the Nusselt number does not show any variation with increase in Lewis number whereas the Sherwood number continuously increases with increase in Lewis number and buoyancy ratio. When the Lewis number is increased by one order of magnitude the average Nusselt number does not vary much on both the hot and cold walls of the cavity whereas the average Sherwood number increases by three times on the hot wall and two times on the cold wall. In the case of Rayleigh number variation, as the Rayleigh number is increased from 1.0e3 to 1.0e06, the increase in Sherwood number is observed to be more than that in Nusselt number because L=2 is used in the computations.

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Table 1	Compa	rison o	f average	Nusselt	number	for v	validation cas	se
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	Average Nusselt		
Surface	Present work	Ref.[7]	% of error
Hot wall	18.3	18.42	0.6
Cold wall	18.3	18.51	1.0

Table 2 Average Nusselt and Sherwood numbers on hot and cold wall

Parameter	Average Nu	sselt number	Average Sherwood number				
	Hot wall	Cold wall	Hot wall	Cold wall			
Le	Ra=1e04, N=1						
1	2.8061	2.8061	2.8061	2.8061			
10	2.33384	2.34461	6.72213	6.21964			
50	2.21499	2.22406	12.29947	9.88366			
100	2.1065	2.11249	16.1605	11.62844			
500	2.14022	2.13056	32.56528	15.21870			
Ra	Le=2, N=1						
1e03	1.26883	1.26921	1.7447	1.72603			
1e04	2.61804	2.61804	3.70173	3.70167			
1e05	5.34081	5.34081	7.36004	7.36004			
1e06	10.33362	10.33362	13.98575	13.98574			
Ν	Ra=1e04, Le=50						
-25	1.10951	1.10951	18.10793	18.10780			
-10	1.05552	1.05553	13.58626	13.56604			
1	2.21499	2.22406	12.29947	9.88366			
10	1.16825	1.16896	15.39293	14.97196			
25	1.15518	1.15552	18.96766	18.78978			