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Numerical Study of the Mass Transfer Effects on the Flow and Thermal Fields Structures under the Influence of Natural Convection

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ABSTRACT: In this paper, a numerical study has been carried out for coupled mass, momentum and heat transfer in the field under effects of natural convection. For this purpose, the unsteady incompressible Navier-Stokes equations with the terms of the Buoyancy forces (due to temperature gradients), energy conservation and concentration (mass) transfer equations have been simultaneously solved using appropriate numerical methods. In order to discretize spatial terms, a combined formulation contains a second-order central difference method and the first-order upwind scheme has been used. Time integration of the governing equation has been performed using the fourth order Runge-Kutta method. The effect of variations of the mass of contaminant has been studied in changing the flow and thermal fields structure. It is concluded from obtained results, an increase in mass flow rate of secondary (mass) injection, alters the structure of the flow and thermal fields. Comparison of the results obtained from the numerical model with appropriate reference data shown that the model has relatively good accuracy.

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Introduction

Discernment of substantial structures and changes in fluid flow, heat and mass transfer for improving the design processes of energy production and conversion systems, studying about environmental problems (e.g. Air and Water pollution) is very important. It is clear that for this purpose we can choose two approaches, experimental and (or) computational methods. For numerical approach, a set of governing equations which are nonlinear and coupled partial differential equations and called transport equations, such as mass and momentum conservation equations should be solved. If the flow is a mixture which contains two or more components, the mass transport should be also mentioned. The interaction of each phase particles with other ones will be done in three ways, one-way coupling, two way coupling and four-way coupling. In one-way mode, the flow is sufficiently dilute such that fluid feels no effect from presence of particles. Particles move in dynamic response to fluid motion and no influence is available between particulate phase and the continuous phase. In two-way coupling, enough particles are present such that momentum exchange between dispersed and carrier phase interfaces alters dynamics of the carrier phase. Fluid phase influences particulate phase via aerodynamic drag and turbulence transfer and particulate phase reduces mean momentum and turbulent kinetic energy in fluid phase. In four-way coupling, flow is dense enough that dispersed phase collisions are significant momentum exchange mechanism and particle-particle collisions create particle pressure and viscous stresses. Energy conservation equation must be added to this set of equations to calculate temperature or any thermodynamics variables changes. Heat transfer which is a form of energy transfer occurs in three different forms as conduction, convection, and radiation. When the continues medium is a fluid, the convective heat transfer is very significant Convection heat transfer usually is generated between a solid surface and an adjacent moving fluid[1]. This type of heat transfer contains heat conveying from one point to another point due to fluid flow and it means that the heat transfer was done due to mass transfer[2]. Obviously, the heat transfer rate is dependent on the flow rate of the fluid. Convection heat transfer occurs in two forms: forced and free. If the fluid flow is caused by an external factor, then heat transfer made a forced type and if the fluid motion is occured by the buoyancy force, due to density differences (as a result of temperature gradient), the free convection heat transfer creates[3]. Convection heat transfer has a wide range of applications in heating and cooling systems, heat transfer systems, industrial ventilation, mining industry, chemical industry, combustion engines, etc.

Similar to other cases in fluid mechanics and heat transfer, experimental, analytical and computational approach can be used for studying the natural convection. Some of the researches in this area have been performed using analytical methods such as similarity solution methods. Guha and Pradhan studied about a unified integral theory for laminar

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natural convection on an arbitrarily inclined surface, both for specified variation in surface temperature and surface heat flux. Their results also agree well with previous computational and experimental results at intermediate angles of inclination between the vertical and the horizontal [4]. The natural convection phenomenon is often occurred due to a temperature gradient between a cooled and heated surfaces and the numerical methods is a good choice to study this flow field. Shi studied about free natural convection in a square cavity contains a vibrated thin blade. This study shows an oscillatory flow was created due to periodic increasing and reduction of blade length[5]. Hasnaoui investigated about natural convection behavior of a heated plate in a square cavity. The oscillatory flow at high Rayleigh number was shown in their results[6]. The effects of three heated plates in a closed area on natural convection heat transfer have been studied by Oosthuizen et al. Also, their results show the oscillatory behavior of the flow field at high Rayleigh number[7]. Numerical study of natural convection phenomenon close to a cooling stage has been investigated in a two-dimensionally controlled environment by Haque and Betz. Their study was conducted for ambient air at constant temperature and Prandtl number of the Newtonian fluid [8]. Lei et al. developed a numerical simulation for the natural convection of a three-dimensional hermetic cavity. A finite element model and a hyper mesh framework have been used for this simulation [9].

Hua Shu et al. investigated the physical mechanism of flow instability and heat transfer of natural convection in a cavity with thin fin using a numerical method. The wall faces of the cavity are differentially heated. They concluded from the simulation results that the positions where instabilities take place in the temperature contours accord well with those of higher thermal conductivity value, which demonstrates that the energy gradient theory reveals the physical mechanism of flow instability. Also, the effects of the fin length, the fin position, the fin number, and Rayleigh number on heat transfer are investigated [10].

Lee studied about the effect of a three-dimensional obstacle of natural convection in a horizontal enclosure. The enclosure was heated from the bottom wall and then was cooled down from above. An obstacle was located in the middle of the enclosure to examine its effect. They concluded that at a low Rayleigh number, thermal behavior in three-dimensional enclosure showed a steady invariant two-dimensional result. After undergoing periodically oscillatory phase, a chaotic flow transition occurred. At a high Rayleigh number, three-dimensional thermal plume oscillates freely consequently yields a higher heat transfer rate [11]. Yildiz et al. studied about natural convection heat transfer along a vertical plate with different values of uniform heat fluxes using numerical approach. They used computational analysis to determine the local wall temperatures for natural convection [12].

Taymourtash studied about natural convection heat transfer from the vertical non-isothermal plate in a supercritical fluid. It is to be noted that the viscosity is changed by pressure and temperature in supercritical fluids. The outcome results for a perfect gas and a gas which follow-up by van der Waals equation has been studied and show good agreement[13]. Moayyedi studied the effect of the temperature gradient on the mass transfer (pollutant) using direct numerical simulation. In this research, the time-dependent behavior of fluid flow, heat and mass transfer were investigated simultaneously[14]. Moayyedi developed a reduced order model based on proper orthogonal decomposition to simulate mass, momentum and energy transfer. In this model, the spatial and temporal variables were separated and the dynamics of coupled flow system simultaneously investigated with a high speed reduced order computational model[15]. Natural convection is a phenomenon which is occurred due to the temperature gradient and therefore a density difference in the flow field is created. It is clear that the density is the representation of the mass field. Variations of mass balance in the field can be an effective parameter to change the buoyancy force in the term of floatability effects. In this research a coupled framework for numerical simulation of the mass, momentum and heat transfer is presented. In this model the effects of mass transfer in changing the structure of flow and thermal field is investigated.

In the sequel, the mathematical formulation of the governing equations is presented. Then, the problem statement and the relared boundary condtions have been presented. Finally, the discretization of the equation in time and space and the results are discussed in the next sections.

Governing Equations

The governing equations of fluid flow contain continuity and linear momentum equations with a term due to the effects of temperature gradients (Boussinesq approximation) as follow:

$$\nabla.\mathbf{u} = 0, \tag{1}$$

$$\frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\mathbf{u} + g\beta\left(\tilde{T} - \tilde{T}_c\right) \tag{2}$$

Where **u** is velocity vector, p is pressure, ρ, is density ν, kinematic viscosity, β thermal expansion coefficient, and g, is gravity acceleration. $\frac{\mathrm{D}}{\mathrm{D}t}$, is the material derivative operator. The continuity and momentum equations can be expressed in vorticity-stream function form as:

$$\nabla^2\psi = -\omega, \tag{3}$$

$$\frac{\partial\omega}{\partial t} + (\mathbf{u}.\nabla)\omega = \frac{1}{\mathrm{Re}}\nabla^2\omega + \frac{\mathrm{Ra}}{\mathrm{Re}^2\times\mathrm{Pr}}\left(\frac{\partial T}{\partial x} - \mathrm{N}\frac{\partial C}{\partial x}\right), \tag{4}$$

where Re, is Reynolds number, N, is floatability number and Ra, is Rayleigh number which are defined as:

$$\mathrm{Ra} = \mathrm{Gr} \times \mathrm{Pr}, \qquad \mathrm{N} = \frac{\mathrm{D} \times \Delta C_0}{\beta \times \Delta T_0},$$

Gr, is Grashof number Pr, is Prandtl number, ΔC_0, is the difference between initial and source dose, D, is the mass diffusion coefficient. The energy and contaminat concentraiton equaitons are spotted as:

$$\frac{\partial T}{\partial t} + (\mathbf{u}.\nabla)T = \frac{1}{\mathrm{Re}\times\ \mathrm{Pr}} \nabla^2 T, \tag{5}$$

$$\frac{\partial C}{\partial t} + (\mathbf{u}.\nabla)C = \frac{1}{\mathrm{Re}\times\ \mathrm{Pr}\times\ \mathrm{Le}} \nabla^2 C + S, \tag{6}$$

Where, S is source term and Le, is Lewis number which is defined as:

$$\mathrm{Le} = \frac{\alpha}{D}$$

Problem Statement and Boundary Conditions

The case study is the natural convection flow from the heated horizontal surface that its configuration is demonstrated in Fig. **1**. As shown in this Fig., at the top, bottom, left and right boundaries, the no-slip boundary condition is applied for the velocity vector. For heat transfer in the domain, at the right and left boundaries, adiabatic wall boundary condition has been used. Also, the wall temperature boundary condition applied to the top side and heated horizontal plate. Also, for two sides near to the horizontal heated plate, adiabatic wall boundary condition has been performed.

For the contaminant transport model, a source is considered over the horizontal heated plate and at all of the boundaries, the derivative of concentration along a perpendicular to the wall has been assumed to be zero (No mass flow through boundaries).

Computational Approach

The governing equations are discretized in both time and space and then used a time-marching approach for the solution of them (except for the stream-function equation). For the stream-function equation used a conventional iterative solution method for elliptic equations (Such as SOR algorithm in explicit or implicit forms) [16].

Spatial discretization

For spatial discretization of the vorticity transport, energy and mass transfer equations used a combined form of the second order finite difference and first-order upwind methods. In this way, the convective terms have been discretized using a first-order upwind scheme that is closely compatible with the physical nature of these terms:

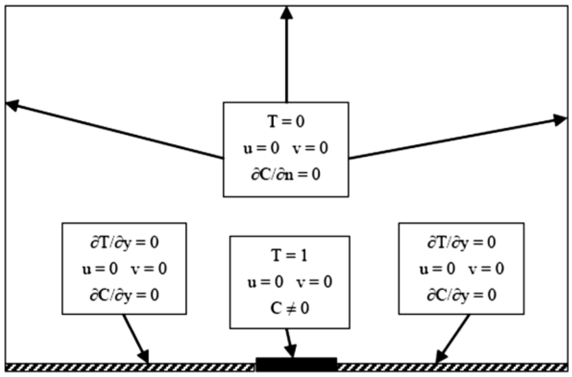

Fig. 1. The geometry of the computational domain and related boundary conditions.

$$u\frac{\partial u}{\partial x} = \begin{cases} u_{i,j}\dfrac{u_{i,j} - u_{i-1,j}}{\Delta x} & if \quad u_{i,j} > 0 \\ u_{i,j}\dfrac{u_{i+1,j} - u_{i,j}}{\Delta x} & if \quad u_{i,j} < 0 \end{cases}, \tag{7}$$

The discretization of the diffusion terms have been carried out using second order central differencing method as follows:

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2}, \tag{8}$$

for the points on the boundaries a forward or backward second-order differential formula is used for first-order derivatives, (e.g. implementation of such boundary conditions), as follows:

$$\begin{aligned} \frac{\partial F}{\partial x} &= \frac{-3F_{i,j} + 4F_{i+1,j} - F_{i+2,j}}{2\Delta x}, \\ \frac{\partial F}{\partial x} &= \frac{3F_{i,j} - 4F_{i-1,j} + F_{i-2,j}}{2\Delta x}, \end{aligned} \tag{9}$$

Time Integration

Time integration of all transport equations is performed using fourth order Explicit Runge-Kutta method. This method is a convenient and accurate way for time marching solution of the governing equations of unsteady problems.

Results and discussion

In this section, the results of this research will be presented. The case study is the natural convection flow from the heated horizontal surface that its configuration is demonstrated in Fig. **1**. To verify the accuracy of the numerical model, the obtained results have been compared with the benchmark data using flow conditions have been listed in Table **1**[17].

Table1. Natural convection problem and contaminant transport conditions

Lewis Number	Prandtl Number	Rayleigh Number	Reynolds Number
1.4	0.72	4.75×10^6	1000

Fig. **2** shows the compared results between local Nusselt Number along heated plate with reference data. It is clear that numerical model data have good accuracy compared to benchmark results. A numerical model was run for free natural convection problem (see Fig. 1) in accordance with Table **1**.

After verification, the validity of the computer code, the model has been used to simulate natural convection flow coupled to mass transfer model. Due to the physics of the problem at this flow statement, the field has a time-dependent behavior. As long as the behavior of the problem obtains an oscillatory response with the identical range, the numerical solution will continue. The criterion to study the behavior of the flow field is the total kinetic energy, which is defined as the square of the velocity magnitude.

$$K.E. = \int_{\partial V} \frac{1}{2}(u^2 + v^2 + w^2)\,\mathrm{dV}, \tag{10}$$

Where u , v and w are velocity vector components. Next, the numerical model of mass transfer is performed for the existing (periodic) solution of the flow field based on an accurate time marching procedure.

Fig. **3** shows the contours of temperature for four different values of floatability number. In the first, which is shown in the left image, there is no contaminant diffusion and the right-top image is related to a second test case which is demonstrated the distribution of temperature under effects of contaminant diffusion with a floatability factor of 0.4. In the third and fourth images, temperature distribution has been shown under the effects of mass diffusion with respect to floatability coefficient equals to 0.7 and 1.2. It is clear from this Fig.s that the secondary mass flow influenced flow field structures. These changes are caused by high variations in the velocity field and therefore the convection part of heat transfer will be greater than other parts. Finally, the temperature field behavior will be changed. To discuss more about the effective parameters of the flow field, the distribution of these variables has been considered. Fig. **4**, demonstrates the distribution of both velocity components, temperature and concentration along a horizontal line located at y = 1.048, and near to upper boundary and for the final time step (t=48 second).

All Fig.s have been presented for four values of the floatability number. Variations of velocity components show that the structure of the flow field is changed related to secondary mass transfer. This variation will be increased for the greater value of the floatability number (N=1.2). It is clear that the variations of the velocity field will be affected on both temperature and concentration field. This is shown in Fig. 4, and the nonlinearity of these changes is more clear for the temperature field. The concentration distribution for

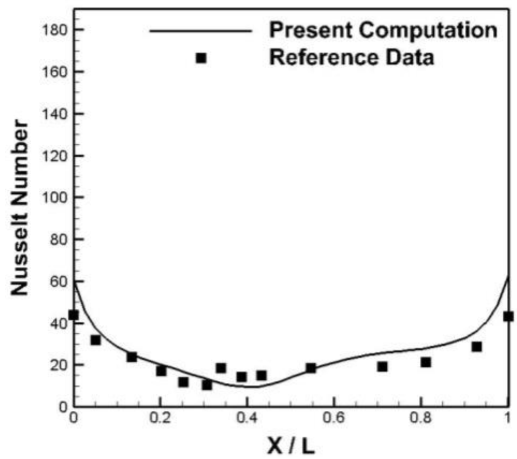

Fig. 2. Distribution of local Nusselt number along horizontal heated plate compared experimental results[17], for conditions listed in Table 1.

the floatability number which is equal to zero, has very few variations. Then, the floatability number is increased, the behavior of concentration distribution due to velocity field changes, will show more variations.

Distribution of temperature, concentration along horizontal center line and local Nusselt number along horizontal heated plate at the final time step, is shown in the Fig. **5**. It is clear by increasing the floatability number (related to mass injection rate), the minimum temperature and concentration inside of the field occurs at a higher distance from the horizontal heated plate. Also, the distribution of the local Nusselt number indicates that its minimum value occurs in the middle of the horizontal plate, and its value will have small

change due to floatability number increasing. But, the slope of the Nusselt number distribution over plate increases before its minimum value point when the floatability number increases. This indicates the increase of local heat flux over the plate surface due to changes in the mass source floatability number. It is clear that the flow field structure is revolved due to mass transport and related influenced force.

In Fig. **6** streamlines in the flow field has been shown at the final time step and for different values of mass flotability number. For N = 0, the flow field contains three vortical structures which are created due to velocity field gradients. When the floatability number is increased these vortical structures will be changed. Especially for N =1.2, the third small vortical structure due to the revolution of the velocity field is merged to another large vortex. Also, for the lower amount of floatability number, the small vortical structure is moved near to upper boundary due to increasing the velocity gradient across the horizontal axis.

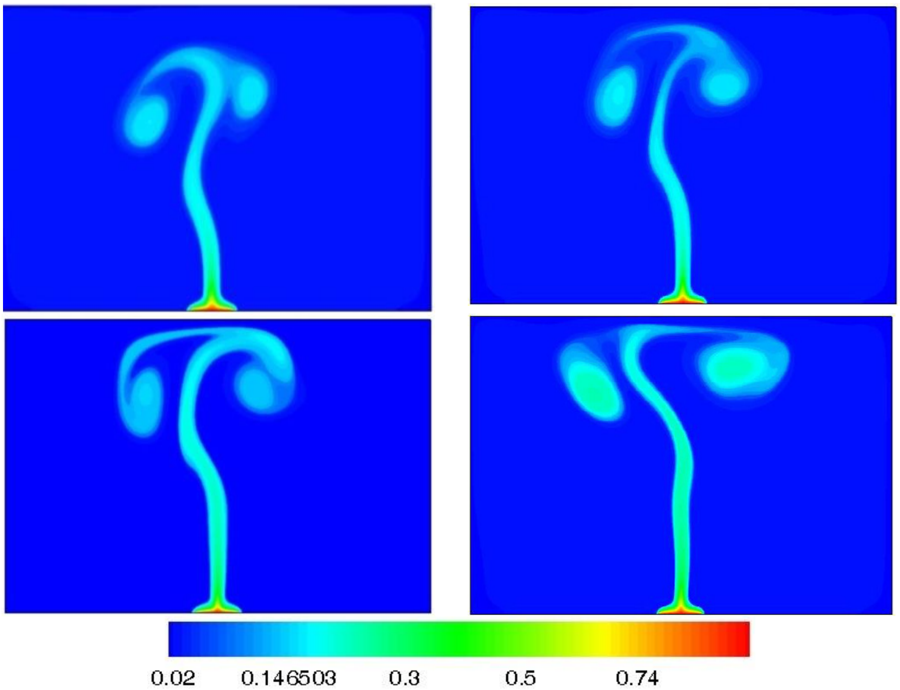

Fig. 3. Contours of temperature(Non-dimensional) in the field without mass diffusion(left),with mass diffusion N = 0.4(right-top), N = 0.7(left-bottom) and N = 1.2 (right-bottom) at t = 48s.

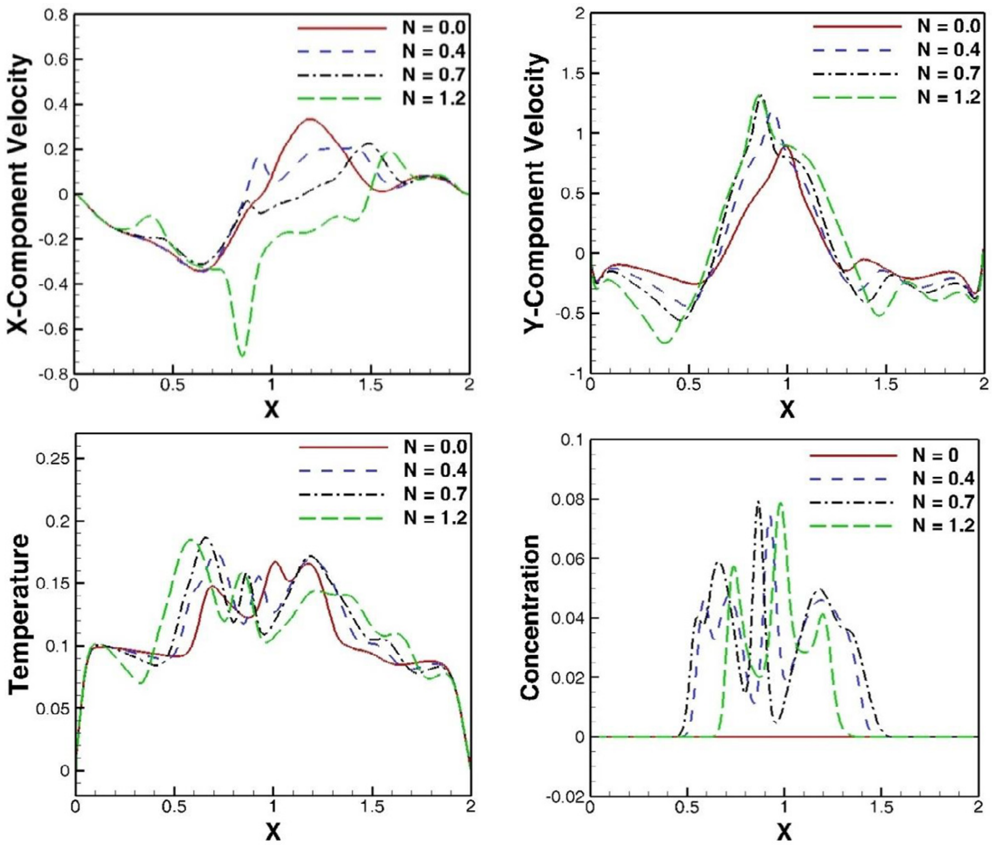

Fig. 4. Distribution of non-dimensional X-Compoent Velocity (top=left), Y-Component Velocity (top-ritght), Temperature (bottom-left) and Concentration(right-bottom) along horizontal line on y=1.048, at t = 48s, for different values of flotability number.

Fig. 7 shows the velocity magnitude contours at the final time step, for different values of the mass flotability number. It is obvious by increasing the floatability number, the maximum velocity magnitude parts are spread. This is caused that the

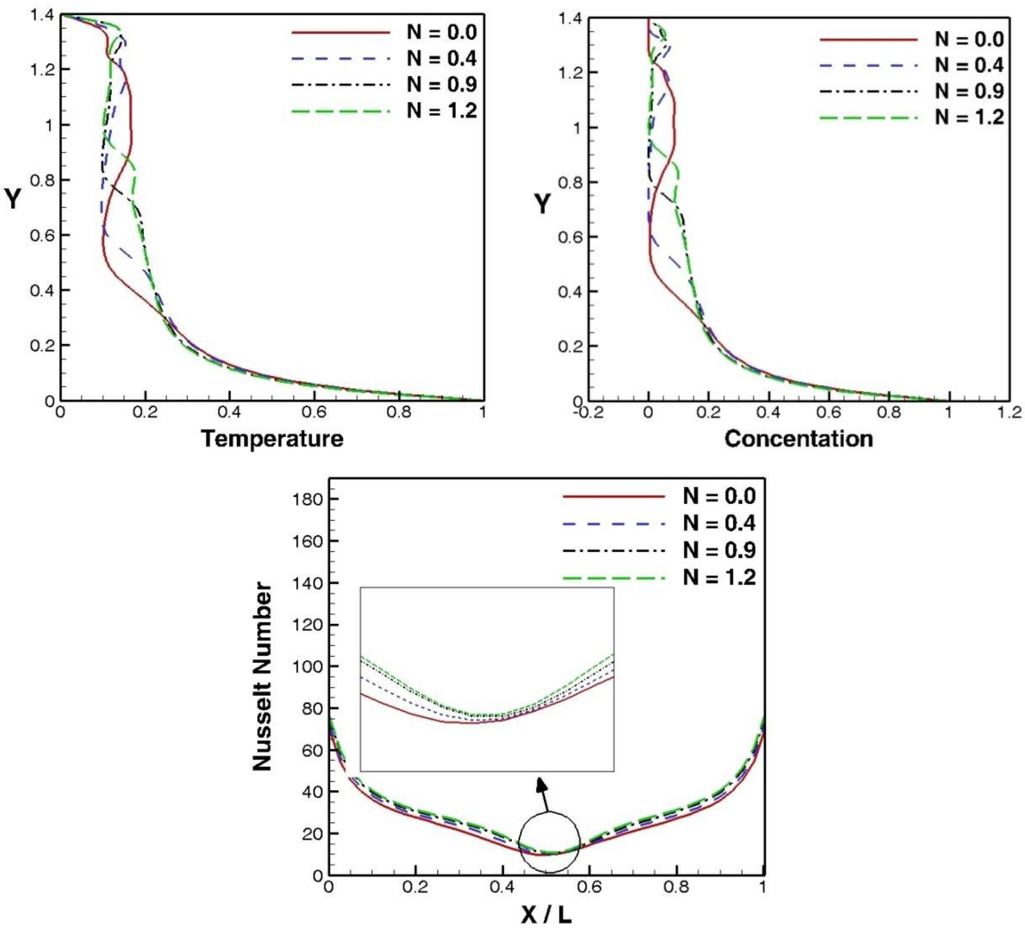

Fig. 5. Distribution of non-dimensional temperature (left) and concentration (right) along the horizontal center line and local Nusselt number along horizontal heated plate surface (bottom) at t = 48s, for different values of flotability number.

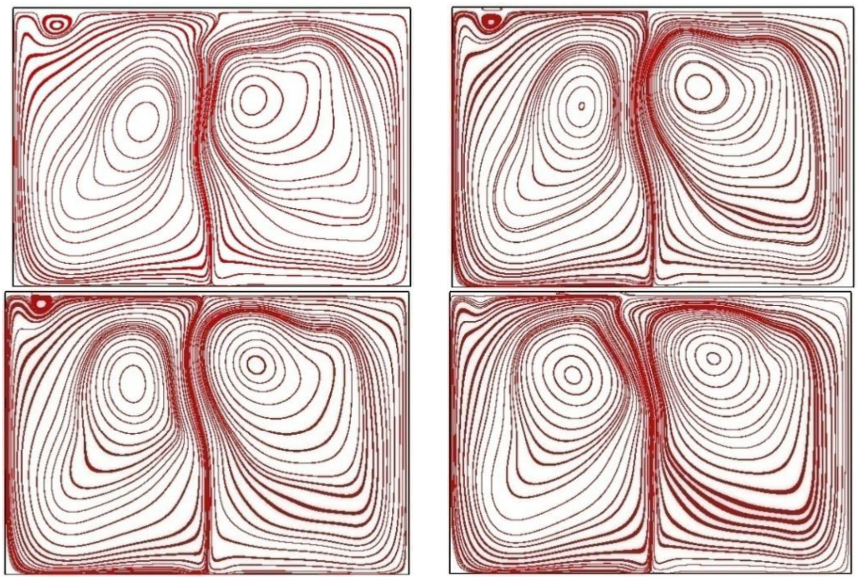

Fig. 6. Streamlines of the field without mass diffusion(left-top),with mass diffusion N = 0.4(right-top), N = 0.7(left-bottom) and N = 1.2 (right-bottom) at t = 48s.

convection part of the mass transfer to be an important role. On the other hand, increasing the velocity at these parts of the flow field caused that the temperature varies due to convective heat transfer. The temperature gradient enhances buoyancy forces and therefore influences on the momentum and mass transfer via convective effects.

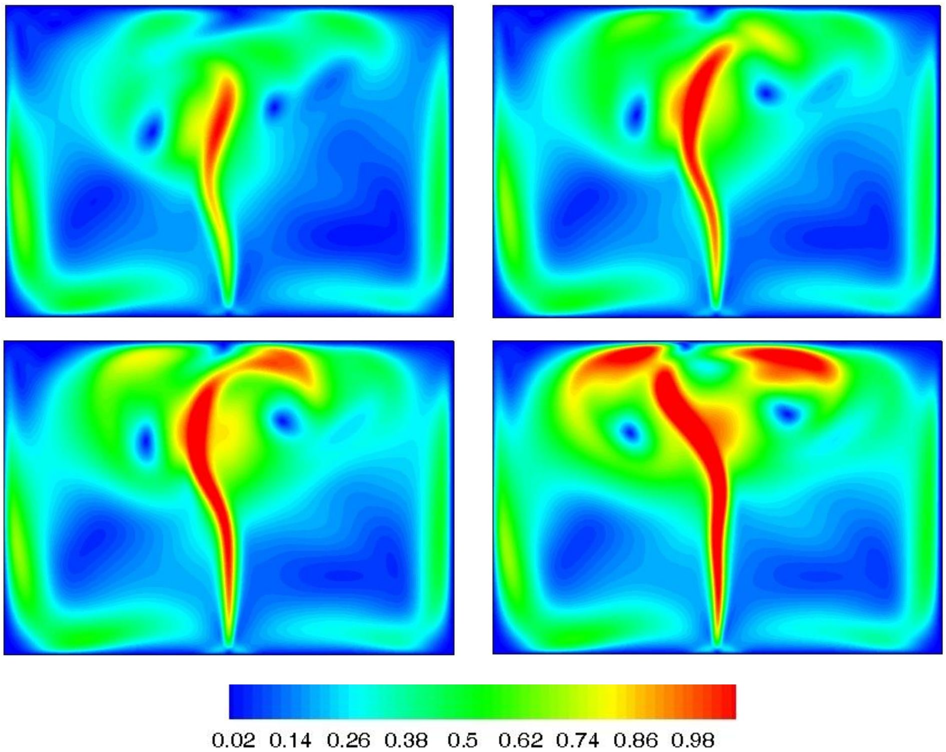

Fig. 7. Velocity magnitude(Non-dimensional) contours in the field without mass diffusion(left-top),with mass diffusion N = 0.4(right-top), N = 0.7(left-bottom) and N = 1.2 (right-bottom) at t = 48s.

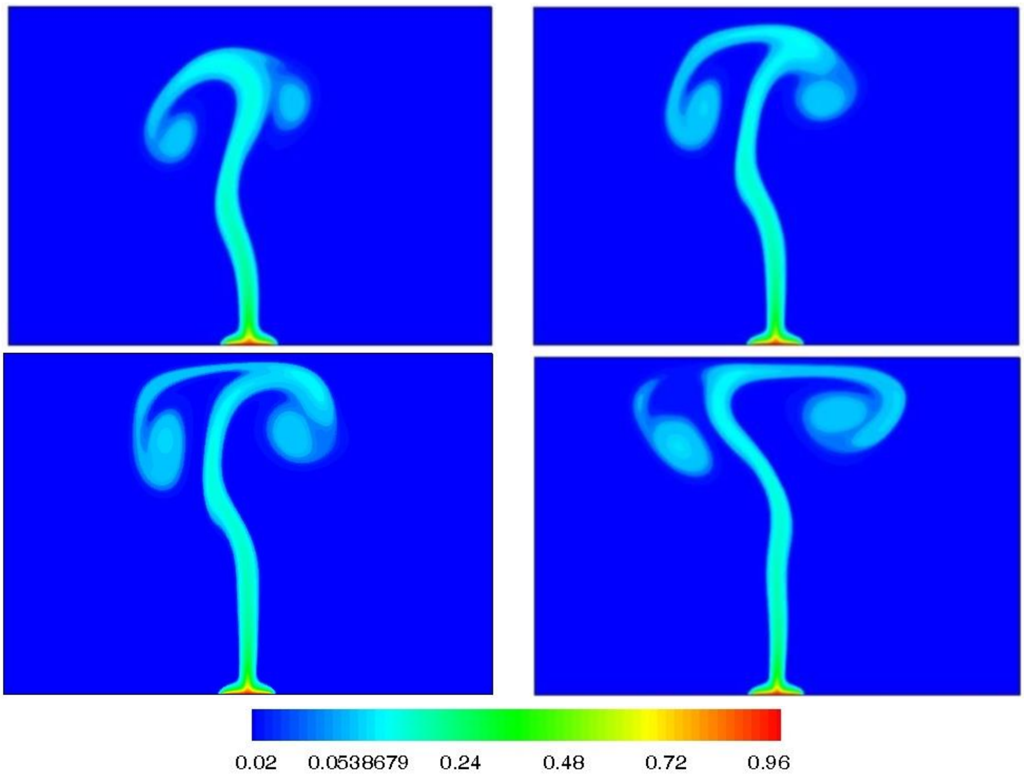

Fig. 8. Contaminat(Non-dimensional) concentration contours in the field without mass diffusion(left-top), with mass diffusion N = 0.4(right-top), N = 0.7(left-bottom) and N = 1.2 (right-bottom) at t = 48s.

Fig. **8** shows the contaminant concentration contours at t = 48 seconds, for different values of the mass flotability number. Variation of diffusion and convection processes of mass transfer is seen in this Fig.. It is clear by increasing the floatability number, the convection part will be an important role in the mass transfer process. But, mass diffusion in the smaller values of the floatability number will play a more important role in the mass transfer phenomenon. This behavior of mass transfer is due to changes in the fluid velocity field and therefore variations of the contaminant concentration. It is clear the velocity field variations effect on temperature field changes.

Conclusions

In this study, the simulation of flow and mass transfer in a field under the effect of natural convection has been studied. Determination of distribution and concentration of contaminants in the field and studying about the influence of the effective parameters can be performed well using numerical methods. For this purpose, the governing equations of the fluid flow, conservation of energy and mass transfer in the unsteady form (time-dependent) are solved simultaneously to analyze the selected problem. The results show that the mass transfer in the domain can change the structure of the flow field by increasing the floatability number. This is arising from a change in the convection and diffusion parts of transport phenomena due to an increase in the mass floatability of pollutants. It caused more changes in the velocity and temperature distribution and therefore the distribution of contaminant will be changed.

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