CHAPTER 3

CHEMICAL REACTION EFFECTS ON NATURAL CONVECTIVE FLOW OVER AN IMPULSIVELY STARTED SEMI-INFINITE VERTICAL PLATE

3.1 INTRODUCTION

Chemical reaction effect on natural convection over a vertical plate in the presence of porous medium has wide range of real time applications. Mainly in the fields of geothermal systems, underground energy storage and transport systems, heating of ground water by vertical intrusive, polymer production, manufacturing of ceramic, packed-bed catalytic reactors, food processing, chemical processing equipment, formation and dispersion of fog, distribution of temperature and moisture over agricultural fields and groves of fruit trees, damage of crops due to freezing, cooling of nuclear reactors, enhanced oil recovery, and the dispersion of chemical contaminants through water-saturated soil.

Moreover, in practical applications such as electrochemical processes and reactors, occurrence of chemical reaction is anticipated the most. Particularly, the effect of electrophoresis with chemical reaction can be applied in the analysis of control of aerosol particles in an environment that may otherwise lead to great climatic changes resulting in natural disaster. The presence of foreign mass in the fluid causes some kind of chemical reaction, such as exothermic or endothermic, which may alter the diffusion rate
tremendously. The effects of a chemical reaction depend on whether the reaction is heterogeneous or homogeneous. A chemical reaction between a foreign mass and the fluid in which the plate is moving is a common phenomenon in chemical engineering process.

The fluids considered in this study are air and water. However, in nature, availability of pure air or water is very difficult. Air and water are usually contaminated with impurities like CO$_2$, O$_2$ and NH$_3$ or salts in water. The effect of the presence of such impurities is studied in scientific literature by considering it as a foreign mass. It is usually a very complicated phenomenon. However, by introducing suitable assumptions, the governing equations can be simplified. These simplified equations were derived by Gebhart (1971) by assuming the concentration level to be very low. Natural convective flow with mass transfer past a semi-infinite vertical plate was presented by Gebhart & Pera (1971). In which a similarity solutions were presented assuming concentration level at the plate to be constant and at low level, which is true in some cases.

Cheng & Minkowycz (1972) presented the similarity solution to free convective flow in a porous medium adjacent to a vertical plate, where the wall temperature is considered as a power function of distance from the leading edge. An exact solution to the mass transfer effects past an impulsively started infinite vertical plate with constant mass flux was presented by Das et al (1996). Most common phenomenon is, mass is supplied at the plate at constant rate in the presence of species concentration, such a situation will be found useful in chemical, aerospace and other engineering applications.

Effects of homogeneous first order chemical reaction on the flow past an impulsively started vertical plate with constant heat flux and mass transfer was investigated by Soundalgekar et al (1994). The solutions are
presented by Laplace transform technique. An impulsive motion of a semi-infinite vertical plate with heat flux and diffusion of chemically reactive species was analyzed by Muthukumaraswamy & Ganesan (2000) with finite difference scheme of Crank Nicolson type. A numerical solution of the transient natural convection flow of an incompressible viscous fluid past an impulsively started semi-infinite vertical plate with uniform heat and mass flux with the homogeneous chemical reaction of first order is discussed by Muthukumaraswamy & Ganesan (2001).

Perturbation method is used to study the influence of chemical reaction and radiation on an unsteady magnetohydrodynamic free convective viscous incompressible fluid flow past a heated vertical porous plate immersed in porous medium by Sharma et al (2011). Loganathan & Golden Stepha (2012) analyzed the effects of chemical reaction and mass transfer on flow of micropolar fluid past a moving porous plate with variable viscosity. An investigation was performed by Ganesan et al (2013) to study the influence of thermo-diffusion and diffusion-thermo effects in the transient, free convective flow of a viscous, incompressible, and doubly stratified fluid past an isothermal vertical plate in the presence of first-order chemical reaction.

In this chapter unsteady, laminar, natural convective flow over an impulsively started vertical plate in the presence of porous medium with first order chemical reaction is investigated. A graphical representation of velocity, temperature and concentration for various values of permeability parameter, chemical reaction parameter, Prandtl number, thermal Grashof number, mass Grashof number and Schmidt number are presented. Also the local skin friction, local Nusselt number, local Sherwood number, average skin friction, average Nusselt number and average Sherwood number are presented graphically.
3.2 FORMULATION OF THE PROBLEM

An unsteady, laminar, two-dimensional, viscous incompressible fluid flow past a moving semi-infinite vertical plate in the presence of porous medium is considered with chemical reaction and mass transfer. The physical model is shown in Figure 2.1. The x-axis is taken along the direction of the vertical plate and y-axis is taken normal to the plate. The properties of the fluid are assumed to be constant. The Darcy’s resistance term is considered with constant permeability of the porous medium. Initially, the fluid and the plate are assumed to be of same temperature and concentration. Later, as time increases the plate is given an impulsive motion with constant velocity $u_0$. The temperature and concentration of the plate are raised to $T_w'$ and $c_w'$ respectively. The governing boundary layer equations by usual Boussinesq's approximation are as follows

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0
\]  
(3.1)

\[
\frac{\partial u}{\partial t'} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = g \beta (T' - T'_{\infty}) + g \beta^* (c' - c'_{\infty}) + \nu \frac{\partial^2 u}{\partial y^2} - \frac{\nu}{\lambda} u
\]  
(3.2)

\[
\frac{\partial T'}{\partial t'} + u \frac{\partial T'}{\partial x} + v \frac{\partial T'}{\partial y} = \alpha \frac{\partial^2 T'}{\partial y^2}
\]  
(3.3)

\[
\frac{\partial c'}{\partial t'} + u \frac{\partial c'}{\partial x} + v \frac{\partial c'}{\partial y} = D \frac{\partial^2 c'}{\partial y^2} - k_i (c' - c'_{\infty})
\]  
(3.4)

The corresponding initial and boundary conditions are

\[
t' \leq 0, \quad u = 0, \quad v = 0, \quad T' = T'_{\infty}, \quad c' = c'_{\infty} \quad \text{for all } x \text{ and } y
\]

\[
t' > 0, \quad u = u_0, \quad v = 0, \quad T' = T'_{w}, \quad c' = c'_{w} \quad \text{at } y = 0
\]

\[
u = 0, \quad v = 0, \quad T' = T'_{\infty}, \quad c' = c'_{\infty} \quad \text{at } x = 0
\]

\[
u \to 0, \quad T' \to T'_{\infty}, \quad c' \to c'_{\infty} \quad \text{as } y \to \infty
\]  
(3.5)
Now introducing the following non-dimensional quantities

\[
X = \frac{xu_0}{v}, \quad Y = \frac{yu_0}{v}, \quad U = \frac{u}{u_0}, \quad V = \frac{v}{u_0}, \quad t = \frac{t'u_0^2}{v}, \quad T = \frac{T' - T'_\infty}{T'_w - T'_\infty}, \quad C = \frac{c' - c'_w}{c'_w - c'_\infty}, \quad Gr = \frac{\nu g \beta (T'_w - T'_\infty)}{u_0^3}, \quad k_c = \frac{k_l v}{u_0^2}
\]  

(3.6)

\[
Gc = \frac{\nu g \beta^* (c'_w - c'_\infty)}{u_0}, \quad Pr = \frac{\nu}{\alpha}, \quad Sc = \frac{\nu}{D}, \quad \lambda = \frac{\lambda' u_0^2}{v^2}
\]

The governing equations and its boundary conditions in dimensionless form are as follows

\[
\frac{\partial U}{\partial X} + \frac{\partial V}{\partial Y} = 0
\]  

(3.7)

\[
\frac{\partial U}{\partial t} + U \frac{\partial U}{\partial X} + V \frac{\partial U}{\partial Y} = Gr \ T + Gc \ C + \frac{\partial^2 U}{\partial Y^2} - \left( \frac{1}{\lambda} \right) U
\]  

(3.8)

\[
\frac{\partial T}{\partial t} + U \frac{\partial T}{\partial X} + V \frac{\partial T}{\partial Y} = \frac{1}{Pr} \frac{\partial^2 T}{\partial Y^2}
\]  

(3.9)

\[
\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial X} + V \frac{\partial C}{\partial Y} = \frac{1}{Sc} \frac{\partial^2 C}{\partial Y^2} - k_c C
\]  

(3.10)

Initial and boundary conditions in dimensionless form are

\[
t \leq 0, \quad U = 0, \quad V = 0, \quad T = 0, \quad C = 0 \text{ for all } X \text{ and } Y
\]

\[
t > 0, \quad U = 1, \quad V = 0, \quad T = 1, \quad C = 1 \quad \text{at } Y = 0
\]

\[
U = 0, \quad V = 0, \quad T = 0, \quad C = 0 \quad \text{at } X = 0
\]

\[
U \rightarrow 0, \quad T \rightarrow 0, \quad C \rightarrow 0 \quad \text{as } Y \rightarrow \infty
\]  

(3.11)
3.3 METHOD OF SOLUTION

The two-dimensional, unsteady, coupled, non-linear partial differential Equations (3.7) to (3.10) subject to the boundary conditions in Equation (3.11) are discretized with Crank Nicolson implicit finite difference scheme which converges faster and is unconditionally stable. After some preliminary investigations, the region of integration is decided as \( X_{\text{max}} = 1 \) and \( Y_{\text{max}} = 14 \), where \( Y_{\text{max}} \) corresponds to \( Y = \infty \). Here the subscript \( i \) designates the grid points in the direction of \( X \), \( j \) designates the grid points in the direction of \( Y \), and \( n \) along the t-direction. The equations at every internal nodal point for a particular \( i \)-level constitute a tridiagonal system.

The system of tridiagonal matrix can be solved by applying Thomas algorithm. Hence the values of \( U, V, T, \) and \( C \) are known at all nodal points in the region at \((n+1)^{th}\) time level. Computations are carried out for all the time levels until the steady state is reached. The scheme is proved to be unconditionally stable using the Von Neumann technique. The local truncation error for the scheme is \( O(\Delta t^2 + \Delta Y^2 + \Delta X) \) and it approaches zero as \( \Delta t, \Delta Y \) and \( \Delta X \) tends to zero. Stability and compatibility ensures the convergence of the scheme. The finite difference scheme for the governing boundary layer equations are as follows

\[
\frac{1}{4\Delta X} \left[ U_{i,j}^{n+1} - U_{i-1,j}^{n+1} + U_{i,j}^n - U_{i-1,j}^n + U_{i,j+1}^{n+1} - U_{i,j+1}^{n+1} + U_{i,j+1}^n - U_{i,j+1}^n \right] + \frac{1}{2\Delta Y} \left[ V_{i,j}^{n+1} - V_{i,j-1}^{n+1} + V_{i,j}^n - V_{i,j-1}^n \right] = 0
\] (3.12)
These Equations (3.12) to (3.15) at every nodal point for a particular $i^{th}$ level constitute a tridiagonal system of equations. In order to get the physical insight into the problem the numerical values of $U$, $V$, $T$ and $C$ are computed for different values of thermal Grashof number, mass Grashof number, Prandtl number, Schmidt number, permeability parameter and chemical reaction parameter. Knowing the velocity, temperature and
concentration it is interesting to calculate the skin friction coefficient, local Nusselt number, local Sherwood number, average skin friction, average Nusselt number and average Sherwood number. Five point approximation is used to approximate the derivatives in local skin friction, local Nusselt number and local Sherwood number. Newton Cotes formula is used to calculate the average skin friction, average Nusselt number and average Sherwood number.

3.4 RESULTS AND DISCUSSION

Numerical solution of finite difference scheme for an unsteady natural convective flow over a semi-infinite vertical plate in the presence of porous medium with chemical reaction is discussed. The Prandtl number is chosen to be 0.73 for air and 7 for water. The species concentration are considered as \( Sc = 0.16, 0.60, 0.78, 0.94 \) and 2 which corresponds to hydrogen, water vapor, ammonia, carbon dioxide and ethyl benzene respectively. The velocity, temperature, concentration, local skin friction, local Nusselt number, local Sherwood number, average skin friction, average Nusselt number and average Sherwood number for different values of flow parameters are computed. The results are shown graphically and the nature of the profiles is explained with its physical significance.

In order to ascertain the accuracy of the numerical results, the present study is compared with the exact solution available in the literature. In the absence of porous medium and taking the chemical reaction parameter as zero, the velocity profile for \( Gr = 2, Gc = 5, Pr = 0.71 \) and \( Sc = 0.16 \) are compared with the exact solution of Soundalgekar et al (1979) at \( t = 0.2 \) in Figure 3.1 and they are found to be in good agreement.
Figure 3.1 Comparison of velocity profiles

Figure 3.2 Velocity profiles for different values of $k_c$ & Pr

$t = 0.2$, $Pr = 0.71$, $k_c = 0$
$Gr = 2$, $Gc = 5$, $Sc = 0.16$
Figure 3.2 shows the velocity profile for different values of chemical reaction parameter and permeability parameter. An increase in the chemical reaction parameter decreases the velocity boundary layer thickness. Also the velocity profile for air is higher when compared to water. The heat diffusion becomes slow due to an increase in Prandtl number which in turn reduces the velocity of the flow. It is also observed that the time taken to reach the steady state is reduced with increasing values of chemical reaction parameter.

![Figure 3.2 Velocity profile](image)

**Figure 3.3 Velocity profiles for different values of $\lambda$.**

From Figure 3.3 it is observed that the velocity boundary layer increases with increasing values of permeability parameter. The velocity boundary layer grows in the direction of the vertically moving plate and gradually reduces to the free stream boundary conditions. This is due to the Darcy's law, which relates the flow rate and the fluid properties to the pressure gradient applied to the porous medium. Hence there is an increase in velocity boundary layer thickness.
In Figures 3.4 and 3.5, velocity profile for Prandtl number and Schmidt numbers are presented respectively. An increase in the Prandtl number decreases the velocity boundary layer thickness. It is also observed that irrespective of the variation in the Prandtl number, the steady state is common for all the Prandtl numbers. In Figure 3.5, velocity profile for various values of Schmidt number is plotted. The velocity boundary layer increases with decreasing values of Sc. The time taken to reach the steady state increases with increasing values of Schmidt number. This describes that the contribution of mass diffusion to the buoyancy force increases the velocity significantly.

Figure 3.4 Velocity profiles for different values of Pr
Figure 3.5 Velocity profiles for different values of Sc

Figure 3.6 Temperature profiles for various values of $\lambda$. 
In Figures 3.6 and 3.7, thermal boundary layer for various values of permeability and Prandtl number are shown respectively. The thermal boundary layer is reduced with increasing values of permeability. The permeability being the measure of the ability of a porous material allows the fluids to pass through the pores. When this parameter is increased there will be a free flow of fluid through it. Hence there is a reduction in the thermal boundary layer.

![Figure 3.7 Temperature profiles for various values of Pr](image)

**Figure 3.7 Temperature profiles for various values of Pr**

In Figures 3.8, 3.9 and 3.10, concentration boundary layer for various effects of permeability, chemical reaction and Schmidt numbers are presented respectively. Concentration boundary layer decreases for increasing values of the permeability parameter. Also the time taken to reach the steady state decreases with increasing values of permeability.

In Figure 3.9, the concentration decreases with increasing values of chemical reaction parameter. The chemical reaction reduces the local
concentration thereby increasing its concentration gradient and its flux. Thus it is observed that there is a fall in concentration due to the increasing values of chemical reaction parameter.

Figure 3.8 Concentration profiles for various values of $\lambda$

Figure 3.9 Concentration profiles for various values of $k_c$
In Figure 3.10, effect of Schmidt number on concentration profile is shown. Concentration boundary layer decreases with increasing values of Schmidt number. As Schmidt number is the ratio of the momentum diffusivity to species diffusivity, it physically relates the relative thickness of the viscous boundary layer and concentration boundary layer. Hence there is an increase in the concentration boundary layer with decreasing Sc. The time taken to reach the steady state also increases with decreasing values of Schmidt number.
Figure 3.11 Local skin friction for various values of $k_c$

Figure 3.12 Local Nusselt number for various values of $k_c$
In Figures 3.11 and 3.12, Local skin friction and average skin friction are presented for various values of chemical reaction parameter. A reduction in the chemical reaction parameter decreases the local skin friction. The presence of chemical reaction reduces the velocity boundary layer. This deceleration in the velocity of the flow reduces the shear stress along the wall which leads to a decrease in the local skin friction. The average skin friction decreases with increasing values of chemical reaction parameter. From Figure 3.2, it is clear that the velocity of the fluid decreases with increasing values of chemical reaction parameter. The deceleration in the velocity reduces the wall friction and hence there is a decrease in the rate of shear stress.

In Figures 3.12 and 3.15, Local Nusselt number and average Nusselt number for various values of chemical reaction parameter are presented. It is observed that an increase in the chemical reaction parameter reduces the local Nusselt number. Also, the average Nusselt number decreases with increasing chemical reaction parameter. It is observed that at initial times, there is no heat transfer this is because, the heat transfer is only by pure conduction.

In Figures 3.13 and 3.16, local Sherwood number and average Sherwood number for various values of chemical reaction parameter is presented. The local Sherwood number and average Sherwood number increases with increasing values of chemical reaction. The chemical reaction parameter induces the rate of mass transfer. From Figure 3.9, it is clear that in the presence of porous medium, increase in the chemical reaction parameter reduces the concentration boundary layer. A decrease in the concentration profile increases the concentration gradient. Hence, there is a rise in the rate of mass transfer.
Figure 3.13  Local Sherwood number for various values of $k_c$

Figure 3.14  Average skin friction for various values of $k_c$
Figure 3.15  Average Nusselt number for various values of $k_c$

Figure 3.16  Average Sherwood number for various values of $k_c$
3.5 CONCLUSION

In the present work, a numerical study of natural convective flow past an impulsively started vertical plate in the presence of porous medium with chemical reaction is analyzed. The non-dimensionl governing partial differential equations are discretized by finite difference scheme of Crank Nicolson type. The results are summarized as follows.

- In the presence of chemical reaction, an increase in permeability increases the velocity boundary layer.

- An increase in permeability and Prandtl number reduces the thermal boundary layer thickness.

- Concentration boundary layer decreases with increasing values of chemical reaction and Schmidt number, where as a reverse process is seen for increasing values of permeability.

- An increase in the chemical reaction parameter decreases the local skin friction, the local Nusselt number and average Nusselt number.

- Local Sherwood number and average Sherwood number increases with increasing values of chemical reaction.