2. Mathematical Analysis

In this chapter we discuss the basic equations, the boundary conditions, the dimensionless parameters, Lie group analysis and the method of solution related to the problems considered for the investigation.

2.1 Basic Equations

Consider the heat and mass transfer by natural convection of two-dimensional steady laminar boundary layer flow of an incompressible viscous fluid along a semi-infinite inclined surface with an acute angle α from the vertical. The x axis is taken along the surface and the y axis is taken normal to the surface. The surface is maintained at a constant temperature $T_w$ which is higher than the constant temperature $T_{\infty}$ of the surrounding fluid. The concentration $C_w$ at the surface is greater than the constant surrounding concentration $C_{\infty}$. The governing equations of the mass, momentum, energy and concentration for the steady flow are:

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \quad (2.1)
\]
\[
\frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = \nu \frac{\partial^2 u}{\partial y^2} + g\beta (T - T_{\infty}) \cos \alpha - g\beta \gamma (C - C_{\infty}) \cos \alpha, \quad (2.2)
\]
\[
\frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \frac{k}{\rho c_p} \frac{\partial^2 T}{\partial y^2}, \quad (2.3)
\]
\[
\frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} = D \frac{\partial^2 C}{\partial y^2}, \quad (2.4)
\]

(For nomenclature see Appendix)

2.2 Boundary Conditions

The no-slip boundary conditions are applied on the surface. The temperature of the surface is maintained at a constant temperature $T_w$ and the constant concentration $C_w$ is maintained at the surface.

\[
u = v = 0, \quad T = T_w, \quad C = C_w \quad \text{at} \ y = 0 \quad (2.5)
\]
The boundary conditions outside the boundary layer (free stream) are

\[ u = 0, \quad T = T_\infty, \quad C = C_\infty \quad \text{as} \quad y \to \infty, \quad (2.6) \]

2.3 Dimensionless Parameters

The individual quantities encountered in a physical problem can be made into dimensionless ones, using dimensional analysis and complicated differential equations governing the fluid flow can be recast into simpler dimensionless forms using this method. The dimensionless quantities are the parameters of the solutions and are the key factors in determining the quantitative and qualitative nature of the flow phenomena.

The following dimensionless parameters are used in this thesis:

**Grashof number**

The ratio of buoyancy force to the viscous force is Grashof number. This number may be constructed either by temperature gradients or concentration gradients or by both and is defined accordingly as

The thermal Grashof number

\[ Gr = \frac{g \beta (T_w - T_\infty) \nu}{U_\infty^3} \]

and the solutal Grashof number

\[ Gc = \frac{g \beta (C_w - C_\infty) \nu}{U_\infty^3} \]

**Prandtl number**

Prandtl number is the ratio of the kinematic viscosity to the thermal diffusivity of the fluid and is given by

\[ Pr = \frac{\nu \rho c_p}{k} \]

**Schmidt number**

This parameter appears when mass transfer process is encountered. The Schmidt number, denoted by \( Sc \), like Prandtl number, gives the ratio of kinematic viscosity
to mass diffusivity of the fluid and is defined by

\[ Sc = \frac{\nu}{D} \]

**Radiation parameter**

The radiation parameter is defined as

\[ R = \frac{4\sigma_0 T_\infty^3}{3kk^*} \]

**Dimensionless chemical reaction parameter**

The non-dimensional chemical reaction parameter is defined as

\[ \gamma = \frac{\nu K_i}{U_\infty^2} \]

**Thermal conductivity parameter**

The thermal conductivity parameter is defined as

\[ A = b(T_w - T_\infty) \]

**Porosity parameter**

The dimensionless permeability of porous medium is given by

\[ K = \frac{k'U_\infty^3}{\nu^3} \]

**Heat generation parameter**

The heat generation parameter is denoted by \( S \) and is defined by

\[ S = \frac{Q \nu}{\rho c_p U_\infty^2} \]

**2.4 Lie Group Analysis**

In this section, we first consider some preliminary notions necessary for the following analysis.
The infinitesimal generator of the one-parameter Lie group of transformation

\[ x^* = \mathcal{X}(\varepsilon) \]  

(2.7)
is the operator

\[ X(x) = \xi(x) \nabla = \sum_{i=1}^{n} \xi_i(x) \frac{\partial}{\partial x_i}, \quad \text{where} \quad \xi_i(x) = \left. \frac{\partial x}{\partial \varepsilon} \right|_{\varepsilon = \text{identity}}. \]  

(2.8)

The components \( \xi_i \) provide the infinitesimals of the transformation group, that is, (2.7) can be written as

\[ x^* = x + \xi(x) + o(\varepsilon^2). \]  

(2.9)

Let \( F(\varepsilon) = F(x_1, x_2, ..., x_n) \) be any differentiable function. Then

\[ X F(x) = \xi(x) \nabla F(x) = \sum_{i=1}^{n} \xi_i(x) \frac{\partial F(x)}{\partial x_i}. \]  

(2.10)

If \( X F = 0 \), then \( F \) is invariant under the action of the associated transformation group.

Now consider a system of \( m \) partial differential equations with \( n \) independent variables \( x = (x_1, x_2, ..., x_n) \) and \( m \) dependent variables \( u = (u^1, u^2, ..., u^m) \).

\[ F^\mu(x, u, u_1, u_2, ..., u_k) = 0, \quad \mu = 1, 2, ..., m \]  

(2.11)

We assume that each partial differential equation in system (2.11) can be written in solved form. In particular

\[ F^\mu(x, u, u_1, u_2, ..., u_k) = u^\nu_{i_1i_2...i_\mu} - f^\mu(x, u, u_1, u_2, ..., u_k) = 0 \]  

(2.12)
in terms of some \( l_\mu \)th order partial derivative of \( u^\nu \) for some \( \nu_\mu = 1, 2, ..., m \) where \( f^\mu(x, u, u_1, u_2, ..., u_k) \) does not depend explicitly on any of \( u^\nu_{i_1i_2...i_\mu}, \mu = 1, 2, ..., m \).

Then the one-parameter Lie group of transformation is of the form

\[ x^* = X(x, u; \varepsilon) \]

\[ u^* = U(x, u; \varepsilon). \]  

(2.13)
The corresponding infinitesimal generator is

\[ X = \xi_i(x, u) \frac{\partial}{\partial x_i} + \eta^\sigma(x, u) \frac{\partial}{\partial u^\sigma}. \]  

(2.14)

The \( k \)th extended infinitesimal generator of (2.14) is

\[ X^{(k)} = \xi_i(x, u) \frac{\partial}{\partial x_i} + \eta^\mu(x, u) \frac{\partial}{\partial u^\mu} + \eta_i^{(1)\mu}(x, u, u_1) \frac{\partial}{\partial u_i^\mu} + \ldots + \eta_{i_1, i_2, \ldots, i_k}^{(k)\mu}(x, u, u_1, u_2, \ldots, u_k) \frac{\partial}{\partial u_{i_1, i_2, \ldots, i_k}^\mu}. \]  

(2.15)

where

\[ \eta_i^{(1)\mu} = D_i \eta^\mu - (D_i \xi_j) u_j^\mu \]  

(2.16)

and

\[ \eta_{i_1, i_2, \ldots, i_k}^{(k)\mu} = D_{i_k} \eta_{i_1, i_2, \ldots, i_{k-1}}^{(k-1)\mu} - (D_{i_k} \xi_j) u_{i_1, i_2, \ldots, i_{k-1}, j}^\mu, \quad \mu = 1, 2, \ldots, m \]  

and

\[ i_j = 1, 2, \ldots, n \]  

for \( j = 1, 2, \ldots, k \)  

(2.17)

Let us now associate with the partial differential equation (2.11) the boundary conditions

\[ B_\alpha(x, u, u_1, u_2, \ldots, u_k) = 0 \]  

(2.18)

prescribed on the boundary

\[ w_\alpha(x) = 0, \quad \alpha = 1, 2, \ldots, s. \]  

(2.19)

The one-parameter Lie group of transformations given by the equations (2.13) is a symmetry group for the boundary value problem prescribed by (2.11), (2.18) and (2.19) if and only if

(i) \( X^{(k)} F^\mu(x, u, u_1, u_2, \ldots, u_k) = 0 \) when \( F^\mu(x, u, u_1, u_2, \ldots, u_k) = 0 \)

(ii) \( X w_\alpha(x) = 0 \) when \( w_\alpha(x) = 0 \).
(iii) $X^{(k-1)}B_\alpha(x,u,u_1,u_2,\ldots,u_{k-1}) = 0$ when $B_\alpha(x,u,u_1,u_2,\ldots,u_{k-1}) = 0$

on $w_\alpha(x) = 0$

From (2.17) $\eta^{(p)}_{\gamma_1,\gamma_2,\ldots,\gamma_p}$ is a polynomial in $u_1,u_2,\ldots,u_p$ whose coefficients are linear homogeneous in $\xi(x,u)$, $\eta(x,u)$ and their partial derivatives upto $p$th order. We eliminate $u^{\delta_\sigma}_{i_1,i_2,\ldots,i_\sigma}$, $\sigma = 1,2,\ldots,m$ by using (2.11). Consequently we obtain a linear homogeneous system of partial differential equations for $\xi$ and $\eta$. These are called the determining equations. In general the number of determining equations is greater than $n+m$, which is the number of unknowns $\xi$, $\eta$ and hence the determining equations are over determined. Solving this overdetermined system, we get the infinitesimals $\xi$ and $\eta$.

The corresponding characteristic equations are given by

$$
\frac{dx_1}{\xi_1(x,u)} = \frac{dx_2}{\xi_2(x,u)} = \cdots = \frac{dx_n}{\xi_n(x,u)} = \frac{du^1}{\eta^1(x,u)} = \frac{du^2}{\eta^2(x,u)} = \cdots = \frac{du^m}{\eta^m(x,u)} \tag{2.20}
$$

If $X_1(x,u), X_2(x,u), \ldots, X_{n-1}(x,u), v^1(x,u), v^2(x,u), \ldots, v^m(x,u)$ are $n+m-1$ independent invariants of (2.20) with the Jacobian

$$
\frac{\partial(v^1,v^2,\ldots,v^m)}{\partial(u^1,u^2,\ldots,u^m)} \neq 0,
$$

then the solution is given implicitly by the invariant form

$$
v^\nu(x,u) = \phi^\nu(X_1(x,u), X_2(x,u), \ldots, X_{n-1}(x,u)) \tag{2.21}
$$

where $\phi^\nu$ is an arbitrary function of $X_1, X_2, \ldots, X_{n-1}$ for $\nu = 1,2,\ldots,m$. Substituting (2.21) into (2.11), we get the reduced system of partial differential equations. If $n = 2$, the reduced system of partial differential equations is a system of ordinary differential equations.

For example, we consider the system of equations

$$
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{2.22}
$$

$$
\frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = \frac{\partial^2 u}{\partial y^2} \tag{2.23}
$$
with the boundary conditions

\begin{align*}
  u &= v = 0, \quad \text{at } y = 0, \\
  u &= 0, \quad \text{as } y \to \infty. \tag{2.24}
\end{align*}

Suppose the system of equations (2.22) and (2.23) admits an infinitesimal generator of the form

\begin{align*}
  X &= \xi_1 \frac{\partial}{\partial x} + \xi_2 \frac{\partial}{\partial y} + \eta^1 \frac{\partial}{\partial u} + \eta^2 \frac{\partial}{\partial v} \tag{2.25}
\end{align*}

where \( \xi_1, \xi_2, \eta^1 \) and \( \eta^2 \) are functions of \((x, y, u, v)\).

The invariance condition (i) become

\begin{align*}
  \eta_1^{(1)1} + \eta_2^{(1)2} &= 0 \tag{2.26} \\
  \eta^1 u_1 + u \eta_1^{(1)1} + \eta^2 u_2 + v \eta_2^{(1)1} &= \eta_2^{(2)1} \tag{2.27}
\end{align*}

when \( v_2 = -u_1 \) and \( u_{22} = uu_1 + vv_2 \). Substituting (2.17) into (2.26) and (2.27) and then eliminating \( v_2 \) and \( u_{22} \) through substitution of (2.22) and (2.23), we obtain

\begin{align*}
  (\eta_x^1 + \eta_y^2) + (\eta_x^1 - \xi_{1x} - \eta^2 - \xi_{2y})u_1 + (\eta_y^1 - \xi_{1y})v_1 \\
  - (\xi_{1u} + \xi_{2v})u_1 + (\eta_x^1 - \xi_{2x})u_2 - (\xi_{1u} + \xi_{2v})v_1 u_2 &= 0, \tag{2.28} \\
  (u \eta_x^1 + \eta_y^1 - \eta_{yy}) + (\eta^2 - u \xi_{1x} - u \eta_x^1 - 2 \eta_{yy} - \xi_{1yy} - 2u \xi_{2y})u_1 \\
  (\eta^1 - u \xi_{2x} - 2 \eta_y^1 + \xi_{2yy} + v \xi_{2y})u_2 + (v \xi_{1u} - 2 \xi_{1yu} - \eta_{uu} - 2u \xi_{2u})u_1 &= 0, \\
  (u \eta_y v) - (u \xi_{1v}) u_1 v_1 - (u \xi_{2v}) u_2 v_1 + (2 \xi_{2yu} - \eta_{uu} + 2v \xi_{2v})u_1 u_2 \\
  + (u \eta_x v) - (u \xi_{1v}) u_1 v_1 - (u \xi_{2v}) u_2 v_1 + (2 \xi_{2yu} - \eta_{uu} + 2v \xi_{2v})u_1 u_2 \\
  + (u \xi_{1uu} - 2 \xi_{2uu}) u_1 u_2^2 + (u \xi_{2uu} - 2 \xi_{1uu}) u_1 u_2^2 + (\xi_{2uu} \xi_3^3 + \xi_{1uu} \xi_1) \\
  + (2 \xi_{1y} + \eta_y^1) u_{21} + (2 \xi_{1u} - \xi_{2v}) u_{21} u_2 - 3 \xi_{1v} u_{21} u_1 &= 0. \tag{2.29}
\end{align*}

Each of the above equations must be an identity for all values of \((x, y, u, v, u_1, u_2, u_{21})\).

Consequently we obtain the determining equations for \((\xi_1, \xi_2, \eta^1, \eta^2)\) which simplify to

\begin{align*}
  \eta_x^1 + \eta_y^2 &= 0
\end{align*}
\begin{align*}
\eta^1_u - \xi_{1x} - \eta^2_v + \xi_{2y} &= 0 \\
\eta^1_v - \xi_{1y} &= 0 \\
\xi_{1u} + \xi_{2v} &= 0 \\
\eta^2_u - \xi_{2x} &= 0 \\
\xi_{1u} + \xi_{2v} &= 0 \\
u \eta^1_x + v \eta^1_y - \eta^1_{yy} &= 0 \\
\eta^1 - u \xi_{1x} - v \eta^1_v - 2 \eta^1_{yv} - \xi_{1yy} - 2u \xi_{2y} &= 0 \\
\eta^2 - u \xi_{2x} - 2 \eta^1_{yu} + \xi_{2y} + v \xi_{2y} &= 0 \\
v \xi_{1v} - 2 \xi_{1yv} - \eta^1_{vy} - 2u \eta_{2v} &= 0 \\
v \xi_{2v} - u \xi_{2v} - v \xi_{1u} + 2 \xi_{1yv} - 2 \xi_{2y} + 2 \eta^1_{uv} + 3u \xi_{2u} + v \xi_{1u} - 2v \xi_{2v} &= 0 \\
u \eta^1_u &= 0 \\
u \xi_{1v} &= 0 \\
u \xi_{2v} &= 0 \\
2 \xi_{2yu} - \eta^1_{uv} + 2v \xi_{2v} &= 0 \\
\xi_{1uu} - 2 \xi_{2uv} &= 0 \\
\xi_{2vv} - 2 \xi_{1uv} &= 0 \\
\xi_{2wu} &= 0 \\
\xi_{1vv} &= 0 \\
2 \xi_{1y} + \eta^1_u &= 0 \\
2 \xi_{1u} - \xi_{2v} &= 0 \\
3 \xi_{1v} &= 0.
\end{align*}

The solution of the above system is

\begin{align}
\xi_1(x, y, u, v) &= c_1 x - 2c_2 x - c_3 \\
\xi_2(x, y, u, v) &= -c_2 y - f(x) \\
\eta_1(x, y, u, v) &= c_1 u \\
\eta_2(x, y, u, v) &= -uf'(x) + c_2 v. \quad (2.30)
\end{align}
We now find the subgroup of (2.30) leaving invariant the boundary condition
\( u(x,0) = v(x,0) = 0 \) prescribed on \( y = 0 \). Invariance of \( y = 0 \) implies that
\( y^* = y + \epsilon \xi_2(x,y,u,v) \) when \( y = 0 \)
which gives \( \xi_2 = 0 \)
and hence \( f(x) = 0 \).

Then (2.29) becomes
\[
\begin{align*}
\xi_1 &= c_1 x - 2c_2 x - c_3 \\
\xi_2 &= -c_2 y \\
\eta_1 &= c_1 u \\
\eta_2 &= c_2 v
\end{align*}
\]
(2.31)
where the parameters \( c_1 \) and \( c_2 \) represent the scaling transformation and parameter
\( c_3 \) represents the translation in the \( x \) coordinate.

The parameter \( c_1 \) is taken to be arbitrary and all other parameters are taken zero
in (2.31). The characteristic equations are
\[
\frac{dx}{x} = \frac{dy}{0} = \frac{du}{u} = \frac{dv}{0}. 
\]
(2.32)
The similarity variable and functions are
\[
\eta = y, \quad u = x F_1(\eta), \quad v = F_2(\eta). 
\]
(2.33)
Substituting (2.33) into equations (2.22) and (2.23), we finally obtain the system of
nonlinear ordinary differential equations
\[
\begin{align*}
F_1 + F_2' &= 0 \\
F_1^2 + F_1' F_2 &= F_1''.
\end{align*}
\]
(2.34)
The appropriate boundary conditions are expressed as
\[
\begin{align*}
F_1 &= F_2 = 0, & \text{at } \eta = 0, \\
F_1 &= 0, & \text{as } \eta \to \infty.
\end{align*}
\]
(2.35)
2.5 Numerical Method for Solution

The equations are highly nonlinear. Therefore analytical solutions may not be found and hence we go in for numerical solution of the problem. Of many numerical methods available for solving a boundary value problem, Runge-Kutta method with shooting technique is used widely.

The shooting method replaces the given boundary value problem by a sequence of initial value problems for the same ordinary differential equations with initial conditions. The solution of the boundary value problem is a linear combination of the solutions of the two initial value problems. The shooting method employs an iterative method for solving nonlinear equations. For example consider the boundary value problem \( f(x, y, y', y'') = 0, \ y(a) = y_a, \ y(b) = y_b. \) In the shooting method, we solve several initial problems iteratively by getting the value \( y'(a) \) in order to get a solution which satisfies \( y(b) = y_b. \) The guess is refined by secant method during the iterations.

The system of transformed ordinary differential equations together with the boundary conditions is numerically solved by employing a Runge-Kutta method and shooting technique with systematic guessing. The numerical computations have been done by the symbolic computation software Mathematica. The value of \( y_{\text{max}}, \) the edge of the boundary layer, is ranging from 10 to 15. The procedure is repeated until we get the results up to the desired degree of accuracy, namely, \( 10^{-5}. \) The results are presented graphically in the form of velocity, temperature and concentration profiles.
Fig. 2.1 The physical configuration and coordinate system