4.1 Navier-Stokes Equations

Computational Fluid Dynamics (CFD) involves numerical solution of the equations governing fluid flow. These equations in their complete form are called the Navier-Stokes equations. Due to the complex nature of these non-linear equations, it is not possible to solve them using the present day computer hardware, except for some simple cases. Instead, approximated forms of these equations, called model equations, are usually solved in CFD. The Navier-Stokes equations form a coupled system of nonlinear partial differential equations describing the conservation of mass, momentum and energy for a viscous, heat conducting fluid. These equations are based on the statement that the net quantity out of a control volume \( V(t) \) through the bounding surface \( S(t) \), minus the quantity produced within the control volume, is equal to the time rate of decrease of the quantity within the control volume.

4.1.1 Equation of Mass Conservation (Continuity Equation)

For an unsteady flow of a compressible fluid, the conservation of mass applied to a fluid passing through an infinitesimal, fixed control volume, yields the continuity equation

\[
\frac{\partial}{\partial t} \iiint_V \rho dV + \iint_S \rho \mathbf{v} \cdot d\mathbf{S} = 0
\]

and in differential form

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = \frac{D \rho}{Dt} + \rho (\nabla \cdot \mathbf{v}) = 0
\]

The first term in Eq. (4.2) represents the rate of increase of density in the control volume and the second term represents the rate of mass flux passing out of the control surface (which surrounds the control volume) per unit volume. The symbol \( D/Dt \) denotes the substantial derivative, which
consists of the local contribution (in unsteady flow) \( \partial / \partial t \), and the convective contribution (due to translation) \( \mathbf{v} \cdot \nabla \).

### 4.1.2 Equation of Momentum Conservation (Equation of Motion)

From Newton's second law, it is known that the sources influencing the variation of momentum are the forces acting on the system. Applying this law to a fluid passing through an infinitesimal, fixed control volume yields the following momentum equation

\[
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{v}) = -\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} + \rho f_x \tag{4.3}
\]

where, for a Newtonian fluid

\[
\tau_{xx} = \lambda (\nabla \cdot \mathbf{v}) + 2\mu \frac{\partial u}{\partial x} \tag{4.4}
\]

\[
\tau_{yx} = \tau_{xy} = \mu \frac{\partial y}{\partial x} + \frac{\partial u}{\partial y} \tag{4.5}
\]

\( \mu \) is the dynamic viscosity and \( \lambda \) is the second coefficient of viscosity.

Using the compact tensor notation for representing the equation, we have:

\[
\frac{\partial (u_i)}{\partial t} + \frac{\partial (u_i u_j)}{\partial x_j} = \frac{\partial \sigma_{ij}}{\partial x_j} + \rho f_i . \tag{4.6}
\]

where

\[
\sigma_{ij} = -p \delta_{ij} + \tau_{ij} \tag{4.7}
\]

is the stress tensor acting on a plane normal to the \( i \) axis in the direction of the \( j \) axis, \( \delta_{ij} \) is the Kronecker delta function, equal to unity if \( i = j \) and zero otherwise, \( p \) is the pressure (normal stress), \( \tau_{ij} \) is the shear stress acting in the \( x_i \) direction on a plane normal to the \( x_j \) direction and equal to

\[
\tau_{ij} = \mu (\partial u_i / \partial x_j + \partial u_j / \partial x_i) + \lambda \delta_{ij} \partial u_k / \partial x_k \tag{4.8}
\]

Combining Eqs. (3.6) and (3.7), we have
\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j} \rho u_j = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} \rho \psi_i \quad (4.9)
\]

Using Stokes relation \(2\mu + 3\lambda = 0\), we have

\[
\tau_{ij} = \mu \left[ (\partial u_i / \partial x_j + \partial u_j / \partial x_i) - \frac{2}{3} \delta_{ij} \partial u_k / \partial x_k \right] \quad (4.10)
\]

The first term on the left hand side in Eq. (4.6) represents the rate of increase of momentum per unit volume in the control volume. The second term represents the rate of momentum lost by convection (per unit volume) through the control surface. The first term on the right hand side represents the surface forces per unit volume. These forces are applied by the external stresses (normal and shear) on the fluid element. The second term on the right hand side is the body force per unit volume.

The integral form of the momentum equation can be written as

\[
\frac{\partial}{\partial t} \iiint_V \rho v dV + \iint_S \rho v \cdot dS = \iiint_V \rho \mathbf{f} \cdot dV + \iint_S \sigma 
\cdot dS
\]

\[
= \iiint_V \rho \mathbf{f} \cdot dV - \iint_S p \cdot dS + \iint_S \tau_{ij} \cdot dS \quad (4.11)
\]

4.1.3 Equation of Energy Conservation

The energy content of a system is measured by its internal energy per unit mass \(E\). In a fluid, the total energy \(e\) to be considered in the conservation equation is the sum of its internal energy and its kinetic energy per unit mass \(v^2/2\). The energy equation is simply the First law of Thermodynamics applied to a control volume. That is, the increase in energy in the system is equal to the heat added to the system plus the work done on the system.

The energy conservation equation in integral form is

\[
\frac{\partial}{\partial t} \iiint_V \rho e dV + \iint_S \rho \mathbf{v} \cdot dS = \iint_S k \nabla T \cdot dS + \iiint_V (W_f + q_m) dV + \iiint_S (\sigma 
\cdot \mathbf{v}) dS \quad (4.12)
\]

In differential form the equation can be written as:
\[
\frac{\partial}{\partial t}(\rho e) + \nabla \cdot (\rho \mathbf{v} e) = q_h + \nabla \cdot q + \nabla \cdot (\sigma_{ij} \cdot \mathbf{v}) + W_f
\]  
(4.13)

Where

\[
q = -\kappa \nabla T = -\frac{\mu}{\text{Pr}} \frac{\partial h}{\partial x_j}
\]  
(4.14)

\[
h = C_p T = \frac{\gamma}{\gamma - 1} \frac{p}{\rho}
\]  
(4.15)

\[
e = E + \frac{u_i u_i}{2}
\]  
(4.16)

\[
E = C_v T = \frac{1}{\gamma - 1} \frac{p}{\rho}
\]  
(4.17)

\[
\text{Pr} = \frac{C_p H}{\kappa}
\]  
(4.18)

\[
W_f = \rho \mathbf{f}_e \cdot \mathbf{v}.
\]  
(4.19)

\[
\kappa = \frac{\mu C_p}{\text{Pr}}
\]  
(4.20)

The first term on the LHS of Eq. 4.13 represents the rate of increase of total energy per unit volume in the control volume while the second term represents the rate of total energy lost by convection (per unit volume) through the control surface. The first term on the RHS is the rate of heat produced per unit volume by external agencies while the second term is the rate of heat lost by conduction (per unit volume) through the control surface. The third term on the RHS is the work done on the control volume (per unit volume) by the surface forces while the last term is the work done by the body forces.

4.2 Approximated Forms of Navier-Stokes Equations

The model equations are approximated, simplified forms of the Navier-Stokes equations developed because the full Navier-Stokes equations cannot be solved for most practical cases. These equations isolate certain aspects of the physics contained in the complete set of equations. Although the model equations are simple and relatively easy to solve, they have to be carefully
selected to representative the complexities that arise in realistic two- and three-dimensional fluid flow simulations. Some of the important model equations are discussed in the following paragraphs.

4.2.1 Boundary-Layer Equations

At high Reynolds numbers, the effects of viscosity are concentrated within a region close to the surface of the body (i.e., within the boundary layer). Hence in all cases where these viscous regions remain close to the body surfaces (that is, in the absence of separation) the calculation of the pressure field may be separated from that of the viscous velocity field. Within the boundary layer, a reduced form of the Navier-Stokes equations could be used by systematically employing two constraints, namely, the viscous layer must be thin relative to the characteristic streamwise dimension of the body, and that the largest viscous term must be of the same approximate magnitude as any inertia (particle acceleration) term. This implies that the second derivatives of the velocity components in the streamwise direction are negligible compared to the corresponding derivatives transverse to the main flow direction, and that the entire momentum equation for the transverse direction could be neglected. Though these concepts were first developed for boundary layer flow, a similar reduction could be made in the governing equations for other flows in which a primary flow direction can be identified. These flows include jets, wakes, mixing layers, and the developing flow in pipes and other internal passages. Thus the terminology boundary-layer approximation has taken on a more general meaning which refers to circumstances which permit the neglect of the transverse momentum equation and the streamwise second derivative term in the remaining momentum equations. These conditions, with y-direction considered normal to the wall, lead to the following boundary layer equations:

Continuity Equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) + \frac{\partial}{\partial y} (\rho v) + \frac{\partial}{\partial z} (\rho w) = 0 \quad (4.21)$$

Momentum equation:
\[
\begin{align*}
\rho \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} + \rho w \frac{\partial u}{\partial z} = & - \frac{\partial p_e}{\partial x} + \frac{\partial}{\partial y} \left( \mu \frac{\partial u}{\partial y} \right) \\
\rho \frac{\partial w}{\partial t} + \rho u \frac{\partial w}{\partial x} + \rho v \frac{\partial w}{\partial y} + \rho w \frac{\partial w}{\partial z} = & - \frac{\partial p_e}{\partial z} + \frac{\partial}{\partial y} \left( \mu \frac{\partial w}{\partial y} \right)
\end{align*}
\] (4.22) (4.23)

Energy Equation:
\[
\begin{align*}
\rho \frac{\partial H}{\partial t} + \rho u \frac{\partial H}{\partial x} + \rho v \frac{\partial H}{\partial y} + \rho w \frac{\partial H}{\partial z} = & \frac{\partial}{\partial y} \left[ \mu \left( 1 \frac{\partial H}{\partial y} + \left( 1 - \frac{1}{p_r} \right) \left( u \frac{\partial u}{\partial y} + w \frac{\partial w}{\partial y} \right) \right) \right] + \frac{\partial p_e}{\partial t}
\end{align*}
\] (4.24)

where, the enthalpy \( H \) is given by
\[
H = C_p T + \frac{u^2}{2} + \frac{w^2}{2}
\] (4.25)

The inviscid pressure gradient, which is obtained from inviscid calculations prior to the solution of the boundary layer equations, acts as an external force on the viscous region. The same inviscid computation also provides the velocities \( u_e(x, y) \) and \( v_e(x, y) \) at the edge of the boundary layer, connected to the pressure field \( p_e \) by the inviscid equation
\[
\rho \frac{\partial v_e}{\partial t} + \rho (v_e \cdot \nabla) v_e = -\nabla p_e
\] (4.26)

Eqs. (4.22) and (4.23) are to be solved by additional boundary conditions \( u = u_e \) and \( v = v_e \) at the edge of the boundary layer. The inviscid region is limited by the edge of the boundary layer, which is initially unknown, since the computation process has to start by the calculation of the pressure field. In the classical boundary layer approximation, the limits of the inviscid region are taken on the surface, which is justified for small boundary layer thicknesses. This leads to a complete separation of the velocity and pressure fields, since the pressure in Eqs. (4.22) and (4.23) will be equal to the inviscid pressure field at the wall, which will be known when these equations are to be solved. The system of equations obtained in this way has only the velocities as unknowns, and hence is a great simplification over the Navier-Stokes equations. When the
influence of the boundary layer on the inviscid flow-field is non-negligible this interaction can be taken into account in an iterative way by recalculating the inviscid pressure field with the limits of the inviscid region located at the edge of the boundary layer obtained at the previous iteration. This procedure is applied for thick boundary layer and for small region of separated flows and is called the ‘Viscid-Inviscid Interaction’. It should be noted that the equations given above are of first order. It is also possible to obtain second order boundary layer equations. These can take into account the transverse and longitudinal curvature of the body. For semi-infinite flat-plates this might not be important, but when the flow over blunt body is considered, the body curvature must be taken into account. The boundary layer approximation can be used in high Reynolds number flow and to resolve flow-fields having little or no separation.

4.2.2 Euler Equations

The Euler equations describe the flow of a non-viscous, non heat-conducting fluid. If we neglect viscosity and heat conduction in the Navier-Stokes equations, the Euler equations are obtained. They are given by:

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} + \frac{\partial \mathbf{H}}{\partial z} = \mathbf{P}$$  \hspace{1cm} (4.27)

in which we redefine the column vectors $\mathbf{F}$, $\mathbf{G}$, $\mathbf{H}$ as

$$\mathbf{F} = \begin{cases} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ \left(\rho e + p\right)u \end{cases}$$  \hspace{1cm} (4.28)

$$\mathbf{G} = \begin{cases} \rho v \\ \rho vu \\ \rho v^2 + p \\ \rho vw \\ \left(\rho e + p\right)v \end{cases}$$  \hspace{1cm} (4.29)
and keep the source ‘P’ and the solution vector ‘Q’ the same. The importance of the Euler equations lies in the fact that at sufficiently large Reynolds numbers, the effect of the viscosity is limited to the boundary layer only; the remaining flow-field is inviscid and can be solved independently of the boundary layer. However, this approach is applicable only if the boundary layer is very thin compared to the characteristic length of the flow field so that the interaction between the boundary layer and the inviscid portion of the flow field is negligible. Nearly all of the Navier-Stokes solvers for high Reynolds numbers are based on Euler solvers extended by the viscous terms. This approximation introduces a drastic change in the formulation of the mathematical models, as the PDE describing the fluid flow reduces from second order to first order. This fact is of paramount importance since it will determine the numerical and physical approach to the computation of these flows.

4.2.3 Parabolized Navier-Stokes Equations

The boundary layer equations can be utilised to solve many viscous flow problems. There are, however, a number of problems where the boundary layer assumptions are not valid. For example, if the inviscid flow is fully merged with the viscous flow, like in a shock layer, the two flows cannot be solved independently of each other. For many of such problems, it is possible to solve a reduced set of equations that fall between the complete Navier-Stokes equations and the boundary layer equations in terms of complexity. These reduced equations belong to a class of equations referred to as the “thin layer” or “parabolised” Navier-Stokes equations. These equations are characterised by the fact that they are applicable to both inviscid and viscous flow regions. In addition, the equations all contain a non-zero normal pressure gradient, which is a necessary requirement if viscous and inviscid flows are to be solved simultaneously. The biggest advantage of most of these equations is that for a steady flow, they are a mixed set of hyperbolic-parabolic equations in the streamwise direction, provided some conditions are met. These conditions are that the inviscid outer region is supersonic and the streamwise velocity component...
is positive everywhere. As a consequence, the equations can be solved using a boundary layer type of marching technique so that a typical problem is reduced from four to three dimensions. In two-dimensional flow, the Parabolized Navier-Stokes (PNS) equations would read:

\[
\frac{\partial M}{\partial x} + \frac{\partial (N - R)}{\partial y} = 0
\]

(4.31)

where the viscous terms R contain only terms with derivatives normal to the main flow. This approximation is directed towards flow situations with a predominant main flow direction, as in the case of a channel flow, whereby the cross-flow components are of a lower order of magnitude. In addition, along the solid boundaries the viscous regions are assumed to be dominated by the normal gradients and hence, the streamwise diffusion of momentum and energy can be neglected. This approximation breaks down if the streamwise flow velocity is not dominant compared to cross flow components (for e.g., if there is a region of reverse flow of the streamwise velocity component).

The PNS equations can be solved using a space-marching technique as opposed to the time-marching technique normally employed for the complete Navier-Stokes equations. In fact, efficient space marching methods are the motivation for using this approximation. Space marching is well suited for stationary, supersonic flow, where all the information is transported downstream within the Mach cone. But in subsonic regions, this assumption fails, since the stationary equations become elliptic and upstream influence occurs in main flow direction. Since only a single space marching sweep is employed in fully parabolic approximation procedures, the computation becomes very efficient with respect to the computation time. The application of parabolic procedures requires initial conditions in two or three cross sections, and has to be taken from other solutions or from experiments. Different versions of PNS equations are available in literature since their derivation from Navier-Stokes equations is not very rigorous. The three dimensional PNS equations of Lubard and Helliwell are obtained by assuming that the streamwise viscous derivative terms are negligible compared to the normal and transverse viscous derivative terms. In other words, the equations are derived by simply dropping all viscous terms containing partial derivatives with respect to the streamwise \((x)\) direction from the steady Navier-Stokes equations.
Continuity Equation:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) + \frac{\partial}{\partial z}(\rho w) = 0 \tag{4.32}
\]

Momentum equations:

\[
\rho \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} + \rho w \frac{\partial u}{\partial z} = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial y} \left( \mu \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu \frac{\partial u}{\partial z} \right) \tag{4.33}
\]

\[
\rho \frac{\partial v}{\partial t} + \rho u \frac{\partial v}{\partial x} + \rho v \frac{\partial v}{\partial y} + \rho w \frac{\partial v}{\partial z} = -\frac{\partial p}{\partial y} + \frac{\partial}{\partial x} \left( \mu \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial z} \left( \mu \frac{\partial v}{\partial z} \right) - \frac{2}{3} \frac{\partial}{\partial y} \left( \frac{\mu}{\partial y} \right) \tag{4.34}
\]

\[
\rho \frac{\partial w}{\partial t} + \rho u \frac{\partial w}{\partial x} + \rho v \frac{\partial w}{\partial y} + \rho w \frac{\partial w}{\partial z} = -\frac{\partial p}{\partial z} + \frac{\partial}{\partial x} \left( \mu \frac{\partial w}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial w}{\partial y} \right) - \frac{2}{3} \frac{\partial}{\partial z} \left( \frac{\mu}{\partial z} \right) \tag{4.35}
\]

Energy Equation:

\[
\rho C_v \frac{\partial T}{\partial t} + \rho u C_v \frac{\partial T}{\partial x} + \rho v C_v \frac{\partial T}{\partial y} + \rho w C_v \frac{\partial T}{\partial z} = -p_e \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) + \frac{\partial}{\partial y} \left( k \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) \\
+ \mu \left[ \left( \frac{\partial u}{\partial y} \right)^2 + \left( \frac{\partial u}{\partial z} \right)^2 \right] + \mu \left[ \left( \frac{\partial v}{\partial y} \right)^2 + \left( \frac{\partial v}{\partial z} \right)^2 \right] \tag{4.36}
\]

### 4.2.4 Reynolds Averaged Navier-Stokes Equations

The Navier-Stokes equations govern laminar as well as turbulent flows. However, solution of the unsteady equations for turbulent flow requires very small time steps and a large number of grid points, which puts the practical computation of turbulent flows by this means
outside the realm of possibility for present computers. The main thrust of present day research in
turbulent flows is through the time-averaged Navier-Stokes equations, called Reynolds Averaged
Navier-Stokes (RANS) equations. These equations are derived by decomposing the randomly
changing flow variables in the Navier-Stokes equations into time averages and fluctuations about
the average, and then time-averaging the entire equation. The averaging process can be
introduced for any quantity ‘A’ by writing
\[ A = \bar{A} + A' \]  \hspace{1cm} (4.37)

where
\[ \bar{A}(x,t) = \frac{1}{T} \int_{-T/2}^{T/2} A(x,t + \tau) d\tau \]  \hspace{1cm} (4.38)
is the mean quantity, and ‘A’ is the instantaneous fluctuating value.

For compressible flows, the averaging process leads to products of fluctuation between
density and other variables such as velocity or internal energy. In order to avoid their explicit
occurrence, a density-weighted average can be introduced through
\[ \tilde{A} = \frac{A}{\bar{\rho}} \]  \hspace{1cm} (4.39)

Performing the averaging process for the continuity equation, we are led to
\[ \frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_j) = 0 \]  \hspace{1cm} (4.40)

Applied to the momentum equations, we are led to the following equation for turbulent
mean momentum in the absence of body forces
\[ \frac{\partial}{\partial t} (\bar{\rho} \tilde{u}_i) + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_i \tilde{u}_j) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_i} (\tilde{\tau}_{ij} - \rho u_i u_j^* ) \]  \hspace{1cm} (4.41)

where
\[ \bar{\tau}_{ij} = \mu \left[ \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \frac{\partial \tilde{u}_k}{\partial x_k} \right] + \mu \left[ \left( \frac{\partial u_i^*}{\partial x_j} + \frac{\partial u_j^*}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \frac{\partial u_k^*}{\partial x_k} \right] \]  \hspace{1cm} (4.42)
4.3 Turbulence Modelling

Turbulence may be defined as a fluid motion involving random macroscopic mixing, with a large range of length and time scales. The wide range of length scales involved in turbulence implies that numerical solutions of the full time-dependant Navier-Stokes equations for turbulence require extremely large number of mesh points. Techniques like Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES) may be used to predict turbulent flows. However, both the approaches are very costly in terms of computing time and memory. In practice, the mean effect of the turbulent quantities is of interest, and not the instantaneous fluctuation quantities. Thus, an alternative to the solution of the complete time-dependant eddies of turbulent flow is Reynolds-averaged modelling, in which a suitable statistical average, commonly a time average, of the Navier-Stokes equations is taken (RANS equations). Comparing Eqs. (4.9) and (4.41), it can be seen that time-averaging the equations of motion gives rise to new terms, which could be interpreted as “apparent” stress gradients associated with the turbulent motion. Thus, Eq. (3.40) could be written as

\[
\rho \frac{D\bar{u}_i}{Dt} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial (\bar{\tau}_{ij})_{\text{Lam}}}{\partial x_j} + \frac{\partial (\bar{\tau}_{ij})_{\text{Turb}}}{\partial x_j} \quad (4.43)
\]

where,

\[
(\bar{\tau}_{ij})_{\text{Turb}} = -\rho \bar{u}_i \bar{u}_j + \mu \left[ \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right] - \frac{2}{3} \delta_{ij} \frac{\partial \bar{u}_k^2}{\partial x_k} \quad (4.44)
\]

are commonly called Reynolds stresses. The second term in RHS of Eq. (4.44) is much smaller than the first term, and is usually neglected. A similar analysis may be performed on the Reynolds averaged energy equation and certain terms involving temperature or enthalpy fluctuations may be identified as apparent heat-flux, \(-\rho \bar{u}_i \bar{T}_i\).

The Reynolds equations cannot be solved in the form given above because the Reynolds stresses and heat-flux terms must be viewed as new unknowns. To proceed with the solution,
additional equations linking these unknowns with the flow variables must be found. This information is contained in the turbulent models, to be added to the averaged Navier-Stokes equations. The expressions for these unknowns, i.e., $\overline{u_i'u_j''}$, $\overline{u_i'T''}$ etc are called turbulence transport equations. These transport equations are obtained by algebraic manipulation of the Navier-Stokes and the Averaged Navier-Stokes equations. Some of the commonly used transport equations are Reynolds stress transport equation, turbulent KE (k) equation, Rate of dissipation ($\varepsilon$) equation and Reynolds turbulent heat-flux equation.

4.3.1 Turbulence Models

In nearly all cases of interest, the Reynolds stresses and other turbulence transport rates are much larger than the viscous stresses and molecular transport rates: this is why turbulence is of such great practical importance. The goal of turbulence modelling is to relate the Reynolds stresses to known mean flow quantities such as velocity.

One classification of turbulence modelling distinguishes between models that employ the basic eddy viscosity concept and those that solve for the Reynolds stresses and fluxes directly. The former category, called eddy viscosity models, includes algebraic (zero-equation) models for the eddy viscosity (e.g., Mixing length and two-layer models), as well as one-equation and two-equation models (e.g., k-$\varepsilon$ models) that compute the eddy viscosity as a function of one or two turbulent quantities governed by partial differential transport equations. The latter category, called stress transport models, includes models with coupled partial differential equations for each Reynolds stress and flux (Direct stress models), as well as simplified or truncated models using algebraic relations (Algebraic stress models) to compute the individual stresses and fluxes.

Eddy-viscosity models relate the Reynolds stresses to strain rate (or velocity derivatives) in a manner identical with molecular stresses. Eddy viscosity models are the simplest turbulent models in the sense that they model the turbulent stresses and fluxes by analogy to molecular stresses and fluxes. The models may be expressed in terms of an eddy viscosity function, $\mu_T$ and a turbulent Prandtl number $Pr_T$, defined by

$$Pr_T = \frac{C_p \mu_T}{\kappa_T}$$

(4.45)
The eddy viscosity function may be expressed in terms of length and velocity scale functions, \( l \) and \( q \), as follows:

\[
\mu_T = \rho l q
\]

The way \( l \) and \( q \) are determined defines the type of model to be used. If \( l \) and \( q \) are determined algebraically from mean flow data, we have the zero-equation models (e.g., Cebeci-Smith and Baldwin-Lomax models). These are the simplest of eddy viscosity models, in which the eddy viscosity is modelled algebraically in terms of flow geometry and mean flow variables. The algebraic eddy viscosity models generally are based upon the Prandtl mixing-length concept and are well adapted to simple attached flows where a single well-defined shear layer is easily identified. As a result, they are the most widely used class of turbulence models. In complex or separated flows, it is difficult to define appropriate velocity and length scales because several such scales are usually present in the flow. These models in general have a low prediction capability, but possess the advantage of simplicity. For simple flows without separation, such as boundary layer flow or pipe flow, the zero-equation models may be used with some degree of success. For complex flows involving multiple strain rates, the mixing-length concept derived for a simple shear layer becomes inadequate.

If \( l \) is determined algebraically, but \( q \) is determined from a field equation such as the TKE equation, the model is referred to as one-equation model. If both \( l \) and \( q \) are determined from field equations, we have the two-equation model (e.g., high Reynolds number \( k-\varepsilon \) and low Reynolds number \( q-\omega \) models). One-equation models usually involve a transport equation for the turbulent kinetic energy, and require the specification of a turbulent length scale to complete the model. The transport equation allows the computed eddy viscosity to include some non-local effects, but the required specification of a length scale inhibits the generality of these models. Two-equation models involve a second transport equation for a dissipation-related turbulence quantity, usually the dissipation rate of the turbulent kinetic energy. They can be considered complete turbulence models, since they require no further specification of any turbulent quantity. Two-equation models provide a more general specification of turbulent length and velocity scales than zero-equation models, but often display numerical stability problems which are not common to zero-equation models.
4.3.1.1 Two Equation $k$-$\varepsilon$ Model

The turbulent KE ($k$) transport equation is well established as providing a reasonable turbulent velocity scale. This is obtained by subtracting the Reynolds-averaged momentum equation from the instantaneous momentum equation and then Reynolds averaging the result. The equation is given by

$$\frac{\partial k}{\partial t} + u_j \frac{\partial k}{\partial x_j} = -u_i u'_i - \varepsilon + \frac{\partial}{\partial x_j} \left[ \nu \frac{\partial k}{\partial x_j} - \frac{1}{2} u'_i u'_i = \frac{1}{\rho} \rho' u'_i \right]$$

(4.47)

Where $k \equiv (u'u' + v'v' + w'w')/2$ is the turbulent kinetic energy and $\varepsilon$ is the rate of dissipation.

Two equation models supply a transport equation for a second variable, apart from $k$, to establish the turbulent length scale. The most popular choice for this variable is $\varepsilon$, which appears directly in the $k$-$\varepsilon$ equation. The standard $k$-$\varepsilon$ model of Jones and Launder consists of the following equations:

$$\nu = \frac{c_\mu k^2}{\varepsilon}$$

(4.48)

$$\frac{\partial k}{\partial t} + u_j \frac{\partial k}{\partial x_j} = \nu \left( \frac{\partial u_i}{\partial x_j} \right)^2 - \varepsilon + \frac{\partial}{\partial x_j} \left[ \nu + \frac{\nu}{\sigma_k} \frac{\partial k}{\partial x_j} \right]$$

(4.49)

$$\frac{\partial \varepsilon}{\partial t} + u_j \frac{\partial \varepsilon}{\partial x_j} = C_{\varepsilon 1} \frac{\varepsilon}{k} \nu \left( \frac{\partial u_i}{\partial x_j} \right)^2 - C_{\varepsilon 2} \frac{\varepsilon^2}{k} + \frac{\partial}{\partial x_j} \left[ \nu + \frac{\nu}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_j} \right]$$

(4.50)

where $C_\mu = 0.09$, $C_{\varepsilon 1} = 1.44$, $C_{\varepsilon 2} = 1.93$, $\sigma_k = 1.0$ and $\sigma_\varepsilon = 1.3$.

Even though the model includes viscous diffusion terms, the constants were evaluated for high Reynolds number flows, a typically decaying turbulence, and in the logarithmic region of the boundary layer. It does not give accurate results close to the wall with no-slip boundary conditions. In these regions, the models are modified by employing one of the following schemes:

(a) Using algebraic wall functions that specify values for $k$ and $\varepsilon$ in terms of friction velocity and distance from the wall for the first grid point off the wall, presumably located in the logarithmic region.
(b) Using robust mixing length models for the near-wall region, which computes eddy viscosity. The two-equation model is matched to the mixing length model at a point generally specified in terms of a fixed $y^+$ within the logarithmic region. The eddy viscosity is used to compute the boundary values for $k$ and $\varepsilon$ at the match point.

(c) Modifying the transport equations of the standard $k$-$\varepsilon$ model and allow integration right down to the wall with appropriate boundary conditions. This requires more grid points in the near-wall region than the other two schemes.

4.4 Discretisation

Discretisation is the process by which a closed-form mathematical expression, such as a function or a differential or integral equation involving functions, all of which are viewed as having an infinite continuum of values throughout some domain, is approximated by analogous expressions which prescribe values at only a finite number of discrete points or values in the domain. All methods in CFD utilize some form of discretisation. Discretization involves two components – space discretisation and equation discretisation.

(a) **Space discretisation.** This consists of setting up a mesh by which a continuum of space is replaced by a finite number of points where the numerical values of the variables will have to be determined. The solution will depend on the form of the mesh and its size (smaller the mesh, better the discretized space approaches continuum, and hence better is the accuracy). FVM is currently the most popular discretisation technique in CFD.

(b) **Equation discretisation.** This is the transformation of the integral or differential equations into an algebraic, linear or non-linear, system of equations, involving the values of the unknowns at the mesh points. The code used for the present work STAR-CCM+, uses implicit schemes based on the density Correction Method to solve the FVM equations.

4.4.1 Finite Volume Method

The basic conservation laws are expressed in terms of conservation of mass, momentum and energy in a volume closed by a surface. To correctly represent discontinuities in the flow, these laws have to be in integral form. In FVM, the integral form of the equations is discretized, and not differential form. In this method, the flow field or domain is subdivided into a set of non-
over lapping cells that cover the whole domain. On each cell the conservation laws are applied to
determine the flow field variables at some discrete points of the cells, called nodes. These nodes
are at typical locations of the cells such as cell centres and cell vertices.

In FVM, the grid may be structured (i.e., all mesh points lie on the intersection of two or
three families of lines, considered as defining curvilinear coordinate lines) or unstructured (mesh
points cannot be identified with coordinate lines, hence they cannot be represented by a set of
integers, such as \(i, j, k\) in three dimensions, but have to be numbered individually in a certain
order). This is perhaps the biggest advantage of FVM. Although requiring a more complicated
bookkeeping, unstructured meshes can offer greater flexibility for complicated geometrical
configurations. In addition, by discretizing the integral form of the conservation equations, we
ensure that the conserved quantities of mass, momentum and energy will also be conserved at the
discrete level. This means that for an arbitrary subdivision of the volume \(V\) into three sub-
volumes \(V_1, V_2\) and \(V_3\), we can write the conservation law for each sub-volume and recover the
global conservation law by adding up the three sub-volume laws. When summing up the surface
integrals, the flux contributions from the surfaces common to adjacent sub-volumes will be of
opposite signs and will cancel out. For e.g., a control volume may be divided into three sub-
volumes as shown in Figure 4.1.

![Figure 4.1 Conservation laws for sub-volumes of volume V](image)

The general conservation laws for the sub-volumes may be written as:

\[
\frac{\partial}{\partial t} \iiint_{V_i} Q dV + \oint_{\partial V_i} \mathbf{F} \cdot \mathbf{dS} = \iiint_{V_i} P dV
\]
\[ \frac{\partial}{\partial t} \iiint_Q dV + \iint_{\partial V^i} \mathbf{F} \cdot d\mathbf{S} = \iiint_P dV \tag{4.57} \]

\[ \frac{\partial}{\partial t} \iiint_Q dV + \iint_{\partial V^i} \mathbf{F} \cdot d\mathbf{S} = \iiint_P dV \tag{4.58} \]

When summing the surface integrals, the contributions of the internal lines ADB and DE always appear twice but with opposite signs. Thus, the sum of the three laws gives the global law

\[ \frac{\partial}{\partial t} \iiint_Q dV + \iint_{\partial V^i} \mathbf{F} \cdot d\mathbf{S} = \iiint_P dV \]

This essential property has to be satisfied for the numerical scheme to be conservative. When this is not the case, i.e., when the resulting equation contains flux contributions from inside the total cell, the discretizing is said to be non-conservative, and the internal flux contributions appear as internal volume sources. In FVM, the user has to define, for a selected sub volume, how to estimate the volume and cell face areas and how to approximate the fluxes at the faces.

### 4.5 Choice of Numerical Method

The numerical methods that are available in the literature for solving the Navier-Stokes equations are generally classified into Density-based and Pressure-based methods.

#### 4.5.1 Density-Based Methods

In this method the density field is obtained by solving the continuity equation. The pressure field is then computed by using the equation of state. Once the pressure field is known the velocity field is obtained by solving the momentum equations. The temperature field is then obtained by solving the energy equation. The density based methods work well for compressible flows but it cannot be extended to the incompressible flows in a straightforward manner. This is because the relationship between the density and pressure become weak as the Mach number of the flow decreases. Thus the density based method loses its generality. However, attempts were made to solve the incompressible flow by using this approach with some modifications.
4.5.2 Pressure-Based Methods

The pressure based methods were developed to solve the incompressible flows. By taking effect of compressibility into account these methods were extended to compressible flows as well. In this class of methods the pressure field is obtained by solving the pressure or pressure correction equation. The pressure correction equation is derived using continuity and the momentum equations. These pressure correction equations are then solved to obtain new pressure corrections. These corrections are then used to updates the pressure and the velocity components. The procedure of updating the pressure and velocity is continued until the correct field of flow variables are obtained.

4.5.3 Treatment of Density Correction

In the compressible flows the density is a strong function of the pressure. It is therefore necessary to correct the density as well as velocity component in order to satisfy the continuity equation. Since pressure is considered as the primary variable, the density corrections are incorporated in the pressure correction equation via the equation of state. If $\rho^*$ and $\rho'$ are the guessed density field and its correction respectively, then the corrected density field is

$$\rho = \rho^* + \rho'$$

(4.59)

The density correction is expressed in terms of the pressure correction via the equation of state as

$$\rho' = \frac{\rho}{RT}$$

(4.60)

4.5.4 Treatment of Pressure Correction

This implicit scheme, used for resolution of Ordinary Differential Eqns, is an iterative method where some innovative physical reasoning is used to construct the next iteration from the results of the previous iteration. The basic sequence of the Pressure Correction method is as follows:

(a) Start the iteration by guessing the pressure field. Let $p^*$ be the guessed pressures.

(b) Using $p^*$, solve for the velocity components $u$, $v$ and $w$ from the momentum equations. Let these be denoted by $u^*$, $v^*$ and $w^*$. 
(c) As the velocity field must satisfy the continuity equation, substitute these obtained values of $u^*$, $v^*$ and $w^*$ in the continuity equation. Since they were obtained from the guessed value $p^*$, the equation will not necessarily be satisfied.

(d) Determine $p'$ correction which, when added to $p^*$, will result in $u$, $v$ and $w$ to be in agreement with the continuity equation, where $u = u^* + u'$, $v = v^* + v'$ and $w = w^* + w'$. Towards this, use the value of $p = p^* + \hat{p}$ in step 2 and repeat the process until a velocity field is found which satisfies the continuity equation.

Sometimes, an under-relaxation factor ($\alpha_p \sim 0.8$) is used to prevent divergence, such that

$$p^{n+1} = p^n + \alpha_p \hat{p}$$

(4.61)

In some cases, it may also be helpful to under relax the values of $u^*$, $v^*$ and $w^*$.

### 4.6 Turbulence Modelling Options

STAR-CCM+ employs mathematical models of turbulence to determine the Reynolds stresses and turbulent scalar fluxes. Special models are also employed to characterize the flow in wall boundary layers. The turbulence models incorporated in the current version of STAR-CCM+ are listed below:

#### 4.6.1 K-Epsilon Turbulence Models

A K-Epsilon turbulence model is a two-equation model in which transport equations are solved for the turbulent kinetic energy ($k$) and its dissipation rate ($\varepsilon$). Various forms of the K-Epsilon model have been in use for several decades, and it has become the most widely used model for industrial applications. Since the inception of the K-Epsilon model, there have been countless attempts to improve it. The most significant of these improvements have been incorporated into STAR-CCM+

In its original form, the K-Epsilon turbulence model was applied with wall functions, but was later modified to use the following approaches for resolving the viscous sublayer.

- Low-Reynolds number
- Two-layer
STAR-CCM+ has a choice of seven different K-Epsilon turbulence models:

- Standard K-Epsilon
- Standard Two-Layer K-Epsilon
- Standard Low-Reynolds number
- Realizable K-Epsilon
- Realizable Two-Layer K-Epsilon
- Abe-Kondoh-Nagano low-Reynolds number
- V2F low-Reynolds number

Non-linear constitutive relations are available in conjunction with the three standard K-Epsilon turbulence model variants. In present investigation Realizable K-Epsilon Two-layer all y+ wall treatment model is used. This model is discussed in detail.

4.6.2 Realizable Two-Layer K-Epsilon Model

The Realizable Two-Layer K-Epsilon model combines the Realizable K-Epsilon model with the two-layer approach. The coefficients in the models are identical, but model gains the added flexibility of an all y+ wall treatment. One of the more successful recent developments is the realizable K-Epsilon model developed by Shih et al. [81]. This model contains a new transport equation for the turbulent dissipation rate. Also, a critical coefficient of the model, $C_\mu$, is expressed as a function of mean flow and turbulence properties, rather than assumed to be constant as in the standard model. This allows the model to satisfy certain mathematical constraints on the normal stresses consistent with the physics of turbulence (realizability). The concept of a variable $C_\mu$ is also consistent with experimental observations in boundary layers.

The realizable K-Epsilon model is substantially better than the standard K-Epsilon model for many applications, and can generally be relied upon to give answers that are at least as accurate. Both the standard and realizable models have been implemented in STAR-CCM+ with a two-layer approach, which enables them to be used with fine meshes that resolve the viscous sublayer.
4.6.2.1 Two-Layer All \( y^+ \) Wall Treatment

The Two-Layer All \( y^+ \) Wall Treatment is a hybrid approach that seeks to recover the behaviors of the other two wall treatments in the limit of very fine or very coarse meshes. It contains a wall boundary condition for \( \varepsilon \) that is consistent with the two-layer formulation. Apart from the specification of the Reynolds stresses in the wall cell, the formulation is identical to the two-layer all-\( y^+ \) wall treatment used for the K-Epsilon model. It is a design goal that this wall treatment should give results similar to the low-\( y^+ \) treatment as \( y^+ \rightarrow 0 \) and to the high-\( y^+ \) treatment for \( y^+ > 30 \). It will also give reasonable results for intermediate meshes where the cell centroid falls in the buffer layer.

4.7 Boundary Conditions

The hypersonic free stream flow is defined by specifying the boundary conditions given in Table 4.1. The outflow being predominantly supersonic, the variables are completely extrapolated from interior to the outlet boundary. The air is assumed to be a calorically perfect gas with constant specific heat ratio, \( \gamma = 1.4 \). At solid walls no-slip adiabatic boundary condition is imposed.

**Table 4.1. Inflow boundary conditions**

<table>
<thead>
<tr>
<th>Cases</th>
<th>( M_\infty )</th>
<th>( T_\infty )</th>
<th>( P_\infty )</th>
<th>( k_\infty )</th>
</tr>
</thead>
<tbody>
<tr>
<td>WF, WS &amp; WOF</td>
<td>6.5</td>
<td>237K</td>
<td>830Pa</td>
<td>0.05</td>
</tr>
</tbody>
</table>

4.8 Validation of Turbulence Model and Code

Suitability of the CFD solver to predict a complex high speed flow through a scramjet inlet was evaluated by comparing the results obtained by the present solver with the experimental results already available in the literature for flow through a dual-mode scramjet at Mach number 4 [45]. Figure 4.2 shows the comparison of variation of pressure along the ramp side of dual-mode scramjet at Mach number 4. The present computational results are also compared with computational result for the same geometry and flow conditions [82]. The present computational results show good agreement with the already available experimental as well as computational results. However discrepancy on the ramp side pressure distribution can be observed in the shock boundary layer interaction region and expansion region. The probable reason for this discrepancy could be deficiency of the turbulence model used, assumed calorically perfect gas condition and
Figure 4.2 Comparison of present computation with experimental and other computational results

Figure 4.3 Grid distribution for validation of turbulence model
the differences between experimental and numerical simulation conditions or the measurement error of the sensors. It indicates the sufficiency of grid distribution, turbulence modelling, boundary conditions etc., being adopted in present computations.

Based on reasonably good comparison achieved, further computations are made for present hypersonic intake geometry with similar grids, boundary conditions and turbulence modelling. Figure 4.3 shows a typical grid distribution showing the overall computational domain with necessary boundary conditions.

4.9 Computational Setup and Grid Sensitivity Analysis

A rectangular computational domain was chosen for the all cases of simulations. The computations were performed on a 16 core cluster. The cluster was connected to a SAN to store large amount of data generated. To monitor convergence of the numerical solution, axial force, normal force and pitching moment plots were monitored. The solutions were converged after about 20,000 iterations. An additional criterion enforced in the current analysis required the difference between computed inflow and outflow mass to drop to 0.5%.

![Figure 4.4 Pressure distribution on forebody lower and the intake upper surface for different grids](image)

Grid sensitivity analysis to study the effect of fence, confirmed that the grid resolution used is sufficient to capture the relevant physical features. The axial force, normal force and pitching moment obtained with different grid refinement levels were compared. Mesh level-1
(total polyhedral cells 4,36,234), mesh level-2 (total polyhedral cells 8,24,234) and mesh level-3 (total polyhedral cells 11,71,113), the maximum discrepancy between the three mesh levels was found to be less than 3%. Figure 4.4 shows computed pressure along the vehicle forebody lower and the intake upper surface for these three grids. Out of these analyses, mesh level-3 was selected, and all results of without fence and with fence intake cases are computed applying this resolution.

Analysis of grid sensitivity to study the influence of bluntness effect and intake strake, also confirmed that the grid resolution used is sufficient to capture the relevant physical features. The axial force, normal force and pitching moment obtained with different grid refinement levels were compared. Coarse Mesh (total Hexahedral cells 3,85,851), medium mesh (total hexahedral cells 19,94,337) and fine mesh (total hexahedral cells 34,09,251), the maximum discrepancy between the three mesh levels was found to be less than 3%. Figure 4.5 shows computed pressure along the vehicle forebody lower and the intake upper surface for these three grids. Out of these analyses, medium mesh was selected, and all results of without fence and with fence intake cases are computed applying this resolution.

![Figure 4.5 Pressure distribution on forebody lower and the intake upper surface for different grids](image)

Figure 4.5 Pressure distribution on forebody lower and the intake upper surface for different grids
4.10 Accuracy

The convergence, consistency and stability have been primarily concerned with the solution behaviour where the finite quantities, such as time step $\nabla t$ and mesh spacing $\nabla x, \nabla y, \text{and } \nabla z$ diminish. In the discretised forms of the transport equations, governing the flow and energy transfer are always solved numerically on a finite grid layout and the effects of turbulence are generally modelled through approximate theories, the solution obtained is always approximate. The corresponding issue of accuracy therefore becomes another important consideration. The truncation error represents the difference between the discretized equation and the exact one and it provides a means of evaluating the accuracy of the solution for partial differential equations. The order of truncation error coincides with the order of the solution error if the grid spacing’s are sufficiently small and if the initial and auxiliary boundary conditions are sufficiently smooth. It is commonly implied that an improvement in accuracy (from the truncation error) of high order approximations can be achieved for a sufficiently fine grid. Refining the grid will often produce a superior accuracy for high order approximations over low order approximations. However, at an absolute accuracy level, justification for more expensive computations may not demonstrate the desired superior accuracy due to limited computing capacity.

4.10.1 Sources of Solution Error

The user should aware of existence of errors in computational solutions but more importantly the user must attempt to distinguish one from another. This section serves to address the possible sources of errors that the user is likely to encounter applying CFD methodologies. Errors are introduced because the numerical solutions of the fluid flow and heat transfer problems are only approximate solutions. Some prevalent sources of errors dealing with numerical solutions include the following classification:

- Discretization error
- Round off error
- Iteration or convergence error
- Physical modelling error
- Human error
Before we elaborate the sources of these errors in CFD, we should like to establish a clear and logical distinction between error and uncertainty that is based on the publication of AIAA guide for verification and validation of Computational Fluid Dynamics Simulations [83]. Error can be defined as a recognizable deficiency that is not due to lack of knowledge while uncertainty can be defined as a particular deficiency that is due to lack of knowledge. Although these definitions appear to be rather philosophical, they will become clearer as the origin of these errors in CFD is further explored.

4.10.1.1 Discretization Error

These errors are due to the difference between the exact solution of the modelled equations and a numerical solution with a limited time and space resolution. They arise because an exact solution to the equation being solved is not obtained but numerically approximated. For a consistent discretization of the algebraic equations, the computed results are expected to become closer to the exact solution of the modelled equations as the number of grid cells is increased. However results are strongly affected by the density of mesh and the distribution of grid nodal points.

Discretization errors can be classified in two types: local and global (or accumulated). To have an idea about the local error and global error, consider the finite difference formulation of the derivatives for the transport variable \( \phi \) in space and time at a specified grid nodal point expressed through the Taylor series expansion,

\[
\frac{\partial \phi}{\partial x} = \frac{\phi_{i+1,j} - \phi_{i,j}}{\Delta x} + 0(\Delta x) \rightarrow (\text{Truncation error})
\]  

Spatial derivative \hspace{1cm} (4.62)

\[
\frac{\partial \phi}{\partial t} = \frac{\phi_{i,j}^{n+1} - \phi_{i,j}^{n}}{\Delta t} + 0(\Delta t) \rightarrow (\text{Truncation error})
\]  

Time derivative \hspace{1cm} (4.63)

Termination of the Taylor series expansion in Eqs (4.62) and (4.63) results in the so called truncation error involved in the approximation.
Figure 4.6 Local and global discretization error resulting from the finite difference method at a specified grid nodal point.

The local error is the formulation associated with single step and provides an idea about accuracy of the method used. For this error, the accuracy of the numerical solution concerns mainly the approximation of the spatial derivative. The solution accuracy for a transient problem, however, focuses on the advancement of the transport variable $\phi$ through time usually characterised by the global error. The representation of the local error and global error are illustrated as shown in Figure 4.6. It is observed that the smaller the mesh size or time step in transient problems, the smaller the error and thus more accurate the approximation.

4.10.1.2 Round–Off Error

These errors exist due to the difference between the machine accuracy of a computer and the true value of variable. Every computer represents numbers that have a finite number of significant figures. The default value of the number of significant digits for many computers is seven and this is commonly referred to as single precision. However, calculations can also be performed using 15 significant figures, which is referred as double precision. The error due to
retaining of limited number of computer digits available for storage of a given physical value is therefore called the round off error. This error is naturally random and there is no easy way of predicking it. It depends on the number of calculations, rounding off method, rounding off type, and even sequence of calculations.

4.10.1.3 Iteration or Convergence Error

These errors occur due to the difference between a fully converged solution of a finite number of grid points and a solution that has not fully achieved convergence. The majority of commercial CFD software solve the discretized equations iteratively for steady state solution at a given time step, this is solved iteratively in transient methods. It is expected that progressively better estimates of the solution are generated as the iteration step proceeds and ideally satisfies the imposed boundary conditions and equations in each local grid cell and globally over the whole domain. However, if the iterative process is terminated prematurely then errors arise. Convergence error therefore can occur because of either being impatient to allow the solution algorithm to complete its progress to the final converged solution or applying to large convergences to half the iteration process when the CFD solution may still be considerably far from its converged state.

4.10.1.4 Physical-Modelling Error

These errors are due to uncertainty in the formation of the mathematical models and deliberate simplifications of the models. Here, we reinforce the definition of uncertainty, where the Navier- Stokes equations can be considered to be exact and solving them is impossible for most flows of engineering interest because of lack of sufficient knowledge to model them. The sources of uncertainty in physical models are:

1. The phenomenon is not thoroughly understood
2. Parameters employed in the model are known to possess some degree of uncertainty
3. Appropriate models are simplified thus uncertainty is introduced
4. Experimental confirmation of the models is not possible or is incomplete

Physical modelling errors are examined by performing validation studies that focuses on certain models.
### 4.10.1.5 Human Error

There are two types of error associated with human error. First, computer programming errors involve human mistakes made in programming, which are the direct responsibility of the programmer. These errors can be removed by systematically performing verification studies of subprograms of the computer code and the entire code, reviewing the details inserted into the code, and performing the validation studies of the code. Second, usage errors are due to application of the code in a less than accurate or improper manner.

### 4.10.2 Controlling the Solution error

Numerical error are primarily concerned with discretization and round-off errors. They have tendency to accumulate through computational processes that they may yield unphysical CFD solutions. Controlling the solution errors therefore represents a crucial step towards obtaining reliable and meaningful CFD solutions.

The contribution of the discretization and round-off errors obtained through numerical methods is shown in Figure 4.7. As the mesh or time step size decreases, the discretization error decreases with step size while the round-off error increases. For the total error it is considered as the sum of the discretization and round-off errors, it is evident that continually decreasing the step size does not necessarily mean that more accurate results are obtained. The opposite is true at small step sizes, where less accurate results are obtained because of the quicker increase in the round-off error. In order to reduce this error, we should therefore avoid a large number of computations with very small numbers. In actual practice, we will not able to determine the magnitude of the error involved in the numerical method. As shown in Figure 4.7, the knowledge of discretization error alone is meaningless without a true estimate of the round-off error. To better assess the accuracy of the results obtained, some practical guidelines are recommended.
4.10.2.1 Grid Independence

To study this issue, we can start by solving the flow problem with reasonable mesh sizes of $\Delta x, \Delta y,$ and $\Delta z$ (and a time step of $\Delta t$ for transient problem) based on acquired experience. The computational results may look qualitatively good but let us assume that the problem is repeated with twice as many grid points, therefore halving the mesh sizes in each direction by $\Delta x/2$, $\Delta y/2$, and $\Delta z/2$. If the results obtained do not differ significantly from those obtained in the original grid layout, we can conclude the discretization error is at an acceptable level. But if the values of transport variables are quite different for this second calculation, then the solution is a function of the number of grid points. In all practical cases, the grid needs to be refined by increasing the number of grid points until a solution is achieved where no significant changes in the results occur. This indicates that the discretization error is reduced to an acceptable level and grid independence is reached.
4.10.2.2 Precision of Computation

The majority of calculations are usually performed in single precision to avoid overburdening of the computational resources. Nevertheless, if the round-off error is found to be significant, the flow calculations can be repeated by using double precision while holding the mesh size constant. If the results do not change considerably, we conclude that the round-off error is not a problem to the CFD solution. However, if the changes are larger than expected, we may attempt to reduce the total number of calculations by either increasing the mesh size or changing the order of computations such as adopting a higher approximation to evaluate the first order spatial derivatives of the convective term and / or the first order time derivative in the conservation equations. Figure 4.7 shows the discretization error increases with increasing mesh size, the user should therefore acknowledge this important trend and seek some reasonable compromise.

4.10.2.3 Selection of Turbulence Model

The selection of turbulence models or other approximate models can be daunting task especially attempting to minimise the physical-modeling errors. The desired level of simplification that can be accepted to adequately model the physical-flow problem is not straightforward, as it depends on the choice of models that govern and characterize flow physics. Also, carelessness in setting up a feasible geometrical model and an improper choice of boundary conditions are some of the human errors that frequently arises in CFD.