CHAPTER 3

COMPUTATIONAL FLUID DYNAMICS METHODOLOGY

3.1 INTRODUCTION

In-cylinder fluid dynamics exerts significant primary influence on the performance and various emissions of Direct Injection (DI) diesel engines. The flow simulation inside the cylinder of a DI diesel engine especially during reaction periods is a complex process involving turbulence and fluid dynamics motion. With the advent of high-speed digital computer and the advancement in numerical techniques in recent years there has been a major impact on the design process, greatly increasing the understanding of complex flow by reducing the amount of trial and error required. Computational Fluid Dynamics (CFD) is considered as connector between the experimental and theoretical fluid dynamics relations. The capability of numerical tools (CFD code) in treating complex geometries and complex turbulence has been drastically improved by the development of computer programs for accurate mesh generation required for it.

CFD is an area in which the governing equations for fluid flows are solved in discrete form on computers by simulating the fluid flow problem. This helps in reducing the time and effort required in narrowing down on the design configurations of various engineering components. The use of CFD can also help in enhancing the quality of the products, as the designers can look at the product from all possible angles before prototyping it. A realistic CFD problem simulation to resolve all possible phenomena places very high
demands on speed and memory of the computer systems. Due to the capability of handling complex flow situations, CFD has become an essential design tool in every branch of engineering related to fluid dynamics.

- CFD is concerned with replacing the governing partial differential equations of fluid flow with manageable algebraic equations and to obtain final numerical description of the complex flow field of interest. Numerical solution procedure requires the repetitive manipulation of numbers. These facts are highlighted by Versteeg and Malalasekara (1995). Advances in numerical procedures and its application to problem of more and more details and sophistication are intimately related to advances in computer hardware, particularly with regard to storage and execution speed.

- The numerical simulation of the flow region of interest requires:
  (i) Modeling and formulating the problem in mathematical form
  (ii) Choice of numerical method
  (iii) Programming
  (iv) Execution for obtaining results
  (v) Interpretation of the results

3.2 BASIC STRUCTURE OF A CFD CODE

CFD codes are structured around the numerical algorithms that can tackle fluid flow and combustion problems. In order to provide easy access to their solving power, all commercial CFD packages include sophisticated user
interfaces to input problem parameters and examine results. Hence all codes contain three main elements

1. Pre-Processor
2. Solver
3. Post-Processor

3.2.1 Pre-processor

Pre-processing consists of the input of a flow problem to a CFD program by means of a user-friendly interface and the subsequent transformation of the input into a form suitable for use by the solver. The user activities at the pre-processing stage involve:

(i) Definition of the geometry of the region of interest – the computational domain

(ii) Grid generation – the sub-division of the domain into a number of smaller, non-overlapping sub-domains – a grid or mesh of cells

(iii) Selection of the physical and chemical phenomena that need to be modeled

(iv) Specification of appropriate boundary conditions at cells which coincide with the domain boundary

The solution to a flow problem i.e., velocity, pressure, temperature, species concentrations, etc., is defined at nodes inside each cell. The number of cells in the grid is major factor for the accuracy of a CFD solution. In general, optimum number of cells results better solutions. Over 50% of the time spent on a CFD project is devoted to the definition of the domain
geometry and grid generation. In order to maximize productivity of CFD personnel, all the major codes now include their own CAD-style interface and/or facilities to import data from proprietary surface modelers and mesh generators like HYPER MESH, ANSA, PATRAN, I-DEAS and GAMBIT. Up-to-date pre-processors also give the user to access the libraries of material properties for common fluids and a facility to invoke special physical and chemical process models such as turbulence models, spray models, droplet drag and break up models, combustion models, emission models etc. along with the main fluid flow equations

3.2.2 Solver

In outline, the numerical methods that form the basis of the solver perform the following steps:

- Approximation of the unknown flow variables by means of simple functions
- Discretisation by substitution of the approximations into the governing flow equations and subsequent mathematical manipulations
- Solution of the algebraic equations

There are three distinct streams of numerical solution techniques:

1. Finite difference method
2. Finite element method and
3. Finite volume method
The main differences between the three separate streams are associated with the way in which the flow variables are approximated and with the discretisation processes.

3.2.2.1 Finite difference method

Finite difference methods describe the unknowns \( \varphi \) of the flow problem by means of point samples at the node points of a grid of co-ordinate lines. Truncated Taylor series expansions are often used to generate finite difference approximations of derivatives of \( \varphi \) at each grid point and its immediate neighbours. Those derivatives appearing in the governing equations are replaced by finite differences yielding an algebraic equation for the values of \( \varphi \) at each grid point.

3.2.2.2 Finite element method

Finite element methods use simple piecewise functions valid on elements to describe the local variations of unknown flow variables \( \varphi \). The governing equation is precisely satisfied by the exact solution \( \varphi \). If the piecewise approximating functions for \( \varphi \) are substituted into the equation, it will not hold exactly and a residual is defined to measure the errors. Next, the residuals and hence the errors are minimized in some sense by multiplying them by a set of weighting functions and integrating. As a result, we obtain a set of algebraic equations for the unknown coefficients of the approximating functions.

3.2.2.3 Finite volume method

The finite volume method, based upon which the thesis was undertaken, was originally developed as a special finite difference formulation. The numerical algorithm consists of the following steps:
• Formal integration of the governing equations of fluid flow over all the finite control volumes of the solution domain

• Discretisation involving the substitution of a variety of finite difference type approximations for the terms in the integral equation representing flow processes such as convection, diffusion and sources. This converts the integral equations into a system of algebraic equations

• Solution of the algebraic equations by an iterative method

The first step, the control volume integration, distinguishes the finite volume method from all other CFD techniques. The resulting statements express the exact conservation of relevant properties for each finite size cell. This clear relationship between the numerical algorithm and the underlying physical conservation principle forms one of the main attractions of the finite volume method and makes its concepts much more simple to understand than finite element and spectral methods. The conservation of a general flow variable \( \phi \) within a finite control volume can be expressed as a balance between the various processes tending to increase or decrease it, i.e.,

\[
\begin{bmatrix}
\text{Rate of change of } \phi \\
\text{in the control volume}
\end{bmatrix}_{\text{w.r.t. time}} =
\begin{bmatrix}
\text{Net flux of } \phi \text{ due to convection into the control volume}
\end{bmatrix} +
\begin{bmatrix}
\text{Net flux of } \phi \text{ due to diffusion into the control volume}
\end{bmatrix} +
\begin{bmatrix}
\text{Net rate of creation of } \phi \text{ inside the control volume}
\end{bmatrix}
\]

The CFD codes contain discretisation technique suitable for the treatment of the key transport phenomena, convection and diffusion as well as for the source terms (\( \phi \)) and the rate of change with respect to time.
3.2.3 **Post-processor**

Owing to the increased popularity of engineering workstations, many of which have outstanding graphics capabilities, the leading CFD packages are now equipped with versatile data visualisation tools. These include:

- Domain geometry and grid display
- Vector plots
- Line and shaded contour plots
- 2D and 3D surface plots
- Particle tracking
- View manipulation and colour postscript output

More recently these facilities also include animation for dynamic result display. In addition to graphics, all codes produce trusty alphanumeric output and have data export facilities for further manipulation external to the code.

### 3.3 GOERING EQUATIONS

The governing equations of fluid flow represent mathematical statements of the conservation laws of physics, i.e.,

- The mass of a fluid is conserved.
- The rate of change of momentum equals the sum of the forces on a fluid particle (Newton’s second law).
The rate of change of energy is equal to the sum of the rate of heat addition to and the rate of work done on a fluid particle (first law of thermodynamics).

### 3.3.1 Conservation Equations for the Flow Field

The mass and momentum equations solved for the unsteady, compressible / incompressible, three-dimensional in-cylinder flow in Cartesian tensor notation are represented as (Warsi (1981)):

\[
\begin{align*}
\text{Rate of increase of mass in fluid element} & = \text{Net rate of flow of mass into fluid element} \\
\text{Rate of increase of momentum of fluid particle} & = \text{Sum of forces on fluid particle}
\end{align*}
\]

\[\text{i.e.,} \quad \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j) = s_m \quad (3.1) \]
\[\frac{\partial (\rho u_j)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j u_i - \tau_{ij}) = -\frac{\partial p}{\partial x_i} + s_i \quad (3.2) \]

where  
\( t \) - time \\
\( x_i \) - Cartesian coordinate ( \( i = 1,2,3 \) ) \\
\( u_i \) - absolute fluid velocity component in direction \( x_i \) \\
\( p \) - piezometric pressure = \( p_s \rho_0 g_m x_m \) where \( p_s \) is static pressure, \( \rho_0 \) is reference density, \( g_m \) are gravitational acceleration components and \( x_m \) are coordinates relative to a datum where \( \rho_0 \) is defined.
\[ \rho - \text{density}, = \left( \frac{p}{RT\sum_{m} \frac{m_m}{M_m}} \right) \]

where \( m_m \) - mass fraction of a constituent with molecular weight \( M_m \),
\( T \) - temperature
\( R \) - universal gas constant.
\( \tau_{ij} \) - stress tensor components
\( s_m \) - mass source
\( s_i \) - momentum source components (assumed to be negligible)

The flow is assumed to be Newtonian, the following constitutive relation is specified connecting the components of the stress tensor \( \tau_{ij} \) to the velocity gradients:

\[ \tau_{ij} = 2\mu s_{ij} - \frac{2}{3}\mu \frac{\partial u_k}{\partial x_k} \delta_{ij} - \bar{\rho} u_i u_j \]  

(3.3)

where \( \mu \) - molecular dynamic fluid viscosity
\( \delta_{ij} \) - the Kronecker delta ( = 1 when \( i = j \), and 0 otherwise)

\[ S_{ij} \] - Rate of strain tensor \[ = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \]  

(3.4)

The rightmost term in equation (3.3) represents the additional Reynolds stresses due to turbulent motion and \( u' \) are the fluctuations about the ensemble average velocity. The Reynolds stresses are linked to the mean velocity fields via turbulent models.
Conservation Equation for heat Transfer

Heat transfer is implemented through the following general forms of the enthalpy conservation equation for a fluid mixture (Jones 1980) depending on the value of Eckert number.

\[ Ec = \frac{U^2}{c_p T} \]

The value of Eckert number of the order of 1.0 or more recommends the solution of a transport equation for total enthalpy and if the Eckert number is less than 1.0, the solution of transport equation for static enthalpy will suffice. The energy equation derived from the first law of thermodynamics states that,

\[
\text{Rate of increase of energy of fluid particle} = \text{Net rate of heat added to fluid particle} + \text{Net rate of work done on fluid particle}
\]

The mathematical forms are represented as follows.

3.3.2.1 Static Chemico-thermal Enthalpy

\[
\frac{\partial h}{\partial t} + \frac{\partial}{\partial x_j} \left( \rho u_j - F_{h,j} \right) + \frac{\partial p}{\partial t} + u_j \frac{\partial p}{\partial x_j} + \tau_{ij} \frac{\partial u_i}{\partial x_j} + s_h = 0
\]

where \( h \) is the static enthalpy defined by:

\[
h = c_p T - c_p T_0 + \sum Y_m H_m h_i + \sum Y_m H_m
\]

and

\(-\quad\)

- Temperature

\(-\quad\)

- Reference Temperature

\(-\quad\)

- mass fraction of mixture constituent \( m \)
\( H_m \) - heat of formation of constituent \( m \) \\
\( \sum \) - summation over all mixture constituents \\
\( \bar{c}_p \) - mean constant – pressure specific heat at temperature \( T \) \\
\( c_p^0 \) - reference specific heat at temperature \( T_0 \) \\
\( F_{hj} \) - diffusional energy flux in direction \( x_j \) \\
\[ \begin{align*}
F_{hj} &= \frac{k}{\rho} \frac{\partial T}{\partial x_j} - \bar{c}_p \overline{u_j h^*} + \sum_m \rho D_m \frac{\partial m_m}{\partial x_j} 
\end{align*} \]
\( s_h \) - energy source \\
\( h_t \) - thermal enthalpy \\

The static enthalpy, \( h \), is defined as the sum of the thermal and chemical components, the latter being included to cater for chemically reacting flows.

### 3.3.2.2 Total Chemico – thermal Enthalpy

A governing equation for the total chemico-thermal enthalpy (\( H \)) may be formed by summing the equation for mechanical energy conservation equation (3.2) and static chemico-thermal enthalpy equation (3.5).

\[
\frac{\partial \rho H}{\partial t} + \frac{\partial}{\partial x_j} \left( \rho u_j H + F_{hj} - \overline{u_j r_j} \right) = \frac{\partial p u_j}{\partial x_j} + s_i u_i + s_h \tag{3.7}
\]

where \( \rho H = \frac{1}{2} u_i u_i + h \)

### Species Conservation Equation

Each constituent \( m \) of a fluid mixture, whose local concentration is expressed as a mass fraction \( Y_m \), is assumed to be governed by a species conservation equation of the form:
\[
\frac{\partial}{\partial t}(\rho Y_m) + \frac{\partial}{\partial x_j}(\rho u_j Y_m - F_{m,j}) = s_m
\]  

(3.8)

where \( F_{m,j} \) is diffusional flux component.

Here \( F_{m,j} \equiv \rho Y_m V_{m,j} - \bar{\rho} u_j Y_m \)  

(3.9)

\( s_m \) is rate of mass production or consumption

In equation (3.9) the rightmost term represents turbulent mass flux. Whose models is given later in the chapter.

**TURBULENCE MODELING**

The in-cylinder flow is turbulent in nature at all speeds and dimensions of the engine. It is necessary to model the turbulence to capture properties of in-cylinder fluid dynamics. Out of the many different linear models available, the following models were focused on:

1. The ‘standard’ model (EI Tahry (1983), Launder and Spalding (1974) and Rodi (1979)) in which the high (turbulent) Reynolds number forms of the \( k \) and \( \varepsilon \) equations are used in conjunction with algebraic ‘law of the wall’ representations of flow for the near wall region

2. The ‘Renormalization group’ (RNG) version of the \( k-\varepsilon \) model (Yakhot and Orszag (1986), Yakhot et al (1992)) denoted as RNG \( k-\varepsilon \) model is employed in high Reynolds number form in conjunction with ‘law of the wall’ functions.

All forms of the \( k-\varepsilon \) models assume that the turbulent Reynolds stresses and scalar fluxes are linked to the ensemble averaged flow properties
in an analogous fashion to their laminar flow counterparts as (Launder and Spalding (1974)):

\[
\begin{align*}
-\rho \frac{\partial u_i u_j}{\partial x_j} &= 2\mu_t s_{ij} - \frac{2}{3} \left( \mu_t \frac{\partial u_k}{\partial x_k} + \rho k \right) \delta_{ij} \\
\frac{\partial \rho u_j h}{\partial x_j} &= -\frac{\mu_t}{\sigma_{h,t}} \frac{\partial h}{\partial x_j} \\
\frac{\partial \rho u_j m}{\partial x_j} &= \frac{\mu_t}{\sigma_{m,t}} \frac{\partial m}{\partial x_j}
\end{align*}
\]

where

- \( k \) - turbulent kinetic energy
- \( \mu_t \) - turbulent viscosity
- \( \sigma_{h,t} \) - turbulent Prandtl number
- \( \sigma_{m,t} \) - turbulent Schmidt number
- \( \mu_t \) - turbulent viscosity = \( f_\mu \frac{C_\mu \rho k^2}{\varepsilon} \) where \( C_\mu \) is a constant empirical coefficient and \( f_\mu \) is another coefficient to be defined in the individual model variants

**3.4.1 Standard k-ε Model Equations**

The particular high Reynolds number form of the k-ε model is appropriate to fully turbulent, compressible or incompressible flows. The transport equations are as follows:

**3.4.1.1 Turbulence Energy**

\[
\begin{bmatrix}
\text{Rate of change of } k \\
\text{by convection}
\end{bmatrix}
+ \begin{bmatrix}
\text{Transport of } k \\
\text{by diffusion}
\end{bmatrix}
= \begin{bmatrix}
\text{Transport of } k \\
\text{by diffusion}
\end{bmatrix}
+ \begin{bmatrix}
\text{Net rate of production} \\
\text{of } k
\end{bmatrix}
- \begin{bmatrix}
\text{Rate of destruction} \\
\text{of } k
\end{bmatrix}
\]
where

\[
P = S_i \frac{\partial u_i}{\partial x_i}
\]

\[
P_B = - \frac{g_i}{\sigma_{h,t}} \frac{1}{\rho} \frac{\partial \rho}{\partial x_i}
\]

\[
P_{NL} = - \frac{\rho_i}{\mu} u_i u_j \left[ P - \frac{2}{3} \left( \frac{\partial u_i}{\partial x_i} + \frac{\rho k}{\mu} \frac{\partial u_i}{\partial x_i} \right) \right]
\]

\[P_{NL} = 0 \text{ for linear models and } \sigma_k \text{ is the turbulent Prandtl number.}
\]

The first term on the right-hand side of equation 3.13 represents the turbulent generation by shear and normal stresses and buoyancy forces, the second viscous dissipation, and the third amplification or attenuation due to compressibility effects. The last term accounts for the non-linear contributions.

### 3.4.1.2 Turbulence Dissipation Rate

\[
\begin{bmatrix}
\text{Rate of change of } \varepsilon \\
\text{Transport of } \varepsilon \text{ by convection} \\
\text{Transport of } \varepsilon \text{ by diffusion} \\
\text{Net rate of production of } \varepsilon \\
\text{Rate of destruction of } \varepsilon
\end{bmatrix} = \begin{bmatrix}
\text{of } \varepsilon \\
\text{by convection} \\
\text{by diffusion} \\
\text{of } \varepsilon \\
\text{of } \varepsilon
\end{bmatrix}
\]
\[
\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_j} \left[ \rho u_j \varepsilon - (\mu + \frac{\mu_t}{\sigma_\varepsilon}) \frac{\partial \varepsilon}{\partial x_j} \right] = \\
C_{\varepsilon 1} \frac{\varepsilon}{k} \left[ \mu_t \left( \frac{2}{3} \left( \mu_t \frac{\partial u_i}{\partial x_i} + \rho k \right) \frac{\partial u_i}{\partial x_j} \right) \right] + C_{\varepsilon 3} \frac{\varepsilon}{k} \mu_t P_{\varepsilon} - \\
C_{\varepsilon 2} \rho \frac{\varepsilon^2}{k} + C_{\varepsilon 4} \rho \frac{\partial u_i}{\partial x_i} + C_{\varepsilon 1} \frac{\varepsilon}{k} \mu_t P_{NL}
\]

(3.14)

where \( \sigma_\varepsilon \), \( C_{\varepsilon 1} \), \( C_{\varepsilon 2} \), \( C_{\varepsilon 3} \), and \( C_{\varepsilon 4} \) are empirical coefficients, whose values taken from (EI Tahry (1983), Launder and Spalding (1974), Rodi (1979)) are given in Table 3.1. The turbulent viscosity \( \mu_t \) is obtained with \( f_\mu \) set equal to unity.

<table>
<thead>
<tr>
<th>( C_\mu )</th>
<th>( \sigma_k )</th>
<th>( \sigma_\varepsilon )</th>
<th>( \sigma_m )</th>
<th>( C_{\varepsilon 1} )</th>
<th>( C_{\varepsilon 2} )</th>
<th>( C_{\varepsilon 3} )</th>
<th>( C_{\varepsilon 4} )</th>
<th>( K )</th>
<th>( \varepsilon )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.09</td>
<td>1.0</td>
<td>1.22</td>
<td>0.9</td>
<td>0.9</td>
<td>1.44</td>
<td>1.92</td>
<td>1.44</td>
<td>-0.33</td>
<td>0.419</td>
</tr>
</tbody>
</table>

### 3.4.2 RNG k-\( \varepsilon \) Model Equations

The procedure in this model systematically removes the small scales of motion from the governing equations by expressing their effects in terms of large-scale motions and a modified viscosity (Yakhot et al (1992)). They claim that the RNG theory is more fundamental than previous approaches and produce a version that is more general and accurate. The equations of the model are quoted below.
3.4.2.1 Turbulence energy

\[
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_j} \left( \rho u_j k - \left( \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right) = \\
\mu_t (P + P_B) - \rho \varepsilon - \frac{2}{3} \left( \frac{\mu_t}{\sigma_k} \right) \frac{\partial u_i}{\partial x_i} \frac{\partial u_i}{\partial x_i} \tag{3.15}
\]

i.e.,

\[
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_j} \left( \rho u_j k - \left( \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right) = \\
\mu_t (P + P_B) - \rho \varepsilon - \frac{2}{3} \left( \frac{\mu_t}{\sigma_k} \right) \frac{\partial u_i}{\partial x_i} \frac{\partial u_i}{\partial x_i} \tag{3.15}
\]

3.4.2.2 Turbulence dissipation rate

\[
\frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_j} \left( \rho u_j \varepsilon - \left( \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right) = \\
C_{\varepsilon 1} \frac{\varepsilon}{k} \left[ \mu_t P - \frac{2}{3} \left( \frac{\mu_t}{\sigma_k} \right) \frac{\partial u_i}{\partial x_i} \frac{\partial u_i}{\partial x_i} \right] + C_{\varepsilon 2} \frac{\varepsilon}{k} \mu_t P_B \tag{3.16}
\]

\[
- C_{\varepsilon 2} \frac{\rho \varepsilon^2}{k} + C_{\varepsilon 4} \rho \varepsilon \frac{\partial u_i}{\partial x_i} \frac{\partial u_i}{\partial x_i} - C_m \eta^3 \frac{(1 - \eta_0)}{1 + \beta \eta^3} \frac{\rho \varepsilon^2}{k}
\]

where \( \eta \equiv S \frac{k}{\varepsilon} \)

\( \eta_0 \) and \( \beta \) are empirical coefficients given in Table 3.2
Comparison of equations (3.15) and (3.16) with their counterparts equations (3.13) and (3.14) in the standard model reveals that the obvious distinctive feature of the RNG k-ε version is the additional last term in the dissipation equation, which represents the effect of mean flow distortion on $\varepsilon$. The coefficients of the model are fixed empirically as in (Launder and Spalding (1974), Rodi (1979)) and recorded in Table 3.2. The $f_\mu$ coefficient is set to unity and $\mu_\tau = f_\mu \frac{C_\mu \rho k^2}{\varepsilon}$

Table 3.2 Values assigned to RNG k-ε turbulence model coefficients

<table>
<thead>
<tr>
<th>$C_\mu$</th>
<th>$\sigma_k$</th>
<th>$\sigma_\varepsilon$</th>
<th>$\sigma_h$</th>
<th>$\sigma_m$</th>
<th>$C_{r1}$</th>
<th>$C_{r2}$</th>
<th>$C_{r3}$</th>
<th>$C_{r4}$</th>
<th>$k$</th>
<th>$E$</th>
<th>$\eta_0$</th>
<th>$\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.085</td>
<td>0.719</td>
<td>0.719</td>
<td>0.9</td>
<td>0.9</td>
<td>1.42</td>
<td>1.68</td>
<td>1.42</td>
<td>-0.38</td>
<td>0.4</td>
<td>9</td>
<td>4.38</td>
<td>0.012</td>
</tr>
</tbody>
</table>

3.5 COMBUSTION AND IGNITION MODELS

The simulation of diesel engines involves modeling several processes such as spray dynamics, auto-ignition, chemistry, turbulence, etc. as well as the interactions between them such as turbulence-chemistry etc. Ignition and combustion are represented as two separate processes. Two models that are normally considered combustion simulation are:

1. Magnussen model
2. Laminar-and-turbulent characteristic-time model

3.5.1 Laminar-and-Turbulent Characteristic- Time Model

This combustion model is based on the works of Magnussen (Magnussen and Hjertager (1976)), Abraham (Abraham et al (1985)) and Patterson (Patterson et al (1994)).
Magnussen (Magnussen and Hjertager (1976)) presented a model based on an eddy break-up (EBU) concept, which relates the rate of combustion to the rate of dissipation of eddies and expresses the rate of reaction by the mean concentration of a reacting species, the turbulent kinetic energy and the rate of dissipation of this energy.

Abraham (Abraham et al (1985)) presented a laminar-and-turbulent characteristic-time combustion model for spark ignition engines. Patterson (Patterson et al (1994)) extended this concept to model diesel engines. In diesel engines, a significant portion of the combustion is thought to be mixing controlled and therefore Magnussen’s model should be able to describe the rate of combustion in a better way. However, it is recognised that the initiation of combustion relies on laminar chemistry (Patterson et al (1994)). Turbulence starts playing its influence only after combustion events have already been observed. Eventually, combustion will be dominated by turbulent mixing effects in the regions of $\tau_l<<\tau_t$, where $\tau_l$ is the laminar (or chemical) time scale and $\tau_t$ is the turbulent (or mixing) time scale.

However, the laminar time scale is not negligible near the injector regions (where the high injection velocity makes the turbulent time scale very small), in shear layers generated by the fuel sprays and in near-wall regions. Hence, the laminar-and-turbulent characteristic-time combustion model is used for the present work in preference to the EBU combustion model. According to Magnussen et al (1976).

\[ R_f = \frac{\rho A}{\tau_t} \min \left( \frac{Y_f, Y_{O_2}}{r_t}, \frac{BY_p}{1 + r_t} \right) \text{kg m}^{-3} \text{s}^{-1} \]  \hspace{1cm} (3.17)

where $\tau_t = k/\varepsilon$, the turbulent time scale.
As mentioned earlier, Patterson (Patterson et al (1994)) recognised that the laminar time scale cannot be assumed to be negligible in a number of important regions of the diesel engine combustion chamber. Hence, the turbulent time scale in equation (3.17) is to be replaced by a characteristic time $\tau_c$ to give:

$$R_f = \frac{\rho A}{\tau_c} \min \left( \frac{Y_{f,l}}{r_f}, \frac{Y_{O_2}}{r_f}, \frac{BY_p}{1+r_f} \right)$$

(3.18)

where $\tau_c = \tau_l + f \tau_t$  

(3.19)

$A = 4, B = 0.5, Y_f, Y_{O_2}$ and $Y_p$ are the fuel, oxygen and product mass fractions respectively and $r_f$ is the oxygen to fuel mass fraction

$$r_f = \frac{n_{O_2} M_{O_2}}{n_f M_f}$$

(3.20)

The laminar time scale $\tau_l$ is derived from an Arrhenius type reaction rate (Mehta and Bhaskar (2001)) with the pre-exponential constant $A = 2.0 \times 10^{10}$ sec$^{-1}$ as:

$$\tau_l = A^{-1} \left[ C_7H_{16} \right]^{0.25} \left[ O_2 \right]^{1.5} \exp \left( \frac{E}{R_m T} \right)$$

(3.21)

where $E$ the activation energy equal to 150.78 KJ/mol for Dodecane, the fuel used in the present work and $A$ is the pre-exponential constant.

The turbulent time scale $\tau_t$ is proportional to the eddy turnover time

$$\tau_t = C_2 \left( \frac{k}{\varepsilon} \right)$$

(3.22)
where \( C_2 = 0.142 \) (Patterson et al (1994)).

The delay coefficient \( f \), present in equation (3.19) was chosen to simulate the increasing influence of turbulence on combustion after ignition has occurred and has the form (Patterson et al (1994)):

\[
f = \frac{1 - e^{-c}}{0.632}
\]  

(3.23)

where the parameter \( c \) is a reaction progress variable given by

\[
C = \frac{Y_{ft} - Y_f}{Y_{ft} - Y_{res}}
\]  

(3.24)

\( Y_{ft} \) and \( Y_{res} \) are the total fuel mass fraction and the amount of fuel left at the end of combustion respectively. The characteristic combustion time scale is given by

\[
\tau_c = \begin{cases} 
\tau_l & \text{at the limit of no combustion} \\
\tau_l + \tau_i & \text{at the limit of complete combustion}
\end{cases}
\]  

(3.25)

3.5.2 Ignition Model

The ignition model used is Shell auto-ignition model developed for study of knock in gasoline engines (Halstead et al (1975)), appropriately modified to predict ignition for fuels of higher molecular weight typical of diesel fuels (Theobald and Cheng (1987)).

The chain-propagation cycle provides the framework for the mathematical model. It is assumed that the reaction chain may be propagated by any number of radical reactions, but each propagation step shows a first-order dependence on the radicals involved. It is further assumed that the radical concentrations are in a steady state relation to each other.
In the model, generic molecular species are introduced. Species play a similar role in the ignition chemistry. However, varying detailed structure are combined and accounted for as a single entity. The model is capable of simulating the cool flame phenomenon, a sharp well defined two-stage ignition, a rapid acceleration of the reaction rate after the onset of ignition and a transition from two-stage to single-stage ignition with increasing temperature (Theobald and Cheng (1987)) The Shell auto-ignition model makes use of the following generic molecules:

RH - Hydrocarbon fuel of nominal composition \( C_nH_{2n+2} \)

\( R^* \) - Radical formed from the fuel (* denotes radical)

B - Branching agent

Q - Intermediate species

P - Products consisting of CO, CO\(_2\) and H\(_2\)O

The chemical model consists of the following set of equations:

Primary initiation \[ \text{RH} + \text{O}_2 \rightarrow 2R^* \quad (3.26) \]

Radical propagation \[ R^* \rightarrow R^* + P \quad (3.27) \]

\[ R^* \rightarrow R^* + B \quad (3.28) \]

\[ R^* \rightarrow R^* + Q \quad (3.29) \]

\[ R^* + Q \rightarrow R^* + B \quad (3.30) \]

Branching \[ B \rightarrow 2R^* \quad (3.31) \]

Linear termination \[ R^* \rightarrow \text{inert products} \quad (3.32) \]

Quadratic termination \[ 2R^* \rightarrow \text{inert products} \quad (3.33) \]
The non-reactive species (inert products) in the termination equations are assumed to be equivalent to nitrogen.

The rate coefficients of the above reactions take the Arrhenius form:

\[ K = Ae^{(-E_{RT}/RT)} \]  \hspace{1cm} (3.34)

As generic species are used in the model, the above reactions as written would not conserve mass. To use the reaction set, the equations are mass balanced. This is achieved by appropriately defining the molecular weights of the generic species \( R^* \), \( B \), \( Q \) and \( P \).

The mathematical model for the above simultaneous reactions comprises the following set of differential equations (Theobald and Cheng (1987)):

\[
\begin{align*}
\frac{1}{V}\frac{dn_{R}}{dt} & = 2 \left\{ k_{Q}[R]H[O]_{2} + k_{B}[B] - k_{f}[R]^{2} \right\} - f_{p}[R] \left( R \right) & (3.35) \\
\frac{1}{V}\frac{dn_{B}}{dt} & = f_{1}[R] + f_{2}[Q][R] - k_{B}[B] & (3.36) \\
\frac{1}{V}\frac{dn_{Q}}{dt} & = f_{1}[R] + f_{2}[Q][R] & (3.37) \\
\frac{1}{V}\frac{dn_{O}}{dt} & = -p_{k}[R] & (3.38) \\
n_{RH} & = \frac{n_{o_{2}}(t = 0) - n_{o_{2}}(t = 0)}{pm} + n_{RH}(t = 0) \hspace{1cm} (3.39)
\end{align*}
\]
Steady state radical hypothesis used to get equation (3.35) through (3.39) give the local reaction rates for the ignition species, which are general functions of the rates of transport by convection and diffusion from other parts of the flow. Thus, for each of the species \( \Phi(\Phi \equiv R', B, \text{or } Q) \), a transport equation of the form

\[
\frac{\partial \rho Y_\Phi}{\partial t} \nabla (\rho U Y_\Phi - \Gamma \nabla Y_\Phi) = S_\Phi
\]

(3.40)
is solved in conjunction with the other species equations (3.8), with the appropriate \( S_\Phi \) term inserted from one of equations (3.35) through (3.39). A new enthalpy source related to temperature rise caused by the ignition model equation (3.40) is also calculated and used as a source term in the thermal enthalpy transport equation.

3.6 NOx MODEL

Nitrogen oxides are important air pollutants, mainly produced by combustion devices. The time scale for NO\(_x\) reactions is larger than the time scales for the turbulent mixing process and the combustion of hydrocarbons that control the heat-releasing reactions. Hence, the computations of NO\(_x\) can be decoupled from the main reacting flow field predictions. Three different mechanisms have been identified for the formation of nitric oxides during the combustion of hydrocarbons, namely thermal, prompt and fuel NO\(_x\). Out of these three two mechanisms have been widely used in the literature for simulating nitric oxide during the combustion of hydrocarbons, namely:

(i) Thermal NO\(_x\)

(ii) Prompt NO\(_x\)
3.6.1 Thermal NOx

Thermal NOx is formed by high temperature oxidation of atmospheric nitrogen and is strongly temperature dependent. For thermal nitric oxide, the principle reactions are generally recognised to be those proposed by the following three extended Zeldovich mechanisms:

\[ \text{N}_2 + O \xrightleftharpoons[k_i]{k_{-i}} \text{NO} + N \]  \hspace{1cm} (3.41)

\[ N + O_2 \xrightleftharpoons[k_{-2}]{k_2} \text{NO} + O \]  \hspace{1cm} (3.42)

\[ N + \text{OH} \xrightleftharpoons[k_{-3}]{k_3} \text{NO} + H \]  \hspace{1cm} (3.43)

OH radicals are derived from shell auto ignition model. At high temperature inside cylinder the oxygen molecules is broken into O radicals. These radicals participate in further reaction creating NOx. and the equilibrium O atom concentration is obtained based on the following equations. (Westenberg(1971)).

\[ \langle O \rangle = K_p (O_2)^{1/2} \text{ kg mol m}^{-3} \text{ and } Y_0 = \langle O \rangle \frac{M_w}{\gamma} \]  \hspace{1cm} (3.44)

where

\[ K_p = \frac{1.255 \times 10^4}{T^{3/2}} \exp \left( -\frac{31090}{T} \right) (\text{kg mol})^{1/2} \text{ m}^{-3/2} \]  \hspace{1cm} (3.45)

The rate constants for these reactions have been measured in numerous experimental studies (Flowers et al (1975), Monat et al (1979)), and the data obtained from these studies have been critically evaluated by Baulch
The expressions for rate coefficients for reactions equations (3.41) to (3.43) based on (Baulch et al (1973)) are given below:

\[
K_1 = 1.8 \times 10^{11} \exp\left(-\frac{38370}{T}\right) \text{m}^3(\text{kg mol})^{-1}\text{s}^{-1} \quad (3.46)
\]

\[
K_{-1} = 3.8 \times 10^{10} \exp\left(-\frac{425}{T}\right) \quad (3.47)
\]

\[
K_2 = 1.8 \times 10^7 T \exp\left(-\frac{4680}{T}\right) \quad (3.48)
\]

\[
K_{-2} = 3.8 \times 10^6 \exp\left(-\frac{20820}{T}\right) \quad (3.49)
\]

\[
K_3 = 7.1 \times 10^9 \exp\left(-\frac{450}{T}\right) \quad (3.50)
\]

\[
K_{-3} = 1.7 \times 10^{11} \exp\left(-\frac{24560}{T}\right) \quad (3.51)
\]

where \(K_1\), \(K_2\) and \(K_3\) are the forward and \(K_{-1}\), \(K_{-2}\) and \(K_{-3}\) are the backward rate constants for reactions equation (3.41) to (3.43) respectively.

The rate of formation of NO\(_x\) is significant only at high temperatures since the thermal fixation of nitrogen requires the breaking of a strong N\(_2\) bond. This effect is represented by the high activation energy of reaction equation (3.41), which makes this reaction the rate limiting step of the Zeldovich mechanism. The activation energy for oxidation of N is small, hence a quasi-steady state can be established. Based on this assumption (Baulch et al (1973)) the instantaneous rate of formation of NO\(_x\) is:
Assumptions have to be made to obtain the concentration of radicals O, OH and H, if these are not calculated by the combustion model.

3.6.2 Prompt NO\textsubscript{x}

Prompt NO\textsubscript{x} is formed from the reaction of hydrocarbon fragments and molecular nitrogen. It has a weak temperature dependence and a lifetime of only several microseconds. The contribution to NO\textsubscript{x} emission in diesel engines from this mechanism can be significant from regions of rich mixtures in the combustion chamber such as in the proximity of the fuel spray.

The production rate of prompt NO\textsubscript{x} is given by De Soete (De Soete (1975)) as,

\[ R_{NO,pt} = K_{pt}M_{NO} \text{ kg m}^{-3}\text{s}^{-1} \]  \hspace{1cm} (3.53)

where \( K_{pt} \) is a rate constant and is defined as:

\[ K_{pt} = k_r [O_2]^b [N_2] [Fuel] \text{exp} \left( \frac{-F_a}{RT} \right) \text{ kg mole m}^{-3}\text{s}^{-1} \]  \hspace{1cm} (3.54)
[O\textsubscript{2}], [N\textsubscript{2}] and [Fuel] are species concentrations in kg mole m\textsuperscript{-3} s\textsuperscript{-1}. The oxygen reaction order \( b \) depends on experimental conditions. According to De Soete (De Soete (1975)), \( b \) varies with the oxygen mole fraction \( X_{o_2} \) as follows:

\[
\begin{align*}
b & = 1.0, & X_{o_2} & \leq 0.0041 \\
b & = -3.95 - 0.9 \ln X_{o_2}, & 0.0041 & \leq X_{o_2} \leq 0.0111 \\
b & = -0.35 - \ln X_{o_2}, & 0.0111 & \leq X_{o_2} \leq 0.03 \\
b & = 0.0, & X_{o_2} & \geq 0.03
\end{align*}
\]

3.7 SOOT MODELING

The formation and emission of carbonaceous particles is a process that is often observed during the combustion of hydrocarbons. The particulates, called soot, are identified in flames and fires as yellow luminescence. In gas turbines, internal combustion engines and other practical combustion devices, the formation of soot is mostly a product of incomplete combustion. Apart from the resulting loss in combustion efficiency, a particularly serious effect of soot formation is the health hazard from a typical diesel engine emitting soot at the rate of 0.2 to 0.6 g/km. Hence, there are strict legislative demands to produce cleaner engines. The soot has to be oxidized before the exhaust is released into the environment. Hence, a detailed knowledge of the different mechanisms leading to soot formation is needed. It is widely accepted that the formation of soot is a complex process, which consists of

- fuel pyrolysis and oxidation reactions;
- formation of polycyclic and aromatic hydrocarbons;
• inception of first particles;
• growth of soot particles due to reaction with gas phase species;
• coagulation of particles;
• oxidation of soot particles and intermediates.

The soot emission model written in the Arrhenius single step form considers the rate of change of soot mass to be equal to the rate of formation less the rate of oxidation (Han et al (1996)):

\[
\frac{dM_{\text{soot}}}{dt} = \frac{dM_{\text{form}}}{dt} - \frac{dM_{\text{oxid}}}{dt} \tag{3.55}
\]

\[
\frac{dM_{\text{form}}}{dt} = K_f M_{\text{fv}} \tag{3.56}
\]

where

\[
K_f = A_f P^{0.5} \exp \left( \frac{-E_f}{RT} \right) \tag{3.57}
\]

\(M_{\text{fv}}\) is the fuel vapour mass, \(P\) is the pressure in bar, \(A_f = 300\), \(E_f = 12500\) cal / mole.

The oxidation rate is adopted from the Nagle Strickland-Constable oxidation model (Nagle and Strickland-Constable (1962)) and is given by,

\[
\frac{dM_{\text{oxid}}}{dt} = \frac{6M_c}{\rho_s D_s} M_{\text{form}} R_T \tag{3.58}
\]

where \(M_c\) is the molecular weight of carbon, \(\rho_s\) is the soot density (2 g/ cm\(^3\)), \(D_s\) is the soot diameter (30 nm) and,
\[ R_T = \left( \frac{K_A P_{O_2}}{1 + K_z P_{O_2}} \right) x + K_B P_{O_2} (1 - x) \] 

where \[ x = \frac{P_{O_2}}{P_{O_2} + \frac{K_T}{K_B}} \] 

\( P_{O_2} \) is the partial pressure of oxygen and the rate constants in \( g/\text{cm}^2\text{s} \) are:

\[ K_A = 20 \exp \left( \frac{-30000}{RT} \right) \] 

\[ K_B = 4.46 \times 10^{-3} \exp \left( \frac{-15200}{RT} \right) \] 

\[ K_T = 1.51 \times 10^5 \exp \left( \frac{-97000}{RT} \right) \] 

\[ K_z = 21.3 \exp \left( \frac{4100}{RT} \right) \]

### 3.8 MULTIPHASE MODELING

The domain of the diesel engine in-cylinder consists of a continuous phase, which is air, and a dispersed phase in the form of liquid fuel droplets. In general, the motion of the dispersed phase will be influenced by that of the continuous one and vice versa via displacement and interphase momentum, mass and heat transfer effects. The strength of the interactions will depend on the dispersed particle’s size, density and number density.

Individual fuel droplets introduced into the turbulent airflow will each have their own random path due to interaction with the fluctuating
turbulent velocity field. The droplets may also interact with each other, i.e., through collision. As diesel fuel, the dispersed phase becomes volatile and reactive as temperatures corresponding to its latent heat of vapourisation is reached, mass transfer occurs between the phases. This is accompanied by interphase heat and mass transfer, which causes size changes (polydispersed) in the liquid fuel droplets. The size change may also be produced by fluid-dynamic forces acting on the dispersed elements, causing them to break up into smaller elements. Inter-element collision processes may produce the opposite effect, i.e., size increase due to coalescence or agglomeration. In the case of the fuel droplets striking the walls, bouncing or shattering according to the impact conditions may result.

The Lagrangian / Eulerian framework (Bracco (1985)) is used to express the conservation equations of mass, momentum and energy for each fuel droplet. As the number of droplets in the calculation is generally large, a statistical approach has been used, where the total population is represented by a finite number of computational parcels or samples, each of which represents a group or cluster of droplets having the same properties. The random walk technique (Mashayek (2001)) is employed to introduce the fluctuating nature of the turbulent velocity field, which results in turbulent dispersion of the droplets.

3.8.1 Basic Conservation Equations for the Dispersed Phase

The instantaneous fluid velocity and droplet velocity are denoted by \( \bar{u} \) and \( \bar{u}_d \) respectively, and the droplet position vector is denoted by \( \bar{x}_d \). The conservation equations for droplets in the Lagrangian framework are as follows:
3.8.1.1 Momentum

The momentum equation for a droplet of mass $m_d$ is

$$m_d \frac{d\vec{u}_d}{dt} = \vec{F}_{dr} + \vec{F}_p + \vec{F}_{am} + \vec{F}_b \quad (3.65)$$

$\vec{F}_{dr}$ is the drag force (ref. Figure 3.1) given by

$$\vec{F}_{dr} = \frac{1}{2} C_d \rho A_d |\vec{u} - \vec{u}_d| (\vec{u} - \vec{u}_d) \quad (3.66)$$

where $C_d$ is the drag coefficient, a function of the droplet Reynolds number given by

$$C_d = \begin{cases} 
24(1 + 0.15 \text{Re}_d^{0.687}) / \text{Re}_d, & \text{Re}_d \leq 10^3 \\
0.44, & \text{Re}_d > 10^3
\end{cases} \quad (3.67)$$
and $Re_d$ is the droplet Reynolds number defined as

$$Re_d \equiv \frac{\rho |\vec{u} - \vec{u}_d| D_d}{\mu}$$  \hspace{1cm} (3.68)$$

and $A_d$ the droplet cross-sectional area.

$\vec{F}_p$ is the pressure force given by

$$\vec{F}_p = V_d \nabla p$$  \hspace{1cm} (3.69)$$

where $V_d$ is the droplet volume and $\nabla p$ the pressure gradient in the carrier fluid, i.e., air. $p$ includes any hydrostatic component.

$\vec{F}_{am}$ is the ‘virtual mass’ force required to accelerate the carrier fluid ‘entrained’ by the droplet, given by

$$\vec{F}_{am} = -C_{am} \rho V_d \frac{d(\vec{u}_d - \vec{u}_d)}{dt}$$  \hspace{1cm} (3.70)$$

where $C_{am}$ is the virtual mass coefficient usually set to 0.5 (Milne-Thompson (1966)).

$\vec{F}_b$ is a general body force term which represents the effect of gravity in the present work. The expression for this is

$$\vec{F}_b = m_d \vec{g}$$  \hspace{1cm} (3.71)$$

where $\vec{g}$ is the gravitational acceleration vector.
Knowledge of the droplet velocity allows its instantaneous position vector $\mathbf{x}_d$ to be determined by integrating:

$$\frac{d\mathbf{x}_d}{dt} = \mathbf{u}_d$$  \hspace{1cm} (3.72)

From equation (3.73), the momentum relaxation time scale $\tau_M$ can be identified as

$$\tau_M = \frac{m_d |\mathbf{u} - \mathbf{u}_d|}{C_d \rho A_d |\mathbf{u} - \mathbf{u}_d|} = \frac{4\rho_d D_d}{3C_d \rho |\mathbf{u} - \mathbf{u}_d|}$$  \hspace{1cm} (3.73)

### 3.8.1.2 Mass

In the presence of mass transfer at a rate $F_m$ per unit surface area, the droplet mass rate of change is given by

$$\frac{dm_d}{dt} = -A_s F_m$$  \hspace{1cm} (3.74)

where $A_s$ is the droplet surface area. For an evapourating / condensing single-component droplet, $F_m$ is expressed as (Bird et al (1966))

$$F_m = K_g \left[ \ln \left( \frac{p_t - p_{v,\infty}}{p_t - p_{v,s}} \right) \right]$$  \hspace{1cm} (3.75)

where $p_t$, $p_{v,\infty}$ and $p_{v,s}$ are the gas pressure and partial pressures of the vapour in the droplet surroundings and at its surface ($p_{v,s}$ is assumed to be equal to the saturation pressure at the droplet temperature $T_d$) respectively, and $K_g$ is the mass transfer coefficient given by
\[ K_g = \frac{\text{Sh}D_m}{R_m T_m D_d} \]  

(3.76)

in which \( R_m \) is the mixture gas constant, \( D_m \) is the vapour diffusivity, \( T_m \) is the mean temperature and \( \text{Sh} \) is the Sherwood number given by (Ranz and Marshall (1952))

\[ \text{Sh} = 2(1 + 0.3 \text{Re}^{1/2} \text{Sc}^{1/3}) \]  

(3.77)

From equations (3.74) and (3.75), the mass relaxation time scale \( \tau_m \) may be defined as

\[ \tau_m = m_d \frac{\rho_d D_d}{A_s |F_m|} = \frac{\rho_d D_d}{6 |F_m|} = \frac{\rho_d D_d}{6K_g p_l \ln \left( \frac{p_l - p_v,\infty}{p_l - p_v,s} \right)} \]  

(3.78)

3.8.1.3 Energy

The droplet energy balance takes into account the mechanisms of surface heat transfer rates \( q_{d}^{*} \) per unit surface area and loss / gain due to phase change, thus:

\[ m_d \frac{d(c_{p,d}T_{d*})}{dt} = A_s q_{d}^{*} + h_{lg} \frac{dm_d}{dt} \]  

(3.79)

where \( A_s \) is the droplet surface area, \( c_{p,d} \) the droplet specific heat and \( h_{lg} \) the latent heat of phase change, the surface heat flux \( q_{d}^{*} \) is given by the following relation:

\[ q_{d}^{*} = h(T_{d} - T) \]  

(3.80)

in which \( h \) is the heat transfer coefficient obtained via the correlation (El Wakil et al (1954))
Here, the Nusselt number $\text{Nu}$ is obtained from the following Ranz-Marshall correlation (Ranz and Marshall (1952)):

$$\text{Nu} = 2(1 + 0.3 \text{Re}^{1/2} \text{Pr}^{1/3})$$  \hspace{1cm} (3.82)

in which $\text{Pr}$ is the Prandtl number. The quantity $Z$ is defined as

$$Z = \frac{c_p (dm_d / dt)}{\pi D_d k_m \text{Nu}}$$  \hspace{1cm} (3.83)

From equations (3.80) and (3.81), the thermal relaxation time scale for droplets $\tau_T$ can be identified as

$$\tau_T = \frac{c_{p,d} T_d m_d}{A_s |q|} = \frac{c_{p,d} \rho_d D_d}{6h} = \frac{c_{p,d} \rho_d D_d^2}{6k_m \text{Nu}}$$  \hspace{1cm} (3.84)

### 3.8.2 Droplet Break-Up Modeling

The injected fuel droplets become unstable under the action of the interfacial forces induced by their motion relative to the in-cylinder air. The model employed to determine the size rate of change of the droplets is that of Reitz and Diwaker (1986). According to this model, droplet break-up due to aerodynamic forces occurs in one of the following modes:

1. ‘Bag break-up’, in which the non-uniform pressure field around the droplet causes it to expand in the low-pressure wake region and eventually disintegrate when surface tension forces are overcome.
2. ‘Stripping break-up’, a process in which liquid is sheared or stripped from the droplet surface.

In each case, theoretical studies have provided a criterion for the onset of break-up and concurrently an estimate of the stable droplet diameter \( D_{d, \text{stable}} \) and the characteristic time scale \( \tau_b \) of the break-up process. This allows the break-up rate to be calculated from

\[
\frac{dD_d}{dt} = -\frac{(D_d - D_{d, \text{stable}})}{\tau_b} \tag{3.85}
\]

where \( D_d \) is the instantaneous droplet diameter. The criteria and time scales are as follows:

**3.8.2.1 Bag break-up**

Here, instability is determined by a critical value of the Weber number \( W_e \), thus:

\[
W_e \equiv \frac{\rho|\vec{u} - \vec{u}_d|^2}{2\sigma_d} \geq C_{bl} \tag{3.86}
\]

where \( \sigma_d \) is the surface tension coefficient and \( C_{bl} \) is an empirical coefficient having a value in the range of 3.6 to 8.4 (Reitz and Diwakar (1986)). A mean value of \( C_{bl} = 6 \) is chosen. The stable droplet size is that which satisfies the equality in equation (3.86). The associated characteristic time is

\[
\tau_b = \frac{C_{b2}D_d^{3/2}}{4\sigma_d^{1/2}} \tag{3.87}
\]

in which \( C_{b2} \approx \pi \).
3.8.2.2 **Stripping break-up**

The criterion for the onset of this regime is

\[
\frac{\text{We}}{\sqrt{\text{Re}_d}} \geq C_{s1}
\]  

(3.88)

where \( C_{s1} \) is a coefficient with the value 0.5 (Reitz and Diwakar (1986)). The characteristic time scale for this regime is

\[
\tau_b \frac{C_{s2}}{2} \left( \frac{\rho_d}{\rho} \right)^{1/2} \frac{D_d}{|\vec{u} - \vec{u}_d|}
\]  

(3.89)

Here the empirical coefficient \( C_{s2} \) is in the range of 2 to 20 (Reitz and Diwakar (1986)), and is presently taken to be 20.

3.8.2.3 **Inter-droplet collisions**

The model for droplet-droplet collisions follows that of O’Rourke (O’Rourke (1981)). It distinguishes the following three types of interaction:

- Coalescence
- Separation
- Bouncing

During these processes, droplets from the participating parcels can exchange mass, momentum and energy. A statistical, rather than a deterministic approach is used to avoid creating an excessive new number of parcels. The number of parcels hence remains constant unless the smaller diameter droplets are all absorbed by coalescence. Once the type of collision has been resolved, then all the droplets in the parcel with the larger diameter
(collectors) undergo collisions with the droplets from parcels with smaller diameter (donors). For each pair of parcels, collisions only occur if they lie in the same computational cell. The droplets are considered to be uniformly distributed throughout the cell so that the collision frequency \( \nu \) of a collector droplet with all droplets in the other parcel is given by:

\[
\nu = \frac{\pi}{4} (D_{d,1} + D_{d,2})^2 |u_{d,1} - u_{d,2}| E_{1,2} \frac{N_{d,2}}{\delta V} \tag{3.90}
\]

Here the subscripts 1 and 2 refer to the collector and donor parcels respectively, \( N_{d,2} \) is the number of parcels in the second parcel and \( \delta V \) is the cell volume. The collision efficiency \( E_{1,2} \) is evaluated from:

\[
E_{1,2} = \left( \frac{0.75 \ln(2w)}{2 - 1.214} \right)^{-2} ; w > 1.214 \tag{3.91}
\]

Otherwise \( E_{1,2} = 0 \). In this equation, \( W \) is a dimensionless parameter given by:

\[
w = \frac{D_{d,2} \left| u_{d,1} - u_{d,2} \right| D_{d,2}^2}{9 \mu D_{d,1}} \tag{3.92}
\]

The probability that the collector undergoes \( n \) collisions with droplets from a donor parcel during the time interval \( \delta \tau \) is taken to follow a Poisson distribution, with the mean value \( n' = \nu \delta \tau \), i.e.,

\[
P_n = \left( \frac{n'}{n!} \right) e^{-n'} \tag{3.93}
\]

To determine whether collisions take place between individual droplets, a random number \( N_{r,1} \) is chosen in the interval \( (0 - 1) \). If \( N_{r,1} < P_0 \), no
collision occurs. If a collision occurs, the probability that the outcome is coalescence of the droplets is given in (Brazier-Smith (1972)) by:

\[ E_{\text{coal}} = \min \left[ \frac{2.4f(\gamma)}{W_{\text{e}_L}}, 1 \right] \]  

(3.94)

where \( f(\gamma) = \gamma^3 - 2.4\gamma^2 + 2.7\gamma \), \( \gamma = D_{d,1}/D_{d,2} \) and \( W_{\text{e}_L} \) is the droplet Weber number defined as:

\[ W_{\text{e}_L} = \frac{\rho_d |u_{d,1} - u_{d,2}|^2 D_{d,2}}{2\sigma} \]  

(3.95)

To determine whether an individual collision results in coalescence or separation, a second random number \( N_{r,2} \) is chosen. If \( N_{r,2} < E_{\text{coal}} \), coalescence occurs and the number of droplets \( m \) which take part in the coalescence with each collector droplet is:

\[ \sum_{i=0}^{i=m-1} \frac{P_i}{P_0} < \frac{N_{r,1}}{P_0} < \sum_{i=0}^{i=m-1} \frac{P_i}{P_0} \]  

(3.96)

Thus the new number of droplets in the donor parcel is \( N_{d,2}^a = N_{d,2} - mN_{d,1} \). The properties of the collector droplets are recomputed so that mass, momentum and energy are conserved. In the case when the condition \( N_{r,2} < E_{\text{coal}} \) and the additional requirement \( W_{\text{e}_L} < W_{\text{e}_{\text{bou}}} \) are satisfied, another type of collision called ‘bouncing’ occurs, where \( W_{\text{e}_{\text{bou}}} \) is obtained from:

\[ W_{\text{e}_{\text{bou}}} = 2.4f(\gamma)N_{r,2}^3 \]  

(3.97)

When separation or bouncing occurs, only momentum is exchanged and thereby conserved overall.
3.8.2.4 Turbulent dispersion

A droplet in a turbulent flow experiences a randomly varying velocity field to which it responds according to its inertia. This process is modelled by a stochastic approach described in (Gosman and Ioannides (1983)). The stochastic model assumes that as a droplet traverses the turbulent flow field, it interacts with a sequence of eddies. It is assumed that the fluctuating velocity within each eddy is isotropic and obeys a Gaussian probability density function. Moreover the interaction time\( \tau_i \) is assumed to be sufficiently short that the fluid velocity in a given eddy is effectively constant during the process. The interaction time is taken to be the smaller of the eddy lifetime \( \tau_e \) and the time \( \tau_i \) required for the droplet to traverse the eddy. Following these assumptions, the droplet experiences an instantaneous fluid velocity \( \bar{u} \) in each eddy given by

\[
\bar{u} + \bar{U} + u'
\]  

(3.98)

where \( \bar{u} \) is the local time averaged velocity and \( u' \) is the random perturbation. The latter is calculated from a Gaussian probability function with zero mean value and a standard deviation of \( (2k/3)^{1/2} \) as follows:

\[
u' = (2k/3)^{1/2}\text{sign}(N_r)\text{erfc}^{-1}(N_r)
\]  

(3.99)

where \( k \) is the turbulent energy, \( N_r \) is a random number in the range \(-1 \) to \(+1\) and \( \text{erfc}^{-1}(N_r) \) is the inverse complementary error function. Thus \( \bar{u} \) is the quantity as detailed above used in the droplet equations for turbulent flow calculations. The interaction time \( \tau_i \) is evaluated as

\[
\tau_i = \min(\tau_e, \tau_i)
\]  

(3.100)

with the eddy lifetime estimated from
\[ \tau_e = \frac{1}{|\bar{u}|} \]  
\[ (3.101) \]

where \( l \) is the turbulence integral length scale. The transit time is estimated from

\[ \tau_i = \frac{1}{|\bar{u} - \bar{u}_d|} \]  
\[ (3.102) \]

### 3.8.2.5 Droplet boundary conditions

The Lagrangian nature of the dispersed phase equations require ‘inlet’ and wall boundary conditions as discussed below:

**Inlets**

The injected spray being modelled approximates the flow at the nozzle exit and its subsequent atomisation. The latter gives rise to a fuel droplet spray represented by a set of computational parcels each containing a number of droplets with the same properties. Nozzle exit droplet size is fixed constant. These properties are calculated on the basis of the Reitz-Diwakar atomisation model. The histories of the computational parcels are obtained from the Lagrangian conservation equations of mass, momentum and energy in the normal way. In the nozzle flow model used, the injection velocity \( u_{ch} \) is calculated from,

\[ \dot{Q} = c_d A_0 \sqrt{\frac{2}{\rho_d}} \Delta_p \]  
\[ (3.103) \]

where \( \dot{Q} \) is the volume flow rate through the injector, \( c_d \) is the coefficient of discharge through the nozzle, \( A_0 \) is the nozzle cross sectional area, \( \rho_d \) is the fuel density and \( \Delta_p \) is the pressure drop across the injector.
Walls

The impact of droplets on the walls may produce a wide variety of consequences according to the size, velocity and material of the impacting elements and the nature of the surface (Naber et. al. (1988)) such as adhere, bounce or shatter. The perfect rebound phenomenon has been adopted in the present work, which imposes the condition that the impinging droplet bounces off the wall after impact. The transition criteria are given below:

\[ \text{We}_d \leq 5 \]

3.8.2.6 Droplet post-impingement characteristics

The normal and tangential components of droplet post-impingement rebound velocity to the wall \( \vec{V}_{d,n}^p \) and \( \vec{V}_{d,t}^p \) are given by:

\[
\vec{V}_{d,n}^p = -e_n \vec{V}_{d,n} \tag{3.104}
\]
\[
\vec{V}_{d,t}^p = -e_t \vec{V}_{d,t} \tag{3.105}
\]

where \( e_n \) and \( e_t \) are the normal and tangential restitution coefficients respectively. The former depends on the droplet incidence angle \( \theta \) measured from the wall as:

\[
e_n = 0.993 - 1.76 \theta + 1.56 \theta^2 - 0.49 \theta^3 \tag{3.106}
\]
\[
e_t = \frac{5}{7} \tag{3.107}
\]

3.8.3 Basic Conservation Equations for the Continuous Phase

The continuous phase conservation equations are essentially equations (3.1) through (3.8) with modifications whose origins and nature are as follows:
1) Account is taken of the displacement of the carrier fluid by the dispersed phase, measured by the fractional volume $\alpha$ occupied by the former. The necessary modifications to the fluid equations are:

a) Replacement of the density $\rho$ and effective viscosity $\mu_{\text{eff}}$ in the transport terms on the left-hand side by the products $\alpha \rho$ and $\alpha \mu_{\text{eff}}$ respectively.

b) Multiplication of the right-hand side terms representing volume-integrated sources and other effects by $\alpha$.

2) Interphase transfer effects are allowed for by including the appropriate source / sink terms derived from the Lagrangian equations.

3.9 DISCRETISATION SCHEMES

The differential equations governing the conservation of mass, momentum, energy, etc. within the fluid are discretised by the finite volume (FV) method (Gosman et. al (1969), Patankar (1980)). They are first integrated over the individual computational cells and over finite time increment, and then approximated in terms of the cell-centred nodal values of the dependant variables.

The general conservation equation of any flow property $\phi$ in Cartesian coordinate system has the general form:

$$ \frac{\partial}{\partial t} (\rho \phi) + \text{div}(\rho \vec{u} \phi) = \text{div}(\Gamma \text{grad}\phi) + S_\phi $$

(3.108)

where $\phi$ is any one of the dependent variables $u, m, k, \varepsilon, m_s$, etc., and $\Gamma_\phi, S_\phi$ are the associated diffusion and source terms. The finite volume integration of
equation (3.108) over a control volume (CV) must be augmented with further integration over a finite time step $\Delta t$. By replacing the volume integrals of the convective and diffusive terms with surface integrals and changing the order of integration in the rate of change term, the following integral form of equation (3.110) can be obtained:

$$\int_{CV} \left( \int_{t}^{t+\Delta t} \frac{\partial}{\partial t} (\rho \phi) dt \right) dv + \int_{t}^{t+\Delta t} \left( \int_{A} \nabla \cdot (\rho \vec{u} \phi) dt \right) dA = \int_{t}^{t+\Delta t} \left( \int_{CV} \int_{t}^{t+\Delta t} \Gamma \nabla \phi dA dt \right) + \int_{t}^{t+\Delta t} \int_{CV} S_{\phi} dv dt$$

(3.109)

Equation (3.109) can be applied to every control volume and discretized so as to obtain a set of linear equations, which can be solved algebraically. The choice of discretization scheme will affect the convergence rate and accuracy of the final solution. Lower order schemes tend to be more stable, while higher order schemes are more accurate but require more computer time to solve and also less stable. As already noted, the finite volume equation applies over an arbitrary time increment $\Delta t$ spanning the old and new time levels. Two options are available for temporal discretization; the fully implicit scheme and the second order Crank-Nicholson scheme. In the present work the fully implicit scheme is used. This method avoids the stability related time step restrictions, which becomes particularly onerous in regions of small mesh spacing and high velocity or diffusion rate. Under this formulation, the fluxes prevailing over time interval are calculated from the new time-level values of the variables. For spatial discretization of $u$, $v$, $w$, $k$ and $\varepsilon$, the first order Upwind Differencing (UD) scheme is used, which accounts for the direction of flow. For spatial discretization of density second-order central differencing (CD) scheme is used which simply interpolates linearly on nearest neighbor values, irrespective of flow direction.
3.10 SOLUTION ALGORITHM FOR PRESSURE-VELOCITY COUPLING

The continuity and momentum equations, which govern the flow, are intricately coupled because every velocity component appears in each momentum and continuity equations. The most complex issue to resolve is the role played by the pressure. It appears in all the momentum equations but there is no equation for pressure. The basic algorithm used for pressure-velocity coupling for transient computations is PISO, which stands for Pressure Implicit with Splitting Operators (Issa (1986)).

3.11 SELECTION OF SUITABLE CFD PACKAGE FOR IN-CYLINDER ENGINE ANALYSIS

In-cylinder analysis for diesel engines requires the dynamic meshing capability such as grid translation, compression, expansion and grid deformation with cell layer activation and deactivation in order to simulate the rate of volume change with time, and the movements of boundaries – the piston head and valves. The choice was available between two commercial codes, FLUENT and STAR-CD. The limitation of FLUENT towards handling dynamic meshing capability is realized. Since the dynamic meshing capabilities of the other available CFD software STAR-CD was well acknowledged in the open literature (Auriemma et al (1998), Okazaki et al (1999)), the package is chosen for the project.

STAR-CD permits a full transient simulation of engine in-cylinder flows by enabling cells to be removed or added during the transient calculation. The average cell size is hence maintained roughly constant. STAR-CD also allows sliding interface that enables cells to change their connectivity during the solution process (Figure 3.2)
STAR CD can only generic heat and fluid flow analysis. In this work it is required to move the piston as well as valve motion. It is also necessary to customize the software for various injection profile mentioned in Tables 4.2 and 4.3. It can thoroughly be seen the above can be made possible by writing as a separate UDF using fortran – language. The author has written the UDF for the purpose of customization and same is presented in Appendix 1.

**Figure 3.2 Illustration of sliding mesh procedure**

<table>
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<tr>
<th>Mesh block</th>
<th>1</th>
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<th>3</th>
<th>4</th>
<th>5</th>
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<td>13</td>
<td>14</td>
<td>15</td>
<td>16</td>
<td></td>
</tr>
</tbody>
</table>

1. Lower mesh block moves, distorting the mesh
2. The interface slides to a new position
3. Lower mesh block moves, reducing the distortion
4. Figure 3.2 Illustration of sliding mesh procedure