CHAPTER 5

CFD METHODOLOGY AND MODELING

5.1 INTRODUCTION

The simulation of flow in internal combustion engines is a complex process involving fluid dynamics and turbulent motion. Any physical fluid flow problem can be solved either experimentally or numerically. The numerical simulation is more suitable for parametric studies and it also gives accurate results by solving governing equations in each and every cell of the fluid domain. In the recent years there were tremendous improvement in the field of numerical techniques, which made a great impact on the evaluation of complex flow problems and achieving their solution. Computational Fluid Dynamics (CFD) has grown from a mathematical curiosity to an essential tool in almost every branch of fluid dynamics. CFD is considered as a bridge between the pure experimental fluid dynamics and pure theoretical fluid dynamics. Until recently, researchers had to mainly depend on time consuming and costly experimentations for studying complex flow problems. With the advent of powerful digital computers and numerical simulation techniques, the extent of experimentation required for analysing complex engineering problems has been reduced considerably.

Computational Fluid Dynamics (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. In the present work a three dimensional numerical simulation was carried out to study the effects of different combustion chamber geometry on the in-cylinder flow process of a four stroke DI diesel engine using commercially available CFD software.

5.2 BASIC STRUCTURE OF A CFD CODE

To write a CFD code to deliver a solution for every new fluid flow case would be time consuming and unforgiving. Due to this, general commercial CFD codes have evolved, such as KIVA, AVL FIRE, STAR-CD, Fluent, ANSYS CFX and Open Foam. They provide user friendly GUIs (graphical user interfaces) to allow the user to utilize an inbuilt code with a variety of problem solving facilities to deliver a solution for problems associated with fluid flow, heat transfer etc. The process of generating a solution to a fluid problem using a general CFD code is described in three stages viz.

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

5.2.1 Pre-Processor

The first step involved in the pre-processor stage is to define a suitable geometry in which the fluid flow problem is to be analysed. Defining the geometry can be achieved by replicating a known geometry through computer aided design (CAD). Once the geometry has been created a suitable mesh can be constructed. A mesh can be described as a volume which has been discretized into a series of smaller volumes or elements. Once a workable mesh has been created, additional known quantities of the fluid are defined such as density, viscosity and turbulent quantities. Boundary conditions are applied to cell faces in the form of a flux adjacent to an
inlet/exit or wall such as temperature, pressure, velocity profile etc. Pre-processing is the most crucial stage in the development of a solution, as the determination of a realistic answer is highly dependent on the mesh quality.

5.2.2 Solver

The solver is considered as the calculation process that ultimately leads to a solution of the transport equations. 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
- Discretization 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 discretization processes.

5.2.3 Post-Processor

For design analysis, secondary variables such as stresses and fluxes must be computed. Most of the commercial CFD codes provide their own post-processor which compute the secondary variables and provide variety of
plots (contour as well as line diagrams) based on the nodal data obtained from simulation. These include:

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

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.

5.3 GOVERNING EQUATIONS

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

1. The mass of a fluid is conserved.
2. The rate of change of momentum equals the sum of the forces on a fluid particle (Newton’s second law).
3. 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).

5.3.1 Conservation Equations for the Flow Field

The mass and momentum equations (5.1) and (5.2) solved for the unsteady, compressible / incompressible, three-dimensional in-cylinder flow in Cartesian tensor notation are represented as (Warsi (1981)): 
\[
\begin{bmatrix}
\text{Rate of increase of mass in fluid element}
\end{bmatrix} = \begin{bmatrix}
\text{Net rate of flow of mass into fluid element}
\end{bmatrix}
\]

\[
\begin{bmatrix}
\text{Rate of increase of momentum of fluid particle}
\end{bmatrix} = \begin{bmatrix}
\text{Sum of forces on fluid particle}
\end{bmatrix}
\]

i.e.

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j) = s_m \tag{5.1}
\]

\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j u_i - \tau_{ij}) = - \frac{\partial p}{\partial x_i} + s_i \tag{5.2}
\]

where

- \( t \) - time
- \( x_i \) - Cartesian coordinate \( (i = 1, 2, 3) \)
- \( u_i \) - absolute fluid velocity component in direction \( x_i \)
- \( p \) - piezometric pressure = \( p_s - \rho \beta_g \) \( g_m \) \( x_m \) where \( p_s \) is static pressure, \( \rho \beta_g \) is reference density, \( g_m \) are gravitational acceleration components and \( x_m \) are coordinates relative to a datum where \( \rho \beta_0 \) is defined

\[
\rho = \left( \frac{p}{RT \sum_{m} \frac{m}{M_m}} \right)
\]

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:

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

(5.3)

where

- \( \mu \) - molecular dynamic fluid viscosity

- \( \delta_{ij} \) - the Kronecker delta ( = 1 when \( i = j \), and 0 otherwise)

\( S_{ij} \) - Rate of strain tensor

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

(5.4)

The right most term in Equation (5.3) 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.

5.4 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)):

\[
\frac{-\rho \overline{u_i u_j}}{\overline{u_i u_j}} = 2 \mu_t \delta_{ij} - \frac{2}{3} \left( \mu_t \frac{\partial u_k}{\partial x_k} + \rho \right) \delta_{ij}
\]  

\[
\frac{-\rho \overline{u_j h}}{\overline{u_j h}} = - \frac{\mu_t}{\sigma_{h,t}} \frac{\partial h}{\partial x_j}
\]  

\[
\frac{-\rho \overline{u_j m}}{\overline{u_j m}} = - \frac{\mu_t}{\sigma_{m,t}} \frac{\partial m}{\partial x_j}
\]

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
5.5 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:

\[
\frac{\partial}{\partial t} \left( \rho \phi \right) + \nabla \cdot \left( \rho \mathbf{u} \phi \right) = \nabla \cdot \left( \Gamma \nabla \phi \right) + S_{\phi} \tag{5.8}
\]

where \( \phi \) is any one of the dependent variables \( u, m, k, \varepsilon, m_i, \) etc., and \( \Gamma, S_{\phi} \) are the associated diffusion and source terms. The finite volume integration of equation (5.8) 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 (5.9) can be obtained:

\[
\int_{CV} \left( \int_{\bar{t}}_{\bar{t}+\Delta t} \left( \rho \phi \right) dt \right) dV + \int_{\bar{t}}_{\bar{t}+\Delta t} \int_{\Lambda} n \cdot (\rho \mathbf{u} \phi) dA dt = \int_{\bar{t}}_{\bar{t}+\Delta t} \int_{\Lambda} n \cdot (\Gamma \nabla \phi) dA dt + \int_{CV} S_{\phi} dV dt \tag{5.9}
\]

Equation (5.9) 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 ε, 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.

5.6 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 (Issa (1986)).

5.7 NUMERICAL SIMULATION

In the present work, simulation studies have been carried out with five different combustion chamber geometries to investigate their effect on flow characteristics under transient operating conditions. The simulation was carried out for a constant engine speed at non reacting condition. Simulation results obtained for these combustion chamber geometries are presented and discussed in Section 6.2 of Chapter 6. Further, in order to attain consistency of in-cylinder flow analysis results; a grid independence study was conducted to arrive at the optimum grid density that can be used for accurate simulation results.
5.8 METHODOLOGY AND PROCEDURE

A commercially available CFD code, was used in this study. Flow conditions inside the cylinder were predicted by solving momentum, continuity and energy equations. The governing equations to be solved are already mentioned in this Chapter. The RNG k–ε model with standard wall function was employed for physical modeling. The program was based on the pressure-correction method and used the PISO algorithm. The first order upwind differencing scheme (UD) was used for the momentum, energy and turbulence equations and the temporal discretization was implicit. Spatial discretization was done using the upwind differencing scheme for momentum, turbulent kinetic energy/dissipation and temperature, and central differencing scheme for density. Temporal discretization was done using the implicit scheme.

The calculations began at TDC of the intake stroke and completed at 30 degrees after TDC (aTDC) of compression. In order to study the average transverse fluid flow behaviour in the analysis, a quantity known as Swirl Ratio (SR) was computed for the in-cylinder flow field about the cylinder axis. It is expressed as,

\[
SR = \frac{60 \ H_\text{Z}}{2 \pi M_\text{Z} \ \Omega_\text{cs}} 
\]

\[
H_\text{Z} = \sum_{i=1}^{N\text{cells}} \{v_i (x_i - x) - (u_i (y_i - y))\} m_i \quad \text{and} 
\]

\[
M_\text{Z} = \sum_{i=1}^{N\text{cells}} \{(x_i - x)^2 + (y_i - y)^2\} m_i 
\]

where \(H_\text{Z}\) represents the total angular momentum of the in-cylinder fluid about the cylinder axis, \(M_\text{Z}\) is the total moment of inertia of the fluid about the cylinder axis, \(\Omega_\text{cs}\) is the angular speed of the crankshaft in rpm, \(u_i\) and \(v_i\) represent the local components of velocity in the x and y directions respectively and \(m_i\), the mass accumulated in each cell.
5.9 GEOMETRIC AND NUMERICAL MODELING

The engine studied in this work was a stationary, single-cylinder, DI diesel engine with five different piston shapes. These shapes are representative of the geometries usually employed for the optimum combustion process in real engines. The piston named HCC had a Hemispherical Combustion Chamber and used as a baseline model. Two pistons having open combustion geometries namely Shallow depth Combustion Chamber and Toroidal Combustion Chamber (named SCC and TCC respectively) and two other pistons having re-entrant combustion geometries namely Shallow depth Re-entrant Combustion Chamber and Toroidal Re-entrant Combustion Chamber (named SRCC and TRCC respectively) were used. In order to maintain the compression ratio of the engine under consideration, while modeling, the bowl volumes for all the combustion chamber configurations, were kept constant. The bowl volumes of different combustion chamber configurations employed are given in Table 5.1. Figure 5.1 shows the shapes and dimensions of five combustion chamber geometries used. The inlet valve axis

![Figure 5.1 Schematic diagram of combustion chambers employed](image-url)
is offset from the cylinder axis by 18.5 mm in the x direction and 2.0 mm in the y direction. The detailed specification of the base engine selected for the simulation is given in Appendix-1

**Table 5.1 Volume of bowls of different combustion chambers employed**

<table>
<thead>
<tr>
<th>Combustion Chamber</th>
<th>Bowl Volume in CC</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCC</td>
<td>35.759</td>
</tr>
<tr>
<td>SCC</td>
<td>35.756</td>
</tr>
<tr>
<td>TCC</td>
<td>35.754</td>
</tr>
<tr>
<td>SRCC</td>
<td>35.760</td>
</tr>
<tr>
<td>TRCC</td>
<td>35.752</td>
</tr>
</tbody>
</table>

5.9.1 **Preprocessing and Grid Generation**

In order to solve the governing equations, approximations for the partial differential equations are required. In finite volume methods, all the differentials are reduced to algebraic expressions by integrating the governing equations over sub domains and in this sub domain the equations are solved subsequently. The preprocessing mainly involves creation of the basic 3D model, grid generation and fixing of the boundary conditions. A hexahedral block structured mesh is employed for the entire computational domain of the engine. A pre-processor was used to create the entire computational domain of the engine including intake and exhaust ports and a commercial CFD code was used for the solution of governing equations and post processing the results. The computational meshes employed for the simulation of different combustion chamber geometries are shown in Figure 5.2

5.9.2 **Boundary Conditions**

The boundary and initial conditions employed are given in Table 5.2. Constant pressure boundary conditions were assigned to both intake and
Figure 5.2  Computational domains of different combustion chamber geometries
### Table 5.2 Boundary and initial conditions

<table>
<thead>
<tr>
<th>BOUNDARY CONDITIONS</th>
<th>INITIAL CONDITIONS</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Intake Manifold</strong></td>
<td><strong>Intake Manifold</strong></td>
</tr>
<tr>
<td>Type</td>
<td>constant pressure</td>
</tr>
<tr>
<td>Pressure</td>
<td>1.01 bar</td>
</tr>
<tr>
<td>Temperature</td>
<td>303 K</td>
</tr>
<tr>
<td>Turb intensity</td>
<td>5%</td>
</tr>
<tr>
<td>Length scale</td>
<td>1 mm</td>
</tr>
<tr>
<td><strong>Exhaust Manifold</strong></td>
<td><strong>Exhaust Manifold</strong></td>
</tr>
<tr>
<td>Type</td>
<td>constant pressure</td>
</tr>
<tr>
<td>Pressure</td>
<td>1.01 bar</td>
</tr>
<tr>
<td>Temperature</td>
<td>303 K</td>
</tr>
<tr>
<td>Turb intensity</td>
<td>5%</td>
</tr>
<tr>
<td>Length scale</td>
<td>1 mm</td>
</tr>
<tr>
<td><strong>Valve – Cylinder interface</strong></td>
<td><strong>Cylinder</strong></td>
</tr>
<tr>
<td>Type</td>
<td>attach</td>
</tr>
<tr>
<td>Wall Type</td>
<td>smooth wall, no slip</td>
</tr>
<tr>
<td>Wall Pressure</td>
<td>1 bar</td>
</tr>
<tr>
<td>Temperature</td>
<td>303 K</td>
</tr>
<tr>
<td>Wall heat type</td>
<td>fixed temperature</td>
</tr>
<tr>
<td>Temperature / Thermal resistance</td>
<td>303 K / 0.01565 m² K/W</td>
</tr>
<tr>
<td>Length scale</td>
<td>1 mm</td>
</tr>
</tbody>
</table>
exhaust ports, so the dynamic effects were neglected. The smooth wall option for turbulent flow boundary condition was used. Adiabatic wall for heat transfer was assumed. The initial values of pressure and temperature were considered as homogeneous in the whole domain. As the residual swirl of the flow in the cylinder at the end of the exhaust stroke was not taken into account, the flow was supposed to be quiescent initially. The initial turbulent intensity was set at 5% of the mean flow, and the integral length scale was estimated with the mixing length model of Prandtl. The walls of the intake ports, the lateral walls of the valves and the cylinder head, the cylinder wall and the piston crown that form the walls of the combustion chamber were considered adiabatic.

5.10 SUMMARY

Geometrical details of the base engine and creation of grid for various combustion chambers employed were discussed. The geometrical modeling and the inputs needed for the simulation of in-cylinder air motion in a DI diesel engine were also highlighted in this section. The results of the study are analyzed and presented in the next chapter.