Chapter 2

CFD MODELING OF MULTIPHASE FLOWS
Computational Fluid Dynamics (CFD) is a body of knowledge and technique used to solve mathematical models of fluid dynamics on digital computers. The three major tasks involved in CFD are mathematical modeling of fluid flows, numerical solution of model equations and computer implementation of numerical techniques. CFD requires relatively few restrictive assumptions and gives a complete description of the flow field for all variables. Quite complex configurations can be treated and the methods are relatively easy to apply. It can incorporate a variety of processes simultaneously. CFD simulations serve as a bridge between the theory and reality. The detailed predicted flow field gives an accurate insight to the fluid behavior and can, sometimes, give information which cannot be obtained from experiments.

Computational Fluid Dynamics (CFD) is the science of predicting the fluid flow, heat transfer, mass transfer, chemical reactions and related phenomena by solving the mathematical equations that govern these processes using a numerical algorithm (that is, on a computer). CFD methods are based on the first principles of mass, momentum and energy conservation, as described by the Navier-Stokes equation. These methods involve the solution of conservation equations of mass, momentum, energy and species at thousands of locations within the flow domain. The computed solution provides flow variables such as velocity, pressure, temperature, density, concentration, etc., within the domain.

There are two different approaches in deriving the governing equations. In the Eulerian approach, an arbitrary control volume in a stationary reference frame is used to derive the basic governing equations. In the Lagrangian approach, equations are...
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derived by considering a control volume (material volume) such that the velocity of the control volume surface always equals the local fluid velocity.

When two or more phases move relative to each other in multiphase flow reactors, these phases exhibit different flow regimes. There are different ways of classifying these multiphase flows. The simplest classification is based on the thermodynamic state of phases like gas–solid, gas–liquid and gas–liquid–solid phases. Each component of these classes is then grouped according to the flow regimes which are generally classified as dispersed flows, mixed flows and separated flows. Dispersed multiphase flows occur in a number of industrially important reactors including stirred tank reactors, fluidised bed reactors, bubble column reactors, combustors and so on.

In CFD modeling of these dispersed multiphase flow processes, in general, there are three main issues:

- Definition of ‘phase’/flow regime/required resolution
- Formulation of governing equations
- Solution of governing equations

In dispersed flows, all the phases except one exist as dispersed (discontinuous) particles flowing through the continuous fluid. For many gas–liquid or gas–liquid–solid reactors, the liquid phase is a continuous phase in which gas bubbles and solid particles are dispersed (bubble column or stirred tank reactors). Since dispersed multiphase flows exhibit complex flow behavior, depending upon the situation one deals with, the coupling between the continuous phase and dispersed phase has to be considered while modeling multiphase flow process.
The simplest situation is a one-way calculation, where the prediction of particle trajectories or distribution is sought in a known single-phase flow field. However, dispersed phase particles may influence the flow of the continuous phase and the level of interaction becomes especially complex for a turbulent flow field. When the size of the dispersed phase particle is very small or the mass loading of the particles is small, the influence of dispersed phase particles on the flow field of the continuous phase may be neglected. This is called one-way coupling. When the dispersed phase volume fraction is increased, the presence of dispersed phase will significantly affect the continuous phase flow field. This is called two-way coupling. If the particle number density is sufficiently large to allow direct particle–particle interactions, the modeler is faced with four-way coupling: continuous phase–dispersed phase particles–dispersed phase particles–continuous phase. It is essential to examine the extent of coupling between the dispersed and continuous phase to select an appropriate modeling approach.

There are three main approaches for modeling disperse multiphase flows:

(a) Eulerian framework for all phases (without explicitly accounting for the interface between phases).

(b) Eulerian framework for the continuous phase and Lagrangian framework for all the dispersed phases.

(c) Volume of fluid approach (Eulerian framework for both the phases with reformulation of interface between the phases on volumetric basis).

2.2. Eulerian–Eulerian Model

The Eulerian–Eulerian approach models the flow of all phases in Eulerian framework on the interpenetrating continuum assumption. The discrete character of the underlying process is, therefore, averaged out to provide a model involving a
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continuum associated with the dispersed phase particles. This approach is the most difficult one to understand conceptually, requiring extensive modeling efforts. Various averaging issues will have to be addressed while formulating the governing equations in this approach. If modeled successfully, this approach can be applied to multiphase flow processes containing large volume fractions of dispersed phase. It may, therefore, be extended to the simulation of complex industrial multiphase reactors consisting of a large number of dispersed particles.

This is the most general model for multiphase flows. In this approach, each phase is treated as an interpenetrating continua. The phases share the same volume and penetrate each other in space and exchange mass, momentum and energy. Each phase is described by its distinctive physical properties and has its own velocity, pressure, concentration and temperature field. Conservation equations for each phase are derived based on the principles of mass, momentum and energy. The interphase transfer between the different phases is computed using empirical closure relations (van Wachem et al., 2003).

If the multiphase system has k phases, then the volume-averaged continuity equation for each phase is given by

\[
\frac{\partial}{\partial t} (\varepsilon_k \rho_k) + \nabla \cdot (\rho_k \varepsilon_k \vec{u}_k) = \sum_{p=1}^{n} m_{pk} \hspace{1cm} (2.1)
\]

where \(\rho_k\) is the density and \(\varepsilon_k\) is the volume fraction of k\(^{th}\) phase respectively and \(m_{pk}\) is the mass transfer from p\(^{th}\) to the k\(^{th}\) phase. The momentum balance for the phase k can be written as

\[
\frac{\partial}{\partial t} (\rho_k \varepsilon_k \vec{u}_k) + \nabla \cdot (\rho_k \varepsilon_k \vec{u}_k \vec{u}_k) = -\varepsilon_k \nabla P + \nabla \cdot (\varepsilon_k \sigma_k) + \rho_k \varepsilon_k \vec{g} + \mathbf{M}_{ik} \hspace{1cm} (2.2)
\]
It should be noted that pressure, $P$, is regarded as being shared by all the phases and, therefore, appears in the governing equations of all phases. $M_{i,k}$ denotes the interphase momentum exchange terms between phase $k$ and all other phases present in the system. $\tau_k$ is the viscous stress tensor of the $k^{th}$ phase which is given by

\[
\tau_k = \varepsilon_k \mu_k \left( \nabla \vec{u}_k + \nabla \vec{u}_k^T \right) + \varepsilon_k \left( \frac{2}{3} \lambda_k \mu_k \right) \nabla \cdot \vec{u}_k I
\]

where $\mu_k$ and $\lambda_k$ are the shear and bulk viscosity of phase $k$ and $I$ is unit vector. When particle–particle interactions play a substantial role, it is necessary to introduce additional terms in the basic governing equations.

The Eulerian–Eulerian model is applicable for continuous–dispersed and continuous–continuous systems. For continuous–dispersed systems, the dispersed phase can be in the form of particles, drops or bubbles. The forces acting on the dispersed phase are modeled using empirical correlations and are included as part of the interphase momentum exchange terms. Drag, lift, gravity, buoyancy and virtual-mass effects are some of the forces that might be acting on the dispersed phase. These forces are computed for an individual particle and then scaled by the local volume fraction to account for multiple particles. If the dispersed phase is in the form of bubbles, then appropriate correlations for bubble distortion effects also are required. Correlations based on a single particle are not appropriate when the local volume fraction of the dispersed phase is high. Multi particle effects and corrections based on the presence of multiple particles in the vicinity of a single particle have to be applied.

This approach is more suitable for modeling dispersed multiphase systems where the dispersed phase volume fraction is greater than 10%. The accuracy of the Eulerian–Eulerian approach mainly depends on the empirical constitutive equations.
used. Although it requires significantly fewer computational recourses (which make it more effective for simulating the large individual reactions), it does not provide information about the hydrodynamics of individual bubbles and particles and thus has limitations in predicting certain discrete flow characteristics such as particle size effect, particle agglomeration or bubble coalescence and break up (Ranade, 2002).

In recent years, a number of simulation results have been presented on the hydrodynamics of multiphase reactors using Eulerian–Eulerian approach. Among these contributions, Lia and Salcudean (1987) simulated the bubble rise behavior using Eulerian–Eulerian approach and obtained good agreement between experimental and predicted velocity field. Ranade (1992) used Eulerian approach to investigate the flow field in a bubble column reactor. The same author (Ranade, 1997) later reported a new model (based on Eulerian approach) to include a radially varying slip velocity. Becker et al. (1994) simulated the 2D dynamic behavior of a relatively large laboratory bubble column with an Eulerian–Eulerian approach. The same case was the subject of study by Sokolichin and Eigenberger (1994). They used laminar flow conditions and concluded that unsteady-state simulations of gas liquid flow are essential in order to resolve the prevailing oscillating structures. The same authors (Sokolichin and Eigenberger, 1999), in a later communication, reported Eulerian simulation results with turbulent flow conditions in both 2D and 3D geometries. They inferred that it was not possible to reproduce the dynamic nature of bubble column using 2D simulations and emphasised the need for 3D dynamic simulation. Dudukovic and co-workers (Pan et al. 1999) used an Eulerian–Eulerian approach description to simulate the flow structures in a gas–liquid bubble column reactor. The simulated velocity field was compared with the experimental observations using
radioactive particle tracking. Mudde and Simonin (1999) reported two and three-dimensional simulations of a meandering bubble plume using the Eulerian–Eulerian approach that included the $k-\varepsilon$ turbulence model.

Krishna and co-workers (Krishna et al., 2000; van Baten and Krishna, 2002) used an Eulerian–Eulerian approach to simulate a bubble column reactor operating in the churn-turbulent regime. Because of varying size (1–5 cm) of bubbles in the churn-turbulent regime, the authors characterised the gas phase as two different phases – ‘small bubbles’ (1–6 mm) and ‘large bubbles’ (20–80 mm). Using 2D and 3D simulations, they obtained good agreement between the predicted and experimental gas holdup. Pfleger and co-workers (Pfleger et al. 1999; Pfleger and Becker 2001) carried out a transient three-dimensional Eulerian–Eulerian simulation of a bubble column reactor. They used the $k-\varepsilon$ model to simulate the turbulent phenomena in the continuous phase. The dispersed phase was modeled using laminar flow conditions. The authors compared the dynamic and time-averaged prediction with the experimental data obtained from a 28.8 cm OD bubble column reactor and obtained good agreement for gas hold-up and velocity profiles. Buwa and Ranade (2004) have recently presented an extensive experimental investigation of a rectangular column with varying parameters such as sparger design, gas flow rate and coalescing properties. The plume oscillating period was shown to decrease with increasing gas flow rate. Although the period of oscillation was somewhat unpredicted, the 3D numerical simulations still exhibited reasonable agreement with experiments.

Gas–solid/gas–solid–liquid simulations with Eulerian–Eulerian approach is an emerging important research area in the last two decades. Gidaspow (1994) provided a comprehensive summary of the numerical models of gas–solid fluidised bed
systems. Most of the effort was primarily focused on 2D simulations. Taghipour and co-workers (2005) have recently applied multi-fluid Eulerian model to simulate gas–solid fluidised bed. Comparison of their model predictions and experimental measurements on the time-averaged bed pressure drop, bed expansion, and qualitative gas–solid flow pattern has indicated reasonable agreement for different operating conditions. While there is an extensive literature on the two-phase flow model, studies of three-phase flow hydrodynamics are rather limited.

Rampure et al. (2003) studied both experimentally and computationally the effects of gas superficial velocity, H/D ratio and solid loading on the dynamic and time averaged flow behavior which provides a basis for further development of CFD models for three-phase systems. In spite of all these recent progresses in the applications of Eulerian–Eulerian approach for two and three-phase flows, experimental validation of these simulation results is still required.

2.3. Eulerian–Lagrangian model

In this approach, motion of the continuous phase is modeled using a conventional Eulerian framework. Depending on the degree of coupling (one-way, two-way or four-way), solutions of both phases interact with each other. For two-way or four-way coupling, an iterative solution procedure needs to be adopted. For four-way coupling, additional models to simulate particle–particle interactions have to be incorporated while simulating the trajectories of dispersed phase particles. In simple, one-way coupling, a continuous phase flow field can be obtained independent of the motion of the dispersed phase. Using such a flow field, the trajectories of dispersed phase particles can be obtained by solving the equations of motion for dispersed phase particles.

The continuous phase flow is described using the volume-averaged (overall) mass and momentum conservation equations:

The continuity equation for the continuous phase is

\[
\frac{\partial}{\partial t} (\epsilon_f \cdot \rho_f) + \nabla \cdot (\rho_f \cdot \epsilon_f \cdot \vec{u}_f) = 0 
\]

\[
\text{..........................(2.4)}
\]

and the momentum balance equation is
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\[
\frac{\partial}{\partial t} (\rho_f \epsilon_f \tilde{u}_f) + \nabla \cdot (\rho_f \epsilon_f \tilde{u}_f \tilde{u}_f) = - \epsilon_f \nabla P + \nabla \cdot \mathbf{\tau}_f + \rho_f \epsilon_f \mathbf{g} - \frac{\sum_{i=1}^{K} V_{s,i} \delta(u_f - u_{s,i})(x - x_{s,i})}{\sum_{i=1}^{K} V_{s,i}} 
\]

\[\text{……………(2.5)}\]

where the fluid phase stress tensor is defined as

\[
\mathbf{\tau}_f = \epsilon_f \mu_f \left( \nabla \tilde{u}_f + \left( \nabla \tilde{u}_f \right)^T \right) + \epsilon_f \left( \lambda_f - \frac{2}{3} \mu_f \right) \nabla \cdot \mathbf{u}_f \mathbf{I} 
\]

\[\text{……………(2.6)}\]

where \( \mu_f \) is fluid viscosity. The last term of equation (2.5) represents the interphase momentum transfer between the fluid phase and each individual particle, \( \delta \) represents a pulse function, which is one, if its argument is zero and zero otherwise. The last term is to ensure that the interphase momentum transfer is only taken into account in the fluid-phase momentum equation at the location of the corresponding particle.

A general force balance over a single dispersed phase particle is written in Lagrangian reference frame. This force balance equates the particle inertia with forces acting on the particle using Newton's second law

\[
m_p \frac{dU_p}{dt} = F_p + F_D + F_{VM} + F_L + F_H + F_G 
\]

\[\text{……………….}(2.7)\]

Here \( m_p \) and \( U_p \) represent the mass and velocity vector of the particle, respectively. The right-hand side represents the total force acting on the dispersed phase particle. The sum of forces due to continuous phase pressure gradient, \( F_p \), and due to gravity, \( F_G \), can be written as

\[
F_p + F_G = V_p \nabla P - \rho_p V_p g 
\]

\[\text{……………….}(2.8)\]
where $p$ is pressure in the continuous phase and $V_p$ is the volume of the particle. The drag force, $F_D$, can be written as

$$F_D = -\frac{\pi}{8} C_D \rho_c D_i^2 [U_p - U_c][U_p - U_c]$$

where the subscript C denotes the continuous phase and P denotes the particulate phase. The drag force has been studied extensively. The drag coefficient, $C_D$, depends on the flow regime (particle Reynolds number) and the properties of the continuous phase. Several empirical correlations have been proposed for the estimation of the drag coefficient. For a single rigid sphere, the drag coefficient is usually approximated by the correlation proposed by Schiller and Naumann (1935):

$$C_D = \begin{cases} 
\frac{24}{Re} \left(1 + 0.15 Re^{0.687}\right) & \text{if } Re_p < 1000 \\
0.44 & \text{if } Re_p > 1000
\end{cases}$$

where $Re_p$ is the particle Reynolds number

$$Re_p = \frac{\rho_c d_p |U_p - U_c|}{\mu_c}$$

$|U_p - U_c|$ represents the slip velocity between the continuous phase and dispersed phase. Apart from the drag force, there are three other important forces acting on a dispersed phase particle, namely lift force, virtual mass force and Basset history force. When the dispersed phase particle is rising through the non-uniform flow field of the continuous phase, it will experience a lift force due to vorticity or shear in the continuous phase flow field. Auton (1983) showed that the lift force is proportional to the vector product of the slip velocity and the curl of the liquid velocity and acts in a
direction perpendicular to both, the direction of slip velocity and the direction of the curl of the continuous phase velocity field.

When a dispersed phase particle accelerates relative to the continuous phase, some part of the surrounding continuous phase is also accelerated. This extra acceleration of the continuous phase has the effect of added inertia or ‘added mass’ or virtual mass force. There may be some additional forces, such as Basset force (due to development of a boundary layer around the dispersed phase particles), thermophoretic force (due to large temperature gradient) and Brownian force. The Basset force denoted by $F_B$ in equation (2.7) is relevant only for unsteady flows and in most cases, its magnitude is much smaller than the interphase drag force. Basset force involves a history integral, which is time-consuming to evaluate. Moreover, Basset force decays as $t^{-n}$ with $n > 2$ (Mei, 1993) for an intermediate time. Therefore, it is very often neglected while integrating the equation of motion of the particle. Picart et al. (1982) discussed specific conditions under which the Basset term may be neglected. For most reactor engineering flows, the other two forces, viz., thermophoretic and Brownian forces, are also quite small compared to some of the terms discussed earlier.

Basically different approaches have been made to simulate a large number of dispersed phase particles, i.e., hard sphere approach, soft sphere approach and Monte Carlo techniques. In a hard sphere approach, particles are assumed to interact through instantaneous binary collisions. This means particle interaction times are much smaller than the free flight time and, therefore, hard particle simulations are event (collision) driven. In a soft sphere approach, particles are allowed to overlap slightly. The contact forces are then calculated from the deformation history of the contact,
using say a linear spring/dashpot model. In Monte Carlo simulations, a new overlap-free particle configuration is generated at each time step. The new configuration is accepted based on the change in the system energy.

The advantage of Eulerian–Lagrangian approach is that the dynamics of the individual bubbles or particles can be assessed; however, in the case of turbulent flows, it is necessary to simulate a very large number of particle trajectories to obtain meaningful averages. Even though this approach gives useful information about particle–particle interaction, it is still difficult to apply this approach for large industrial multiphase reactors. This is due to the fact that for large size reactors, the tracking process of thousands of particles becomes highly memory-intensive and this approach is, therefore, suitable for simulating multiphase flows containing a low (<10%) volume fraction of the dispersed phases (Ranade, 2002). In literature, many papers have been published on the hydrodynamic modeling of multiphase reactors with Eulerian–Lagrangian approach.

Grevet et al. (1982) were among the first researchers to theoretically investigate the bubble rise phenomenon using Eulerian–Lagrangian approach in a bubble plume. The authors obtained a reasonably good agreement with experimental observations. van Swaaij and co-workers (Delnoij et al. 1997a; Delnoij et al. 1997b) used the same approach to simulate bubble trajectories in a bubble column reactor. Using 2D simulation, they obtained good agreement with the experimental observations of Becker et al. (1994). Delnoij et al. (1999) reported a 3D simulation of bubble rise in a rectangular bubble column reactor. They studied the effect of aspect ratio of the bubble column reactor on the flow pattern. As expected, they observed significantly complex flow patterns with 3D simulations. Lain et al. (1999) developed
an Eulerian–Lagrangian approach including the $k$-$\varepsilon$ turbulence model. Their model, however, neglected the effect of phase volume fractions. In a recent effort (Lain et al., 2002) a similar approach was applied for turbulence modeling in a cylindrical bubble column reactor with 14 cm diameter and 65 cm height. Bubble source term was included for hydrodynamic modeling and numerical results were confirmed with the experimental measurements using the phase-Doppler anemometer.

More recently, by ignoring the bubble–bubble interactions, Lapin et al. (2002) reported their Eulerian–Lagrangian simulations for slender bubble columns. They observed that the flow moves downwards near the axis and rises close to the wall in the lower part of the column, but in the upper part, the opposite trend is observed. When one or more dispersed phases are present as solid particles, the implementation of an Eulerian–Lagrangian approach is still straightforward.

Tsuji et al. (1993) developed an alternate Eulerian–Lagrangian method that used the discrete element method (DEM) for the solid phase coupled with the Eulerian equations for the fluid phase and studied 2D fluidisation of particles by a jet of gas at the inlet. Li et al. (1999) performed a series of simulations of gas–liquid–solid flows in fluidised beds using Eulerian–Lagrangian approach. Their study, however, was limited to the consideration of only a single bubble rising in liquid–solid fluidised bed. The predicted bubble rise velocity and bubble size compared very well with experimental data.

More recently, Zhang and Ahmadi (2005) have used similar approach to study the transient characteristics of gas–liquid–solid phase flows in three-phase slurry reactors. In addition to considering the interactions between particle–particle,
bubble–bubble, and particle–bubble, bubble coalescence is also included and the effects of bubble size variation on the flow pattern was also included.

2.4. Volume of Fluid (VOF) Approach

The VOF is one of the simplest and conceptually simple approach. In this approach, the motion of all phases is modeled by formulating local, instantaneous conservation equations for mass, momentum and energy. Such local instantaneous conservation equations can be solved using appropriate jump boundary conditions at the interface. However, the interface between different phases may not remain stationary and imposing boundary conditions at such an interface becomes a very complicated moving boundary problem. To avoid this, instead of directly tracking the deforming and moving interface, the VOF approach tracks the motion of all the phases, from which motion of the interface is inferred indirectly. All the interfacial forces, therefore, have to be replaced by smoothly varying volumetric forces. If the shape and flow processes occurring near the interface are of interest, the VOF approach should be used.

In VOF approach, the tracking of the interface between the phases is accomplished by the solution of a continuity equation for the volume fraction of one (or more) of the phases. For the q\textsuperscript{th} phase, this equation has the following form:
\begin{equation}
\frac{d \varepsilon_q}{dt} + \nabla \cdot \varepsilon_q \mathbf{F} = 0
\end{equation}

A single momentum equation, which is solved throughout the domain and shared by all the phases, is given by
\begin{equation}
\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla P + \nabla \cdot \mathbf{t} + \rho g + \mathbf{F}
\end{equation}
Whenever the shape and flow processes occurring near the interface are of interest, the VOF approach is useful. Some interface related forces, such as surface or adhesion forces can be modeled accurately using this approach (van Wachem et al., 2003). The only drawback of VOF method is the so-called artificial (or numerical) coalescence of gas bubbles which occurs when their mutual distances is less than the size of the computational cell, which also make this approach memory intensive for simulation of dispersed multiphase flows in large equipment (Ranade 2002). The first VOF type approach was suggested by Hirt and Nichols (1981). Although this scheme is still considered one of the simplest and well known methods for volume tracking, it performs badly due to large amount of smearing at the interface. The application of the so-called surface sharpening or reconstruction models, which are present in some commercial CFD codes, can somewhat prevent the smearing of the interface.

Hydrodynamic modeling of multiphase reactors with VOF is so far limited. The motion of single bubble in liquid is relatively well understood and extensive experimental data on shape and terminal velocity are available in the literature (Clift et al., 1978). Using these experimental data, 2D VOF simulations have been carried out for a single bubble rising in a stagnant fluid by many researchers (Krishna and van Baten, 1999; Essemiani et al., 2001; Liu et al., 2005) and few simulations have been carried out in three-dimensions (Olmos et al., 2001; van Sint Annaland et al., 2005). The rise trajectories of bubbles, their size and shape, rise velocity; effect of fluid properties on bubble dynamics and gas holdup were largely discussed. Among these studies, the efficiency of VOF approach was proved for the calculation of air bubble terminal velocities and shapes in stagnant water by Rudman (1997) and Krishna and van Baten (1999). For a precise prediction of ellipsoidal bubble properties, a three-
dimensional system with sufficient small grid scales was considered by Olmos et al. (2001) and small spherical bubbles were simulated using two-dimensional axisymmetric models. Chen et al. (2004) has applied level set formulation of VOF to simulate bubble motion for two and three-phase fluidised bed. More recent studies (Bertola et al., 2004) predict the influence of bubble diameter and gas holdup on the hydrodynamics of bubble column reactor using VOF approach. Even though VOF simulations have shown significant improvements, there are still a lot of problems to be sorted out before implementing VOF simulations for large scale dispersed multiphase flow simulation.

2.5. Overview of ANSYS CFX Package

Since in the present work, the main emphasis is on understanding the complex flow structure of multiphase flow reactors using CFD as a tool, we have not attempted to develop an in-house code. Instead we have used one of the available commercial CFD code for our study in this thesis. There are many general purpose commercial software codes available in the market like, ANSYS CFX, FLUENT, STAR-CD, CHAM etc., Ranade (2002) in his book has devoted a separate chapter discussing in length about the capabilities of these commercial codes. For our investigations we have used ANSYS CFX software package.
The major modules available in ANSYS CFX are shown in Figure 2.1

![Diagram showing the modules of ANSYS CFX Software Package]

**Figure 2.1.** Modules of ANSYS CFX Software Package

### 2.5.1. Pre-Processor

In the preprocessor module the following tasks are carried out:

a) Creation of geometry under investigation (Geometry);

b) Dividing the geometry into smaller non-overlapping control volumes or meshing (Meshing);

c) Defining the material properties, inlet and outlet conditions and specifications of boundary and initial conditions (ANSYS CFX-Pre);

d) Setting up of the governing equations (ANSYS CFX-Pre).
The ANSYS Workbench for CFD Applications module from ANSYS, Inc. offers a viable alternative approach for creating the geometry. The meshing application within the ANSYS Workbench environment provides access to swept, hex-dominant, tetrahedral and prism meshing technologies in a single location that can be applied on a part-by-part basis. ANSYS ICEMCFD meshing tools are available that include mesh editing capabilities as well as structured hexahedral meshing. After users have completed meshing, ANSYS CFX-Pre offers a modern, consistent and intuitive interface for the definition of complex CFD problems. ANSYS CFX-Pre can read one or more meshes from a variety of sources. Once meshes have been loaded, the user also has greater flexibility in assigning meshes to domains. In ANSYS CFX-10 multiple meshes can be put into a single domain, or a single mesh can be split into multiple domains, depending on the demands of the physics of the problem. Users are guided through physics definition by moving along the ‘Define’ toolbar, which presents the key steps in problem set-up. Existing cases may be loaded directly from CFX-5 DEF or RES files, ensuring consistent problem definition no matter how the problem may have been modified.

The creation and modification of physics objects is presented through a user interface with tabbed panels providing easy access to model details. The evolving problem definition is displayed in the object selector, which shows the key objects that can be selected to access any part of the problem definition. Errors or inconsistencies that occur during the problem setup/modification are shown through color coding in the object selector, or via descriptive messages in the Physics Message panel. Double-clicking in any one of the location will automatically open a panel to correct the problem.
Once the problem definition is complete, hitting the ‘Go’ button will write a definition file for the CFX-5 solver.

### 2.5.2. Solver

Solving the governing conservation equations quickly and efficiently is a vital aspect of any CFD code. ANSYS CFX-10 uses a unique solution strategy, based on coupled multigrid solver technology, that surpasses existing CFD methods in speed and robustness. It produces accurate solutions to the linear algebraic equations with fast and reliable convergence.

The salient features of the ANSYS CFX solver are

- Fully automatic and requires no user input.
- Fully scalable achieving linear increase in CPU time with problem size.
- Representative of true physics.
- Easy to set up in both serial and parallel.
- Insensitive to mesh aspect ratio; so it reliably converges even with high refinement of boundary layer.

ANSYS CFX-10 radically improves the performance of the solver by solving the full hydrodynamic system of equations simultaneously across all grid nodes. This technique provides a robust and reliable solver, which requires far fewer iterations to converge. The coupled solver delivers better performance on all types of problems, but is particularly powerful in flows where inter-equation coupling is significant. The second important aspect of the ANSYS CFX-10 solver is its multigrid approach. While the coupled aspect of the solver deals with local effects, the multigrid solver effectively deals with the long distance or 'long wavelength' effects. This approach automatically generates a cascade of successively coarser grids, which allows the
solution information to propagate rapidly across the entire computational domain. The solutions on the coarser meshes are used to accelerate the original fine grid solution. Also, iterations performed on the coarse mesh are proportionally less expensive than finer grid iterations, so it is clear that these accelerations are also economical. The ANSYS CFX-10 solver provides high memory efficiency. One million unstructured tetrahedral mesh element problems can be run in 400 MB RAM. The software intelligently uses the memory available in order to dynamically optimise the balance of resource usage against computational speed. The advanced numeric of ANSYS CFX-10’s default “High-Resolution” discretisation delivers both of these. This adaptive numeric scheme locally adjusts the discretisation to be as close to Second-Order as possible, while ensuring the physical boundedness of the solution.

ANSYS CFX-10 has a large number of physical models like heat transfer, multiphase flow etc., to provide accurate simulation of a wide variety of industrial applications. Accurate simulation is enhanced because almost all the physical models inter operate with each other and in conjunction with all element types, across all grid interfaces, connection types, using the coupled multigrid solver, in parallel, with accurate numerics.

2.5.3. Post-Processor

Post-processing is a key step in the CFD analysis process. The large quantities of data generated by the solver must be clearly presented and help the analyst make valuable engineering decisions about their application. A good post-processing tool should allow the user to not only examine qualitative flow visualisation, but also to extract quantitative numbers for performance comparison and prediction. ANSYS
CFX Post is a powerful graphical and quantitative post-processing tool that allows users to quickly extract useful information from ANSYS CFX-10. Its intuitive user interface makes it easy to use even for the casual user. In the standard interactive mode, ANSYS CFX Post also easily execute post-processing session files in batch mode to quickly reproduce the output for a series of runs.

ANSYS CFX Post provides flexible and accurate quantitative post-processing of ANSYS CFX-10 results. CFX-Post enables the full power of the CFX Expression Language within the post-processor, and extends it with a range of post-processing specific functions such as exact mass flow, area, length and volume-based integrals and averages of any quantity. Expressions can also be used to define new variables for the presentation of user specified quantities.