Chapter 3

Governing Equations and Numerical Methods

3.1 Introduction

The need for full Navier-Stokes simulation of complex fluid flows arises in numerous engineering problems. Over the last two or three decades, Computational Fluid Dynamics (CFD) method has matured in several aspects and has been used widely in the industry. Several different algorithms have been proposed and developed by various researchers. At the present, no single approach or method can be fully considered to be robust for all flow situations and applications from the point of view of numerical and modeling accuracy as well as efficiency.

For turbulent flows, several approaches have evolved based on the level of resolution of the length scales (or the size of the resolved eddies) in the flow. The so-called Direct Numerical Simulation (DNS) methods resolve all the length scales by solving the instantaneous form of the Navier-Stokes equations for turbulent flows. The next level of methods are the Large Eddy Simulation (LES) methods which resolve the large eddies in the flow and use modeling to resolve the sub-grid scales; the grid requirement is not as stringent as the DNS methods but is still prohibitively expensive for practical engineering flows. The most commonly used methods are based on the Reynolds-Averaged Navier-Stokes (RANS) equations which resolve only the mean flow by modeling all turbulent fluctuations using turbulence models of varying complexity.

At the beginning of this chapter, the governing equations of turbulence flow are presented, particularly for natural convection flow. Moreover, for turbulence flow, the turbulence models are necessarily presented to solve additional parameter. Finally, numerical methods of this CFD technique are also presented.

3.2 Governing Equations

The fluid flow field can be described by the conservation of mass, momentum and energy. Given the boundary conditions, the resulting flow and temperature patterns are determined by solving these equations all together. In turbulent flow, the governing equations preferred are the time averaged equations, called Reynolds-averaged Navier-Stokes. For an incompressible fluid, and natural convection flow these are given by:

Continuity equation

$$\frac{\partial}{\partial x_i}\left(\rho\overline{u_i}\right)=0 \tag{2.1}$$

Averaged Navier-Stokes equations

$$\frac{\partial}{\partial x_i}\left(\rho\overline{u_j u_i}\right)=-\frac{\partial\overline{\mathrm{P}}}{\partial x_i}+\frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial\overline{u}_i}{\partial x_j}+\frac{\partial\overline{u}_j}{\partial x_i}\right)-\rho\overline{u_i' u_j'}\right]-\rho g_i\beta\left(\overline{T}-\overline{T}_{ref}\right) \tag{2.2}$$

Energy equation

$$\frac{\partial}{\partial x_i}\left(\rho\overline{u_i T}\right)=\frac{\partial}{\partial x_i}\left[\frac{\mu}{\mathrm{Pr}}\frac{\partial\overline{T}}{\partial x_i}-\rho\overline{u_j' T'}\right] \tag{2.3}$$

Where, $\overline{u}$ is the mean velocity components (u, v, w), $\overline{u_i'}$ is the velocity fluctuation and $\overline{\mathrm{P}}$ is the pressure. Here, x_i is the coordinate axis (x, y, z), ρ is the density, g_i is the gravitational acceleration vector and β is the thermal expansion coefficient. The diffusion term is indicated by viscosity μ. The Boussinesq approximation is employed in the last term of Eq. (2.2), where $T_{ref}=\frac{1}{2}(T_h+T_c)$ is the reference temperature, $\overline{T}$ is the mean temperature, and $\overline{T'}$ is the temperature fluctuation.

The averaging process results in new unknowns, $-\overline{\rho u_i' u_j'}$ and $-\overline{\rho u_i' T'}$, so called Reynolds terms. The first term is called the Reynolds stress (τ_{ij}). The latter can be considered as a diffusion term for the enthalpy. The determination of the Reynolds terms requires extra equations. The correlation of the Reynolds terms to the mean flow field is resolved by turbulence models. Most turbulence models are based on the concept proposed by Boussinesq [15] who assumed that the turbulent stresses are proportional to the mean velocity gradients:

$$\tau_{ij}=-\rho\overline{u_i' u_j'}=\mu_t\frac{\partial u_i}{\partial x_j}\left(\frac{\partial\overline{u}_i}{\partial x_j}+\frac{\partial\overline{u}_i}{\partial x_i}\right)-\frac{2}{3}\delta_{ij}\rho k \tag{2.4}$$

$$-\rho\overline{u_i' T'}=\Gamma_t\frac{\partial\overline{T}}{\partial x_i} \tag{2.5}$$

Where μ_t is the turbulent or eddy viscosity, a property of the flow, Γ_t the turbulent scalar diffusivity (also given as μ_t/σ_H, where σ_H is the turbulent-Prandtl number), δ_{ij} the

Kronecker delta, and k is the turbulent kinetic energy. The second term on the right hand side of equation 2.4, which can be considered as a dynamic pressure, will be ignored because it is small [16].

Different turbulence models are available to determine the unknown variable μ_t [17]. These models vary greatly in their level of complexity and generality. Some are quite simple mathematically but rely heavily on experimental data and, as a consequence, are useful only in flows similar to those upon which they are based. Other turbulence models are more general or more accurate, but involve the repeated, expensive solution of complex equations. The best turbulence model for a given simulation is often a compromise between accuracy, cost, and depends heavily on the degree of accuracy required for the particular simulation [18]. The turbulence models will be discussed in the next section.

3.3 Turbulence models

For most engineering purposes, it is unnecessary to resolve the details of the turbulent fluctuations. To be useful in a general purpose CFD code, the turbulence model must have wide applicability, and be accurate, simple and economical to run. The most common turbulence models are classified in Table 3.1.

Table 3.1 Turbulence models

Classical model (RANS)	Based on Reynolds equations
	1. Zero-equation model - mixing length model.
	2. Two-Equation model the $k-\varepsilon$ model
	3. Reynolds stress model
	4. Algebraic stress model
Large eddy simulation (LES)	Based on space-filtered equations

The classical models use the Reynolds equations developed and form the basis of turbulence calculation in currently available commercial CFD codes. The mixing length and $k-\varepsilon$ models are presently by far the most widely used and validated. Two transport equations, one for the turbulent kinetic energy and the other one for the rate of dissipation of turbulent kinetic energy, are solved. The underlying assumption of both these models is

that the turbulent viscosity is isentropic. In other words, the ratio between the Reynolds stress and mean rate of deformation is the same in all directions.

Large eddy simulations (LES) are turbulence models where the time-dependent flow equations are solved for the mean flow and largest eddies. It was argued earlier that the largest eddies interact strong with the mean flow and contain most of the energy. So this approach results in a good model of the main effects of turbulence. LES are at present at the research stage and the calculations are too costly to merit consideration in general purpose computation. Although anticipated improvement in computer hardware may change this perspective in the future, we will not discuss these models further.

3.3.1 Mixing length model

This approach was first proposed by Prandtl in the 1920s. It is based on the analogy between the mixing by molecular motion and by turbulent eddies. In a broader sense, the concept of the eddy viscosity is also based on this analogy. The mixing-length model by Balwin and Lomax developed for boundary layer flows has been very popular in aerodynamics up to the 1990s [19].

The mixing length formulation is based upon an analogy between the motion of eddies in a turbulent fluid and the motion of molecules in a gas, as explained by the kinetic theory of gases and, in this formulation, turbulent eddies are considered to behave like molecules in some hypothetical gas [20]. The mixing length represents an effective interaction distance between eddies, similar to a mean free path of molecules [21]. In eddy viscosity models, we want an expression for the turbulent viscosity $\mu_t = \rho\nu_t$. The dimension of kinematics turbulent viscosity (ν_t) is m^2/s (same as ν), it can be expressed as product of a turbulent velocity scale ϑ (m/s) and a length scale ℓ (m) [22]. If one velocity scale and one length scale suffice to describe the effects of turbulent, dimensional analysis yields

$$\nu_t = C\vartheta\ell \tag{2.6}$$

where C is a dimensionless constant of proportionality and the dynamic turbulent viscosity is then given by

$$\mu_t = C\rho\vartheta\ell \tag{2.7}$$

Most of the kinetic energy of turbulence is contained in the largest eddies and the turbulence length scale ℓ is therefore characteristic of these eddies which interact with the mean flow. The Reynolds stress is $\tau_{xy} = \tau_{yx} = -\rho\overline{u'v'}$ and the mean velocity gradient is $\partial\bar{u}/\partial y$. The eddies length scale is ℓ.

$$\vartheta = c\ell\left|\frac{\partial\bar{u}}{\partial y}\right| \tag{2.8}$$

Combining (2.6) and (2.8) and absorbing the two constants C and c which appear in these formulae into a new length scale ℓ_m we obtain

$$\nu_t = \ell_m^2\left|\frac{\partial\bar{u}}{\partial y}\right| \tag{2.9}$$

where y is the coordinate normal to the wall, and where ℓ_m is the mixing length, and the model is called Prandtl's mixing length model. The turbulence Reynolds stress is described by

$$\tau_{xy} = \tau_{yx} = -\rho\overline{u'v'} = \rho\ell_m^2\left|\frac{\partial\bar{u}}{\partial y}\right|\frac{\partial\bar{u}}{\partial y} \tag{2.10}$$

Turbulence is a function of the flow and if the turbulence changes it is necessary to account for this within the mixing length model by varying ℓ_m. Some examples are given in Table 3.2. The mixing length model can also be used to predict turbulent transport of scalar quantities [23].

$$-\overline{\rho v'T'} = \Gamma_t\frac{\partial\bar{T}}{\partial y} \tag{2.11}$$

where $\Gamma_t = \mu_t/\sigma_H$ and ν_t is found from (2.9). Rodi [23] recommends value for σ_t of 0.9 in near wall flows, 0.5 for jets and mixing layers and 0.7 for axisymmetric jets.

The mixing length is clearly very useful in flow where the turbulent properties develop in proportion to mean flow length scale, so that ℓ_m can be described as a function of position by means of a simple algebraic formula. An overall assessment of the mixing length model is given in Table 3.3

Table 3.2 Mixing lengths for two-dimensional turbulent flows.

Flow	Mixing length ℓ_m	L
Mixing layer	$0.07L$	Layer width
Jet	$0.09L$	Jet half width
Wake	$0.16L$	Wake half width
Axisymmetric jet	$0.075L$	Jet half width
Boundary layer $(\partial p/\partial x = 0)$		
viscous sub-layer and		
log-law layer $(y/L \le 0.22)$	$\kappa y[1-\exp(-y^+/26)]$	Boundary layer
outer layer $(y/L \ge 0.22)$	$0.09L$	thickness
Pipes and channels (fully developed flow)	$L[0.14-0.08(1-y/L)^2 - 0.06(1-y/L)^4]$	Pipe radius or channel half width

Where y is the distance from the floor and $\kappa = 0.41$ is von Karman's constant
Ref. (Rodi, W.(1980)).

Table 3.3 Mixing length model assessments.

Advantages

- easy to implement and cheap in terms of computing resources
- good predictions for thin shear layers: jets, mixing layers, wakes and boundary layer
- well established

Disadvantages

- completely incapable of describing flows with separation and recirculation
  only calculates mean flow properties and turbulent shear stress

3.3.2 The $k-\varepsilon$ model

Launder and Spalding's two-equation $k-\varepsilon$ model is unarguably the most widely used and validated model employed for turbulent fluid dynamics to date [24]. The model is favored for industrial applications due to its relatively low computational expense and generally better numerical stability than more complex turbulence models [25]. The

predominant drawback of the standard $k-\varepsilon$ turbulence model, for this application area, is that the model was designed for high Reynolds number flows therefore resulting poorly in terms of model accuracy when considering fluid flow over populated Printed Circuit Boards (PCB) which is usually classified as being low Reynolds number flow due to the small velocities and length scales encountered [26].

The high Reynolds number version is obtained by neglecting all the terms containing the kinematics viscosity. In the proximity of solid walls, viscous effects become important and this assumption no longer holds. Several modifications have been proposed: in the two-layer formulation [27], and then the eddy viscosity is patched at a certain distance from the wall. The eddy viscosity (μ_t) is defined from dimensional analysis as:

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \tag{2.5}$$

Where ε is the rate of dissipation of turbulent kinetic energy and C_μ is an empirically determined constant (C_μ = 0.09; Launder and Spalding 1974).

The calculation of the turbulent viscosity requires the derivation of two additional equations to determine k and ε. The standard $k-\varepsilon$ model, therefore, is called a two-equation model. The derivation of these equations can be found in for example Nieuwstadt (1992). The equations for the kinetic energy of turbulence (k) and its dissipation rate (ε) are given by:

k Equation:

$$\rho u_i \frac{\partial k}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_i}\right] + P + G - \rho\varepsilon \tag{2.6}$$

ε Equation:

$$\rho u_i \frac{\partial \varepsilon}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_i}\right] + C_1 \frac{\varepsilon}{k}\left(P + C_3 G\right) - C_2 \rho \frac{\varepsilon^2}{k} \tag{2.7}$$

The model constants are

$$C_\mu = 0.09, C_1 = 1.44, C_2 = 1.92, C_3 = 1.0, \sigma_k = 1.0, \sigma_\varepsilon = 1.217$$

The last term in equation (2.4), $\rho\varepsilon$ is the destruction rate, and P is the shear production and G is the buoyancy production term, which are given by:

$$P = \mu_t \frac{\partial u_i}{\partial x_j}\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_i}{\partial x_i}\right) \tag{2.8}$$

$$G = g_i \beta \frac{\mu_t}{\sigma_t}\left(\frac{\partial \bar{T}}{\partial x_i}\right) \tag{2.9}$$

Due to the no-slip condition at the wall and the resulting damping, close to the wall a laminar flow is found. The standard $k-\varepsilon$ model (Equation 2.6 and 2.7) however is only valid for flow regions where the turbulent transport is dominating. An overall assessment of the $k-\varepsilon$ model is given in Table 3.4

Table 3.4 The $k-\varepsilon$ model assessment.

Advantages

- simplest turbulence model for which only initial and/or boundary conditions need to be supplied
- excellent performance for many industrially relevant flows
- well established; the most widely validated turbulence model

Disadvantages

- more expensive to implement than mixing length model (two extra PDEs)
- poor performance in variety of important cases such as
  - (i) some unconfined flows
  - (ii) flows with large extra strains
  - (iii) rotating flows
  - (iv) fully developed flows in non-circular ducts

3.3.3 Reynolds stress model

The most complex classical turbulence is the Reynolds stress model (RSM), also called the second-order closure model. The modeling strategy originates from work reported in Launder et al (1975). We follow established practice in the literature by calling $R_{ij} = -\tau_{ij}/\rho = \overline{u_i' u_j'}$ the Reynolds stress, although the term kinematics Reynolds stress would be more precise. The exact equation for equation for the transport of R takes the following form:

$$\frac{DR_{ij}}{Dt} = P_{it} + D_{ij} - \varepsilon_{ij} + \Pi_{ij} + \Omega_{ij} \qquad (3.45)$$

Equation 3.45 describes six partial differential equations: one for the transport of each of six independent Reynolds stress ($\overline{u_1'^2}, \overline{u_2'^2}, \overline{u_3'^2}, \overline{u_1'u_2'}, \overline{u_1'u_3'}$ and $\overline{u_2'u_3'}$, since $\overline{u_2'u_1'} = \overline{u_1'u_2'}$, $\overline{u_3'u_1'} = \overline{u_1'u_3'}$ and $\overline{u_3'u_2'} = \overline{u_2'u_3'}$). Two new physical processes appear in the Reynolds stress equations: the pressure-strain correlation term Π_{ij} whose effect on the kinetic energy can be shown to be zero, and the rotation term Ω_{ij} .

$$P_{it} = -\left(R_{im}\frac{\partial U_j}{\partial x_m} + R_{jm}\frac{\partial U_i}{\partial x_m} \right) \qquad (3.46)$$

The diffusion term D_{it} can be modeled by the assumption that the rate of transport of Reynolds stresses by diffusion is proportional to the gradients of Reynolds stresses. Commercial CFD codes often favour the simplest form.

$$D_{it} = \frac{\partial}{\partial x_m}\left(\frac{\nu_t}{\sigma_k}\frac{\partial R_{ij}}{\partial x_m} \right) \qquad (3.47)$$

with $\nu_t = C_\mu \frac{k^2}{\varepsilon}$; $C_\mu = 0.09$ and $\sigma_k = 1.0$.

The dissipation rate is modelled by assuming isotropy of the small dissipative eddies. It is set so that it affects the normal Reynolds stress ($i = j$) only and in equal measure. This can be achieved by

$$\varepsilon_{ij} = \frac{2}{3}\varepsilon\delta_{ij}$$

Where ε is the dissipation rate of turbulent kinetic energy. The Kronecker delta, δ_{ij} is given by $\delta_{ij} = 1$ if $i = j$ and if $i \neq j$.

Corrections are needed to account for the influence of wall proximity on the pressure-strain terms. These corrections are different in nature from the wall-damping functions encountered in the $k-\varepsilon$ model and need to be applied irrespective of the value of the mean flow Reynolds number. Measurements indicate that the wall effect increase the anisotropy of normal Reynolds number by damping out fluctuation in the direction normal to the wall and decreases the magnitude of the Reynolds stresses. The following simpler form is favored by some commercial available CFD codes:

$$\Pi_{ij} = -C_1 \frac{\varepsilon}{k}\left(R_{ij} - \tfrac{2}{3}k\delta_{ij}\right) - C_2\left(P_{ij} - \tfrac{2}{3}P\delta_{ij}\right) \qquad (3.49)$$

with $C_1 = 1.8$ and $C_2 = 0.6$

The rotational term is given by

$$\Omega_{ij} = -2\omega_k\left(R_{jm}e_{ikm} + R_{im}e_{jkm}\right) \qquad (3.50)$$

Here ω_k is the rotational vector and e_{ijk} is the alternating symbol; $e_{ijk} = +1$ if i, j and are different and in cyclic order, $e_{ijk} = -1$ if i, j and k are different and in anti-cyclic order and $e_{ijk} = 0$ if any two indices are the same.

Turbulent kinetic energy k is needed in the above formulae and can be found by adding the three normal stresses together:

$$k = \frac{1}{2}\left(R_{11} + R_{22} + R_{33}\right) = \frac{1}{2}\left(\overline{u_1'^2} + \overline{u_2'^2} + \overline{u_3'^2}\right)$$

The six equations for Reynolds stress transport are solved along with a model equation for the scalar dissipation rate ε.

$$\frac{D\varepsilon}{Dt} = div\left(\frac{\nu_t}{\sigma_\varepsilon} grad\varepsilon\right) + C_{1\varepsilon}\frac{\varepsilon}{k}2\nu_t E_{ij}\cdot E_{ij} - C_{2\varepsilon}\frac{\varepsilon^2}{k} \qquad (3.51)$$

where $C_{1\varepsilon} = 1.44$ and $C_{2\varepsilon} = 1.92$

The usual boundary conditions for elliptic flows are required for the solution of the Reynolds stress transport equations:

- inlet: specified distributions of R_{ij} and ε
- outlet: $\partial R_{ij} / \partial n = 0$ and $\partial\varepsilon / \partial n = 0$
- free stream: $R_{ij} = 0$ and $\varepsilon = 0$
- solid wall: wall functions

In the absence of any information approximate inlet distribution for R_{ij} may be calculated from the turbulence intensity T_i and a characteristic length L of the equipment (e.g. equipment pipe radius) by means of the following assumed relationships:

$$k = \frac{3}{2}\left(U_{ref}T_i\right)^2; \qquad \varepsilon = C_\mu^{3/4}\frac{3}{2}\frac{k}{l}^{3/2}; \qquad l = 0.07L; \qquad \overline{u_1'^2} = k;$$

$$\overline{u_2'^2} = \overline{u_3'^2} = \frac{1}{2}k; \qquad \overline{u_i'u_j'} = 0 (i \neq j)$$

RSMs are clearly quiet complex, but it is generally accepted that they are the 'simplest' type of the model with the potential to describe all the mean flow properties and Reynolds stress without case-by-case adjustment (Table 3.5). The RSM is by no mean as well validated as the $k-\varepsilon$ model. The extension and improvement of theses model is an area of very active research.

Table 3.5 Reynolds stress equation model assessment

Advantages
- potentially the most general of a classical turbulence model
- only initial and/or boundary conditions need to be supplied
- very accurate calculation of mean flow properties and all Reynolds stress for many simple and more complex flows including wall jets, asymmetric channel and non-circular duct flows and cured flows
Disadvantages
- very large computing costs(seven extra PDEs)
- not as widely validated as mixing length and $k-\varepsilon$ models
- performs just as poorly as the $k-\varepsilon$ model in some flows owing to identical problem with equation modeling (e.g. axisymmetric jets and unconfined recirculating flow)

3.3.4 Algebraic stress model

The algebraic stress model (ASM) is an economical way of accounting for the anisotropy of Reynolds stresses without going to the full length of solving the Reynolds stress transport equations. The huge computational cost of solving the RSM is caused by the fact that gradients of the Reynolds stress R_{ij} etc. appear in the convective (D/D_t) and diffusive transport term D_{ij} of 3.47 and 3.49 respectively.

The simplest method is to neglect the convection and diffusion terms altogether. In some cases this appears to be sufficiently accurate (Naot and Rodi, 1982; Demuren and Rodi, 1984). A more generally applicable method is to assume that the sum of the convection and diffusion terms of Reynolds stresses is proportional to the sum of the convection and diffusion terms of turbulent kinetic energy.

$$\frac{D\overline{u_i' u_j'}}{Dt} - D_{ij} = \frac{\overline{u_i' u_j'}}{k} \cdot \left(- \overline{u_i' u_j'} . E_{ij} - \varepsilon \right) \qquad (3.52)$$

The term in the brackets on the right side comprise the sum of the rate of production. The rate of dissipation of turbulent kinetic energy from the exact $k - \varepsilon$ equation and the rate of dissipation of turbulent kinematics energy are both turbulence properties and are closely related, so 3.52 is likely not to be too bad an approximation provided that the ratio $\overline{u_i' u_j'} / k$ does not vary too rapidly across the flow. Further refinements may be obtained by relating the transport by convection and diffusion independently to the transport by convection and diffusion independently to the transport of turbulent kinetic energy.

$$R_{ij} = \overline{u_i' u_j'} = \frac{2}{3} k \delta_{ij} + \left(\frac{C_D}{C_1 - 1 + \frac{P}{\varepsilon}} \right) \left(P_{ij} - \frac{2}{3} P \delta_{ij} \right) \frac{k}{\varepsilon} \qquad (3.53)$$

Reynolds stress appears on both sides of the equation. On the right side they are contained within P_{ij} . Eq. (3.53) is set of six simultaneous algebraic equations for six unknown Reynolds stress R_{ij} that can be solved by matrix inversion or iterative technique if k and ε are unknown. The constant C_D is adjustable to make up for the physics 'lost' in the approximation. One commercial CFD code recommends ASM for swirling flows with the following constant:

$$C_D = 0.55 \qquad \text{and} \qquad C_D = 0.55$$

Demuren and Rodi [28] reported the computation of the secondary flow in non-circular ducts with a somewhat more sophisticated version of this model that includes wall corrections for the pressure-strain term and modified values of adjustable constants to get a good match with measured data in nearly homogenous shear flows and channel flows. They achieved realistic predictions of the primary flow distortions and secondary flow in square and rectangular ducts. These effects are caused by anisotropy of the normal Reynolds stress and can therefore not be represented in simulations of the same situation with the standard $k-\varepsilon$ model.

The algebraic stress model is an economical method of incorporating the effects of anisotropy into the calculations of Reynolds stresses. The model is not as well validated as the $k-\varepsilon$ model but can be used in flows where the latter is known to perform poorly and

where the transport assumptions made do not compromise too severely the calculation accuracy (Table 3.6).

Table 3.6 Algebraic stress model assessment.

Advantages
- cheap method to account for Reynolds stress anisotropy
- combines the generality of approach of the RSM (good modeling of buoyancy and rotation effects possible) with the economy of the $k-\varepsilon$ model
- successfully applied to isothermal and buoyant thin shear layers
- if convection and diffusion term are negligible the ASM performs as well as the RSM
Disadvantages
- only slightly more expensive than model (two PDEs and a system of algebraic equations)
- not as widely validated as mixing length and $k-\varepsilon$ models
- model is severely restricted in flow where the transport assumptions for convective and diffusive effects do not apply-validation is necessary to define the performance limits

3.4 Numerical Methods

An analytic solution of the coupled, non-linear, partial differential equations for a three-dimensional, turbulent flow field is not possible. The use of numerical methods is inevitable and therefore the calculation of a flow problem requires the discretization of that flow field into space and time. Finite volume methods are used to obtain a numerical solution for three-dimensional convection-diffusion problem. In this method the discretized equations represent the flow problem in each control volume. Detail of this method includes the following procedure:

Discretization - Discretization in space requires the flow field to be divided in small control volumes. Types of possible control volumes are hexahedral and tetrahedral. Integration over the control volume in order to balance the conservation equations requires the calculation of the cell face values of the scalar variable ϕ so that the convective and

diffusive fluxes can be determined. This requires an interpolation from the ϕ value at the cell centre to the cell face. Different interpolation schemes are available [29]. The application of a specific scheme for a variable (among others) depends on the grid alignment to the flow field. Higher order schemes present a better accuracy as a first order scheme introduces numerical diffusion when the flow field is oblique to the grid alignment. Higher order schemes however show a less stable solution procedure.

Solver - Solving the equations on a structured grid allows the application of line-iterative methods as the line Gauss-Seidel (LGS) method. The equations for a variable are solved directly along one line of control volumes applying the tri-diagonal matrix algorithm (TDMA) [30]. The calculation proceeds with the next line by applying the latest available boundary values. The solution process can be improved via block correction along a line of control volumes. The added correction satisfies the balance over the control volume block [31]. A further improvement can be obtained by applying a multigrid solver. Corrections are determined from a successively coarser grid which is constructed from a block of control volumes. These corrections are added to the fine grid solution during the iteration process [32]. The Gauss-Seidel solution process is combined with the multigrid technique. An algebraic scheme is then used to determine the coarse level mesh.

An iterative approach is required to obtain the separate but coupled flow field variables from an initial guessed flow field. The solution of the flow field is complicated by the pressure source term in the momentum equation. The pressure field cannot be determined from a separate equation. Patankar [31] describes a procedure in which the pressure field is obtained via the continuity equation, the Semi-Implicit Method for Pressure-Linked Equations (SIMPLE). Given an initial pressure field, the momentum equations are solved. A pressure correction is obtained from the revised continuity equation and the velocity component values are corrected subsequently. After calculation of the coupled flow field variables, as temperature and turbulent quantities, the corrected pressure is taken as the new pressure field and the operation is repeated until a converged solution is obtained as shown in Fig.3.1.

All flow field variables are stored in the cell centre of the control volume. A linear interpolation procedure is applied to obtain the pressure value at the face of the control volume, as is necessary for solving the momentum equation [33]. In this way an oscillatory pressure field is prevented without the application of a staggered grid. This approach is useful when boundary fitted coordinates are used for non-orthogonal boundaries of a flow

problem. For large local gradients of the pressure, as with large buoyant forces, the discretization should be refined. Also a staggered grid approach may be re-introduced for the calculation of the face pressure. To prevent a similar oscillatory solution for the flow field when solving the continuity equation, a momentum-weighted averaging is applied for the velocity that is based on the convection and diffusion effects [34].

When the buoyancy force is of the same order of magnitude as the pressure gradient the convergence is poor because of the relatively small contribution of the convective and viscous terms. This results from the sequential solving process of the SIMPLE-algorithm. A correction term can be incorporated in the revised continuity equation that accounts for the buoyancy force.

Convergence - Because of the non-linearity of the problem the solution process is controlled via relaxation factors. A relaxation factor controls the change of a variable as calculated at each iteration. The convergence is checked by several criteria: the mass and heat conservation should be balanced; the residuals of the discretized conservation equations must steadily decrease; and the change in field values between two iterations should be very small.