CHAPTER 4

GOVERNING EQUATIONS AND NUMERICAL METHODS

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4.1. Introduction

In this chapter, the computational fluid dynamics ”CFD” modeling is well defined. The governing equations of the flow are presented. In addition, the turbulence models and numerical methods are illustrated. The modeling process of the flow is divided into a number of steps which are preprocess, process and post process steps. These steps are illustrated by defining the meshing criteria, different types of meshes used, the recommended types of turbulence models for turbomachinery applications and the recommended values for post process step.

4.2 Governing equations and numerical methods

4.2.1 Equations of motion for fluid flow

The conservation of mass, momentum and energy are considered as the main equations to describe any fluid flow field. The continuity equation for an incompressible Newtonian fluid is derived from the conservation of mass in vector form to be:

$$\nabla.\vec{U} = 0 \tag{4-1}$$

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{4-2}$$

After defining the continuity equation, the conservation of momentum is defined for steady, incompressible flow can be expressed as:

The momentum equation could be described in vector form as:

$$\rho \frac{DU}{Dt} = f - \nabla P + \nabla.T \tag{4-3}$$

Or in tensor form as:

$$\rho \frac{\partial u_i u_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \rho g_i + \mu\left(\frac{\partial^2 u_i}{\partial x_j x_j}\right) \tag{4-4}$$

where $\boldsymbol{\rho}$ is the density of the fluid, $\boldsymbol{p}$ is the pressure, $\boldsymbol{f}$ is the body force (per unit volume) and $\boldsymbol{T}$ is the stress tensor.

4.2.2. Equations of motion in a rotating frame of reference

There are a lot of methods to solve any computational problems such as; Stationary reference frame (SRF), moving reference frame (MRF) dynamic mesh and other methods. The criterion of selecting a specific method of these is that the applicability in the problem, the accuracy and the available computational resources. Using a stationary reference frame is dominated in analyzing uttermost of engineering problems. However, solving equations in a moving reference frame is sometimes advantageous for some applications. On the other hand, using dynamic mesh method is preferable as it would eliminate the interpolation errors introduced in the MRF method but it needs a powerful computational resources and much time which is not often available.

The mathematical modeling of rotating flow can be formulated, as seen by a stationary observer. All equations of motion is modified to incorporate the moving frame. The modification is presented in adding new terms in the equations corresponding to the acceleration terms appeared due to the transformation from the stationary to the moving reference frame. The different zones of the flow and the boundary conditions governing the flow would however, be specified in terms of the rotating frame. This is applicable in applications such as rotating machines which consists of a rotor which rotates in a specific RPM and surrounded by a stationary casing, in which case it is favorable to view the flow from a coordinate system fixed to the rotating parts. This provides flow motion that is predominantly steady relative to the rotating components.

Childs [21] described the velocity vector, U_a, in a stationary frame of reference which is related to the relative velocity vector U, in a rotating reference frame by

$$\boldsymbol{U_a} = \boldsymbol{U} + (\boldsymbol{\Omega} \times \boldsymbol{r}) \tag{4-5}$$

Where Ω is the angular velocity of the system and r is a position vector from the origin of rotation to the point of interest. The components of the relative velocity vector are $u, v, and\ w$.

For an arbitrary vector, X:

$$\left(\frac{\boldsymbol{dX}}{\boldsymbol{dt}}\right)_{\boldsymbol{stationary\ frame}} = \left(\frac{\boldsymbol{dX}}{\boldsymbol{dt}}\right)_{\boldsymbol{rotating\ frame}} + \boldsymbol{\Omega} \times \boldsymbol{X} \tag{4-6}$$

Similarly, for the material derivative

$$\left(\frac{\boldsymbol{DX}}{\boldsymbol{Dt}}\right)_{\boldsymbol{stationary\ frame}} = \left(\frac{\boldsymbol{DX}}{\boldsymbol{Dt}}\right)_{\boldsymbol{rotating\ frame}} + \boldsymbol{\Omega} \times \boldsymbol{X} \tag{4-7}$$

Differentiating the left-hand side of equation (4-5) and using equation (4-6) yields

$$\left(\frac{\boldsymbol{DU_a}}{\boldsymbol{Dt}}\right) = \left(\frac{\boldsymbol{DU}}{\boldsymbol{Dt}}\right) + \boldsymbol{\Omega} \times \boldsymbol{U} \tag{4-8}$$

Substituting from equation (4-5) into equation (4-8) yields to

$$\left(\frac{\boldsymbol{DU_a}}{\boldsymbol{Dt}}\right) = \left(\frac{\boldsymbol{DU}}{\boldsymbol{Dt}}\right) + \boldsymbol{\Omega} \times \frac{\boldsymbol{Dr}}{\boldsymbol{Dt}} + \boldsymbol{\Omega} \times (\boldsymbol{U} + \boldsymbol{\Omega} \times \boldsymbol{r}) \tag{4-9}$$

$$\left(\frac{\boldsymbol{DU_a}}{\boldsymbol{Dt}}\right) = \left(\frac{\boldsymbol{DU}}{\boldsymbol{Dt}}\right) + 2\boldsymbol{\Omega} \times \boldsymbol{U} + \boldsymbol{\Omega} \times (\boldsymbol{\Omega} \times \boldsymbol{r}) \tag{4-10}$$

$$\left(\frac{\boldsymbol{DU_a}}{\boldsymbol{Dt}}\right) = \left(\frac{\boldsymbol{DU}}{\boldsymbol{Dt}}\right) + 2\boldsymbol{\Omega} \times \boldsymbol{U} - \boldsymbol{\Omega}^2 \boldsymbol{r} \tag{4-11}$$

Thus, the momentum equation in a reference frame rotating at constant angular velocity Ω is given by:

$$\boldsymbol{\rho} \left(\frac{\boldsymbol{DU}}{\boldsymbol{Dt}}\right) + 2\boldsymbol{\Omega} \times \boldsymbol{U} - \boldsymbol{\Omega}^2 \boldsymbol{r} = -\boldsymbol{\nabla P} + \boldsymbol{\rho g} + \boldsymbol{\mu \nabla^2 U} \tag{4-12}$$

$$\boldsymbol{\rho} \left(\frac{\boldsymbol{DU}}{\boldsymbol{Dt}}\right) = -\boldsymbol{\nabla P} + \boldsymbol{\rho g} + \boldsymbol{\mu \nabla^2 U} - 2\boldsymbol{\Omega} \times \boldsymbol{U} + \boldsymbol{\Omega}^2 \boldsymbol{r} \tag{4-13}$$

Concerning equations (4-12) and (4-13), two acceleration terms are added which are the Coriolis acceleration term, $2\Omega \times U$, and the centrifugal acceleration, $\Omega^2 r$.

Moreover, the continuity equation in a rotating reference frame is given by equation (4-14) taking a form similar to that for a stationary reference frame.

$$\boldsymbol{\nabla . \vec{U}} = \mathbf{0.0} \tag{4-14}$$

Reynolds-Averaged Navier-Stokes Equations

The common approach to the modeling of turbulence is to assume that the motion is random and adopt a statistical treatment. In this method of averaging two components of the velocity appear due to the decomposition of the instantaneous Navier-Stokes equations. These components are the mean and fluctuating components as follows:

$$\boldsymbol{u_i} = \boldsymbol{\bar{u}_i} + \boldsymbol{u'_i} \tag{4-15}$$

Where $\bar{u}_i$ and u'_i are the mean and fluctuating velocity components (i = 1, 2, 3).

Similarly, for other scalar quantities:

$$\emptyset = \overline{\emptyset} + \emptyset' \tag{4-16}$$

where $\emptyset$ denotes a scalar quantity such as pressure, energy, or species concentration.

Using equation (4-15) and applying Reynolds time-averaging to the incompressible form of the continuity equation yields:

$$\frac{\partial(\overline{u_i + u_i'})}{\partial x_i} = 0 \tag{4-17}$$

Then,

$$\frac{\partial \overline{u_i'}}{\partial x_i} = 0 \tag{4-18}$$

As a result,:

$$\frac{\partial \overline{u_i}}{\partial x_i} = 0 \tag{4-19}$$

The ensemble-averaged momentum equations are resulted from the substitution of the previous expressions for the flow variables into the instantaneous continuity and momentum equations and taking a time (or ensemble) average (and dropping the over bar on the mean velocity,$\bar{u}$). These equations can be written in tensor form as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0 \tag{4-20}$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial u_1}{\partial x_1}\right)\right] + \frac{\partial}{\partial x_j}\left(-\rho\overline{u_i' u_j'}\right) \tag{4-21}$$

The previous equations are called *Reynolds-averaged Navier-Stokes* (RANS) equations. These equations are the same as the instantaneous Navier-Stokes equations form but with the velocities and other solution variables representing ensemble-averaged (or time-averaged) values. The effect of turbulence appeared in the additional terms.

Substituting Reynolds decomposition into momentum equation and take time averaging to obtain the RANs equations:

$$\rho\,\frac{\partial \overline{u_i u_j}}{\partial x_j} = -\frac{\partial \bar{P}}{\partial x_i} + \rho g_i + \mu\left(\frac{\partial^2 \overline{u_i}}{\partial x_j x_j}\right) - \rho\frac{\partial}{\partial x_j}\overline{u_i' u_j'} \tag{4-22}$$

It is noticed that, after the time averaging process, the continuity equation has remained unchanged, but additional terms, comprising products of the fluctuating components, have appeared in Navier–Stokes equations. These terms have arisen from the non-linear convection term and are called the Reynolds or turbulent stresses.

The Reynolds Averaged Navier-Stokes (RANS) equations form a closed set of four-solver equations with ten unknowns, namely, u, v, w, P and six additional terms denoted as Reynolds stresses. It is clear that the number of unknowns is more than the number of equations available and this is called the turbulence closure problem. The main task of turbulence modeling is to develop mathematical models of sufficient accuracy and generality to predict the Reynolds stresses in terms of the mean flow variables. There are several approaches for Reynolds stresses modeling, such as algebraic (zero equation) models, one equation models, two equation models and Reynolds stress models, ordered according to complexity, accuracy and computational cost. Since two-equation models are the most commonly used in practical applications, they would be used to model turbulence in the present study.

4.3 Turbulence model

Turbulence is defined as the three-dimensional unsteady random motion observed in fluids at moderate to high Reynolds numbers. Most of technical flows are based on low viscous fluids which are considered turbulent.

Navier-Stokes equations NSE are the equations which describe the turbulence flows. Albeit, solving these equations fully in time and space is not feasible by Direct Numerical Simulation (DNS) because of computational resources which may exceed the maximum limit. As a result, an averaging procedures are applied to NSE to simplify turbulent terms is the equations.

There are two methods of averaging: Reynolds-averaging (which, for all practical purposes is time-averaging) of the equations and Scale-Resolving Simulation (SRS) models. The most recommended turbulence models for turbomachinery applications are k - ε, k - ω and *Spalart-Allmaras* [22]

The three models have the same forms with transport equations for k and ε. On the other hand, there are differences in these models as follows:

- The method of calculating turbulent viscosity
- The turbulent Prandtl numbers governing the turbulent diffusion of k and
- The generation and destruction terms in the equation

1. Standard k - ε Model

It is a two-equation model in which just two transport equations are solved to determine the turbulent velocity and length scales.
It is commonly used in different applications such as industrial flow and heat transfer simulations due to its robustness, economy, and reasonable accuracy for a wide range of turbulent flows.
It is a semi-empirical model, and the derivation of the model equations relies on phenomenological considerations and empiricism.

Improvements of the model led to the appearance of two new models: the RNG k-model and the realizable k - ε model. The standard k - ε model is a semi-empirical model based on model transport equations for the turbulence kinetic energy (k) and its dissipation rate

(ε). The model transport equation for k is derived from the exact equation, while the model transport equation for ε was obtained using physical reasoning and bears little resemblance to its mathematically exact counterpart. The assumption is that the flow is fully turbulent, and the effects of molecular viscosity are negligible while the derivation of the k - ε model. The standard k - ε model is therefore valid only for **fully turbulent flows.**

Transport Equations for the Standard k - ε Model

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + G_k + G_b - \rho\epsilon - Y_\mu + S_k \quad (4\text{-}23)$$

$$\frac{\partial}{\partial t}(\rho\epsilon) + \frac{\partial}{\partial x_i}(\rho\epsilon u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon}\right)\frac{\partial \epsilon}{\partial x_j}\right] + C_{1\epsilon}\frac{\epsilon}{k}(G_k + C_{3\epsilon}G_b) - C_{2\epsilon}\rho\frac{\epsilon^2}{k} + S_\epsilon \quad (4\text{-}24)$$

Where G_k represents the generation of turbulence kinetic energy due to the mean velocity gradients. G_b is the generation of turbulence kinetic energy due to buoyancy. Y_μ represents the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate. $C_{1\epsilon}$, $C_{2\epsilon}$, and $C_{3\epsilon}$ are constants. σ_k and σ_ϵ are the turbulent Prandtl numbers for k and ε respectively. S_k and S_ϵ are user-defined source terms.

Modeling the Turbulent Viscosity

The turbulent (or eddy) viscosity, μ_t, is computed by combining k and ε as follows:

$$\mu_t = \rho C_\mu \frac{k^2}{\epsilon} \quad (4\text{-}25)$$

Where C_μ is a constant.

Model Constants

The model constants $C_{1\epsilon}$, $C_{2\epsilon}$, C_μ, σ_k, and σ_ϵ have the following default values[22]:

$C_{1\epsilon}$ = 1.44, $C_{2\epsilon}$ = 1.92, C_μ = 0.09, σ_k= 1.0, σ_ϵ = 1.3

These values were determined according to experiments with air and water for fundamental turbulent shear flows including homogeneous shear flows and decaying isotropic grid turbulence. These values are accepted for a wide range of wall bounded and free shear flows.

2. RNG k - ε Model

The RNG model is similar to the standard k - ε model with some modifications. It is based on a statistical technique called renormalization group theory

3. Realizable k - ε Model

The realizable k- ϵ is considered an advanced model which differs from the standard one in two main things:

- It includes a new formulation for the turbulent viscosity.
- The transport equation for the dissipation rate, ε, is derived from an exact equation for the transport of the mean-square vorticity fluctuation.

The term "realizable" refers to that certain mathematical constraints on the Reynolds stresses, consistent with the physics of turbulent flows are satisfied in it.
One more advantage of this model is that the spreading rate of both planar and round jets is accurately predicted. It is well suited for flows involving rotation, boundary layers under strong adverse pressure gradients, separation, and recirculation which is the case in the present work.

The following expression describes the normal Reynolds stress in an incompressible strained mean flow:

$$\overline{u^2} = \frac{2}{3}k - 2\nu_t \frac{\partial U}{\partial x} \tag{4-26}$$

$$\frac{k}{\epsilon}\frac{\partial U}{\partial x} > \frac{1}{3C_\mu} \approx 3.7 \tag{4-27}$$

Both the realizable and RNG k - ε models have shown substantial improvements over the standard k- ϵ model where the flow features include strong streamline curvature, vortices, and rotation. Initial studies have shown that the realizable model provides the best performance of all the k - ε model versions for several validations of separated flows and flows with complex secondary flow features [22].

The realizable k - ε model proposed by Shih et al. [23] was intended to address these deficiencies of traditional k-models by adopting the following:

• A new eddy-viscosity formula involving a variable Cμ originally proposed by Reynolds [24].
• A new model equation for dissipation (ε) based on the dynamic equation of the mean-square vorticity fluctuation.

One limitation of the realizable k-ϵ model is that it produces non-physical turbulent viscosities in situations when the computational domain contains both rotating and stationary fluid zones (e.g., multiple reference frames, rotating sliding meshes). This is due to the fact that the realizable k - ε model includes the effects of mean rotation in the definition of the turbulent viscosity.

Transport Equations for the Realizable *k* - *ε* Model

The modeled transport equations for k and ϵ in the realizable k - ε model are:

$$\frac{\partial}{\partial t}(\rho k)+\frac{\partial}{\partial x_{ij}}(\rho k u_j)=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]+G_k+G_b-\rho\epsilon-Y_\mu+S_k \tag{4-28}$$

and

$$\frac{\partial}{\partial t}(\rho\epsilon)+\frac{\partial}{\partial x_j}(\rho k u_j)=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_\epsilon}\right)\frac{\partial \epsilon}{\partial x_j}\right]+\rho C_1 S_\epsilon-\rho C_2\frac{\epsilon^2}{k+\sqrt{\nu\epsilon}}+C_{1\epsilon}\frac{\epsilon}{k}C_{3\epsilon}G_b+S_G \tag{4-29}$$

Where

$$C_1=\max\left[0.43,\frac{\eta}{\eta+5}\right],\eta=S\frac{k}{\epsilon},S=\sqrt{2S_{ij}S_{ij}}$$

In these equations, G_k represents the generation of turbulence kinetic energy due to the mean velocity gradients. G_b is the generation of turbulence kinetic energy due to buoyancy. Y_μ represents the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate. C_2 and $C_{1\epsilon}$ are constant values. σ_k and σ_ϵ are the turbulent Prandtl numbers for k and ϵ, respectively. S_k and S_ϵ are user-defined source terms[22].

This model has been extensively validated for a wide range of flows, including rotating homogeneous shear flows, free flows including jets and mixing layers, channel and boundary layer flows, and separated flows. For all these cases, the performance of the model has been found to be substantially better than that of the standard k - ε model.
Especially noteworthy is the fact that the realizable k-ϵ model resolves the round-jet anomaly; i.e., it predicts the spreading rate for axisymmetric jets as well as that for planar jets.

Modeling the Turbulent Viscosity

As in other k - ε models, the eddy viscosity is computed from

$$\mu_t = \rho C_\mu \frac{k^2}{\epsilon}$$

The difference between the realizable k-ϵ model and the standard and RNG k - ε models is that C_μ is no longer constant. It is computed from

$$C_\mu = \frac{1}{A_o + A_s\, k \frac{U^*}{\epsilon}}$$

Where

$$U^* = \sqrt{S_{ij}S_{ij} + \tilde{\Omega}_{ij}\tilde{\Omega}_{ij}}$$

And

$$\tilde{\Omega}_{ij} = \Omega_{ij} - 2\epsilon_{ijk}\omega_k$$

$$\Omega_{ij} = \bar{\Omega}_{ij} - \epsilon_{ijk}\omega_k$$

Where $\bar{\Omega}_{ij}$ is the mean rate-of-rotation tensor viewed in a rotating reference frame with the angular velocity ω_k. The model constants A_o and A_s are given by

$$A_o = 4.04, A_s = \sqrt{6}\, cos\phi$$

Where

$$\phi = \frac{1}{3}\cos^{-1}(\sqrt{6}\, W),$$

$$W = \frac{S_{ij}S_{jk}S_{ki}}{\breve{S}^3}, \breve{S} = \sqrt{S_{ij}S_{ij}},$$

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

Model Parameters

The term G_k, representing the production of turbulence kinetic energy, is modeled identically for the standard, RNG, and realizable k-ϵ models. From the exact equation for the transport of k, this term may be defined as

$$G_k = -\rho \overline{u_i' u_j'} \frac{\partial u_j}{\partial x_i}$$

To evaluate G_k in a manner consistent with the Boussinesq hypothesis,

$$G_k = \mu_t S^2$$

where S is the modulus of the mean rate-of-strain tensor, defined as

$$S \equiv \sqrt{2S_{ij}S_{ij}}$$

4.4 CFD modelling procedure

CFD modelling consists of a number of steps which are: pre-processor, solver and postprocessor

1. Pre-processor

Preprocessor means the step of creating the geometry of the problem and creating the mesh i.e. Design Modeler and ANSYS meshing application. This involves the following steps:

- Definition of the geometry, i.e. the computational domain, by creating volumes, surfaces, edges and points.
- Generation of the grid, i.e. sub-division of the computational domain into smaller sub-domains. Meshes can be both triangular and quadrilateral.
- Specification of boundaries and continuum zone types.

2. Solver

Once the mesh is created, the user defines models for solver, energy, viscosity and turbulence. Initial and boundary conditions are specified, as well as properties of the different fluids present in the system.

The scheme for spatial discretization of the convection terms is then selected. The user also selects the desired level of convergence. Before the iteration process can start, it is necessary to initialize the entire flow field, such as ambient pressure, velocity and temperature. The residuals for continuity, momentum equations and turbulence model equations are calculated after each iteration step. In the present study, the convergence criteria is set to 1e-4.

3. Post-processor

Once the solution has converged, the post-processor provides plotting and animation of contours and vectors, tracking of particles in the flow and several other visualization tools. Most CFD packages, such as FLUENT, are equipped with such tools.