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2 Background on Computational Fluid Dynamics

2.1 Introduction

Computational Fluid Dynamics (CFD) is, in part, the art of replacing the governing partial differential equations of fluid flow with numbers, and advancing these numbers in space and/or time to obtain a final numerical description of the complete flow field of interest [**1**].

The governing equations for flows of practical interest are usually so complicated that an exact solution is unavailable and it is necessary to seek a computational solution. Computational techniques replace the governing non-linear partial differential equations with systems of algebraic equations, so that a computer can be used to obtain the solution [**2**].

CFD provides four major advantages compared to experimental fluid dynamics [**2**]:

- Lead-time in design and development is significantly reduced.
- CFD can simulate flow conditions not reproducible in experimental model tests.
- CFD provides more detailed and comprehensive information.
- CFD is more cost-effective than wind tunnel or scale-model testing.

To obtain a well-posed problem, three conditions must be met: the solution must exist, the solution must be unique, and the solution must depend continuously on the initial and boundary conditions [**2**].

The commercial CFD solver STAR-CD is used in this study to solve the Reynolds-Averaged Navier-Stokes equations [**3**]. STAR-CD can handle complex phenomena in the flow field such as chemical reactions, combustion, dispersed multiphase flow, thermal radiation and distributed resistances.

2.2 The Basic Equations

There are three basic non-linear partial differential equations of conservation for physical fluid systems:

- Conservation of mass (Equation of continuity)
- Conservation of momentum (Navier-Stokes equations)
- Conservation of energy

In these equations there are three unknown variables, i.e. velocity, V, thermodynamic pressure, p, and absolute temperature, T. Variables like ρ, h, μ and k can be uniquely determined from the independent variables p and T. Refer to the List of Symbols for the definition of these variables.

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When diffusion and chemical reactions are involved in the flow, there are at least two extra basic equations that must be considered:

- Conservation of species
- Conservation of chemical reaction

The first three equations above are now stated mathematically.

2.2.1 *Equation of Continuity*

$$\frac{D\rho}{Dt} + \rho div\overline{V} = 0 \tag{2-1}$$

2.2.2 *The Navier-Stokes Equations*

$$\begin{aligned}
\rho\frac{Du}{Dt} &= \rho g_x - \frac{\partial p}{\partial x} + \frac{\partial}{\partial x}\left(2\mu\frac{\partial u}{\partial x} + \lambda div\overline{V}\right) + \frac{\partial}{\partial y}\left[\mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)\right] + \frac{\partial}{\partial z}\left[\mu\left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z}\right)\right] \\
\rho\frac{Dv}{Dt} &= \rho g_y - \frac{\partial p}{\partial y} + \frac{\partial}{\partial x}\left[\mu\left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right)\right] + \frac{\partial}{\partial y}\left(2\mu\frac{\partial v}{\partial y} + \lambda div\overline{V}\right) + \frac{\partial}{\partial z}\left[\mu\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right)\right] \\
\rho\frac{Dw}{Dt} &= \rho g_z - \frac{\partial p}{\partial z} + \frac{\partial}{\partial x}\left[\mu\left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z}\right)\right] + \frac{\partial}{\partial y}\left[\mu\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right)\right] + \frac{\partial}{\partial z}\left(2\mu\frac{\partial w}{\partial z} + \lambda div\overline{V}\right)
\end{aligned} \tag{2-2}$$

2.2.3 *The Energy Equation*

$$\rho\frac{D}{Dt}\left(e + \frac{p}{\rho}\right) = \frac{Dp}{Dt} + div\left(k\nabla T\right) + \tau_{ij}\frac{\partial u_i}{\partial x_j} \tag{2-3}$$

2.3 Modelling of Turbulence

As far as we know, the Navier-Stokes equations do apply to turbulent flow [**4**]. Direct numerical simulation is a technique to solve turbulent flow directly with the Navier-Stokes equations. The solution grid used must be infinitesimally small because the smallest eddy size is about 0.04mm. Presently, the computational power does not exist to implement direct numerical simulation for practical applications, because literally millions of mesh points would be needed to solve a small domain of a few cubic centimeters.

To implement turbulence practically, there exist a few empirical modelling ideas for certain mean statistical properties of turbulent shear flows. These can be classified as zero-equation, one-equation, two-equation and Reynolds stress models.

Reynolds averaging of the Navier-Stokes equations leads to extra stress terms called Reynolds stresses. These stresses can be modelled as 'viscous' stresses with an eddy viscosity in the same way as laminar shear stresses, e.g.

$$\tau_t = -\rho\overline{u'v'} = \mu_t\frac{\partial\overline{u}}{\partial y} \tag{2-4}$$

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The eddy viscosity, μ_t, varies with flow conditions and geometry and is not a fluid property although it has the same dimensions as fluid viscosity. In the class of eddy-viscosity turbulence models, the models are constructed to find a description of the eddy viscosity μ_t, i.e. an 'equivalent' viscosity due to turbulence.

2.3.1 Zero-Equation Models

The mixing-length theory of Prandtl proposes that each turbulent fluctuation can be related to a length scale and a velocity gradient. Iteration is required to find the edge of the boundary layer. Different zero-equation models exist, e.g. Cebeci-Smith[**5**], and van Driest[**6**]. Most of these models require a specification of the outer edge of the boundary layer. A model that circumvents this problem is the Baldwin-Lomax[**7**] model.

2.3.2 One-Equation Models

These are usually models that describe the transport of turbulent kinetic energy. The turbulent kinetic energy equation can be described as follows [**4**]:

The rate of chance of turbulent energy =
convective diffusion + production +
work done by turbulent viscous stresses +
turbulent viscous dissipation.

The terms in this relation are so complex that they cannot be computed from first principles, therefore the one-equation model combines features of eddy-viscosity modelling with that of Reynolds stress models.

2.3.3 Two-Equation Models

If a second equation modelling rate of change is coupled with the turbulent energy equation described above, better results are usually obtained because the convection of turbulence is accounted for. The second rate of change can be that of turbulence dissipation, turbulent length scale, or vorticity, but dissipation is more commonly used. From there the k-ε model, where k is the turbulent kinetic energy and ε the turbulence dissipation.

2.3.4 Reynolds Stress Models

Turbulence can also be modelled using Reynolds stresses (like the one shown in Equation (2-4)), with additional partial differential equations describing the stresses. The modelling of Reynolds stresses is more complex than the previous models and is called a second-order closure. The stresses are computed directly and therefore the usage of the eddy viscosity and velocity gradient approaches are discarded.

2.4 Boundary Conditions

Any CFD model is as good as the assumptions it is based on. One can have a sufficiently converged solution, but if the boundary conditions do not resemble reality, the solution is useless. Thus, it is very important to apply the correct boundary conditions. The following are some of the boundary conditions that

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can be applied to a CFD model. As STAR-CD is used in this study, the boundary conditions implemented in STAR-CD are described below.

2.4.1 Prescribed Flow or Inlet

This can be used for an inlet where the fluid properties and mass flux properties are known.

2.4.2 Outlet

The mass flow rate at this exit boundary is fixed from continuity considerations and all the variables' gradients are taken to be zero in the direction of the local flow direction at the exit boundary.

2.4.3 Prescribed Pressure

The static pressure at this boundary is specified and, unlike the outlet boundary condition, the direction and magnitude of the flow must be determined to describe the near-wall region [**4**].

2.4.4 Impermeable Wall and Baffle Surfaces

The no-slip condition next to the wall is applied and 'wall functions' are applied with certain turbulence models.

2.4.5 Symmetry Plane

When the flow domain is symmetrical relative to a plane, great simplifications can be made to the CFD model regarding grid size. At the symmetry plane the normal velocity and the normal gradients of all other variables are zero.

2.5 Computational Grids

A grid is generated in the domain where the fluid flow equations are solved through computational techniques. To obtain good results the grid must meet certain requirements:

- The grid points must be clustered near solid boundaries to provide high resolution of the viscous boundary layer.
- The grid resolution must be the highest in expected areas of high gradients of the flow variables.
- Excessive skewness of the grid must be avoided.

Body-fitted grids are generated in this study using either an algebraic method or a scheme based on elliptical partial differential equations.

2.5.1 Algebraic Grid Generation

Algebraic grid generation is computationally inexpensive and very simple to implement. After the grid points on the boundaries are obtained with stretching functions such as Vinokur[**8**] stretching, the interior grid is obtained by transfinite interpolation. After this, the gridlines can be blended to be orthogonal near the boundary walls. This was done in this study using the SURCH-algorithm in Fletcher[**9**].

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2.5.2 Elliptic Grid Generation

As was the case with algebraic grid generation, the grid points on the boundary can also be obtained using stretching functions. Solving the transformed Poisson equations generates the interior of the grid [**10**]. For 2D grids, the Poisson equations are:

$$\begin{aligned} \alpha x_{\xi\xi} - 2\beta x_{\xi\eta} + \gamma x_{\eta\eta} &= -J^2\left(Px_\xi + Qx_\eta\right) \\ \alpha y_{\xi\xi} - 2\beta y_{\xi\eta} + \gamma y_{\eta\eta} &= -J^2\left(Py_\xi + Qy_\eta\right) \end{aligned} \qquad (2\text{-}5)$$

where (ξ,η) represent the coordinates in the computational domain, and P and Q are terms which control the point spacing in the interior of the domain. α, β and γ are metric coefficients and J is the Jacobian of the transformation.

2.6 Conclusion

CFD is a powerful tool to perform simulations of complex flow phenomena in a very economical manner. Computational techniques make it possible to solve the non-linear partial differential governing equations. CFD has major advantages compared with experimental fluid dynamics. One such advantage is the application of boundary conditions to a CFD model that will be very difficult or even impossible to apply in experimental fluid dynamics. Turbulence can be modelled in CFD using one of several turbulence models that differ in complexity. In this study CFD is used in Chapter 4 for a parametric study of boiler operational conditions and in Chapter 5 for the investigation of remedial measures for boiler tube failures due to particle impingement erosion.