Introduction

1 What is a fluid?

Fluids are easily recognized because they readily adopt the shape of the recipient or vessel that contains them. More exactly, a fluid is a material that has the ability to deform even under zero applied stress. Fluids are made up of atomic particles but this feature can be safely ignored for many practical purposes by studying fluids from a macroscopic point of view, regarding the fluid as a continuum formed by an infinite collection of fluid particles with each particle containing a very large number of fluid atoms or molecules. This is what is usually done in the study of fluid dynamics.

Newtonian fluids are an important group of fluids characterized for a linear constitutive relationship between the stress tensor and the rate of strain in the fluid. Many fluids of engineering importance can be regarded as Newtonian. The focus of CFD here is the study of flows of incompressible Newtonian fluids.

Density ρ and viscosity μ are the most important macroscopic properties determining the deformation behavior of Newtonian fluids. Surface tension may also play a role. Thermo-physical and mass transport properties are important for convective heat and mass transfer. Furthermore, turbulent kinetic energy and dissipation rate are important quantities involved in the analysis of turbulent flows.

2 Conservation Principles

Computational Fluid Dynamics (CFD) is the investigation of the detailed flow behavior of fluids using numerical methods, computational algorithms and powerful computing machines. The equations solved in CFD are mathematical representation of conservation principles which have been observed to be fairly universally satisfied.

The first conservation principle is the statement of conservation of mass also called the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = \frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0$$

where $\mathbf{u} = u_i = (u_1, u_2, u_3)$ is the velocity vector giving the magnitude and direction of the fluid velocity at all points inside the fluid at time t. The u_i's are the components of the velocity vector along the three coordinate directions and the presence of the repeated subscripts in the last term in multiplicative suggestive form imply summation over the coordinate directions, i.e. for a rectangular Cartesian system of coordinates $(x_1, x_2, x_3) = (x, y, z)$ with $(u_1, u_2, u_3) = (u, v, w)$

$$\frac{\partial(\rho u_i)}{\partial x_i} = \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z}$$

A fluid with constant density is called incompressible. In this case, the continuity equation reduces to

$$\nabla \cdot \mathbf{u} = \frac{\partial u_i}{\partial x_i} = 0$$

and in rectangular Cartesian coordinates

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

The second conservation principle is the principle of conservation of momentum. For any fluid, this is given as

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial p}{\partial x_i} + \rho g_i$$

in so called "conservative" form. A useful but non-conservative form of the momentum conservation equation is given by

$$\rho\frac{\partial u_i}{\partial t} + \rho(\mathbf{u} \cdot \nabla)u_i = \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial p}{\partial x_i} + \rho g_i$$

where τ_{ij} are the components of the viscous stress tensor.

In a Newtonian fluid the viscous stress tensor components are linearly related to the components of the strain rate tensor $D_{ij} = \mu(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i})$ as follows

$$\tau_{ij} = \mu D_{ij} - \frac{2}{3}\mu\delta_{ij}\nabla \cdot \mathbf{u} = \mu(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}) - \frac{2}{3}\mu\delta_{ij}\nabla \cdot \mathbf{u}$$

Moreover p is the pressure (an important quantity to be determined by computation), $\mathbf{g} = g_i$ is the gravitational acceleration vector and δ_{ij} is the Kronecker symbol ($= 1$ if $i = j$, zero otherwise).

Since momentum is a vectorial quantity, the momentum conservation equation is a vector equation. In a rectangular Cartesian system of coordinates, for any fluid, the components are:

$$\rho\frac{\partial u}{\partial t} + \rho u\frac{\partial u}{\partial x} + \rho v\frac{\partial u}{\partial y} + \rho w\frac{\partial u}{\partial z} = \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} - \frac{\partial p}{\partial x} + \rho g_x$$

$$\rho\frac{\partial v}{\partial t}+\rho u\frac{\partial v}{\partial x}+\rho v\frac{\partial v}{\partial y}+\rho w\frac{\partial v}{\partial z}=\frac{\partial \tau_{yx}}{\partial x}+\frac{\partial \tau_{yy}}{\partial y}+\frac{\partial \tau_{yz}}{\partial z}-\frac{\partial p}{\partial y}+\rho g_y$$

and

$$\rho\frac{\partial w}{\partial t}+\rho u\frac{\partial w}{\partial x}+\rho v\frac{\partial w}{\partial y}+\rho w\frac{\partial w}{\partial z}=\frac{\partial \tau_{zx}}{\partial x}+\frac{\partial \tau_{zy}}{\partial y}+\frac{\partial \tau_{zz}}{\partial z}-\frac{\partial p}{\partial z}+\rho g_z$$

For incompressible fluids the components of the viscous stress tensor in Cartesian coordinates are given by

$$\tau_{xx}=2\mu\frac{\partial u}{\partial x}\qquad \tau_{yy}=2\mu\frac{\partial v}{\partial y}\qquad \tau_{zz}=2\mu\frac{\partial w}{\partial z}$$

$$\tau_{xy}=\tau_{yx}=\mu(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x})$$

$$\tau_{yz}=\tau_{zy}=\mu(\frac{\partial v}{\partial z}+\frac{\partial w}{\partial y})$$

$$\tau_{zx}=\tau_{xz}=\mu(\frac{\partial w}{\partial x}+\frac{\partial u}{\partial z})$$

Introducing the above into the momentum conservation equations yields the equations of motion of a Newtonian fluid of constant density and viscosity, namely

$$\rho\frac{\partial u}{\partial t}+\rho u\frac{\partial u}{\partial x}+\rho v\frac{\partial u}{\partial y}+\rho w\frac{\partial u}{\partial z}=\mu(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2})-\frac{\partial p}{\partial x}+\rho g_x$$

$$\rho\frac{\partial v}{\partial t}+\rho u\frac{\partial v}{\partial x}+\rho v\frac{\partial v}{\partial y}+\rho w\frac{\partial v}{\partial z}=\mu(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}+\frac{\partial^2 v}{\partial z^2})-\frac{\partial p}{\partial y}+\rho g_y$$

$$\rho\frac{\partial w}{\partial t}+\rho u\frac{\partial w}{\partial x}+\rho v\frac{\partial w}{\partial y}+\rho w\frac{\partial w}{\partial z}=\mu(\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial y^2}+\frac{\partial^2 w}{\partial z^2})-\frac{\partial p}{\partial z}+\rho g_z$$

Using vector notation, the above equations simplify to

$$\rho\frac{\partial u_i}{\partial t}+\rho(\mathbf{u}\cdot\nabla)u_i=\mu\nabla^2 u_i-\nabla p+\rho\mathbf{g}$$

In the above equations, the first term on the left hand side represents the time rate of change of momentum along a particular coordinate direction $(x, yorz)$ at a fixed point in the fluid. The next three terms on the left hand side are rate of change of momentum in the fluid, in the same coordinate direction, due to the three vector components of the fluid motion (i.e the rate of change of momentum induced by the convective motion of the fluid). The four terms on the left hand side represent the inertial effect of fluid motion. The first three terms on the right hand side are the time rate change of momentum in the fluid associated with the internal viscous forces in the fluid. The fourth term on the right hand side is the rate of change of momentum due to spatial pressure variations in the fluid and the last term is the rate of change of momentum due to the action of gravity. Note that the units of all terms in the equations are momentum per unit time per unit volume, which are equivalent to force per unit volume. Therefore the equations can be regarded as representing the conservation of the components of momentum or the balance of force components at all points in the fluid.

Additional conservation equations must be invoked when in addition to fluid flow, transport of energy, mass or turbulent kinetic energy are involved. The generic conservation principle for a transported scalar quantity ϕ is

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial(\rho u_j \phi)}{\partial x_j} = \frac{\partial}{\partial x_j}(\Gamma \frac{\partial \phi}{\partial x_j}) + q_\phi$$

in conservative form, or

$$\rho\frac{\partial \phi}{\partial t} + \rho u_j \frac{\partial \phi}{\partial x_j} = \frac{\partial}{\partial x_j}(\Gamma \frac{\partial \phi}{\partial x_j}) + q_\phi$$

in non-conservative form, where Γ and q_ϕ are, respectively, the (molecular) diffusivity and the internal rate of generation (source) or consumption (sink) of ϕ in the fluid. This important equation is called the generalized convection-diffusion equation because of the presence of the convective term on the left hand side and the diffusive term on the right hand side.

Note that the mass conservation and momentum conservation equations above are particular cases of the generic conservation equation above. Specifically, the mass conservation equation is obtained by making $\phi = 1$ and $\Gamma = q_\phi = 0$, and the momentum conservation equation is obtained by making $\phi = u_i$, $\Gamma = \mu$ and $q_\phi = -\frac{\partial p}{\partial x_i} + \rho g_i$.

Moreover, the generic conservation equation becomes the convective-diffusive heat transfer equation governing the transport of thermal energy in the flow when $\phi = H$, the enthalpy of the fluid and $\Gamma = k$, its thermal conductivity. And it becomes the convective-diffusive mass transfer equation governing the transport of a dissolved substance in the fluid when $\phi = C$, the concentration of dissolved substance in the fluid and $\Gamma = \rho D$, where D is the mass diffusivity of the dissolved substance.

3 Reduced Models

From the above, various useful simplifications of the momentum conservation equation can be obtained that are appropriate for the analysis of important special cases.

If the flow of an incompressible Newtonian fluid does not change with time (steady flow), the momentum equation becomes

$$\rho(\mathbf{u} \cdot \nabla) u_i = \mu \nabla^2 u_i - \nabla p + \rho \mathbf{g}$$

For situations where the effect of viscosity can be neglected (inviscid flows or Euler flows), the momentum equation is

$$\rho \frac{\partial u_i}{\partial t} + \rho(\mathbf{u} \cdot \nabla) u_i = -\nabla p + \rho \mathbf{g}$$

and if the flow does not change with time (steady inviscid flow) this reduces to

$$\rho(\mathbf{u} \cdot \nabla) u_i = -\nabla p + \rho \mathbf{g}$$

If for an inviscid steady flow the velocity field is irrotational (i.e. $\nabla \times \mathbf{u} = 0$), the velocity is given by the gradient of a potential Φ, i.e. $\mathbf{u} = -\nabla \Phi$ and the flow can be simply modeled by the potential equation

$$\nabla^2 \Phi = 0$$

such flows are called potential flows.

If viscosity is important but inertia effects are negligible (creeping flows), the momentum equation becomes

$$\rho \frac{\partial u_i}{\partial t} = \nabla \cdot (\mu \nabla u_i) - \nabla p + \rho \mathbf{g}$$

For steady state creeping flows with constant viscosity and when the effect of gravity is negligible, the momentum equation reduces to (lubrication flows)

$$\mu \nabla^2 u_i = \nabla p$$

When the flow is mainly unidirectional and the flow geometry changes gradually, one obtains the boundary layer approximation. In non-isothermal flows, if the density is not constant but changes little with temperature, one can regard density as constant in all terms of the momentum equation except the gravitational term. This is called the Boussinesq approximation.

The various reduced models are important in their own right and are the focus of intensive study. In CFD one generally aims to develop the ability to solve three-dimensional problems involving of the flow of incompressible Newtonian fluids.

4 Initial and Boundary Conditions

Specific problems in CFD involve the solution of the momentum conservation equations subject to the constraint imposed by the principle of mass conservation (equation of continuity)as well as the associated initial and boundary conditions prevailing in any particular problem.

An initial condition is the specification of the value of the velocity components in the entire fluid domain at time $t = 0$, i.e.

$$\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0$$

Boundary conditions constitute statements about the particular values acquired by the velocity components, their derivatives or combinations of these at the bounding surfaces of the fluid. Commonly used boundary conditions are the no-slip condition at fluid-solid interfaces, i.e.

$$\mathbf{u} = \mathbf{u}_{wall}$$

and the no-shear condition at liquid-gas interfaces

$$D_{ij} t_i n_j = 0$$

where $t_i = \mathbf{t}$ and $n_j = \mathbf{n}$ are, respectively, the tangent and normal vectors to the interface.

Finally, at fluid-fluid interfaces where the effects of shear and surface tension cannot be neglected, both tangential and normal forces must be in equilibrium at the interface, e.g. for Newtonian incompressible fluids labelled ' and "

$$\mu' D'_{ij} t_i n_j = \mu" D_{ij}" t_i n_j$$

and

$$p" - \mu" D_{ij}" n_i n_j = p' - \mu' D'_{ij} n_i n_j + \gamma(\frac{1}{R_1} + \frac{1}{R_2})$$

where γ is the surface tension and R_1, R_2 are the principal radii of curvature of the interface.

Two important additional types of boundary conditions are associated with fluid domains containing inlets and outlets. At an inlet, one usually assigns (known) values to the velocity vector, i.e.

$$\mathbf{u} = \mathbf{u}_{inlet}$$

At an outlet, a reference value of pressure (usually zero) is specified, i.e.

$$p = 0$$

5 Obtaining Solutions ot Flow Problems

Exact solutions of the equations governing the flow of incompressible Newtonian fluids exist only for a very small number of special, simplified situations. Therefore the calculation of approximate, numerical solutions is necessary, hence CFD.

There are several methods of computing approximate solutions. The ones most commonly used include, finite differences, finite volumes and finite elements. Alternative approaches include various types of particle methods, lattice Boltzmann methods, and cellular automata among others.