2 Modelling

In CFD the equations for continuity, momentum, energy and species are solved. These coupled partial nonlinear differential equations are in general not easy to solve numerically and analytical solutions are available for only very few limited cases. The reader is expected to have a basic knowledge of transport phenomena but, since all CFD is based on these few equations, they are given here in tensor notation so that the reader can become familiar with this notation.

A general balance formulation in tensor notation for a scalar, vector or tensor ϕ can be formulated as

$$\frac{\partial \phi}{\partial t} + U_i \frac{\partial \phi}{\partial x_i} = D \frac{\partial^2 \phi}{\partial x_i \partial x_i} + S(\phi), \tag{2.1}$$

where the terms have the following meanings:

$$\left\{ \begin{array}{l} \text{rate of} \\ \text{accumulation} \end{array} \right\} + \left\{ \begin{array}{l} \text{transport by} \\ \text{convection} \end{array} \right\} = \left\{ \begin{array}{l} \text{transport by} \\ \text{diffusion} \end{array} \right\} + \left\{ \begin{array}{l} \text{source} \\ \text{terms} \end{array} \right\}$$

This notation will be used throughout the book and the reader must be familiar with this notation. In this convention there is an understood summation that is written explicitly below (see the appendix for further information):

$$\frac{\partial \phi}{\partial t} + \sum_i U_i \frac{\partial \phi}{\partial x_i} = \sum_i D \frac{\partial^2 \phi}{\partial x_i^2} + S(\phi)$$

In 3D Cartesian coordinates i can take the values 1, 2 and 3, and for a scalar ϕ the equation above becomes

$$\frac{\partial \phi}{\partial t} + U_1 \frac{\partial \phi}{\partial x_1} + U_2 \frac{\partial \phi}{\partial x_2} + U_3 \frac{\partial \phi}{\partial x_3} = D \left(\frac{\partial^2 \phi}{\partial x_1^2} + \frac{\partial^2 \phi}{\partial x_2^2} + \frac{\partial^2 \phi}{\partial x_3^2} \right) + S(\phi). \tag{2.2}$$

Note that since ϕ is a scalar there is only one equation describing how ϕ is distributed in the three dimensions x_1, x_2 and x_3. The easiest way to understand the notation is to identify whether the dependent variable is a scalar, vector or tensor. When ϕ is a scalar, e.g. temperature, T, only one equation is possible, since there is only one temperature at a given position. When ϕ is a vector, e.g. $\phi = [U_1 U_2 U_3]^{\mathrm{T}}$, there will be one equation for each of the three velocities. Equation (2.21) below is a tensor notation of the three momentum equations written in Eq. (2.20). For a tensor τ_{ij} there will be nine equations in three dimensions, cf. Eq. (2.7) below.

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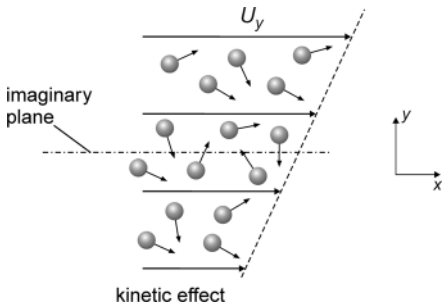

Figure 2.1 The effect of random movement of molecules on momentum transfer.

Accumulation, convection, diffusion and a source term will appear in many equations, and by identifying these terms it will be easier to refer to the various parts in the equations. The accumulation is recognized from the time derivative, the convection term from the velocity term and the first-order derivative, and the diffusion term from the second-order derivative and the transport coefficient, e.g. diffusivity, conductivity, or viscosity. The source term is a function solely of the local variables.

2.1 Mass, heat and momentum balances

All modelling is easier when the underlying physics can be understood and momentum balances are the basis of all fluid dynamics. Transport of mass, heat and momentum occurs by convection of the mean flow and by random movement of molecules or in turbulent flow by random movement of fluid elements. Viscous transport of momentum is due to the random movement of molecules carrying their average momentum in all directions as shown in Figure 2.1.

2.1.1 Viscosity, diffusion and heat conduction

There are many similarities among viscosity, diffusion and heat conduction in fluids. The mechanism for transport in all these cases is random movement of molecules or fluid elements. According to the kinetic theory of gases a molecule moves randomly in all directions, giving a mean velocity of $\overline{u} = \sqrt{8RT/(\pi M_v)}$. This molecule will move a distance corresponding to the mean free path $\lambda = k_B T/(\sqrt{2\pi d^2 P})$ before it collides with another molecule and transfers momentum and heat to that molecule. For oxygen at room temperature and atmospheric pressure, $\overline{u} = 444$ m s^{-1} and $\lambda = 71.4$ nm. For an ideal gas the kinetic viscosity, the diffusivity and the heat diffusivity are all of the same order, $\nu \approx D \approx D_H \approx \frac{1}{3}u\lambda$. Heat conduction is related to heat diffusivity by the amount of energy that each molecule carries, $k = \rho c_p D_H$. From this simple model one can also observe that, for gases, the viscosity depends on the temperature, pressure, relative molecular mass, M_v, and size of the molecule, d. The Schmidt number $Sc = \nu/D$

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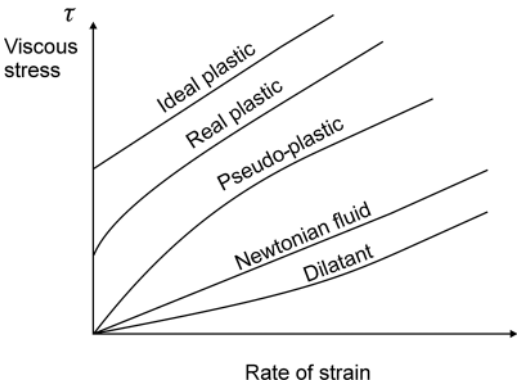

Figure 2.2 The viscous stress for Newtonian and non-Newtonian fluids.

and the Prandtl number $Pr = \rho c_p \nu / k$ describe the ratio between viscosity and diffusivity and that between viscosity and heat conduction, respectively. Both Sc and Pr are of the order of 0.7 for air.

In liquids, the transport is somewhat different. The molecules are in close contact with neighbouring molecules and the movement of the molecules can be modelled as movement with viscous drag. Momentum and heat are transported much faster than mass, because the momentum and heat can be transferred to other molecules by collisions, while diffusion is limited to the movement of the single molecules. This difference can be seen by noting that $Sc \approx 1000$ while $Pr \approx 7$ for transport in water.

The mechanism for momentum, mass and heat transport is similar in turbulent flow. Here the random movement of turbulent eddies will transfer fluid elements containing momentum, species and energy. The turbulent viscosity is of the order of the turbulent velocity times the average distance travelled by a turbulent eddy. Since all transport is by the turbulent eddies, the turbulent Sc and Pr numbers are all of the order of unity, both for gases and for liquids. The kinetic theory of gases is also the governing idea in some of the models for viscosity in multiphase flow, e.g. the kinetic theory for granular flow (KTGF).

Newton's law of viscosity

The viscous stress as a function of velocity gradients can vary significantly for different fluids depending on how the molecules arrange themselves when exposed to strain, as shown in Figure 2.2.

The simplest fluid is the Newtonian fluid, and fortunately many of the common fluids are very close to Newtonian, e.g. gases, water and other simple liquids. In Newtonian fluids the viscous stress is a linear function of the rate of strain. In Figure 2.3 a simple laminar flow with velocity U_1 flows in only one dimension x_1. The resistance of the flow that is observed in a pressure drop is due to the fact that the momentum in the velocity direction x_1 is transported in the x_2 direction due to viscous forces.

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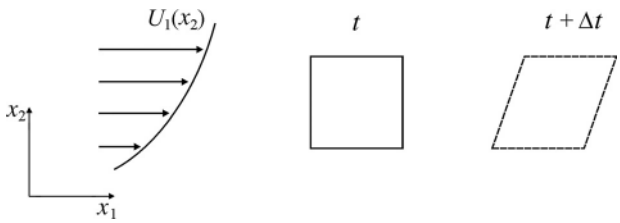

Figure 2.3 The distortion of a fluid element due to strain rate dU_1/dx_2.

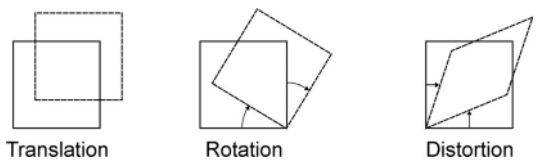

Figure 2.4 Translation, rotation and distortion of a fluid element.

For a Newtonian fluid the linear dependence between stress and the velocity gradient is expressed as

$$\tau_{21} = \mu \frac{\mathrm{d}U_1}{\mathrm{d}x_2}. \tag{2.3}$$

Here the first index of τ_{21} denotes the direction of transport and the second the direction of the momentum. Note that the stress tensor is written with a positive sign. There is a tradition in chemical engineering of viewing the stress tensor as the transport of momentum and consequently defining it with a negative sign since the direction of momentum transport is opposite to the direction of the gradient analogous to heat and mass transfer.

The velocity gradient in itself does not cause the stresses, but rather the stresses arise due to the distortion of the fluid element. A pure translation or rotation of the element will not give rise to viscous stress (Figure 2.4).

In a 2D case, the viscous stress will depend on distortion of the fluid element and the viscous stress becomes a linear function of the strain rate

$$\tau_{12} = \tau_{21} = \mu \left(\frac{\partial U_1}{\partial x_2} + \frac{\partial U_2}{\partial x_1} \right). \tag{2.4}$$

The expression is symmetric in the two dimensions and the two stresses must be equal, $\tau_{12} = \tau_{21}$.

The normal stresses are also affected by the compression of the fluid elements,

$$\tau_{11} = 2\mu \frac{\partial U_1}{\partial x_1} - \left(\tfrac{2}{3}\mu - \kappa\right) \left(\frac{\partial U_1}{\partial x_1} + \frac{\partial U_2}{\partial x_2} \right) \tag{2.5}$$

and

$$\tau_{22} = 2\mu \frac{\partial U_2}{\partial x_2} - \left(\tfrac{2}{3}\mu - \kappa\right) \left(\frac{\partial U_1}{\partial x_1} + \frac{\partial U_2}{\partial x_2} \right). \tag{2.6}$$

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In 3D the nine possible stresses become

$$\tau_{ij} = \tau_{ji} = \mu \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \left(\tfrac{2}{3}\mu - \kappa \right) \delta_{ij} \left(\frac{\partial U_k}{\partial x_k} \right), \tag{2.7}$$

where δ_{ij} is the Kronecker delta

$$\delta_{ij} = (\mathbf{I})_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases}$$

Sometimes the pressure is added to the normal stresses and the stress tensor is written

$$\sigma_{ij} = \mu \left(\frac{\partial U_1}{\partial x_1} + \frac{\partial U_2}{\partial x_2} \right) - \left(\tfrac{2}{3}\mu - \kappa \right) \delta_{ij} \left(\frac{\partial U_k}{\partial x_k} \right) - \delta_{ij} P. \tag{2.8}$$

The dilatational viscosity κ is important only for shock waves and sound waves. From the kinetic theory of gases it has also been shown that κ is zero for monatomic gases at low pressure. In this book we will mostly describe non-compressible fluids, for which the term $\partial U_k / \partial x_k$ on the right-hand side is zero and the viscous stress for a Newtonian fluid is described by

$$\tau_{ij} = \tau_{ji} = \mu \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right). \tag{2.9}$$

2.2 The equation of continuity

A material balance over a stationary fluid element $\Delta x_1 \Delta x_2 \Delta x_3$ is written

$$\{\text{accumulation}\} = \{\text{transport in}\} - \{\text{transport out}\},$$

$$\begin{aligned} \Delta x_1\, \Delta x_2\, \Delta x_3 \frac{\partial \rho}{dt} = {} & \Delta x_2\, \Delta x_3 \left[(\rho U_1)|_{x_1} - (\rho U_1)|_{x_1 + \Delta x_1} \right] \\ & + \Delta x_1\, \Delta x_3 \left[(\rho U_2)|_{x_2} - (\rho U_2)|_{x_2 + \Delta x_2} \right] \\ & + \Delta x_1\, \Delta x_2 \left[(\rho U_3)|_{x_3} - (\rho U_3)|_{x_3 + \Delta x_3} \right]. \end{aligned} \tag{2.10}$$

See Figure 2.5. This formulation corresponds to the finite-volume formulation of the continuity equation for a hexahedral mesh aligned with the coordinate axis. Dividing by $\Delta x_1\ \Delta x_2\ \Delta x_3$ and taking the limit $\Delta x \to 0$ gives the continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho U_1}{\partial x_1} + \frac{\partial \rho U_2}{\partial x_2} + \frac{\partial \rho U_3}{\partial x_3} = 0 \qquad \text{or} \qquad \frac{\partial \rho}{\partial t} = -(\nabla \cdot \rho \mathbf{U}). \tag{2.11}$$

Tensor notation is mostly applied to equations in the book and the equation above is written

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho U_j}{\partial x_j} = 0. \tag{2.12}$$

In 3D the index j is 1, 2 and 3, giving Eq. (2.11).

The continuity equation is difficult to solve numerically. In CFD programs, the continuity equation is often combined with the momentum equations (see below) to form

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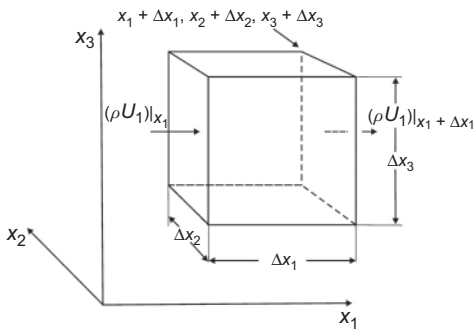

Figure 2.5 A material balance over a fluid element.

a Poisson equation for pressure. For constant density and viscosity the new equation will be

$$\frac{\partial}{\partial x_i}\left(\frac{\partial P}{\partial x_i}\right) = -\frac{\partial}{\partial x_i}\left[\frac{\partial\left(\rho U_i U_j\right)}{\partial x_j}\right]. \tag{2.13}$$

This equation has more suitable numerical properties and can be solved by proper iteration methods. The Navier–Stokes equations are used for simulation of velocity and pressure. The Poisson formulation introduces pressure as a dependent variable, and the momentum equations can be formulated to solve for velocity. The Poisson equation and other methods to solve the continuity are discussed in Chapter 3.

In many cases it is more convenient to describe the change in flow of a fluid element that moves with the flow. On performing the derivation in Eq. (2.12) we obtain

$$\frac{\partial \rho}{\partial t} + U_1\frac{\partial \rho}{\partial x_1} + U_2\frac{\partial \rho}{\partial x_2} + U_3\frac{\partial \rho}{\partial x_3} = -\rho\left(\frac{\partial U_1}{\partial x_1} + \frac{\partial U_2}{\partial x_2} + \frac{\partial U_3}{\partial x_3}\right). \tag{2.14}$$

The left-hand side is the substantial derivative of density, i.e. the time derivative for a fluid element that follows the fluid motion. The equation can be abbreviated as

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} = -\rho\frac{\partial U_i}{\partial x_i} \tag{2.15}$$

and the substantial operator defined as

$$\frac{\mathrm{D}}{\mathrm{D}t} \equiv \frac{\partial}{\partial t} + U_1\frac{\partial}{\partial x_1} + U_2\frac{\partial}{\partial x_2} + U_3\frac{\partial}{\partial x_3}. \tag{2.16}$$

Incompressible flow is defined by having constant density along the streamline, i.e. the left-hand side of Eq. (2.15) is zero and

$$\frac{\partial U_i}{\partial x_i} = 0. \tag{2.17}$$

The assumption of incompressible flow will simplify the modelling substantially, and we will use it throughout the book. Truly incompressible flow does not exist, but the assumption of incompressible flow is valid for most engineering applications. A local change in pressure will spread with the speed of sound, and, when modelling phenomena

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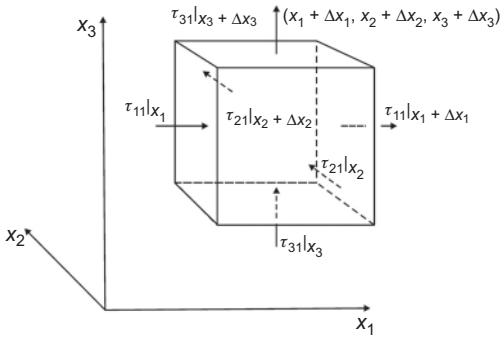

Figure 2.6 Momentum balance over a fluid element.

much slower than the speed of sound, we can safely assume that the new pressure is reached in each time step, i.e. compressible flows can be characterized by the value of the Mach number $M = U/c$. Here, c is the speed of sound in the gas $c = \sqrt{\gamma RT}$, where γ is the ratio of specific heats c_p/c_v. At Mach numbers much less than 1.0 ($M < 0.1$), compressibility effects are negligible and the variation of the gas density due to pressure waves can safely be ignored in the flow modelling. The density change due to pressure drops and temperature variations will automatically be compensated for by the state equation that describes how the density is related to pressure and temperature.

2.3 The equation of motion

The momentum balance for the U_1 momentum over the volume $\Delta x_1 \Delta x_2 \Delta x_3$ is given by

$$\left\{\begin{array}{l}\text{rate of}\\ \text{momentum}\\ \text{accumulation}\end{array}\right\} = \left\{\begin{array}{l}\text{rate of}\\ \text{momentum}\\ \text{in}\end{array}\right\} - \left\{\begin{array}{l}\text{rate of}\\ \text{momentum}\\ \text{out}\end{array}\right\} + \left\{\begin{array}{l}\text{sum of forces}\\ \text{acting on}\\ \text{the system}\end{array}\right\}. \tag{2.18}$$

Newton's law requires that the change in momentum in each direction should be balanced by the forces acting in that direction. The arrows in Figure 2.6 describe the direction of viscous transport of U_i momentum. A balance for the momentum of the velocity component in the x_1 direction, i.e. U_1, is written

$$\begin{aligned}\Delta x_1\,\Delta x_2\,\Delta x_3 \frac{\partial \rho U_1}{\partial x_1} = {} & \Delta x_2\,\Delta x_3 \left[(\rho U_1 U_1)|_{x_1} - (\rho U_1 U_1)|_{x_1+\Delta x_1}\right] - \tau_{11}|_{x_1} + \tau_{11}|_{x_1+\Delta x_1} \\ & + \Delta x_1\,\Delta x_3 \left[(\rho U_2 U_1)|_{x_2} - (\rho U_2 U_1)|_{x_2+\Delta x_2}\right] - \tau_{21}|_{x_2} + \tau_{21}|_{x_2+\Delta x_2} \\ & + \Delta x_1\,\Delta x_2 \left[(\rho U_3 U_1)|_{x_3} - (\rho U_3 U_1)|_{x_3+\Delta x_3}\right] - \tau_{31}|_{x_3} + \tau_{31}|_{x_3+\Delta x_3} \\ & + \Delta x_2\,\Delta x_3 \left[(P)|_{x_1} - (P)|_{x_1+\Delta x_1}\right] + \Delta x_1\,\Delta x_2\,\Delta x_3\,\rho g_1. \end{aligned} \tag{2.19}$$

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From our definition of τ it is $-\tau$ that denotes the momentum that is transported into the fluid element at x. Equation (2.19) corresponds to a finite-volume formulation of the momentum equations for a hexahedral mesh aligned with the coordinate axis. Dividing by $\Delta x_1\ \Delta x_2\ \Delta x_3$ and taking the limit $\Delta x \to 0$ gives for all three components the Navier–Stokes equations

$$\begin{aligned}
\frac{\partial U_1}{\partial t} + U_1\frac{\partial U_1}{\partial x_1} + U_2\frac{\partial U_1}{\partial x_2} + U_3\frac{\partial U_1}{\partial x_3} &= -\frac{1}{\rho}\frac{\partial P}{\partial x_1} + \frac{1}{\rho}\frac{\partial \tau_{11}}{\partial x_1} + \frac{1}{\rho}\frac{\partial \tau_{21}}{\partial x_2} + \frac{1}{\rho}\frac{\partial \tau_{31}}{\partial x_3} + g_1,\\
\frac{\partial U_2}{\partial t} + U_1\frac{\partial U_2}{\partial x_1} + U_2\frac{\partial U_2}{\partial x_2} + U_3\frac{\partial U_2}{\partial x_3} &= -\frac{1}{\rho}\frac{\partial P}{\partial x_2} + \frac{1}{\rho}\frac{\partial \tau_{12}}{\partial x_1} + \frac{1}{\rho}\frac{\partial \tau_{22}}{\partial x_2} + \frac{1}{\rho}\frac{\partial \tau_{32}}{\partial x_3} + g_2,\\
\frac{\partial U_3}{\partial t} + U_1\frac{\partial U_3}{\partial x_1} + U_2\frac{\partial U_3}{\partial x_2} + U_3\frac{\partial U_3}{\partial x_3} &= -\frac{1}{\rho}\frac{\partial P}{\partial x_3} + \frac{1}{\rho}\frac{\partial \tau_{13}}{\partial x_1} + \frac{1}{\rho}\frac{\partial \tau_{23}}{\partial x_2} + \frac{1}{\rho}\frac{\partial \tau_{33}}{\partial x_3} + g_3.
\end{aligned} \tag{2.20}$$

These three equations can be rewritten as

$$\frac{\partial U_i}{\partial t} + \sum_j U_j\frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \sum_j \frac{1}{\rho}\frac{\partial \tau_{ji}}{\partial x_j} + g_i.$$

Note that there is no summation over i, since i represents the three equations. In tensor notation these three equations are written

$$\frac{\partial U_i}{\partial t} + U_j\frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \frac{1}{\rho}\frac{\partial \tau_{ji}}{\partial x_j} + g_i, \tag{2.21}$$

which for a Newtonian fluid becomes

$$\frac{\partial U_i}{\partial t} + U_j\frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \nu\frac{\partial}{\partial x_j}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) + g_i. \tag{2.22}$$

Equation (2.22) can be written in different forms since

$$\nu\frac{\partial}{\partial x_j}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) = \nu\frac{\partial^2 U_i}{\partial x_j \partial x_j}$$

in incompressible flow with constant ρ and ν. In addition to gravity, there are additional external sources that may affect the acceleration of the fluid, e.g. electrical and magnetic fields. When reading Eq. (2.21) note that j should be summed over all dimensions, i.e. $j = 1$, 2 and 3, and i appears in all terms and for three dimensions, constituting the three equations as in Eq. (2.20).

Strictly it is the momentum equations that form the Navier–Stokes equations, but sometimes the continuity and the momentum equations together are called the Navier–Stokes equations. The Navier–Stokes equations are limited to macroscopic conditions. In reality the molecules move some distance before they collide, and the kinetic energy and consequently the velocity of the individual molecules are Boltzmann distributed. These effects must be accounted for at low pressures and in very small volumes. The Knudsen number relates the mean free path, λ, to the system dimension, $Kn = \lambda/L$. The average distance between collisions, i.e. the mean free path, in air at 1 atm and room temperature is ~80 nm, and a correction of the Navier–Stokes equations and the

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boundary conditions is required for Knudsen numbers larger than ~0.02. Simulation of microfluids at dimensions below 5 μm at atmospheric pressure will require special boundary conditions [1].

2.4 Energy transport

Energy is present in many forms in flow, e.g. as kinetic energy due to the mass and velocity of the fluid, as thermal energy and as chemically bounded energy. We can then define the enthalpy as

$$\begin{aligned} h &= h_m + h_T + h_C + \Phi && \text{total energy,} \\ h_m &= \tfrac{1}{2}\rho U_i U_i && \text{kinetic energy,} \\ h_T &= \sum_n m_n \int_{T_{\text{ref}}}^{T} c_{p,n}\,\mathrm{d}T && \text{thermal energy,} \\ h_C &= \sum_n m_n h_n && \text{chemical energy,} \\ \Phi &= \rho g_i x_i && \text{potential energy,} \end{aligned}$$

where m_n is the mass fraction, $c_{p,n}$ the heat capacity and h_n the standard state enthalpy (heat of formation) for species n. The potential energy is often included in the kinetic energy.

The balance equation for total energy is

$$\frac{\partial h}{\partial t} = -\frac{\partial}{\partial x_j}\left[hU_j - k_{\text{eff}}\frac{\partial T}{\partial x_i} + \sum_n m_n h_n j_n - \tau_{kj}U_k\right] + S_h. \tag{2.23}$$

Here j_n is the diffusional flux of species n,

$$j_n = -D_n \frac{\partial C_n}{\partial x_j}.$$

The couplings between the energy equations and the momentum equations are weak for incompressible flows, and the equations for kinetic, thermal and chemical energies can be written separately.

2.4.1 The balance for kinetic energy

An equation for the kinetic energy including the potential energy can be deduced from the momentum equation by multiplying by velocity U_i:

$$U_i\frac{\partial U_i}{\partial t} + U_i U_j \frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho}U_i\frac{\partial P}{\partial x_i} + \frac{U_i}{\rho}\frac{\partial \tau_{ij}}{\partial x_j} + U_i g_i. \tag{2.24}$$

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By using

$$U_i \frac{\partial U_i}{\partial x_i} = \frac{1}{2} \frac{\partial U_i^2}{\partial x_i}$$

and defining $e \equiv \frac{1}{2}(U_1^2 + U_2^2 + U_3^2)$ [J kg^{-1} fluid] we obtain

$$\frac{\partial e}{\partial t} + U_j \frac{\partial e}{\partial x_j} = -\frac{1}{\rho} U_i \frac{\partial P}{\partial x_i} + \frac{1}{\rho} U_i \frac{\partial \tau_{ij}}{\partial x_j} + U_i g_i. \tag{2.25}$$

Note that this is a scalar equation and the expanded equation is obtained by summation over i and j. On multiplying by the density of the fluid and defining $h_m = \rho e$ [J m^{-3} fluid] and using the relations

$$\frac{\partial (P U_i)}{\partial x_i} = U_i \frac{\partial P}{\partial x_i} + P \frac{\partial U_i}{\partial x_i} \qquad \text{and} \qquad \frac{\partial (\tau_{ij} U_i)}{\partial x_i} = U_i \frac{\partial \tau_{ij}}{\partial x_i} + \tau_{ij} \frac{\partial U_i}{\partial x_i}$$

we obtain

$$\frac{\partial (h_m)}{\partial t} = -U_j \frac{\partial (h_m)}{\partial x_j} + P \frac{\partial U_i}{\partial x_i} - \frac{\partial (P U_i)}{\partial x_i} + \frac{\partial (\tau_{ij} U_i)}{\partial x_i} - \tau_{ij} \frac{\partial U_i}{\partial x_i} + \rho g U_i. \tag{2.26}$$

The accumulation and convection terms (the first two terms on the right-hand side) are straightforward and need no further comments. The work done by the gravity force (the sixth term on the right-hand side) is the change in potential energy due to gravity. Reversible conversion to heat (the third term on the right-hand side) stems from the thermodynamic cooling when a gas expands or heating when it is compressed. The work done by viscous forces (the fourth term on the right-hand side) is the accumulation of strain in some fluids, e.g. a rubber band. The irreversible conversion of kinetic energy into heat (the fifth term on the right-hand side) is, for Newtonian fluids,

$$\varepsilon = -\frac{1}{\rho} \tau_{ij} \frac{\partial U_i}{\partial x_j} = \frac{1}{2} \nu \left[\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \frac{\partial U_i}{\partial x_i} \right]^2. \tag{2.27}$$

Owing to the fact that this is a squared term, the viscous dissipation term is always positive for Newtonian fluids. Heat is actually random movement of molecules or atoms, i.e. translational, rotational and vibrational movement. The difference between kinetic energy and heat is that kinetic energy has an average direction of movement whereas heat is random movement. With this perspective the dissipation term can be seen as viscous transport of fast molecules into areas with low average velocity and of slow molecules into areas with high average velocity. The molecules will collide with other molecules, transferring their average momentum, but will very soon lose their directional average and the movement is defined as heat.

The dissipation term is usually small and only with a very high velocity gradient will it be possible to measure the temperature increase due to viscous dissipation. In a stirred-tank reactor the power input by the impeller is of the order of 1 kW m^{-3}, which corresponds to a temperature increase of about 1 K h^{-1}. However, in turbulent flow this

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term becomes very important since it describes the decay of turbulence when the energy in the turbulent eddies is transferred into heat.

2.4.2 The balance for thermal energy

A balance for heat can be formulated generally by simply adding the source terms from the kinetic-energy balance and from chemical reactions:

$$\frac{\partial(\rho c_p T)}{\partial t} = -U_j \frac{\partial(\rho c_p T)}{\partial x_j} + k_{\text{eff}} \frac{\partial^2 T}{\partial x_j \, \partial x_j} - P \frac{\partial U_j}{\partial x_j} + \tau_{kj} \frac{\partial U_k}{\partial x_j} + \sum_m R_m(C, T)(-\Delta H_m) + S_T, \tag{2.28}$$

where the terms on the right-hand side are for accumulation, convection, conduction, expansion, dissipation and the reaction source.

Here the terms in the equation for transformation between thermal and kinetic energy, i.e. expansion and dissipation, occur as source terms. The relation to change in chemical energy is seen in the term for heat formation due to chemical reactions. Examples of the source term S_T are absorption and emission of radiation.

2.5 The balance for species

The balance for transport and reaction for species in constant-density fluids is described by

$$\frac{\partial C_n}{\partial t} + U_j \frac{\partial C_n}{\partial x_j} = \frac{\partial}{\partial x_j} \left(D_n \frac{\partial C_n}{\partial x_j} \right) + R(C, T) + S_n. \tag{2.29}$$

In most CFD programs, the concentration is replaced with the mass fraction

$$y_n = \frac{M_{v,n} C_n}{\rho}. \tag{2.30}$$

Transport and reaction will be discussed further in Chapter 5.

2.6 Boundary conditions

The 3D Navier–Stokes equations contain four dependent variables, U_1, U_2, U_3 and P. Depending on the conditions of the flow, we can define the boundary conditions in many different ways. The boundary conditions are just as important as the differential equations that determine the system, and the results of the simulations depend on the inlet and outlet conditions and the conditions at the walls as well as on the differential equations. We may also introduce boundary conditions due to simplifications of the computational domain, e.g. symmetry.

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2.6.1 Inlet and outlet boundaries

The inlet velocity can be defined in terms of velocities or mass flow rate. In most CFD programs it is possible to enter the inlet condition as an average flow perpendicular to the surface or as a velocity-component distribution over the inlet surface. The way we define boundaries may affect the results, e.g. defining the inlet by an average velocity or by a parabolic laminar flow distribution will give the flow different momentum distributions and the total energy added by the inlet flow will be different in these two cases. An alternative to defining inlet velocities is the pressure inlet boundary condition that can be used when the inlet pressure is known without knowledge of the flow rate. The pressure inlet boundary condition is also useful when it is unknown whether the flow enters or exits at this position.

The standard outlet boundary condition is the zero-diffusion flux condition applied at outflow cells, which means that the conditions of the outflow plane are extrapolated from within the domain and have no impact on the upstream flow, i.e.

$$\phi|_{L-} = \phi|_{L+} \,. \tag{2.31}$$

The pressure outlet boundary condition is often the default condition used to define the static pressure at flow outlets. The use of a pressure outlet boundary condition instead of an outflow condition often results in a better rate of convergence when backflow occurs during iteration. Pressure outflow is also useful when there are several outflows. Specified outflow boundary conditions are used to model flow exits where the details of the inlet flow velocity and pressure are not known prior to solution of the flow problem. They are appropriate where the exit flow is close to a fully developed condition, since the standard outflow boundary condition assumes a normal gradient of zero for all flow variables except pressure.

Scalars, e.g. temperature and species, are usually defined as temperature and mass fractions in the inlet flow. Standard outlet conditions are usually the default.

2.6.2 Wall boundaries

The usual boundary condition for velocity at the walls is the 'no-slip condition', i.e. the relative velocity between the wall and the fluid is set to zero. For high-Reynolds-number turbulent flow the no-slip condition is still valid but the grid resolution is usually too coarse to specify the no-slip condition. In this case the velocity and shear close to the wall are modelled using a wall function. (See Chapter 4 for further details.) The no-slip condition may be inappropriate for non-Newtonian and multiphase flow and at large Knudsen numbers ($Kn > 0.02$), i.e. for low pressure or small dimensions.

For heat transfer, walls can be considered insulated or heat may be transferred through the walls. For heat there are several choices for boundary conditions, e.g. fixed heat flux, fixed temperature, convective heat transfer, radiation heat transfer or a combination of these boundary conditions. Heat transfer by radiation occurs mainly between solid surfaces, and the CFD program must be able also to calculate view angles in order to obtain accurate radiation boundary conditions.

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The boundary conditions for species are usually termed 'no penetration', but diffusion to and reaction at the walls can occur. Evaporation and condensation are also possible wall boundary conditions.

2.6.3 Symmetry and axis boundary conditions

The time taken for simulations can be reduced significantly by using the geometrical symmetry of the problem. Mirror symmetry can halve or even further reduce the calculation region, and rotational symmetry, by defining a rotation axis, reduces a problem from 3D to 2D, which can decrease the time taken for simulation by several orders of magnitude. Symmetric initial and boundary conditions do not guarantee that the solution is symmetric, e.g. buoyancy-driven flows have a tendency to have several possible solutions depending on the initial conditions, and enforced symmetry conditions can produce erroneous results. Two-dimensional simulations may give very misleading results, e.g. the bubbles appearing in a simulation of a fluidized bed are cylinders in 2D and toroids in rotational symmetry. It should also be recognized that no net transport is allowed across a symmetry plane.

Periodic boundaries are convenient for DNS and LES simulations of turbulent flows since time-resolved inlet conditions are required. In periodic boundaries the inlet is set to the outlet. In this way the time-resolved solution will transfer the outlet solution to the inlet. However, to avoid having the boundary condition affect the simulation results, the residence time in the simulation domain should be long compared with the lifetime of the turbulent eddies. Periodic boundaries are also useful for rotating systems when only a fraction of the tangential direction is resolved, e.g. in simulation of turbines.

2.6.4 Initial conditions

Since the Navier–Stokes equations are nonlinear it is necessary to have an initial guess from which the solver can start the iterations. The better the initial conditions, the faster the final solution will convergence. It is also possible that the specified problem has multiple solutions and that the solution will converge to different solutions depending on the initial guess. It is always recommended that different initial conditions should be tested to evaluate convergence and to determine whether there are multiple stationary solutions. When multiple solutions are possible, the simulations must be transient, starting from correct initial conditions.

If a time-dependent solution is required, the actual initial conditions must be specified. Initial conditions for all variables that are to be solved must be specified. For example, in turbulence modelling the initial conditions for the variables describing the turbulence, e.g. the turbulence kinetic energy and the rate of dissipation, must also be set.

Owing to the numerical properties in transient simulations, it is in some cases more efficient to solve a steady-state case by transient simulations. In this case, we are not interested in accurate simulation of the transient behaviour, but only in obtaining a reliable steady-state solution. Exact initial conditions are not necessary, and it is possible to use larger time steps to obtain faster convergence.

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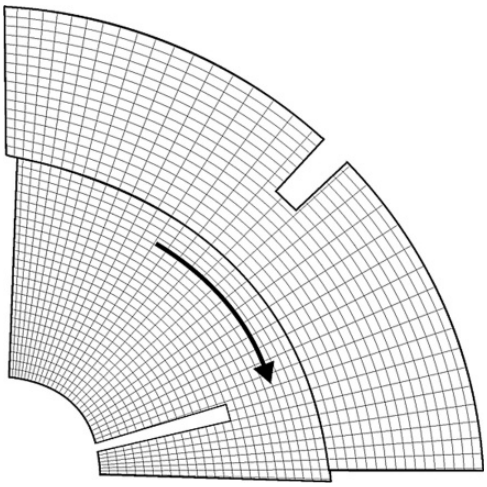

Figure 2.7 A mesh with a rotating and a stationary part.

2.6.5 Domain settings

There are occasions when we are interested only in relative velocities, e.g. flow through rotor blades in a compressor or flow in a centrifuge. We can then define the flow relative to the moving surfaces, and the CFD program will add volume forces due to acceleration, e.g. the centrifugal force.

It is also possible to have rotational parts together with stationary parts, e.g. in a stirred-tank reactor the impeller is rotating and the walls and baffles are stationary. We can then define a cylindrical volume around the impeller that is moving with the impeller and define the rest of the tank as stationary as shown in Figure 2.7.

In this model we do not have to specify the fluid velocities at the moving walls. Standard wall boundary conditions, e.g. no-slip conditions, are sufficient. By choosing the boundary between the moving and stationary parts at a point where the change in flow in the tangential direction is small, it is possible to obtain very good time-resolved flow simulations. The inner volume is stepped in time and the flow is distributed to the connecting cells in the outer volume. In some CFD programs it is also possible to use the average flow to obtain a steady-state solution. By proper choice of a rotating or sliding mesh it is even possible to obtain good average properties of a stirred-tank reactor.

2.7 Physical properties

Most physical properties of fluids, e.g. viscosity, density, diffusion, heat conductivity and surface tension, will vary locally due to variations in temperature, pressure and composition of the fluid. Algebraic equations describing these properties must be specified in the CFD program.

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2.7.1 The equation of state

The relations among density, temperature, pressure and composition are described by the equation of state. For gases at low pressure the ideal-gas law can be used for compressible flows:

$$\rho = \frac{P}{RT \sum_n y_n / M_{w,n}}. \tag{2.32}$$

The ideal-gas law is also an option for incompressible flow if the pressure variation is moderate. The model will then correctly express the relationship between density and temperature required for e.g. natural convection problems.

For non-ideal gases many choices can be found in the literature, the most common of which are the law of corresponding states and the cubic equations of state. The law of corresponding states is defined as

$$Z = \frac{PV}{RT}, \tag{2.33}$$

where Z is a function of the reduced temperature and pressure. The cubic equations are in the form

$$P = \frac{RT}{V - b} - \frac{a}{V^2 + ubV + wb^2}, \tag{2.34}$$

where a, b, u and w are parameters. Depending on the parameters, they form van der Waals, Redlich–Kwong, Soave and Peng–Robinson equations of state.

For liquids the pressure dependence can often be neglected and a simple polynomial can describe the temperature dependence:

$$\rho = A + BT + CT^2 + DT^3 + \cdots. \tag{2.35}$$

2.7.2 Viscosity

At low pressure the viscosity increases slowly with temperature but there is only a small pressure dependence. The Chapman–Enskog theory provides an expression for the gas viscosity:

$$\mu_{\text{gas}} = \frac{5}{16} \frac{\sqrt{\pi m k_{\text{B}} T}}{\pi \sigma^2 \Omega T^*}. \tag{2.36}$$

A more compressed form is Sutherland's law,

$$\mu = \frac{C_1 T^{3/2}}{T + C_2}, \tag{2.37}$$

where C_1 and C_2 are constants. For a multi-component system the total viscosity depends in a nonlinear fashion on the individual viscosities μ_i and mole fractions X_i:

$$\mu = \sum_i \frac{X_i \mu_i}{\sum_j X_i \phi_{ij}}, \tag{2.38}$$

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where

$$\phi_{ij} = \left[1 + \left(\frac{\mu_i}{\mu_j}\right)^{1/2} \left(\frac{M_{w,j}}{M_{w,i}}\right)^{1/4}\right]^2 \Bigg/ \left[8\left(1 + \frac{M_{w,i}}{M_{w,j}}\right)\right]^{1/2}. \tag{2.39}$$

The viscosity increases with temperature for gases, whereas the viscosity decreases exponentially with temperature for liquids. The temperature dependence for liquid viscosity is often written as

$$\mu_{\text{liq}} = a\mathrm{e}^{b/T}. \tag{2.40}$$

For non-Newtonian fluids there are several models available. In this book we will cover only Newtonian fluids, but the interested reader can find additional theories in standard textbooks [2]. The standard models for turbulent flows assume Newtonian fluids, and empirical models are required for modelling turbulent viscosity.

Questions

(1) Why are diffusivity, kinematic viscosity and thermal diffusion similar in gases at low pressure?
(2) What is the molecular mechanism for viscous transport of momentum in gases?
(3) Why is it necessary to rewrite the continuity equation in CFD software?
(4) Why can a gas be treated as incompressible when there is a pressure drop?
(5) Why does viscous dissipation of kinetic energy form heat?
(6) What are standard outlet conditions?
(7) What is a no-slip condition at the wall and when can it be used?
(8) What is a periodic boundary condition?
(9) What are symmetry and axis boundary conditions?
(10) What is an equation of state?

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