1 Introduction

The purpose of this chapter is to explain the input needed to solve CFD problems, e.g. CAD geometry, computational mesh, material properties, boundary conditions etc. The difficulty and accuracy of CFD simulations for various applications, such as laminar and turbulent flows, single-phase and multiphase flows and reactive systems are discussed briefly.

1.1 Modelling in engineering

Traditional modelling in engineering is heavily based on empirical or semi-empirical models. These models often work very well for well-known unit operations, but are not reliable for new process conditions. The development of new equipment and processes is dependent on the experience of experts, and scaling up from laboratory to full scale is very time-consuming and difficult. New design equations and new parameters in existing models must be determined when changing the equipment or the process conditions outside the validated experimental database. A new trend is that engineers are increasingly using computational fluid dynamics (CFD) to analyse flow and performance in the design of new equipment and processes. CFD allows a detailed analysis of the flow combined with mass and heat transfer. Modern CFD tools can also simulate transport of chemical species, chemical reactions, combustion, evaporation, condensation and crystallization.

1.2 CFD simulations

Simple, single-phase laminar flow can be simulated very accurately, and for most single-phase turbulent flows the simulations are reliable. However, many systems in engineering are very complex, and simulations of multiphase systems and systems including very fast reactions are at present not very accurate. For these systems, the traditional models using well-proven design equations that have been verified over many years are more accurate than the best CFD simulations. However, design equations are available only for existing equipment and for a limited range of process conditions, and CFD simulations can be very useful even when no accurate predictions are possible, e.g. by calibrating the model to get a solution that is verified experimentally. From this simulation we can

Table 1.1 Potential CFD simulations in engineering

Flow	Mass transfer	Heat transfer
Laminar	Convection	Convection
Turbulent	Diffusion	Conduction
Single-phase	Reaction	Radiation
Multiphase	Phase transfer	

do parameter studies by implementing small changes in the parameters, e.g. to assess what will result from changes in temperature, flow, viscosity etc.

One advantage using CFD is that it is possible to obtain detailed local information on the simulated system. In a fluidized bed it is possible to simulate not only the conversion but also the local temperature, the entrainment of particles, the backmixing and bubble formation. This detailed information will help by building a qualitative understanding of the process, and a parameter study can reveal additional information such as the bottle necks and the operational limits of the equipment.

CFD simulation without proper knowledge can be a very uncertain tool. The commercial CFD programs have many default settings and will almost always give results from the simulations, but, to obtain reliable results, the model must be chosen with a logical methodology. A converged solution displays the results of the specific chosen model with the given mesh; however, it does not reveal the truth. Without proper understanding of the CFD program and the modelling theory behind it, CFD can become limited to 'colourful fluid display'.

1.3 Applications in engineering

Virtual prototyping is now the standard method to develop new products in e.g. the automotive industry. This very effective method is now being introduced into other fields of engineering. Within chemical engineering we find applications in most fields, e.g. reactor modelling, separations and heat transfer. Unfortunately, we seldom have single-phase laminar flow that can easily be simulated. Chemical reactors are almost always turbulent and often multiphase. Mixing of the reactants and removal of the heat produced are the main objectives for typical reactors such as stirred-tank reactors, bubble columns, trickle beds and fluidized beds. Almost all separations are multiphase, e.g. distillations, extractions, filtering and crystallization. Most heat-transfer equipment involves single-phase flow, yet boiling and condensation are also commonly used. Modern CFD programs can simulate a very wide range of systems and Table 1.1 lists possible simulations in CFD.

1.4 Flow

It is useful to separate the properties of fluids and flows. The properties of fluids, e.g. viscosity, density, surface tension, diffusivity and heat conduction, are intrinsic properties

that can be described as functions of temperature, pressure and composition. Properties that depend on the flow include pressure, turbulence and turbulent viscosity.

From a CFD modelling point of view it is useful to separate possible flows into the following categories:

laminar–turbulent
steady–transient
single-phase–multiphase

1.4.1 Laminar flow

In laminar flow the Navier–Stokes equations describe the momentum transport of flow that is dominated by viscous forces. It is possible with CFD to obtain very accurate flow simulations for single-phase systems, provided that the flow is always laminar. The transitions between laminar and turbulent flow, both from turbulent to laminar and from laminar to turbulent, are difficult to simulate accurately. In this region the flow can fluctuate between laminar and turbulent and turbulent slugs can frequently appear in laminar flow far below the critical Reynolds number for transition to turbulent flow.

Simulation of heat transfer is also often very accurate and a good prediction of temperature can easily be obtained. Mass transfer in the gas phase is also quite straightforward. However, the diffusivities in liquids are about four orders of magnitude lower than those in the gas phase at atmospheric pressure and accurate mass-transport simulations in laminar liquids are difficult. An estimation of the transport distance due to diffusion in laminar flow can be calculated from $x = \sqrt{Dt}$. The diffusivity in liquids is of the order of 10^{-9} m^2 s^{-1} and the average transport distance in 1 s is about 3 μm, i.e. very dense grids are required. The corresponding transport distance in the gas phase is 300 μm, with a gas-phase diffusivity of 10^{-5} m^2 s^{-1}.

1.4.2 Turbulent flow

The Navier–Stokes equations describe turbulent flows, but, due to the properties of the flow, it is seldom possible to solve the equations for real engineering applications even with supercomputers. In a stirred-tank reactor the lifetime and size of the smallest turbulent eddies, the Kolmogorov scales, are about 5 ms and 50 μm, respectively. A very fine time and space resolution is needed when solving the Navier–Stokes equations and it is at present not possible. Direct solution of the Navier–Stokes equations (DNS) for small systems is, however, very useful for developing an understanding of turbulence, and for developing new models.

A more cost-effective method is to resolve only the large-scale turbulence, by filtering out the fine-scale turbulence, and model these small scales as flow-dependent effective viscosity. This method, large-eddy simulation (LES), is growing in popularity since it makes it possible to simulate simple engineering flows on a fast PC. The simulations are, however, very time consuming on a PC, and several weeks can often be needed to obtain good statistical averages even for rather simple flows.

For more complex flows, it is not possible to resolve the turbulence fluctuations at all. Most engineering simulations are done with Reynolds-averaged Navier–Stokes (RANS) methods. In these models the turbulent fluctuations are time averaged, yet reasonable velocity averages can be simulated from these models. However, there are important properties of the flow that are not resolved. Everything that occurs on a scale below the size of the grid is not resolved, e.g. mixing of chemical species or the break-up and coalescence of bubbles and drops in multiphase flow. Additional models must be added to the RANS models in order to include these phenomena.

1.4.3 Single-phase flow

In single-phase laminar flow we can obtain very accurate solutions and in turbulent flow we can in most cases obtain satisfactory flow simulations. The main problem is usually simulation of the mixing of reactants for fast reactions in laminar or turbulent flow. When the reaction rate is fast compared with mixing, there will be strong concentration gradients that cannot be resolved in the grid, and a model for mixing coupled with a chemical reaction must be introduced. Combustion in the gas phase and ion–ion reactions in the liquid phase belong to this category.

1.4.4 Multiphase flow

Multiphase flow may consist of gas–liquid, gas–solid, liquid–liquid, liquid–solid or gas–liquid–solid systems. For a multiphase system containing very small particles, bubbles or drops that follow the continuous phase closely, reasonable simulation results can be obtained. Systems in which the dispersed phase has a large effect on the continuous phase are more difficult to simulate accurately, and only crude models are available for multiphase systems with a high load of the dispersed phase. At the moment, the quality of the simulations is limited not by the computer speed or memory but by the lack of good models for multiphase flow. However, multiphase flows are very important in engineering since many common processes involve multiphase flow.

The mass and heat transfer between the phases are of interest in many applications, e.g. in boiling, heterogeneous catalysis and distillation. For these simulations we must introduce empirical or semi-empirical correlations to describe mass and heat transfer. The mass- and heat-transfer coefficients are usually calculated from the traditional correlations for the Sherwood, Sh, and Nusselt, Nu, numbers. The advantage with CFD is that Sh and Nu can be computed using local flow properties. The mass and heat transfer are also affected by the coalescence and break-up of bubbles and drops. The phenomenon of break-up and coalescence is not included in this book since only very simple models are available for simulation of the effect of turbulence and shear rate on drop or bubble size distributions.

1.5 CFD programs

There are many commercial general-purpose CFD programs available, e.g. Fluent, CFX, Star-CD, FLOW-3D and Phoenics. There are also some very specialized programs

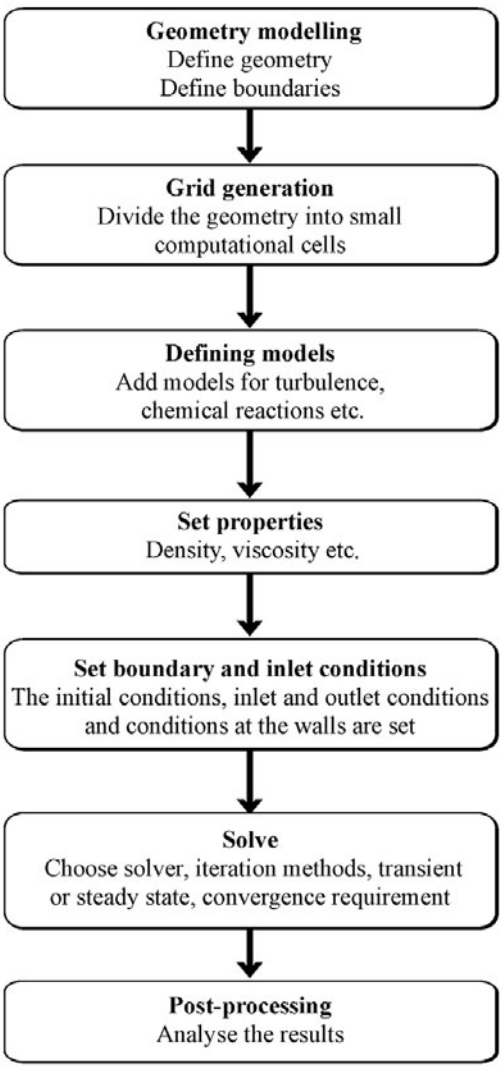

Figure 1.1 Steps in CFD simulations.

simulating combustion in engines, cooling of semiconductors and simulation of weather. A very useful open-source program that can handle most CFD problems is OpenFoam. However, the documentation and the user interface are not as well developed as those for the commercial codes.

Commercial CFD packages contain modules for CAD drawing, meshing, flow simulations and post-processing. In solving a problem using CFD there are many steps that must be defined, as is illustrated in Figure 1.1.

Geometry modelling

Solving a CFD problem starts with a two-dimensional (2D) or three-dimensional (3D) drawing of the geometry of the system. A CAD program is included in all commercial

CFD programs but the geometry of the system can usually be drawn in any CAD program and imported into the grid-generation program. However, CAD programs not designed for CFD often contains details that cannot be included in CFD drawings, e.g. nuts and bolts. These drawings must be cleaned before they can be used in a meshing program.

Grid generation (meshing)

The equations for momentum transport are nonlinear, which means that the computational volume must be discretized properly to obtain an accurate numerical solution of the equations. Accurate meshing of the computational domain is as important as defining the physical models. An ill-conditioned mesh can give rise to very inaccurate results, so the quality of the mesh, e.g. its aspect ratio and skewness, must be evaluated prior to the simulations. Most CFD programs have also the possibility of adaptation, which, after a preliminary result has been obtained, enables local refinement of the grid where necessary.

Define models

For single-phase laminar flow, the Navier–Stokes equations can be solved directly, but for turbulent and multiphase flows the user must select the most appropriate model. There are few generally accepted models for turbulence and multiphase flow, but there are hundreds of models to choose from. For each model there are also several parameters that must be set. Usually the default values are the best choice, but in some cases the user can find more suitable parameters. In most commercial CFD programs it is also possible to write your own model as a user-defined subroutine/function (UDS/UDF) in Fortran or C. Not all properties are resolved in the CFD program, and many semi-empirical models must be defined. The momentum, heat and mass transfer between the dispersed and continuous phases in multiphase flow are defined by empirical models for drag and Sherwood and Nusselt numbers as functions of the local particle Reynolds number or turbulence intensity.

Set properties

All physical properties of the fluids must be defined, e.g. the viscosity and density and their temperature, composition and pressure dependence. Some are built into the CFD software or easily found in available databases. The programs also provide polynomials for which you can add your own constants. It is also possible to write a UDS/UDF that is added to the CFD program for calculating the properties.

Set boundary and initial conditions

All inlet and outlet conditions must be defined, as must conditions on the walls and other boundaries. Rotational symmetry and other symmetries, e.g. periodic induced boundary conditions, must also be defined. Periodic boundary conditions are very useful with rotating equipment, e.g. a turbine, when only a part is modelled. Initial conditions for transient simulations or an initial guess to start the iterations for steady-state simulations must also be provided.

Solve

For the solver you can choose either a segregated or a coupled solver, pressure- or density-based, and for unsteady problems you must choose either implicit or explicit time-stepping methods. Numerical schemes to enhance convergence, e.g. multigrid, upwind schemes or under-relaxation factors, must be defined. The quality of an acceptable solution in terms of the convergence criteria must also be defined.

Post-processing/analysis

The first objective in the post-processing is to analyse the quality of the solution. Is the solution independent of the grid size, the convergence criterion and the numerical schemes? Have the proper turbulence model and boundary conditions been chosen, and is the solution strongly dependent on those choices?

Analysis of the final simulation results will then give local information about flow, concentrations, temperatures, reaction rates etc.

For very complex systems the results are not very accurate, but CFD can still be very useful in answering the question 'What if?'. Starting with an adjusted CFD simulation that fits the available experimental results, a parameter study can reveal how e.g. the mixing is affected by an increase in molecular viscosity.

Questions

(1) What can be simulated in a CFD program?
(2) Why is it not possible to solve Navier–Stokes equations for turbulent flows for typical engineering applications?
(3) What steps are involved in solving a typical CFD problem?

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:

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

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.

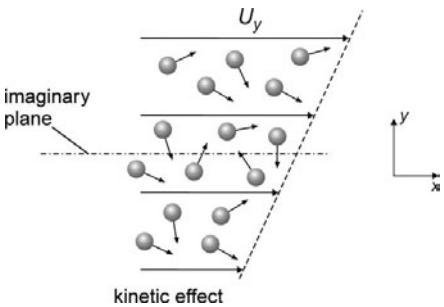

Figure 2.1 The effect of random movement of molecules on momentum transfer.

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 $Sc = \nu/D$

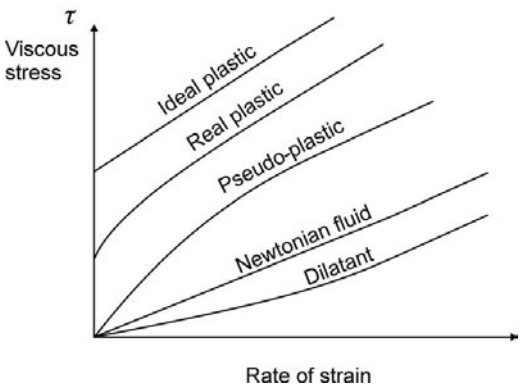

Figure 2.2 The viscous stress for Newtonian and non-Newtonian fluids.

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.