1 Introduction

1.1 CFD Activity

Computational fluid dynamics (CFD) is concerned with numerical solution of differential equations governing transport of mass, momentum, and energy in moving fluids. CFD activity emerged and gained prominence with availability of computers in the early 1960s. Today, CFD finds extensive usage in basic and applied research, in design of engineering equipment, and in calculation of environmental and geophysical phenomena. Since the early 1970s, commercial software packages (or computer codes) became available, making CFD an important component of engineering practise in industrial, defence, and environmental organizations.

For a long time, design (as it relates to sizing, economic operation, and safety) of engineering equipment such as heat exchangers, furnaces, cooling towers, internal combustion engines, gas turbine engines, hydraulic pumps and turbines, aircraft bodies, sea-going vessels, and rockets depended on painstakingly generated empirical information. The same was the case with numerous industrial processes such as casting, welding, alloying, mixing, drying, air-conditioning, spraying, environmental discharging of pollutants, and so on. The empirical information is typically displayed in the form of *correlations* or tables and nomograms among the main influencing variables. Such information is extensively availed by designers and consultants from handbooks [55].

The main difficulty with empirical information is that it is applicable only to the limited range of scales of fluid velocity, temperature, time, or length for which it is generated. Thus, to take advantage of economies of scale, for example, when engineers were called upon to design a higher capacity power plant, boiler furnaces, condensers, and turbines of ever higher dimensions had to be designed for which new empirical information had to be generated all over again. The generation of this new information was by no means an easy task. This was because the information applicable to bigger scales had to be, after all, generated via laboratory-scale models. This required establishment of *scaling laws* to ensure geometric, kinematic, and dynamic similarities between models and the full-scale equipment. This activity

required considerable experience as well as ingenuity, for it is not an easy matter to simultaneously maintain the three aforementioned similarities. The activity had to, therefore, be supported by flow-visualization studies and by simple (typically, one-dimensional) analytical solutions to equations governing the phenomenon under consideration. Ultimately, experience permitted judicious compromises. Being very expensive to generate, such information is often of a proprietary kind. In more recent times, of course, scaling difficulties are encountered in the opposite direction. This is because electronic equipment is considerably miniaturised and, in materials processing, for example, the more relevant phenomena occur at microscales (even molecular or atomic scales where the continuum assumption breaks down). Similarly, small-scale processes occur in biocells.

Clearly, designers need a design tool that is *scale neutral*. The tool must be scientific and must also be economical to use. An individual designer can rarely, if at all, acquire or assimilate this scale neutrality. Fortunately, the fundamental laws of mass, momentum, and energy, in fact, do embody such scale-neutral information. The key is to solve the differential equations describing these laws and then to interpret the solutions for practical design.

The potential of fundamental laws (in association with some further empirical laws) for generating widely applicable and scale-neutral information has been known almost ever since they were invented nearly 200 years ago. The realisation of this potential (meaning the ability to solve the relevant differential equations), however, has been made possible only with the availability of computers. The past five decades have witnessed almost exponential growth in the speed with which arithmetic operations can be performed on a computer.

By way of reminder, we note that the three laws governing transport are the following:

1. the law of conservation of mass (transport of mass),
2. Newton's second law of motion (transport of momentum), and
3. the first law of thermodynamics. (transport of energy).

1.2 Transport Equations

The aforementioned laws are applied to an infinitesimally small *control volume* located in a moving fluid. This application results in partial differential equations (PDEs) of mass, momentum and energy transfer. The derivation of PDEs is given in Appendix A.[1] Here, it will suffice to mention that the law of conservation of mass is written for a single-component fluid or for a mixture of several species. When applied to a single species of the mixture, the law yields the equation of *mass transfer* when an empirical law, namely, Fick's law of mass diffusion ($m_i'' = -\rho D\, \partial\omega/\partial x_i$),

[1] The reader is strongly advised to read Appendix A to grasp the main ideas and the process of derivations.

is invoked. Newton's second law of motion, combined with Stokes's stress laws, yields three momentum equations for velocity in directions x_j ($j = 1, 2, 3$). Similarly, the first law of thermodynamics in conjunction with Fourier's law of heat conduction ($q_{i,\text{cond}} = -K\,\partial T/\partial x_i$) yields the so-called energy equation for the transport of temperature T or enthalpy h. Using tensor notation, we can state these laws as follows:

Conservation of Mass for the Mixture

$$\frac{\partial \rho_m}{\partial t} + \frac{\partial (\rho_m u_j)}{\partial x_j} = 0, \tag{1.1}$$

Equation of Mass Transfer for Species *k*

$$\frac{\partial (\rho_m \omega_k)}{\partial t} + \frac{\partial (\rho_m u_j \omega_k)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\rho_m D_{\text{eff}} \frac{\partial \omega_k}{\partial x_j}\right] + R_k, \tag{1.2}$$

Momentum Equations u_i ($i = 1, 2, 3$)

$$\frac{\partial (\rho_m u_i)}{\partial t} + \frac{\partial (\rho_m u_j u_i)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\mu_{\text{eff}} \frac{\partial u_i}{\partial x_j}\right] - \frac{\partial p}{\partial x_i} + \rho_m B_i + S_{u_i}, \tag{1.3}$$

Energy Equation – Enthalpy Form

$$\frac{\partial (\rho_m h)}{\partial t} + \frac{\partial (\rho_m u_j h)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\frac{k_{\text{eff}}}{C_{pm}} \frac{\partial h}{\partial x_j}\right] + Q''', \tag{1.4}$$

where enthalpy $h = C_{pm}(T - T_{\text{ref}})$, and

Energy Equation – Temperature Form

$$\frac{\partial (\rho_m T)}{\partial t} + \frac{\partial (\rho_m u_j T)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\frac{k_{\text{eff}}}{C_{pm}} \frac{\partial T}{\partial x_j}\right] + \frac{Q'''}{C_{pm}}. \tag{1.5}$$

In these equations, the suffix m refers to the fluid mixture. For a single-component fluid, the suffix may be dropped and the equation of mass transfer becomes irrelevant. Similarly, the suffix *eff* indicates *effective* values of mass diffusivity D, viscosity μ, and thermal conductivity k. In laminar flows, the values of these *transport* properties are taken from property tables for the fluid under consideration. In turbulent flows, however, the transport properties assume values much in excess of the values ascribed to the fluid; moreover, the effective transport properties turn out to be properties *of the flow* [39], rather than those of the fluid.

From the point of view of further discussion of numerical methods, it is indeed a happy coincidence that the set of equations [(1.1)–(1.5)] can be cast as a single equation for a general variable Φ. Thus,

$$\frac{\partial (\rho_m \Phi)}{\partial t} + \frac{\partial (\rho_m u_j \Phi)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\Gamma_{\text{eff}} \frac{\partial \Phi}{\partial x_j}\right] + S_\Phi. \tag{1.6}$$

Table 1.1: Generalised representation of transport equations.

Equation	Φ	Γ_{eff} (exch. coef.)	S_Φ (net source)
1.1	1	0	0
1.2	ω_k	$\rho_{\text{m}}\, D_{\text{eff}}$	R_k
1.3	u_i	μ_{eff}	$-\partial p/\partial x_i + \rho_{\text{m}}\, B_i + S_{u_i}$
1.4	h	$k_{\text{eff}} / C_{p\text{m}}$	Q'''
1.5	T	$k_{\text{eff}} / C_{p\text{m}}$	$Q''' / C_{p\text{m}}$

The meanings of Γ_{eff} and S_Φ for each Φ are listed in Table 1.1. Equation 1.6 is called the *transport equation* for property Φ. The rate of change (or time derivative) term is to be invoked only when a transient phenomenon is under consideration. The term $\rho_{\text{m}}\, \Phi$ denotes the amount of *extensive* property available in a unit volume. The convection (second) term accounts for transport of Φ due to bulk motion. This first-order derivative term is relatively uncomplicated but assumes considerable significance when stable and convergent numerical solutions are to be economically obtained. This matter will become clear in Chapter 3. Both the transient and the convection terms require no further modelling or empirical information.

The greatest impediment to obtaining physically accurate solutions is offered by the diffusion and the net source (S) terms because both these terms require empirical information. In laminar flows, the diffusion term represented by the second-order derivative offers no difficulty because Γ, being a fluid property, can be accurately determined (via experiments) in *isolation* of the flow under consideration. In turbulent (or transitional) flows, however, determination of Γ_{eff} requires considerable empirical support. This is labelled as *turbulence modelling*. This extremely complex phenomenon has attracted attention for over 150 years. Although turbulence models of adequate generality (at least, for specific classes of flows) have been proposed, they by no means satisfy the expectations of an equipment designer. These models determine Γ_{eff} from simple algebraic empirical laws. Sometimes, Γ_{eff} is also determined from other scalar quantities (such as turbulent kinetic energy and/or its dissipation rate) for which differential equations are constituted. Fortunately, these equations often have the form of Equation 1.6.

The term *net source* implies an algebraic sum of sources and sinks of Φ. Thus, in a chemically reacting flow (combustion, for example), a given species k may be generated via some chemical reactions and destroyed (or consumed) via some others and R_k will comprise both positive and negative contributions. Also, some chemical reactions may be exothermic, whereas others may be endothermic, making positive and negative contributions to Q'''. Similarly, the term B_i in the momentum equations may represent a buoyancy force, a centrifugal and/or Coriolis force, an electromagnetic force, etc. Sometimes, B_i may also represent resistance forces. Thus, in a mixture of gas and solid particles (as in pulverised fuel combustion), B_i will represent the drag offered by the particles on air, or, in a fluid flow through a

densely filled medium (a porous body or a shell-and-tube geometry), the resistance will be a function of the porosity of the medium. Such empirical resistance laws are often determined from experiments. The S_{u_i} terms represent viscous terms arising from Stokes's stress laws that are not accounted for in the $\frac{\partial}{\partial x_j}[\mu_{\text{eff}} \frac{\partial u_i}{\partial x_j}]$ term in Equation 1.3.

1.3 Numerical Versus Analytical Solutions

Analytical solutions to our transport equations are rarely possible for the following reasons:

1. The equations are three-dimensional.
2. The equations are strongly coupled and nonlinear.
3. In practical engineering problems, the solution domains are almost always complex.

The equations, however, can be made amenable to analytical solutions when simplified through assumptions. In a typical undergraduate program, students develop extensive familiarity with such analytical solutions that can be represented in *closed form*. Thus, in a fluid mechanics course, for example, when fully developed laminar flow in a pipe is considered, a student is readily able to *integrate* the simplified (one-dimensional) momentum equation to obtain a closed-form solution for the streamwise velocity u as a function of radius r. The assumptions made are as follows: The flow is steady and laminar, it is fully developed, it is axisymmetric, and fluid properties are uniform. The solution is then interpreted to yield the scale-neutral result $f \times Re = 16$. The friction factor f is a practically useful quantity that enables calculation of pumping power required to force fluid through a pipe. Similarly, in a heat transfer course, a student learns to calculate reduction of heat transfer rate when insulation of a given thickness is applied to a pipe. In this case, the energy equation is simplified and the assumptions are as follows: Heat transfer is radial and axi symmetric, steady state prevails, and the insulation conductivity may be constant and there is no generation or dissipation of energy within the insulation.

In both these examples, the equations are one dimensional. They are, therefore, *ordinary differential equations* (ODEs), although the original transport equations were PDEs. In many situations, in spite of the assumptions, the governing equations cannot be rendered one dimensional. Thus, the equations of a steady, two-dimensional velocity boundary layer or that of one-dimensional *unsteady* heat conduction are partial differential equations. It is important to recognise, however, that there are no direct solutions to partial differential equations. To obtain solutions, the PDEs are always first converted to ODEs (usually more in number than the original PDEs) and the latter are solved by integration. Thus, in an unsteady conduction problem, the ODEs are formed by the method of separation of variables, whereas, for the two-dimensional velocity boundary layer, the ODE is

formed by invoking a *similarity* variable. In such circumstances, often the solution is in the form of a series. We assume, of course, that the reader is familiar with the restrictive circumstances (often of significant practical consequence) under which such analytical solutions are constructed.

Analytical solutions obtained in the manner described here are termed *exact* solutions. They are applicable to every point of the time and/or space domain. The solutions are also called continuous solutions. All the aforementioned solutions are well covered in an undergraduate curriculum and in textbooks (see, for example, [34, 80, 88]).

Unlike analytical solutions, numerical solutions are obtained at a few *chosen points* within the domain. They are therefore called *discrete* solutions. Numerical solutions are obtained by employing numerical methods. The latter are really an intermediary between the physics embodied in the transport equations and the computers that can unravel them by generating numerical solutions. The process of arriving at numerical solutions is thus quite different from the process by which analytical solutions are developed.

Before describing the essence of numerical methods, it is important to note that these methods, in principle, can overcome all three aforementioned impediments to obtaining analytical solutions. In fact, the history of CFD shows that numerical methods have been evolved precisely to overcome the impediments in the order of their mention. Thus, the earliest numerical methods dealt with one-dimensional equations for which analytical solutions may or may not be possible. Methods for two-dimensional transport equations, however, had to incorporate substantially new features. In spite of these new features, many methods applicable to two-dimensional coupled equations could not be extended to three-dimensional equations. Similarly, the earlier methods were derived for transport equations cast in only orthogonal co-ordinates (Cartesian, cylindrical polar, or spherical). Later, however, as computations over complex domains were attempted, the equations were cast in completely arbitrary curvilinear (ξ_1, ξ_2, ξ_3) coordinates. This led to development of an important branch of CFD, namely, *numerical grid generation*. With this development, domains of arbitrary shape could be mapped such that the coordinate lines followed the shape of the domain boundary. Today, complex domains are mapped by yet another development called *unstructured mesh generation*. In this, the domain can be mapped by a completely arbitrary distribution of points. When the points are connected by straight lines, one obtains polygons (in two dimensions) and polyhedra (in three dimensions). Several methods (as well as packages) for unstructured mesh generation are now available.

1.4 Main Task

It is now appropriate to list the main steps involved in arriving at numerical solutions to the transport equation. To enhance understanding, an example of an *idealised*

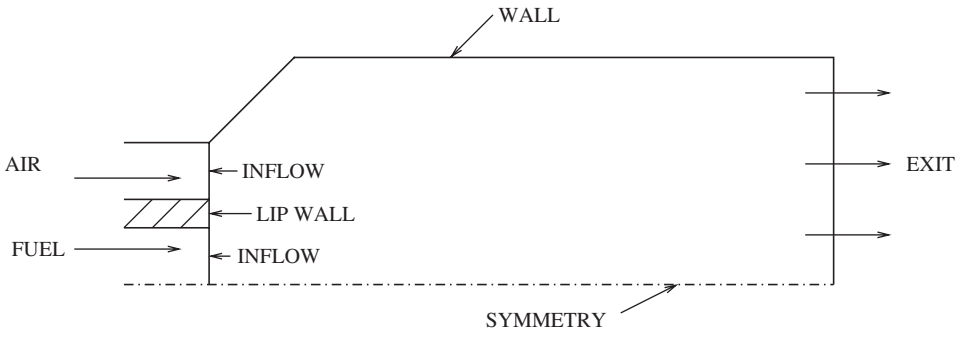

Figure 1.1. Typical two-dimensional domain.

combustion chamber of a gas-turbine engine will be considered.

1. *Given the flow situation of interest, define the physical (or space) domain of interest.* In unsteady problems, the time domain is *imagined*. Figure 1.1 shows the domain of interest of the idealised chember. Fuel and air streams, separated by a lip wall, enter the chamber at the *inflow* boundary. The cross section of the chamber is taken to be a perfect circle so that a *symmetry* boundary coinciding with the axis is readily identified. The enclosing *wall* is solid and the burnt products of combustion leave through the *exit* boundary. Because the situation is idealised as a two-dimensional axisymmetric domain that will involve fluid recirculation, there are four boundaries of interest: inflow, wall, symmetry, and exit.
2. *Select transport equations with appropriate diffusion and source laws. Define boundary conditions on segments of the domain boundary for each variable* Φ. *Also, define the fluid properties*. The boundary segments have already been identified in Figure 1.1. Now, since air and fuel mix and react chemically, equations for $\Phi = u_1, u_2, u_3$ (swirl velocity), T or h, and several mass fractions ω_k must be solved. The choice of ω_k will of course depend on the *reaction model* postulated by the analyst. Further, additional equations must be solved to capture effects of turbulence via a *turbulence model*. This matter will become clear in later chapters.
3. *Select points (called nodes) within the domain so as to map the domain with a grid. Construct control volumes around each node*. In Figure 1.2, the domain of interest is mapped by three types of grids: Cartesian, Curvilinear, and Unstructured. The hatched portions show the control volumes and the filled circles are the nodes. Note that in the Cartesian grids, the control volumes near the slanted wall are not rectangular as elsewhere. This type of difficulty is overcome in the curvilinear grids where all control volumes are quadrilaterals and the grid lines follow the contours of the domain boundary as required. The unstructured grid is completely arbitrary. Although most control volumes are triangular, one can also

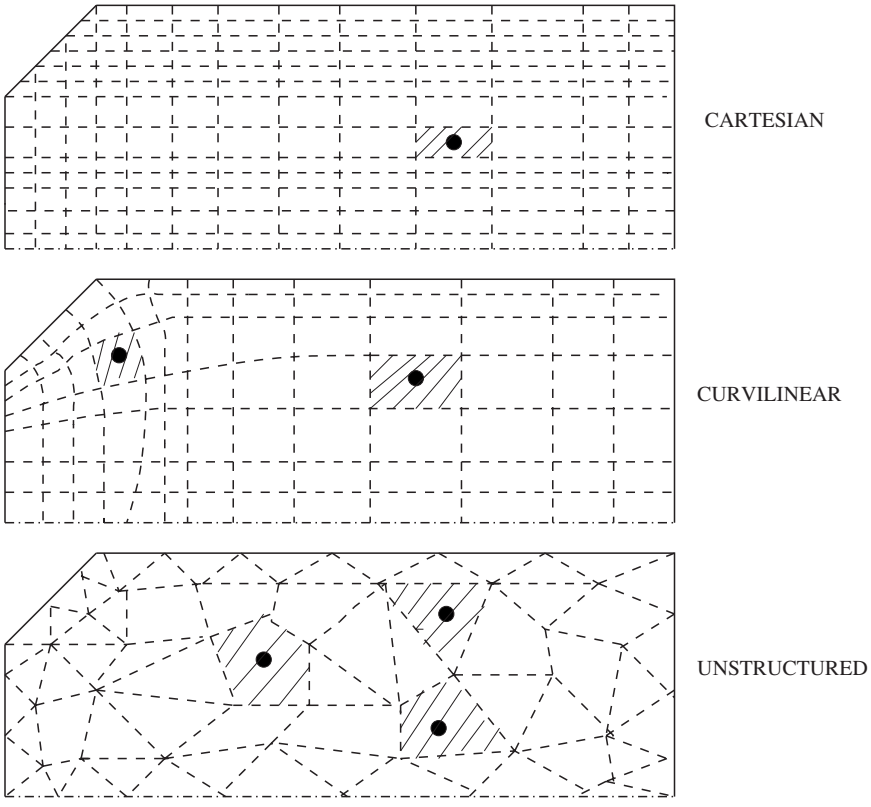

Figure 1.2. Different types of grids.

have polygons of any number of sides. This activity of specifying coordinates of nodes and of specification of control volumes is called *grid generation*.

4. *Integrate Equation 1.6 over a typical control volume so as to convert the partial differential equation into an algebraic one*. This is unlike the analytical solutions in which the original PDEs are converted to ordinary ones. Thus, if there are NV variables of interest and the number of nodes chosen is NP, one obtains a set of $NV \times NP$ algebraic equations. The process of converting PDEs into algebraic equations is called *discretisation*.
5. *Devise a numerical method to solve the set of algebraic equations*. This can be done sequentially, so that NP equations are solved for each Φ in succession. Alternatively, one may solve the entire set of $NV \times NP$ equations simultaneously. The construction of the overall calculation sequence is called an *algorithm*.
6. *Devise a computer program to implement the numerical method on a computer*. Different numerical methods require different amounts of computer storage and different amounts of computer time to arrive at a solution. Aspects such as economy in terms of number of arithmetic operations, convergence rate, and stability of the numerical method are thus important.

7. "*Interpret the solution*:" The numerical solution results in values of each Φ at each node. Such a Φ field provides the distribution of Φ over the domain. The task now is to interpret the solution to retrieve quantities of engineering interest such as the friction factor, a Nusselt number at the wall, or average concentrations of CO, fuel, and NO_x at the exit from a combustion chamber. Sometimes the field may be curve-fitted to take the appearance of an analytical solution. Similarly, the derived quantities may also be curve-fitted to take the appearance of an experimentally derived correlation for ready use in further design work.
8. "*Display of results*:" Since a numerical solution is obtained at discrete points, the solution comprises numbers that can be printed in tabular forms. The inconvenience of reading numbers can be circumvented by plotting results on a graph or by displaying the Φ fields by means of contour or vector plots. Fortunately, such graphic displays can now be made using computers. This activity is called *postprocessing* of results. The commercial success of computer codes often depends on the quality and flexibility of their *postprocessors*.

The primary focus of this book is to explain procedures for executing these steps. Computer code developers and researchers adopt a variety of practices to implement the procedures depending on their background, familiarity, and notions of convenience. Clearly biases are involved.

In this book, emphasis is laid on physical principles. In fact, the attitude is one of relearning fluid mechanics and heat and mass transfer by obtaining numerical (as opposed to restrictive analytical) solutions. The book is not intended to provide a survey of all numerical methods; rather, the objective is to introduce the reader to a few specific methods and procedures that have been found to be robust in a wide variety of situations of a specific class. The emphasis is on skill development, skills required for problem formulation, computer code writing, and interpretation of results.

1.5 A Note on Navier–Stokes Equations

The law of conservation of mass for the bulk fluid together with Newton's second law of motion constitutes the main laws governing fluid motion. As shown in Appendix A, the equations of motion are written in *differential form* and, therefore, assume existence of a fluid continuum. In this section, attention is drawn to an often overlooked requirement that assumes considerable importance in the context of CFD in which numerical solutions are obtained at *discrete points* rather than at every point in space as in a continuum.

Attention is focussed primarily on the normal stress expressions given in Appendix A (see Equations A.15). As presented in Schlichting [65], the normal

stresses are given by

$$\sigma_x = -p + \sigma'_x = -p + q + \tau_{xx} = -p + q + 2\mu \frac{\partial u}{\partial x}, \tag{1.7}$$

$$\sigma_y = -p + \sigma'_y = -p + q + \tau_{yy} = -p + q + 2\mu \frac{\partial v}{\partial y}, \tag{1.8}$$

$$\sigma_z = -p + \sigma'_z = -p + q + \tau_{zz} = -p + q + 2\mu \frac{\partial w}{\partial z}. \tag{1.9}$$

In these normal stress expressions, σ' is called the deviotoric stress and the significance of quantity q in its definition requires elaboration. Schlichting [65] and Warsi [86], for example, define a space-averaged pressure $\overline{p}$ as

$$\overline{p} = -\frac{1}{3}(\sigma_x + \sigma_y + \sigma_z). \tag{1.10}$$

Now, an often overlooked *requirement* of the Stokes's relations is that, in a continuum, $\overline{p}$ must equal the point value of pressure p and the latter, in turn, must equal the thermodynamic pressure p_{th}. Thus,

$$\overline{p} = p = p_{\text{th}} = p - q - \frac{2}{3}\mu \bigtriangledown \cdot V. \tag{1.11}$$

In the context of this requirement, we now consider different flow cases to derive the significance of q.

1. *Case 1* ($V = 0$): In this *hydrostatic case*,

$$\overline{p} = p - q. \tag{1.12}$$

But in this case, p can only vary linearly with x, y, and z and, therefore, the point value of p exactly equals its space-averaged value $\overline{p}$ in both continuum as well as discretised space and hence $q = 0$ exactly.

2. *Case 2* ($\mu = 0$ or $\bigtriangledown \cdot V = 0$): Clearly when $\mu = 0$ (inviscid flow) or $\bigtriangledown . V = 0$ (constant-density incompressible flow) Equation 1.12 again holds. But, in this case, since fluid motion is considered, p can vary arbitrarily with x, y, and z and, therefore, p may not equal $\overline{p}$ in a discrete space. To understand this matter, consider a case in which pressure varies arbitrarily in the x direction, whereas its variation in y and z directions is constant or linear (as in a hydrostatic case). Such a variation is shown in Figure 1.3. Now consider a point P. According to Stokes's requirement p_{P} must equal $\overline{p}_{\text{P}}$ in a continuum. However, in a discretised space, the values of pressure are available at points E and W only, and if these points are equidistant from P then $\overline{p}_{\text{P}} = 0.5\,(p_{\text{W}} + p_{\text{E}})$. Now, this $\overline{p}_{\text{P}}$ *will not equal* p_{P}, as seen from the figure, and therefore the requirement of the Stokes's relations is not met.

However, without violating the continuum requirement, we may set

$$q = \lambda_1 (p - \overline{p}), \tag{1.13}$$