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An Introduction to COMPUTATIONAL FLUID DYNAMICS

The Finite Volume Method

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An Introduction to Computational Fluid Dynamics

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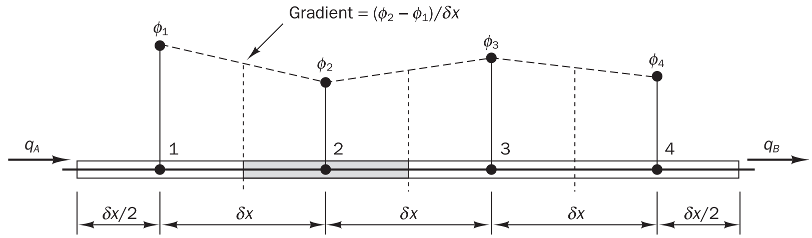


Figure 5.7 Example of consistent specification of diffusive fluxes

The fluxes across the domain boundaries are denoted by q_A and q_B. Let us consider four control volumes and apply central differencing to calculate the diffusive flux across the cell faces. The expression for the flux leaving the element around node 2 across its west face is $\Gamma_{w_2}(\phi_2 - \phi_1)/\delta x$ and the flux entering across its east face is $\Gamma_{e_2}(\phi_3 - \phi_2)/\delta x$. An overall flux balance may be obtained by summing the net flux through each control volume, taking into account the boundary fluxes for the control volumes around nodes 1 and 4:

$$\left[\Gamma_{e_1}\frac{(\phi_2-\phi_1)}{\delta x} - q_A\right] + \left[\Gamma_{e_2}\frac{(\phi_3-\phi_2)}{\delta x} - \Gamma_{w_2}\frac{(\phi_2-\phi_1)}{\delta x}\right]$$
$$+\left[\Gamma_{e_3}\frac{(\phi_4-\phi_3)}{\delta x} - \Gamma_{w_3}\frac{(\phi_3-\phi_2)}{\delta x}\right] + \left[q_B - \Gamma_{w_4}\frac{(\phi_4-\phi_3)}{\delta x}\right]$$
$$= q_B - q_A \tag{5.21}$$

Since $\Gamma_{e_1} = \Gamma_{w_2}$, $\Gamma_{e_2} = \Gamma_{w_3}$ and $\Gamma_{e_3} = \Gamma_{w_4}$ the fluxes across control volume faces are expressed in a consistent manner and cancel out in pairs when summed over the entire domain. Only the two boundary fluxes q_A and q_B remain in the overall balance, so equation (5.21) expresses overall conservation of property ϕ. Flux consistency ensures conservation of ϕ over the entire domain for the central difference formulation of the diffusion flux.

Inconsistent flux interpolation formulae give rise to unsuitable schemes that do not satisfy overall conservation. For example, let us consider the situation where a quadratic interpolation formula, based on values at 1, 2 and 3, is used for control volume 2, and a quadratic profile, based on values at points 2, 3 and 4, is used for control volume 3.

As shown in Figure 5.8, the resulting quadratic profiles can be quite different.

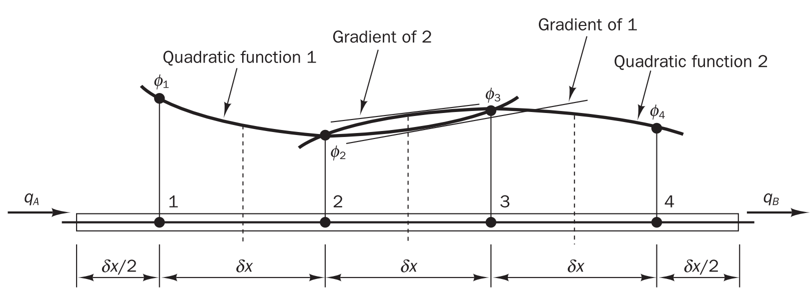


Figure 5.8 Example of inconsistent specification of diffusive fluxes

Consequently, the flux values calculated at the east face of control volume 2 and the west face of control volume 3 may be unequal if the gradients of the two curves are different at the cell face. If this is the case the two fluxes do not cancel out when summed and overall conservation is not satisfied. The example should not suggest to the reader that quadratic interpolation is entirely bad. Further on we will meet a quadratic discretisation practice – the so-called QUICK scheme – that *is* consistent.

5.4.2 Boundedness

The discretised equations at each nodal point represent a set of algebraic equations that needs to be solved. Normally iterative numerical techniques are used to solve large equation sets. These methods start the solution process from a guessed distribution of the variable ϕ and perform successive updates until a converged solution is obtained. Scarborough (1958) has shown that a **sufficient condition for a convergent iterative method** can be expressed in terms of the values of the coefficients of the discretised equations:

$$\boxed{\frac{\sum|a_{nb}|}{|a'_P|} \begin{cases} \leq 1 \text{ at all nodes} \\ < 1 \text{ at one node at least} \end{cases}} \tag{5.22}$$

Here a'_P is the net coefficient of the central node P (i.e. $a_P - S_P$), and the summation in the numerator is taken over all the neighbouring nodes (nb). If the differencing scheme produces coefficients that satisfy the above criterion the resulting matrix of coefficients is **diagonally dominant**. To achieve diagonal dominance we need large values of net coefficient ($a_P - S_P$) so the **linearisation** practice of **source terms** should ensure that $\boldsymbol{S_P}$ is always **negative**. If this is the case $-S_P$ is always positive and adds to a_P.

Diagonal dominance is a desirable feature for satisfying the 'boundedness' criterion. This states that in the **absence of sources** the internal nodal values of **property** ϕ should be **bounded by its boundary values**. Hence in a steady state conduction problem without sources and with boundary temperatures of 500°C and 200°C, all interior values of T should be less than 500°C and greater than 200°C. Another essential requirement for boundedness is that **all coefficients of the discretised equations should have the same sign** (usually all positive). Physically this implies that an increase in the variable ϕ at one node should result in an increase in ϕ at neighbouring nodes. If the discretisation scheme does not satisfy the boundedness requirements it is possible that the solution does not converge at all, or, if it does, that it contains 'wiggles'. This is powerfully illustrated by the results of Case 2 of Example 5.1. In all other worked examples we have developed discretised equations with positive coefficients a_P and a_{nb}, but in Case 2 most of the east coefficients were negative (see Table 5.3), and the solution contained large under- and overshoots!

5.4.3 Transportiveness

The transportiveness property of a fluid flow (Roache, 1976) can be illustrated by considering the effect at a point P due to two constant sources of ϕ at nearby points W and E on either side as shown in Figure 5.9. We define the non-dimensional cell Peclet number as a measure of the relative strengths of convection and diffusion:

$$\boxed{Pe = \frac{F}{D} = \frac{\rho u}{\Gamma/\delta x}} \quad (5.23)$$

where δx = characteristic length (cell width)

The lines in Figure 5.9 indicate the general shape of contours of constant ϕ (say $\phi = 1$) due to both sources for different values of Pe. The value of ϕ at any point can be thought of as the sum of contributions due to the two sources.

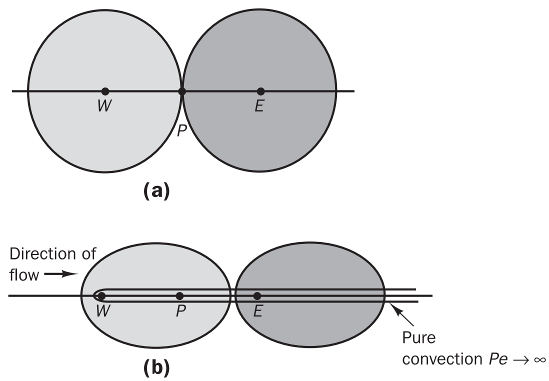


Figure 5.9 Distribution of ϕ in the vicinity of two sources at different Peclet numbers: (a) pure convection, $Pe \to 0$; (b) diffusion and convection

Let us consider two extreme cases to identify the extent of the influence at node P due to the sources at W and E:

- no convection and pure diffusion ($Pe \to 0$)
- no diffusion and pure convection ($Pe \to \infty$)

In the case of pure diffusion the fluid is stagnant ($Pe \to 0$) and the contours of constant ϕ will be concentric circles centred around W and E since the diffusion process tends to spread ϕ equally in all directions. Figure 5.9a shows that both $\phi = 1$ contours pass through P, indicating that conditions at this point are influenced by both sources at W and E. As Pe increases the contours change shape from circular to elliptical and are shifted in the direction of the flow as shown in Figure 5.9b. Influencing becomes increasingly biased towards the upstream direction at large values of Pe, so, in the present case where the flow is in the positive x-direction, conditions at P will be mainly influenced by the upstream source at W. In the case of pure convection ($Pe \to \infty$) the elliptical contours are completely stretched out in the flow direction. All of property ϕ emanating from the sources at W and E is immediately transported downstream. Thus, conditions at P are now unaffected by the downstream source at E and completely dictated by the upstream source at W. Since there is no diffusion ϕ_P is equal to ϕ_W. If the flow is in the negative x-direction we would find that ϕ_P is equal to ϕ_E. It is very important that the relationship between the directionality of influencing and the flow direction and magnitude of the Peclet number, known as the **transportiveness**, is borne out in the discretisation scheme.

5.5 Assessment of the central differencing scheme for convection–diffusion problems

Conservativeness: The central differencing scheme uses consistent expressions to evaluate convective and diffusive fluxes at the control volume faces. The discussions in section 5.4.1 show that the scheme is conservative.

Boundedness:

(i) The internal coefficients of discretised scalar transport equation (5.14) are

a_W	a_E	a_P
$D_w + \dfrac{F_w}{2}$	$D_e - \dfrac{F_e}{2}$	$a_W + a_E + (F_e - F_w)$

A steady one-dimensional flow field is also governed by the discretised continuity equation (5.10). This equation states that $(F_e - F_w)$ is zero when the flow field satisfies continuity. Thus the expression for a_P in (5.14) becomes equal to $a_P = a_W + a_E$. The coefficients of the central differencing scheme satisfy the Scarborough criterion (5.22).

(ii) With $a_E = D_e - F_e/2$ the convective contribution to the east coefficient is negative; if the convection dominates it is possible for a_E to be negative. Given that $F_w > 0$ and $F_e > 0$ (i.e. the flow is unidirectional), for a_E to be positive D_e and F_e must satisfy the following condition:

$$F_e/D_e = Pe_e < 2 \tag{5.24}$$

If Pe_e is greater than 2 the east coefficient will be negative. This violates one of the requirements for boundedness and may lead to physically impossible solutions.

In the example of section 5.3 we took $Pe = 5$ in Case 2 so condition (5.24) is violated. The consequences were evident in the results, which showed large ‘undershoots’ and ‘overshoots’. Taking Pe less than 2 in Cases 1 and 3 gave bounded answers close to the analytical solution.

Transportiveness: The central differencing scheme introduces influencing at node P from the directions of all its neighbours to calculate the convective and diffusive flux. Thus the scheme does not recognise the direction of the flow or the strength of convection relative to diffusion. It does not possess the transportiveness property at high Pe.

Accuracy: The Taylor series truncation error of the central differencing scheme is second-order (see Appendix A for further details). The requirement for positive coefficients in the central differencing scheme as given by formula (5.24) implies that the scheme will be stable and accurate only if $Pe = F/D < 2$. It is important to note that the cell Peclet number, as defined by (5.23), is a combination of fluid properties (ρ and Γ), a flow property (u) and a property of the computational grid (δx). So for given values of ρ and Γ it is only possible to satisfy condition (5.24) if the velocity is small, hence in diffusion-dominated low Reynolds number flows, or if the grid spacing is small. Owing to this limitation central differencing is not a suitable discretisation practice for general-purpose flow calculations. This creates the need for discretisation schemes which possess more favourable properties. Below we discuss the upwind, hybrid, power-law, QUICK and TVD schemes.

5.6 The upwind differencing scheme

One of the major inadequacies of the central differencing scheme is its inability to identify flow direction. The value of property ϕ at a west cell face is always influenced by both ϕ_P and ϕ_W in central differencing. In a strongly convective flow from west to east, the above treatment is unsuitable because the west cell face should receive much stronger influencing from node W than from node P. The upwind differencing or 'donor cell' differencing scheme takes into account the flow direction when determining the value at a cell face: the convected value of ϕ at a cell face is taken to be equal to the value at the upstream node. In Figure 5.10 we show the nodal values used to calculate cell face values when the flow is in the positive direction (west to east) and in Figure 5.11 those for the negative direction.

Figure 5.10

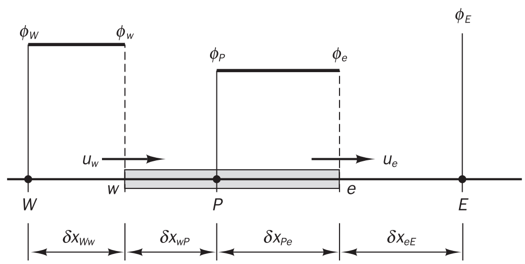
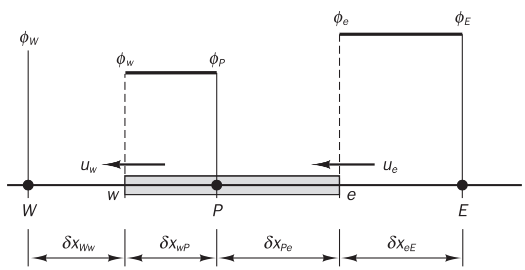


Figure 5.11



When the flow is in the positive direction, $u_w > 0$, $u_e > 0$ ($F_w > 0$, $F_e > 0$), the upwind scheme sets

$$\phi_w = \phi_W \quad \text{and} \quad \phi_e = \phi_P \tag{5.25}$$

and the discretised equation (5.9) becomes

$$F_e\phi_P - F_w\phi_W = D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W) \tag{5.26}$$

which can be rearranged as

$$(D_w + D_e + F_e)\phi_P = (D_w + F_w)\phi_W + D_e\phi_E$$

to give

$$[(D_w + F_w) + D_e + (F_e - F_w)]\phi_P = (D_w + F_w)\phi_W + D_e\phi_E \tag{5.27}$$

When the flow is in the negative direction, $u_w < 0$, $u_e < 0$ ($F_w < 0$, $F_e < 0$), the scheme takes

$$\phi_w = \phi_P \quad \text{and} \quad \phi_e = \phi_E \tag{5.28}$$

Now the discretised equation is

$$F_e\phi_E - F_w\phi_P = D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W) \tag{5.29}$$

or

$$[D_w + (D_e - F_e) + (F_e - F_w)]\phi_P = D_w\phi_W + (D_e - F_e)\phi_E \quad (5.30)$$

Identifying the coefficients of ϕ_W and ϕ_E as a_W and a_E, equations (5.27) and (5.30) can be written in the usual general form

$$\boxed{a_P\phi_P = a_W\phi_W + a_E\phi_E} \quad (5.31)$$

with central coefficient

$$\boxed{a_P = a_W + a_E + (F_e - F_w)}$$

and neighbour coefficients

	a_W	a_E
$F_w > 0, F_e > 0$	$D_w + F_w$	D_e
$F_w < 0, F_e < 0$	D_w	$D_e - F_e$

A form of notation for the **neighbour coefficients of the upwind differencing method** that covers both flow directions is given below:

a_W	a_E
$D_w + \max(F_w, 0)$	$D_e + \max(0, -F_e)$

Example 5.2

Solve the problem considered in Example 5.1 using the upwind differencing scheme for (i) $u = 0.1$ m/s, (ii) $u = 2.5$ m/s with the coarse five-point grid.

Solution

The grid shown in Figure 5.3 is again used here for the discretisation. The discretisation equation at internal nodes 2, 3 and 4 and the relevant neighbour coefficients are given by (5.31) and its accompanying tables. Note that in this example $F = F_e = F_w = \rho u$ and $D = D_e = D_w = \Gamma/\delta x$ everywhere.

At the boundary node 1, the use of upwind differencing for the convective terms gives

$$F_e\phi_P - F_A\phi_A = D_e(\phi_E - \phi_P) - D_A(\phi_P - \phi_A) \quad (5.32)$$

And at node 5

$$F_B\phi_P - F_w\phi_W = D_B(\phi_B - \phi_P) - D_w(\phi_P - \phi_W) \quad (5.33)$$

At the boundary nodes we have $D_A = D_B = 2\Gamma/\delta x = 2D$ and $F_A = F_B = F$, and as usual the boundary conditions enter the discretised equations as source contributions:

$$\boxed{a_P\phi_P = a_W\phi_W + a_E\phi_E + S_u} \quad (5.34)$$

with

$$\boxed{a_P = a_W + a_E + (F_e - F_w) - S_P}$$