Lecture 5 - The Finite Volume Method for Convection-Diffusion Problems

Considering the steady convection-diffusion equation:

$$\cancel{\frac{\partial(\rho\phi)}{\partial t}} + div(\rho\phi\mathbf{u}) = div\left(\Gamma\, grad\ \phi\right) + S_\phi$$

- The control volume integration gives:

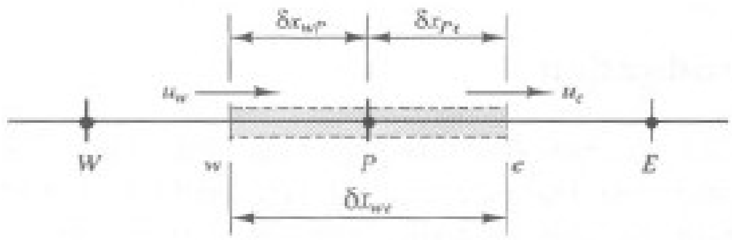
$$\int_A \mathbf{n}\cdot(\rho\phi\ \mathbf{u})dA = \int_A \mathbf{n}\cdot(\Gamma\, grad\ \phi)dA + \int_{CV} S_\phi dV$$

- Apply the central differencing method of obtaining discretised equations for the diffusion?
- Not the same, since the diffusion process affects the distribution of a transported quantity along its gradient in all directions, whereas convection spreads influence only in the flow direction (i.e. the grid size is dependent on the relative strength of convection and diffusion)

1. Steady one-dimensional convection and diffusion

Consider the steady state convection and diffusion of a property φ in a one-dimensional domain:

Fig. 5.1 A control volume around node P



- In the absence of sources, the process in a given one-dimensional flow field u is:

$$\frac{d}{dx}(\rho u\phi) = \frac{d}{dx}\left(\Gamma\frac{d\phi}{dx}\right)$$

where Γ is the diffusion coefficient.

- This flow also satisfies continuity:

$$\frac{d}{dx}(\rho u) = 0$$

- Integration of transport equation over the control volume gives:

  $$\left(\rho uA\phi\right)_e - \left(\rho uA\phi\right)_w = \left(\Gamma A\frac{d\phi}{dx}\right)_e - \left(\Gamma A\frac{d\phi}{dx}\right)_w$$

- Integration of continuity equation over the control volume gives:

  $$\left(\rho uA\right)_e - \left(\rho uA\right)_w = 0$$

- Define the convective mass flux per unit area, F, and diffusion conductance at cell faces, D:

  $$F = \rho u$$

  $$D = \frac{\Gamma}{\delta x}$$

  with

  $$F_w = \left(\rho u\right)_w$$

  $$F_e = \left(\rho u\right)_e$$

  $$D_w = \frac{\Gamma_w}{\delta x_{WP}}$$

  $$D_e = \frac{\Gamma_e}{\delta x_{PE}}$$

  ✓ Assuming $A_e = A_w = A$ and the central differencing approach, the transport equation is:

  $$F_e\phi_e - F_w\phi_w = D_e\left(\phi_E - \phi_P\right) - D_w\left(\phi_P - \phi_W\right)$$

  and the continuity equation is:

  $$F_e - F_w = 0$$

2. The central differencing scheme

✓ The central differencing scheme has been used to represent the diffusion terms and it seems logical to try linear interpolation to compute the cell face values for the convective terms. For a uniform grid:

$$\phi_e = \frac{\left(\phi_P + \phi_E\right)}{2} \text{ and } \phi_w = \frac{\left(\phi_P + \phi_W\right)}{2}$$

✓ The transport equation becomes:

$$\frac{F_e}{2}\left(\phi_P + \phi_E\right) - \frac{F_w}{2}\left(\phi_W + \phi_P\right) = D_e\left(\phi_E - \phi_P\right) - D_w\left(\phi_P - \phi_W\right)$$

re-arranging,

$$\left[\left(D_w - \frac{F_w}{2}\right) + \left(D_e + \frac{F_e}{2}\right)\right]\phi_P = \left(D_w + \frac{F_w}{2}\right)\phi_W + \left(D_e - \frac{F_e}{2}\right)\phi_E$$

or

$$\left[\left(D_w+\frac{F_w}{2}\right)+\left(D_e-\frac{F_e}{2}\right)+\left(F_e-F_w\right)\right]\phi_P=\left(D_w+\frac{F_w}{2}\right)\phi_W+\left(D_e-\frac{F_e}{2}\right)\phi_E$$

- ✓ In central differencing expression:

$$a_P\phi_P=a_W\phi_W+a_E\phi_E$$

where

$$a_W=\left(D_w+\frac{F_w}{2}\right)$$

$$a_E=\left(D_e-\frac{F_e}{2}\right)$$

$$a_P=a_W+a_E+\left(F_e-F_w\right)$$

Examples: one-dimensional steady states convection and diffusion

A property φ is transported by means of convection and diffusion through the one-dimensional domain. The equation governing is:

$$\frac{d}{dx}(\rho u\phi)=\frac{d}{dx}\left(\Gamma\frac{d\phi}{dx}\right)$$

Boundary conditions are:

$$\phi_0=1\big|_{x=0}\quad and \quad \phi_L=0\big|_{x=L}$$

Using 5 equally spaced cells and the central differencing scheme for convection and diffusion, calculate the distribution of φ as a function of x for,

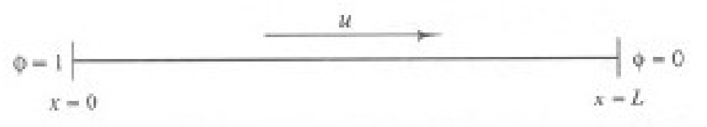
(1) Case 1: u = 0.1 m/s

(2) Case 2: u = 2.5 m/s

(3) Case 3: u = 2.5 m/s with 20 grid nodes

L = 1.0 m, ρ = 1.0 kg/m^3, Γ = 0.1 x 10^{-3} kg/m/s.

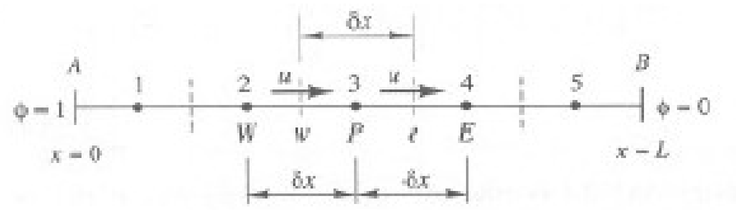
Fig. 5.2



Ans:

- ✓ Divide the length into 5 equal control volumes. This gives δx = 0.2 m.

Fig. 5.3 The grid used for discretisation



- For nodes 2, 3, and 4
  - ✓ Compared with the general form:

$$a_P\phi_P = a_W\phi_W + a_E\phi_E$$

where

$$a_W = \left(D_w + \frac{F_w}{2}\right)$$

$$a_E = \left(D_e - \frac{F_e}{2}\right)$$

$$a_P = a_W + a_E + (F_e - F_w)$$

  - ✓ For the boundary nodes 1 and 5, from:

$$\frac{F_e}{2}(\phi_P + \phi_E) - \frac{F_w}{2}(\phi_W + \phi_P) = D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W)$$

→ For node 1, we have:

$$\frac{F_e}{2}(\phi_P + \phi_E) - F_A\phi_A = D_e(\phi_E - \phi_P) - D_A(\phi_P - \phi_A)$$

→ For node 5, we have:

$$F_B\phi_B - \frac{F_w}{2}(\phi_P + \phi_W) = D_B(\phi_B - \phi_P) - D_w(\phi_P - \phi_W)$$

→ Noting that $D_A = D_B = 2D$ and $F_A = F_B = F$

→ Compared with the general form:

$$a_P T_P = a_W T_W + a_E T_E + S_u$$

with

$$a_P = a_W + a_E + (F_e - F_w) - S_P$$

we have

Node	a_W	a_E	S_P	S_u
1	*0*	*D-F/2*	*-(2D+F)*	*(2D+F)φ_A*
2,3,4	*D+F/2*	*D-F/2*	*0*	*0*
5	*D+F/2*	*0*	*-(2D+F)*	*(2D-F)φ_B*

- Case 1, the values for each discretised equation are

Table 5.1

Node	a_W	a_E	S_u	S_p	$a_P = a_W + a_E - S_p$
1	0	0.45	$1.1\phi_A$	−1.1	1.55
2	0.55	0.45	0	0	1.0
3	0.55	0.45	0	0	1.0
4	0.55	0.45	0	0	1.0
5	0.55	0	$0.9\phi_B$	−0.9	1.45

✓ The resulting set of algebraic equations:

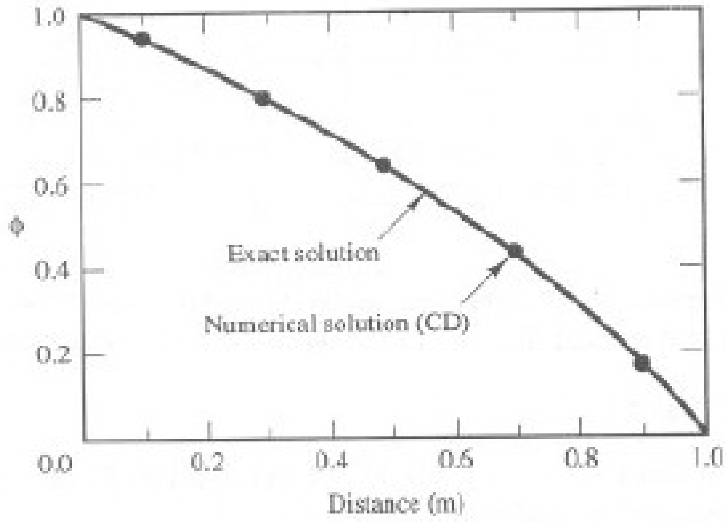
$$\begin{bmatrix} 1.55 & -0.45 & 0 & 0 & 0 \\ -0.55 & 1.0 & -0.45 & 0 & 0 \\ 0 & -0.55 & 1.0 & -0.45 & 0 \\ 0 & 0 & -0.55 & 1.0 & -0.45 \\ 0 & 0 & 0 & -0.55 & 1.45 \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \end{bmatrix} = \begin{bmatrix} 1.1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

✓ The solution of the system:

$$\begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \end{bmatrix} = \begin{bmatrix} 0.9421 \\ 0.8006 \\ 0.6276 \\ 0.4163 \\ 0.1579 \end{bmatrix}$$

✓ Compared with the exact solution (i.e. $\dfrac{\phi - \phi_0}{\phi_L - \phi_0} = \dfrac{\exp\left(\dfrac{\rho u x}{\Gamma}\right) - 1}{\exp\left(\dfrac{\rho u L}{\Gamma}\right) - 1}$)

Fig. 5.4 Comparison of numerical and analytical solutions for Case 1



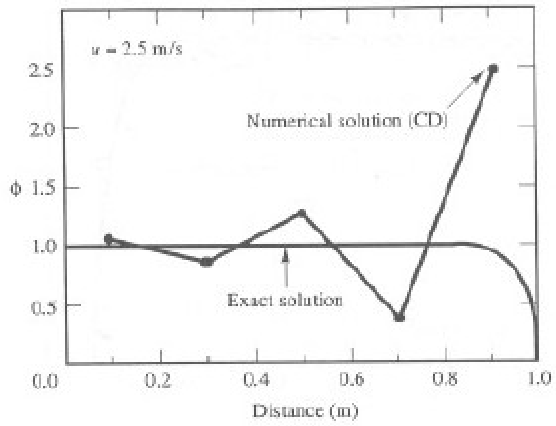
- Case 2, the values for each discretised equation are

Table 5.3

Node	a_W	a_E	S_u	S_p	$a_P = a_W + a_E - S_p$
1	0	−0.75	$3.5\phi_A$	−3.5	2.75
2	1.75	−0.75	0	0	1.0
3	1.75	−0.75	0	0	1.0
4	1.75	−0.75	0	0	1.0
5	1.75	0	$-1.5\phi_B$	1.5	0.25

✓ Compared with the exact solution

Fig. 5.5 Comparison of numerical and analytical solutions for Case 2



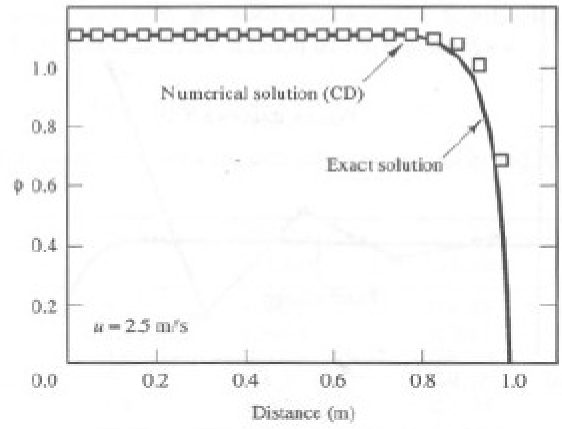
- Case 3, the values for each discretised equation are

Table 5.5

Node	a_W	a_E	S_u	S_p	$a_P = a_W + a_E - S_p$
1	0	0.75	$6.5\phi_A$	−6.5	7.25
2–19	3.25	0.75	0	0	4.00
20	3.25	0	$5\phi_B$	−1.5	4.75

✓ Compared with the exact solution

Fig. 5.6 Comparison of numerical and analytical solutions for Case 3

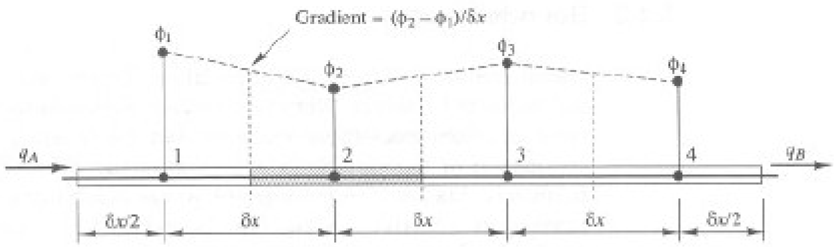


3. Properties of discretisation schemes

- ✓ The numerical results will only be physically realistic when the discretisation scheme has certain fundamental properties: Conservativeness, Boundedness and Transportiveness

- Conservativeness

Fig. 5.7 Example of consistent specification of diffusive fluxes



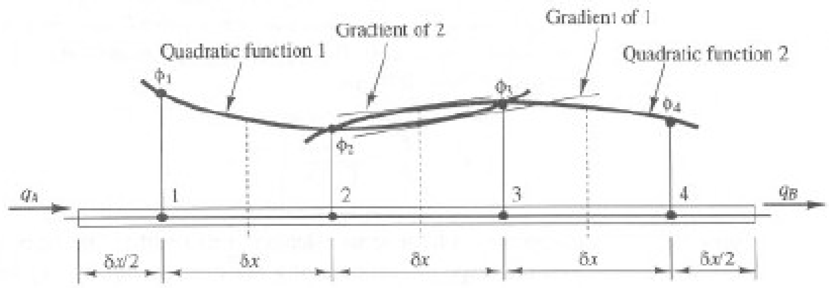
An overall flux balance:

$$\left(\Gamma_{e1}\frac{(\phi_2-\phi_1)}{\delta x}-q_A\right)+\left(\Gamma_{e2}\frac{(\phi_3-\phi_2)}{\delta x}-\Gamma_{w2}\frac{(\phi_2-\phi_1)}{\delta x}\right)$$
$$+\left(\Gamma_{e3}\frac{(\phi_4-\phi_3)}{\delta x}-\Gamma_{w3}\frac{(\phi_3-\phi_2)}{\delta x}\right)+\left(q_B-\Gamma_{w4}\frac{(\phi_4-\phi_3)}{\delta x}\right)$$
$$=q_B-q_A$$

- ✓ Flux consistency ensures conservation of φ over the entire domain for the central difference formulation of the diffusion flux.
- ✓ In consistent flux interpolation formulae give rise to unsuitable schemes that do not satisfy overall conservation.
- ✓ 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 gradient 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.
- ✓ This should not suggest that the quadratic interpolation is entirely bad. A

popular quadratic discretisation practice, the so-called QUICK scheme.

Fig. 5.8 Example of inconsistent specification of diffusive fluxes



- Boundedness
  - ✓ When solving a set of algebraic equations, normally iterative numerical techniques are used. Scarborough (1958) has shown that a sufficient condition for a convergent iterative method can be expressed in terms of the values of the coefficient of the discretised equations:

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

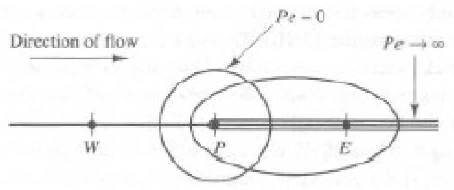
    a'_P is the net coefficient of the central node P (i.e. $a_P - S_P$) and the summation in the numerator is taken over all the neighbouring nodes (nb).
  - ✓ If the differencing scheme produces coefficients that satisfy the criterion, the resulting matrix of coefficients is diagonally dominated.
  - ✓ For diagonally dominance, we need large values of net coefficient ($a_P - S_P$). (i.e. the linearisation practice of source terms should ensure that S_P is negative.)
  - ✓ Diagonal dominance states that in the absence of sources the internal nodal values of the 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 A 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.
- Transportiveness
  - ✓ Define the non-dimensional cell Peclet number as a measure of the relative strengths of convection and diffusion:

$$Pe = \frac{F}{D} = \frac{\rho u}{\Gamma / \delta x}$$

    where δx = characteristic length (cell width).

- ✓ Two extreme cases: (1) no convection and pure diffusion ($Pe = 0$) and (2) no diffusion and pure convection ($Pe \to \infty$)
- ✓ It is very important that the relationship between the magnitude of the Peclet number and the directionality of influencing, known as the transportiveness, is borne out in the discretisation scheme.

Fig. 5.9 Distribution of ϕ in the vicinity of a source at different Peclet numbers



4. 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.
- Boundedness
  - ✓ The internal coefficients of discretised scalar transport equation are:

a_W	a_E	a_P
$D_w+F_w/2$	$D_e-F_e/2$	$a_W+a_E+(F_e-F_w)$

  - ✓ The expression for $a_P = a_W+a_E$ which satisfies the Scarborough criterion.
  - ✓ With $a_E = D_e-F_e/2$, given that $F_w > 0$ and $F_e > 0$ (i.e. the flow is unidirectional), for a_E to be positive: $F_e/D_e = Pe_e < 2$.
    - → The previous example case 2 with $Pe = 5$ gave bad result while cases 1 and 3 gave bounded answers with $Pe < 2$
- 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 recongnise the direction of the flow or the strength of convection relative to diffusion.
  - ✓ It does not possess the transportiveness property at high Pe.
- Accuracy
  - ✓ $$Pe = \frac{F}{D} = \frac{\rho u}{\Gamma/\delta x} < 2$$
  - ✓ For given values of ρ and Γ, it is only possible to satisfy the condition if the velocity is small, hence in diffusion-dominated low Reynolds number flows, or

if the grid spacing is small.

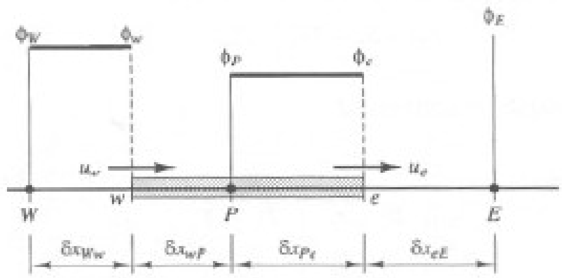
- ✓ Owing to this limitation central differencing is not a suitable discretisation practice for general purpose flow calculations.
- ✓ Other schemes: upwind, hybrid, power-low and QUICK schemes.

5. The upwind differencing scheme

- One major inadequacy of the central differencing scheme is its inability to identify flow direction. In a strong 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 is taken to be equal to the value at the upstream node.

- When the flow is in the positive direction:

Fig. 5.10



✓ $u_w > 0$ and $u_e > 0$ ($F_w > 0$ and $F_e > 0$), the upwind scheme sets:

→ $\phi_w = \phi_W$ and $\phi_e = \phi_P$

→ the discretised equation is:

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

re-arranging

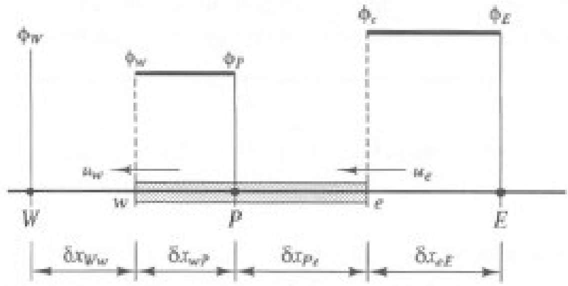
$$(D_w + D_e + F_e)\phi_P = (D_w + F_w)\phi_W + D_e\phi_E$$

or

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

- When the flow is in the negative direction:

Fig. 5.11



- ✓ $u_w < 0$ and $u_e < 0$ ($F_w < 0$ and $F_e < 0$), the upwind scheme sets:
  - → $\phi_w = \phi_P$ and $\phi_e = \phi_E$
  - → the discretised equation is:

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

    re-arranging

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

- Compared with the general form:

  $$a_P\phi_P = a_W\phi_W + a_E\phi_E$$

  with central coefficient

  $$a_P = a_W + a_E + (F_e - F_w)$$

  we have

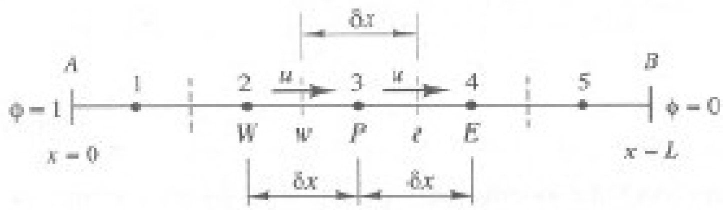
	a_W	a_E
$F_w > 0$ $F_e > 0$	D_w+F_w	D_e
$F_w < 0$ $F_e < 0$	D_w	D_e-F_e

or

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

Example: the same example as the previous one.

Fig. 5.3 The grid used for discretisation



- Internal nodes 2, 3 and 4
  - ✓ Since $F = F_e = F_w = \rho u$ and $D = D_e = D_w = \Gamma/\delta x$, the discretised equation at and the relevant neighbour coefficients are given by the above accompany tables.
- Boundary nodes 1 and 5
  - ✓ At the boundary node 1, the upwind scheme gives:

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

  - ✓ At the boundary node 5, the upwind scheme gives:

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

  - ✓ Since at the boundary nodes: $F_A = F_B = F = \rho u$ and $D_A = D_B = 2\Gamma/\delta x = 2D$, compared with the general form:

$$a_P\phi_P = a_W\phi_W + a_E\phi_E + S_u$$

with

$$a_P = a_W + a_E + (F_e - F_w) - S_P$$

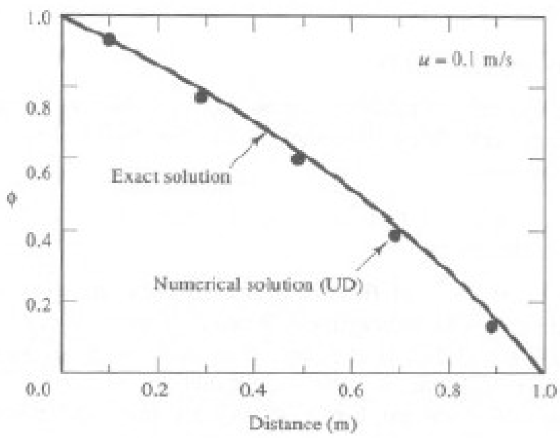
- We have:

Node	a_W	a_E	S_P	S_u
1	0	D	$-(2D+F)$	$(2D+F)\varphi_A$
2,3,4	$D+F$	D	0	0
5	$D+F$	0	$-2D$	$2D\varphi_B$

- Case 1: $u = 0.1\ m/s$, $F = \rho u = 0.1$, $D = \Gamma/\delta x = 0.1/0.2 = 0.5$, $Pe = F/D = 0.2$.

  → Comparison:

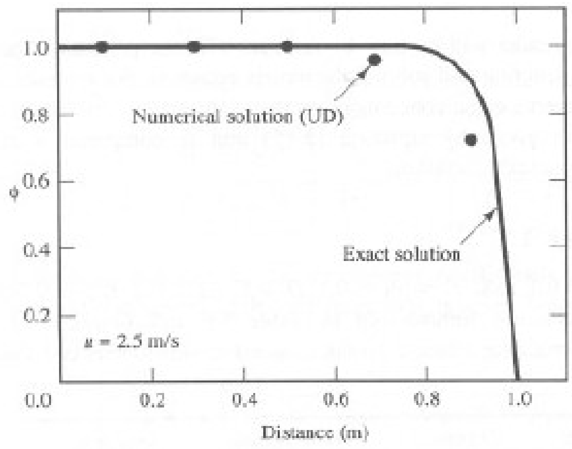
Fig. 5.12 Comparison of the upwind difference numerical results and the analytical solution for Case 1



- Case 2: $u = 2.5\ m/s$, $F = \rho u = 2.5$, $D = \Gamma/\delta x = 0.1/0.2 = 0.5$, $Pe = F/D = 5$.

  → Comparison:

Fig. 5.13 Comparison of the upwind difference numerical results and the analytical solution for Case 2



- Assessment of the upwind differencing scheme
  - ✓ Conservativeness: Calculate fluxes through cell faces and the formulation is conservative.
  - ✓ Boundedness: All the coefficients are positive and the coefficient matrix is diagonally dominated.
  - ✓ Transportiveness: Accounts for the direction of flow.
  - ✓ Accuracy:
    - → Based on the backward differencing formula, the accuracy is first order on the basis of the Taylor series error.
    - → It can be easily extended to multi-dimensional problems.
    - → A major drawback is that it produces erroneous results when the flow is not aligned with the grid lines. The resulting error has a diffusion-like appearance and is referred to as "false diffusion".

Fig. 5.14 Flow domain for the illustration of false diffusion

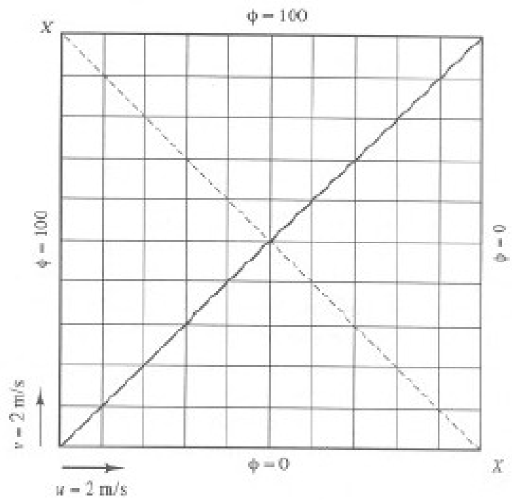
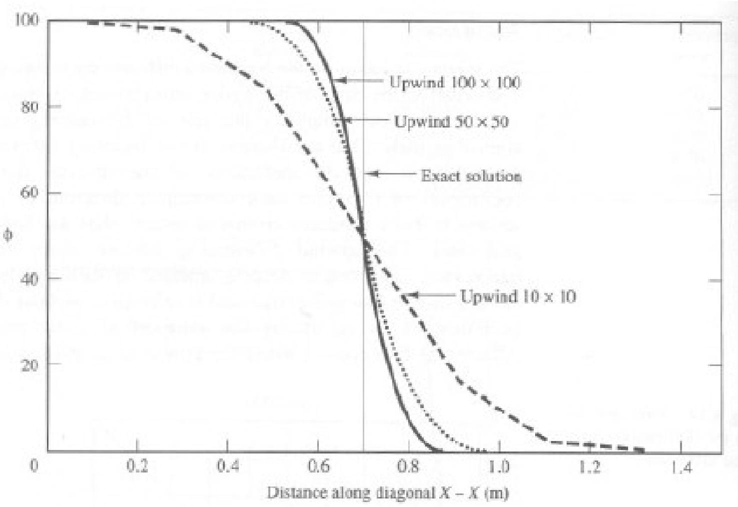


Fig. 5.15



→ The error is large for the coarsest grid and that refinement of the grid can, in principle, overcome the problem of false diffusion.

→ The upwind differencing scheme is not entirely suitable for accurate flow calculations.

6. The hybrid differencing scheme

- The hybrid differencing scheme of Spalding (1972) is based on a combination of central and upwind differencing schemes.
  - ✓ The central differencing scheme, which is accurate to second-order, is employed for small Peclet numbers (Pe < 2).
  - ✓ The upwind scheme, which is accurate to first order but accounts for transportiveness, is employed for large Peclet number (Pe $\geq$2).
- The hybrid differencing scheme uses pieces formulae based on the local Peclet number to evaluate the net flux through each control volume face:

$$q_w = F_w\left[\frac{1}{2}\left(1+\frac{2}{Pe_w}\right)\phi_W + \frac{1}{2}\left(1-\frac{2}{Pe_w}\right)\phi_P\right] \qquad \text{for } -2 < Pe_w < 2$$

$$q_w = F_w A_w \phi_W \qquad \text{for } Pe_w \geq 2$$

$$q_w = F_w A_w \phi_P \qquad \text{for } Pe_w \leq -2$$

- The general form of the discretised equation is:

  $$a_P\phi_P = a_W\phi_W + a_E\phi_E$$

  with central coefficient

  $$a_P = a_W + a_E + (F_e - F_w)$$

  For steady one-dimensional convection-diffusion, we have

a_W	a_E
$\max\left[F_w, \left(D_w + \frac{F_w}{2}\right), 0\right]$	$\max\left[-F_e, \left(D_e - \frac{F_e}{2}\right), 0\right]$

Example: Solve the problem in case 2 using the hybrid scheme.

- Case 2: *$u = 2.5$ m/s, $F = F_e = F_w = \rho u = 2.5$, $D = D_e = D_w = \Gamma/\delta x = 0.1/0.2 = 0.5$, $Pe_w = Pe_e = F/D = 5$.*
- Boundary nodes 1 and 5
  - ✓ At the boundary node 1, the hybrid scheme gives:

    $$F_e(\phi_P) - F_A(\phi_A) = 0 - D_A(\phi_P - \phi_A)$$

  - ✓ At the boundary node 5, the hybrid scheme gives:

    $$F_B(\phi_P) - F_w(\phi_W) = D_B(\phi_B - \phi_P) - 0$$

  - ✓ Since at the boundary nodes: $F_A = F_B = F = \rho u$ and $D_B = 2\Gamma/\delta x = 2D$, compared with the general form:

    $$a_P\phi_P = a_W\phi_W + a_E\phi_E + S_u$$

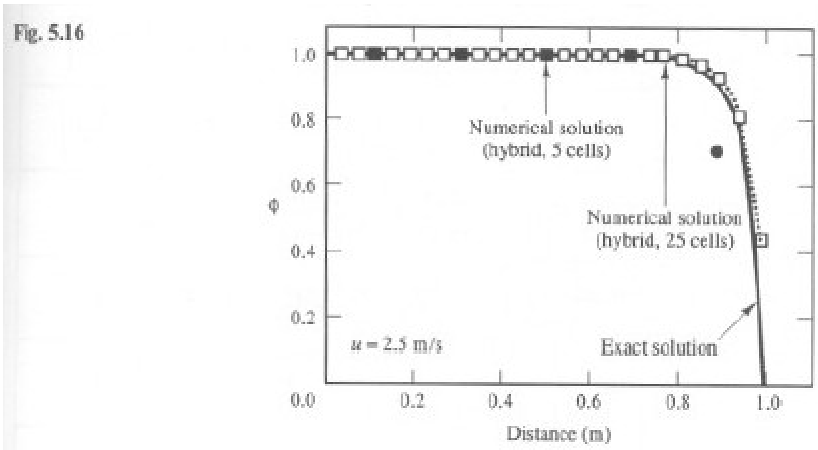
with

$$a_P = a_W + a_E + (F_e - F_w) - S_P$$

- We have:

Node	a_W	a_E	S_P	S_u
1	0	0	$-(2D+F)$	$(2D+F)\varphi_A$
2,3,4	F	0	0	0
5	F	0	$-2D$	$2D\varphi_B$

- Comparison:



- Assessment of the hybrid differencing scheme
  - ✓ The scheme is fully conservative and since the coefficients are always positive it is unconditionally bounded.
  - ✓ It satisfies the transportiveness requirement by using upwind formulation for large values of Peclet number.
  - ✓ Widely used in various CFD procedures.
  - ✓ The disadvantage is that the accuracy in terms of Taylor series truncation error is only first-order
- For multi-dimensional convection-diffusion
  - ✓ Repeated application of the derivation in each new coordinate direction.
  - ✓ The discretised equation that covers all cases is given by:

$$a_P\phi_P = a_W\phi_W + a_E\phi_E + a_S\phi_S + a_N\phi_N + a_B\phi_B + a_T\phi_T$$

with

$$a_P = a_W + a_E + a_S + a_N + a_B + a_T + \Delta F$$

✓ The values of F and D are:

Face	*w*	*e*	*s*	*n*	*b*	*t*
F	$(\rho u)_w A_w$	$(\rho u)_e A_e$	$(\rho u)_s A_s$	$(\rho u)_n A_n$	$(\rho u)_b A_b$	$(\rho u)_t A_t$
D	$\frac{\Gamma_w}{\delta x_{WP}} A_w$	$\frac{\Gamma_e}{\delta x_{PE}} A_e$	$\frac{\Gamma_s}{\delta y_{SP}} A_s$	$\frac{\Gamma_n}{\delta y_{PN}} A_n$	$\frac{\Gamma_b}{\delta z_{BP}} A_b$	$\frac{\Gamma_t}{\delta z_{PT}} A_t$

✓ The coefficients of the hybrid differencing scheme are:

	One-dimensional flow	Two-dimensional flow	Three-dimensional flow
a_W	$\max\left[F_w, \left(D_w + \frac{F_w}{2}\right), 0\right]$	$\max\left[F_w, \left(D_w + \frac{F_w}{2}\right), 0\right]$	$\max\left[F_w, \left(D_w + \frac{F_w}{2}\right), 0\right]$
a_E	$\max\left[-F_e, \left(D_e - \frac{F_e}{2}\right), 0\right]$	$\max\left[-F_e, \left(D_e - \frac{F_e}{2}\right), 0\right]$	$\max\left[-F_e, \left(D_e - \frac{F_e}{2}\right), 0\right]$
a_S	–	$\max\left[F_s, \left(D_s + \frac{F_s}{2}\right), 0\right]$	$\max\left[F_s, \left(D_s + \frac{F_s}{2}\right), 0\right]$
a_N	–	$\max\left[-F_n, \left(D_n - \frac{F_n}{2}\right), 0\right]$	$\max\left[-F_n, \left(D_n - \frac{F_n}{2}\right), 0\right]$
a_B	–	–	$\max\left[F_b, \left(D_b + \frac{F_b}{2}\right), 0\right]$
a_T	–	–	$\max\left[-F_t, \left(D_t - \frac{F_t}{2}\right), 0\right]$
ΔF	$F_e - F_w$	$F_e - F_w + F_n - F_s$	$F_e - F_w + F_n - F_s + F_t - F_b$

7. The power-law scheme

- The powder-law differencing scheme of Patankar (1980) is a more accurate approximation to the one-dimensional exact solution than the hybrid scheme.
- Diffusion is set to zero when cell *Pe* exceeds 10.
- If $0 < Pe < 10$, the flux is evaluate by using a polynomial expression.
- The net flux per unit area at the west control volume face:

✓ $q_w = F_w[\phi_W - \beta_w(\phi_P - \phi_W)]$ for $0 < Pe < 10$

where

$$\beta_w = {(1-0.1Pe_w)^5}/{Pe_w}$$

✓ $q_w = F_w\phi_W$ for $Pe > 10$

- The coefficients of the one-dimensional discretised equation for steady one-dimensional convection-diffusion are given by:

  central coefficient

  $$a_P = a_W + a_E + (F_e - F_w)$$

  and

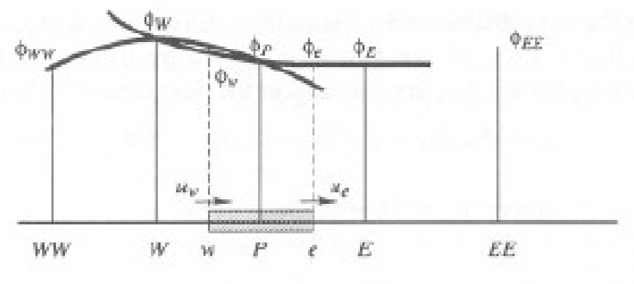
a_W	a_E
$D_w \max\left[0, \left(1 - 0.1\|Pe_w\|^5\right)\right] + \max[F_w, 0$	$D_e \max\left[0, \left(1 - 0.1\|Pe_e\|^5\right)\right] + \max[-F_e$

- The scheme has proved to be useful in practical flow calculations (Fluent V4.22)

8. Higher order differencing schemes for convection-diffusion problems

- Higher order schemes involve more neighbour points and reduce the discretisation errors by bringing in a wider influence.
- Quadratic upwind differrencing scheme: the QUICK scheme
  - ✓ The quadratic upstream interpolation for convective kinetics (QUICK) scheme of Leonard (1979) uses a three-point upstream-weighted quadratic interpolation for cell face values.
  - ✓ The face value of φ is obtained from a quadratic function passing through two bracketing nodes (on each side of the face) and a node on the upstream side:

Fig. 5.17 Quadratic profiles used in the QUICK scheme



→ The cell face between two bracketing nodes i and i -1 and upstream node i -2: $\phi_{face} = \frac{6}{8}\phi_{i-1} + \frac{3}{8}\phi_i - \frac{1}{8}\phi_{i-2}$

→ When $u_w > 0$ and $u_e > 0$, a quadratic fit through WW, A and P is used to evaluate φ_w, and a further quadratic fit through W, P and E to calculate φ_e:

$$\phi_w = \frac{6}{8}\phi_W + \frac{3}{8}\phi_P - \frac{1}{8}\phi_{WW}$$

$$\phi_e = \frac{6}{8}\phi_P + \frac{3}{8}\phi_E - \frac{1}{8}\phi_W$$

→ When $u_w < 0$ and $u_e < 0$, a quadratic fit through W, P and E is used to evaluate φ_w, and a further quadratic fit through P, E and EE to calculate φ_e.

→ If $F_w > 0$ and $F_e > 0$, the discretised form of the one-dimensional convection-diffusion transport equation is:

$$\left[F_e\left(\frac{6}{8}\phi_P + \frac{3}{8}\phi_E - \frac{1}{8}\phi_W\right) - F_w\left(\frac{6}{8}\phi_W + \frac{3}{8}\phi_P - \frac{1}{8}\phi_{WW}\right)\right] = D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W)$$

re-arranging:

$$\left[D_w - \frac{3}{8}F_w + D_e + \frac{6}{8}F_e\right]\phi_P = \left[D_w + \frac{6}{8}F_w + \frac{1}{8}F_e\right]\phi_W + \left[D_e - \frac{3}{8}F_e\right]\phi_E - \frac{1}{8}F_w\phi_{WW}$$

→ The standard general form:

$$a_P\phi_P = a_W\phi_W + a_E\phi_E + a_{WW}\phi_{WW}$$

with

a_W	a_E	a_{EE}	a_P
$\left[D_w + \frac{6}{8}F_w + \frac{1}{8}F_e\right]$	$\left[D_e - \frac{3}{8}F_e\right]$	$-\frac{1}{8}F_w$	$a_W + a_E + a_{WW} + (F_e - F_w)$

→ The QUICK scheme for one-dimensional convection-diffusion problems:

$$a_P\phi_P = a_W\phi_W + a_E\phi_E + a_{WW}\phi_{WW} + a_{EE}\phi_{EE}$$

with central coefficient

$$a_P = a_W + a_E + a_{WW} + a_{EE} + (F_e - F_w)$$

and neighbour coefficients

a_W	a_{WW}	a_E	a_{EE}
$\left[D_w + \frac{6}{8}\alpha_w F_w + \frac{1}{8}\alpha_e F_e + \frac{3}{8}(1-\alpha_w)F_w\right]$	$-\frac{1}{8}\alpha_w F_w$	$\left[D_e - \frac{3}{8}\alpha_e F_e - \frac{6}{8}(1-\alpha_e)F_e - \frac{1}{8}(1-\alpha_w)F_w\right]$	$\frac{1}{8}(1-\alpha_e)F_e$

where

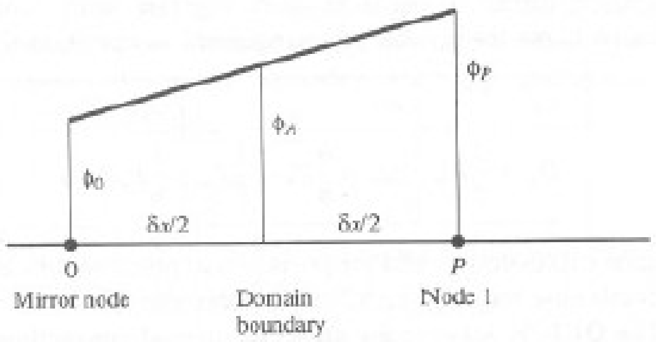
$\alpha_w = 1$ for $F_w > 0$ and $\alpha_e = 1$ for $F_e > 0$

$\alpha_w = 0$ for $F_w < 0$ and $\alpha_e = 0$ for $F_e < 0$

Example: using the QUICK scheme solve the problem for u = 0.2 m/s on a 5-point grid.

- *u = 0.2 m/s, $F = F_e = F_w = \rho u = 0.2$, $D = D_e = D_w = \Gamma/\delta x = 0.1/0.2 = 0.5$, $Pe_w = Pe_e = F/D = 0.4$.*
- the discretisation equation with the QUICK scheme at internal nodes 3 and 4 is given by the previous table.
- Nodes 1, 2 and 5 are all affected by the domain boundaries. Leonard (1979) suggests a linear extrapolation to create a "mirror" node at a distance δx/2 to the west of the physical boundary.

Fig. 5.18 Mirror node treatment at the boundary



- At node 1
  - ✓ φ_e at the east face of control volume 1:

$$\phi_e = \frac{6}{8}\phi_P + \frac{3}{8}\phi_E - \frac{1}{8}\phi_0 = \frac{6}{8}\phi_P + \frac{3}{8}\phi_E - \frac{1}{8}(2\phi_A - \phi_P) = \frac{7}{8}\phi_P + \frac{3}{8}\phi_E - \frac{2}{8}\phi_A$$

  - ✓ The diffusive flux through the west boundary is:

$$\Gamma\frac{\partial\phi}{\partial x}\Big|_A = \frac{D_A}{3}(9\phi_P - 8\phi_A - \phi_E)$$

  - ✓ The discretised equation at node 1 is:

$$F_e\left[\frac{7}{8}\phi_P + \frac{3}{8}\phi_E - \frac{2}{8}\phi_A\right] - F_A\phi_A = D_e(\phi_E - \phi_P) - \frac{D_A}{3}(9\phi_P - 8\phi_A - \phi_E)$$

- At node 5
  - ✓ The diffusive flux through the east boundary is:

$$\Gamma\frac{\partial\phi}{\partial x}\Big|_B = \frac{D_B}{3}(8\phi_B - 9\phi_P + \phi_W)$$

  - ✓ The discretised equation at node 5:

$$F_B\phi_B - F_w\left[\frac{6}{8}\phi_W + \frac{3}{8}\phi_P - \frac{1}{8}\phi_{WW}\right] = \frac{D_B}{3}(8\phi_B - 9\phi_P + \phi_W) - D_w(\phi_P - \phi_W)$$

- At node 2
  - ✓ The discretised equation at node 2:

$$F_e\left[\frac{6}{8}\phi_P+\frac{3}{8}\phi_E-\frac{1}{8}\phi_W\right]-F_w\left[\frac{7}{8}\phi_W+\frac{3}{8}\phi_P-\frac{2}{8}\phi_A\right]=D_e(\phi_E-\phi_P)-D_w(\phi_P-\phi_W)$$

- Compared with the general form:

$$a_P\phi_P = a_W\phi_W + a_E\phi_E + a_{WW}\phi_{WW} + S_u$$

with central coefficient

$$a_P = a_W + a_E + a_{WW} + (F_e - F_w) - S_P$$

and neighbour coefficients

Node	a_{WW}	a_W	a_E	S_P	S_u
1	*0*	*0*	$\left[D_e+\frac{1}{3}D_A-\frac{3}{8}F\right.$	$-\left[\frac{8}{3}D_A+\frac{2}{8}F_e+F\right.$	$\left[\frac{8}{3}D_A+\frac{2}{8}F_e+F_A\right]$
2	*0*	$\left[D_w+\frac{7}{8}F_w+\frac{1}{8}F\right.$	$\left[D_e-\frac{3}{8}F_e\right]$	$\frac{1}{4}F_w$	$-\frac{1}{4}F_w\phi_A$
5	$-\frac{1}{8}F$	$\left[D_w+\frac{1}{3}D_B+\frac{6}{8}F\right.$	*0*	$-\left[\frac{8}{3}D_B-F_B\right]$	$\left[\frac{8}{3}D_B-F_B\right]\phi_B$

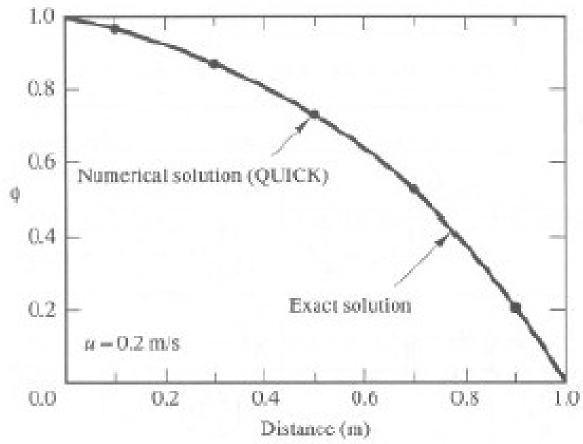
- Substitute the numerical values:

Table 5.10

Node	a_W	a_E	a_{WW}	S_u	S_P	a_P
1	0	0.592	0	$1.583\phi_A$	−1.583	2.175
2	0.7	0.425	0	$-0.05\phi_A$	0.05	1.075
3	0.675	0.425	−0.025	0	0	1.075
4	0.675	0.425	−0.025	0	0	1.075
5	0.817	0	−0.025	$1.133\phi_B$	−1.133	1.925

- Comparison

Fig. 5.19 Comparison of QUICK solution with the analytical solution



- Assessment of the QUICK scheme
  - ✓ The cell face values of fluxes are conservative.
  - ✓ Its accuracy in terms of the Taylor series truncation error is third order on a uniform mesh.
  - ✓ The transportiveness property is built into the scheme using two upstream and one downstream nodal values.

- ✓ Boundedness:
  - → If the flow field satisfies continuity, the coefficient a_P equals the sum of all neighbour coefficient which is desirable for bounded.
- ✓ The main coefficients (E and W) are not guaranteed to be positive and the coefficients a_{WW} and a_{EE} are negative. This give rise to stability problems and unbounded solutions under certain flow conditions.
- ✓ Since the discretised equations involve not only immediate-neighbour nodes but also nodes further away. Tri-diagonal matrix solution (TDMA) methods are not directly applicable.
- ✓ The QUICK scheme is conditionally stable:
  - → The Hayase et al. (1990) QUICK scheme:

$$\phi_w = \phi_W + \frac{1}{8}(3\phi_P - 2\phi_W - \phi_{WW}) \qquad \text{for } F_w > 0$$

$$\phi_e = \phi_P + \frac{1}{8}(3\phi_E - 2\phi_P - \phi_W) \qquad \text{for } F_e > 0$$

$$\phi_w = \phi_P + \frac{1}{8}(3\phi_W - 2\phi_P - \phi_E) \qquad \text{for } F_w < 0$$

$$\phi_e = \phi_E + \frac{1}{8}(3\phi_P - 2\phi_E - \phi_{EE}) \qquad \text{for } F_e < 0$$

  - → The discritised equation:

$$a_P\phi_P = a_W\phi_W + a_E\phi_E + \bar{S}$$

with central coefficient

$$a_P = a_W + a_E + (F_e - F_w)$$

a_W	a_E	$\bar{S}$
$D_w + \alpha_w F_w$	$D_e - (1-\alpha_e)F$	$\frac{1}{8}(3\phi_P - 2\phi_W - \phi_{WW})\alpha_w F_w + \frac{1}{8}(\phi_W + 2\phi_P - 3\phi_E)\alpha_e F_E$ $+\frac{1}{8}(3\phi_W - 2\phi_P - \phi_E)(1-\alpha_w)F_w + \frac{1}{8}(2\phi_E + \phi_{EE} - 3\phi_P)(1$

where

$\alpha_w = 1$ for $F_w > 0$ and $\alpha_e = 1$ for $F_e > 0$

$\alpha_w = 0$ for $F_w < 0$ and $\alpha_e = 0$ for $F_e < 0$

9. Summary

- The crucial issue of discrettising the convection-diffusion equation is the formulation of suitable expressions for the values of the transported property φ at cell faces when accounting for the convective contribution in the equation.
- Discretisation scheme that posses conservativeness, boundedness and

transportiveness give physically realistic results and stable iterative solutions.

- ✓ The central differencing scheme lacks transportiveness and gives unrealistic solutions at large values of the cell Peclet number.
- ✓ Upwind, hybrid and power-law differencing scheme possess conservativeness, boundedness and transportiveness and are hightly stable, but suffer from false diffusion in multi-dimensional flows if the velocity vectors is not parallel to one of the co-ordinate directions.

- Higher order schemes, such as QUICK, can minimise false diffusion errors but are less computationally stable. This causes small over- and undershoots in the solutions of some problems including those with large gradients of φ.