Convection and Diffusion

General Differential Equation

$$\frac{\partial}{\partial t}(\rho\Phi) + div(\rho\, u\, \Phi) = div(\gamma\ grad\ \Phi) + S$$

Where

$\frac{\partial}{\partial t}(\rho\Phi)$ ➔Unsteady term

$div(\rho\, u\, \Phi)$ ➔Convective term

$div(\gamma\ grad\ \Phi)$ ➔Diffusion term

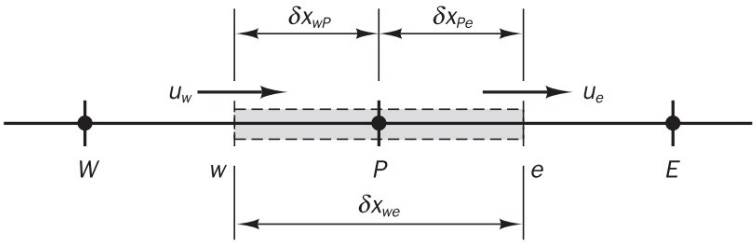
S ➔Source term

Φ ➔Dependent variable (example mass, pressure, temperature, etc.)

$$\frac{d}{dx}(\rho\, u\, \Phi) = \frac{d}{dx}\left(\gamma\ \frac{d\Phi}{dx}\right)$$

This is the governing equation of steady state 1D convection diffusion of a property Φ

For flow, continuity equation also must be satisfied $\frac{d}{dx}(\rho\, u\ ) = 0$



Integration of transport equation over control volume is

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

$$\int_{w}^{e}\left(\frac{\mathrm{d}}{\mathrm{dx}}\left(\Gamma\frac{\mathrm{d}\phi}{dx}\right)A\ dx\right) = \int_{w}^{e}\left(\frac{\mathrm{d}}{\mathrm{dx}}(\rho u\phi)\ A\ dx\right)$$

$$(\rho uA\phi)_w^e = \left(\Gamma A\frac{\mathrm{d}\phi}{\mathrm{d}x}\right)_w^e$$

$$(\rho u\phi)_e - (\rho u\phi)_w = \left(\Gamma \frac{\mathrm{d}\phi}{\mathrm{d}x}\right)_e - \left(\Gamma \frac{\mathrm{d}\phi}{\mathrm{d}x}\right)_w$$

And integration of continuity equation yields

$$(\rho u A)_e - (\rho u A)_w = 0$$

To obtain discretised equations for the convection-diffusion problem we must approximate the terms in equation. It is convenient to define two variables F and D to represent the convective mass flux per unit area and diffusion conductance at cell faces:

$$F = \rho u \text{ and } D = \frac{\Gamma}{\delta x}$$

The cell face values of the variables F and D can be written as

$$F_w = (\rho u)_w \quad F_e = (\rho u)_e$$
$$D_w = \frac{\Gamma_w}{\delta x_{WP}} \quad D_e = \frac{\Gamma_e}{\delta x_{PE}}$$

$$Pe = \frac{F}{D}$$

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

$$F_e - F_w = 0$$

Central difference scheme for convective term on cell face

Using central difference scheme in a uniform grid linearly interpolated values for ϕ_w and ϕ_e are given by

$$\phi_e = (\phi_P + \phi_E)/2$$
$$\phi_w = (\phi_W + \phi_P)/2$$

Hence, the CD expression becomes

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

On rearranging, we get

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

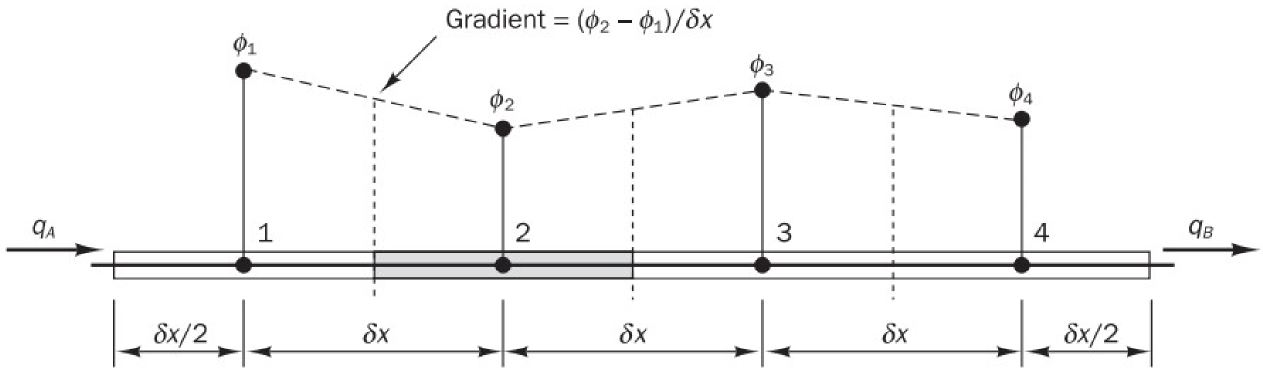
$$a_P\phi_P = a_W\phi_W + a_E\phi_E$$

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

Properties of Discretization Scheme

1 - Conservativeness

Integration of the convection–diffusion equation over a finite number of control volumes yields a set of discretised conservation equations involving fluxes of the transported property φ through control volume faces. To ensure conservation of φ for the whole solution domain the flux of φ leaving a control volume across a certain face must be equal to the flux of φ entering the adjacent control volume through the same face. To achieve this the flux through a common face must be represented in a consistent manner by the same expression in adjacent control volumes.



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. 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 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’.

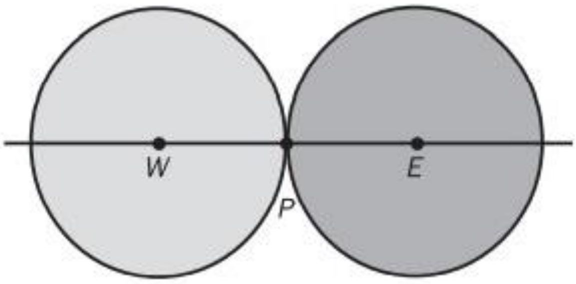
3 - Transportiveness

We define the non-dimensional cell Peclet number as a measure of the relative strengths of convection and diffusion:

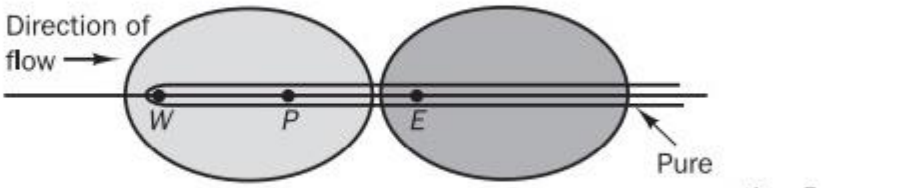
$$Pe = \frac{F}{D} = \frac{\rho u}{\gamma/\delta x}$$

where δx = characteristic length (cell width)

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



(a)



(b)

- no convection and pure diffusion (Pe → 0)
- no diffusion and pure convection (Pe → ∞)

In the case of pure diffusion the fluid is stagnant (Pe → 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 (a) shows that both φ = 1 contours pass through P, indicating that conditions at this point are influenced by both sources at W and E.

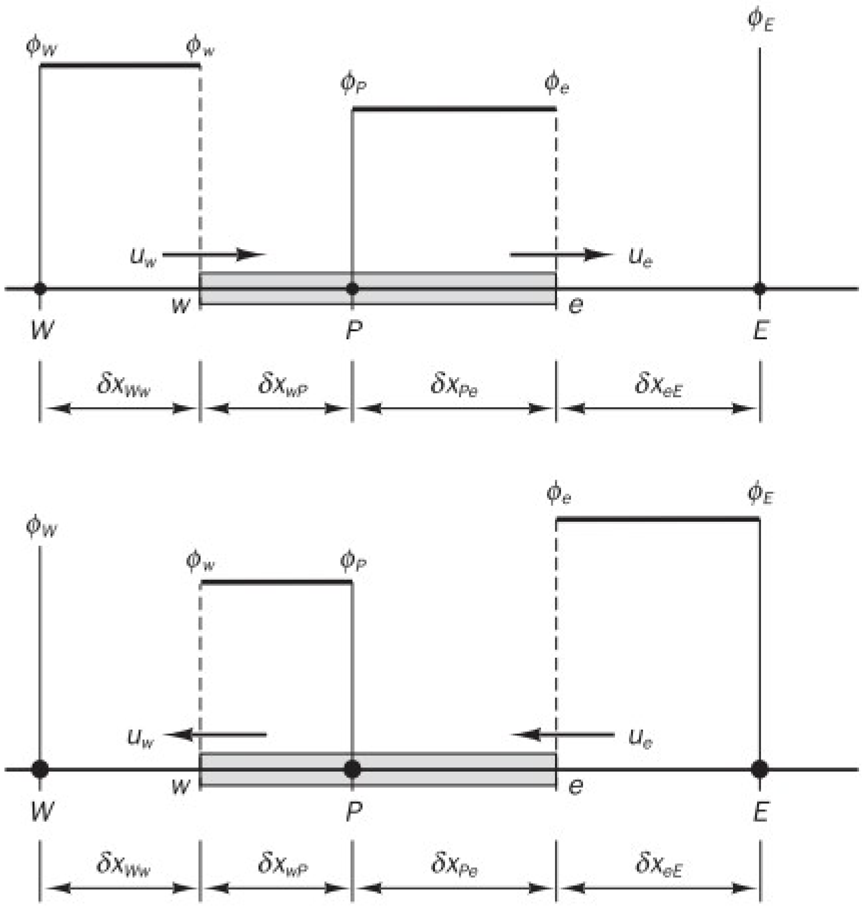
As Pe increases the contours change shape from circular to elliptical and are shifted in the direction of the flow as shown in Figure (b). Influencing becomes increasingly biased towards the upstream direction at large values of Pe, so, in the present case where the flow is in the positive x-direction, conditions at P will be mainly influenced by the upstream source at W. In the case of pure convection

(Pe → ∞) 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.

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.

Upwind

The upwind differencing or 'donor cell' differencing scheme takes into account the flow direction



When the flow is in the positive direction,

$$u_w > 0, u_e > 0 \left(F_p > 0, F_e > 0\right)$$

the upwind scheme sets $\phi_w = \phi_W$ and $\phi_e = \phi_P$

and the discretised equation becomes

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

which can be rearranged as

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

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

When the flow is in the negative direction

$$u_w < 0, u_e < 0(F_w < 0, F_e < 0)$$

the scheme takes

$$\phi_w = \phi_P \text{ and } \phi_e = \phi_E$$

Now the discretised equation is

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

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

Both equation can be written in general form as

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

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

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

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 second-order accurate, is employed for small Peclet numbers (Pe < 2) and the upwind scheme, which is first-order accurate but accounts for transportiveness, is employed for large Peclet numbers (Pe ≥ 2). As before, we develop the discretisation of the one-dimensional convection– diffusion equation without source terms. This equation can be interpreted as a flux balance equation. The hybrid differencing scheme uses piecewise formulae based on the local Peclet number to evaluate the net flux through each control volume face. The Peclet number is evaluated at the face of the control volume. For example, for a west face,

$$Pe_m = \frac{F_w}{D_w} = \frac{(\rho u)_w}{\Gamma_w/\delta x_{WP}}$$

The hybrid differencing formula for the net flux per unit area through the west face is as follows:

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

It can be easily seen that for low Peclet numbers this is equivalent to using central differencing for the convection and diffusion terms, but when |Pe| > 2 it is equivalent to upwinding for convection and setting the diffusion to zero. The general form of the discretised equation is

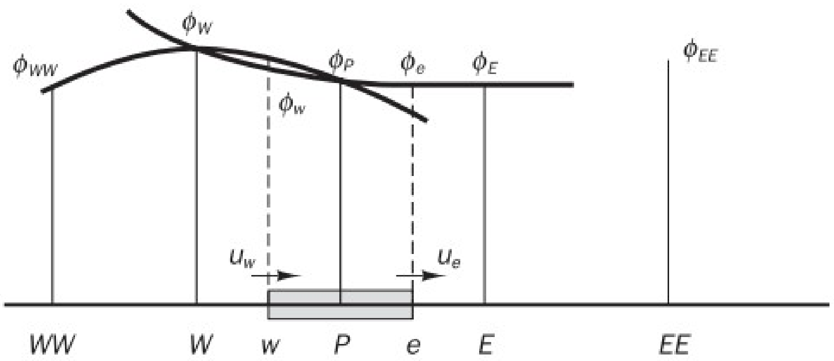
$$a_P\phi_P = a_W\phi_W + a_E\phi_E$$

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

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

Quadratic upwind differencing 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.



For example, when $u_w > 0$ and $u_e > 0$ a quadratic fit through WW, W and P is used to evaluate ϕ_w, and a further quadratic fit through W, P and E to calculate ϕ_e. For $u_w < 0$ and $u_e < 0$ values of ϕ at

W, P and E are used for ϕ_m and values at P, E and EE for ϕ_e. It can be shown that for a uniform grid the value of ϕ at the cell face between two bracketing nodes i and $i-1$ and upstream node $i-2$ is given by the following formula:

$$\phi_{\text{face}} = \frac{6}{8}\phi_{i-1} + \frac{3}{8}\phi_i - \frac{1}{8}\phi_{i-2}$$

When $u_w > 0$, the bracketing nodes for the west face w are W and P, the upstream node is WW (Figure 5.17) and

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

When $u_e > 0$, the bracketing nodes for the east face e are P and E, the upstream node is W, so

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

The diffusion terms may be evaluated using the gradient of the approximating parabola (It is same expressions as central differencing for diffusion). If $F_w > 0$ and $F_c > 0$, and if we use equations for the convective terms and central differencing for the diffusion terms, the discretised form of the one-dimensional convection diffusion transport equation may be written as

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

which can be rearranged to give

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

This is now written in the standard form for discretised equations:

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

where

a_W	a_E	a_{WW}	a_P
$D_m + \frac{6}{8}F_w + \frac{1}{8}F_e$	$D_e - \frac{3}{8}F_e$	$-\frac{1}{8}F_w$	$a_W + a_E + a_{WW} + (F_e - F_m)$

For $F_x < 0$ and $F_e < 0$ the flux across the west and east boundaries is given by the expressions

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

Substitution of these two formulae for the convective terms in the discretised convection-diffusion equation (5.9) together with central differencing for the diffusion terms leads, after rearrangement as above, to the following coefficients:

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

General expressions, valid for positive and negative flow directions, can be obtained by combining the two sets of coefficients above.

The QUICK scheme for one-dimensional convection-diffusion problems can be summarised as follows:

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

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

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