Temporal Discretisation

The temporal discretisation is carried out by choosing a time stepsize δt and letting $t_n = n\delta t$ for $n = 0, 1, \ldots$. Returning to (7), one way to proceed is to integrate from time t_n to t_{n+1} to obtain

$$\int_{t_n}^{t_{n+1}} \frac{\mathrm{d}\varphi_P}{\mathrm{d}t}\,\mathrm{d}t = \int_{t_n}^{t_{n+1}} \frac{1}{\Delta x_P}(J_w - J_e)\,\mathrm{d}t + \int_{t_n}^{t_{n+1}} S_P\,\mathrm{d}t\,.$$

We consider a general **theta method** for approximating the integrals in time:

$$\varphi_P^{n+1} - \underbrace{\varphi_P^n}_{=\,\varphi_P(t_n)} = \frac{\delta t}{\Delta x_P}\left[\theta_1\left(J_w^{n+1} - J_e^{n+1}\right) + (1-\theta_1)\,(J_w^n - J_e^n)\right]$$
$$+\,\delta t\left[\theta_2 S_P^{n+1} + (1-\theta_2) S_P^n\right]. \qquad (12)$$

$\varphi_P(t)$

$\varphi_P(t_{n+1}) := \varphi_P^{n+1}$

left-hand rule.

The above exercise allows us to conclude that if $\theta = 0$, which is known as the **forward Euler method**, then

Explicit

$$\int_{t_n}^{t_{n+1}} f(t)\,\mathrm{d}t = \delta t\, f(t_n) + \mathcal{O}(\delta t^2)$$

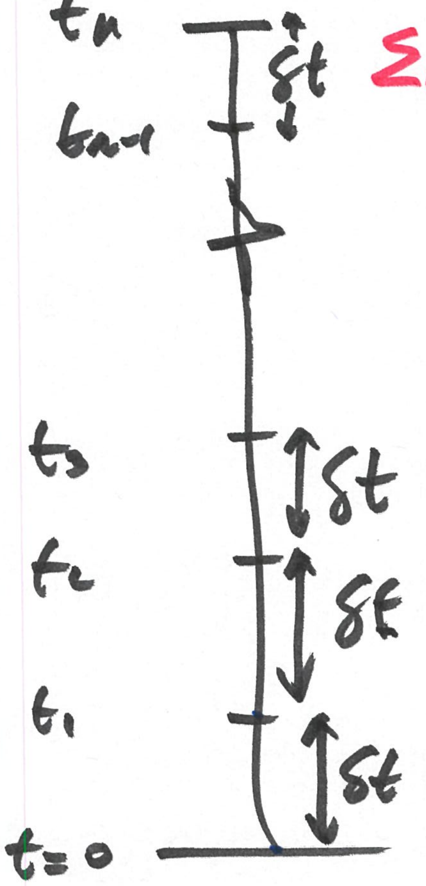
and the *local* error associated with the temporal discretisation is $\mathcal{O}(\delta t^2)$, and hence the *global* error is $\mathcal{O}(\delta t)$: it is *first order in time*.

right-hand rule.

The same is true for the choice $\theta = 1$, which is known as the **backward Euler method**, where

Implicit.

$$\int_{t_n}^{t_{n+1}} f(t)\,\mathrm{d}t = \delta t\, f(t_{n+1}) + \mathcal{O}(\delta t^2).$$



$\varepsilon_n = C\,\delta t^2 f''(\eta_n)$

$$\int_{t_n}^{t_{n+1}} f(t)\,dt \simeq \delta t\, f(t_{n+1}) \quad . \quad O(\delta t^2)$$

local error.

$\varepsilon_3 = C\,\delta t^2 f''(\eta_3)$

$\varepsilon_2 = C\,\delta t^2 f''(\eta_2) \leftarrow$ local error.

$\varepsilon_1 = C\,\delta t^2 f''(\eta_1) \leftarrow$ local error

Global Error

$t_n = \underbrace{n\,\delta t}$.

$$E = \sum_{i=1}^{n} \varepsilon_i = c\,\delta t^2 \sum_{i=1}^{n} f''(\eta_i)$$

$$= c\,\delta t^2 n \left[\frac{1}{n}\sum_{i=1}^{n} f''(\eta_i)\right] = \overline{f''}(\eta^*).$$

$$E = C^* \overline{f''}(\eta^*)\,\delta t$$

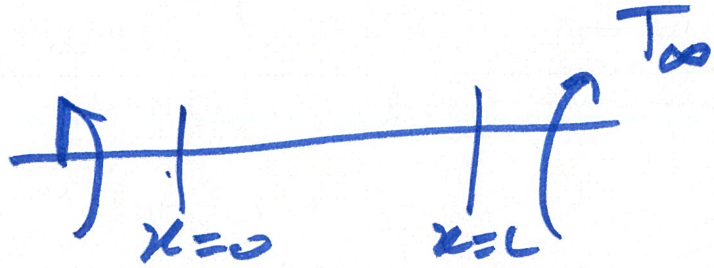
$O(\delta t)$.

MXB324 Prac 1

Finite Volume Method for Diffusion Equations

Topics:

- Diffusion Equation.
- Heating of Wood.
- Finite Volume Methods.
- Separation of Variables.



1.1 The Heating of Wood

The temperature within a piece of wood initially at some prescribed temperature T_0 being heated by hot convected air at temperature T_∞ over its boundaries at $x = 0$ and $x = L$ is governed by the following model:

$$\rho c \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2}, \qquad 0 < x < L, \qquad t > 0$$

subject to

$$\text{at } x = 0, \quad -k\frac{\partial T}{\partial x} + hT = hT_\infty, \quad t > 0$$

$$\text{at } x = L, \quad k\frac{\partial T}{\partial x} + hT = hT_\infty, \quad t > 0$$

$$\theta = \frac{T - T_\infty}{T_0 - T_\infty}$$

and

$$T(x, 0) = T_0, \quad 0 \leq x \leq L.$$

1. (OPTIONAL) Show that the analytical solution to this problem is given by

$$T(x,t) = T_\infty + (T_0 - T_\infty)\Theta(\xi, \tau) \qquad \text{where}$$

$$\Theta(\xi, \tau) = \sum_{n=1}^{\infty} \frac{\Psi(\mu_n, \xi)}{N(\mu_n)} \left(\sin\mu_n - \frac{B_i}{\mu_n}\cos\mu_n + \frac{B_i}{\mu_n} \right) e^{-\mu_n^2 \tau}$$

and

$$\Psi(\mu_n, \xi) = \mu_n \cos(\mu_n \xi) + B_i \sin(\mu_n \xi),$$

$$N(\mu_n) = \frac{1}{2}\left[(\mu_n^2 + B_i^2)\left(1 + \frac{B_i}{\mu_n^2 + B_i^2}\right) + B_i \right]$$

with $\xi = \frac{x}{L}$, $B_i = \frac{hL}{k}$, $\tau = \frac{k}{\rho c L^2} t$. The eigenvalues μ_n are the roots of the transcendental equation $\tan\mu_n = \frac{2B_i\mu_n}{\mu_n^2 - B_i^2}$.

2. Write a MATLAB function `ANALYTIC_WOOD` that implements the analytic solution of the diffusion equation.

3. Write a MATLAB function `FVM_WOOD` that implements the finite volume solution of the diffusion equation with options to use either a backward Euler or the Crank-Nicolson time stepping scheme. Use the MATLAB function `fsolve` to obtain the solution at each time step. You may wish to consider implementing generalised boundary conditions into your FVM computational model for easy extension to other diffusion models.

4. Tabulate and compare the solutions for various times and test your code using the parameters $k = 0.159\, W\, m^{-1} C^{-1}$, $\rho = 595\, kg\, m^{-3}$, $c = 1758\, J\, kg^{-1} C^{-1}$, $L = 0.05\, m$, $h = 25\, W\, m^{-2}$, $T_\infty = 140\, C$, and $T_0 = 30\, C$.

Finite Volume Methods

$\boxed{1}$ FVM + B.E.M. $\quad O(\underbrace{\Delta x^2}_{\text{2nd order in space}} + \underbrace{\delta t}_{\text{1st order time}})$

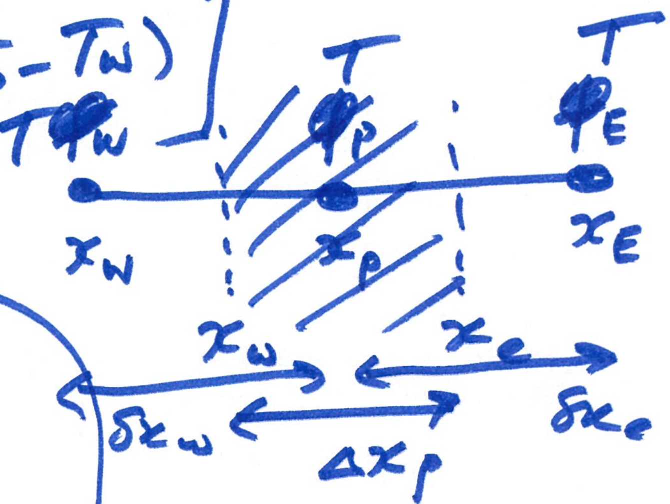
θ-method. uniform grid.

$\boxed{2}$ FVM + C.N. $\quad O(\Delta x^2 + \delta t^2)$

2nd order in time.

$$\cancel{\rho c}\frac{\partial T}{\partial t} = \frac{k}{\rho c}\frac{\partial^2 T}{\partial x^2} = D\frac{\partial^2 T}{\partial x^2}, \quad D = \frac{k}{\rho c}.$$

$$\frac{dT_p}{dt} = \frac{1}{\Delta x_p}\left[\frac{D}{\delta x_e}(T_E - T_p) - \frac{D}{\delta x_w}(T_p - T_W)\right]$$



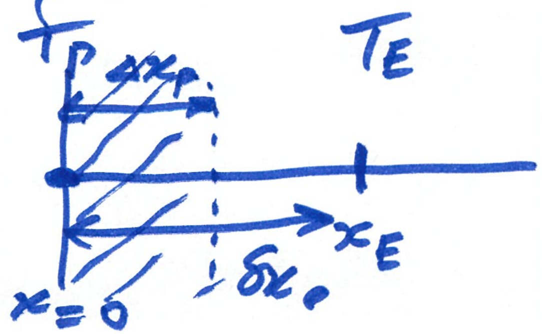
$$= \frac{1}{\Delta x_p}\left[\frac{D}{\delta x_w}T_W - \left(\frac{D}{\delta x_e} + \frac{D}{\delta x_w}\right)T_p + \frac{D}{\delta x_e}T_E\right]$$

Boundary Conditions:

At $x=0$: $$-\frac{k}{\rho c}\frac{\partial T}{\partial x} = \frac{h}{\rho c}(T_\infty - T)$$

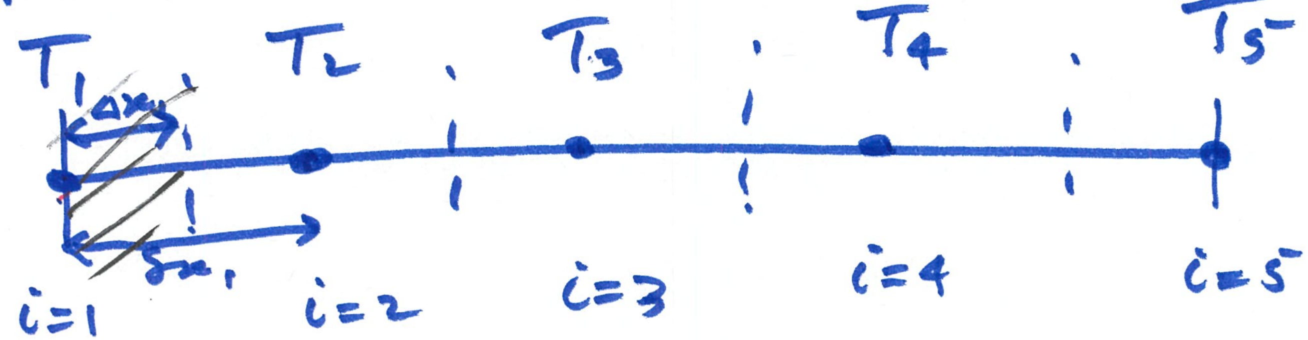
$$-D\frac{\partial T}{\partial x} = H(T_\infty - T), \quad H = \frac{h}{\rho c}.$$

$$\frac{dT_p}{dt} = \frac{1}{\Delta x_p}\left[\frac{D}{\delta x_e}(T_E - T_p) + H(T_\infty - T_p)\right]$$



$$\frac{dT_P}{dt} = \frac{1}{\Delta x_P}\left[-\left(\frac{D}{\delta x_e}+H\right)T_P + \frac{D}{\delta x_e}T_E + HT_\infty\right]$$

At $x = L$: Your job.



$\theta = 1, \frac{1}{2}$
BE CN

Integrate in time :

$$T_1^{n+1} - T_1^{n} = \frac{\boxed{\theta}\,\delta t}{\Delta x_1}\left[-\left(\frac{D}{\delta x_1}+H\right)T_1^{n+1} + \frac{D}{\delta x_1}T_2^{n+1} + HT_\infty\right]$$
$$+\frac{(1-\theta)\delta t}{\Delta x_1}\left[-\left(\frac{D}{\delta x_1}+H\right)T_1^{n} + \frac{D}{\delta x_1}T_2^{n} + HT_\infty\right]$$

$\underline{u}^{n+1}$

T_2 T_1 T_2 T_1

$$f_1(\underline{u}^{n+1}) := T_1^{n+1} - T_1^{n} - \frac{\theta\,\delta t}{\Delta x_1}\left[\cdots\cdots^{n+1}\cdots\right] - \frac{(1-\theta)\delta t}{\Delta x_1}\left[\cdots^{n}\cdots\right]$$

$$\underline{u}^{n+1} = \left(T_1^{n+1}, T_2^{n+1}, \ldots, T_5^{n+1}\right)^T.$$

$$T_i^{n+1} - T_i^{n} = \frac{\theta\,\delta t}{\Delta x_i}\left[\frac{D}{\delta x_{i-1}} T_{i-1}^{n+1} - \left(\frac{D}{\delta x_i} + \frac{D}{\delta x_{i-1}}\right) T_i^{n+1} + \frac{D}{\delta x_i} T_{i+1}^{n+1}\right]$$

$$+ \frac{(1-\theta)\,\delta t}{\Delta x_i}\left[\frac{D}{\delta x_{i-1}} T_{i-1}^{n} - \left(\frac{D}{\delta x_i} + \frac{D}{\delta x_{i-1}}\right) T_i^{n} + \frac{D}{\delta x_i} T_{i+1}^{n}\right],$$

$i = 2, 3, 4.$

$$f_i(\underline{u}^{n+1}) := T_i^{n+1} - T_i^{n} - \frac{\theta\,\delta t}{\Delta x_i}\left[T_{i-1} \cdot T_i^{n+1} \cdot T_{i+1}\right]$$

$$- \frac{(1-\theta)\,\delta t}{\Delta x_i}\left[T_{i-1}\ T_i\ T_{i+1}\right]^{n}.$$

$$f_5(\underline{u}^{n+1}) := T_5^{n+1} - T_5^{n} - \ - \ - \ -$$

$$\underline{F}(\underline{u}^{n+1}) = \begin{pmatrix} f_1(\underline{u}^{n+1}) \\ f_2(\underline{u}^{n+1}) \\ \vdots \\ f_5(\underline{u}^{n+1}) \end{pmatrix}$$

"fsolve"

We must solve $\underline{F}(\underline{u}^{n+1}) = \underline{0}$ to obtain all Temperatures $T_1^{n+1}, T_2^{n+1} - - T_5^{n+1}$ at t_{n+1} timestep.

$$\underline{u}^2 = (T_1^2, T_2^2, T_3^2, T_4^2, T_5^2)^T$$

$$\underline{F}(\underline{u}^2) = \underline{0} \quad \text{fsolve}$$

$t = t_2$

$$\underline{u}^1 = (T_1^1, T_2^1, T_3^1, T_4^1, T_5^1)^T$$

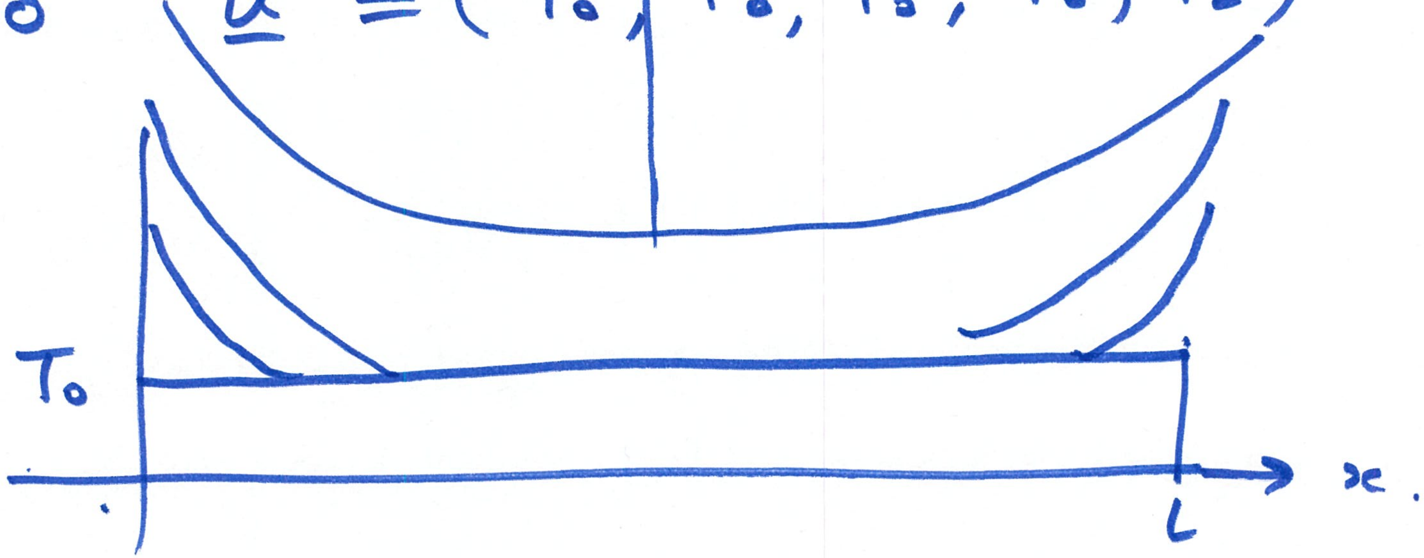
$t = t_1$

$$\underline{F}(\underline{u}^1) = \underline{0} \quad \text{using fsolve} \rightarrow$$

$\updownarrow \delta t$

$t = 0$

$$\underline{u}^0 = (T_0, T_0, T_0, T_0, T_0)^T$$

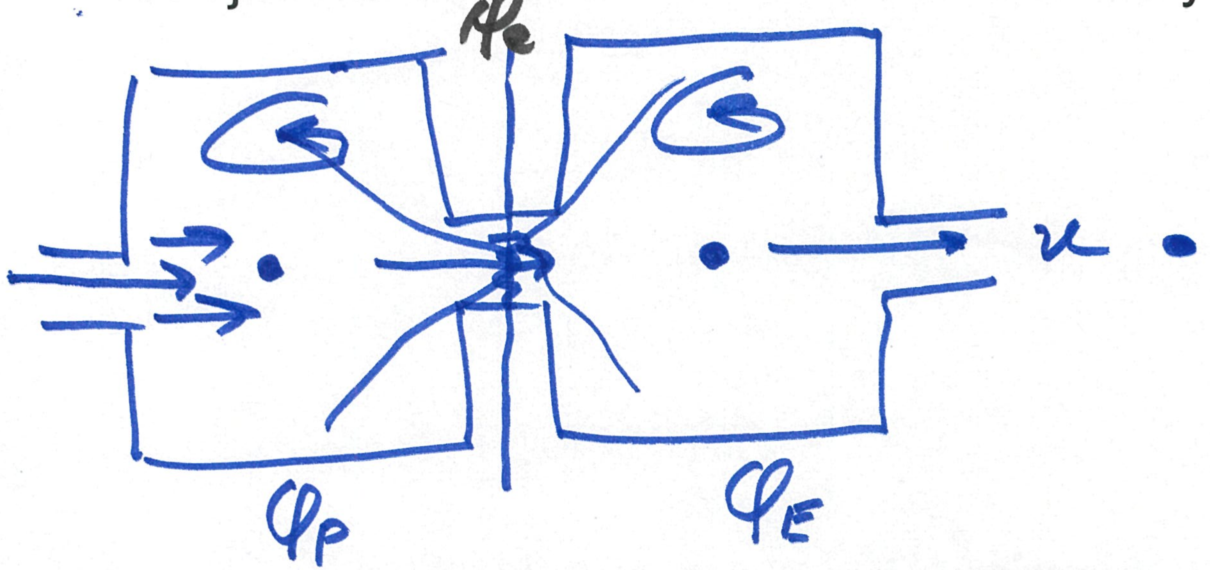


Advection-diffusion Equation

We now consider the linear *advection-diffusion equation with source term*:

$$\frac{\partial \varphi}{\partial t} + \frac{\partial}{\partial x}\underbrace{\left(\boxed{u\varphi} - D\frac{\partial \varphi}{\partial x}\right)}_{J} = S \qquad 0 < x < L, \quad t > 0 \qquad (14)$$

subject to the same initial and boundary conditions as before. $u \approx$



$\varphi_e = \frac{1}{2}(\varphi_E + \varphi_P)$

$u >>$

$\varphi_e = \varphi_P$

$$\frac{\partial \varphi}{\partial t} + \frac{\partial J}{\partial x} = S \quad , \quad J = u\varphi - D\frac{\partial \varphi}{\partial x}$$

FLUX TERM.

Integration over control volume

$$\frac{d\varphi_P}{dt} + \frac{1}{\Delta x_P}\left[J_e - J_w \right] = S_P$$

unknown

$$J_e = u_e \varphi_e - \left[D\frac{\partial \varphi}{\partial x} \right]_e = u_e \varphi_e - \frac{D_e}{\delta x_e}(\varphi_E - \varphi_P)$$

known

unknown

$$J_w = u_w \varphi_w - \left[D\frac{\partial \varphi}{\partial x} \right]_w = u_w \varphi_w - \frac{D_w}{\delta x_w}(\varphi_P - \varphi_W)$$

Averaging

We require approximations for J_w and J_e. The approximation for the diffusive component of the flux has been described in the previous section. For the advective component, we can approximate φ_w by $(\varphi_W + \varphi_P)/2$ and φ_e by $(\varphi_P + \varphi_E)/2$, to give

$$J_w = \left(u\varphi - D\frac{\partial\varphi}{\partial x}\right)_w \approx u\left(\overset{\varphi_w}{\frac{\varphi_P + \varphi_W}{2}}\right) - D\left(\frac{\varphi_P - \varphi_W}{\delta x_w}\right)$$

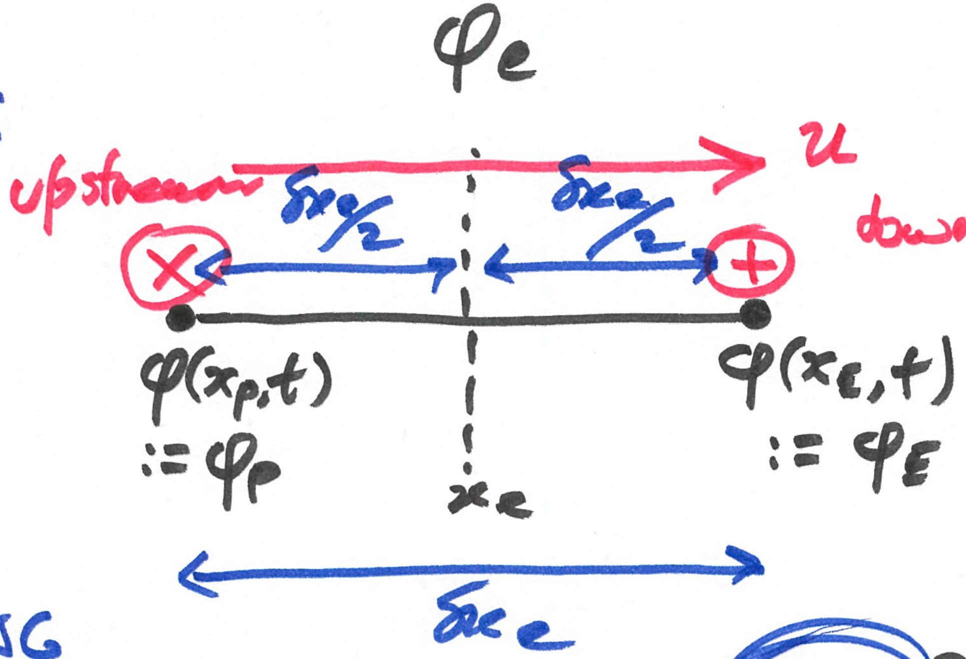
and

$$J_e = \left(u\varphi - D\frac{\partial\varphi}{\partial x}\right)_e \approx u\left(\overset{\varphi_e}{\frac{\varphi_P + \varphi_E}{2}}\right) - D\left(\frac{\varphi_E - \varphi_P}{\delta x_e}\right).$$

UPWINDING

$\varphi_e \simeq \varphi_P$

$O(\delta x_e)$



We need to know the direction of flow.

$x_e < \xi^+ < x_E$

$x_P < \xi^- < x_e$

AVERAGING

$$\varphi_P = \varphi\left(x_e - \frac{\delta x_e}{2}, t\right) = \varphi_e - \frac{\delta x_e}{2}\frac{\partial \varphi}{\partial x}(x_e,t) + \frac{\delta x_e^2}{8}\frac{\partial^2 \varphi}{\partial x^2}(\xi^-,t).$$

$$\varphi_E = \varphi\left(x_e + \frac{\delta x_e}{2}, t\right) = \varphi_e + \frac{\delta x_e}{2}\frac{\partial \varphi}{\partial x}(x_e,t) + \frac{\delta x_e^2}{8}\frac{\partial^2 \varphi}{\partial x^2}(\xi^+,t)$$

$$\frac{\varphi_P + \varphi_E}{2} = \cancel{2}\varphi_e + \frac{\delta x_e^2}{8\cancel{4}}\frac{\partial^2 \varphi}{\partial x^2}(\xi^*,t) \quad ; \quad \text{I.V. Th}^{m}$$

- Assuming continuity of 2^{nd} derivative in space

$x_P < \xi^* < x_E$

i.e., $\varphi_e \simeq \dfrac{\varphi_P + \varphi_E}{2}$ $O(\delta x_e^2)$ second order in space.

Averaging (continued)

$u_{\cdot} = u_e = u_w$

This approach to approximating the advective flux is called **averaging**.

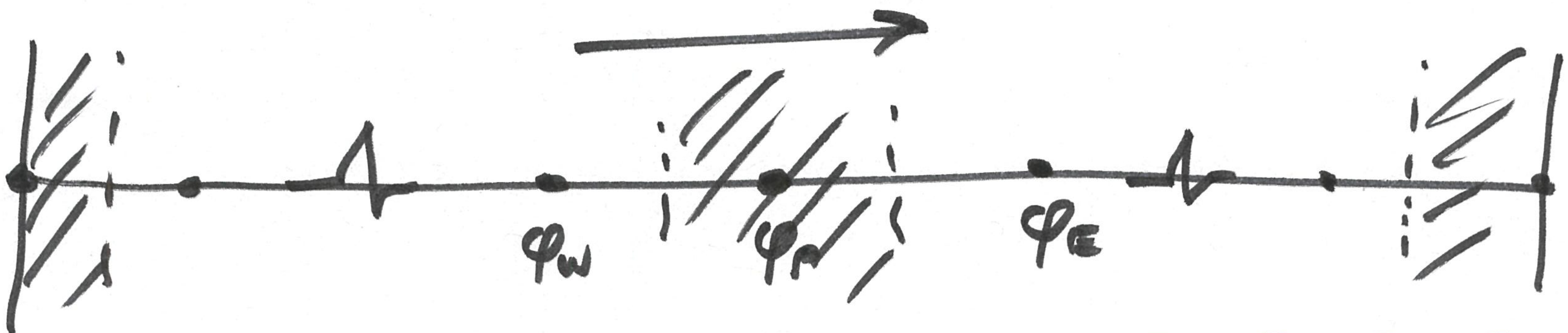
We obtain

$+$ $\quad$ $-ve$

$$\frac{\mathrm{d}\varphi_P}{\mathrm{d}t} = \frac{1}{\Delta x_P}\left[\left(\frac{u}{2} + \frac{D}{\delta x_w}\right)\varphi_W - \left(\frac{D}{\delta x_w} + \frac{D}{\delta x_e}\right)\varphi_P \right. \tag{15}$$

$$\left. + \left(\frac{-u}{2} + \frac{D}{\delta x_e}\right)\varphi_E\right] + S_P \tag{16}$$

$-ve$? Does this cause any problems ?



Boundary Nodes

On a boundary, the control volume node and face coincide. Hence the value of φ is known at boundary faces, so there is no need for any approximation in the advection term there:

$-\frac{u}{2} \mp \frac{D}{\delta x_e} - \frac{A_0 D}{B_0} + u$

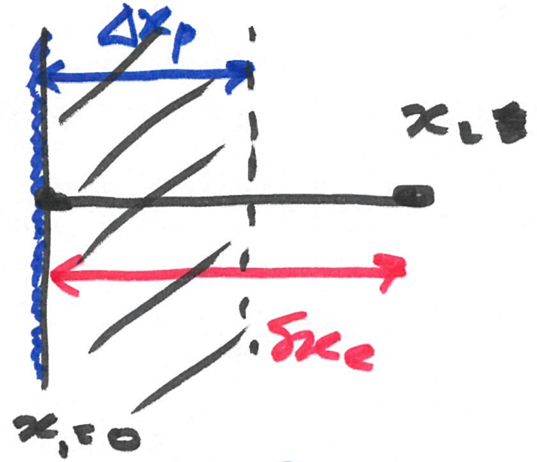
at $x = 0$:

$$\frac{\mathrm{d}\varphi_P}{\mathrm{d}t} = \frac{1}{\Delta x_P}\left[-\left(\frac{-u}{2} + \frac{D}{\delta x_e} + \frac{DA_0}{B_0}\right)\varphi_P + \left(\frac{-u}{2} + \frac{D}{\delta x_e}\right)\varphi_E + \frac{DC_0}{B_0}\right] + S_P$$

at $x = L$:

$$\frac{\mathrm{d}\varphi_P}{\mathrm{d}t} = \frac{1}{\Delta x_P}\left[\left(\frac{u}{2} + \frac{D}{\delta x_w}\right)\varphi_W - \left(\frac{u}{2} + \frac{D}{\delta x_w} + \frac{DA_L}{B_L}\right)\varphi_P + \frac{DC_L}{B_L}\right] + S_P$$

Boundary at $x = 0$:



$$\frac{d\varphi_P}{dt} = \frac{1}{\Delta x_P}\left[-J_e + J_b\right] + S_P$$

$$= \frac{1}{\Delta x_P}\left\{-\frac{u}{2}(\varphi_E + \varphi_P) + \frac{D_e}{\delta x_e}(\varphi_E - \varphi_P) + u\varphi_P + \underbrace{\left[-D\frac{\partial\varphi}{\partial x}\right]_{x=0}}_{\text{we know this from B.C. information.}}\right\} + S_P$$

Given B.C. at $x=0$.

$$\left[-D\frac{\partial\varphi}{\partial x}\right]_{x=0} = \frac{C_0 D}{B_0} - \frac{A_0 D}{B_0}\varphi_P$$

(u constant)

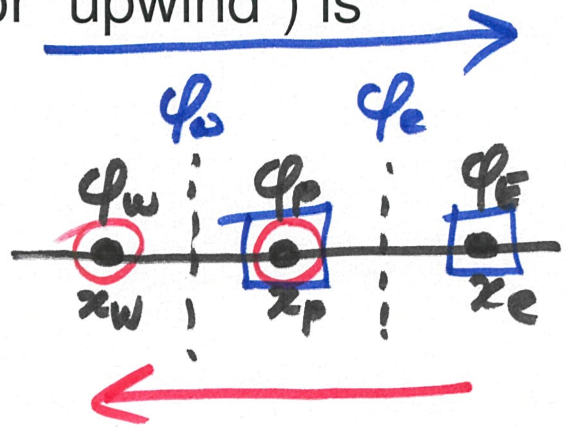
(D constant)

Substitution gives:

$$\frac{d\varphi_P}{dt} = \frac{1}{\Delta x_P}\left\{-\frac{u}{2}(\varphi_E + \varphi_P) + \frac{D_e}{\delta x_e}(\varphi_E - \varphi_P) + u\varphi_P + \frac{C_0 D}{B_0} - \frac{A_0 D \varphi_P}{B_0}\right\} + S_P.$$

Upstream Weighting (continued)

This gives rise to a discretisation known as **upstream weighting** or **upwinding**, where *only* information from upstream (or "upwind") is used to approximate advection terms.



Thus, we use the approximations

$$\varphi_w \approx \begin{cases} \varphi_W, & u > 0 \\ \varphi_P, & u < 0 \end{cases}$$

and

$$\varphi_e \approx \begin{cases} \varphi_P, & u > 0 \\ \varphi_E, & u < 0 \end{cases}.$$

Upstream Weighting (continued)

For the case $u > 0$ this leads to the spatial discretisation for internal nodes

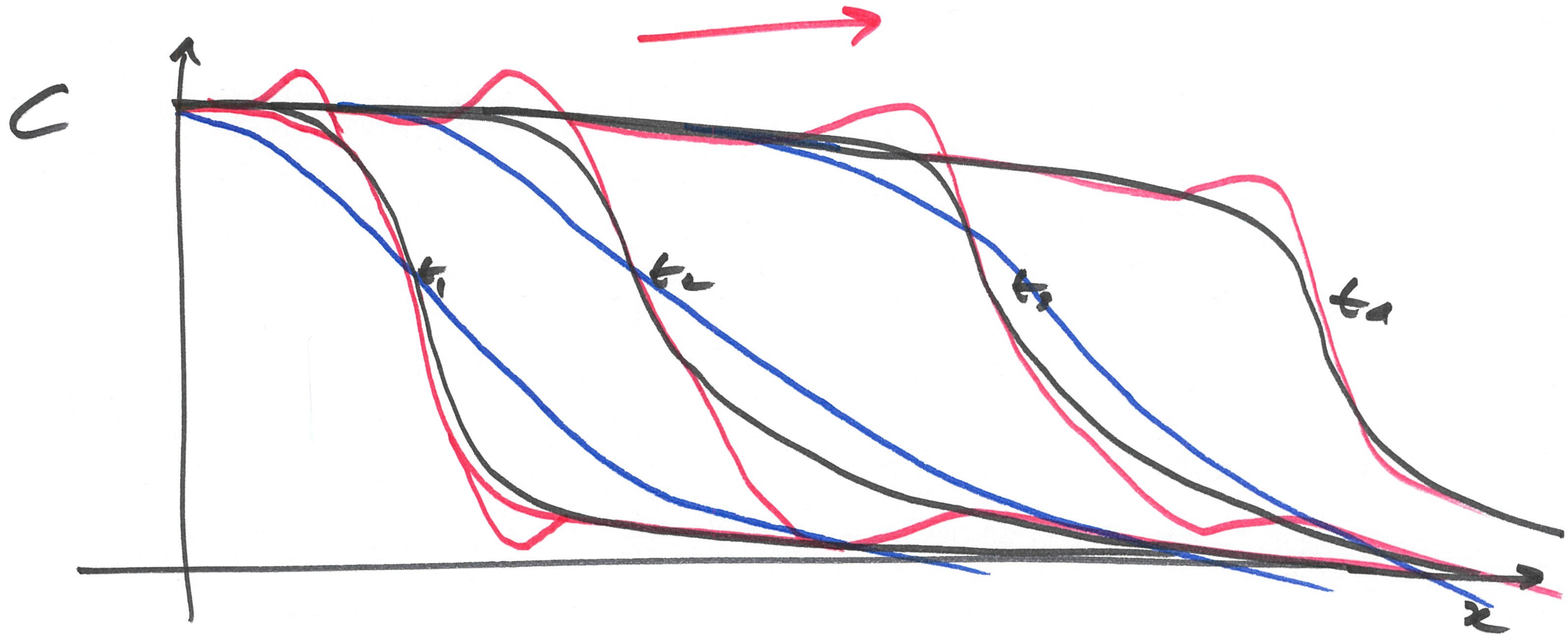
INTERNAL CONTROL VOLUME

$$\frac{d\varphi_P}{dt} = \frac{1}{\Delta x_P}\left[\underbrace{\left(u + \frac{D}{\delta x_w}\right)}_{+ve}\varphi_W - \underbrace{\left(u + \frac{D}{\delta x_w} + \frac{D}{\delta x_e}\right)}_{-ve}\varphi_P + \underbrace{\left(\frac{D}{\delta x_e}\right)}_{+ve}\varphi_E\right] + S_P \quad (17)$$

and at $x = L$

$$\frac{d\varphi_P}{dt} = \frac{1}{\Delta x_P}\left[\left(u + \frac{D}{\delta x_w}\right)\varphi_W - \left(u + \frac{D}{\delta x_w} + \frac{DA_L}{B_L}\right)\varphi_P + \frac{DC_L}{B_L}\right] + S_P\,.$$

First order in space.



SMEARING OF FRONT.

Numerical Diffusion

The upstream weighting discretisation is only first order accurate in space, and the solutions obtained exhibit what is known as **numerical diffusion** or **false diffusion**.

This phenomenon can be understood by considering (15) and (17) for uniform meshes.

$\Delta x_p = \delta x_e = \delta x_w = \Delta x$

Averaging:

$D^* = D + \frac{u\Delta x}{2}$

$\cancel{\frac{u}{2\Delta x}} + \frac{D}{\Delta x^2} + \cancel{\frac{u}{2\Delta x}}$

INTERNAL C.V.s

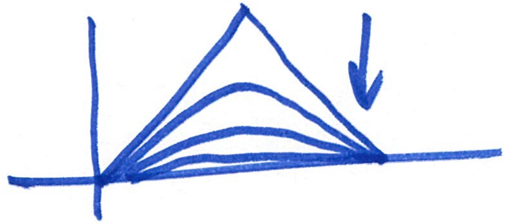
$$\frac{\mathrm{d}\varphi_P}{\mathrm{d}t} = \underbrace{\left(\frac{u}{2\Delta x} + \frac{D^*}{\Delta x^2}\right)}_{+ve}\varphi_W - \underbrace{\frac{2D^*}{\Delta x^2}}_{-ve}\varphi_P + \underbrace{\left(\frac{-u}{2\Delta x} + \frac{D^*}{\Delta x^2}\right)}_{-ve\ ?}\varphi_E + S_P \qquad (18)$$

Upstream weighting:

$$\frac{\mathrm{d}\varphi_P}{\mathrm{d}t} = \underbrace{\left(\frac{u}{\Delta x} + \frac{D}{\Delta x^2}\right)}_{+ve}\varphi_W - \underbrace{\left(\frac{u}{\Delta x} + \frac{2D}{\Delta x^2}\right)}_{-ve}\varphi_P + \underbrace{\frac{D}{\Delta x^2}}_{+ve.}\varphi_E + S_P\,. \qquad (19)$$

Our FVM Schemes

$$\frac{d\underline{u}}{dt} = k A \underline{u} + \underline{b}, \qquad \underline{u}(0) = \underline{u}_0$$



$$(\underline{b} = \underline{0}).$$

$$\frac{\underline{u}^{n+1} - \underline{u}^n}{\cancel{\delta t}} = \delta t\, k A \underline{u}^{n+1},$$

$$(I - \delta t\, k A)\underline{u}^{n+1} = \underline{u}^n.$$

i.e.,

$$\underline{u}^{n+1} = A \underline{u}^n, \qquad A = (I - \delta t\, k A)^{-1}$$

Suppose $\underline{u}^{(0)}$ has some error $\underline{\varepsilon}^{(0)}$.

$$\underline{u}^{(1)} = A(\underline{u}^{(0)} + \varepsilon^{(0)}) = A\underline{u}^{(0)} + A\underline{\varepsilon}^{(0)}$$

$$\underline{u}^{(2)} = A u^{(1)} = A^2 \underline{u}^{(0)} + A^2 \underline{\varepsilon}^{(0)}$$

$\vdots$

$$\underline{u}^{(n)} = A^n \underline{u}^{(0)} + A^n \underline{\varepsilon}^{(0)}$$

Stable scheme we need

$$\lim_{n \to \infty} A^n \underline{\varepsilon}^{(0)} = \underline{0}$$

$\uparrow$

$\rho(A) < 1$

spectral radius

$$\rho(A) = \max_{\lambda \in \sigma(A)} |\lambda|$$

Note:

- When this discretisation is applied to problems exhibiting sharp fronts, these fronts will generally come out smeared, as a result of this numerical diffusion.
- However, provided this phenomenon is understood by those interpreting the numerical results, this outcome is still preferable to obtaining a non-physical oscillatory solution, as from an averaging discretisation on a coarse mesh.
- Hence, if a coarse mesh is all that can be afforded, upstream weighting is the preferred approach.
- If using a fine mesh is possible, then there is no issue with monotonicity, and the averaging discretisation should certainly be used.

Treatment of Nonlinearity

Until now, we have assumed that the finite volume discretisation produces, at each timestep, a linear system of equations for the φ_i^{n+1}.

However, the FVM discretisation produces a *nonlinear* system of equations at each timestep if any of the following conditions are satisfied:

- D is a function of φ
- u is a function of φ
- S is a nonlinear function of φ

$$\frac{\partial \varphi}{\partial t} = \frac{\partial}{\partial x}\left(\underline{D(\varphi)}\frac{\partial \varphi}{\partial x}\right) + \underline{S(\varphi)}$$

Nonlinear PDE

The means for solving nonlinear systems of equations will be investigated in the next chapter. For now, we examine one additional issue that arises with the discretisation itself in the nonlinear case.

Interface Diffusivities

We require the value of the diffusivity D at the control volume faces x_w and x_e.

If D is a function of φ, then values of D are known only at node points x_W, x_P and x_E as $D_W = D(\varphi_W)$, $D_P = D(\varphi_P)$, $D_E = D(\varphi_E)$.

One option is to assume a linear variation of D between nodes, giving the following arithmetic average:

$$D_w = \frac{\delta x_w^+ D_W + \delta x_w^- D_P}{\delta x_w} \quad \text{and} \quad D_e = \frac{\delta x_e^+ D_P + \delta x_e^- D_E}{\delta x_e}. \qquad (20)$$

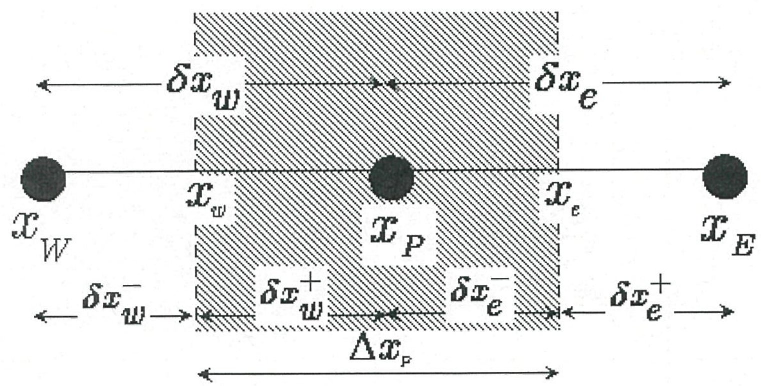
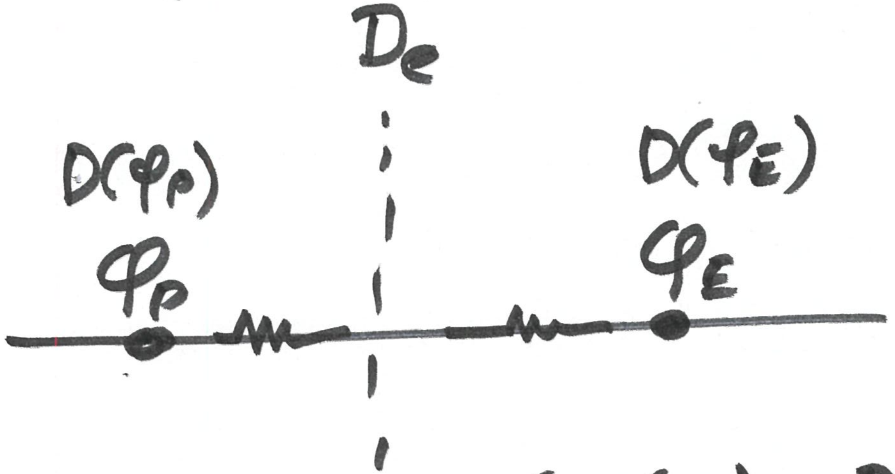


Figure: Control volume in one dimension

$$\frac{d\varphi_P}{dt} = \frac{1}{\Delta x_P}\left\{ \frac{D_e}{\delta x_e}(\varphi_E - \varphi_P) - \frac{D_w}{\delta x_w}(\varphi_P - \varphi_W) \right\} + S_P .$$

How do we evaluate this term at CV face.



$D(\varphi)$.

$$D_e = \frac{1}{2}\left(D(\varphi_P) + D(\varphi_E) \right)$$

ARITHMETIC AVERAGING

HARMONIC AVERAGING

$$\frac{\cancel{\delta x_e}}{D_e} = \frac{\frac{\cancel{\delta x_e}}{2}}{D_E} + \frac{\frac{\cancel{\delta x_e}}{2}}{D_P}$$

$$\frac{1}{D_e} = \frac{D_P + D_E}{2 D_E D_P} \Rightarrow D_e = \frac{2 D_P D_E}{D_P + D_E}$$

Interface Diffusivities continued

However, in some problems, particularly those involving heterogeneous materials where there are abrupt changes of diffusivity, a *harmonic* average is more appropriate than an arithmetic one.

In this case, we obtain

$$D_w = \delta x_w \left[\frac{\delta x_w^-}{D_W} + \frac{\delta x_w^+}{D_P} \right]^{-1} \quad \text{and} \quad D_e = \delta x_e \left[\frac{\delta x_e^-}{D_P} + \frac{\delta x_e^+}{D_E} \right]^{-1} . \tag{21}$$