□ Dispersion

① $$\frac{\partial AC}{\partial t} = \frac{\partial}{\partial x}\left(AK \frac{\partial C}{\partial x} \right)$$

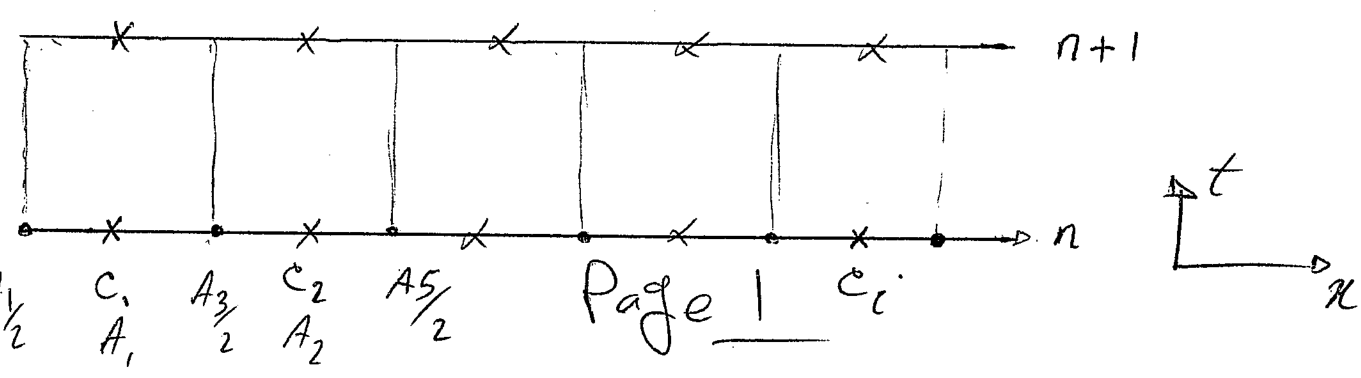
② $$\frac{AC_i^{n+1} - AC_i^{n}}{\Delta t} = \theta \left[\frac{AK_{i+\frac{1}{2}}^{n+1}\left(\frac{\partial C}{\partial x}\right)_{i+\frac{1}{2}}^{n+1} - AK_{i-\frac{1}{2}}^{n+1}\left(\frac{\partial C}{\partial x}\right)_{i-\frac{1}{2}}^{n+1}}{\Delta x} \right]$$

$$(1-\theta)\left[\frac{AK_{i+\frac{1}{2}}^{n}\left(\frac{\partial C}{\partial x}\right)_{i+\frac{1}{2}}^{n} - AK_{i-\frac{1}{2}}^{n}\left(\frac{\partial C}{\partial x}\right)_{i-\frac{1}{2}}^{n}}{\Delta x} \right]$$

②-1 Recast

$$\left.\begin{array}{l} A^n,\ A^{n+1} \\ A_{i\mp\frac{1}{2}}^{n},\ A_{i\mp\frac{1}{2}}^{n+1} \\ C^n \\ \Delta t,\ \theta,\ \Delta x \\ K_{i\pm\frac{1}{2}}^{n},\ K_{i\pm\frac{1}{2}}^{n+1} \end{array}\right\} \text{Known}$$

C^{n+1} ↳ ?



$$AK \frac{\partial C}{\partial n}\Big|_{i\pm 1/2}^{n} \longleftrightarrow F_{i\pm 1/2}^{n}$$

$\Rightarrow$

(3) $$AC_i^{n+1} = AC_i^{n} + \theta\Delta t\left[\frac{F_{i+1/2}^{n+1} - F_{i-1/2}^{n+1}}{\Delta n}\right] + \Delta t(1-\theta)\times\cdots$$

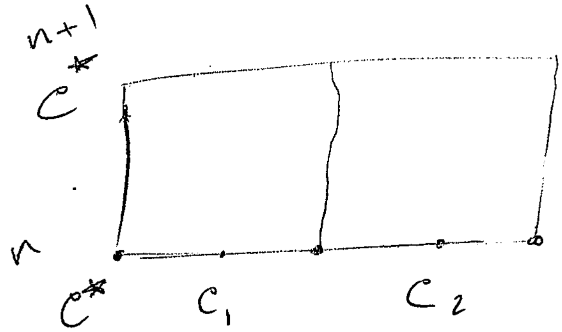
$$\cdots\left[\frac{F_{i+1/2}^{n} - F_{i-1/2}^{n}}{\Delta n}\right]$$

For BC:

(1) Nuemann $\frac{\partial C}{\partial n}$ is known on the boundary

$$\Rightarrow F_{\text{Boundary}} = \underbrace{AK}_{\text{Known}} \times \underbrace{\frac{\partial C}{\partial x}}_{\text{Known}}$$

(2) Dirichlet C is known on the center of first / last cell C^* or leftside of first cell ?



□ $C(x) = a + bx$ Linear

$$\begin{cases} @\ x = 0 \longrightarrow C(0) = a + b(0) = C^* = a \\ @\ x = \dfrac{dx}{2} \longrightarrow C(1/2) = a + \dfrac{b(dx)}{2} = C^* + \dfrac{b\,dx}{2} \end{cases}$$

$$\Longrightarrow \quad b = \frac{2}{\Delta x}\left(C_{1/2} - C_0\right) = \frac{2}{\Delta x}\left(C_{1/2} - C^*\right)$$

Center of cell one

unknown

$$F^t_{first} = Ak^t \frac{\partial C^t}{\partial x} = Ak^t b^t = \frac{2Ak^t}{\Delta x}\left(C_1^t - C^{t*}\right)$$

□ at the Rigth

$$b = \frac{2}{\Delta x}\left(C^* - C_{end/cell/center}\right)$$

$$F^t_{end} = Ak \left.\frac{\partial C}{\partial x}\right|^t_{end} = Akb^t_{end} = \frac{2Ak}{\Delta x}\left(C^{*t} - C^t_{end}\right)$$

unknown

$$AC_i^{n+1} = AC_i^n + \theta\Delta t\left[\frac{F^{n+1}_{i+1/2} - F^{n+1}_{i-1/2}}{\Delta x}\right] + \Delta t(1-\theta)\left[\frac{F^n_{i+1/2} - F^n_{i-1/2}}{\Delta x}\right]$$

□ Mid row

$$AC_i^{n+1} - \frac{\theta\Delta t}{\Delta x} F_{i+1/2}^{n+1} + \frac{\theta\Delta t}{\Delta n} F_{i-1/2}^{n+1} = AC_i^{n} + \underbrace{\frac{\Delta t(1-\theta)}{\Delta x}\left[\frac{F_{i+1/2}^{n} - F_{i-1/2}^{n}}{\Delta x}\right]}_{rhs}$$

$$A_i^{n+1} - \frac{\theta\Delta t}{\Delta n^2}\left(AK_{i+1/2}^{n+1} - AK_{i-1/2}^{n+1}\right)$$

$$C_i^{n+1} \qquad C_{i+1/2}^{n+1} \qquad C_{i-1/2}^{n+1}$$

$$C_{i+1} - C_i \qquad C_i - C_{i-1}$$

$$\hookrightarrow \left(-\frac{\theta\Delta t}{\Delta x^2} AK_{i-1/2}^{n+1} \quad A_i^{n+1} + \frac{\theta\Delta t}{\Delta x^2}\left(AK_{i+1/2}^{n+1} + AK_{i-1/2}^{n+1}\right) \quad -\frac{\theta\Delta t}{\Delta x^2} AK_{i+1/2}^{n+1}\right) \begin{pmatrix} C_{i-1}^{n+1} \\ C_i^{n+1} \\ C_{i+1}^{n+1} \end{pmatrix}$$

$$= AC_i^{n} + \Delta t(1-\theta)\left(\frac{F_{i+1/2}^{n} - F_{i-1/2}^{n}}{\Delta x^2}\right)$$

↳ explicit diffusive operator

☒ First row:

$$\underbrace{AC_i^{n+1} - \frac{\theta\Delta t}{\Delta x} F_{i+1/2}^{n+1}}_{\text{unknown}} + \frac{\theta\Delta t}{\Delta x}\frac{2AK}{\Delta x}\left(\underset{\text{unknown}}{C_1} - \overset{\text{known}}{C^*}\right)^{n+1} =$$

$$AC_i^n + \frac{\Delta t(1-\theta)}{\Delta x}\left[\frac{F_{i+1/2}^n - F_{i-1/2}^n}{\Delta x}\right]$$

$$\frac{2AK}{\Delta x}^n\left(\underset{\text{known}}{C_1} - \underset{\text{known}}{C^*}\right)^n$$

$$AC_1^{n+1} - \frac{\theta\Delta t}{\Delta x^2}\left(AK_{3/2}^{n+1}(C_2 - C_1) + \frac{\theta\Delta t}{\Delta x^2} 2 AK_{1/2}^{n+1} C_1\right) =$$

$$AC_1^n + \frac{\Delta t(1-\theta)}{\Delta x}\left[\frac{F_{3/2}^n - F_{1/2}^n}{\Delta x}\right] \rightarrow \frac{2AK_{1/2}^n}{\Delta x}\left(C_1^n - C^{*n}\right)$$

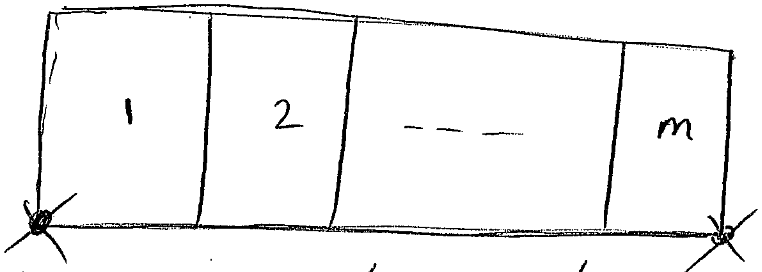
All known

additional term $+\frac{\theta\Delta t}{\Delta x^2} 2AK_{1/2} C^{*n+1}$

$$\left[A + \frac{\theta\Delta t}{\Delta x^2} AK_{3/2}^{n+1} + 2\frac{\theta\Delta t}{\Delta x^2} AK_{1/2}^{n+1} \quad -\frac{\theta\Delta t}{\Delta x^2} AK_{3/2}^{n+1}\right] \times \begin{Bmatrix} C_1^{n+1} \\ C_2^{n+1} \end{Bmatrix} =$$

$$AC_1^n + \frac{\Delta t(1-\theta)}{\Delta x^2}\left(F_{3/2}^n - F_{1/2}^n\right) + \frac{2\theta\Delta t}{\Delta x^2} AK_{1/2}^{n+1} C^{*n+1}$$

▯ note for Eli



In Dirichlet BC I assumed we know the value of c at the edge ($C_{1/2}$ = known, $C_{m+1/2}$ = known)

▯ last row (m is $\underline{\underline{10}}$)

$$AC_m^{n+1} - \frac{\theta\Delta t}{\Delta x}F^{n+1}_{10+1/2} + \frac{\theta\Delta t}{\Delta x}F^{n+1}_{10-1/2} = AC_m^{n} + \frac{\Delta t(1-\theta)}{\Delta x^2}\left[F^{n}_{10+1/2} - F^{n}_{10-1/2}\right]$$

✗ ✗ ✗ ✓ ✓ ✓ ✓

from prev step

$$AC_{10}^{n+1} - 2\frac{\theta\Delta t}{\Delta x^2}AK_{10+\frac{1}{2}}\left(\underbrace{C_*^{n+1}}_{\text{Known}} - C_{10}^{n+1}\right) + \frac{\theta\Delta t}{\Delta x^2}AK_{10-\frac{1}{2}}\left(C_{10}^{n+1} - C_9^{n+1}\right) =$$

$$AC_{10}^{n} + \frac{\Delta t(1-\theta)}{\Delta x^2}\left[F^{n}_{10+1/2} - F^{n}_{10-1/2}\right]$$

$$\frac{2AK_{10+1/2}}{\Delta x}\left[C_*^{n} - C_{10}^{n}\right]$$

$$\left[-\frac{\theta \Delta t}{\Delta x^2} Ak^{n+1}_{10-\frac{1}{2}} \;/\; A^{n+1}_{10} + \frac{\theta \Delta t}{\Delta x^2} \left[Ak^{n+1}_{10-\frac{1}{2}} + 2\, Ak^{n+1}_{10+\frac{1}{2}} \right] \right] \times \begin{Bmatrix} C_9^{n+1} \\ C_{10}^{n+1} \end{Bmatrix} =$$

$$AC_{10}^{n} + \frac{\Delta t (1-\theta)}{\Delta x^2} \left[F^{n}_{10+\frac{1}{2}} - F^{n}_{10-\frac{1}{2}} \right] + \frac{2\,\theta \Delta t}{\Delta x^2} Ak_{10+\frac{1}{2}} C_*^{n+1}$$

1. I think we may Make_diffusive_flux inside explicit_diffusion_operator

2. Right hand side is not only a function of explicit_diffuse_op in case of Dirichlet boundary condition, do we need change in the structure? How we should impose D_BC?