2*.

a) From Taylor

$$\left.\frac{\partial u}{\partial t}\right|_i^{n+1} = \frac{u_i^{n+1} - u_i^n}{\Delta t} + O(\Delta t) \quad \text{(Backward in time)}$$

$$\left.\frac{\partial u}{\partial x}\right|_i^{n+1} = \frac{u_i^{n+1} - u_{i-1}^{n+1}}{\Delta x} + O(\Delta x) \quad \text{(Backward in space)}$$

$$\frac{u_i^{n+1} + u_i^n}{\Delta t} + a\,\frac{u_i^{n+1} - u_{i-1}^{n+1}}{\Delta x} + \underbrace{O(\Delta t, \Delta x)}_{\tau_i^n \text{ truncation error}} = 0$$

Neglecting the truncation error

$$\boxed{U_i^{n+1} + a\frac{\Delta t}{\Delta x}\left(U_i^{n+1} - U_{i-1}^{n+1}\right) = U_i^n}$$

$$U_i^{n+1}\left(1 + a\frac{\Delta t}{\Delta x}\right) - a\frac{\Delta t}{\Delta x}U_{i-1}^{n+1} = U_i^n$$

If we use centered in space we get second order in space

So we have to use backward.

b) $i = 0 \Rightarrow U_0^{n+1}\left(1 + a\frac{\Delta t}{\Delta x}\right) - a\frac{\Delta t}{\Delta x}U_{-1}^{n+1} = U_0^n$ $\quad \rightarrow U_0 = U_{M+1}$

$i = M+1 \Rightarrow U_{M+1}^{n+1}\left(1 + a\frac{\Delta t}{\Delta x}\right) - a\frac{\Delta t}{\Delta x}U_M^{n+1} = U_{M+1}^n$ $\quad U_{-1} = U_M$

$$U_0^{n+1}\left(1 + a\frac{\Delta t}{\Delta x}\right) - a\frac{\Delta t}{\Delta x}U_M^{n+1} = U_0^n$$

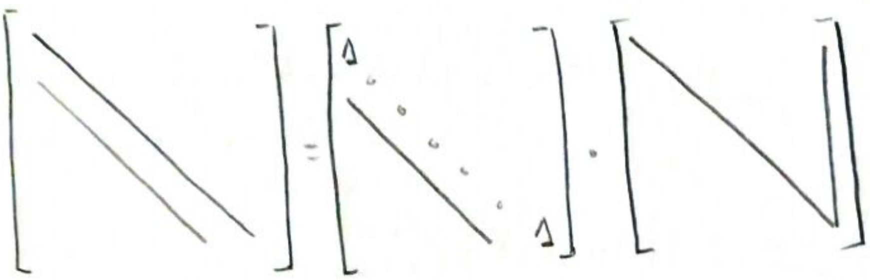
$$\Rightarrow AU^{n+1} = \overset{\rightarrow \text{Identify matrix}}{I}U^n$$

$$\begin{bmatrix} 1+a\frac{\Delta t}{\Delta x} & 0 & \cdots & \cdots & 0 & -a\frac{\Delta t}{\Delta x} \\ -a\frac{\Delta t}{\Delta x} & 1+a\frac{\Delta t}{\Delta x} & 0 & \cdots & \cdots & 0 \\ 0 & -a\frac{\Delta t}{\Delta x} & 1-a\frac{\Delta t}{\Delta x} & 0 & \cdots & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & \cdots & -a\frac{\Delta t}{\Delta x} & 1+a\frac{\Delta t}{\Delta x} \end{bmatrix} \begin{bmatrix} u_0^{n+1} \\ u_1^{n+1} \\ \vdots \\ \vdots \\ u_M^{n+1} \end{bmatrix} = \begin{bmatrix} u_0^n \\ u_1^n \\ \vdots \\ \vdots \\ u_M^n \end{bmatrix}$$

c) A matrix is diagonally dominant

- Iterative method → Gauss-Seidel (converges faster than Jacobi)
- Direct method → Doolittle

d)



4*. FTCS → Forward in time centered in space

$$FT \rightarrow \left.\frac{\partial u}{\partial t}\right|_i^n = \frac{u_i^{n+1} - u_i^n}{\Delta t} + O(\Delta t)$$

$$CS \rightarrow \left.\frac{\partial^2 u}{\partial x^2}\right|_i^n = \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} + O(\Delta x^2)$$

Neglecting the truncation error

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} = v \frac{U_{i+1}^n - 2U_i^n + U_{i-1}^n}{\Delta x^2} + \sigma U_i^n$$

$$\boxed{U_i^{n+1} = v\frac{\Delta t}{\Delta x^2} U_{i+1}^n + \left(\sigma \Delta t - 2v\frac{\Delta t}{\Delta x^2} + 1\right) U_i^n + v\frac{\Delta t}{\Delta x^2} U_{i-1}^n} \quad i = 1, \dots, n, \; n \geq 0$$

BC: Dirichlet → $U_0^{n+1} = 0 \quad n \geq 0$

Neumann → $U_{n+1}^{n+1} = v\frac{\Delta t}{\Delta x^2} U_{n+2}^n + \left(\sigma \Delta t - 2v\frac{\Delta t}{\Delta x^2} + 1\right) U_{n+1}^n + v\frac{\Delta t}{\Delta x^2} U_n^n$

approximation of the boundary condition

$$\left.\frac{\partial u}{\partial x}\right|_{n+1}^p = \frac{U_{n+2}^p - U_n^p}{2\Delta x} = 0 \Rightarrow U_{n+2}^p = U_n^p$$

$$\rightarrow U_{n+1}^{n+1} = 2v\frac{\Delta t}{\Delta x^2} U_n^n + \left(\sigma \Delta t - 2v\frac{\Delta t}{\Delta x^2} + 1\right) U_{n+1}^n \quad n \geq 0$$

$$IC: U_i^0 = \begin{cases} 0 & \text{for } x < 1/4 \\ 4x - 1 & \text{for } 1/4 \leq x < 1/2 \\ -4x + 3 & \text{for } 1/2 \leq x \leq 3/4 \\ 0 & \text{for } 3/4 < x \end{cases} \quad i = 1, \dots, n$$

b) <u>Diffusion eq</u> $(\sigma = 0)$

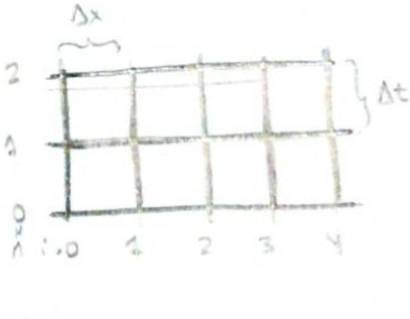
$$\begin{cases} U_i^{n+1} = \nu \frac{\Delta t}{\Delta x^2} U_{i-1}^n + \left(1 - 2\nu \frac{\Delta t}{\Delta x^2}\right) U_i^n + \nu \frac{\Delta t}{\Delta x^2} U_{i+1}^n & i = 1, \ldots, M \ , n \geq 0 \\ U_0^{n+1} = 0 & n \geq 0 \\ U_{M+1}^{n+1} = 2\nu \frac{\Delta t}{\Delta x^2} U_M^n + \left(1 - 2\nu \frac{\Delta t}{\Delta x^2}\right) U_{M+1}^n & n \geq 0 \\ U_i^0 = \begin{cases} 0 & \text{for } x < 1/4 \\ 4x - 1 & \text{for } 1/4 \leq x < 1/2 \\ -4x + 3 & \text{for } 1/2 \leq x \leq 3/4 \\ 0 & \text{for } 3/4 < x \end{cases} & i = 1, \ldots, M+1 \end{cases}$$

<u>Reaction eq</u> $(\nu = 0)$

$$\begin{cases} U_i^{n+1} = (\sigma \Delta t + 1) U_i^n & i = 1, \ldots, M \ , n \geq 0 \\ U_0^{n+1} = 0 & n \geq 0 \\ U_{M+1}^{n+1} = (\sigma \Delta t + 1) U_{M+1}^n & n \geq 0 \\ U_i^0 = \begin{cases} 0 & \text{for } x < 1/4 \\ 4x - 1 & \text{for } 1/4 \leq x \leq 1/2 \\ -4x + 3 & \text{for } 1/2 \leq x < 3/4 \\ 0 & \text{for } 3/4 \leq x \end{cases} & i = 1, \ldots, M+1 \end{cases}$$

c) $\nu = 0'1 \quad \sigma = -0'1 \quad \Delta x = 0'25 \quad \Delta t = 0'1$

$$\begin{cases} U_i^{n+1} = \frac{4}{25} U_{i-1}^n + \frac{67}{100} U_i^n + \frac{4}{25} U_{i+1}^n & i = 1, 2, 3 \ , n \geq 0 \\ U_0^{n+1} = 0 & n = 1, 2 \\ U_4^{n+1} = \frac{8}{25} U_3^n + \frac{67}{100} U_4^n & n = 1, 2 \\ U_i^0 = f(x) & i = 1, 2, 3, 4 \end{cases}$$



IC

Dirichlet BC

Neumann BC

$$\begin{array}{ccccc} \boxed{U_0^0 = 0} & U_1^0 = 0 & U_2^0 = 1 & U_3^0 = 0 & U_4^0 = 0 \\ U_0^1 = 0 & U_1^1 = \frac{4}{25} & U_2^1 = \frac{67}{100} & U_3^1 = \frac{4}{25} & U_4^1 = 0 \\ U_0^2 = 0 & U_1^2 = \frac{134}{625} & U_2^2 = \frac{5001}{10000} & U_3^2 = \frac{134}{625} & U_4^2 = \frac{32}{625} \end{array}$$

(graphic of the profile of u is attached at the end)

$\nu > 0$ generates a diffusion effect, that is why the profile becomes wider over the time.

Also, a lost of contaminant occurs as $\sigma < 0$.

d) BTCS → Backward in time centered in space

$$BT \rightarrow \left.\frac{\partial u}{\partial t}\right|_i^{n+1} = \frac{u_i^{n+1} - u_i^n}{\Delta t} + O(\Delta t)$$

$$CS \rightarrow \left.\frac{\partial^2 u}{\partial x^2}\right|_i^{n+1} = \frac{u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1}}{\Delta x^2} + O(\Delta x^2)$$

Neglecting the truncation error

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \nu \frac{u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1}}{\Delta x^2} + \sigma u_i^{n+1}$$

$$\boxed{\frac{\nu \Delta t}{\Delta x^2} u_{i-1}^{n+1} + \left(1 + \frac{2\nu\Delta t}{\Delta x^2} - \sigma \Delta t\right) u_i^{n+1} - \frac{\nu \Delta t}{\Delta x^2} u_{i+1}^{n+1} = u_i^n} \quad i = 1, \dots, n, \quad n > 0$$

BC: Dirichlet → $U_0^{n+1} = 0 \quad n \geq 0$

Newmann → $-\frac{\nu\Delta t}{\Delta x^2} u_n^{n+1} + \left(1 + \frac{2\nu\Delta t}{\Delta x^2} - \sigma \Delta t\right) u_{n+1}^{n+1} - \frac{\nu\Delta t}{\Delta x^2} u_{n+2}^{n+1} = u_{n+1}^n$

approximation of the boundary condition

$$\left.\frac{\partial u}{\partial x}\right|_{n+1}^p = \frac{u_{n+2}^p - u_n^p}{2\Delta x} = 0 \rightarrow u_{n+2}^p = u_n^p$$

$$\rightarrow -2\frac{\nu\Delta t}{\Delta x^2} u_n^{n+1} + \left(1 + \frac{2\nu\Delta t}{\Delta x^2} - \sigma\Delta t\right) u_{n+1}^{n+1} = u_{n+1}^n \quad n \geq 0$$

IC: $u_i^0 = f(x) \quad i = 0, \dots, n+1$

$$\Rightarrow A \cdot u^{n+1} = I u^n$$

$$A = \begin{bmatrix} 1+\frac{2\nu\Delta t}{\Delta x^2}-\sigma\Delta t & -\frac{\nu\Delta t}{\Delta x^2} & 0 & \cdots & \cdots & 0 \\ -\frac{\nu\Delta t}{\Delta x^2} & 1+\frac{2\nu\Delta t}{\Delta x^2}-\sigma\Delta t & -\frac{\nu\Delta t}{\Delta x^2} & \cdots & & 0 \\ \vdots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & -\frac{\nu\Delta t}{\Delta x^2} & 1+\frac{2\nu\Delta t}{\Delta x^2}-\sigma\Delta t & & -\frac{\nu\Delta t}{\Delta x^2} \\ 0 & \cdots & \cdots & 0 & -\frac{\nu\Delta t}{\Delta x^2} & 1+\frac{2\nu\Delta t}{\Delta x^2}-\sigma\Delta t \end{bmatrix}$$

Thomas Algorithm would be the most suitable method (fewer number of opperations than Gauss or Doolittle)

4^*. c) profile of u