1-D Polar Diffusion Equation with Constant Diffusion Equation

(Heat Equation)

① $$\frac{\partial C}{\partial t} = D \nabla^2 C - S$$

② $$\frac{\partial C}{\partial t} = D \left[\frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} \right] - kC$$

③ FTCSish scheme :

$$\left.\begin{aligned} \frac{\partial C}{\partial t} &= \frac{c_i^{n+1} - c_i^n}{\Delta t} \\ \frac{\partial^2 C}{\partial r^2} &= \frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{(\Delta r)^2} \\ \frac{\partial C}{\partial r} &= \frac{c_{i+1}^n - c_i^n}{\Delta r} \end{aligned}\right\}$$

Refer to Pascal's Triangle for Factors

Important! r_i is local polar position

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} = D \left[\frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{(\Delta r)^2} + \frac{1}{r_i} \frac{c_{i+1}^n - c_i^n}{\Delta r} \right] - kc_i^n$$

$$c_i^{n+1} = c_i^n + \left(D \left[\frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{(\Delta r)^2} + \frac{1}{r_i} \frac{c_{i+1}^n - c_i^n}{\Delta r} \right] - kc_i^n \right) \Delta t$$

④ Boundary Conditions

- Neumann BC at $r = 0$ $\longrightarrow$ $\frac{\partial C}{\partial r} = 0$

$$c_1^{n+1} = c_i^n + \left(D \left[\frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{(\Delta r)^2} \right] - kc_i^n \right) \Delta t$$

- Dirichlet BC at $r = r_{max}$ $\longrightarrow$ $c_I^{n+1} = C_e$

$$c_I^{n+1} = C_e$$

⑤ Matrix Form

$$[\,M\,]\cdot[\,C^n\,] = [\,C^{n+1}\,]$$

- M-elements

subdiagonal : $A_i \equiv c_{i-1}^n \longrightarrow A_i = D\left(\frac{1}{\Delta r^2}\right)\Delta t$

diagonal : $B_i \equiv c_i^n \longrightarrow B_i = 1 + \left(D\left[\frac{-2}{\Delta r^2} \frac{-1}{r_i \Delta r}\right] - k\right)\Delta t$

superdiagonal : $C_i \equiv c_{i+1}^n \longrightarrow C_i = D\left[\frac{1}{\Delta r^2} + \frac{1}{r_i \Delta r}\right]\Delta t$

Not the same as concentration!

- Neumann BC

$$B_1 = 1 + \left(D\left[\frac{-2}{\Delta r^2}\right] - k\right)\Delta t$$

$$C_1 = D\left[\frac{1}{\Delta r^2}\right]\Delta t$$

Need to ask David about this

$$\begin{bmatrix} B_1 & C_1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ A_2 & B_2 & C_2 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & A_3 & B_3 & C_3 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & A_4 & B_4 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & A_{I-2} & B_{I-2} & C_{I-2} & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & A_{I-1} & B_{I-1} & C_{I-1} \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} C_1^n \\ C_2^n \\ C_3^n \\ C_4^n \\ \vdots \\ C_{I-2}^n \\ C_{I-1}^n \\ C_e \end{bmatrix} = \begin{bmatrix} C_1^{n+1} \\ C_2^{n+1} \\ C_3^{n+1} \\ C_4^{n+1} \\ \vdots \\ C_{I-2}^{n+1} \\ C_{I-1}^{n+1} \\ C_I^{n+1} \end{bmatrix}$$

⑥ Solve the System of Equations

- Direct : Thomas
- Iterative : Gauss-Seidel (Hard)

⑦ FTCS scheme:

$$\frac{\partial C}{\partial t} = \frac{c_i^{n+1} - c_i^n}{\Delta t}$$

$$\frac{\partial^2 C}{\partial r^2} = \frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{(\Delta r)^2}$$

$$\frac{\partial C}{\partial r} = \frac{c_{i+1}^n - c_{i-1}^n}{2\Delta r}$$

$$c_i^{n+1} = c_i^n + \left(D\left[\frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{(\Delta r)^2} + \frac{1}{r_i}\frac{c_{i+1}^n - c_{i-1}^n}{2\Delta r} \right] - kc_i^n \right)\Delta t$$

- M-elements

subdiagonal : $A_i \equiv c_{i-1}^n \longrightarrow A_i = D\left(\frac{1}{\Delta r^2} - \frac{1}{r_i 2\Delta r}\right)\Delta t$

diagonal : $B_i \equiv c_i^n \longrightarrow B_i = 1 + \left(D\left[\frac{-2}{\Delta r^2}\right] - k\right)\Delta t$

superdiagonal : $C_i \equiv c_{i+1}^n \longrightarrow C_i = D\left[\frac{1}{\Delta r^2} + \frac{1}{r_i 2\Delta r}\right]\Delta t$

Not the same as concentration!

- Neumann BC

$$B_1 = 1 + \left(D\left[\frac{-2}{\Delta r^2}\right] - k\right)\Delta t$$

$$C_1 = D\left[\frac{1}{\Delta r^2}\right]\Delta t$$

Need to ask David about this

$$\begin{bmatrix} B_1 & C_1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ A_2 & B_2 & C_2 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & A_3 & B_3 & C_3 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & A_4 & B_4 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & A_{I-2} & B_{I-2} & C_{I-2} & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & A_{I-1} & B_{I-1} & C_{I-1} \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} c_1^n \\ c_2^n \\ c_3^n \\ c_4^n \\ \vdots \\ c_{I-2}^n \\ c_{I-1}^n \\ C_e \end{bmatrix} = \begin{bmatrix} c_1^{n+1} \\ c_2^{n+1} \\ c_3^{n+1} \\ c_4^{n+1} \\ \vdots \\ c_{I-2}^{n+1} \\ c_{I-1}^{n+1} \\ c_I^{n+1} \end{bmatrix}$$

(8) Analytical Solution at Steady-State

1. $\frac{\partial C}{\partial t} = D\left[\frac{\partial^2 C}{\partial r^2} + \frac{1}{r}\frac{\partial C}{\partial r}\right] - kC$

2. $\frac{\partial C}{\partial t} = 0$

3. find $\frac{\partial C}{\partial r}$ & $C(r)$ by integrating twice

4. $\frac{\partial C}{\partial r}(r=0) = 0$ & $C(r = r_{max}) = C_e$

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