CL249: ASSIGNMENT 9

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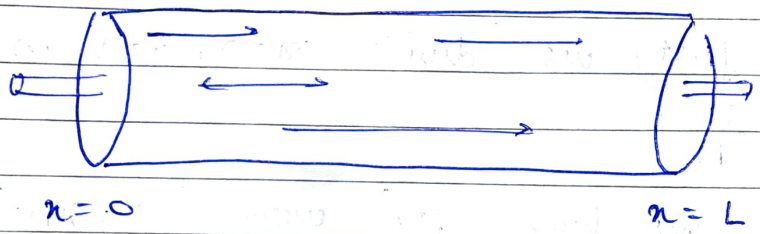
PROBLEM

We have to solve the following diff. eqn which describes the steady state conc. of substance that reacts with 1st order kinetics in an axially-dispersed plug flow reactor.



$$D\frac{d^2C}{dx^2} - U\frac{dc}{dx} = KC$$

D = diffusion const = 5000 m^2/hr

C = conc. of subs.

U = Axial velocity = 100 m/hr

K = Rate const = $2h^{-1}$

C_{inlet} = 100 mol/L

① $UC_{inlet} = UC_{x=0} - D\frac{dC}{dx}\Big|_{x=0}$

② $\frac{dC}{dx}\Big|_{x=L} = 0$

L = length = 100 m

We have to submit plot of y vs x for diff. h.

Description of method

Boundary value problem

We have a diff. eqn

$$D\frac{d^2C}{dx^2} - v\frac{dc}{dx} = kc$$

Now, first, we divide $x=0, x=1$ in N part

$h = \frac{L}{N}$;

then we have for every $[x_i, x_{i+1}]$

$$\frac{d^2C}{dx^2} = \frac{C_{i+1} - 2C_i + C_{i-1}}{h^2}$$

$$\frac{dC}{dx} = \frac{C_{i+1} - C_{i-1}}{2h}$$

$$D\left(\frac{C_{i+1} - 2C_i + C_{i-1}}{h^2}\right) - v\left(\frac{C_{i+1} - C_{i-1}}{2h}\right) = kC_i$$

$$2D(C_{i+1} - 2C_i + C_{i-1}) - 2hv(C_{i+1} - C_{i-1}) = 2h^2kC_i$$

$$(2D + hv)C_{i-1} - (2h^2k + 4D)C_i + (2D - hv)C_{i-1} = 0 \quad -(1)$$

and Bound. cond.

$$UC_{in} = UC_1 - D\left(\frac{C_2 - C_0}{2h}\right)$$

$$2hUC_{in} = 2hUC_1 - DC_2 + DC_0 \quad \text{—— (2)}$$

and $$\frac{C_{n+2} - C_n}{2h} = 0 \quad \text{—— (3)}$$

We can define matrix in which

$$\begin{bmatrix} D & -2hv & -D & 0 & \cdots & 0 \\ 0 & 2D+hv & -2h^2k+hv & 2b+hv & & \\ & \cdots & & & & \\ 0 & 0 & \cdots & 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ \vdots \\ C_{N+1} \end{bmatrix} = \begin{bmatrix} 2h^2 U_{(in)} \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

solve this using gauss elim

Pseudo code

main.m

loop in N to increase values
$N = 2^i$
divide x in parts
get y from solve

error = $\frac{y - y_{pre}}{y}$

get maximum error

if max err > tol
normal plot
else bold plot

solve.m

define constants
take inputs
A, B : zeros

loop to define general matrix
A(i, i+1) = —

define boundary cond. in the matrix
solve using gauss elim
return value