$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - kC$$

IC

initially no conc $\rightarrow C(x, t=0) = 0$

BC1: $C(t, 0) = 0.03\,mol/L$

BC2: $\left.\frac{\partial C}{\partial x}\right|_{x=L} = 0$

(Also expect $C(t, L) = 0$)

MoL $\rightarrow$ write FD in $x$ dir only

$x=0$ — x $i=0$

$0+\Delta x$ — x $i=1$

$0+2\Delta x$ x $i=2$

x

x

$L$ x $n+1$

$n$ = # internal node

$\Rightarrow \Delta x = \frac{L}{n+1}$ $\rightarrow$ # increment = # total − 1

$C = C_i$ at node $i$

$x = i\Delta x$

$$\frac{\partial C}{\partial x} = \frac{C_{i+1} - C_{i-1}}{2\Delta x} \quad O(\Delta x^2)$$

$$\frac{\partial^2 C}{\partial x^2} = \frac{C_{i+1} - 2C_i + C_{i-1}}{\Delta x^2} \quad O(\Delta x^2)$$

Sub FD into the PDE

$$\frac{\partial C_i}{\partial t} = D\frac{C_{i+1} - 2C_i + C_{i-1}}{\Delta x^2} - kC_i$$

appliable to all internal nodes

$i = 1 : n$

Boundaries?

at $x = 0$ $\quad C(t,0) = 0.03\ mol/L = C_0$

$\Rightarrow$ for eqn 1 $\rightarrow$ $\dfrac{\partial C_1}{\partial t} = D\dfrac{C_2 - 2C_1 + C_0}{\Delta x^2} - kC_1$ $\quad$ sub in

either pass $C_0$ to ode func as input or put in C and break apart inside and outside ode func.

at $x = L$ $\quad \left.\dfrac{\partial C}{\partial x}\right|_{x=L} = 0$ $\rightarrow$ we have nodes n+1 and before $\Rightarrow$ ① second order backward diff would change ODE

$\dfrac{\partial C_{n+1}}{\partial x} = \dfrac{C_{n+2} - C_n}{2\Delta x} = 0$ central

② central diff gives us the imaginary node we don't have.

$\Rightarrow C_{n+2} - C_n = 0 \rightarrow C_{n+2} = C_n$

$$\Rightarrow \frac{\partial C_{n+1}}{\partial t} = D\frac{C_{n+2} - 2C_{n+1} + C_n}{\Delta x^2} - kC_{n+1}$$

$$= \frac{D}{\Delta x^2}\left(2C_n - 2C_{n+1}\right) - kC_{n+1}$$

$$= \frac{2D}{\Delta x^2}\left(C_n - C_{n+1}\right) - kC_{n+1}$$

please see code for the rest