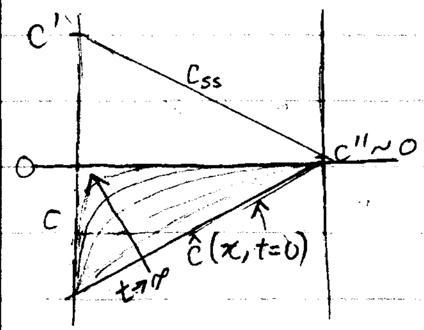
Problem 2.1 BE.430 Homework 2

a)



Assumptions:

- c'' is very small, ~ 0
- c' & c'' are $\sim$ constant
- $c' >> c''$
- $k=1$ for $x=0$, $x=L$

Complete $c(x,t)$ equation:

$$C(x,t) = \underbrace{\hat{c}(x,t)}_{\text{transient}} + \underbrace{C_{ss}(x)}_{\text{st. state}}$$

$$C_{ss}(x) = c' \cdot \left(1 - \frac{x}{L}\right) \text{ if } c''=0$$

or

$$c' - \left(\frac{c'-c''}{L}\right)x \text{ if } c'' \neq 0$$

Boundary conditions:

$c(0,t) = c'$

$c(L,t) = c''$

Initial Condition:

$c(x,0) = 0$

Species Conservation Equation

$$\frac{\partial \hat{c}(x,t)}{\partial t} = \frac{\partial^2 \hat{c}(x,t)}{\partial x^2}$$

$$\hat{c}(x,t) = X(x)T(t)$$

$$X(x)\frac{\partial T(t)}{\partial t} = T(t)\frac{\partial^2 X(x)}{\partial x^2} = -k^2$$

$$\frac{\partial T(t)}{T(t)\partial t} = \frac{\partial^2 X(x)}{X(x)\partial x^2} = -k^2$$

$$T(t) = A_1 e^{-k^2 t} = A_1 e^{-t/\tau};\ k^2 = \frac{1}{\tau}$$

$$X(x) = \cancel{B_1} \overset{0}{\cos}\left(\frac{n\pi x}{L}\right) + B_2 \sin\left(\frac{n\pi x}{L}\right)$$

to meet I.C.

Transient component of $c(x,t)$, $\hat{c}(x,t)$, doesn't contribute to boundary conditions because c' & c'' don't vary much w/ respect to time.

$$\therefore \left.\begin{aligned} \hat{c}(x=0,t) &= 0 \\ \hat{c}(x=L,t) &= 0 \end{aligned}\right\} \text{Homogeneous B.C.}$$

$$\hat{c}(x,t=0) = -C_{ss}(x) \} \text{ I.C.}$$

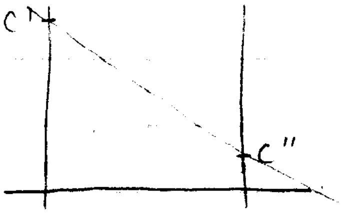
Problem 2.1

b) If $k = 1.4$, it will increase the steady state flux while diffusion time constant remains the same.

$$\boxed{c(x,t) = \sum_{n=1}^{\infty} \left[\frac{-2kC_0'}{n\pi} \sin\left(\frac{n\pi x}{L}\right) \right] e^{\frac{-(n\pi)^2 t}{L^2/D_{eff}}} + C'\left(1 - \frac{x}{L}\right)}$$

Alternative solution to 2.1 if C'' is not assumed to be 0.

$$\frac{L}{2} A_m' = \int_0^L \left[\left(\frac{C' - C''}{L}\, x\right) - C' \right] \sin\left(\frac{m\pi x}{L}\right) dx$$



$$u = \left(\frac{C' - C''}{L}\right) x - C' \qquad dv = \sin\left(\frac{m\pi x}{L}\right) dx$$

$$du = \frac{C' - C''}{L} \qquad V = -\cos\left(\frac{m\pi x}{L}\right)\left(\frac{L}{m\pi}\right)$$

$$\frac{L A_m'}{2} = \left[C' - \left(\frac{C' - C''}{L}\right) x \right] \cos\left(\frac{m\pi x}{L}\right) \frac{L}{m\pi} \Bigg|_0^L + \cancel{\int_0^L \frac{C' - C''}{m\pi} \cos\left(\frac{m\pi x}{L}\right) dx} \to 0$$

$$= \frac{C'' L}{m\pi} \cos(m\pi) - \frac{C' L}{m\pi}$$

- $$A_m' = \frac{(2C'' \cos(m\pi) - 2C')}{m\pi}$$
- $$c(x,t) = \sum_{n=1}^{\infty} \frac{2}{n\pi} \left[C'' \cos(n\pi) - C' \right] \sin\left(\frac{n\pi x}{L}\right) e^{\frac{-(n\pi)^2 t}{L^2/D_{eff}}} + C' - \left(\frac{C' - C''}{L}\right) x$$

b) If $k = 1.4$, it will increase the steady state flux while diffusion time constant remains the same.

- $$c(x,t) = \sum_{n=1}^{\infty} \frac{2k}{n\pi} \left[C'' \cos(n\pi) - C' \right] \sin\left(\frac{n\pi x}{L}\right) e^{\frac{-(n\pi)^2 t}{L^2/D_{eff}}} + kC' - k\left(\frac{C' - C''}{L}\right) x$$

$$\therefore \hat{c}(x,t) = \sum_{n=1}^{\infty} A_n' \sin\left(\frac{n\pi x}{L}\right) e^{-t/\tau}$$

When $t=0$, $\hat{c}(x,t) = \left(\frac{c'-c''}{L}\right)x - c'$ or $-c'\left(1-\frac{x}{L}\right)$ assuming $c''=0$

$$\sum_{n=1}^{\infty} A_n' \sin\left(\frac{n\pi x}{L}\right) = \left(\frac{c'-c''}{L}\right)x - c' \text{ or } ''$$

Using orthogonality of eigenfunctions to extract A_n'

$$① \; \underbrace{\int_0^L \sum_{n=1}^{\infty} A_n' \sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right)dx}_{= C_1 \delta[n-m]} = ② \int_0^L -c'\left(1-\frac{x}{L}\right)\sin\frac{m\pi x}{L}\,dx$$

$$C_1 = \int_0^L A_m' \sin^2\left(\frac{m\pi x}{L}\right)dx$$

$$= \int_0^L A_m' \left[\frac{1}{2} - \frac{1}{2}\cos\left(\frac{2m\pi x}{L}\right)\right]dx$$

$$= \frac{L}{2}A_m'$$

$$u = 1 - \frac{x}{L}$$

$$du = -\frac{1}{L}$$

$$dv = \sin\left(\frac{m\pi x}{L}\right)dx$$

$$v = -\frac{L}{m\pi}\cos\left(\frac{m\pi x}{L}\right)$$

② becomes

$$= -c'\left[\left(1-\frac{x}{L}\right)\left[\frac{-L}{m\pi}\cos\left(\frac{m\pi x}{L}\right)\right]\Bigg|_0^L + \left(\frac{c'}{\cancel{L}}\right)\frac{\cancel{L}}{m\pi}\cancel{\int_0^L \cos\left(\frac{m\pi x}{L}\right)dx}^{\to 0}\right]$$

$$= \frac{-c'L}{m\pi}$$

$\therefore$ for $c''=0$, $A_m' = \frac{-2c'}{m\pi}$ $\Rightarrow$ $\boxed{\hat{c}(x,t) = \sum_{n=1}^{\infty}\left[\frac{-2c_0'}{n\pi}\sin\left(\frac{n\pi x}{L}\right)\right]e^{-t/\tau}}$

$$c(x,t) = \hat{c}(x,t) + c'\left(1-\frac{x}{L}\right) \qquad \tau = \frac{L^2}{(n\pi)^2}\cdot\frac{1}{D_{eff}}$$

Problem 2.2 BE.430 Homework 2

a) $$N(t)\Big|_{x=L} = -D\frac{\partial C}{\partial x} = \frac{DC'}{L} + \frac{2DC'}{L}\sum_{n=1}^{\infty} e^{-\frac{(n\pi)^2 t}{L^2/D_{eff}}}\cos\pi n$$

$$T(t) = \int_0^t N(t)\Big|_{x=L} dt = \int_0^t\left(\frac{DC'}{L} + \frac{2DC'}{L}\sum_{n=1}^{\infty} e^{-\frac{(n\pi)^2 t}{L^2/D_{eff}}}\cos\pi n\right)dt$$

$$= \frac{Dc'}{L}t + \frac{2Dc'}{L}\sum_{n=1}^{\infty}\cos\pi n\int_0^t e^{-\frac{(n\pi)^2 t}{L^2/D_{eff}}}dt$$

$$= \frac{Dc't}{L} + \frac{2Dc'}{L}\sum_{n=1}^{\infty}\cos\pi n\left(-\frac{L^2}{D_{eff}(n\pi)^2}e^{-\frac{(n\pi)^2 t}{L^2/D_{eff}}}\right)\Bigg|_0^t$$

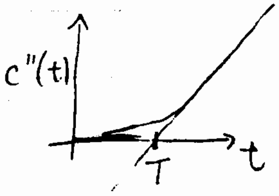
$$= \frac{Dc't}{L} + \frac{2Dc'}{L}\sum_{n=1}^{\infty}\cos\pi n\left(\frac{L^2}{D_{eff}(n\pi)^2} - \frac{L^2}{D_{eff}(n\pi)^2}e^{-\frac{(n\pi)^2 t}{L^2/D_{eff}}}\right)$$

$$C''(t) = \frac{T(t)}{V}\cdot A_c$$ cross-sectional area of tissue.

$$\boxed{C''(t) = \frac{A_c}{V}\frac{Dc'}{L}\left[t + \underbrace{2\sum_{n=1}^{\infty}\cos(\pi n)\left(\frac{L^2}{D_{eff}(n\pi)^2} - \frac{L^2}{D_{eff}(n\pi)^2}e^{-\frac{(n\pi)^2 t}{L^2/D_{eff}}}\right)}_{\hat{C}''(t)}\right.}$$

b) As $t\to\infty$, $\hat{C}''(t) = \frac{2Dc'A_c}{V\cancel{L}}\sum_{n=1}^{\infty}\cos(n\pi)\frac{L^{\cancel{2}}}{D_{eff}(n\pi)^2}$

Find time intercept: T



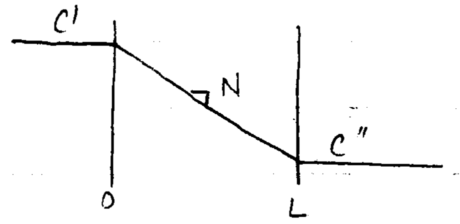
$$C''(T) = 0 = \frac{Dc'T}{L} + \frac{2Dc'}{L}\sum_{n=1}^{\infty}\cos\pi n\left(\frac{L^2}{D_{eff}(n\pi)^2}\right)$$

$$T = \frac{-2L^2}{D_{eff}}\sum_{n=1}^{\infty}\frac{\cos(\pi n)}{(n\pi)^2} = \frac{-2L^2}{D_{eff}}\left(-1 + \frac{1}{4\pi^2} - \frac{1}{9\pi^2} + \dots\right)$$

$$\boxed{T \approx \frac{L^2}{6D_{eff}}}$$

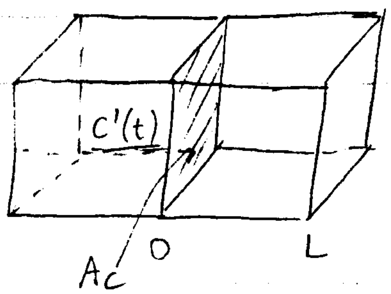
Problem 2.3 BE.430 Homework 2

a)



$$\boxed{N = -\frac{D}{L}\left(c' - c''\right)}$$

b) $Vc'(t) + Vc''(t) = V\beta$



Difference Equation: $Vc'(t) + A_c N \Delta t = Vc'(t+\Delta t)$

$$\frac{\partial c(t)}{\partial t} = \lim_{\Delta t \to 0}\left[\frac{c'(t+\Delta t) - c'(t)}{\Delta t}\right]$$

$$= \frac{AD}{VL}\left(c'' - c'\right)$$

$$= \frac{AD}{VL}\left(-c' + \beta - c'\right)$$

$$= \frac{AD}{VL}\left(-2c' + \beta\right)$$

$$\therefore \frac{\partial c'(t)}{\partial t} + 2c'(t)\frac{D \cdot A}{V \cdot L} = \frac{\beta DA}{VL}$$

c) $$c'(t) = e^{-\frac{2DA}{VL}t}\left[A_1 + \int_0^t e^{\frac{2DA}{VL}t} \cdot \frac{\beta DA}{VL}\, dt\right]$$

$$= A_1 e^{-\frac{2DA}{VL}t} + \frac{\beta}{2} \quad \text{satisfies} \quad c'(t \to \infty) = \frac{\beta}{2}$$

$$c'(0) = \frac{c'(0) + c''(0)}{2} + A_1 \Rightarrow A_1 = \frac{c'(0) - c''(0)}{2}$$

$$c'(t) = \left[\frac{c'(0) - c''(0)}{2} e^{-\frac{2DA}{VL}t}\right] + \frac{\beta}{2} \qquad \tau_{lag} = \frac{LV}{2DA}$$

$$\left.\begin{aligned} \tau_1 &= \frac{LV}{2DA} \\ \tau_{diff} &= \frac{L^2}{\pi^2 D} \end{aligned}\right\} \quad \frac{V}{A} \gg L, \therefore \tau \gg \tau_{diff}$$

Since the time decay constant here is much larger than the diffusion constant, we can assume that C' & C'' remain constant at the boundaries and that it reaches the SS linear concentration profile quickly in the tissue.