Math Modelling & Systems Biology

Assignment 4

1.

$$\left.\frac{\partial c}{\partial x}\right|_{x=0} \quad \left.\frac{\partial c}{\partial x}\right|_{x=l} = 0$$

a) Diffusion equation

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$$

to non dimensionalize the eq we substitute

$$c = c_0 \tilde{c} \qquad x = L\tilde{x}$$
$$t = t_0 \tilde{t}$$
$$x = x_0 \tilde{x}$$

$$\frac{\cancel{c_0}}{t_0}\frac{\partial \tilde{c}}{\partial \tilde{t}} = \frac{D\cancel{c_0}}{x_0^2}\frac{\partial^2 \tilde{c}}{\partial \tilde{x}^2}$$

$$\frac{\partial \tilde{c}}{\partial \tilde{t}} = \frac{D t_0}{x_0^2}\frac{\partial^2 \tilde{c}}{\partial \tilde{x}^2}$$

assuming

$x_0 = L$ and $t_0 = \frac{L^2}{D}$;

Non dimensionized Equation

$$\frac{\partial \tilde{c}}{\partial \tilde{t}} = \frac{\partial^2 \tilde{c}}{\partial \tilde{x}^2}$$

b)

$$c(x,0) = c_0\left[1 + a\cos\left(\frac{\pi x}{l}\right)\right]$$

let $\tilde{c}(x,t) = A(\tilde{x})B(\tilde{t})$

$$\dot{B}(\tilde{t})A(\tilde{x}) = A''(\tilde{x})B(\tilde{t})$$

$$\Rightarrow \frac{\dot{B}(\tilde{t})}{B(\tilde{t})} = \frac{A''(\tilde{x})}{A(\tilde{x})}$$

since the dimensions on both sides don't match

$$\Rightarrow \frac{\dot{B}(\tilde{t})}{B(\tilde{t})} = \frac{A''(\tilde{x})}{A(\tilde{x})} = -\lambda^2 \text{ [constant]}$$

$$\int \frac{dB}{B} = \int -\lambda^2 d\tilde{t}$$

$$\Rightarrow B = B_0 e^{-\lambda^2 \tilde{t}}$$

$$A''(\tilde{x}) + \lambda^2 A(\tilde{x}) = 0$$

let $A(\tilde{x}) = e^{mx}$

$$\Rightarrow e^{m\tilde{x}}(m^2 + \lambda^2) = 0$$

$$\Rightarrow m = \pm \lambda i$$

$A(x)$ is a linear combinations of the two roots

$$\Rightarrow A(x) = c_1\sin(\lambda\tilde{x}) + c_2\cos(\lambda\tilde{x})$$

$$\Rightarrow c(\tilde{x},\tilde{t}) = B_0 e^{-\lambda^2\tilde{t}}(c_1\sin(\lambda\tilde{x}) + c_2\cos(\lambda\tilde{x}))$$

let $c_1' = c_1 B_0$ and $c_2' = c_2 B_0$

$$\Rightarrow c(\tilde{x},\tilde{t}) = e^{-\lambda^2\tilde{t}}(c_1'\sin(\lambda\tilde{x}) + c_2'\cos(\lambda\tilde{x}))$$

$$\frac{\partial \tilde{c}}{\partial \tilde{x}} = e^{-\lambda^2\tilde{t}}\lambda[c_1'\cos(\lambda\tilde{x}) - c_2'\sin(\lambda\tilde{x})]$$

$$\left.\frac{\partial \tilde{c}}{\partial \tilde{x}}\right|_{\tilde{x}=0} = 0 \qquad \left.\frac{\partial \tilde{c}}{\partial \tilde{x}}\right|_{\tilde{x}=\frac{l}{x_0}=1} = 0$$

$$\Rightarrow c_1' = 0 \qquad \Rightarrow \lambda \quad n\pi$$
$$\Rightarrow \lambda = n\pi$$

$$\Rightarrow c(\tilde{x},\tilde{t}) = \sum_{n=0}^{n=\infty} d_n e^{-n^2\pi^2\tilde{t}}\cos(n\pi\tilde{x})$$

$$c(x,0) = c_0\left[1 + a\cos\left(\frac{\pi x}{l}\right)\right]$$

$$\Rightarrow c(\tilde{x},0) = c_0[1 + a\cos(\pi\tilde{x})]$$

$$d_0 + d_1\cos(\pi\tilde{x}) = c_0 + c_0 a\cos(\pi\tilde{x})$$

$$\Rightarrow d_0 = c_0 \text{ \& } d_1 = c_0 a$$

$$\Rightarrow c(\tilde{x},\tilde{t}) = c_0 + c_0 a e^{-\pi^2\tilde{t}}\cos(\pi\tilde{x})$$

$$c(\tilde{x},\tilde{t}) = c_0\left[1 + a e^{-\pi^2\tilde{t}}\cos(\pi\tilde{x})\right]$$

c) The solution is for the non dimensionalized equation

substituting

$\tilde{x} = \frac{x}{x_0}$ & $\tilde{t} = \frac{t}{t_0}$

$$\Rightarrow c(x,t) = c_0\left[1 + a e^{-\frac{\pi^2 D t}{l^2}}\cos\left(\frac{\pi x}{l}\right)\right]$$

$t = 7$ sec

$$c(x,7) = c_0\left[1 + a e^{-\pi^2\frac{30u^2(7s)}{100u^2}}\cos\left(\frac{\pi x}{10u}\right)\right]$$

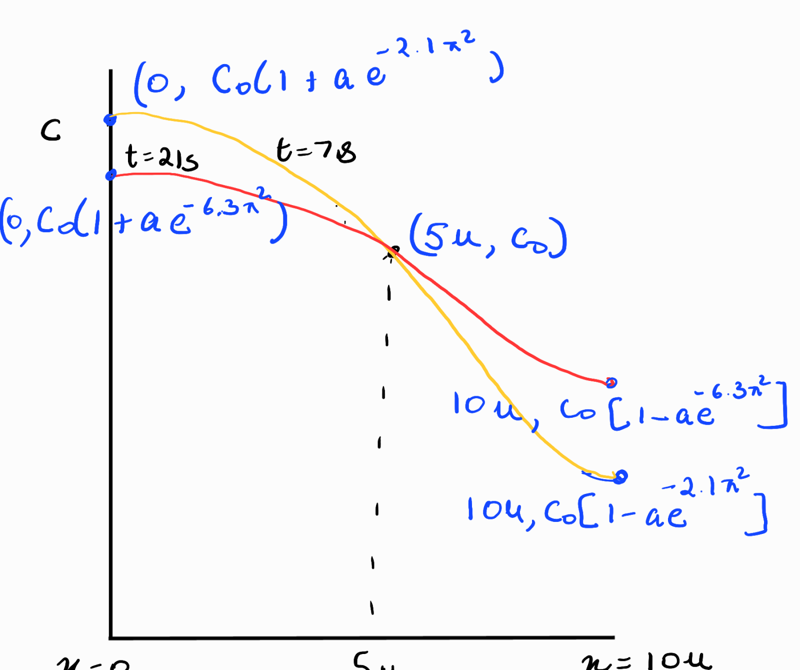
$$\Rightarrow c(x,7) = c_0\left[1 + a e^{-\pi^2(2.1)}\cos\left(\frac{\pi x}{10u}\right)\right]$$

similarly we have

$$c(x,21) = c_0\left[1 + a e^{-\pi^2\frac{(30)(21)}{100}}\cos\left(\frac{\pi x}{10u}\right)\right]$$

$$c(x,21) = c_0\left[1 + a e^{-\pi^2 6.3}\cos\left(\frac{\pi x}{10u}\right)\right]$$

Plotting these curves from $x=0$ to $x=10u$



2. If the molecule is being degraded the differential eq is given by

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - Bc$$

for non dimensionalizing the eq we substitute

$$c = c_0\tilde{c}$$
$$x = x_0\tilde{x}$$
$$t = t_0\tilde{t}$$

$$\Rightarrow \frac{c_0}{t_0}\frac{\partial \tilde{c}}{\partial \tilde{t}} = \frac{D c_0}{x_0^2}\frac{\partial^2 \tilde{c}}{\partial x^2} - B c_0\tilde{c}$$

$$\Rightarrow \frac{\partial \tilde{c}}{\partial \tilde{t}} = \frac{D t_0}{x_0^2}\frac{\partial^2 \tilde{c}}{\partial x^2} - B t_0\tilde{c}$$

now choosing

$x_0 = L$, $t_0 = \frac{L^2}{D}$

Non dimensionalized Equation

$$\frac{\partial \tilde{c}}{\partial \tilde{t}} = \frac{\partial^2 \tilde{c}}{\partial x^2} - \frac{BL^2}{D}\tilde{c}$$

b) assume

$$c(x,t) = A(x)B(t)$$

substituting in the equation

$$\dot{B}(t)A(x) = DA''(x)B(t) - B\,A(x)B(t)$$

$$\Rightarrow \frac{\dot{B}(t)}{B(t)} = \frac{DA''(x)}{A(x)} - B$$

$$\Rightarrow \frac{B(t)}{B(t)} = \frac{DA''(x)}{A(x)} - B = -B - \lambda^2$$

$$\Rightarrow B(t) = B_0 e^{-(\lambda^2+B)t}$$

$$A(x) = c_1\cos\left(\frac{\lambda x}{\sqrt{D}}\right) + c_2\sin\left(\frac{\lambda x}{\sqrt{D}}\right)$$

$$\Rightarrow c(x,t) = e^{-(\lambda^2+B)t}\left[c_1\cos\left(\frac{\lambda x}{\sqrt{D}}\right) + c_2\sin\left(\frac{\lambda x}{\sqrt{D}}\right)\right]$$

we know

$$\left.\frac{\partial c}{\partial x}\right|_{x=0} = \left.\frac{\partial c}{\partial x}\right|_{x=l} = 0$$

$$\Rightarrow c_2 = 0 \qquad \Rightarrow \frac{\lambda l}{\sqrt{D}} = n\pi$$

$$\Rightarrow \lambda = \frac{n\pi\sqrt{D}}{l}$$

$$\Rightarrow c(x,t) = \sum_{n=0}^{\infty} d_n e^{-\left(\frac{n^2\pi^2 D}{l^2} + B\right)t}\cos\left(\frac{n\pi x}{l}\right)$$

given that

$$c(x,0) = c_0\left[1 + a\cos\left(\frac{\pi x}{l}\right)\right]$$

$$\Rightarrow d_0 + d_1\cos\left(\frac{\pi x}{l}\right) = c_0 + c_0 a\cos\left(\frac{\pi x}{l}\right)$$

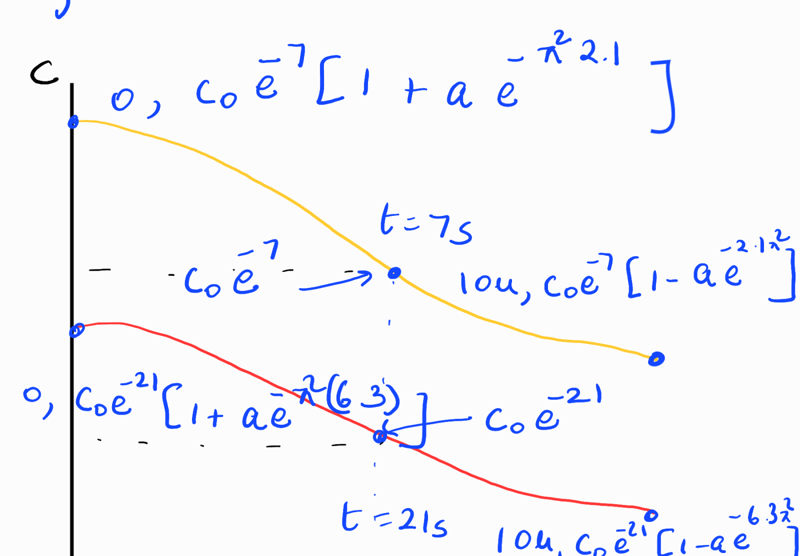
$$d_i = 0 \quad \forall i \geq 2$$
$$d_0 = c_0$$
$$d_1 = c_0 a$$

$$c(x,t) = c_0 e^{-Bt} + c_0 a e^{-\left(\frac{\pi^2 D}{l^2} + B\right)t}\cos\left(\frac{\pi x}{l}\right)$$

$$c(x,t) = c_0 e^{-Bt}\left[1 + a e^{-\frac{\pi^2 D}{l^2}t}\cos\left(\frac{\pi x}{l}\right)\right]$$

$B = 1/s$

c)



d)

By Flicks Law

$$F(x) = \frac{\partial c}{\partial x}$$

→ Physically $\frac{\partial c}{\partial x} = 0$ signifies that there is no outflux or influx of the diffused substance at $x=0$ & $x=l$

→ This indicates the presense of boundries at $x=0$ & $x=L$ that prevent diffusion to the left of 0 and the right of L