BB 101: Physical Biology

TUTORIAL 3: Solutions

1. Energy required to bend DNA in a circle of radius R is given by

$$E = \frac{k_b \pi}{2R}$$

$$= \frac{300\text{ÅKcal } mol^{-1} \times 3.14}{2 \times 45\text{Å}}$$

$$= 20.93/2 \text{ Kcal } mol^{-1}$$

$$\approx 21/2 \text{ Kcal } mol^{-1}$$

$$\approx 7.25 \times 10^{-18}\ J/molecule$$

2. (i) Let's calculate flux which is number of molecules arriving/colliding at the surface of sphere per unit area per unit time

$$J(r) = -D\ \frac{\partial}{\partial r}\left[a(1 - \frac{b}{r})\right]$$

$$= -Da\ \frac{\partial}{\partial r}\left[(1 - \frac{b}{r})\right]$$

$$= Db\ \frac{\partial}{\partial r}\left[\frac{1}{r}\right]$$

$$= Dbr^{-2}$$

Therefore, number of molecules colliding at $r = b$ per unit time is given by

$$I(b) = J(b).\, 4\pi b^2 = -4\pi Dab$$

The minus sign in above expression indicates that flow of molecule or current is towards –r or towards sphere

(ii)The total no. N of molecules colliding the surface between time T_1 and T_2 is given by

$$N = 4\pi Dab(T_2 - T_1)$$

3. Let the concentration of the drug in the tablet be C_0. In this case there are two processes that are happening, diffusion of the drug and reaction of the drug

Therefore, equation capturing both reaction and diffusion is given by

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

We shall solve this equation under steady state condition i.e. $\frac{\partial C}{\partial t} = 0$

Therefore, equation to solve is

$$0 = D\frac{\partial^2 C}{\partial x^2} - kC$$

Or,

$$\frac{\partial^2 C}{\partial x^2} = \frac{k}{D}C \qquad (1)$$

The general solution of this second order differential equation is given by

$$C(x) = A_1 e^{-B_1 x} + A_2 e^{+B_2 x}$$

Let use the boundary condition $C(x) = 0$ at $x = \infty$ and $C(x) = C_0$ at $x = 0$

Let us the first boundary condition $(x) = 0$ at $x = \infty$

$$\Rightarrow A_2 = 0$$

Therefore,

$$C(x) = A_1 e^{-B_1 x}$$

Now let’s use the second boundary condition $C(x) = C_0$ at $x = 0$

$$\Rightarrow A_1 = C_0$$

Therefore,

$$C(x) = C_0 e^{-B_1 x} \qquad (2)$$

To determineB_1, substitute (2) in (1)

$$\Rightarrow B_1^2 = \frac{k}{D}$$

$$\Rightarrow B_1 = \sqrt{\frac{k}{D}}$$

Therefore, $$C(x) = C_0 e^{-\sqrt{\frac{k}{D}}x}$$

To compute the rate at which the drug is being drawn out, we have to calculate flux at $x = 0$

Therefore, $$J(x) = -D\frac{\partial C}{\partial x} = \sqrt{kD}C_0 e^{-\sqrt{\frac{k}{D}}x}$$

$$J(x = 0) = -D\frac{\partial C}{\partial x} = \sqrt{kD}C_0$$

This suggests that flux at $x = 0$ is proportional to both k and D i.e. drug will be drawn out rapidly if either diffusion rate or reaction rate is higher

4. (i) In this case we have to solve the diffusion equation with condition $\frac{\partial C}{\partial t} = -R$

Therefore,

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

Or, $$D\frac{\partial^2 C}{\partial x^2} = -R$$

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

(ii) Integrating w.r.t. x twice we get

$$C(x) = -\frac{R}{2D}x^2 + A_1 x + A_2$$

Where A_1 and A_2 are arbitrary constants

Using condition $C(0) = 0$ gives $A_2 = 0$

Therefore,

$$C(x) = -\frac{R}{2D}x^2 + A_1 x$$

Using condition $C(h) = 0$ gives $A_1 = \frac{R}{2D}h$

Therefore,

$$C(x) = -\frac{R}{2D}x^2 + \frac{Rh}{2D}x$$

$$C(x) = \frac{R}{2D}x(h - x)$$

(iii) Flux out of the tablet is given by

$$J = -D\frac{\partial c}{\partial x} = Rx - \frac{R}{2}h$$

Therefore,

$$J|_{x=0} = -\frac{Rh}{2}$$

$$J|_{x=h} = +\frac{Rh}{2}$$