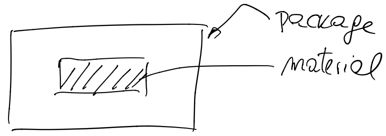
ABE 308 — SOLUTION OF HOMEWORK # 5
SPRING 2018

(1)

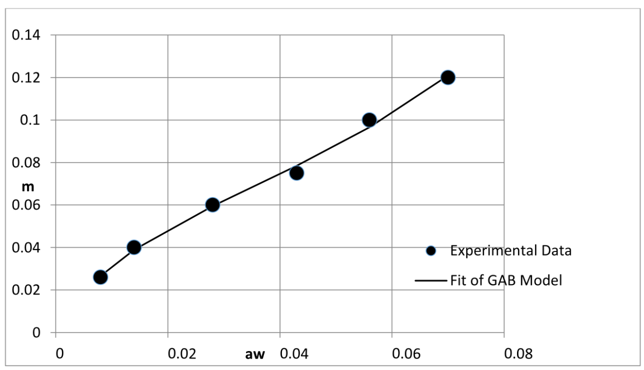
Problem 1

(1)




| RH | m |
|---|---|
| 0.008 | 0.026 |
| 0.014 | 0.040 |
| 0.028 | 0.060 |
| 0.043 | 0.075 |
| 0.056 | 0.10 |
| 0.070 | 0.12 |

A plot of m versus $\frac{RH}{100} = a_w$ is given in the following page. For example the GAB model can be used to get the moisture isotherm parameters. Values of the table are already given as RH/100 so values as given in the table are plotted



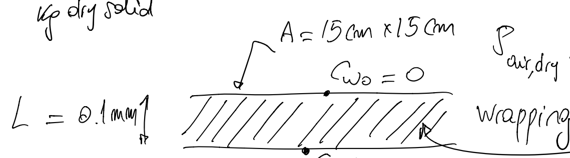

The GAB model is:

$$m = \frac{K C m_1 a_w}{(1 - K a_w)(1 + K C a_w - K a_w)}$$

By using Excel the following parameters can be calculated:

$K = 7.10$
$C = 9.95$
$m_1 = 0.07$

(2) $m = 0.05 \frac{\text{kg water}}{\text{kg dry solid}}$




$\rho_{air,dry} = 1.1 \frac{kg}{m^3}$

$D_{w,film} = D_w = 0.4 \times 10^{-11} \frac{m^2}{s}$

Obviously by assuming steady state, no convection, no chemical reaction, mass transfer in x-direction and no convection inside the package

$$N_{w,x} = D_w A \frac{C_{ws} - C_{wo}}{L} \quad (1)$$

Also assume $K^* = 1$

(2)

we can assume that the concentration of water vapor in equilibrium with the material having a $m = 0.05 \frac{Kg\ water}{Kg\ dry\ solid}$, which can be obtained from the plot above (or by using the GAB model) can be obtained and its value is: $C_{w,air} = C_{ws}$ [Because there is no convection inside the package

From the plot for $m = 0.05 \frac{Kg\ water}{Kg\ dry\ solid} \rightarrow a_w = 0.021$ and $RH = 2.1\%$

at $30°C$ $P_w^o = 0.0424$ bars

and $\frac{RH}{100} = \frac{P_w}{P_w^o} \Rightarrow P_w = \frac{RH \times P_w^o}{100} = \frac{2.1 \times 0.0424}{100}$ bars

$P_w = 8.9 \times 10^{-4}$ bars

By assuming that the water vapor behaves as an ideal gas

$$P_w V_w = n_w RT = \frac{m_w}{M_w} RT$$

and

$$\frac{m_w}{V_w} = C_w = \frac{P_w M_w}{RT} = \frac{8.9 \times 10^{-4} \cancel{bars} \times 18\ g/\cancel{mol}}{83.14 \frac{\cancel{bars} \times cm^3}{\cancel{mol}\ \cancel{K}} \times 303 \cancel{K}} = 6.4 \times 10^{-7} \frac{g}{cm^3}$$

Substituting values into Eq.(1) we can obtain:

$$N_{w,x} = 0.4 \times 10^{-11} \frac{\cancel{m^2}}{s} \times 10^4 \frac{\cancel{cm^2}}{\cancel{m^2}} \times 15 \times 15\ \cancel{cm^2} \times \frac{(6.4 \times 10^{-7} - 0)\ g/\cancel{cm^3}}{0.1 \times 10^{-3}\ \cancel{cm}} \simeq 5.8 \times 10^{-8} \frac{g}{s}$$

$$N_{wx} = 5.8 \times 10^{-8} \frac{g}{s} \times \frac{3600\ s}{1h} \times \frac{24h}{1 day} = 5 \times 10^{-3} \frac{g}{day}$$

$$\boxed{N_{wx} = 5 \times 10^{-3}\ g/day}$$

Problem 2

$$N_A = \frac{C_{A1} - C_{A2}}{Resistance}$$ [This is the objective, i.e. to get an equation like this]

(1) Microscopic Mass Balance for the Component A, assuming no convection no chemical reaction, spherical geometry and radial diffusion

$$\frac{\partial C_A}{\partial t} = D\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial C_A}{\partial r}\right)\right]$$ this equation assumes that $D$ = constant

if we assume steady state the equation simplifies to:

$$\frac{d}{dr}\left[r^2 \frac{dC_A}{dr}\right] = 0 \qquad (1)$$

and the Boundary conditions are:

(3)

$C = C_i$ at $r = R_i$ (1a)

$C = C_o$ at $r = R_o$ (1b)

By integrating Eq. (1) once we get

$$r^2 \frac{dC_A}{dr} = C_1 \quad (2)$$ where $C_2$ is an integration constant

$$\frac{dC_A}{dr} = \frac{C_1}{r^2} \quad (3)$$

By integrating Eq. (3) once more

$$C_A(r) = -\frac{C_1}{r} + C_2 \quad (4)$$

By using the Boundary conditions (1a) and (1b) we obtain:

$$C_A(r = R_i) = C_i = -\frac{C_1}{R_i} + C_2 \quad (5)$$

$$C_A(r = R_o) = C_o = -\frac{C_1}{R_o} + C_2 \quad (6)$$

Substracting Eqs (5) and (6) we obtain

$$C_i - C_o = -C_1\left[\frac{1}{R_i} - \frac{1}{R_o}\right] \Longrightarrow C_1 = \frac{C_i - C_o}{\frac{1}{R_o} - \frac{1}{R_i}} \quad (7)$$

and From Eq. (5) $\quad C_2 = C_i + \frac{C_1}{R_i}$

and $$C_2 = C_i + \frac{C_i - C_o}{R_i\left[\frac{1}{R_o} - \frac{1}{R_i}\right]} = C_i + \frac{C_i - C_o}{\frac{R_i}{R_o} - 1} \quad (8)$$

substituting Eqs (7) and (8) into Eq. (4)

$$C_A(r) = -\frac{C_i - C_o}{\frac{1}{R_o} - \frac{1}{R_i}} \frac{1}{r} + C_i + \frac{C_i - C_o}{\frac{R_i}{R_o} - 1} \quad (9)$$

and $$\frac{dC_A(r)}{dr} = \frac{C_i - C_o}{\frac{1}{R_o} - \frac{1}{R_i}} \frac{1}{r^2} \quad (10)$$

(2) Flow of A through the layer

$$N_A = -DA \frac{dC_A(r)}{dr} \quad (10)$$

(4)

From Eq. (10) $N_A = -DA \cdot \left[ \dfrac{C_i - C_o}{\frac{1}{R_o} - \frac{1}{R_i}} \dfrac{1}{r^2} \right]$ (11)

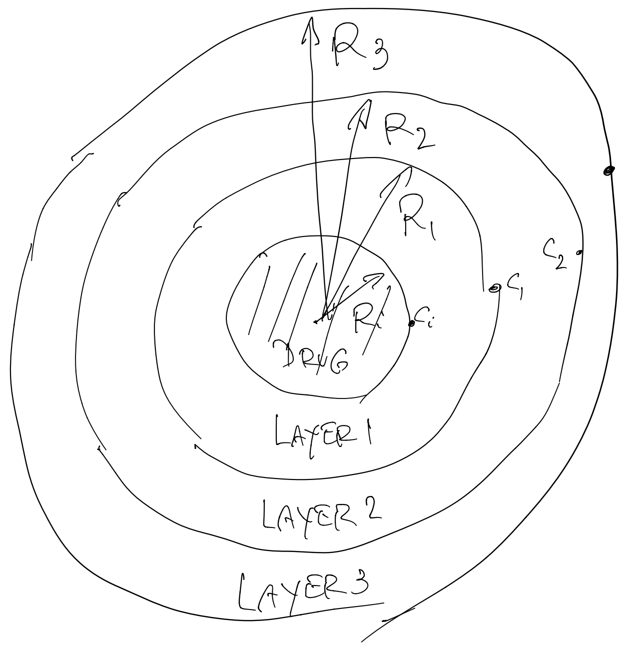
For a sphere $A = 4\pi r^2$ so substituting into Eq. (11) we obtain

$$N_A = -D4\pi \cancel{r^2} \frac{C_i - C_o}{\frac{1}{R_o} - \frac{1}{R_i}} \frac{1}{\cancel{r^2}} = -4\pi D \frac{C_i - C_o}{\frac{R_i - R_o}{R_i R_o}} = \frac{C_i - C_o}{\frac{R_o - R_i}{4\pi D R_i R_o}}$$

$$N_A = \frac{C_i - C_o}{\frac{R_o - R_i}{4\pi D R_i R_o}} \Longrightarrow \text{Resistance} = \frac{R_o - R_i}{4\pi D R_i R_o}$$

(3) $N_A = \dfrac{C_i - C_o}{\text{Resistance Diffusion}}$ (12) $\text{Resistance Diffusion} = \dfrac{R_o - R_i}{4\pi D R_i R_o}$

(4) MULTILAYER TABLET – NO CONVECTION




$R_i = 5\text{mm}$

$R_1 = 6\text{mm}$

$R_2 = 6.9\text{mm}$

$R_3 = 7.05\text{mm}$

By anology with Eq. (12)

$$N_A = \frac{C_i - C_o}{\text{Res layer 1} + \text{Res layer 2} + \text{Res layer 3}}$$

$$N_A = \frac{C_i - C_o}{\frac{R_1 - R_i}{4\pi D_1 R_i R_1} + \frac{R_2 - R_1}{4\pi D_2 R_1 R_2} + \frac{R_3 - R_2}{4\pi D_3 R_2 R_3}} \qquad (13)$$

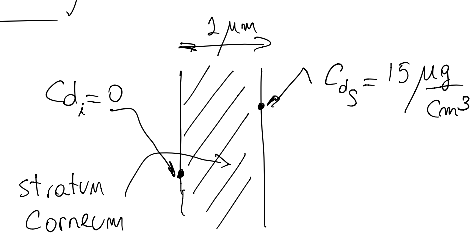
substituting values into Eq. (13)

$$N_A = \frac{1\,mg/mm^3 - 0}{\frac{6-5\ mm}{4\pi \times 10 \times 10^{-2}\frac{mm^2}{s} \times 5 \times 6\ mm^2} + \frac{6.9-6}{4\pi \times 0.2 \times 10^{-2}\frac{mm^2}{s} \times 6.9 \times 6\ mm^2} + \frac{7.05-6.9}{4\pi \times 0.35 \times 10^{-2}\frac{mm^2}{s} \times 7.05 \times 6.9\ mm^2}}$$

$$N_A = \frac{1\,mg/mm^3}{0.0265\frac{s}{mm^3} + 0.865\frac{s}{mm^3} + 0.07\frac{s}{mm^3}} \cong 1.04\frac{mg}{s}$$

$$\boxed{N_A = 1.04\frac{mg}{s}}$$

Problem 3




(1) Flux of drug for steady state

$$n_d = -D\frac{dC_d}{dx} = D\frac{C_{ds} - C_{di}}{\ell} = 10^{-10}\frac{\cancel{cm^2}}{s} \times \frac{(15-0)\,\mu g/\cancel{cm^3}}{0.1\,\cancel{\mu m} \times \frac{1\,\cancel{cm}}{10^4\,\cancel{\mu m}}}$$

$$\boxed{n_d = 1.5 \times 10^{-2}\frac{\mu g}{s}}$$

(2) To know how much medication resides in the stratum corneum we need to determine the concentration profile

By assuming steady state, slab geometry, no convection and no chemical reaction the balance of mass for the drug is:

$$\frac{d^2 C_d}{dx^2} = 0 \qquad (1)$$

$$\text{at } x = 0 \quad C_d = C_{ds} \qquad (1a)$$

$$\text{at } x = \ell \quad C_d = C_{di} \qquad (1b)$$

By integrating Eq.(1) twice

$$C_d(x) = C_1 x + C_2 \qquad (2)$$

and using the boundary conditions

$$C_2 = C_{ds} \quad \text{and} \quad C_1 = \frac{C_{di} - C_{ds}}{l} = -\frac{C_{ds} - C_{di}}{l} \qquad (3)$$

Substituting Eq.(3) into Eq.(2)

$$C_d(x) = C_{ds} - \frac{C_{ds} - C_{di}}{l} x$$

the amount of medication residing in the stratum corneum is:

$$C_{d\,residing} = \frac{1}{l}\int_0^l C_d(x)\,dx \qquad (4)$$

$$C_{d\,residing} = \frac{1}{l}\left[C_{ds}\,l - \frac{C_{ds} - C_{di}}{\cancel{l}} \frac{l^{\cancel{2}}}{2}\right]$$

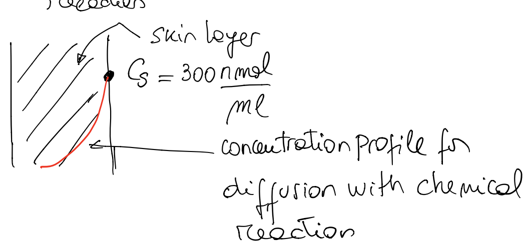
$$C_{d\,residing} = \frac{1}{l}\left[C_{ds}\frac{l}{2} + \frac{C_{di}\,l}{2}\right]$$

$$C_{residing} = \frac{C_{ds} + C_{di}}{2} = 7.5\ \mu g/cm^3$$

## Problem 4

First order reaction $\quad K = 1000\ \frac{1}{m} \quad D = 2\times10^{-10}\ m^2/s$

(1)




For a slab geometry by assuming steady state, no convection the equation simplifies to:

$$0 = D\frac{d^2C}{dx^2} - KC \qquad (1)$$

$$C = C_s \ \text{at}\ x = 0 \qquad (1a)$$

$$C = 0 \ \text{at}\ x = L \qquad (1b)$$

(2) if we define $m^2 = \frac{K}{D}$ or $m = \sqrt{\frac{K}{D}} = \sqrt{\frac{1000\ 1/min \times 1 min/60 s}{2\times10^{-10}\ \frac{m^2}{s}}} \simeq 2.9\times10^{5}\ \frac{1}{m}$ (7)

Solutions were given in lecture 10 as:

$$\frac{C(x)}{C_s} = e^{-mx} - \frac{e^{-mL}}{e^{mL} - e^{-mL}}\left[e^{mx} - e^{-mx}\right] \qquad (2)$$

but as m is large the equation simplifies to:

$$\frac{C(x)}{C_s} = e^{-2.9\times10^5 x} \qquad (3)$$

(3) if $C = 0.10\,C_s$ substituting into Eq.(3)

$$\frac{0.10C_s}{C_s} = e^{-2.9\times10^5 x} \Longrightarrow X_{depth} = -\frac{\ln 0.10}{2.9\times10^5\ 1/m} = 7.94\times10^{-6}\ m$$

$$X_{depth} = 7.9\ \mu m$$

(4) DRUG FLUX [FROM LECTURE 10]

$$n_d = -D\left.\frac{dC(x)}{dx}\right|_{x=0} = -DC_s(-m)\left.e^{-mx}\right|_{x=0} = DC_s m = 2\times10^{-10}\ \frac{m^2}{s} \times 300\ \frac{nmol}{cm^3} \times 2.9\times10^{5}\ \frac{1}{m}$$

$$n_d = 1.74\times10^{-2}\ nmol \times \frac{m}{s} \times \frac{1}{\cancel{cm^3}} \times \frac{10^6\ \cancel{cm^3}}{1\ m^{3}} = 1.74\times10^{-4}\ \frac{nmol}{m^2 s}$$

(5) if $K = 2000\ 1/min$ $\quad m = \sqrt{\frac{K}{D}} = \sqrt{\frac{2000}{60\times2\times10^{-10}}} \simeq 4.1\times10^{5}\ \frac{1}{m}$

$$X_{depth} = -\frac{\ln 0.10}{4.1\times10^5\ 1/m} = 5.6\times10^{-6}\ m$$

$$X_{depth} = 5.6\ \mu m$$

(6) the diffusion coefficient could be changed but it is more practical to change the concentration at the surface. If we want to have the same concentration that will be $0.10\times300\ \frac{nmol}{cm^3}$. Thus,

$$30\ \frac{nmol}{cm^3} = C_{so}\,e^{-7.94\times10^{-6}\ m \times 4.1\ 10^5\ \frac{1}{m}} \Longrightarrow C_{so} = \frac{30\ nmol/cm^3}{3.86\times10^{-2}} \simeq 778\ \frac{nmol}{cm^3}$$