

BMOLE 452-689 – Transport

Chapter 6. Mass Transport in Biological Systems

Text Book: Transport Phenomena in Biological Systems

Authors: Truskey, Yuan, Katz

Focus on what is presented in class and problems...

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Which was Tesla's favorite number?

Non-steady State Diffusion

- Sample Problem: An FCC iron-carbon alloy initially containing 0.20 wt% C is carburized at an elevated temperature and in an atmosphere that gives a surface carbon concentration constant at 1.0 wt%. If after 49.5 h the concentration of carbon is 0.35 wt% at a position 4.0 mm below the surface, determine the temperature at which the treatment was carried out.
- **Solution:** use Eqn.

$$\frac{C(x,t) - C_o}{C_s - C_o} = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

$$\frac{C(x,t) - C_o}{C_s - C_o} = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

- $t = 49.5 \text{ h}$ $x = 4 \times 10^{-3} \text{ m}$
- $C_x = 0.35 \text{ wt\%}$ $C_s = 1.0 \text{ wt\%}$
- $C_o = 0.20 \text{ wt\%}$

$$\frac{C(x,t) - C_o}{C_s - C_o} = \frac{0.35 - 0.20}{1.0 - 0.20} = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) = 1 - \operatorname{erf}(z)$$

$$\therefore \operatorname{erf}(z) = 0.8125$$

Problem 6.1

- *Compare $D_s...$ where $T=298K$, Diameter = 0.3467 nm; For oxygen the partial molar volume is $25.6 \text{ cm}^3/\text{mol}$.*

- *S.E. $\Rightarrow D = \frac{K_B T}{6\pi\mu R}$*

- *Wilkie-Chang (semi-empirical) \Rightarrow*

$$D = 7.4e - 10 \frac{T(\varphi M)^{0.5}}{\mu V_o^{0.6}}; \varphi_{\text{water}} = 2.26$$

Problem 6.1

- Compare $Ds...$ where $T=298K$, Diameter = 0.3467 nm; For oxygen the partial molar volume is $25.6 \text{ cm}^3/\text{mol}$. Ans is $2.1e-5 \text{ cm}^2/\text{s}$

- S.E. $\Rightarrow D = \frac{K_B T}{6\pi\mu R} =$

$$\frac{1.38e-23 \frac{\text{J}}{\text{K}} * 298\text{K}}{6\pi * 0.00089\text{Pa} * \text{s} * 1.7335e-10 \text{ m}} * 100^2 \text{ cm}^2/\text{m}^2 = 1.41e-5 \frac{\text{cm}^2}{\text{s}}$$

Abs(ans-guess)*100/ans = 32.6% error

- Wilkie-Change (semi-empirical; cP and cm^3/mol) \Rightarrow

$$D = 7.4e-10 \frac{\text{cm}^2}{\text{s}} \frac{T(\varphi M)^{0.5}}{\mu V_o^{0.6}} = ; \varphi_{\text{water}} = 2.26$$

$$D = 7.4e-10 \frac{\text{cm}^2}{\text{s}} \frac{298\text{K} \left(2.26 * \frac{18.015\text{g}}{\text{mol}}\right)^{0.5}}{0.0089\text{cP} * \left(\frac{25.6\text{cm}^3}{\text{s}}\right)^{0.6}} = 2.21e-5 \frac{\text{cm}^2}{\text{s}}$$

5.22% error

Problem 6.2

- They want to know what D_2 is of a protein at 25°C. They know D_1 ($6.8e-7$ cm²/s) and R_1 (3 nm)

- $D = \frac{K_B T}{6\pi\mu R}$

- $\frac{D_1}{D_2} = \frac{\left[\frac{K_B T}{6\pi\mu R_1}\right]}{\left[\frac{K_B T}{6\pi\mu R_2}\right]}$ so $D_2 = 1.7e-7$ cm²/s

Problem 6.3

- MatLab:
- Using recursion relations:

$$\langle X^2 \rangle^{1/2} = \left[\langle X_{n-1}^2 \rangle^{1/2} + \frac{1}{n} \sum_{i=1}^n \delta_i^2 \right]^{1/2}$$
$$r_i = r_{i-1} + \delta$$

(The cross term $\sum_{i=1}^n x_{n-1} \delta_i$ is zero because the mean of δ_i is still zero. Substituting for x_{n-1} , the root mean square displacement can be written in terms of x_{n-1} :

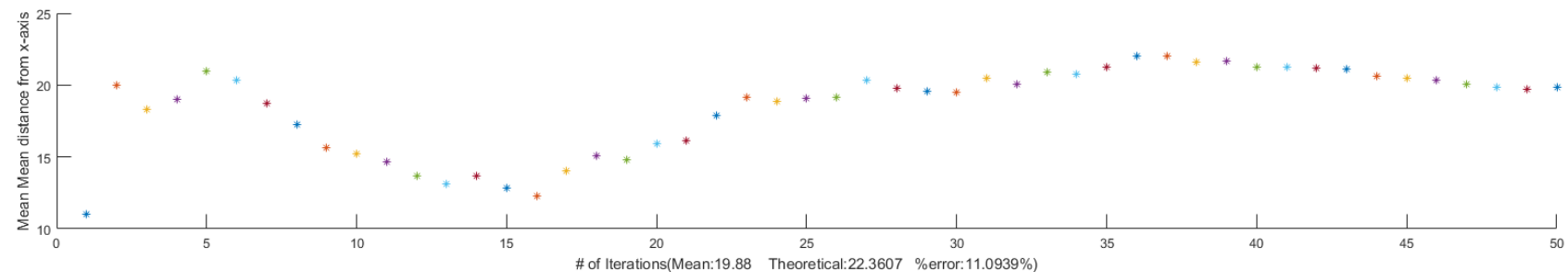
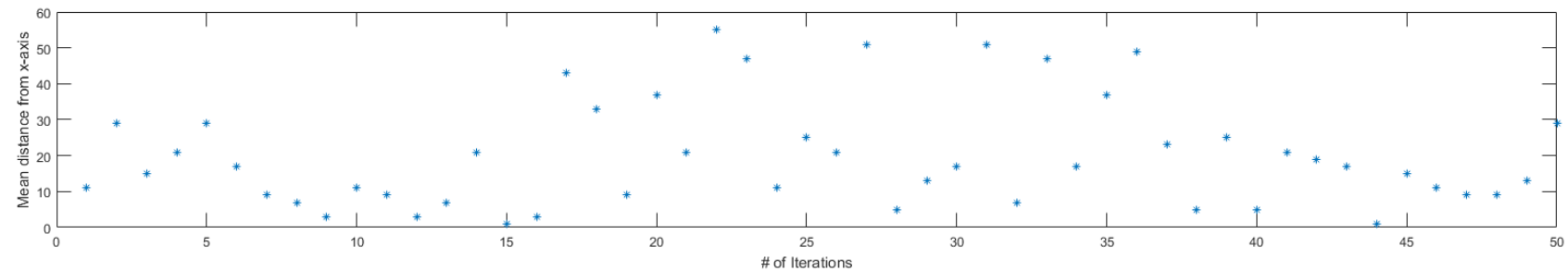
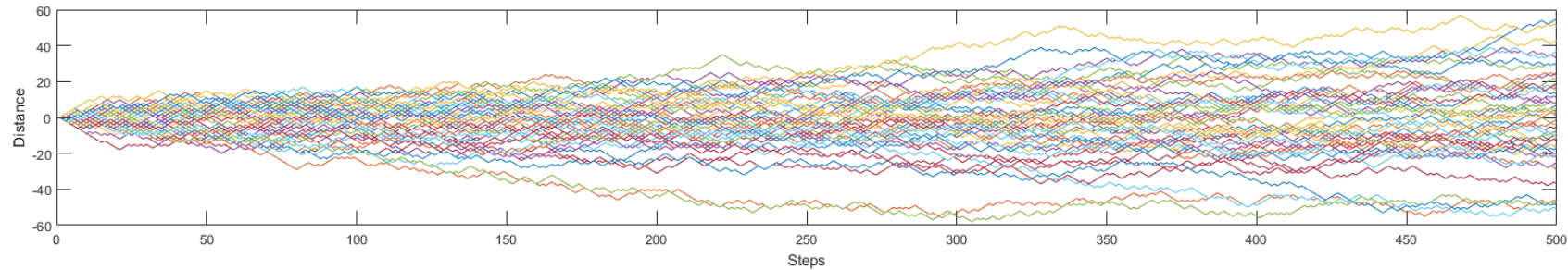
$$\langle X^2 \rangle^{1/2} = \left[\langle X_{n-2}^2 \rangle^{1/2} + \frac{2}{n} \sum_{i=1}^n \delta_i^2 \right]^{1/2}$$

Repeating this procedure until the first term on the right hand side is $x_1 = 0$, the root mean square displacement becomes.

$$\langle X^2 \rangle^{1/2} = \left[\frac{n}{n} \sum_{i=1}^n \delta_i^2 \right]^{1/2} = n^{1/2} \langle \delta^2 \rangle^{1/2}$$

Matlab “RandomWalk.m”

- Create a program that you can input either [-1 0 1] or [-1 1] with any number of steps and have it calculate the error% for each run up to a specified value...



Problem 6.4

- Fibrinogen
- Estimate D if
- A) a prolate ellipsoid
- B) a cylindrical rod

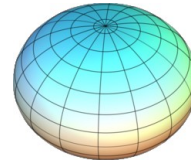
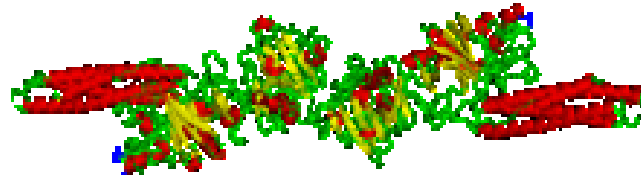


TABLE 6.3

Values of the Mean Frictional Drag Coefficient for Different Shapes [9,10]

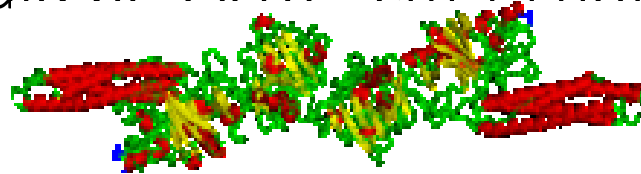
Shape	Frictional drag coefficient
Sphere of radius R	$f = 6\pi\mu R$
Prolate ellipsoid, $p = a/b > 1$, where a is a major axis, b is a minor axis	$\bar{f} = \frac{6\pi\mu b(p^2 - 1)^{1/2}}{p^{1/3}\ln[p + (p^2 - 1)^{1/2}]}$
Oblate ellipsoid, $p = a/b < 1$	$\bar{f} = \frac{6\pi\mu b(1 - p^2)^{1/2}}{p^{1/3}\tan^{-1}[1 - p^2]^{1/2}p^{-1}}$
Thin circular disk of radius a	$\bar{f} = 16\mu a$
Cylinder of radius a and length L	$\bar{f} \approx \frac{4\pi\mu L}{\ln(L/a) + 0.193}$

Source: From Refs [9,10].

Note: $p^{0.333}$ is close to 1 when a and b are similar. Can remove in some cases.

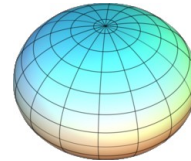
Problem 6.4 (compare to table 6.4)

Note that Table 6.4 should be $2 \times 10^{-7} \text{ cm}^2/\text{s}$ not positive 7...



- Fibrinogen
- Estimate D if
- A) a prolate ellipsoid
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$$D_{ij} = \frac{k_B T}{f}$$



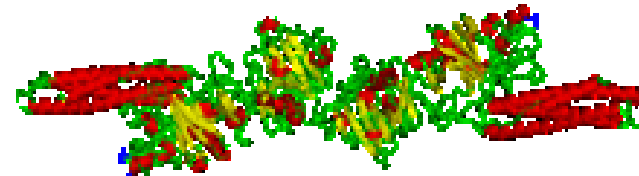
For a prolate ellipsoid ($p=a/b>1$) $\bar{f} = \frac{6\pi\mu b(p^2 - 1)^{1/2}}{\ln[p + (p^2 - 1)^{1/2}]}$

$$\bar{f} \approx \frac{8\pi\mu L}{3\ln(L/a) - 0.94}$$

For a cylinder of radius a and length L

$$S.E. \Rightarrow D = \frac{K_B T}{f_{bar}}; f_{bar} \text{ based on geometry}$$

Problem 6.4



	prolate ellipsoid			cylinder			
	Kb	1.38E-23 J/K		Kb	1.38E-23 J/K		
	T	298 K		T	298 K		
	u	0.00089 Pa*s		u	0.00089 Pa*s		
a>b	a	4.75E-08 m		L	4.75E-08 m		
	a radius	2.38E-08 m		D	9.00E-09 m		
	b	9.00E-09 m		r	4.50E-09 m		
	b radius	4.50E-09 m					
	a/b	5.28E+00		fbar num	0.000000001		
	fbar num	3.91E-10		fbar			
	fbar denom	2.347553949		denom	6.13E+00		
	fbar	1.67E-10		fbar	1.73E-10		
	D	2.47E-07 cm^2/s		D	2.37E-07		
	D table 6.4	2.00E-07 cm^2/s		D table			
	Error%	23.44 %		6.4	2.00E-07 cm^2/s		
				Error%	18.69 %		

Problem 6.6

- NO = potent vasodilator for treating newborns who have pulmonary hypertension
- Examine transport of gas through an alveolus and into the capillaries.
- Gas is added at a $[] < 100$ ppm.
- Alveolus is modeled as a sphere of radius R_a

6.6

- 100 ppm => mole fraction of 0.001. The maximum level of error in the flux is also on this level.
 - $1-x_i=0.9999$.
 - So...
-
- Time to reach steady state is R^2/D_{ij} .
 - Radius of alveolus = 50 μm = $1\text{e-}2$ cm; Diffusivity = 0.2 cm^2/s . so $\text{Time}_{ss} = 1.25\text{e-}4$ s
 - Gas concentration in blood is = 0.
 - Average breath is 5 seconds.

Problem 6.6

6.6 Nitric oxide (NO) is an extremely potent vasodilator that is used to treat newborns who have pulmonary hypertension and adults who have undergone certain operative procedures. We want to examine the transport of the gas through an alveolus and into the capillaries. The gas is added at a concentration of less than 100 parts per million (ppm). The alveolus is modeled as a sphere of radius R_a (see Figure 6.29).

Mole fraction: ?

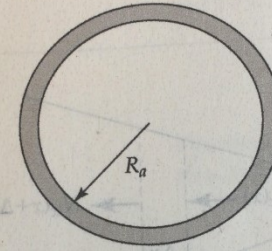


FIGURE 6.29 Diffusion in an alveolus.

- Determine the mole fraction of the gas and assess the maximum error in the flux, assuming that the gas is a dilute solution of NO.
- In each inspiration, the concentration of NO in each alveolus is 30 ppm and the gas is initially uniformly mixed. Is the gas completely removed between breaths? Use the following data:

alveolus radius = $50 \mu\text{m}$ $D_{\text{NO}} = 0.2 \text{ cm}^2 \text{ s}^{-1}$

gas concentration in blood = 0

Problem 6.6

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Mole fraction: 100 parts/million = $100e-6 = 1e-4$
The error is thus?

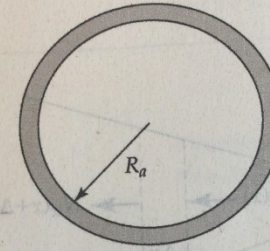


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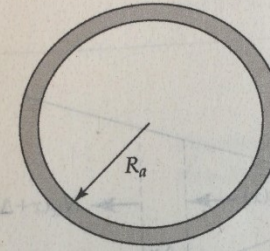


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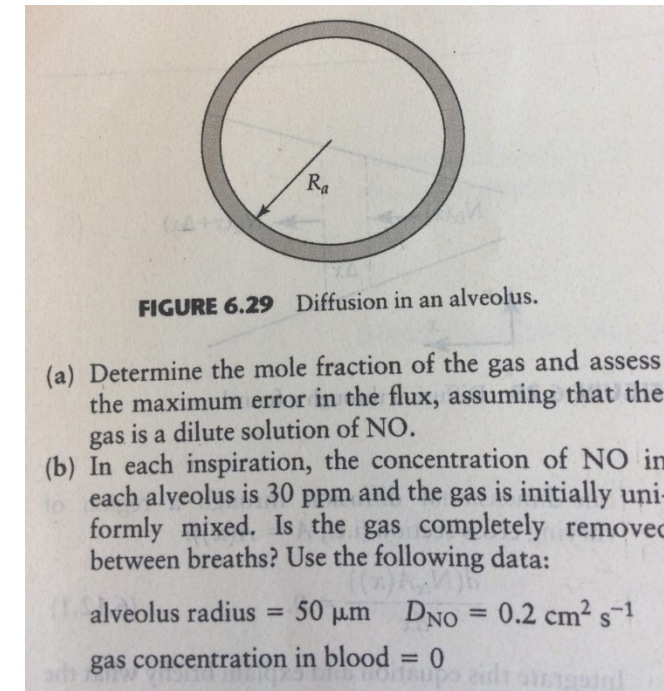
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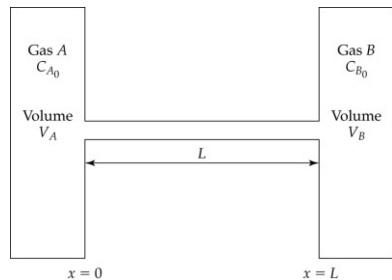
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 Since it is dilute we can assume what?
 And flux is what?

$$N_1 = -CD_{ij}\nabla x_1 + x_1(N_1 + N_2)$$



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$$N_i = -\frac{CD_{ij}}{1-x_i} \frac{dx_i}{dr} \approx CD_{ij} \frac{dx_i}{dr}$$

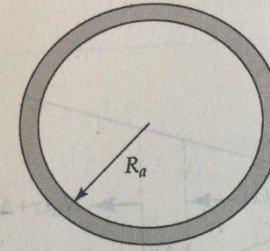
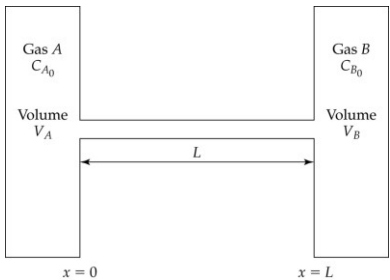


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↑
=?

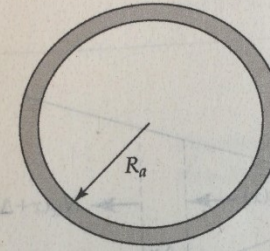


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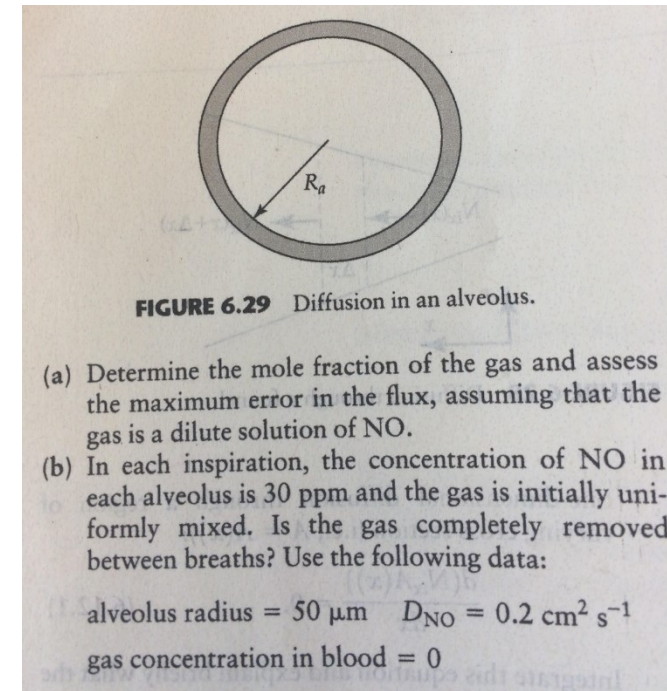
$$N_i = -\frac{CD_{ij}}{1-x_i} \frac{dx_i}{dr}$$



=0.9999 initially and grows because 0.0001 gets smaller(t)...

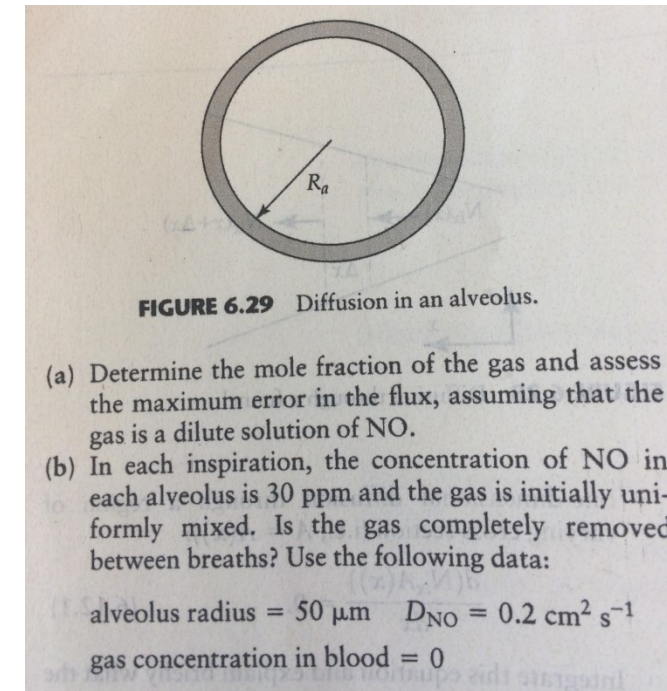
So...

$$\approx CD_{ij} \frac{dx_i}{dr}$$



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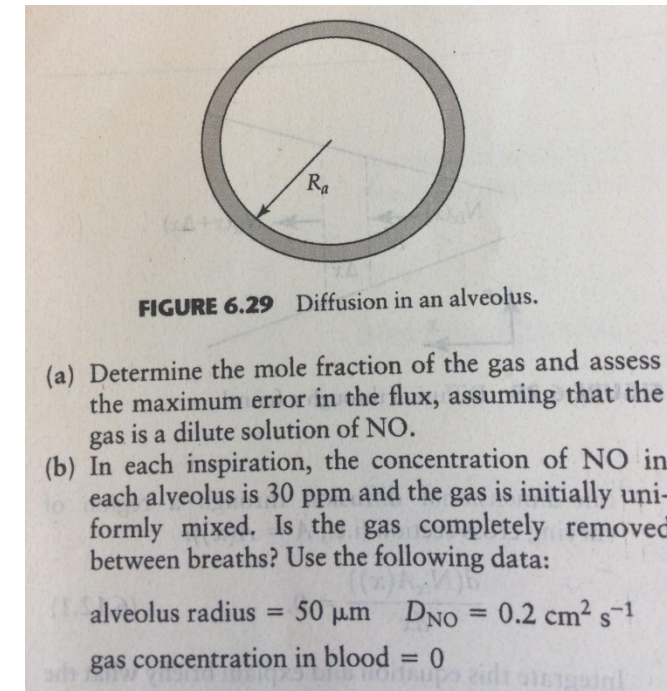
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Proceed to calculate flux from here if that is the objective

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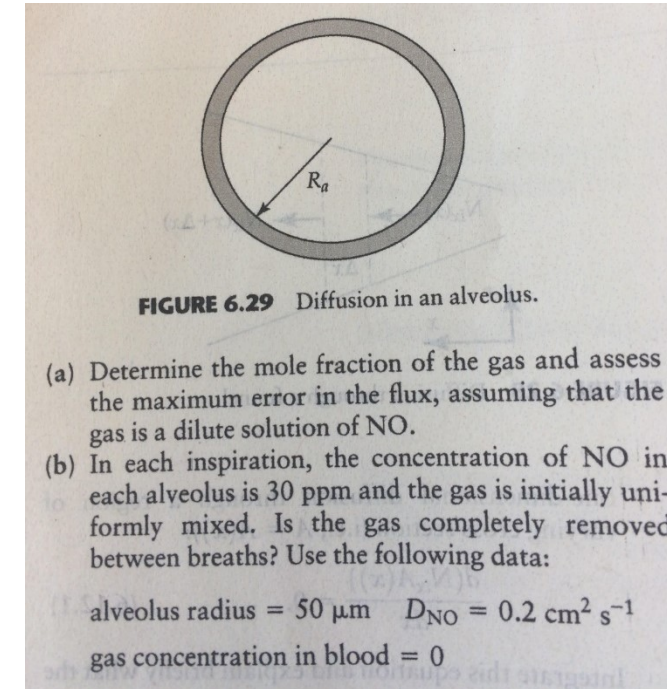
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Mole fraction (ans to part a)



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So...

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Proceed to calculate flux from here if that is the objective

Mole fraction (ans to part a)



Part b.

How long to reach steady state?

$R^2/D_{ij} = 1.25e-4$ s and is much shorter

5 seconds so yes, the gas is completely

Removed between breaths...

Problem 6.7

6.7 An uncharged membrane separates two aqueous salt solutions that contain a protein at concentrations of C_L and C_R , with $C_L > C_R$ (see Figure 6.30). Stirring the solutions reduces, but does not eliminate, mass transfer effects near the membrane surface. The salt concentrations are the same for both solutions, so the potential differences are negligible. Figure 6.30 shows concentration distributions for the protein solutions.

For each sketch, briefly discuss whether the concentration profiles are physically possible, and if they are, determine whether the partition coefficient Φ ($= C_m/C_L$ or C_m/C_R) is greater than, less than, or equal to unity.

Left figure:

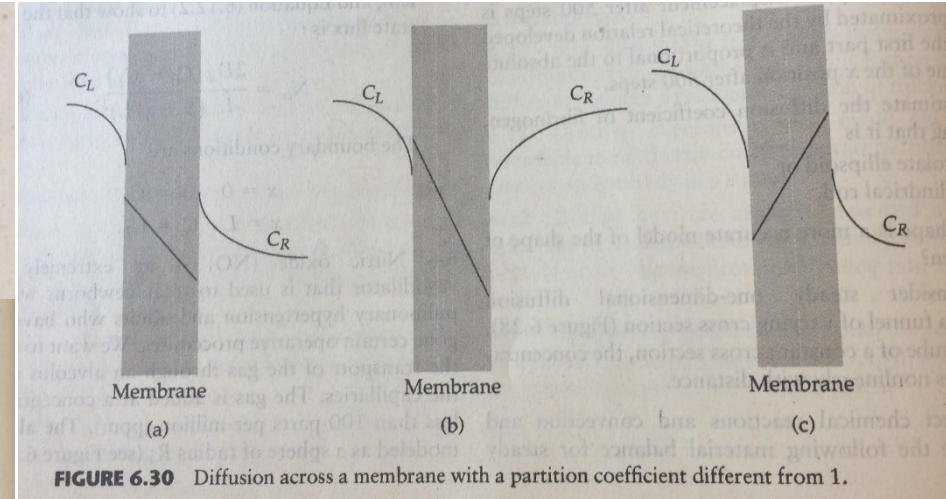
Reason 1 and 2 are satisfied.

Middle figure:

Reasons 1 and 2 are not satisfied.

Right figure:

Reason 2 is not satisfied.



We know flow is occurring from left to right:

Needs to hold true:

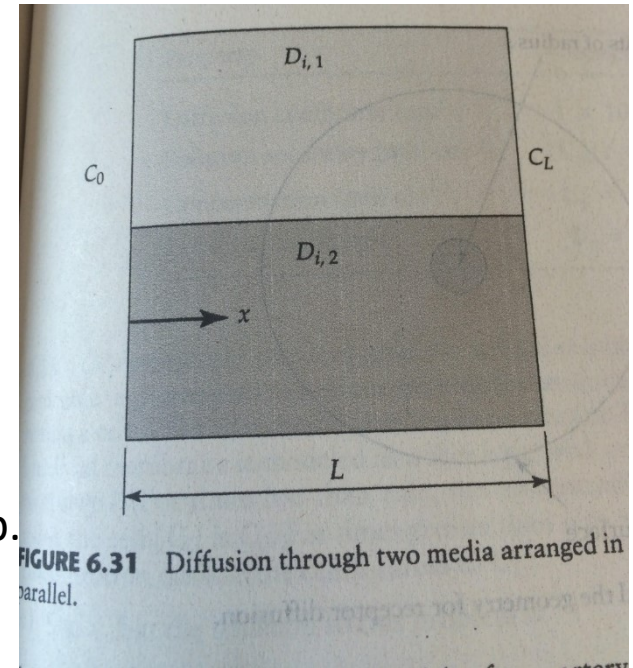
Reason 1: C_L is coming from a source and is expected to be higher on the far left. It also needs to be higher than C_R and C_R needs to continue to drop as you go more to the right.

Reason 2: We know that the partition coefficient is the same on the left side and the right side of the membrane. Thus if the concentration on the far left of the membrane is lower than C_L at the membrane, then the concentration of the membrane also needs to be lower than C_R on the far right of the membrane. Similarly, if the concentration on the far left of the membrane is higher than C_L at the membrane, then the concentration of the membrane also needs to be higher than C_R on the far right of the membrane.

Problem 6.8

6.8 In Section 6.7, diffusion through multiple layers of tissue arranged in series was examined. Now consider steady-state diffusion through two media arranged parallel to each other (see Figure 6.31). Assume that diffusion is one dimensional. At $x = 0$, $C_1 = \Phi_1 C_0$, and $C_2 = \Phi_2 C_0$. At $x = L$, $C_1 = \Phi_1 C_L$ and $C_2 = \Phi_2 C_L$. Develop an expression for the steady-state flux across the two media. Show that the diffusive resistances act in parallel.

What is your assumption based on the previous result the prob. Is referring to?



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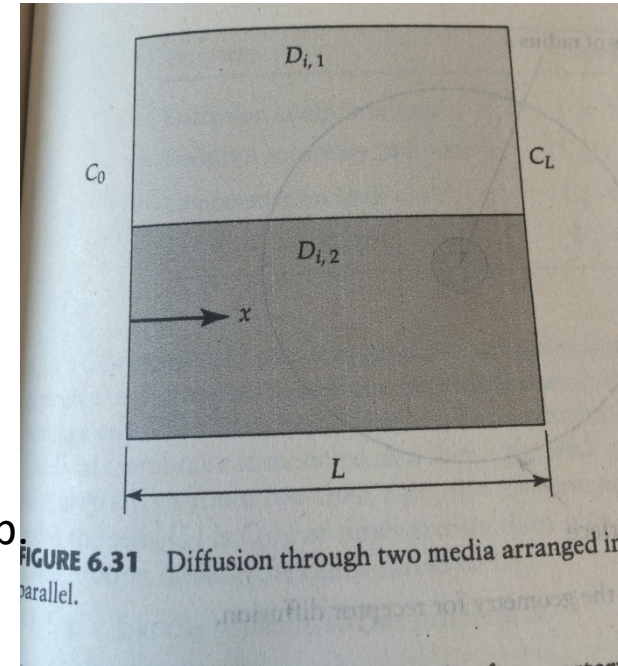


FIGURE 6.31 Diffusion through two media arranged in parallel.

What is your assumption based on the previous result the prob. Is referring to?

$$\frac{d^2 C_i}{dx^2} = 0$$

$$\iint d^2 C_i = \iint 0 dx^2$$

$$C_i = C_1 x + C_2 \Rightarrow C_i = A_1 x + B_1 \Rightarrow 2 \text{ eqns}$$

$$C_1 = A_1 + B_1 x$$

$$C_2 = A_2 + B_2 x$$

$\textcircled{1} x=0 \quad C_1 = \Phi_1 C_0$
 $\textcircled{2} x=L=L_1+L_2 \quad C_2 = \Phi_2 C_L$
 $\textcircled{3} x=L_1 \quad N_{1x} = N_{2x}$
 $\textcircled{4} x=L_1 \quad C_1 = C_2$

1. c. #1 $C_1 = \Phi_1 C_0 = A_1 + B_1(x=0) \Rightarrow A_1 = \Phi_1 C_0$
 #2 $C_2 = \Phi_2 C_L = A_2 + B_2(x=L) \Rightarrow A_2 = \Phi_2 C_L - B_2(L+L_2)$
 #3 $\frac{C_1}{\Phi_1} = \frac{A_1 + B_1 x}{\Phi_1} = \frac{\Phi_1 C_0}{\Phi_1} + \frac{B_1 x}{\Phi_1} = C_0 + \frac{B_1 x}{\Phi_1} = C_0 + B_1 \frac{x}{\Phi_1} = A_1 + B_1 x = \frac{(\Phi_2 C_L - B_2(L+L_2)) + B_2 x}{\Phi_2}$
 #4 $D_{i,1} \frac{dC_1}{dx} = D_{i,2} \frac{dC_2}{dx} = C_0 - B_2 \frac{L+L_2}{\Phi_2}$
 $D_{i,1} \frac{d(A_1 + B_1 x)}{dx} = D_{i,2} \frac{d(A_2 + B_2 x)}{dx} = D_{i,1} B_1 = D_{i,2} B_2$

solving for unknowns yields

$$N_{ix} = \frac{D_{i,1} D_{i,2}}{D_{i,1} L_1 + D_{i,2} L_2} (C_0 - C_L)$$

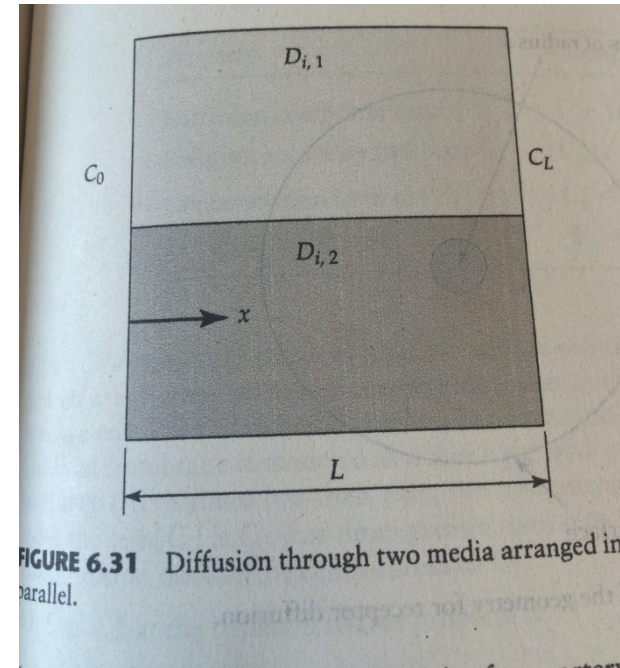
$\frac{1}{\frac{D_{i,1} D_{i,2}}{D_{i,1} L_1 + D_{i,2} L_2}} = \frac{L_1}{D_{i,1}} + \frac{L_2}{D_{i,2}}$ ← diffusive resistances in electrical systems
 generalizing...
 $\frac{L}{D_{i,1} D_{i,2}} = \sum \frac{L_i}{D_{i,i}}$

Reminiscent of resistors in electrical systems!

Problem 6.8

6.8 In Section 6.7, diffusion through multiple layers of tissue arranged in series was examined. Now consider steady-state diffusion through two media arranged parallel to each other (see Figure 6.31). Assume that diffusion is one dimensional. At $x = 0$, $C_1 = \Phi_1 C_0$, and $C_2 = \Phi_2 C_0$. At $x = L$, $C_1 = \Phi_1 C_L$ and $C_2 = \Phi_2 C_L$. Develop an expression for the steady-state flux across the two media. Show that the diffusive resistances act in parallel.

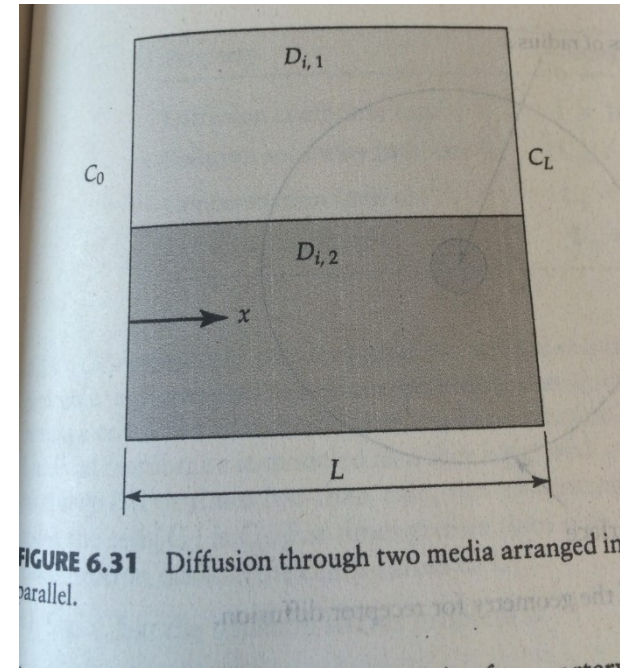
What variables do we need not shown here?



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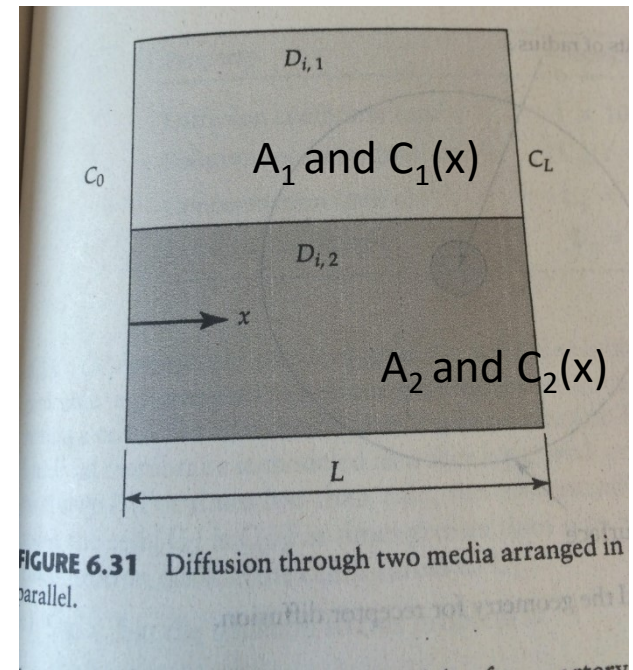
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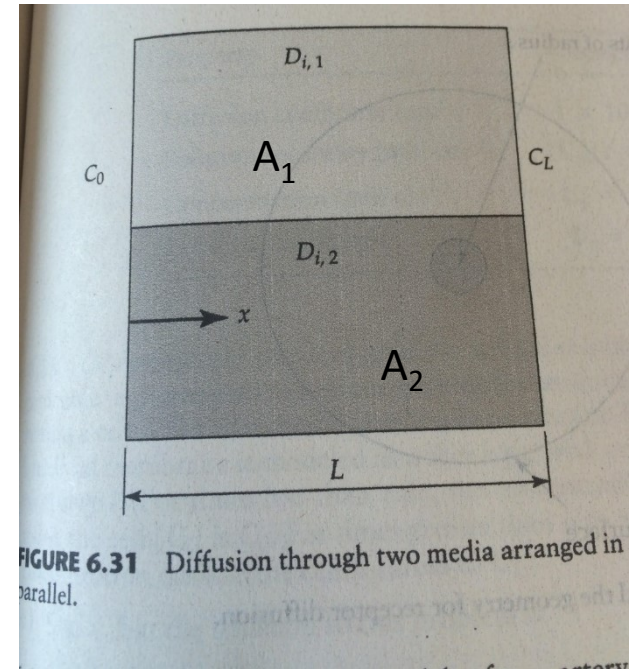
Assuming what about the concentration?



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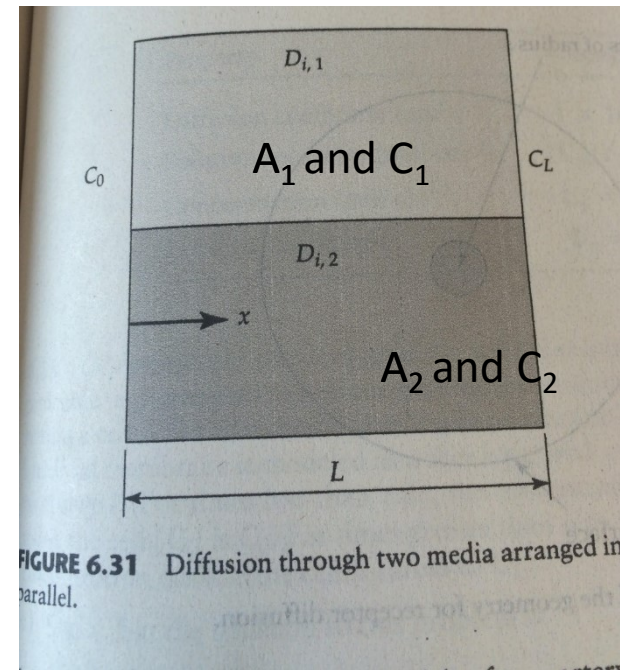
Assuming what about the concentration? It's dilute...



Problem 6.8

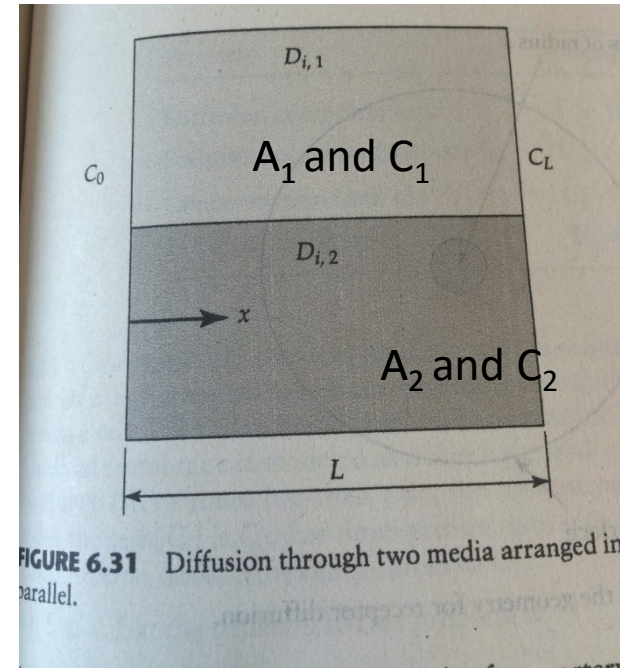
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What are the conservation relations for each phase?



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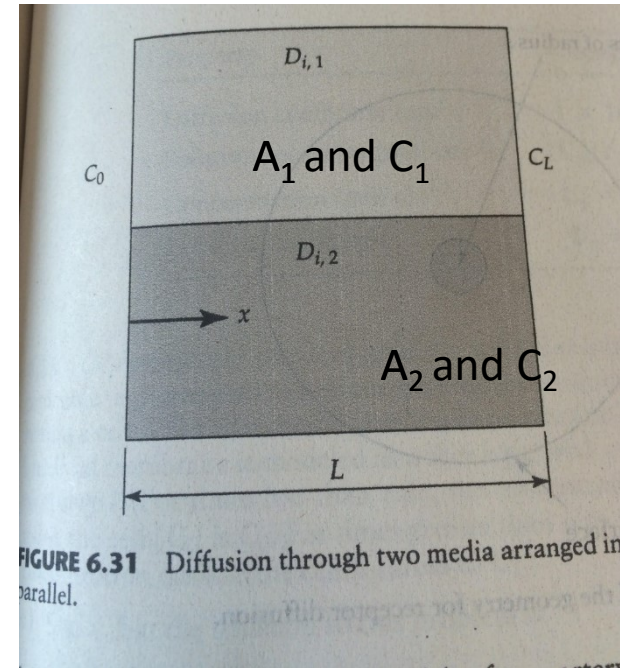
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What does this mean physically?

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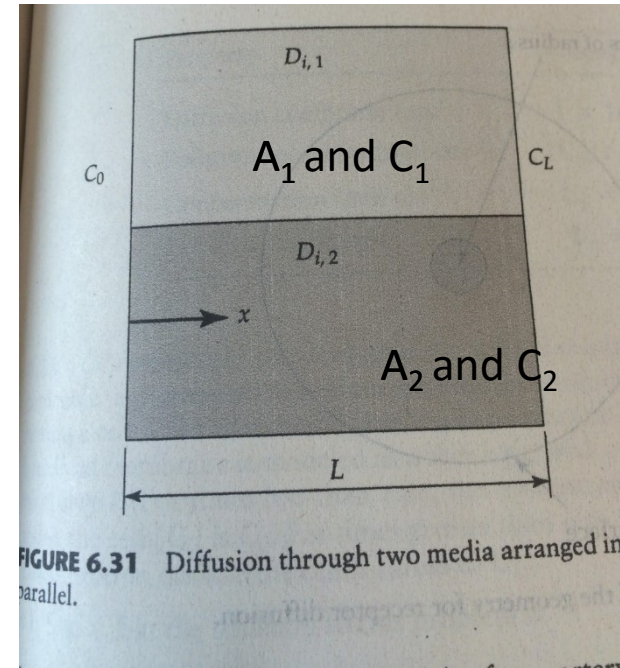
$$\frac{d^2 C_1}{dx^2} = 0 \qquad \frac{d^2 C_2}{dx^2} = 0$$

What does this mean physically?

$C(x)$ changes linearly with x or $C(x) = 0$... when would $C(x)=0$?

Problem 6.8

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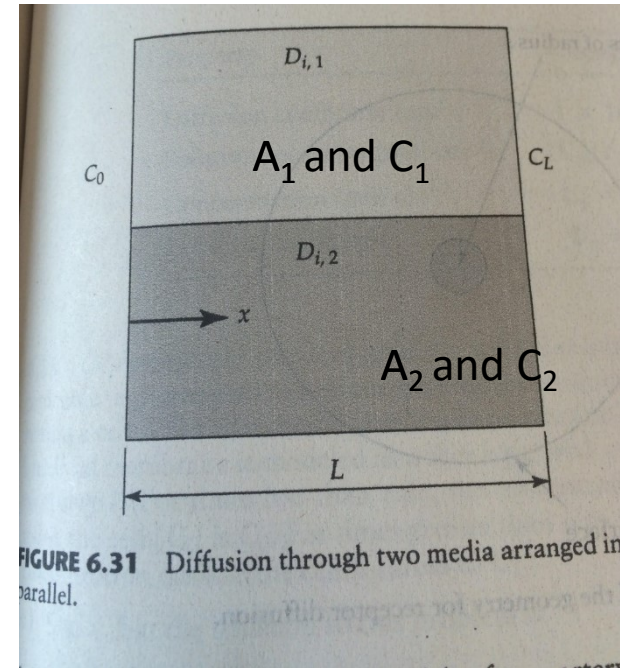
What does this mean physically?

$C(x)$ changes linearly with x or $C(x) = 0 \dots$ when would $C(x) = 0 \dots$ for long time $t (> 5\tau)$

So what does this mean for our solutions of this problem in terms of $C(x)$?

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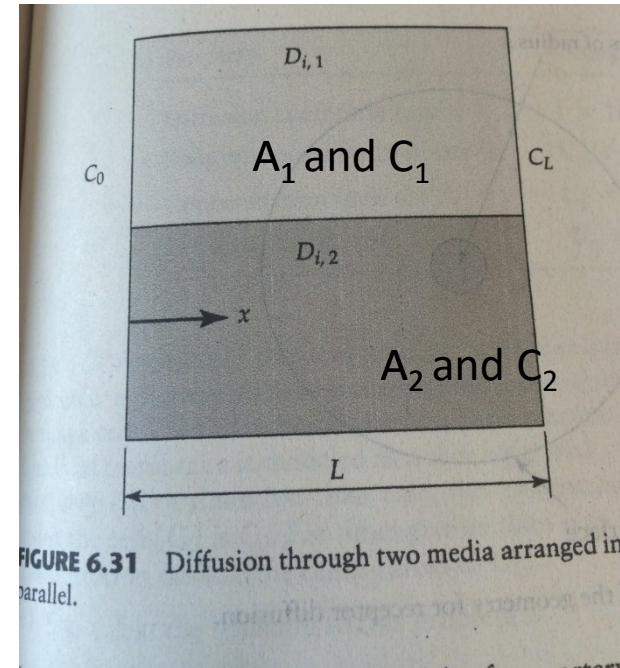
$C_1 = A_1 x + B_1$ and $C_2 = A_2 x + B_2$ but let's actually show this mathematically...

Now what?

$$\begin{aligned} \frac{d^2 c}{dx^2} &= 0 \\ d^2 c &= 0 \cdot dx^2 \\ \int \int d^2 c &= \int \int 0 \cdot dx^2 \\ C &= \int \text{constant} \cdot dx \\ C &= \text{constant}_1 x + \text{constant}_2 \\ C &= Ax + B \quad (A \neq \text{Area}) \end{aligned}$$

Problem 6.8

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$C_1 = A_1 x + B_1$ and $C_2 = A_2 x + B_2$ but let's actually show this mathematically...

Now what? Apply B.C.s

$$\begin{aligned} \frac{d^2 c}{dx^2} &= 0 \\ d^2 c &= 0 \cdot dx^2 \\ \int \int d^2 c &= \int \int 0 \cdot dx^2 \\ c &= \int \text{constant}_1 dx \\ c &= \text{constant}_1 x + \text{constant}_2 \\ c &= Ax + B \quad (A \neq \text{Area}) \end{aligned}$$

Problem 6.8

generally...

$$C = Ax + B$$

$$\textcircled{a} x=0: C = A \cdot 0 + B = \Phi \cdot C_0 \text{ so } B = \Phi C_0$$

$$\textcircled{b} x=L: C = AL + \Phi C_0 = \Phi C_L \text{ so } A = \frac{\Phi C_L - \Phi C_0}{L}$$

$$\text{so } C = \left(\frac{\Phi C_L - \Phi C_0}{L} \right) x + \Phi C_0$$

B.C. $\textcircled{a} x=0, C_1 = \Phi_1 C_0, C_2 = \Phi_2 C_0$

$\textcircled{b} x=L, C_1 = \Phi_1 C_L, C_2 = \Phi_2 C_L$

more specifically...

$$C_1 = \frac{\Phi_1 (C_L - C_0)}{L} x + \Phi_1 C_0$$

$$C_2 = \frac{\Phi_2 (C_L - C_0)}{L} x + \Phi_2 C_0$$

$$\frac{dc_1}{dx} = \frac{\Phi_1 (C_L - C_0)}{L}$$

$$\frac{dc_2}{dx} = \frac{\Phi_2 (C_L - C_0)}{L}$$

$$N_1 = -D_{i1} \frac{dc_1}{dx} = -D_{i1} \frac{\Phi_1 (C_L - C_0)}{L} \quad N_2 = -D_{i2} \frac{dc_2}{dx} = -D_{i2} \frac{\Phi_2 (C_L - C_0)}{L}$$

mass balance moles of i entering = moles of i in phase 1 & 2

$$N_{i \text{ total}} \underbrace{(A_1 + A_2)}_{\text{Area}} = A_1 N_{i1} + A_2 N_{i2}$$

$$N_{i \text{ total}} = \frac{A_1 N_{i1} + A_2 N_{i2}}{A_1 + A_2} = \frac{\left[-D_{i1} A_1 \frac{\Phi_1 (C_L - C_0)}{L} \right] + \left[-D_{i2} A_2 \frac{\Phi_2 (C_L - C_0)}{L} \right]}{A_1 + A_2}$$

$$N_{i \text{ total}} = \frac{(A_1 \Phi_1 D_{i1} + A_2 \Phi_2 D_{i2}) (C_0 - C_L)}{L (A_1 + A_2)}$$

What is
Conductance of
Each phase?

Problem 6.9

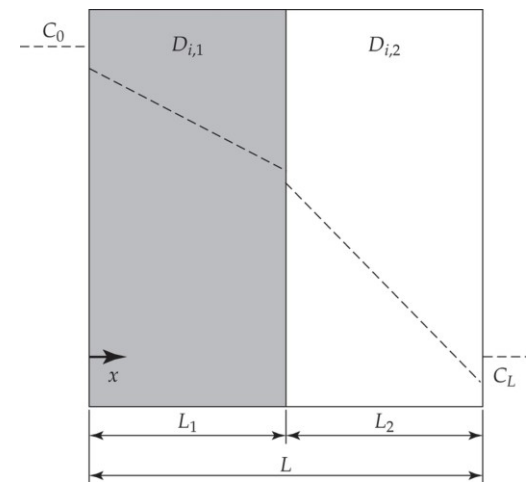
that the diffusive resistance is the same in both layers. Consider a rectangular laminate consisting of two layers, as shown in Figure 6.9. Assume that $\Phi_1 = \Phi_2 = 1$.

(a) For the following values, determine the effective diffusion coefficient:

$$D_{i,1} = 5 \times 10^{-6} \text{ cm}^2\text{s}^{-1} \quad L_1 = 20 \text{ } \mu\text{m}$$

$$D_{i,2} = 7 \times 10^{-7} \text{ cm}^2\text{s}^{-1} \quad L_2 = 80 \text{ } \mu\text{m}$$

(b) Determine conditions for which the two-layer model behaves as an effective one-layer model.



How?

This is from an earlier problem to remind you of the solution, as it is helpful for you for 6.9.

$$\frac{d^2 c_i}{dx^2} = 0$$

$$\int \int d^2 c_i = \int \int 0 \cdot dx^2$$

$$c_i = C_1 x + C_2 \Rightarrow c_i = A x + B \Rightarrow 2 \text{ equations}$$

$$C_1 = A_1 + B_1 x$$

$$C_2 = A_2 + B_2 x$$

$$\textcircled{1} x=0 \quad C_1 = \Phi_1 C_0$$

$$\textcircled{2} x=L=L_1+L_2 \quad C_2 = \Phi_2 C_L$$

$$\textcircled{3} x=L_1 \quad N_{1x} = N_{2x}$$

$$\textcircled{4} x=L_1 \quad \frac{C_1}{\Phi_1} = \frac{C_2}{\Phi_2}$$

$$\text{B.C. \#1: } C_1 = \Phi_1 C_0 = A_1 + B_1(x=0); A_1 = \Phi_1 C_0$$

$$\text{B.C. \#2: } C_2 = \Phi_2 C_L = A_2 + B_2(x=L)$$

$$A_2 = \Phi_2 C_L - B_2(L+L_2)$$

$$\text{\#3} \quad \frac{C_1}{\Phi_1} = \frac{A_1 + B_1 x}{\Phi_1} = \frac{\Phi_1 C_0 + B_1 x}{\Phi_1} = C_0 + \frac{B_1 x}{\Phi_1} = C_0 + \frac{B_1 L_1}{\Phi_1} = \frac{A_2 + B_2 x}{\Phi_2} = \frac{(\Phi_2 C_L - B_2 L) + B_2 L_1}{\Phi_2}$$

$$\text{\#4} \quad D_{i,1} \frac{dc_1}{dx} = D_{i,2} \frac{dc_2}{dx} = \frac{C_1 - B_2 L_2}{\Phi_2}$$

$$D_{i,1} \frac{d(A_1 + B_1 x)}{dx} = D_{i,2} \frac{d(A_2 + B_2 x)}{dx} = D_{i,1} B_1 = D_{i,2} B_2$$

solving for unknowns yields

$$N_{ix} = \frac{\Phi_{\text{eff}} D_{\text{eff}}}{L} (C_0 - C_L)$$

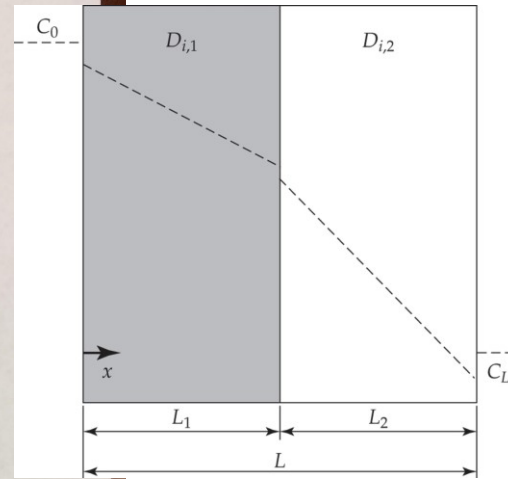
$$\frac{L}{\Phi_{\text{eff}} D_{\text{eff}}} = \frac{L_1}{\Phi_1 D_{i,1}} + \frac{L_2}{\Phi_2 D_{i,2}}$$

← diffusive resistances
electrical systems

generalizing...

$$\frac{L}{\Phi_{\text{eff}} D_{\text{eff}}} = \sum_{j=1}^N \frac{L_j}{\Phi_j D_{i,j}}$$

$$\begin{cases} 0 < x < L_1 : C_1 = ? \\ L_1 < x < L_2 : C_2 = ? \end{cases}$$



Problem 6.9

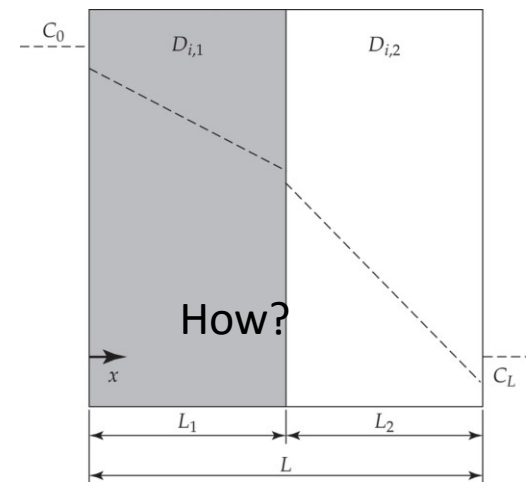
that the diffusive resistance is negligible at the interface between the two layers. Consider a rectangular laminate consisting of two layers, as shown in Figure 6.9. Assume that $\Phi_1 = \Phi_2 = 1$.

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How?

Problem 6.9

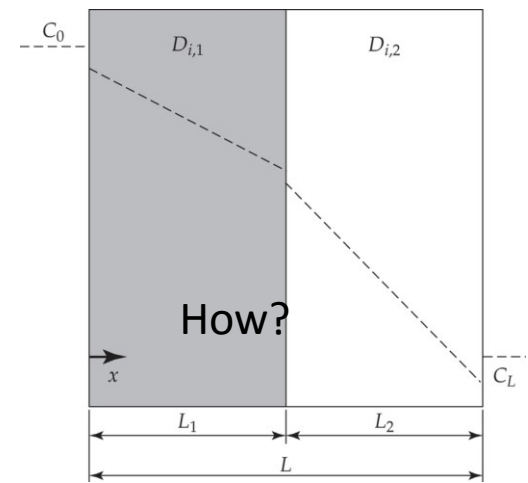
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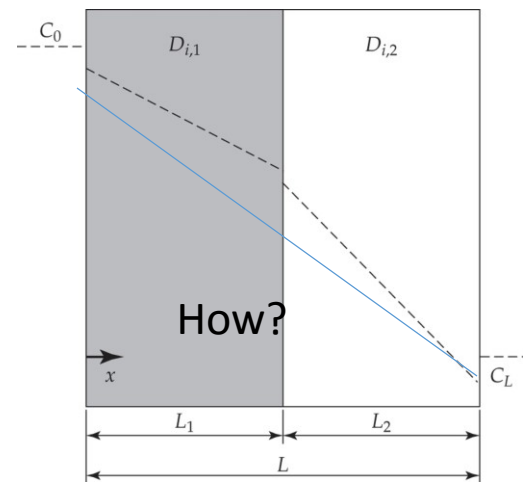
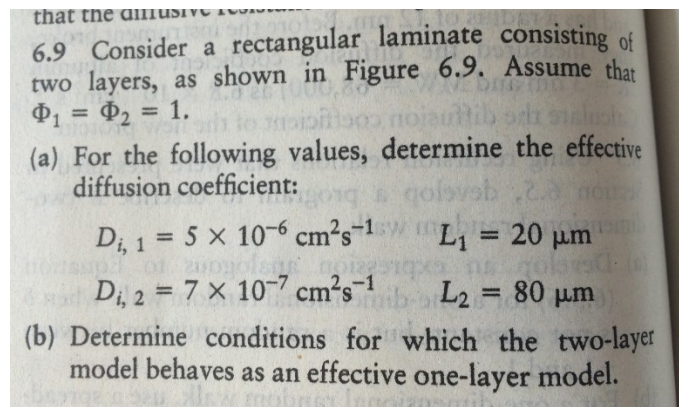
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Function of L ?

Problem 6.9



Function of L ?

How?

Problem 6.9

that the diffusive resistance is the same in both layers.

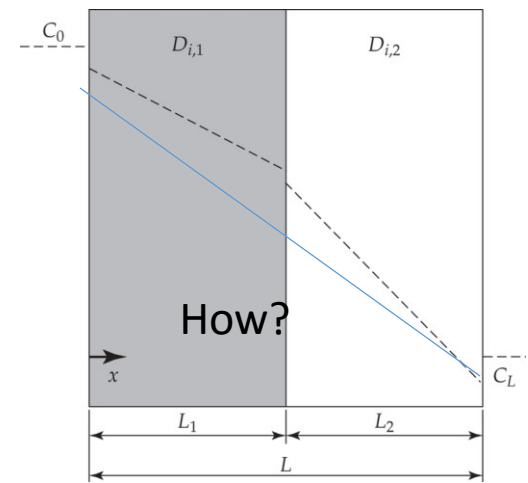
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(b) Determine conditions for which the two-layer model behaves as an effective one-layer model.

How?



Function of L ?
Phi.s and D.s must
Be equal...

Problem 6.10

- Where to start?

6.10 Consider a two-layer model of an artery, as shown in Figure 6.32. The layers are of thickness $R_0 - R_1$ and $R_1 - R_i$. The inner layer has the diffusion coefficient D_i and the outer layer has the diffusion coefficient D_0 . The solute concentration in the lumen (i.e., $0 < r < R_i$) is C_i , and the concentration at R_0 is C_0 . Calculate the effective diffusion coefficient.

6.11 Beginning with Equation (6.8.101), derive a generalized quasi-steady-state relation for transport across a thin membrane when the volumes on the two sides of the membrane differ. Show that the result reduces to Equation (6.8.107) when $V_1 = V_2$.

6.12 Low-density lipoprotein (LDL) is the major cholesterol-carrying lipoprotein in the body. Its entry into cells occurs when LDL binds to receptors that are localized on specialized regions of the cell surface known as

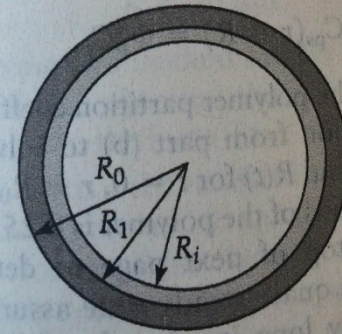


FIGURE 6.32 Diffusion through a cylindrical laminate.

Problem 6.10

- Where to start?
- ss? Using r , it is how many Dimensions?

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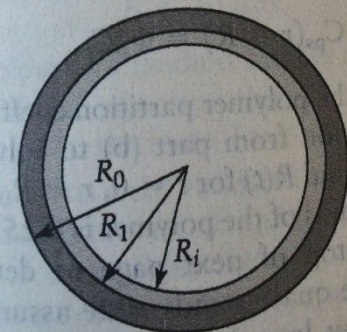


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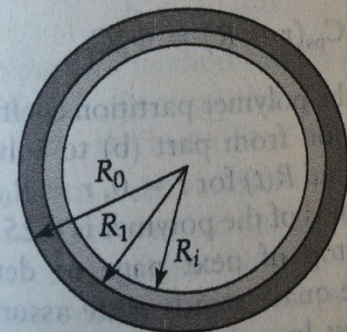


FIGURE 6.32 Diffusion through a cylindrical laminate.

Problem 6.10

- Where to start?
- ss? Using r , it is how many

Dimensions?

1-D

6.10 Consider a two-layer model of an artery, as shown in Figure 6.32. The layers are of thickness $R_0 - R_1$ and $R_1 - R_i$. The inner layer has the diffusion coefficient D_i and the outer layer has the diffusion coefficient D_0 . The solute concentration in the lumen (i.e., $0 < r < R_i$) is C_i , and the concentration at R_0 is C_0 . Calculate the effective diffusion coefficient.

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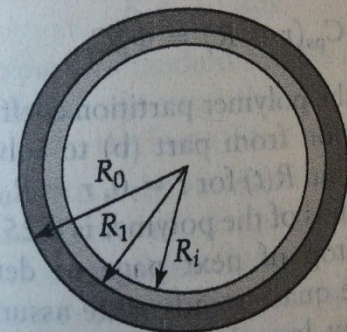


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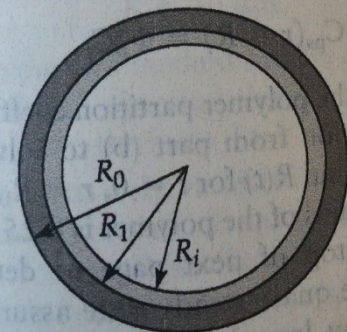


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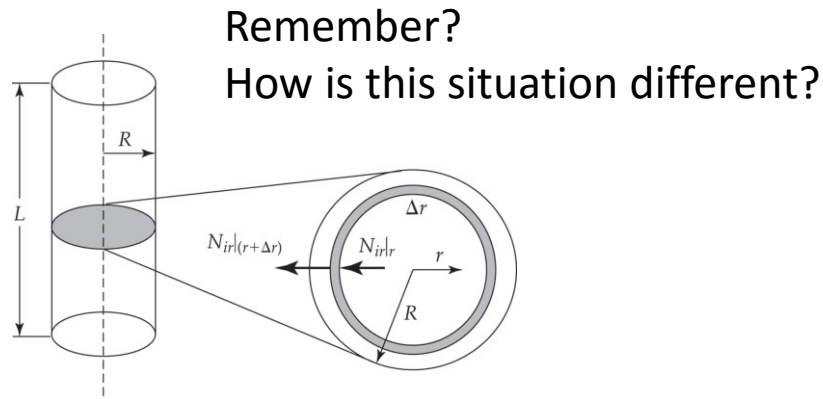
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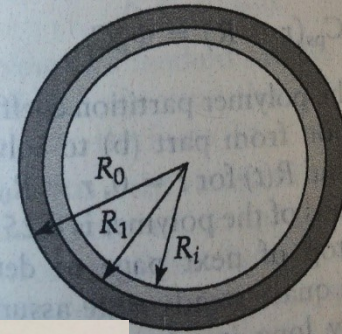
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Example 6.7 Figure 6.13
 Given $\frac{\partial C_i}{\partial t} = -\frac{1}{r} \frac{\partial (r N_{ir})}{\partial r} + R_i$
 Fick's First: $N_{ir} = -D_{ij} \frac{\partial C_i}{\partial r}$
 $\frac{\partial C_i}{\partial t} = \frac{D_{ij}}{r} \frac{\partial}{\partial r} (r \frac{\partial C_i}{\partial r}) + R_i$
 assuming $R_i = \phi \neq s.s.$
 $\phi = \frac{D_{ij}}{r} \frac{\partial}{\partial r} (r \frac{\partial C_i}{\partial r}) + \phi$

on through a cylindrical laminate.

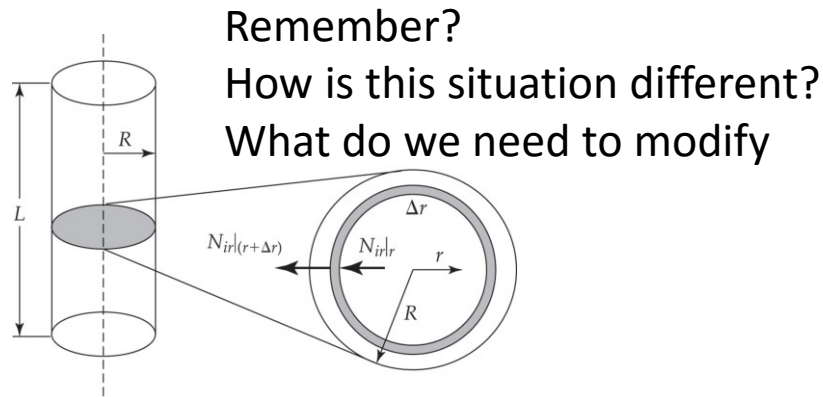
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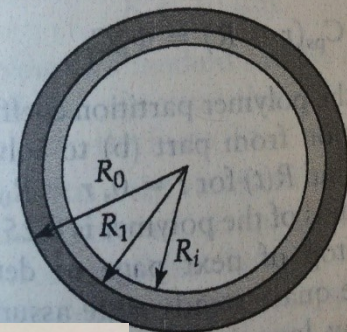
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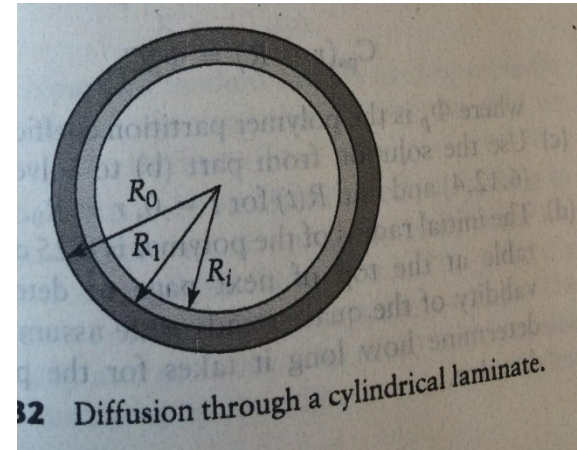
$$\text{Given } \frac{\partial C_i}{\partial t} = -\frac{1}{r} \frac{\partial (r N_{ir})}{\partial r} + R_i$$

$$\text{Fick's First: } N_{ir} = -D_{ij} \frac{\partial C_i}{\partial r}$$

$$\frac{\partial C_i}{\partial t} = \frac{D_{ij}}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C_i}{\partial r} \right) + R_i$$

assuming $R_i = \phi$ s.s.

$$\phi = \frac{D_{ij}}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C_i}{\partial r} \right) + \phi$$



$$\frac{D_{ij}}{r} \frac{d}{dr} \left(r \frac{dc_{ij}}{dr} \right) = 0$$

$$\frac{d}{dr} \left(r \frac{dc_{ij}}{dr} \right) = 0 \quad r \frac{dc_{ij}}{dr} = u$$

$\frac{du}{dr} = 0 \Rightarrow \int du = \int 0 dr$ so $u = \text{const} + \text{constant}$

$$r \frac{dc_{ij}}{dr} = \text{const} +$$

$$\int r \frac{dc_{ij}}{dr} = \int (\text{const} + dr)$$

$$c_{ij} = \text{const} + \ln r + \text{const} +$$

$$c_{ij} = \delta_j \ln r + \phi_j \quad (2 \text{ phases})$$

B.C. 4 equations, 4 unknowns ($\delta_1, \delta_2, \phi_1, \phi_2$)

1) $r=R_0, c_{ij}=C_0$

2) $r=R_i, c_{ij}=C_i$

we know that

$$1) c_{ij} = C_0 = \delta_j \ln R_0 + \phi_j \quad (\text{B.C. 1}) \begin{cases} C_0 = \delta_1 \ln R_0 + \phi_1 \\ C_0 = \delta_2 \ln R_0 + \phi_2 \end{cases}$$

$$2) c_{ij} = C_i = \delta_j \ln R_i + \phi_j \quad (\text{B.C. 2}) \begin{cases} C_i = \delta_1 \ln R_i + \phi_1 \\ C_i = \delta_2 \ln R_i + \phi_2 \end{cases}$$

so we solve for unknowns ($\delta_1, \delta_2, \phi_1, \phi_2$)

after simplification...

solutions for N_{i1} & N_{i2} are similar

$$N_{i1} = -D_{i1} \frac{dc_{i1}}{dr} \quad \& \quad N_{i2} = -D_{i2} \frac{dc_{i2}}{dr}$$

4 eqns.
4 unknowns
w/ drastic
simplification

~~...~~

solutions are of the form...

Takes too much unnecessary time to solve this. You should know how to do this though. For an exam, I would give this soln. to you to proceed so there isn't just 1 problem for the exam.

$$N_{ij} = \frac{-D_{i1} D_{i2} (C_0 - C_i)}{D_{i1} \ln \left(\frac{R_0}{R_i} \right) - D_{i2} \ln \left(\frac{R_i}{R_i} \right)} \cdot \frac{1}{r}$$

& we want a Deff which will be getting rid of R_i
so Deff would be of the form

$$N_{ij} = \frac{-\text{Deff} (C_0 - C_i)}{\ln \left(\frac{R_0}{R_i} \right)} \cdot \frac{1}{r} = \frac{-D_{i1} D_{i2} (C_0 - C_i)}{D_{i1} \ln \left(\frac{R_0}{R_i} \right) - D_{i2} \ln \left(\frac{R_i}{R_i} \right)} \cdot \frac{1}{r}$$

$$\text{so } \frac{\text{Deff}}{\ln \left(\frac{R_0}{R_i} \right)} = \frac{D_{i1} D_{i2} \ln \left(\frac{R_0}{R_i} \right)}{D_{i1} \ln \left(\frac{R_0}{R_i} \right) - D_{i2} \ln \left(\frac{R_i}{R_i} \right)} = \text{Deff}$$

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Problem 6.11

- Moles of solute leaving side 1 per unit time = moles of solute transported across membrane

Diff. statement 6.8.102
$$-V_1 \frac{dC_1}{dt} = A_m D_m K \frac{(C_1 - C_2)}{L}$$

Diff. statement 6.8.103
$$V_1 \frac{dC_1}{dt} = - \left(\frac{V_m}{K} \frac{dC_m}{dt} + V_2 \frac{dC_2}{dt} \right)$$

If $V_m \ll V_2$ and $V_m \ll V_1$ then...

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If $V_m \ll V_2$ and $V_m \ll V_1$ then...

$$\frac{dC_2}{dt} = - \frac{V_1}{V_2} \frac{dC_1}{dt}$$

initial conditions $C_1 = C_0$ and $C_2 = 0$.

$$C_2 = - \frac{v_1 C_0}{V_2} + Cx; Cx = \frac{V_1 C_0}{V_2} \text{ so } C_2 = - \frac{v_1 C_0}{V_2} + \frac{V_1 C_0}{V_2} \text{ so } C_2 = - \frac{v_1}{v_2} (C_1 - C_0)$$

Put C2 into 6.8.102

$$-V_1 \frac{dC_1}{dt} = \frac{A_m D_m K}{L} \left[\left(1 + \frac{V_1}{V_2} \right) C_1 - \frac{V_1}{V_2} C_o \right]$$

Solve this for C1: hint: there are exponentials in the solution...

Hint 2: Use integration factor: know how to convert a first order differential equation and

Solve using the integration factor method...covering on 2.6.17

$$\frac{dy}{dt} + p(t)y = g(t)$$

pretend there is a beautiful fun called $\mu(t) = \text{integrating factor}$
 & multiply everything by it...

$$\frac{dy}{dt} \mu(t) + \mu(t)p(t)y = g(t)\mu(t)$$

We also will magically assume that $\mu(t)p(t) = \mu'(t)$

so...

$$\underbrace{\frac{dy}{dt} \mu(t) + \mu'(t)y}_{\text{what is this?}} = g(t)\mu(t)$$

Chain rule! so...

$$(\mu(t)y(t))' = g(t)\mu(t) = \frac{d[\mu(t)y(t)]}{dt}$$

multiply both sides by dt but don't cancel ... & integrate

$$\int (\mu(t)y(t))' dt = \int g(t)\mu(t) dt$$

$$\mu(t)y(t) + \text{constant} = \int g(t)\mu(t) dt$$

$$y(t) = \frac{\int g(t)\mu(t) dt + \text{constant}}{\mu(t)}$$

How can we calculate $\mu(t)$ based on what we have...

$$p(t) = \frac{\mu'(t)}{\mu(t)} \leftarrow \text{what is this} \quad (\ln \mu(t))' = p(t) = \frac{d(\ln \mu(t))}{dt}$$

$$\int p(t) dt = \int d(\ln \mu(t)) = \ln \mu(t) = \int p(t) dt + \text{constant} +$$

$$\text{so } \mu(t) = e^{\int p(t) dt} \Rightarrow y(t) = \frac{\int g(t) e^{\int p(t) dt} dt + \text{constant}}{e^{\int p(t) dt}} = \int g(t) e^{\int p(t) dt} dt + \frac{C}{e^{\int p(t) dt}}$$

$$-V_1 \frac{dC_1}{dt} = \frac{A_m D_m k}{L} \left[\left(1 + \frac{V_1}{V_2}\right) C_1 - \frac{V_1}{V_2} C_0 \right] \quad \text{make in the form}$$

$$\frac{dy}{dt} + p(t)y = g(t)$$

note: $\Phi = k$

$$-\frac{1}{V_1} \cdot -V_1 \frac{dC_1}{dt} = \frac{A_m D_m \Phi}{-V_1 L} \left(1 + \frac{V_1}{V_2}\right) C_1 - \frac{A_m D_m k}{-V_1 L} \frac{V_1}{V_2} C_0$$

$$\frac{dC_1}{dt} = -\frac{A_m D_m \Phi}{V_1 L} \left(1 + \frac{V_1}{V_2}\right) C_1 + \frac{A_m D_m \Phi V_1 C_0}{V_1 L V_2}$$

$$= \left(-\frac{A_m D_m \Phi}{V_1 L} - \frac{A_m D_m \Phi}{V_1 L V_2} \right) C_1 + \frac{A_m D_m \Phi C_0}{L V_2}$$

$$\frac{dC_1}{dt} = - \underbrace{\left(\frac{A_m D_m \Phi}{V_1 L} + \frac{A_m D_m \Phi}{V_1 L V_2} \right)}_{\sim -p(t)} C_1 + \underbrace{\frac{A_m D_m \Phi C_0}{L V_2}}_{\sim g(t)}$$

$$\text{I.F.} \quad \int p(t) dt = e^{\int \left(\frac{A_m D_m \Phi}{V_1 L} + \frac{A_m D_m \Phi}{V_1 L V_2} \right) dt}$$

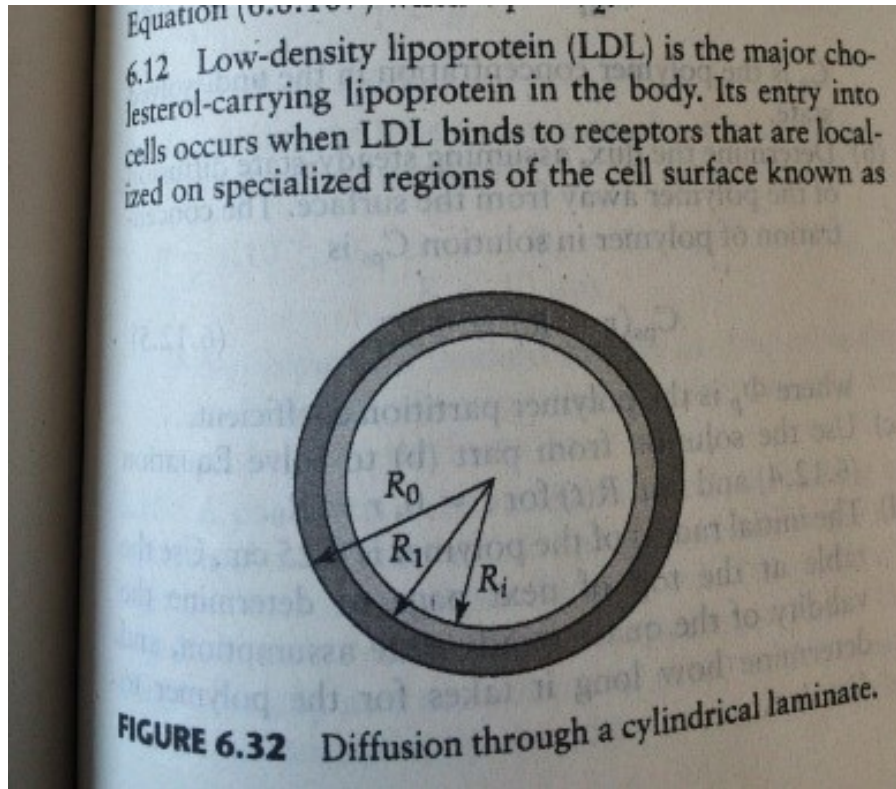
$$C_1(t) = \frac{\int \frac{A_m D_m \Phi C_0}{L V_2} e^{\int \left(\frac{A_m D_m \Phi}{V_1 L} + \frac{A_m D_m \Phi}{V_1 L V_2} \right) dt} dt}{e^{\int \left(\frac{A_m D_m \Phi}{V_1 L} + \frac{A_m D_m \Phi}{V_1 L V_2} \right) dt}}$$

$$= \frac{\int \frac{A_m D_m \Phi C_0}{L V_2} e^{\left(\frac{A_m D_m \Phi}{V_1 L} + \frac{A_m D_m \Phi}{V_1 L V_2} \right) t} dt}{e^{\left(\frac{A_m D_m \Phi}{V_1 L} + \frac{A_m D_m \Phi}{V_1 L V_2} \right) t}}$$

$$= \frac{1}{\left(\frac{A_m D_m \Phi}{V_1 L} + \frac{A_m D_m \Phi}{V_1 L V_2} \right)} \cdot \frac{A_m D_m \Phi C_0}{L V_2} e^{\left(\frac{A_m D_m \Phi}{V_1 L} + \frac{A_m D_m \Phi}{V_1 L V_2} \right) t} + \gamma$$

$$C_1 = \frac{\frac{A_m D_m \Phi C_0}{L V_2} \left[e^{\left(\frac{A_m D_m \Phi}{V_1 L} + \frac{A_m D_m \Phi}{V_1 L V_2} \right) t} = M \right]}{M} = \frac{\left[\frac{V_1}{1+V_2} \right] M C_0 + \gamma}{M}$$

$$k_- = \frac{2D_L}{R_R^2 \ln\left(\frac{b}{R_R}\right)}$$



coated pits. (The name arises from the electron-dense appearance of the membrane in electron micrographs.) A coated pit contains proteins that regulate the binding of receptors and the formation of vesicles. When a coated pit forms a vesicle, LDL molecules are transported to lysosomes. In the lysosome, the cholesterol is esterified and enters the cell cytoplasm; the protein portion is degraded to amino acid.

Determine the rate constant for the diffusion-limited dissociation of LDL receptors from binding sites in coated pits. Binding and dissociation of LDL receptors to coated-pit proteins occurs independently of LDL binding to its receptor. Assume that coated pits have a radius s and are separated by a distance $2b$ (see Figure 6.33), and use the following data to determine k_- for the dissociation of a receptor from a ternary complex in coated pits on the cell membrane surface:

FIGURE 6.33 Schematic of two coated pits

P	0.30 coated pit μm^{-2}	Number density of coated pits
N	100,000 receptors cell $^{-1}$	Number of receptors per cell
A	5,000 μm^2	Surface area of cell
R_R	1 nm	Receptor radius
s	0.10 μm	Radius of a coated pit
D_R	4.5×10^{-11} $\text{cm}^2 \text{s}^{-1}$	Diffusion coefficient of receptor
λ	0.20 min^{-1}	Rate constant for vesicle formation
b	1.0 μm	Half of the separation distance between two coated pits

$$k_- = \frac{2D_L}{R_R^2 \ln\left(\frac{b}{R_R}\right)}$$

- Would a ligand and receptor be more likely to dissociate if the complex were free floating in solution versus on the surface of the cell?
- What does entropy (of what?) have to do with 2 spherical entities in water (i.e., 2 air bubbles or 2 hydrophobic nanoparticles) combining to be one? Why are two bubbles coming together favorable in certain cases?