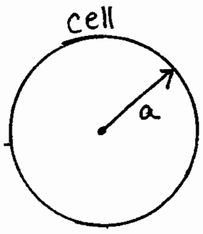
Problem 1 BE.430 Homework 1



Assumptions / Parameters:

a) Steady state (S.S.)

b) Zeroth-order consumption of O_2 in the cell, k_o

c) $r = a$

d) O_2 concentration fi just inside the cell, C_o.

e) Consumption rate is spatially uniform

a) Conservation equation:

$$\frac{\partial c}{\partial t} = -\nabla \cdot N + R. \quad \Rightarrow \quad \underbrace{\cancel{\frac{\partial c}{\partial t}}^{\,0}}_{S.S.} = \frac{D}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial c}{\partial r}\right) - \underbrace{k_o}_{\text{consumption}} = 0$$

Boundary Conditions:

i) $C(r = r_o) = C_o$

ii) $\left.\frac{\partial c}{\partial r}\right|_{r=0} = 0$ due to spherical symmetry.

Solving:

$$\frac{D}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial c}{\partial r}\right) = k_o$$

$$\frac{\partial}{\partial r}\left(r^2 \frac{\partial c}{\partial r}\right) = \frac{k_o r^2}{D}$$

$$\int \partial\left(r^2 \frac{\partial c}{\partial r}\right) = \int \frac{k_o r^2}{D}\,\partial r$$

$$r^2 \frac{\partial c}{\partial r} = \frac{k_o r^3}{3D} + C_1$$

$$\frac{\partial c}{\partial r} = \frac{k_o r}{3D} + \frac{C_1}{r^2}$$

$$\int \partial c = \int \left(\frac{k_o r}{3D} + \frac{C_1}{r^2}\right) \partial r$$

$$\therefore C(r) = \frac{k_o r^2}{6D} - \frac{C_1}{r} + C_2$$

General Equation

Incorporate Boundary Conditions:

$$\frac{\partial c}{\partial r} = \frac{C_1}{r^2} + \frac{k_o r}{3D}\Big|_{r=0} = 0 \quad \text{from ii)}$$

$$\therefore C_1 = 0$$

$$c(r=a) = \frac{K_o a^2}{6D} + C_2 = C_o$$

$$\therefore C_2 = C_o - \frac{k_o a^2}{6D}$$

$$\boxed{c(r) = C_o + \frac{k_o}{6D}(r^2 - a^2)}$$

$$\frac{D}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c}{\partial r}\right) - k_o = \frac{\partial c}{\partial t}$$

• Start with conservation equation.

Scaling Factors: $t^* = \frac{1}{k_o}$, $c^* = C_o$, $r^* = a$

Nondimensionalize: $\tau = \frac{t}{t^*}$, $u = \frac{c}{c^*}$, $\gamma = \frac{r}{r^*}$

$\frac{C_o D}{a^2 k_o} = 0.0036$ ↑ very small

∴ Diffusion limitation negligible

Substitute: $$\frac{C_o D}{\cancel{a^3}\, a\, \gamma^2}\frac{\partial}{\partial \gamma}\left(\frac{\gamma^2 \cdot \cancel{a^2}}{a}\cdot\frac{\partial u}{\partial \gamma}\right) - k_o = \frac{\partial u}{\partial \tau} C_o k_o$$

$\frac{1}{\text{Damcholer \#}} \rightarrow$ $$\boxed{\frac{C_o D}{a^2 K_o}}\frac{1}{\gamma^2}\frac{\partial}{\partial \gamma}\left(\gamma^2\frac{\partial u}{\partial \gamma}\right) - 1 = \frac{\partial u}{\partial \tau} C_o$$

b) "Central core": $c(r=0) = 0$.

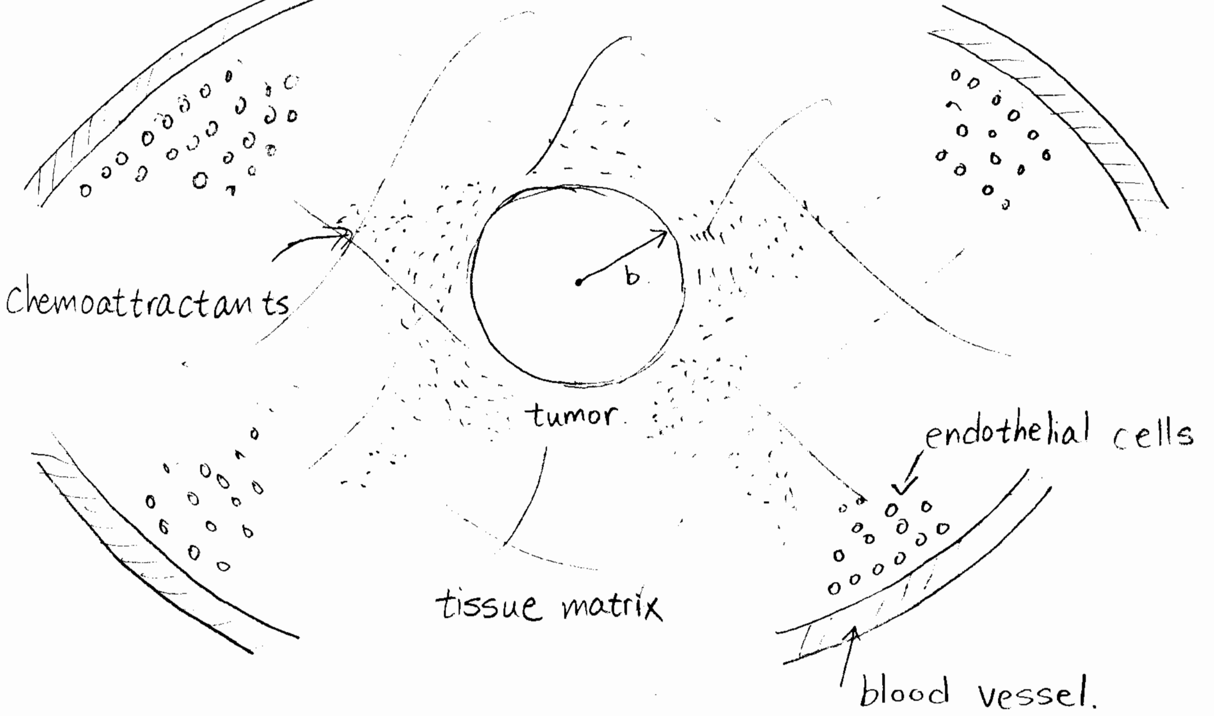
Assumption of zeroth order kinetics is no longer valid.

Find r_c such that $c(r=0) = 0$

$$c(r=0) = C_o \;\; \frac{K_o}{6D} r_c^2 = 0 \Rightarrow \boxed{r_c = \sqrt{\frac{6 C_o D}{k_o}}}$$

Problem 2 BE.430 Homework 1

a)



Situation: tumor generates chemoattractants, which diffuse through the tissue matrix. Then, the endothelial cells on the blood vessel surface proliferate towards the tumor by perceiving a concentration gradient in the chemoattractants.

Assumptions:

- No reactive loss of chemoattractant
- Steady state
- Spherical symmetry
- tissue is of infinite extent

Conservation Equation for tissue:

$$\frac{\partial C_c(r)}{\cancel{\partial t}} \to 0 = \frac{D}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial c}{\partial r}\right) + \cancel{R} \to 0$$

s.s. no reactive loss

Boundary conditions:

i) Flux Matching @ $r=b$: $\underbrace{-4\pi b^2}_{m^2} D \underbrace{\frac{\partial C_c(r)}{\partial r}}_{\frac{moles}{m^2 \cdot s}} + \underbrace{R}_{\frac{moles}{s}} = 0$

ii) Concentration @ $r=\infty$: $C(r=\infty)=0$

Solve:

$$\frac{D}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial c}{\partial r}\right) = 0$$

$$\left(r^2 \frac{\partial c}{\partial r}\right) = B_1$$

$$\frac{\partial c}{\partial r} = \frac{B_1}{r^2}$$

$$\therefore \; C(r) = -\frac{B_1}{r} + B_2$$

$C_c(r=\infty) = B_2 = 0$ using B.C. i)

$$\frac{\partial C_c(r)}{\partial r} = \left.\frac{B_1}{r^2}\right|_{r=b} = \frac{R}{4\pi b^2 D}$$

$B_1 = \frac{R}{4\pi D}$ using B.C. ii)

$$\boxed{C_c(r) = -\frac{R}{4\pi D r}} = -\frac{1.983\times 10^{-12}}{r}$$

$$\boxed{\frac{\partial C_c(r)}{\partial r} = \frac{R}{4\pi D r^2}} = \frac{1.983\times 10^{-12}}{r^2}$$

Substituting in values:

$$\#\text{ of cells in tumor} = \frac{\cancel{\tfrac{4}{3}\pi}(300\,\mu m)^3}{\cancel{\tfrac{4}{3}\pi}(10\,\mu m)^3} = 27000 \text{ cells}$$

$$R: \quad \frac{1000 \text{ molecules}}{\cancel{\text{cell}}\cdot\cancel{\text{min}}} \times \frac{27000\,\cancel{\text{cells}}}{} \times \frac{\cancel{\text{min}}}{60\,s} = 450000\ \frac{\text{molecules}}{s}$$

$$= 7.475\times10^{-19}\ \frac{\text{moles}}{s}$$

$$D: \quad 3\times10^{-7}\,\frac{cm^2}{s} \times \left(\frac{1m}{100cm}\right)^2 = 3\times10^{-11}\ m^2/s$$

$$\frac{\partial C_c(r)}{\partial r} = \frac{7.475\times10^{-19}}{3\times10^{-11}\times1000\times4\pi r^2} = \frac{1.983\times10^{-12}}{r^2}, \quad r \geq b$$

divide from left side to convert $L \rightarrow m^3$

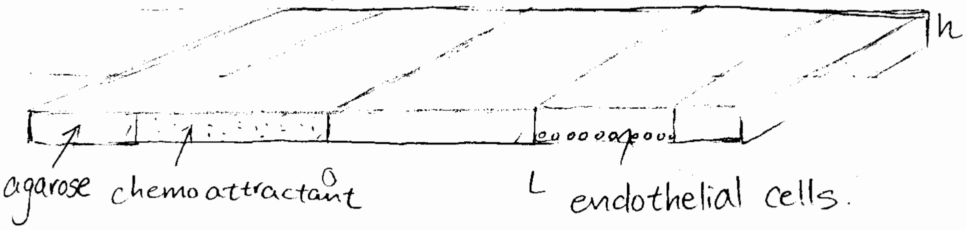
The cell would perceive a 1% gradient in chemoattractant concentration when $\frac{\partial C_c(r)}{\partial r} \geq 0.01 \Rightarrow \boxed{r_g = 14.08\,\mu m}$

The region where concentration goes from $0.3\times10^{-9}\,M \sim 3\times10^{-9}\,M$ is between $r = 6.609\,\mu m$ & $r = 0.661\,\mu m$

for $0.3\times10^{-9}\,M$ for $3\times10^{-9}\,M$

For $0.3\times10^{-9} < C(r) < 3\times10^{-9}$, the possible radius is $\boxed{0.661\,\mu m < r < 6.609\,\mu m}$

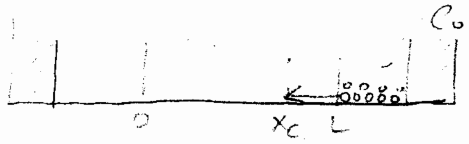
According to the r values, the cells wouldn't be able to detect the Chemoattractants.

b) 

$L >> h$
$h \sim 1\,\mu m$
$L \sim 1\,cm$

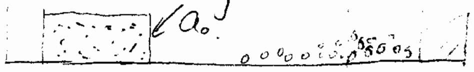
- Prepare a long, thin plate filled w/ agarose gel.
- Carve out two sections from the gel such for depositing chemoattractants and endothelial cells, respectively.
- At time $t=0$, place cells with concentration C_0 in well, mark them with trypan blue.
- At time $t = 2hrs$, calculate D of cells measuring distance that the cells have crawled in agarose gel, assuming cells diffuse slowly.

$\therefore\ D\,(\text{cells}) = \frac{X_c^2}{2\,hrs} \quad \left(\frac{cm^2}{s}\right)$



$t=0$

- At time $t = 2hrs$, place attractants w/ concentration, a_0, in well (marking them w/ flourescent dye). such that $a_0 >>$ cells.

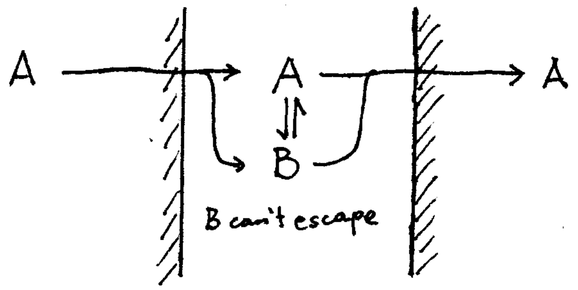


$t = 2hrs.$

- C_0 is constant because cell diffusion is slow
- a_0 is constant because there's an abundance of attractantants.

Assuming chemoattractants diffuse much faster than cells, we can assume quasi-steady state as soon as attractants are placed in the cell, thus inducing a linear concentration profile for the chemoattractants.

Problem 3 - Facilitated Transport



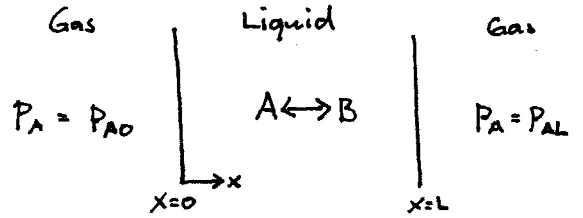
B is an alternative form of A.

Ex. $A = CO_2$

$B = HCO_3^-$

(as in the respiratory system)

Schematic:



Solubility relation: $C_A = \alpha P_A$

For simplicity, assume $D_A = D_B = D$

Reaction: $A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} B \qquad K = \frac{k_{-1}}{k}$

Assumptions:

1. Steady-state $(\frac{\partial}{\partial t} \to 0)$
2. 1-dimensional problem (liquid film of small thickness)
3. constant diffusivities $(D_A = D_B = D \neq f(c))$
4. first-order reversible reaction
5. neglect convection, charge interactions, etc.

a) No reaction! Relate the flux of A to partial pressures and other system parameters

Species conservation of A: $\underbrace{\cancel{\frac{\partial c_A}{\partial t}}}_{st.\,st.}{}^{0} = -\frac{\partial N_{x,A}}{\partial x} + \underbrace{\cancel{R_A}}_{\text{no reaction}}{}^{0}$

Constitutive equation (Fick's Law): $N_A = -D_A \frac{\partial c_A}{\partial x} = -D \frac{dc_A}{dx}$

$$\Rightarrow \quad D \frac{d^2 c_A}{dx^2} = 0$$

Solving the ODE:

$$C_A(x) = Ax + B$$

Boundary conditions:

$P(x=0^-) = P_{A0}$ $\quad\quad$ $P(x=L^+) = P_{AL}$

1. $C(x=0^+) = \alpha P_{A0}$ $\quad\quad$ 2. $C(x=L^-) = \alpha P_{AL}$

Applying B.C.s,

1. $\alpha P_{A0} = A \cdot 0 + B$
   $\Rightarrow B = \alpha P_{A0}$

2. $\alpha P_{AL} = A \cdot L + \alpha P_{A0}$
   $\Rightarrow A = \frac{\alpha}{L}(P_{AL} - P_{A0})$

$$\Rightarrow C_A(x) = \frac{\alpha}{L}(P_{AL} - P_{A0})x + \alpha P_{A0}$$

for no reaction case
(did not need to get here to solve part a))

Flux: $N_{x,A} = -D\frac{dc_A}{dx}$

$$\boxed{N_{x,A} = -D \cdot \frac{\alpha}{L}(P_{AL} - P_{A0})}$$

b) Determine the flux of A under reactive conditions.

$A \underset{k_1}{\overset{k_1}{\rightleftharpoons}} B$ $\quad$ with $K = \frac{k_1}{k_1}$

Set up teaction kinetics:

A: $\frac{\partial C_A}{\partial t} = -k_1 C_A + k_1 C_B = k_1(KC_B - C_A) = R_A$

B: $\frac{\partial C_B}{\partial t} = -k_1 C_B + k_1 C_A = -k_1(KC_B - C_A) = R_B = -R_A$

Species conservation and constitutive equations:

A: $\cancel{\frac{\partial C_A}{\partial t}}^{\,0} = D\frac{\partial^2 C_A}{\partial x^2} + R_A \quad\quad (1)$

B: $\text{st.st.}\ \cancel{\frac{\partial C_B}{\partial t}}^{\,0} = D\frac{\partial^2 C_B}{\partial x^2} + R_B = D\frac{\partial^2 C_B}{\partial x^2} - R_A \quad\quad (2)$

Adding both equations:

$$\cancel{D}\frac{d^2C_A}{dx^2} + \cancel{D}\frac{d^2C_B}{dx^2} = 0 \quad \Rightarrow \frac{d^2}{dx^2}(C_A + C_B) = 0 \qquad (3)$$

Solve the ODE to obtain

$$C_A + C_B = A\frac{x}{L} + B \qquad (4)$$

(We introduce the factor L to simplify things later)

Boundary conditions:

1. $C_A(x=0^+) = \alpha P_{A0}$
2. $C_A(x=L^-) = \alpha P_{AL}$
3. $\left.\frac{dC_B}{dx}\right|_{x=0^+} = 0$
4. $\left.\frac{dC_B}{dx}\right|_{x=L^-} = 0$

(no escape of B allowed ⇒ no flux condition)

Let's try to find another way to solve this problem.

Rearrange (4): $\quad C_B = A\frac{x}{L} + B - C_A \qquad (5)$

Insert (5) into (1): $\quad D\frac{d^2C_A}{dx^2} + k_1\left(K\left(A\frac{x}{L} + B - C_A\right) - C_A\right) = 0$

$$\Rightarrow D\frac{d^2C_A}{dx^2} + k_1\left[K\left(A\frac{x}{L} + B\right) - (1+K)C_A\right] = 0$$

Let $\eta = \frac{x}{L}$ for simplicity:

$$\frac{D}{L^2}\frac{d^2C_A}{d\eta^2} + k_1\left[K(A\cdot\eta + B) - (1+K)C_A\right] = 0$$

$$\Rightarrow \frac{d^2C_A}{d\eta^2} + \frac{k_1L^2}{D}\left[K(A\cdot\eta + B) - (1+K)C_A\right] = 0$$

Let $\quad Da = \frac{k_1L^2}{D}$ (this number will come up later in the semester)

$\lambda^2 = Da(1+K)$ (note that $Da(1+K)$ is always positive)

$$\Rightarrow \frac{d^2C_A}{d\eta^2} - \lambda^2C_A = -\frac{\lambda^2K}{1+K}(A\cdot\eta + B) \qquad (6)$$

This is a non-homogeneous second-order differential equation.

Let $C_A(\eta) = C_A^{homogeneous}(\eta) + C_A^{particular}(\eta)$ where

$C_A^{homog.}(\eta)$ is the solution to the homogeneous equation $\frac{d^2 C_A}{d\eta^2} - \lambda^2 C_A = 0$
Since λ^2 is always positive,

$$C_A(\eta) = C\sinh\lambda\eta + D\cosh\lambda\eta$$

The particular solution can be found by guessing: Let $C_A^{part.}(\eta) = C'(A\eta+B)$
Plug $C_A^{part.}(\eta)$ into (6)

$$\cancel{\frac{d^2}{dx^2}(C'(A\eta+B))}^{\,0} - \lambda^2 C'(A\eta+B) = -\frac{\lambda^2 K}{1+K}(A\cdot\eta+B)$$

$$\Rightarrow C' = \frac{K}{1+K}$$

$$\Rightarrow \quad C_A(\eta) = C\sinh\lambda\eta + D\cosh\lambda\eta + \frac{K}{1+K}(A\cdot\eta+B)$$

Recall boundary conditions (with $\eta = \frac{x}{L}$)

1. $C_A(\eta=0) = \alpha P_{A0}$ 3. $\frac{dC_B}{d\eta}\Big|_{\eta=0} = 0$
2. $C_A(\eta=1) = \alpha P_{AL}$ 4. $\frac{dC_B}{d\eta}\Big|_{\eta=1} = 0$

Applying B.C.s

1. $\alpha P_{A0} = \cancel{C\cdot\sinh\lambda\cdot 0}^{\,0} + D\cosh\lambda\cdot 0 + \frac{K}{1+K}(\cancel{A\cdot 0}^{\,0} + B)$
2. $\alpha P_{AL} = C\cdot\sinh\lambda + D\cdot\cosh\lambda + \frac{K}{1+K}(A\cdot\lambda + B)$

From (4) (with $\eta = \frac{x}{L}$)

$$\begin{aligned} C_B &= A\cdot\eta + B - C_A \\ &= A\cdot\eta + B - C\sinh\lambda\eta - D\cosh\lambda\eta - \frac{K}{1+K}(A\cdot\eta+B) \\ &= -C\sinh\lambda\eta - D\cosh\lambda\eta + \frac{1}{1+K}(A\cdot\eta+B) \end{aligned}$$

$$\Rightarrow \frac{\partial C_B}{\partial \eta} = -C\cdot\lambda\cdot\cosh\lambda\eta - D\lambda\cdot\sinh\lambda\eta + \frac{1}{1+K}\cdot A$$

3. $0 = -C\cdot\lambda\cosh\lambda\cdot 0 - D\lambda\cancel{\sinh\lambda\cdot 0}^{\,0} + \frac{1}{1+K}A$

4. $0 = -C\cdot\lambda\cdot\cosh\lambda - D\lambda\sinh\lambda + \frac{1}{1+K}A$

Rearranging:

from 1. $\quad B = \frac{K+1}{K}(\alpha P_{AO} - D) \qquad (a)$

from 3. $\quad A = (K+1)\lambda\cdot C \qquad (b)$

(b) into 4.

$$0 = -C\cdot\lambda\cdot\cosh\lambda - D\lambda\sinh\lambda + C\lambda$$

$$\Rightarrow C = \frac{D\sinh\lambda}{1-\cosh\lambda} \qquad (c)$$

$$\Rightarrow A = (K+1)\lambda\frac{D\sinh\lambda}{1-\cosh\lambda} \qquad (d)$$

2. and (a), (c), (d)

$$\alpha P_{AL} = \frac{D\sinh\lambda}{1-\cosh\lambda}\sinh\lambda + D\cosh\lambda + \frac{K}{\cancel{1+K}}\cdot\cancel{(K+1)}\lambda^2\frac{D\sinh\lambda}{1-\cosh\lambda} + (\alpha P_{AO} - D)$$

$$\Rightarrow D = \frac{\alpha(P_{AL}-P_{AO})(1-\cosh\lambda)}{\sinh^2\lambda + \cosh\lambda - \cosh^2\lambda + K\lambda^2\sinh\lambda - 1 + \cosh\lambda}$$ (with $\sinh^2\lambda - \cosh^2\lambda = 1$)

$$\Rightarrow D = \frac{\alpha(P_{AL}-P_{AO})(1-\cosh\lambda)}{2(\cosh\lambda - 1) + K\lambda\sinh\lambda}$$

$$C = \frac{\alpha(P_{AL}-P_{AO})\sinh\lambda}{2(\cosh\lambda-1) + K\lambda\sinh\lambda}$$

$$B = \frac{K+1}{K}\left(\alpha P_{AO} - \frac{\alpha(P_{AL}-P_{AO})}{2(\cosh\lambda-1)+K\lambda\sinh\lambda}\right)$$

$$A = (K+1)\lambda\frac{\alpha(P_{AL}-P_{AO})\sinh\lambda}{2(\cosh\lambda-1)+K\lambda\sinh\lambda}$$

Determine the flux of c_A:

$$\frac{dc_A}{d\eta} = C\lambda\cos\lambda\eta + D\lambda\sinh\lambda\eta + \frac{K}{1+K}A$$

$$\Rightarrow \quad N_A = -D^* \frac{dc_A}{d\eta} = -\frac{D^*}{L}\left(C\lambda\cos\lambda\eta + D\lambda\sin\lambda\eta + \frac{K}{1+K}A\right)$$

where $C = \dfrac{\alpha(P_{AL} - P_{A0})\sinh\lambda}{2(\cosh\lambda - 1) + K\lambda\sinh\lambda}$ $\qquad D^* = \text{diffusivity}$

$$D = \frac{\alpha(P_{AL} - P_{A0})(1-\cosh\lambda)}{2(\cosh\lambda-1) + K\lambda\sinh\lambda}$$

$$A = (K+1)\lambda\frac{\alpha(P_{AL} - P_{A0})\sinh\lambda}{2(\cosh\lambda-1)+K\lambda\sinh\lambda}$$

Btw. C and D terms are simplifyable.

c) Instead of simplifying the algebra to find a cleaner flux term, we recognize that the enhancement factor is only meaningful at the boundaries. We choose:

$$E = \frac{N_{x,A}|_{x=0} \text{ (with reaction)}}{N_{x,A} \text{ (w/o reaction)}}$$

We could obtain $N_{x,A}|_{x=0}$ from b); however, this requires tedious algebraic simplifications. So, we will recognize that from (3)

$$\frac{d^2}{dx^2}(C_A + C_B) = 0 \quad \Rightarrow \quad \frac{d}{dx}(C_A + C_B) = A$$

Since at the boundaries,

$$\frac{dc_B}{dx}\Big|_{x=0} = \frac{dc_B}{dx}\Big|_{x=L} = 0$$

$$\Rightarrow \frac{dc_A}{dx}\Big|_{x=0} = \frac{dc_A}{dx}\Big|_{x=L} = A$$

So,

$$N = -D\cdot(K+1)\lambda \frac{\alpha(P_{AL}-P_{A0})\sinh\lambda}{2(\cosh\lambda-1)+K\lambda\sinh\lambda}$$

$$\Rightarrow \boxed{E = \frac{(K+1)\lambda\sinh\lambda}{2(\cosh\lambda-1)+K\lambda\sinh\lambda}}$$

For slow reactions, $\lambda \to 0$ $(k_1 \to 0)$ with K fixed:

$$\sinh\lambda = \frac{e^{\lambda}-e^{-\lambda}}{2} \to \frac{(1+\lambda+\cdots)-(1-\lambda+\cdots)}{2} = \lambda+\cdots$$

$$\cosh\lambda = \frac{e^{\lambda}+e^{-\lambda}}{2} \to \frac{(1+\lambda+\frac{\lambda^2}{2})+(1-\lambda+\frac{\lambda^2}{2})}{2} = 1+\frac{\lambda^2}{2}$$

$$\cosh\lambda - 1 \to \frac{\lambda^2}{2}$$

$$\Rightarrow \lim_{\lambda\to 0} E = \frac{(1+K)\lambda^2}{2(\frac{\lambda^2}{2})+K\lambda^2} = 1$$

(i.e., no enhancement for very slow reaction rate)

For fast reactions, $\lambda \to \infty$ with K fixed:

$$\sinh\lambda \to \frac{e^{\lambda}}{2} \qquad \cosh\lambda \to \frac{e^{\lambda}}{2}$$

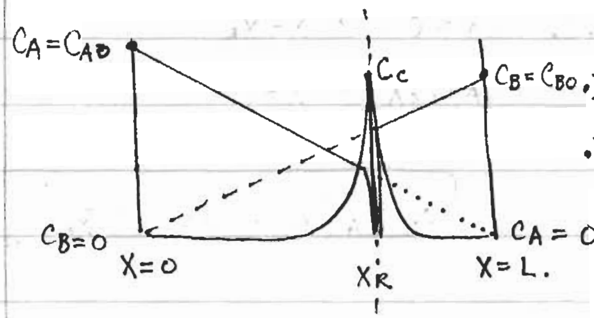
$$\Rightarrow \lim_{\lambda\to\infty} E = \frac{(K+1)\lambda \frac{e^\lambda}{2}}{2(\frac{e^\lambda}{2}-1)+K\lambda\frac{e^\lambda}{2}} \longrightarrow \frac{K+1}{K}$$

Thus, E is largest for $\lambda \gg 1$ (fast reaction) and $K \ll 1$.
At equilibrium ($R_{VA}=0$),

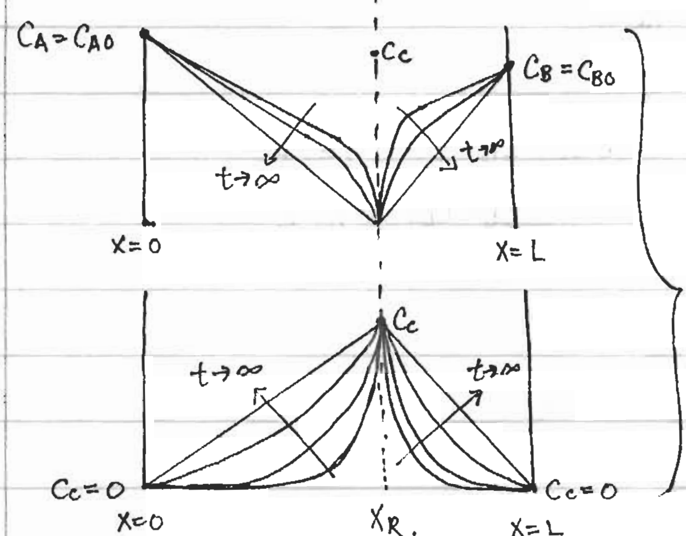
$$\left.\frac{C_B}{C_A}\right|_{eq.} = \frac{1}{K}$$

so that with $K \ll 1$, there is a lot of B present. This is what leads to the large flux enhancements.

Problem 4 (2.12 Deen) BE.430 Homework 1



- Instant that $A + B \to C$, $t = t_0$
- There's very fast reaction, $k \to \infty$, $\therefore C_A = C_B = 0$ @ X_R.
- C_c spikes @ X_R



- As $t \to \infty$, the concentration profile becomes linear for all three species.
- Basically, if you assume s.s. before reaction, A & B both have a linear profile going from 0 to L & vice versa.
- Then, @ $t = t_0$, there's a sink for A & B @ $X = X_R$ where $C_A = C_B = 0$ immediately to form C, causing an impulse of C @ X_R.
- Eventually, depletion of A & B @ X_R forces A & B profiles to be linear again, a new s.s.
- Two boundary conditions @ $X = 0$, $X = L$ for C_c also eventually force C_c to have linear profile on both sides. with $C_c(X_r^+) = C_c(X_r^-)$

Conservation of Species:

$0 < X < X_R$ $$\frac{\partial^2 C_A}{\partial x^2} + \underbrace{R_{AV}}_{\text{no reaction}} \overset{0}{=} \cancel{\frac{\partial C_A}{\partial t}}^{\,0} \quad \text{(steady state)}$$

$X_R < X < X_L$ $$\frac{\partial^2 C_B}{\partial x^2} + \cancel{R_{BV}}^{\,0} = \cancel{\frac{\partial C_B}{\partial t}}^{\,0}$$

Assumptions:

- nonhomogeneous reaction $A + B \to C$ @ $X = X_R$.
- fast reaction @ $X = X_R$, $k \to \infty$
- steady-state
- dilute solution

Solve for $C_A(x)$, $C_B(x)$, X_R, $C_C(x)$

C_A: $D_A \frac{\partial^2 C_A}{\partial x^2} = 0$ B.C. $C_A = 0$ @ $x = X_R$

$C_A = C_{oA}$ @ $x = 0$

$C_A(x) = C_1 x + C_2$

$C_A(x=0) = C_2 = C_{oA}$

$C_A(x = X_R) = C_1 X_R + C_{oA} = 0$

$C_1 = -\frac{C_{oA}}{X_R}$

$\boxed{\therefore C_A(x) = C_{oA}\left(1 - \frac{x}{X_R}\right)}$

C_B: $D_B \frac{\partial^2 C_B}{\partial x^2} = 0$ BC: $C_B = 0$ @ $x = X_R$

$C_B = C_{BL}$ @ $x = L$

$C_B(x) = C_3 x + C_4$

$C_B(x = X_R) = C_3 X_R + C_4 = 0$

$C_B(x = L) = C_3 L + C_4 = C_{BL}$

$C_3(X_R - L) = -C_{BL}$

$C_3 = \frac{-C_{BL}}{X_R - L}$

$C_B(x) = \frac{-C_{BL}}{X_R - L} x + \frac{C_{BL} X_R}{X_R - L}$

$\boxed{C_B(x) = C_{BL}\left(\frac{X_R - x}{X_R - L}\right)}$

X_R: • Use flux matching between C_A & C_B @ $x = X_R$

• If it's counter intuitive why there would be flux although $C_A = C_B = 0$ @ X_R @ S.S., remember the slope (flux) of the respective concentration profiles is NOT 0 @ $x = X_R$ and the heterogeneous reaction is shaping the concentration profile, not vice versa.

Problem 4 (2.12 Deen) BE.430 Homework 1

x_R: $N_A = -N_B$

$$D_A \frac{\partial C_A}{\partial x} = -D_B \frac{\partial C_B}{\partial x}$$

$$D_A\left(-\frac{C_{0A}}{x_R}\right) = -D_B\left(\frac{-C_{BL}}{x_R - L}\right)$$

$$L - x_R = \frac{D_B}{D_A}\frac{C_{BL}\,x_R}{C_{0A}}$$

$$\boxed{x_R = \frac{L}{1 + \frac{D_B}{D_A}\frac{C_{BL}}{C_{0A}}}}$$

Find the x_R such that the flux on both sides will match because you assume everything that comes to x_R reacts completely.

Boundary Conditions

C_C: $D_C \frac{\partial^2 C_C}{\partial x^2} = 0$ for $0 \le x < x_R$, $x_R \le x \le x_L$

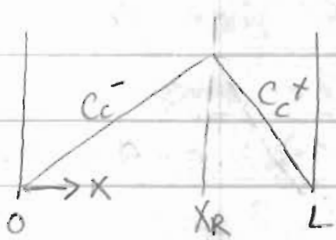
a) $C_C^-(x=0) = C_C^+(x=L) = 0$

b) $C_C^+(x = x_R^+) = C_C^-(x = x_R^-)$

c) $-D_C \frac{\partial C_C^+}{\partial x}(x = x_R^+) + D_C \frac{\partial C_C^-}{\partial x}(x = x_R^-) = R_C$

Since there exists a 1:1:1 ratio in $A + B \rightarrow C$,

$\underbrace{-R_{SA} = -R_{SB} = R_{SC}}_{\text{All @ surface}}$ (Note: $R_V = k C_A C_B$ given was not used)



$$\cancel{N_A\big|_{x=x_R^+}}^{\,0} - N_A\big|_{x=x_R^-} = R_{SA}$$

$$N_B\big|_{x=x_R^+} - \cancel{N_B\big|_{x=x_R^-}}^{\,0} = R_{SB}$$

$$N_C\big|_{x=x_R^+} - N_C\big|_{x=x_R^-} = R_{SC}$$

Flux Matching @ x_R

$$R_{SC} = \frac{D_A C_{0A}}{x_R} = -R_{SA}$$

Solve:

$$C_c^-(x) = \alpha x + \beta$$

$$C_c^+(x) = \xi x + \theta$$

① $C_c^-(0) = \beta = 0$

② $C_c^+(X_L) = \xi X_L + \theta = 0$

$\Big\}$ using B.C. a)

③ $\alpha X_R = \xi X_R + \theta$ using B.C. b)

④ $-D_c \cdot \xi + D_c \alpha = \dfrac{D_A C_{OA}}{X_R}$ using B.C. c)

$$\alpha = \frac{D_A C_{OA}}{D_c X_R} + \xi \quad \text{(i) from ④}$$

$$\theta = -X_L \xi \quad \text{(ii) from ②.}$$

Substitute (i) & (ii) into ③

$$\frac{D_A C_{OA}}{D_c} + \cancel{\xi X_R} = \cancel{\xi X_R} - X_L \xi \Rightarrow \xi = -\frac{D_A C_{OA}}{D_c X_L};$$

$$\theta = \frac{D_A C_{OA}}{D_c}; \quad \alpha = \frac{-D_A C_{OA}}{D_c X_L} + \frac{D_A C_{OA}}{D_c X_R}$$

$$\boxed{C_c(x) = \begin{cases} \dfrac{D_B C_{BL}}{D_c X_L} & 0 < x < X_R \\[2ex] \dfrac{D_A C_{OA}}{D_c}\left(1 - \dfrac{x}{X_L}\right) & X_R < x < L \end{cases}}$$