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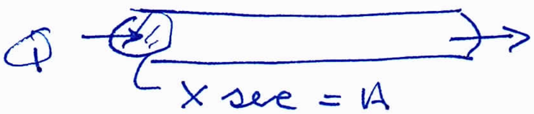
Problem 1. (20 Points)

A liquid containing dissolved component A flows through a pipe of diameter D with a volumetric flow rate Q.

a. (4 points) Write an expression for the flux of A in the axial (z) direction of the pipe and explain what will be the dominant form of mass transfer.



$V_z = Q/A$

$N_{Az} = -D_{AB}\frac{\partial C_A}{\partial z} + C_A V_z$ +2

The ~~diffusive~~ convective flux will dominate and the flux of N_A in the ~~radial~~ axial direction is ~~large~~ small.

$D_{AB}\frac{\partial C_A}{\partial z} \approx 0$ unless

+2

b. (4 points) If mass A does not react in the liquid or adsorb on the pipe wall, what is the flux of A in the radial (r) direction? Be sure to give a short explanation for your result.

+2 The flux of A in the radial direction will be 0 in the absence of a gradient in A

$N_{Ar} = -D_{AB}\frac{\partial C_A}{\partial r} = 0$

+2

c. (4 points) Now assume that A adsorbs on the wall and that the concentration of A very near the wall is nearly zero. How does this change affect your answers to parts i and ii of this problem?

If A is adsorbed on the wall and the rate of adsorption is very rapid $C_A(R,z) = 0$.

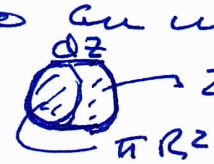
$N_A = -D_{AB}\frac{\partial C_A}{\partial r} \neq 0$ /+4 written w numerical fine

$= k(\langle C_A \rangle - C_{A,w}) \quad C_{A,w} = 0$

d. (4 points) Write down the fluxes of A in the z and r direction and the steady-state mole balance for A using the assumption described in part c of this problem. What are the boundary conditions for the mole balance? Hint: develop the mole balance for A assuming that the concentration of A is constant across the pipe radius and equal to $\langle C_A \rangle$ except at the pipe wall. $\langle C_A \rangle$ is the mixing-cup average concentration of A.

$N_{A_z} = V\langle C_A\rangle$ +1 $\quad N_{A_r} = k\langle C_A\rangle$

For the mole bal., do an integral balance on differential slice



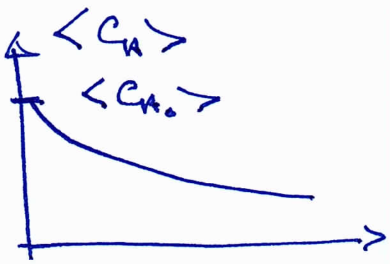
. Then

$$+\pi R^2 \frac{d}{dz}\left(V\langle C_A\rangle\right) + 2\pi R k\langle C_A\rangle = 0$$

or $$V\frac{d\langle C_A\rangle}{dz} + \frac{2}{R}k\langle C_A\rangle = 0$$ +2 $\quad$ B.C. $\langle C_A\rangle = \langle C_{A0}\rangle$ at $z = 0$ +1

• Assumes $V \neq f(z)$

e. (4 points) Sketch the radially averaged concentration of A, $\langle C_A \rangle$, in the z direction.



$$\langle C_A\rangle = \langle C_{A0}\rangle \exp\left(-\frac{k2}{VR}z\right)$$

+2 for intercept

+2 for shape

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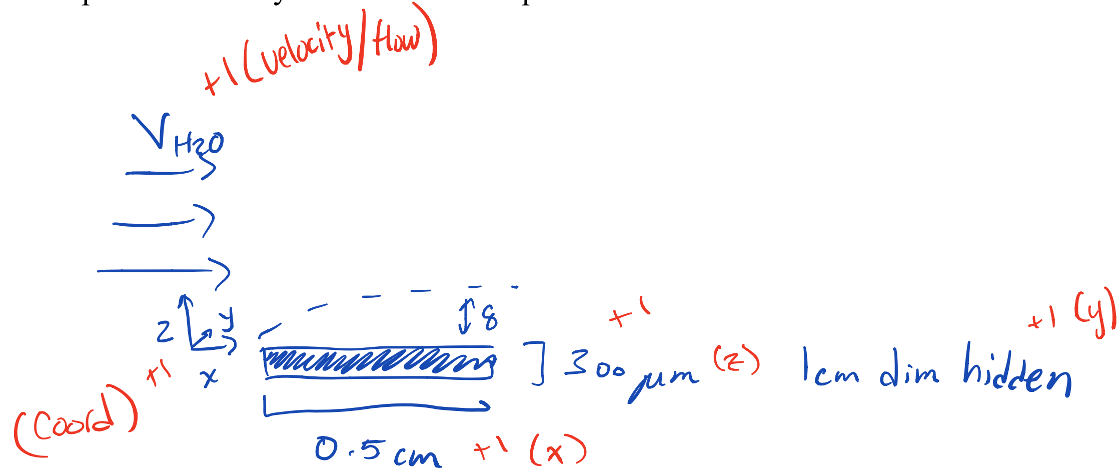
Problem 2. (25 points)

A current field of research is further understanding of dopamine (DA) dynamics in the brain. One way that this can be understood is by obtaining a live brain slice, roughly 300 µm thick, from a mouse. In order to keep the slice alive, researchers flow artificial cerebral spinal fluid (aCSF) over the slice at a rate of 1 cm^3/min. During imaging, the slice (0.5 cm x 1 cm) is placed on a glass slide with the longer dimension (1 cm) placed perpendicular to fluid flow. We can assume the neurons sustain a concentration of 1×10^{-6} mol/L (or 1×10^{-9} mol/cm^3) at all points in the slice and the properties of aCSF are the same as those of pure water. You also know the diffusion coefficient of dopamine in water is 7.6×10^{-10} m^2/s (or 7.6×10^{-6} cm^2/s) and the kinematic viscosity is 1×10^{-6} m^2/s (or 1×10^{-2} cm^2/s). The aim of this experiment is to understand how much dopamine is lost to the flow of aCSF.

Should be cm/min

a. Draw a picture of the system and label all parts and show the dimensions.



b. What is the mole balance that describes the profile of DA in the water and what are the boundary conditions for this balance? Be sure to explain what assumptions you have made in in the equation that you give for the mole balance and why they are made.

Could be more

As for BC, there can be quite a bit in the total solution of B.L. the Below are the Important ones for this problem

(1) Incompressible Newtonian Fluid (water),

+1.5 B.C. (0.75 ea)

(2) All conc is coming from the surface.

(3) Boundary layer is diffusion dominated in Z

$C_{DA}^{BATH}(z=\delta_c)=0$ mol/cm^3

(4) Bath is large enough to sustain a concentration of zero.

$C_{DA}^{Surf}(z=0)=1\times10^{-9}$ mol/cm^3

+2 Assumptions (min of 2 correct)

(5) System is at steady state.

B.L. mole balance. +1.5 for Mol Bal

Solution from Blausius written

(6) Conc only a function of Z

$$V_x\frac{\partial C_{DA}}{\partial x}+V_z\frac{\partial C_{DA}}{\partial z}=D_{DA}\frac{\partial^2 C_A}{\partial z^2}$$

Many other solutions given credit due to the nature of the problem.

(7) No Rxn

for time based mole balance (1/1.5) $\rightarrow$ $\dfrac{dn_{DA}}{dt}=k_c(C_{DA}^S-C_{DA}^B)\cdot S_A$ = total moles lost over time

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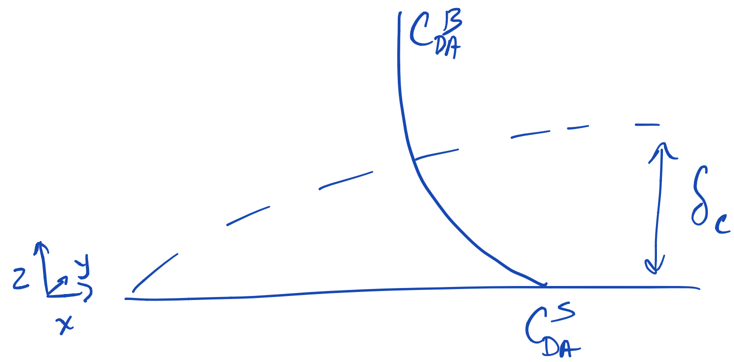
c. Draw a concentration profile for this system.



(+1) Label δ_c

(+3) curvature

(+1) mark conc @ C_{DA}^{B} \$ C_{DA}^{S}

d. Write an expression for the flux of DA from the brain slice for a fixed position (x) in the direction of the flow?

+2 Sherwood Correlation

$$Sh_x = 0.332\, Re^{1/2}\, Sc^{1/3} = \frac{k_c X}{D} \Rightarrow \frac{Sh_x D}{x} = k_c$$

$$N_{Ax} = k_c\left(C_{DA}^{S} - \underbrace{\cancel{C_{DA}^{B}}}_{0}\right)$$ +2 Flux Equation

$$N_{Ax} = \frac{0.332\, D}{x} Re^{1/2} Sc^{1/3} C_{DA}^{S}$$ + 1 Plug in

e. What is the average flux of DA from the surface?

Using a similar Analogy for L

$Sc_L = 1315.79 \rightarrow Sc^{1/3} = 10.958$

$Re_L = 0.833 \rightarrow Re^{1/2} = 0.918$

$$N_{DAL} = \frac{0.664\,(7.6\times10^{-6}\,cm^2/s)}{(0.5\,cm)}(0.918)(10.958)(1\times10^{-9}\,mol/cm^3)$$

$$N_{DA_L} = 1.01\times10^{-13}\ mol/cm^2\cdot s$$

Due to unit error in Problem Statement No Points given for Correct numerical answer

+ 2 for any Sherwood correlation For the Flat Plate.

+ 3 for a

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Problem 3. (30 points)

Liquid A is flowing with velocity v = 0.001 m/s through a cylindrical reactor of length L = 0.5 m and diameter D = 0.1 m that is completely filled with spherical catalyst pellets of diameter D_p = 1 cm. A forms B via the reaction $A \rightarrow B$ at the surface of the catalyst pellets with reaction rate coefficient k = 0.1 $cm^{-2} \cdot s^{-1}$. The concentration of A in the bulk fluid is 1 mol/m^3, and the diffusivity of A is D_{AB} = 1x10^{-2} m^2/s. The kinematic viscosity is ν=1x10^{-5} m^2/s.

a. (5 points) What is the mole balance for this problem in terms of C_A? Neglect radial concentration gradients in the reactor.

Overall mass balance:

+1 $$\cancel{\frac{\partial C_A}{\partial t}} + \cancel{v_r \frac{\partial C_A}{\partial r}} + \cancel{\frac{v_\theta}{r}\frac{\partial C_A}{\partial \theta}} + v_z \frac{\partial C_A}{\partial z} = D_{AB}\left[\cancel{\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_A}{\partial r}\right)} + \cancel{\frac{1}{r^2}\frac{\partial^2 C_A}{\partial \theta^2}} + \frac{\partial^2 C_A}{\partial z^2}\right] + R_A$$

Assumptions: (1) Steady-state +1

(2) Neglect r gradients +1

(3) Neglect θ gradients (symmetry) +1

$$\boxed{v_z \frac{\partial C_A}{\partial z} = D_{AB}\frac{\partial^2 C_A}{\partial z^2} - k C_A}$$ +1

b. (10 points) Nondimensionalize the mole balance and show which term(s) can be neglected based on the parameters given.

Parameters: $\eta = \frac{z}{L}$ +1, $\theta = \frac{C_A}{C_{A0}}$ +1

Don't need Pe and Da explicitly

$$v_z \frac{\partial(\theta \cancel{C_{A0}})}{\partial(L\eta)} = D_{AB}\frac{\partial^2(\cancel{C_{A0}}\theta)}{\partial(L\eta)^2} \quad k\theta\cancel{C_{A0}}$$

$$\frac{v_z}{L}\frac{\partial \theta}{\partial \eta} = \frac{D_{AB}}{L^2}\frac{\partial^2 \theta}{\partial \eta^2} - k\theta$$ +3

$$\underbrace{\frac{v_z L}{D_{AB}}}_{Pe}\frac{\partial \theta}{\partial \eta} = \frac{\partial^2 \theta}{\partial \eta^2} - \underbrace{\frac{kL^2}{D_{AB}}}_{Da}\theta$$

+1 $Pe = \frac{.001 \cdot 0.5}{1 \cdot 10^{-2}} = 0.05$

+1 $Da = \frac{.1 \cdot .5^2}{1 \cdot 10^{-2}} = 2.5$

∴ Neglect convection term (small Pe), and $\boxed{0 = \frac{\partial^2 \theta}{\partial \eta^2} - Da\,\theta}$ +2 for equation

+1 for correct statement

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c. (10 points) Now consider a single catalyst pellet in the reactor. Assume the particles are far enough apart so that C = $C_{A,bulk}$ far from the particle. Assume the fluid around the particle is stagnant (reasonable given the packed nature of the reactor). What is the flux of A at the particle surface assuming the reaction rate is very rapid? Assume the pellet radius is 0.5 cm.

+2 for assumptions

Assumptions: (1) S.S. (2) $C_A(r)$ only (3) No convection (4) No rxn

Option 1: $\int 0 = D_{AB}\frac{1}{r^2}\int\frac{\partial}{\partial r}\left(r^2\frac{\partial C_A}{\partial r}\right)$ +2 for eqn

$\int C_1 = \int r^2\frac{\partial C_A}{\partial r}$

B.C.s: $C_A(r\to\infty) = C_{A\infty}$

$C_A(r=R) = 0$ +2 for B.C.

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

$C_A(r\to\infty) = -\frac{C_1}{\infty} + C_2 = C_{A\infty} \Rightarrow C_{A\infty} = C_2$

$C_A(r=R) = -\frac{C_1}{R} + C_{A\infty} = 0 \Rightarrow C_1 = RC_A$

+1 for C profile

$C_A(r) = \frac{-RC_{A\infty}}{r} + C_{A\infty}$

+2 for flux eqn

$N_A|_{r=R} = \left(-D_{AB}\frac{\partial C_A}{\partial r} + y_A(\cancel{N_A + N_B})\right)\Big|_R = -D_{AB}\frac{\partial C_A}{\partial r}\Big|_R$ EMD

$= -D_{AB}\left(\frac{C_{A\infty}}{R}\right) = 1\cdot10^{-2}\cdot\frac{1}{0.005} = 2$ mol/m²·s

+1 for answer

$\boxed{N_A|_{r=R} = 2 \text{ mol/m}^2\cdot\text{s}}$

Option 2: +2 for eqn

$Sh = (4 + 1.21(ReSc)^{2/3})^{1/2}$

$V=0,\ Re=0$ +2

$\Rightarrow Sh = (4)^{1/2} = 2$

$\frac{k_l D}{D_{AB}} = 2$ +2 for eqn

$\frac{k_l\cdot .01}{1\cdot10^{-2}} = 2$

$k_1 = 2$ m/s +1 answer

$N_A = k_1(C_{A\infty} - C_{AS})$ +2 eqn

$N_A = 2(1-0) = 2$

$\boxed{N_A = 2 \text{ mol/m}^2\text{-s}}$

+1 for answer

d. (5 points) Calculate the mass transfer coefficient, k_l, for this system.

$N_A = k_l(C_{A\infty} - C_{AS})$ +3 for equation

$2 = k_l(1-0)$

$\boxed{k_l = 2 \text{ m/s}}$ +2 correct answer

-1 for units

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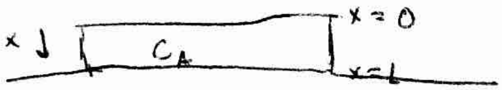
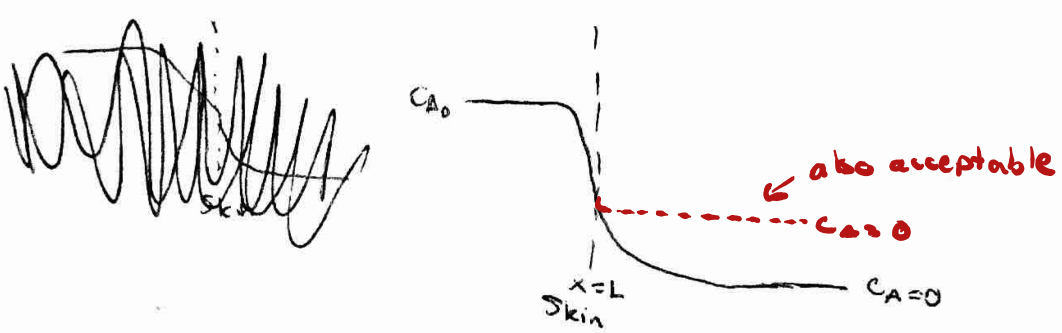
Problem 4. (25 points)

You are designing a drug patch that consists of a thin polymer film loaded with a drug. When applied to the skin, the drug immediately diffuses from the patch-skin interface into the skin with very little resistance in the skin. The initial concentration of the drug in the patch is 0.50 mole/m^3 and the diffusivity of the drug in the polymer is D = 2 x 10^{-11} m^2/s. The thickness of the patch is 0.5 mm.

a. Sketch a concentration profile of the drug within the patch and into the skin layer adjacent to the patch.



Shape (+1)
Direction (+1)
Interface continuous (+1)
Bulk Values (+2)



b. If the mass transfer resistance of the drug in the skin is negligible, what is the drug concentration at the skin/drug patch interface? Explain your answer with a few words.

$N_z = k_c(C_{A_i} - C_{A\infty}) = k_c(C_{A_i})$ +3 $C_i = 0$

Interface conc

In body $= 0$

+1 Mention of flux

+1 Physical intuition

MT Resistance ~ $1/k_c = 0 \rightarrow k_c \rightarrow \infty$

$N_z = k_c C_{A_i} = \infty C_{A_i} \rightarrow C_{A_i} = k_c/\infty = \boxed{0}$

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c. Assuming unidirectional transport of species in the patch, write down the equation governing the concentration of drug in the patch and explain the initial condition and boundary conditions for this equation.

$$\frac{\partial C_A}{\partial t} = D_A \frac{\partial^2 C_A}{\partial x^2} \quad +7$$

$$\left.\frac{\partial C_A}{\partial x}\right|_{x=0} = 0$$ no flux at interface +1

$$C_A\big|_{x=L} = 0 \quad +1$$

$$C_A\big|_{t=0} = C_{A0} \quad +1$$

d. Using the concentration-time charts given at the back of the exam, determine how long it takes for the concentration in the middle of the patch to reach 10% of its initial value.

(+.5)

$n = 0.5$

$m = 0$

(+1)

(+1)

$$Y = \frac{C_A}{C_{A0}} = 0.1$$

From Chart: $X = 0.9 = \frac{Dt}{L^2} \rightarrow t = 0.9\frac{L^2}{D} =$ $\boxed{3.125\text{hrs}}$

(+1) (+1) (+.5)