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Problem 1. (20 Points)

a. (5 points) Consider a pore of average diameter d_p through which O_2 diffuses through Ar. The total pressure is 1 atm, and T = 300 K. Explain what dictates the kind of diffusion that will occur in the pore. Under what circumstances will the diffusion coefficient depend on the total gas pressure?

1st question worth 3 pts

2nd question worth 2 pts

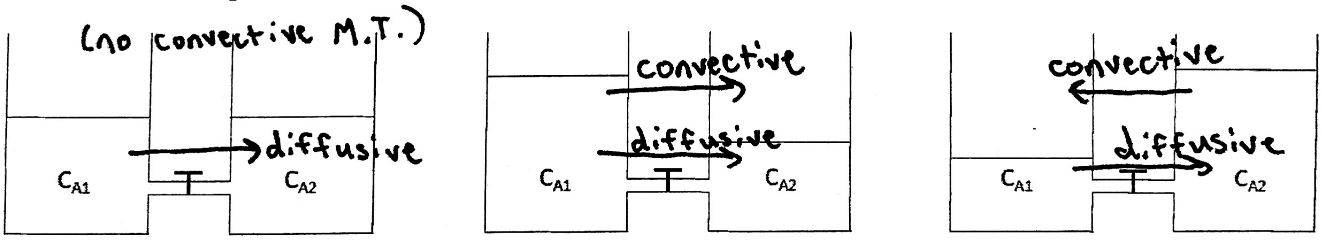
Kn number (Knudsen number) dictates diffusion:

$$Kn = \frac{\lambda}{d_{pore}} \quad \text{where } \lambda = \text{mean free path}$$

+3 pts

+2 pts: Diffusion coefficient depends on total gas pressure ($\propto \frac{1}{P}$) when in molecular diffusion regime ($Kn < 0.1$). $Kn > 10$ means Knudsen diffusion dominates; D_{KA} = Knudsen diffusion coef. does not depend on P.

b. (5 points) Consider two tanks having different concentrations of species A, with $C_{A1} > C_{A2}$. The tanks are connected by a tube with a valve, as shown in the images below. At t=0, the valve is opened such that mass can flow in between the two tanks.



(3 pts) i. Show the direction of diffusive and convective mass transport in each case.

(2 pts) ii. Define and explain the dimensionless number that determines the relative importance of diffusion versus convection.

i. (3 pts) +0.5 pts per arrow

convection → higher fluid level to lower fluid level (due to pressure difference)

diffusion → higher concentration to lower concentration

ii. (2 pts)

$$Pe = \underbrace{\frac{\text{convection}}{\text{diffusion}}}_{+1} = \underbrace{\frac{V_\infty L}{D_{AB}}}_{+1}$$

(Award +1 if Sherwood # given and explained)

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c. (5 points) Explain why a flow of a gas or liquid parallel to a solid surface can enhance mass transfer from a surface. How will the mass transfer flux increase with increasing velocity of the flowing gas or liquid?

Convection enhances mass transport because
(a) limits conc. gradient to B.L.
(b) mass diffusing from surface is immediately removed
(c) additional mass transport mechanism due to convection

+2 for any 1 pt.

$k_c \propto Re_x^{1/2}$ laminar $\Rightarrow$ $k_c \propto v^{1/2}$

$\propto Re_x^{4/5}$ turbulent $\Rightarrow$ $v^{4/5}$

+3 for correct exponents

+2 for qualitative explanation

d. (5 points) Substance A transfers from one liquid (1) to a second liquid (2) that is immiscible (does not mix) with the first liquid. At equilibrium, the distribution of A between the two liquids is given by $C_{A1} = K_A C_{A2}$, where C_{A1} and C_{A2} are the equilibrium concentrations of A in liquid 1 and liquid 2, respectively, and K_A is the equilibrium constant. The mass transfer coefficients in liquids 1 and 2 are k_{c1} and k_{c2}, respectively. How does the value of K_A influence the fraction of the overall mass transfer coefficient, K_{L1}, associated with mass transfer in each liquid phase?

$$\text{Flux} = k_{c1}(C_{A1} - C_{A1}^i) = k_{c2}(C_{A2}^i - C_{A2}) = K_{L1}(C_{A1} - \underbrace{K_A C_{A2}}_{C_{A1}^*})$$

+1 if any of these is written w/ correct conc. and nothing else is done

$C_{A1}^i = K_A C_{A2}^i$ equilibrium at interface

$$\frac{\text{Flux}}{K_{L1}} = C_{A1} - C_{A1}^i + C_{A1}^i - K_A C_{A2}$$

$$= (C_{A1} - C_{A1}^i) + K_A(C_{A2}^i - C_{A2})$$

$$= \frac{\text{Flux}}{k_{c1}} + \frac{\text{Flux} \cdot K_A}{k_{c2}} \Rightarrow \frac{1}{K_{L1}} = \frac{1}{k_{c1}} + \frac{K_A}{k_{c2}}$$ +3

If $K_A \gg 1 \rightarrow$ resistance in phase 2 dominates +1

$$\frac{1}{K_{L1}} \sim \frac{K_A}{k_{c2}}$$

$K_A \ll 1 \rightarrow$ resistance in phase 1 dominates +1

$$\frac{1}{K_{L1}} \sim \frac{1}{k_{c1}}$$

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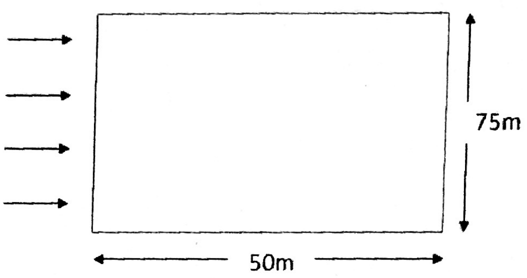
Problem 2. (30 points)

Consider the artificial pond that you have seen in your homework, for which you examined the O_2 availability for fish in the pond by looking at the rate of O_2 mass transfer from air. However, now you are worried about CO_2 released by the fish, since excess dissolved CO_2 can impact the health of the fish. You would like to maintain the concentration of dissolved CO_2 in water at 2×10^{-5} mol/m^3. A fish produces CO_2 at the rate of 2.1×10^{-6} mol/s. Assume the CO_2 concentration in the surrounding air far above the pond is zero. The kinematic viscosity of air is 1.55×10^{-5} m^2/s, and the mass diffusivity of CO_2 in air is 2×10^{-5} m^2/s at T = 300K and P = 1 atm. The Henry's constant for CO_2 in water is H = 0.029 m^3 atm/mol, where $P_{CO_2} = H\, C_{CO_2}$.



a. (20 points) Consider no transport resistance within the pond. Air flows over the surface of the pond at a velocity of 1 m/s. Determine the number of fish that can survive in the pond. Be sure to clearly state any assumptions you make.

Assumptions: (1) Steady state (2) 1-D transport w/ no edge effects
(3) constant T & P (4) No rxn. (+2 for any 2 pts)

Check flow regime, at transition point $Re_x = \frac{v x^*}{\nu} = 2 \times 10^5$ (+1)

$x^* = 3.1$m (+1) (both laminar & turbulent present)

In laminar, $k_c = 0.332\, Re_x^{1/2}\, Sc^{1/3}\, \frac{D_{AB}}{x}$ (+1)

In turbulent, $k_c = 0.0292\, Re_x^{4/5}\, Sc^{1/3}\, \frac{D_{AB}}{x}$ (+1)

$$k_c(\text{avg}) = \frac{1}{L}\left[\int_0^{x^*} 0.332\, Re_x^{1/2}\, Sc^{1/3}\, \frac{D_{AB}\,dx}{x} + \int_{x^*}^{50} 0.0292\, Re_x^{4/5}\, Sc^{1/3}\, \frac{D_{AB}\,dx}{x}\right]$$ +2 for taking avg

$= 2 \times 10^{-3}$ m/s

CO_2 molar flow out $=$ flux x area $= k_c(\Delta C) \times (50 \times 75)$ +1 +2 for area

C_{CO_2} (in air) $= 0$ (+1)

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C_{CO_2} (on surface) = $\underbrace{2\times10^{-5}}_{\text{(bulk water conc.)}}$ (+1) $\times$ $\overbrace{0.029}^{\text{Henry's const.}}$ (+2) = 5.8×10^{-7} atm (+1) (partial pressure)

$= 2.36\times10^{-5}$ mol/m³ (+2) for conversion

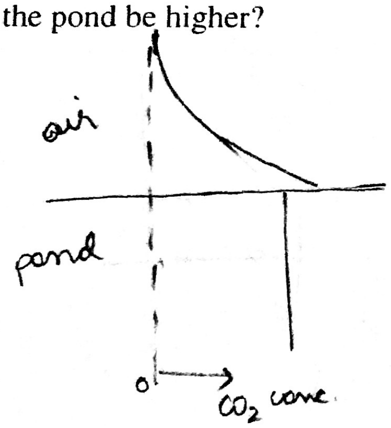
Flux = 4.78×10^{-8} mol/m²/s

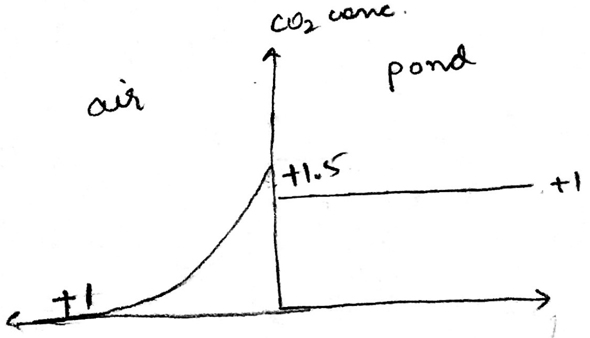
Molar flow = Flux × area = 1.79×10^{-4} mol/s

No. of fish = $\dfrac{\text{molar flow}}{CO_2 \text{ produced by 1 fish}}$ (+1) = 85 (+1)

b. (10 points) Draw the CO_2 concentration profiles for (1) the case of no liquid phase mass transfer resistance as described in part a., and for (2) the case where liquid phase mass transfer becomes significant. In which case would the number of fish that can survive in the pond be higher?

(Case 1)

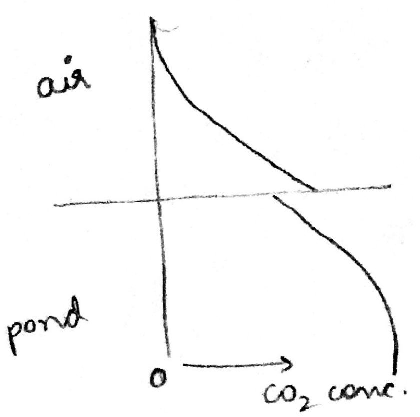


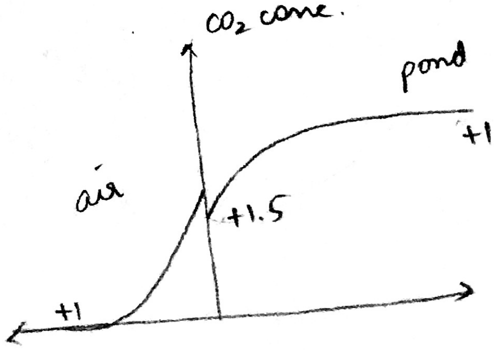


No points for wrong shapes of curves

Half credit if conc. in air doesnot go to zero

(Case 2)





More fish will survive in case 1 +3

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Problem 3. (30 points)

Cd^{2+} cations are present in the wastewater from a zinc smelting plant. Since Cd^{2+} cations are highly toxic, it is very important to dispose of this impurity responsibly. As a recently hired engineer, you discover your company has been continuously disposing the Cd^{2+}-contaminated wastewater by dumping it in an abandoned field, and you need to figure out how much of the underlying soil is contaminated. Their process has operated for 1 year, and the soil at the surface of the field contains 4.5 ppm Cd^{2+} (1 ppm means that the mole fraction of Cd^{2+} is 1×10^{-6}). The Cd^{2+} cations have a diffusion coefficient in soil of 1.5×10^{-9} m^2/s. One meter below the field surface is rock that is impermeable to the diffusion of Cd^{2+}. Cd^{2+} is toxic above 4 ppm in soil. Assume that mass transport only occurs in the direction perpendicular to the field surface.

a. (10 points) Derive an equation for the Cd^{2+} concentration in the soil as a function of depth and time. Justify any simplifying assumptions clearly.

$t = 1\ yr$, so

$$\tau = \frac{\delta^2}{D} = \frac{(1m)^2}{1.5\times10^{-9}\ m^2/s} = 6.67\times10^8 s = 21.14\ yr$$

$t \ll \tau$, assume semi-infinite.

(+3) P.C. possible

$$\frac{\partial C}{\partial t} = D_{AB}\frac{\partial^2 C}{\partial z^2} - \underbrace{v\frac{\partial C}{\partial z}}_{=0,\ \text{no velocity}} + \underbrace{R}_{=0,\ \text{no rxn}}$$

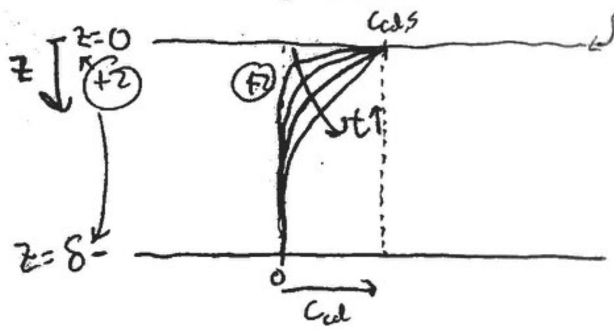
(+1) (+1)

(+2)

$$\frac{\partial C}{\partial t} = D_{AB}\frac{\partial^2 C}{\partial z^2} \xrightarrow[\text{solution}]{\text{semi-infinite}} \boxed{\frac{C_{Cd}}{C_{Cd,s}} = 1 - \text{erf}\left(\frac{z}{\sqrt{4D_{AB}t}}\right)}$$

(+3)

b. (10 Points) Draw a sketch of the Cd^{2+} concentration profile and use it to define the **boundary** conditions for the equation that you developed in response to part (a) of this problem.



$C_{Cd,s} = 4.5\ ppm$

$C_{Cd}(t=0, z) = 0$ (+2)

$C_{Cd}(t, z=0) = C_{Cd,s}$ (+2)

$C_{Cd}(t, z\to\infty) = 0$ (+2)

P.C. possible

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c. (10 Points) Determine how much soil must be removed (that is, at what depth is the soil no longer toxic?).

$$\frac{C_{Cd}}{C_{Cd,s}} = 1 - \mathrm{erf}\left(\frac{z}{\sqrt{4D_{AB}t}}\right) \quad (+2)$$

$$\frac{4\ \text{ppm}}{4.5\ \text{ppm}} = 1 - \mathrm{erf}\left(\frac{z}{\sqrt{4D_{AB}t}}\right)$$

$$\mathrm{erf}\left(\frac{z}{\sqrt{4D_{AB}t}}\right) = 0.11 \quad (+2)$$

From chart,

$$\frac{z}{\sqrt{4D_{AB}t}} = 0.1 \quad (+4)$$

P.C. possible.

$$z = 0.1\sqrt{4(1.5\times10^{-9}\ m^2/s)\left(1y \times 365\left(\frac{d}{y}\right) \times 24\left(\frac{hr}{d}\right) \times 3600\left(\frac{s}{hr}\right)\right)}$$

$$\boxed{z = 4.3\times10^{-2}\ m} \quad (+2)$$

(+2) for Gurney-Lurie method is done properly.

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Problem 4. (20 points)

Microorganisms are often used to bioremediate toxic chemical spills. Your chemical company just spilled trichloroethylene (TCE), a carcinogen, into a nearby pond, forming a TCE concentration of 0.01 mol m^{-3}. To get rid of the TCE, you disperse microorganisms into the pond so that they can break down the TCE. TCE diffuses into the microorganism cell, where it is then decomposed by enzymes in the cell following Michaelis-Menten reaction kinetics:

$$R_{TCE} = \frac{-R_{TCE,max}\, C_{TCE}}{K_M + C_{TCE}},$$

where $R_{TCE,max}$ (3.7×10^{-5} mol m^{-3} s^{-1}) is the maximum possible degradation of TCE, K_M (2.4 mol m^{-3}) is the half-saturation constant for the degradation of TCE, and C_{TCE} is the concentration of TCE. Assume there are no resistances to convective mass transfer across the fluid boundary layer between the bulk fluid and the microorganism surface. The diffusion coefficient for TCE in water is 8.2×10^{-10} m^2/s.

a. (10 points) What is the differential equation for mass transfer in the microorganism in terms of C_{TCE}? Assume the microorganism is spherical with a radius of R = 5 μm. State at least three other reasonable assumptions you made, and state what boundary conditions you would use to solve the differential equation.

Assumptions (3/10 pts, 1 pt per assumption up to 3 pts)

1.) No convection (only diffusion terms in gov. eqn)

2.) Axial symmetry ($\frac{\partial}{\partial\theta} = 0 = \frac{\partial}{\partial\phi}$)

3.) Diffusion only in r-direction ($N_{A,\theta} = 0 = N_{A,\phi}$)

4.) Constant T, P, concentration, D_{AB}, etc.

5.) Steady state

6.) Constant bulk/surface concentration of 0.01 $\frac{mol}{m^3}$

7.) No TCE in cell originally before placed in pond

8.) Degradation product does not affect rxn rate, diffusion, etc.

* Invalid assumptions to earn points: ones already stated in problem (e.g., use spherical coordinates, etc.) or no rxn (R_{TCE} is present!)

Differential Eqn (5/10 pts, see below for pt breakdown)

$$\nabla N_A + \cancel{\frac{\partial C_A}{\partial t}}^{\,S.S.} - R_A = 0 \quad (A = TCE) \quad \boxed{+2} \text{ if only showed this step}$$

$$N_A = -D_{AB}\nabla C_A$$

$$\rightarrow \frac{1}{r^2}\frac{d}{dr}\left(-D_{AB}r^2\frac{dC_A}{dr}\right) = R_A = \frac{-R_{A,max}C_A}{K_M + C_A}$$

$$\boxed{\frac{D_{AB}}{r^2}\frac{d}{dr}\left(r^2\frac{dC_A}{dr}\right) = \frac{R_{A,max}C_A}{K_M + C_A} \approx \frac{R_{A,max}C_A}{K_M}}$$

+5 * Inclusion of $\frac{\partial C_A}{\partial t}$ also accepted

or $$\frac{D_{AB}}{r^2}\left(2r\frac{dC_A}{dr} + r^2\frac{d^2C_A}{dr^2}\right) = \frac{R_{A,max}C_A}{K_M + C_A}$$

Typical deductions:
- → −2 in terms of N_A instead of C_A
- → −1 incorrect ∇ used
- → −0.5 wrong algebra sign (negative)

Boundary conditions (2/10 pts, 1 pt. per correct B.C.)

1.) At $r = R$, $C_A = 0.01\frac{mol}{m^3}$ (no convective M.T. resistance)

2.) At $r = 0$, $\frac{\partial C_A}{\partial r} = 0$ (symmetry)

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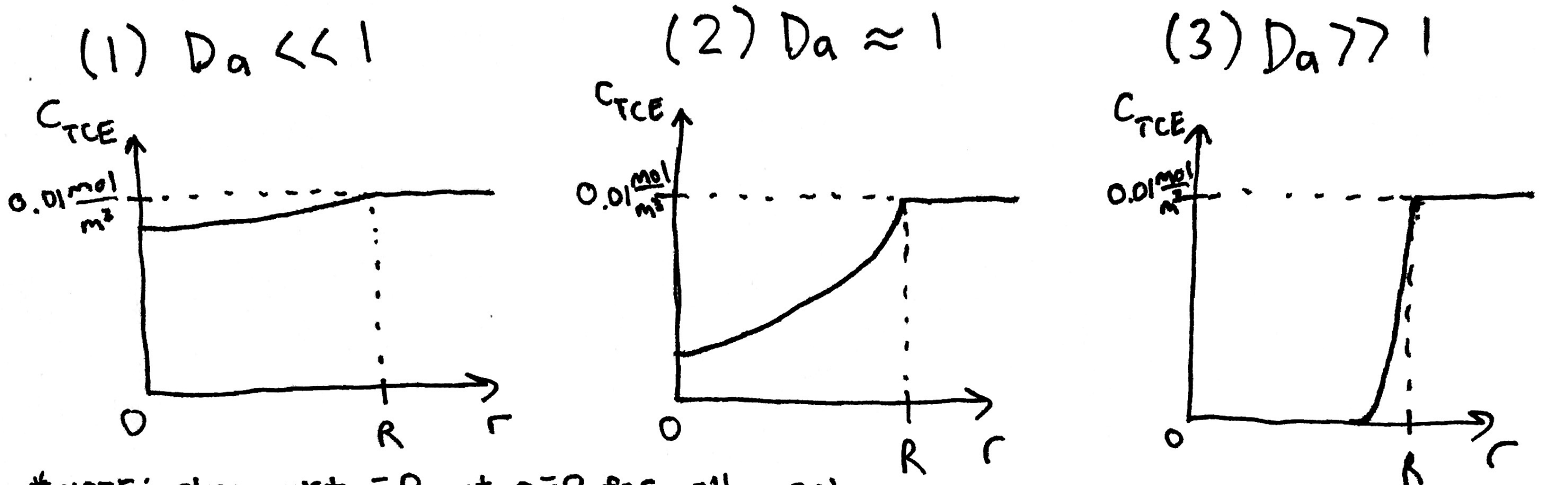
b. (10 points) Draw the concentration profiles of TCE in the cell for the following three cases: (1) Da is very small, (2) Da = 1, and (3) Da is very large, where Da is the Damköhler number in the cell (Da = kR/D_{TCE}, where k is the apparent first-order rate coefficient for the enzymatic consumption of TCE, R is the radius of the microorganism, and D_{TCE} is the diffusion coefficient for TCE).



* NOTE: slope must = 0 at r = 0 for all graphs

Point breakdown

+10 all graphs correct

→ +3.5 each for two graphs correct, +3 for third graph correct

→ +6 if Da≈1 correct but Da<<1 and Da>>1 graphs switched

→ +3 if curves all backwards but correct shapes/positions (max C_{TCE} drawn at r=0, min at r=R)

Typical partial credit

+2 incorrect graphs but explanation that $Da = \frac{\text{rxn rate}}{\text{M.T. (diffusion) rate}}$, when diffusion dominates vs. rxn, etc.

+1 $C_{TCE} = 0.01 \frac{mol}{m^3}$ at $r \geq R$,

Typical deductions

→ −2 if slope ≠ 0 at r = 0 (since $N_{A,r} = -D_{AB}\frac{\partial C_A}{\partial r}$, and $\frac{\partial C_A}{\partial r} = 0$ at $r = 0$)

→ −1 per missing axis label but clear drawing