Problem 1

Two solutions are separated by a thin film 0.3cm thick that can allow diffusion of HCl (A) and water (B). The concentration of HCl at one side of the film at point z_1 is 0.004 mol/cm^3 and the concentration of HCl at the other side of the film at point z_2 is 0.002 mol/cm^3. The total concentration at both points is 0.055 mol/cm^3. The diffusivity of HCl in water in the film is $2.5 * 10^{-5}$ cm^2/s. Assume steady state.

a) Find an expression for the molar flux of HCl assuming that water does not diffuse. Calculate this flux.

b) Find an expression for the molar fluxes of HCl and water assuming that they are related by N_A = -2N_B. Calculate both fluxes.

Solution

a) We can start with the expression for molar flux:

$$
\begin{aligned}
N_A &= -\mathcal{D}_{AB}\frac{dc_A}{dz} + x_A\left(N_A + N_B\right) && (1)\\
&= -\mathcal{D}_{AB}\frac{dc_A}{dz} + \frac{c_A}{c}\left(N_A + N_B\right). && (2)
\end{aligned}
$$

As water does not diffuse $N_B = 0$, and we can rearrange to find an exact expression for N_A:

$$
\begin{aligned}
N_A &= -\frac{\mathcal{D}_{AB}}{1-x_A}\frac{dc_A}{dz} = -\frac{c\mathcal{D}_{AB}}{c-c_A}\frac{dc_A}{dz} && (3)\\
N_A dz &= -\frac{c\mathcal{D}_{AB}}{c-c_A}dc_A. && (4)
\end{aligned}
$$

As we are assuming steady state, N_A is constant and we can integrate the expression from z_1 to z_2 and c_{A1} to c_{A2}:

$$
\begin{aligned}
\int_{z_1}^{z_2} N_A dz &= \int_{c_{A1}}^{c_{A2}} -\frac{c\mathcal{D}_{AB}}{c-c_A}dc_A\\
N_A(z_2 - z_1) &= c\mathcal{D}_{AB}\ln\left(\frac{c-c_{A2}}{c-c_{A1}}\right) = c\mathcal{D}_{AB}\ln\left(\frac{1-x_{A2}}{1-x_{A1}}\right),
\end{aligned}
$$

which gives the final expression as:

$$N_A = \frac{c\mathcal{D}_{AB}}{z_2 - z_1} \ln\left(\frac{c - c_{A2}}{c - c_{A1}}\right) = \frac{c\mathcal{D}_{AB}}{z_2 - z_1} \ln\left(\frac{1 - x_{A2}}{1 - x_{A1}}\right). \tag{5}$$

Plugging in the parameters of the problem:
$c = 0.055$ mol/cm^3
$x_{A2} = c_{A2}/c = 0.002/0.055 = 0.0364$
$x_{A1} = c_{A1}/c = 0.004/0.055 = 0.0727$
$z_2 - z_1 = 0.3$cm
$\mathcal{D}_{AB} = 2.5 * 10^{-5}$ cm^2/s

$$\begin{aligned} N_A &= \frac{c\mathcal{D}_{AB}}{z_2 - z_1} \ln\left(\frac{1 - x_{A2}}{1 - x_{A1}}\right) \\ &= \frac{0.055 * 2.5 * 10^{-5}}{0.3} \ln\left(\frac{1 - 0.0364}{1 - 0.0727}\right) \\ &= 1.76 * 10^{-7} \text{mol/cm}^2\text{s}. \end{aligned} \tag{6}$$

b) As before, we can start with the expression for molar flux using either (1) or (2). The problem statement tells us that N_A = -2N_B, so we can plug in N_B = -1/2 N_A and rearrange:

$$N_A = -\mathcal{D}_{AB}\frac{dc_A}{dz} + x_A\left(N_A - \frac{1}{2}N_A\right) = -\mathcal{D}_{AB}\frac{dc_A}{dz} + \frac{x_A}{2}N_A \tag{7}$$

$$= -\frac{\mathcal{D}_{AB}}{1 - \frac{x_A}{2}}\frac{dc_A}{dz} = -\frac{c\mathcal{D}_{AB}}{c - \frac{c_A}{2}}\frac{dc_A}{dz} \tag{8}$$

$$N_A dz = -\frac{c\mathcal{D}_{AB}}{c - \frac{c_A}{2}} dc_A. \tag{9}$$

As we are assuming steady state N_A is constant and we can integrate the expression from z_1 to z_2 and c_{A1} to c_{A2}:

$$\int_{z_1}^{z_2} N_A dz = \int_{c_{A1}}^{c_{A2}} -\frac{c\mathcal{D}_{AB}}{c - \frac{c_A}{2}} dc_A$$

$$N_A(z_2 - z_1) = 2c\mathcal{D}_{AB} \ln\left(\frac{c - \frac{c_{A2}}{2}}{c - \frac{c_{A1}}{2}}\right) = 2c\mathcal{D}_{AB} \ln\left(\frac{1 - \frac{x_{A2}}{2}}{1 - \frac{x_{A1}}{2}}\right) = 2c\mathcal{D}_{AB} \ln\left(\frac{2 - x_{A2}}{2 - x_{A1}}\right),$$

which gives the final expressions as:

$$N_A = \frac{2c\mathcal{D}_{AB}}{z_2 - z_1} \ln\left(\frac{2c - c_{A2}}{2c - c_{A1}}\right) = \frac{2c\mathcal{D}_{AB}}{z_2 - z_1} \ln\left(\frac{2 - x_{A2}}{2 - x_{A1}}\right) \tag{10}$$

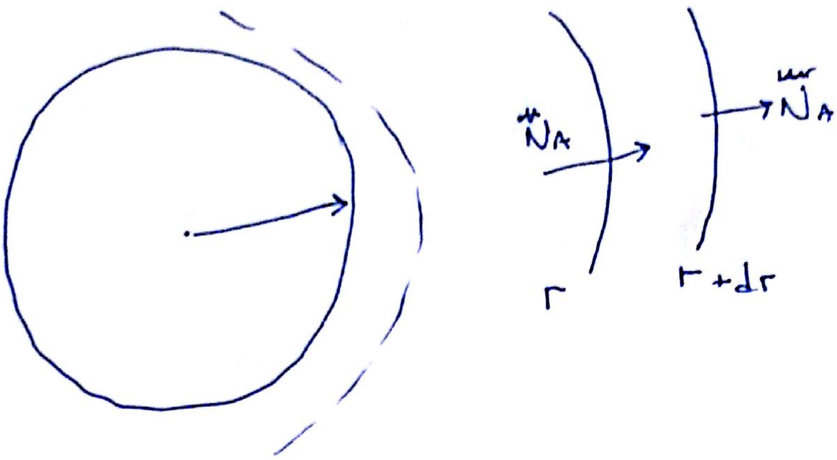
$$N_B = -\frac{N_A}{2} = -\frac{c\mathcal{D}_{AB}}{z_2 - z_1} \ln\left(\frac{2 - x_{A2}}{2 - x_{A1}}\right). \tag{11}$$

Plugging in the parameters of the problem:
$c = 0.055$ mol/cm^3
$x_{A2} = c_{A2}/c = 0.002/0.055 = 0.0364$
$x_{A1} = c_{A1}/c = 0.004/0.055 = 0.0727$
$z_2 - z_1 = 0.3$cm
$\mathcal{D}_{AB} = 2.5 * 10^{-5}$ cm^2/s

$$N_A = \frac{2c\mathcal{D}_{AB}}{z_2 - z_1} \ln\left(\frac{2 - x_{A2}}{2 - x_{A1}}\right) = \frac{2 * 0.055 * 2.5 * 10^{-5}}{0.3} \ln\left(\frac{2 - 0.0364}{2 - 0.0727}\right)$$
$$N_A = 1.71 * 10^{-7} \text{mol/cm}^2\text{s} \tag{12}$$
$$N_B = -\frac{N_A}{2} = -8.55 * 10^{-8} \text{mol/cm}^2\text{s} \tag{13}$$

Problem 2 - PART A [15 pts]

If. Start with shell Balance



$$\frac{d}{dr}\tilde{N}_A = 0 = \nabla N_A \quad \leftarrow \text{constant}$$

OR if you used conservation of species eqn

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

* Steady state
* no bulk flow
* no $\theta, \theta\ \phi$ component

$$N_A = -4\pi r^2 \mathcal{D}\frac{dC_A}{dr}$$

$$\frac{d}{dr}N_A = \mathcal{D}\cdot\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_A}{\partial r}\right) = 0$$

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

Boundary conditions ① $r = R$, $C_A = C_{AR}$
② $r = \infty$, $C_A = 0$

$$r^2 \frac{dC_A}{dr} = A_1$$

$$\frac{dC_A}{dr} = \frac{A_1}{r^2} \Rightarrow C_A = A_2 - \frac{A_1}{r}$$

Evaluating at $r = R \Rightarrow A_1 = -C_{AR} \cdot R$

at $r = \infty \Rightarrow A_2 = 0$

Concentration Profile :- $C_A = C_{AR} \dfrac{R}{r}$

If Start with flux eq$\underline{n}$ (NOT RECOMMENDED)

$$N_A = -\mathcal{D} \frac{dC_A}{dr} + \frac{C_A}{C}\left(N_A + \cancelto{0}{N_B}\right)$$

OR

$$N_A = -\mathcal{D}\, C \frac{dX_A}{dr} + X_A\left(N_A + \cancelto{0}{N_B}\right)$$

OR

$$N_A = -\mathcal{D}\, C \frac{dy_A}{dr} + y_A\left(N_A + \cancelto{0}{N_B}\right)$$

If assuming stagnant film $N_B = 0$

$$N_A = \frac{-\mathcal{D}}{\left(1 - \frac{C_A}{C}\right)} \frac{dC_A}{dr} \overset{\text{OR}}{=} \frac{-\mathcal{D} C}{(1 - X_A)} \frac{\partial X_A}{\partial r} \overset{\text{OR}}{=} -\frac{\mathcal{D} C}{(1 - y_A)} \frac{\partial y_A}{\partial r}$$

$$N_A = \frac{-D}{\left(1-\frac{C_A}{C}\right)} \frac{dC_A}{dr}$$

Boundary cond:

$r = R \quad , \quad C_A = C_{AR}$

$r = \infty \quad , \quad C_A = 0$

$$\int_R^{\infty} N_A \cdot dr = \int_{C_{AR}}^{C_A} \frac{-D}{\left(1-\frac{C_A}{C}\right)} \, dC_A$$

$$N_A \cdot r \Big|_R^{\infty} = N_A (r-R) = -D \ln\left(1-\frac{C_A}{C}\right)\Big|_{C_{AR}}^{C_A}$$

$$N_A(\infty - R) = -D \ln\left[\frac{1-\cancelto{0}{\frac{C_A}{C}}}{1-\frac{C_{AR}}{C}}\right]$$

$$N_A(\infty - R) = -D \ln\left[\frac{1}{1-\frac{C_{AR}}{C}}\right]$$

$$\exp\left[\frac{-N_A}{D}(\cancelto{0}{\infty} - R)\right] = \exp\left[+\frac{N_A \cdot R}{D}\right] = \frac{1}{1-C_{AR}/C}$$

$$1 - \frac{C_{AR}}{C} = \exp\left(-\frac{N_A \cdot R}{D}\right)$$

N_A is constant $\Leftarrow$ $N_A = -\frac{D}{R} \underbrace{\ln\left[1-\frac{C_{AR}}{C}\right]}_{}$ $\approx C_{AR}$ [evaluating $\ln\left(1-\frac{C_{AR}}{C}\right)$]

$$N_A = -\frac{D \, C_{AR}}{R}$$

To find $C_A \rightarrow N_A = \cancel{-D} \frac{dC_A}{dr} = \frac{\cancel{-D} \, C_{AR}}{R}$

doan indefinite integral $\Rightarrow \int dC_A = \int \frac{C_{AR}}{r} dr \Rightarrow \boxed{C_A(r) = \frac{C_{AR} R}{r}}$

Problem 2 Part B Method 1 (20 pts)

use $C_A = C_{AR}\frac{R}{r}$ from part A

Flux N_A @ $r=R$ $\quad -\mathcal{D}\left.\frac{dC_A}{dr}\right|_R = -\mathcal{D}C_{AR}R\left.\frac{-1}{r^2}\right|_{r=R}$

$$\boxed{N_A = C_{AR}\mathcal{D}\frac{1}{R}}$$

Mass Balance

$$\boxed{\begin{aligned} dM &= -N\cdot A\cdot dt \\ \rho dV &= -N\cdot A\cdot dt \end{aligned}}$$

mass balance

$$\rho\frac{4}{3}\pi d r^3 = -C_{AR}\mathcal{D}\frac{1}{r}4\pi r^2 dt$$

substitute + simplify

$$\rho \cancel{4\pi r^2} dr = -C_{AR}\mathcal{D}\cancel{4\pi} r\, dt$$

cancelling

$$\int_R^0 \rho r dr = \int_0^{t_f} -C_{AR}\mathcal{D}dt$$

integration

$$\rho\frac{R^2}{2} = C_{AR}\mathcal{D}t_f$$

$$\boxed{t_f = \frac{\rho R^2}{2C_{AR}\mathcal{D}}}$$

final analytical expression

$$C_{AR} = \frac{74}{101000}\cdot\frac{101000}{8.314\cdot 318} = 2.8\times10^{-2}\ \frac{mol}{m^3}$$

from $C = \frac{P}{RT}$

$$t_f = \frac{0.001^2\cdot 8600}{2\cdot 2.8\times10^{-2}\cdot 6.92\times10^{-6}} = 2.219\times10^4 \text{ seconds}$$

$$\boxed{\begin{array}{c}2.2e4 \text{ seconds} \\ 6.2 \text{ hours}\end{array}}$$

final numerical answer

Problem 2 Part B Method 2 (20 pts)

Flux $N_A = -c\mathcal{D}\frac{dx_A}{dr} + x_A(N_A + \cancel{N_B}^{\,0})$

$N_A = -\frac{P}{RT}\mathcal{D}\frac{dP}{dr}\frac{1}{P} + \frac{P_A}{P}N_A$

$$\boxed{N_A\,dr = \frac{-\mathcal{D}}{RT}\frac{dP_A}{(1-P_A/P)}}$$

$N_A = \frac{\overline{N_A}}{4\pi r^2}$ average flux

$$\int_{r_1}^{r_2}\frac{\overline{N_A}}{4\pi r^2}dr = \int_0^{P_A^{vap}}\frac{-\mathcal{D}\,dP_A}{RT\{1-P_A/P\}}$$ integrate

B.C. $r=r_1$ $P_A = P_A^{vap}$

$r=r_2$ $P_A = 0$

$(r_2 \to \infty)$

$(r_1 = R)$

$$\frac{\overline{N_A}}{4\pi}\left(\frac{1}{r_1} - \cancel{\frac{1}{r_2}}^{\,0}\right) = \frac{-\mathcal{D}}{RT}(-P)\ln(1-P_A/P)$$

$$\boxed{N_A = \frac{\mathcal{D}P}{RTr_1}\ln(1-P_A/P)}$$

set equal to $\boxed{-\rho\frac{dr}{dt}}$

$$\int_0^{t_f}\frac{\mathcal{D}P}{RT}\ln(1-P_A/P)\,dt = \int_R^0 -\rho r\,dr$$ integrate

$$t_f\frac{\mathcal{D}P}{RT}\ln(1-P_A/P) = \rho\frac{R^2}{2}$$

final analytical answer

$$\boxed{t_f = \frac{\rho R^2 R_{gas}T}{2\mathcal{D}P\ln(1-P_A/P)} = \frac{\rho R^2 R_{gas}T\,P_{BM}}{2\mathcal{D}P(P_1-P_2)}}$$

$t_f = 2.219\times10^4$ s

$\boxed{\begin{array}{l}\text{2.2e4 seconds}\\ \text{6.2 hours}\end{array}}$ final numerical answer

Problem 3 Part A (15 pts)

assumptions

- diffusion in z << convection in z
- steady-state
- flow in z only, Concentration function of r, z

Governing Equation

$$\underbrace{\cancel{\frac{\partial C_{O_2}}{\partial t}}}_{0\ \text{S.S.}} + \underbrace{v_r \cancel{\frac{\partial C_{O_2}}{\partial r}}}_{0\ v_r = 0} + v_z \frac{\partial C_{O_2}}{\partial z} = \mathcal{D}_{O_2}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_{O_2}}{\partial r}\right) + \underbrace{\cancel{\frac{\partial^2 C_{O_2}}{\partial z^2}}}_{0\ v_z \gg \mathcal{D}\frac{\partial^2 C_{O_2}}{\partial z^2}}\right] + \underbrace{\cancel{R_{O_2}}}_{0\ \text{no homogenous rxn}}$$

$$\boxed{v_z \frac{\partial C_{O_2 blood}}{\partial z} = \mathcal{D}_{O_2 blood}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_{O_2 blood}}{\partial r}\right)\right)}$$ +6

Boundary Conditions

① @ $z=0$ $\quad C_{O_2 blood} = C_{O_2,0}$ $\quad$ inlet +3

② @ $r=0$ $\quad \frac{\partial C_{O_2 blood}}{\partial r} = 0$ $\quad$ symmetry +3

③ @ $r=R$ $\quad N_{O_2 blood} = -k\, C_{O_2 blood}$

$$\mathcal{D}_{O_2 blood} \frac{\partial C_{O_2 blood}}{\partial r}\bigg|_{r=R} = -k\, C_{O_2 blood}\bigg|_{r=R}$$ +3

Problem 3 Part B (20 pts)

assumptions

- steady-state
- Concentration function of r only
- no bulk flow inside cell, only diffusion + rxn

Governing Equation

$$\underbrace{\cancel{\frac{\partial C_{O_2}}{\partial t}}}_{0 \text{ s.s.}} + \underbrace{\cancel{v} \cdot \nabla C_{O_2}}_{0 \text{ no flow}} = \mathcal{D}_{O_2}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial C_{O_2}}{\partial r}\right)\right] + R_V$$

$$\boxed{0 = \mathcal{D}_{O_2 cell}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial C_{O_2 cell}}{\partial r}\right)\right] - k\, C_{O_2 cell}}$$ +10

Boundary Conditions

① @ $r=0$ $\quad \frac{\partial C_{O_2 cell}}{\partial r} = 0$ symmetry +5

② @ $r=R$ $\quad N_{O_2 cell}\Big|_{r=R} = k_c\left(C_{O_2 toe} - C_{O_2, surf. ext.}\right)$

$$N_{O_2 cell}\Big|_{r=R} = k_c\left(C_{O_2 toe} - \frac{C_{O_2 cell}}{K}\right)$$

$$\mathcal{D}\frac{\partial C_{O_2 cell}}{\partial r}\Big|_{r=R} = k_c\left(C_{O_2 toe} - \frac{C_{O_2 cell}}{K}\right)$$ +5