HW3_1

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1 Problem 1

1.1 Problem 1.1

Starting with the definition,

$$N_A = x_A(N_A + N_B) + J_A \tag{1}$$

derive the expression for n_A with diffusion between concentric spheres but no bulk flow,

$$n_A = -4\pi r_1 r_2 D_{AB}(\frac{c_{A_2} - c_{A_1}}{r_2 - r_1}) \tag{2}$$

n_A is defined as

$$n_A = x_A(n_A + n_B) + AJ_A \tag{3}$$

where A is surface area

Since there is no bulk flow, $N = 0$ and $n = 0$ which means $n_A = -n_B$. $\therefore$

$$n_A = AJ_A \tag{3.1}$$

Fick's law defines J_A as

$$J_A = -cD_{AB}\nabla \cdot x_A \tag{4}$$

and if c is constant

$$J_A = -D_{AB}\nabla \cdot c_A \tag{4.1}$$

For spherical coordinates, ∇ is defined as

$$\nabla \cdot c_A = \frac{\partial c_A}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial c_A}{\partial \theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial c_A}{\partial \phi}\hat{\phi} \tag{5}$$

and in 1D

$$\nabla \cdot c_A = \frac{dc_A}{dr}\hat{r} \tag{5.1}$$

Substituting (4.1) into (3.1) gives

$$n_A = -4\pi r^2 D_{AB}\frac{dc_A}{dr}$$

Separate and integrate

$$\int_{r_2}^{r_1} \frac{dr}{r^2} = -\frac{4\pi D_{AB}}{n}\int_{c_1}^{c_2} dc_A$$

Simplify to get

$$\frac{r_2 - r_1}{r_1 r_2} = \frac{-4\pi D_{AB}}{n_A}(c_{A_2} - c_{A_1})$$

and finally

$$n_A = -4\pi D_{AB} r_1 r_2 \frac{c_{A_2} - c_{A_1}}{r_2 - r_1}$$

1.2 Problem 1.2

Show that

$$N_A = -\frac{D_{AB} r_1 r_2}{r^2} \frac{c_{A_2} - c_{A_1}}{r_2 - r_1} \tag{6}$$

and derive an experession for N_B

For no bulk flow,

$$N_A = J_A$$

and

$$n_A = A J_A$$

$\therefore$

$$N_A = \frac{n_A}{A} = \frac{-4\pi D_{AB} r_1 r_2 \frac{c_{A_2} - c_{A_1}}{r_2 - r_1}}{4\pi r^2} = -\frac{D_{AB} r_1 r_2}{r^2} \frac{c_{A_2} - c_{A_1}}{r_2 - r_1}$$

Given that $N_A + N_B = 0$, N_B must be $-N_A$. $\therefore$

$$N_B = \frac{D_{AB} r_1 r_2}{r^2} \frac{c_{A_2} - c_{A_1}}{r_2 - r_1}$$