EXAMPLE 4 : EQUIMOLAR COUNTERDIFFUSION

"A" DIFFUSES THROUGH A PORE OF LENGTH L TO A CATALYTIC SURFACE WHERE THE FOLLOWING REACTION TAKES PLACE:

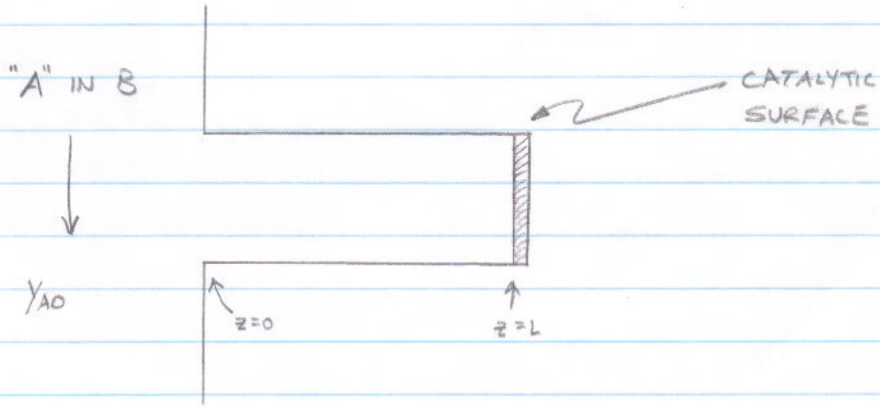
$$A \rightarrow C$$

WITH A SURFACE RATE OF REACTION

$$R_A = k' C_A$$

k' = SURFACE FIRST ORDER RATE CONSTANT $[cm/s]$

SO R_A HAS UNITS OF $[cm/s][mol/cm^3] = mol/cm^2 s$



"B" IS STAGNANT

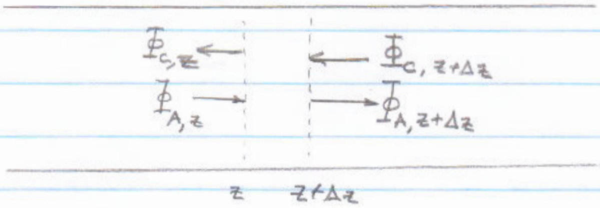
$y_A = y_{A0}$ @ $z = 0$

$y_A = y_{AL}$ @ $z = L$

QUESTIONS:

1) WHAT IS y_{AL}?
2) WHAT IS Φ_A?

STEP 1



"B" IS STAGNANT

STEP 2

MATERIAL BALANCE ON $\underline{\underline{A}}$!

WE HAVE ALREADY SOLVED THIS PROBLEM
IT IS SAME AS EXAMPLE 1A. NOTE THAT
THE REACTION DOES NOT OCCUR
IN "SYSTEM".

$$\Phi_A = C_1$$

STEP 3

$$\vec{\Phi}_A = -cD_{AB}\vec{\nabla}y_A + y_A \Sigma \vec{\Phi}_i$$

$$\Phi_B = 0$$

$$\Phi_C = -\Phi_A \qquad \text{EQUIMOLAR COUNTERDIFFUSION}$$

RECTANGULAR COORDINATE SYSTEM

$$\Phi_A = -cD_{AB}\frac{dy_A}{dz} + y_A\left(\Phi_A + \Phi_B + \Phi_C\right)$$

$$\Phi_A = -cD_{AB}\frac{dy_A}{dz}$$

STEP 4
$$C_1 = -cD_{AB}\frac{dy_A}{dz}$$

$$C_1 z + C_2 = -cD_{AB}\, y_A$$

$$C_2 = -cD_{AB}\, y_{A0}$$

$$C_1 L - cD_{AB}\, y_{A0} = -cD_{AB}\, y_{AL}$$

$$C_1 = \frac{cD_{AB}}{L}\left(y_{A0} - y_{AL}\right)$$

$$\left(y_{A0} - y_{AL}\right)\frac{z}{L} - y_{A0} = -y_A$$

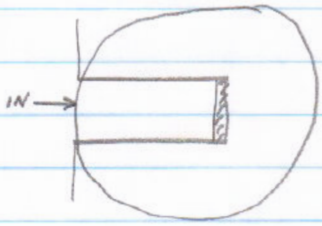
$$y_A = y_{A0} - \frac{z}{L}\left(y_{A0} - y_{AL}\right)$$ CONC. PROFILE

$$\Phi_A = \frac{cD_{AB}}{L}\left(y_{A0} - y_{AL}\right)$$

A) WHAT IS RELATIONSHIP BETWEEN DIFFUSION & REACTION?

B) HOW CAN WE USE THESE EQUATIONS WHEN WE DON'T KNOW y_{AL}?

AT STEADY STATE, MOLAR FLOW RATE OF "A" THROUGH PORE MUST BE EQUAL TO MOLAR REACTION RATE



ACC = IN − OUT − CONS

$$0 = \Phi_A S\Big|_{z=0} - k' c_A S\Big|_{z=L}$$

OR

$$\Phi_A = k' c_{AL} = k' c\, y_{AL}$$

$$\frac{c D_{AB}}{L}\left(y_{A0} - y_{AL}\right) = k' c\, y_{AL}$$

$$\frac{y_{A0} - y_{AL}}{y_{AL}} = \frac{k' c L}{c D_{AB}} = \frac{k' L}{D_{AB}}$$

$$\frac{y_{A0}}{y_{AL}} - 1 = \frac{k' L}{D_{AB}}$$

NOTE $\frac{k' L}{D_{AB}}$ IS DIMENSIONLESS

Let $\frac{k' L}{D_{AB}}$ = DAMKÖHLER NUMBER

$$\frac{k' L}{D_{AB}} = N_{DA} = \frac{\text{RATE OF REACTION}}{\text{RATE OF DIFFUSION}}$$

$$\frac{y_{A0}}{y_{AL}} = N_{DA} + 1$$

$$y_{A0} = \left(N_{DA} + 1\right) y_{AL} \qquad \text{OR} \qquad y_{AL} = \frac{y_{A0}}{N_{DA} + 1}$$

CONSIDER TWO EXTREME CASES:

(A) $k'L \ll D_{AB}$ $\quad N_{DA}$ IS SMALL $\quad Y_{AL} = Y_{A0}$

RATE OF DIFFUSION IS LARGE

SYSTEM IS LIMITED BY REACTION RATE

(B) $k'L \gg D_{AB}$ $\quad N_{DA}$ IS LARGE $\quad Y_{AL} = 0$

RATE OF REACTION IS LARGE

SYSTEM IS LIMITED BY DIFFUSION RATE

NOTE:

$$\Phi_A = \frac{cD_{AB}}{L}\left(Y_{A0} - \frac{Y_{A0}}{N_{DA}+1}\right)$$

$$\Phi_A = \frac{cD_{AB}Y_{A0}}{L}\left(1 - \frac{1}{N_{DA}+1}\right)$$

$$\Phi_A = \frac{cD_{AB}Y_{A0}}{L}\underbrace{\left(\frac{N_{DA}}{N_{DA}+1}\right)}_{\text{VARIES BETWEEN 0 AND 1}}$$

IF N_{DA} IS SMALL (REACTION RATE LIMITED) $\quad \Phi_A \cong 0$

IF N_{DA} IS LARGE (DIFFUSION LIMITED) $\quad \Phi_A \cong \dfrac{cD_{AB}Y_{A0}}{L}$

(MAXIMUM FLUX)

SOME NUMBERS...

1) HOW MUCH "C" IS PRODUCED IN A SINGLE PORE OF 0.1 cm DIAMETER AND 0.1 cm LENGTH WHEN P = 1 atm, T = 298 K, $y_{A0} = 0.1$, $D_{AB} = 0.10\ cm^2/s$, $k' = 0.04\ cm/s$?

$$N_{DA} = \frac{k'L}{D_{AB}} = \frac{(0.04\,cm/s)(0.10\,cm)}{(0.10\,cm^2/s)} = 0.04$$

(REACTION LIMITED!)

$$\frac{y_{A0}}{y_{AL}} = N_{DA} + 1 = 1.04$$

$$y_{AL} = 0.0962$$

$$\Phi_A = \frac{c D_{AB} y_{A0}}{L}\left(\frac{N_{DA}}{N_{DA}+1}\right)$$

$$\Phi_A = \frac{P D_{AB} y_{A0}}{LRT}\left(\frac{N_{DA}}{N_{DA}+1}\right)$$

$$\Phi_A = \frac{(1\,atm)(0.10\,cm^2/s)(0.1)\left(\frac{0.04}{1.04}\right)}{(0.1\,cm)(0.08206\,L\,atm/mol\,K)(298\,K)(1000\,cm^3/L)}$$

$$\Phi_A = 1.57\times10^{-7}\ mol/cm^2 s$$

$$\dot{n}_A = \Phi_A S = (1.57\times10^{-7}\,mol/cm^2 s)\left(\frac{\pi}{4}(0.1\,cm)^2\right)$$

$$\dot{n}_A = 1.23\times10^{-9}\ mol/s$$

$$\dot{n}_C = (-)\,1.23\times10^{-9}\ mol/s$$