Concentration Distribution in Solids and Laminar Flow

The mass transfer problems in this chapter are solved by applying the mass balance

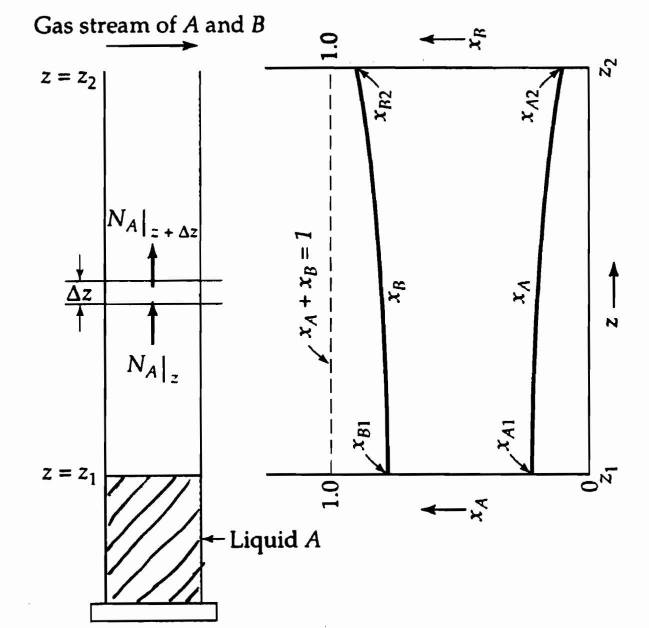
Rate of mass in − Rate of Mass out + Rate of Mass Production due to chemical Reaction (homogeneous) = 0

for simplicity the molar flux of compont A through B is given by

$$\underset{\text{Total flux}}{N_{Az}} = \underset{\text{molecular flux}}{-c D_{AB} \frac{\partial x_A}{\partial z}} + \underset{\text{convective flux}}{x_A (N_{Az} + N_{Bz})}$$

in the above equation N_{Bz} must be eleminated based on the information provided in the problem.

Example 1 Diffusion through Stagnant Gas. ②



Liquid A contained at the bottom of a tube evaporates the diffuses through a stagnant gas ↓ in the tube. Eventually, as A reaches the tip of the tube it is swept away by moving stream of gas B.

containing A & B

(mole)
Mass Balance on differential element Δz :

$$S N_{Az}\big|_{z} - S N_{Az}\big|_{z+\Delta z} = 0 .$$

Note that $N_A = \frac{mole}{m^2\ s}$ flux.

Since the area S is constant along diffusion path, it can be eliminated

$$N_{Az}\big|_z - N_{Az}\big|_{z+\Delta z} = 0 .$$

deride the above equation by Δz and take the limite when $\Delta z \to 0$.

$$\lim_{\Delta z \to 0} \frac{N_{Az}|_z - N_{Az}|_{z+\Delta z}}{\Delta z} = 0 .$$

$$\Rightarrow -\frac{d N_{Az}}{dz} = 0 .$$

recall, $N_{Az} = -c D_{AB} \frac{d x_A}{dz} + x_A (N_{Az} + N_{Bz})$

since component B is not condensing or desolving in liquid A, this imply that on A is moving and B is stagnet $N_{Bz} = 0$.

$$\Rightarrow N_{Az} = -\frac{c D_{AB}}{1 - x_A} \frac{d x_A}{dz}$$

substituting the flux equation in the mass balance yields

since component B is not condensing

$$\frac{d}{dz}\left[\frac{c D_{AB}}{1-x_A}\frac{dx_A}{dz}\right] = 0 .$$

integrating once:

$$\frac{c D_{AB}}{1-x_A}\frac{dx_A}{dz} = C_1$$

integrating twice:

$$-\ln(1-x_A) = \underbrace{\frac{C_1}{c D_{AB}}}_{C_1'} z + C_2 .$$

BC's

$z = z_1 \qquad x_A = x_{A1}$

$z = z_2 \qquad x_A = x_{A2}$.

$$-\ln(1-x_{A1}) = C_1' z_1 + C_2$$

$$-\ln(1-x_2) = C_1' z_2 + C_2 .$$

$$\Rightarrow C_1' = \frac{\ln\left(\frac{1-x_{A1}}{1-x_{A2}}\right)}{z_2 - z_1}$$

$$C_2 = -\ln(1-x_{A1}) - \frac{\ln\left(\frac{1-x_{A1}}{1-x_{A2}}\right)}{z_2 - z_1} z_1$$

$$\Rightarrow -\ln(1-x_A) = \frac{\ln\left(\frac{1-x_{A1}}{1-x_{A2}}\right)}{z_2 - z_1} z - \frac{\ln\left(\frac{1-x_{A1}}{1-x_{A2}}\right)}{z_2-z_1} z_1 - \ln(1-x_{A1})$$

$$\ln\left(\frac{1-x_A}{1-x_{A1}}\right) = \frac{\ln\left(\frac{1-x_{A1}}{1-x_{A2}}\right)}{z_2-z_1} (z_1 - z)$$

$$\frac{1-x_A}{1-x_{A1}} = \left(\frac{1-x_{A_2}}{1-x_{A1}}\right)^{\frac{z-z_1}{z_2-z_1}}$$

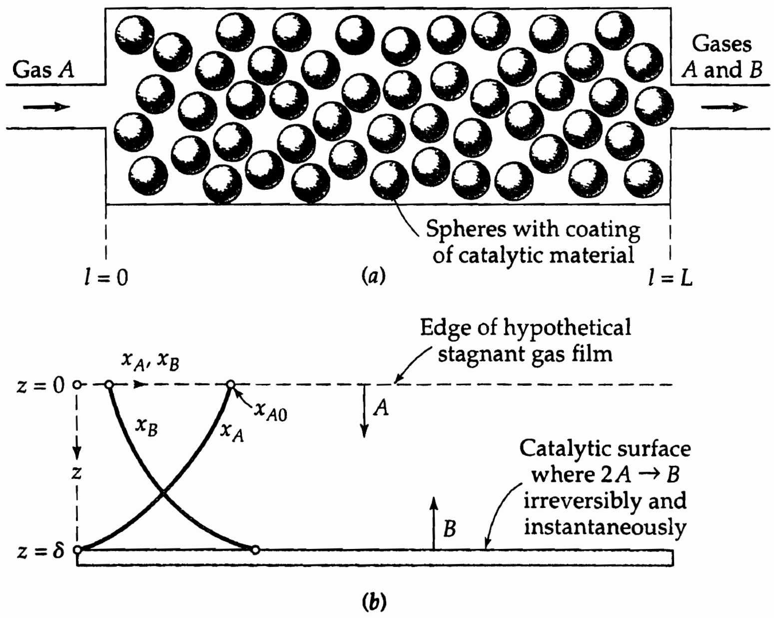
The mole fraction of component B can be obtained: $x_B = 1 - x_A$

The flux of component A, recall:

$$N_A = -\frac{c D_{AB}}{1-x_A}\frac{dx_A}{dz} = C_1 = c D_{AB} C_1'$$

$$= \frac{c D_{AB}}{z_2-z_1} \ln\left(\frac{1-x_{A1}}{1-x_{A2}}\right) \left(\begin{array}{c}\text{constant} \\ \text{independent} \\ \text{of } z\end{array}\right)$$

Example 2 Diffusion with Hetrogeneous Reaction.



Consider the case of hetrogeous raction of component A at the suface of a catalyst to produce component B according to the following stoichiometry

$$2A \longrightarrow B$$

2 moles of A reacting $\Rightarrow$ 1 mole of B produced

$\Rightarrow \quad N_B = -\frac{1}{2} N_A$ Note $-$ve sign because diffusion of B in opposite direction.

$$\Rightarrow \quad N_A = -cD_{AB}\frac{dx_A}{dz} + x_A(N_A + N_B)$$

$$= -cD_{AB}\frac{dx_A}{dz} + \frac{1}{2}x_A N_A$$

$$\Rightarrow N_A = - \frac{c D_{AB}}{1-\frac{1}{2}x_A} \frac{dx_A}{dz}$$

Component A diffuses through a stagnent gas film. Mass balance along diffusion path yields:

$$\frac{d N_{Az}}{dz} = 0$$

$$\Rightarrow \frac{d}{dz}\left(\frac{c D_{AB}}{1-\frac{1}{2}x_A} \frac{dx_A}{dz}\right) = 0 .$$

integrating twice:

$$-2 \ln\left(1-\frac{1}{2}x_A\right) = c_1 z + c_2$$

BC's

$z = 0 \qquad x_A = x_{A0}$

$z = \delta \qquad x_A = 0 \leftarrow$ (assuming A is completely consumed)

Note: if reaction is slow: $N_A\big|_{z=\delta} = k_s C_A\big|_{z=\delta} = k_s C x_A\big|_\delta$

$$\Rightarrow c_2 = -2 \ln\left(1-\frac{1}{2}x_{A0}\right)$$

$$c_1 = -c_2/\delta$$

$$\Rightarrow -2 \ln\left(1-\frac{1}{2}x_A\right) = +2 \ln\left(1-\frac{1}{2}x_{A0}\right)\frac{z}{\delta} - 2\ln\left(1-\frac{1}{2}x_{A0}\right)$$

$$\ln\left(1-\tfrac{1}{2}x_A\right) = \ln\left(1-\tfrac{1}{2}x_{A0}\right)\left(1-\frac{z}{\delta}\right)$$

$$1-\tfrac{1}{2}x_A = \left(1-\tfrac{1}{2}x_{A0}\right)^{1-\frac{z}{\delta}}.$$

$$x_A = 2 - 2\left(1-\tfrac{1}{2}x_{A0}\right)^{1-\frac{z}{\delta}}.$$

Flux of A $\quad N_A = -\dfrac{C D_{AB}}{1-\frac{1}{2}x_A}\dfrac{dx_A}{dz} = -C D_{AB}\, C_1$

$$= \frac{-C D_{AB}}{\delta}\, 2 \ln\left(1-\tfrac{1}{2}x_{A0}\right)$$

$$N_A = \frac{2 C D_{AB}}{\delta} \ln\left(\frac{1}{1-\frac{1}{2}x_{A0}}\right)$$

Example 3 Diffusion with homogeneous Reaction

Consider the diffusion and reaction:

$$A + B \longrightarrow AB$$

According to the following pseudo-first-order reaction $-r_A = k_1''' C_A$ (mole/m$^3 \cdot$s)

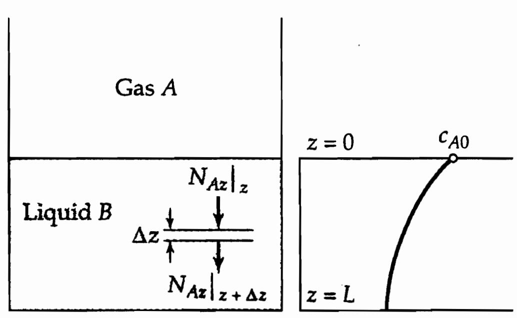
in this case the concentration of A is small to that of B. $\Rightarrow N_A = -c D_{AB} \frac{dx_A}{dz}$

$$= -D_{AB} \frac{dC_A}{dz}$$

mass balance along diffusion path:

$$S N_A\big|_z - S N_A\big|_{z+\Delta z} - k_1''' C_A S \Delta z = 0.$$

$$\Rightarrow \frac{dN_A}{dz} + k_1''' C_A = 0.$$



Substitution of flux into mass ~~bo~~ balance: (10)

$$D_{AB} \frac{d^2 C_A}{dz^2} - k_1''' C_A = 0$$

$z = 0$ $\quad C_A = C_{A0}$

$z = L$ $\quad N_A = 0 \Rightarrow \frac{dC_A}{dz} = 0$

non-dimensionalization:

$$\xi = \frac{z}{L} \qquad \mu = \frac{C_A}{C_{A0}} \qquad \phi^2 = \frac{L^2 k_1'''}{D_{AB}}$$

$$\Rightarrow \frac{d^2\mu}{d\xi^2} - \phi^2 \mu = 0.$$

ϕ is known as Hatta number

$\xi = 0 \quad \mu = 1$

$\xi = 1 \quad \frac{d\mu}{d\xi} = 0.$

$$\mu = C_1 \cosh(\phi\xi) + C_2 \sinh(\phi\xi)$$ see appendix C

$BC1 \Rightarrow 1 = C_1$

$BC2 \Rightarrow 0 = \phi C_1 \sinh(\phi) + C_2 \phi \cosh(\phi)$

$\Rightarrow C_2 = -\tanh(\phi)$

$$\Rightarrow \mu = \cosh(\phi\xi) - \tanh(\phi) \sinh(\phi\xi)$$

$$\bar{\psi} = \frac{C_{A\,avg}}{C_{A0}} = \frac{\int_0^L \psi \, dz}{\int_0^L dz}.$$

$$= \int_0^1 \psi \, d\xi = \frac{1}{\phi} \sinh(\phi) - \tanh(\phi) \frac{1}{\phi} \left[\cosh(\phi) - 1\right].$$

$$= \cancel{\frac{1}{\phi} \sinh(\phi)} - \frac{1}{\phi} \cancel{\tanh(\phi) \cosh(\phi)} + \frac{1}{\phi} \tanh(\phi)$$

$$= \frac{\tanh(\phi)}{\phi}$$

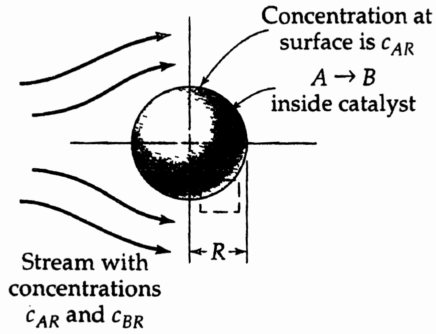
Total flux $\quad N_A\big|_{z=0} = -D_A \frac{dC_A}{dz}\Big|_{z=0}.$

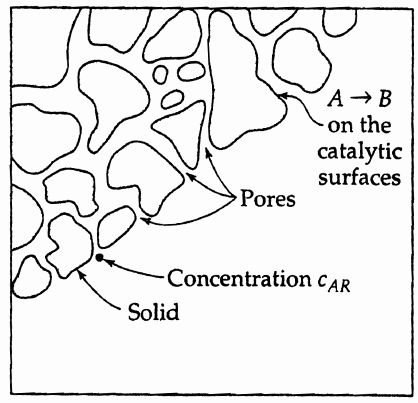
$$= \frac{-D_A C_{A0}}{L} \frac{d\psi}{d\xi}\Big|_{\xi=0}.$$

$$N_A\big|_{z=0} = -\frac{D_A C_{A0}}{L} \left[\phi \sinh(\phi\, 0) - \tanh\phi \; \phi \cosh(\phi\, 0)\right]$$

$$= \frac{D_A C_{A0}}{L} \phi \tanh(\phi)$$

Example 4 Diffusion and Reaction Inside Porous Catalyst.





mass balance on shperical shell :

$$N_{Ar}\Big|_r \cancel{4\pi} r^2 - N_{Ar}\Big|_{r+\Delta r} \cancel{4\pi} (r+\Delta r)^2 -$$

$$k_1'' a \, C_A \quad \cancel{4\pi} r^2 \Delta r = 0$$

$\uparrow$
area/volume of catalyst.

Note $\Delta r^2 \simeq 0$.

deriding by Δr and taking $\lim_{\Delta r \to 0}$

$$-\frac{d}{dr}\left(r^2 N_A\right) - r^2 k_1'' a \, C_A = 0 .$$

for diffusion in solids $N_A = -D_A \frac{dC_A}{dr}$.

$$\Rightarrow \frac{D_A}{r^2} \frac{d}{dr}\left(r^2 \frac{dC_A}{dr}\right) - k_1'' a \, C_A = 0 .$$

$r = 0 \quad \frac{dC_A}{dr} = 0$

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

$$\frac{C_A}{C_{AR}} = \left(\frac{R}{r}\right) \frac{\sinh\left[\sqrt{k_1'' a/D_A}\, r\right]}{\sinh\left[\sqrt{k_1 a/D_A}\, R\right]} \qquad (C.1\text{-}6a)$$

Total molar flow $W_{AR} = 4\pi R^2 N_A|_{r=R}$.

$$W_{AR} = -4\pi R^2 D_A \left.\frac{dC_A}{dr}\right|_{r=R}.$$

$$= 4\pi R D_A C_{AR}\left(1 - \sqrt{\frac{k_1'' a}{D_A}} \coth \sqrt{\frac{k_1'' a}{D_A}}\, R\right)$$

Maximum molar flow (when catalyst is all exposed to gas A)

$$W_{AR0} = \frac{4}{3}\pi R^3 a \left(-k C_{AR}\right)$$

Effectiveness Factor $\eta = \frac{W_{AR}}{W_{AR0}}$

$$\eta = \frac{3}{\phi^2}\left(\phi \coth\phi - 1\right)$$

where $\phi = \sqrt{\frac{k_1'' a}{D_A}}\, R$ Thiele Modulus