CM3120 F. MORRISON 1

Exam 3

31 MAR 2021

Solution

1. Mass transfer of species A only happens if there is both a source of species A and a sink; that is species A that is free to move (source) + a place for it to "disappear" into (sink). If there is no sink, the species will not move (diffuse).

2) Oxygen (A) O_2

Carbon dioxide (B) CO_2

1D - z dir

steady

$\underline{U}^* = 0$

EMCD $N_A = -N_B$

$$\longrightarrow z$$

a) Fick's Law

$$N_{Az} = x_A \underbrace{(N_{Az} + N_{Bz})}_{\substack{=0 \\ \text{(EMCD)}}} - c\mathcal{D}_{AB} \frac{dx_A}{dz}$$

a)

$$N_{Az} = -c\mathcal{D}_{AB} \frac{dx_A}{dz}$$

flux of species A

$[=] \dfrac{\text{moles } A}{\text{area} \cdot \text{time}}$

concentration (A mole fraction) gradient

Diffusion coef

$c = \dfrac{\text{moles mix}}{\text{volume mix}}$

b need to measure
1. $\frac{dX_A}{dz} = \frac{\Delta X_A}{\Delta z}$
2. N_{Az}
3. $\underbrace{c = \frac{n}{V} = \frac{P}{RT}}_{\text{ideal gas, need } P, T}$

3) AIR + WATER MIXTURE

$P_{A,water} = 2.137 \text{ kPa}$

$T = 25.0°C$

$P = 1.00 \text{atm} = 101.325 \text{ kPa}$

$PV = nRT$

$PX_A = P_A$ (definition of partial pressure) (ideal gas)

$\Rightarrow X_A = \frac{P_A}{P} = \frac{2.137 \text{ kPa}}{101.325 \text{ kPA}}$

$X_A = 0.0210906$

$\boxed{X_A = 0.0211}$

3 SIG FIGS
(2 accepted)

b) is the humid air saturated?

ANS: if saturated $p_A = y_A P = p^*$

← vapor pressure of water (steam tables)

$T = 25.0°C$

$p^* = 3.169\ kPa$

but $p_A = 2.137\ kPa$

this is less that p^*

$\Rightarrow$ not saturated

4.) binary mixture, A + B

$T = 310\,K$

$P = 101.325\,kPa$

mixture of A (He) $\quad X_A = 1.1 \times 10^{-2}$

B (N_2) $\quad X_B = 1 - X_A$

$\quad = 0.989$

Ideal gases

steady diffusion

$V_A = 1.34 \times 10^{-4}\ \frac{m}{s}$

$\longrightarrow z$

$V_B = -0.87 \times 10^{-5}\ \frac{m}{s}$

a) calc $V^* = X_A V_A + X_B V_B$

$$= (1.1 \times 10^{-2})(1.34 \times 10^{-4})\frac{m}{s} + (0.989)(-0.87 \times 10^{-5})\frac{m}{s}$$

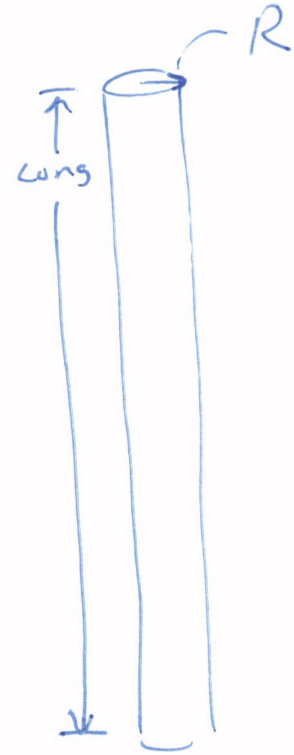
$$= -7.13030 \times 10^{-6}\ \frac{m}{s}$$

$$\boxed{V^* = -7.1 \times 10^{-6}\ \frac{m}{s}}$$ 2 sig figs (mole frac)

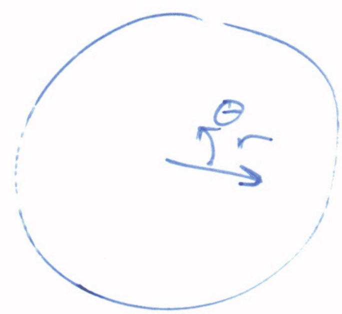
b) $C = \frac{n}{V} = \frac{P}{RT} = \frac{(101.325\,\cancel{kPa})\left(\frac{10^3\,Pa}{\cancel{kPa}}\right)}{\left(8.314\ \frac{\cancel{Pa}\,m^3}{mol\,\cancel{K}}\right)(310\,\cancel{K})}$

$C = 3.931378 \times 10^{1}\ \frac{mol}{m^3} = \boxed{39.3\ \frac{mol}{m^3}}$ 2 or 3 S.F. accepted

5.) Benzoic acid
Water



water water



steady
slow diffusion

$x_A(r, \theta, z) = ?$

Since we want to determine concentration distribution, we must use:

a

$\boxed{\text{microscopic species A mass balance (step 1)}}$

This is followed by (step 2)

$\boxed{\text{Fick's Law of diffusion}}$

b) The calculation domain is the water around the rod:

$$R \le r \le \infty \quad \text{or} \quad R \le r \le \delta$$

BC: assume the water is saturated with benzoic acid at $r=R$:

$r = R$

$x_A = x_A^*$ ← saturated solution at T (liquid phase)

c) Calc $x_A(r)$

$$\underline{N}_A = \begin{pmatrix} N_{Ar} \\ \cancel{N_{A\theta}} \\ \cancel{N_{Az}} \end{pmatrix}$$ } assume 1D diffusion in r-direction

$N_B = 0$ stagnant B

"slash + burn" ⟶

The **Equation of Species Mass Balance in Terms of Combined Molar quantities** in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B.

The general case, where the combined molar flux with respect to molar velocity ($\underline{N}_A$), is given on page 1.

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In terms of total molar flux, $\underline{N}_A$

Microscopic species mass balance, in terms of molar flux; Gibbs notation

$$\frac{\partial c_A}{\partial t} = -\nabla \cdot \underline{N}_A + R_A$$

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Microscopic species mass balance, in terms of combined molar flux; Cartesian coordinates

STEP 1

$$\frac{\partial c_A}{\partial t} = -\left(\frac{\partial N_{A,x}}{\partial x} + \frac{\partial N_{A,y}}{\partial y} + \frac{\partial N_{A,z}}{\partial z}\right) + R_A$$

Microscopic species mass balance, in terms of combined molar flux; cylindrical coordinates

steady

$$\cancel{\frac{\partial c_A}{\partial t}} = -\left(\frac{1}{r}\frac{\partial (rN_{A,r})}{\partial r} + \cancel{\frac{1}{r}\frac{\partial N_{A,\theta}}{\partial \theta}} + \cancel{\frac{\partial N_{A,z}}{\partial z}}\right) + \cancel{R_A}$$

no homogeneous rxn

Microscopic species mass balance, in terms of combined molar flux; spherical coordinates

one-dimensional radial diffusion

$$\frac{\partial c_A}{\partial t} = -\left(\frac{1}{r^2}\frac{\partial (r^2 N_{A,r})}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial (N_{A,\theta}\sin\theta)}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial N_{A,\phi}}{\partial \phi}\right) + R_A$$

Fick's law of diffusion, Gibbs notation: $\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$

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STEP 2

$$= c_A\underline{v}^* - cD_{AB}\nabla x_A$$

Fick's law of diffusion, Cartesian coordinates:

$$\begin{pmatrix} N_{A,x} \\ N_{A,y} \\ N_{A,z} \end{pmatrix}_{xyz} = \begin{pmatrix} x_A(N_{A,x} + N_{B,x}) - cD_{AB}\frac{\partial x_A}{\partial x} \\ x_A(N_{A,y} + N_{B,y}) - cD_{AB}\frac{\partial x_A}{\partial y} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB}\frac{\partial x_A}{\partial z} \end{pmatrix}_{xyz}$$

stagnant

Fick's law of diffusion, cylindrical coordinates:

$$\begin{pmatrix} N_{A,r} \\ \cancel{N_{A,\theta}} \\ \cancel{N_{A,z}} \end{pmatrix}_{r\theta z} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB}\frac{\partial x_A}{\partial r} \\ x_A(\cancel{N_{A,\theta}} + \cancel{N_{B,\theta}}) - \cancel{\frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta}} \\ x_A(\cancel{N_{A,z}} + \cancel{N_{B,z}}) - cD_{AB}\cancel{\frac{\partial x_A}{\partial z}} \end{pmatrix}_{r\theta z}$$

assume 1D radial

Fick's law of diffusion, spherical coordinates:

$$\begin{pmatrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,\phi} \end{pmatrix}_{r\theta\phi} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB}\frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,\phi} + N_{B,\phi}) - \frac{cD_{AB}}{r\sin\theta}\frac{\partial x_A}{\partial \phi} \end{pmatrix}_{r\theta\phi}$$

microscopic species A mass balance:

$$0 = \cancel{-\frac{1}{r}} \frac{d}{dr}\underbrace{\left(r N_{A,r}\right)}_{\equiv \Phi}$$

$$\frac{d\Phi}{dr} = 0$$ integrate:

$$r N_{Ar} = \Phi = c_1$$

$$\boxed{N_{Ar} = \frac{c_1}{r}}$$

Fick's Law: (stagnant B)

$$N_{Ar} = x_A N_{Ar} - c D_{AB} \frac{dx_A}{dr}$$

$\frac{c_1}{r}$ $\Rightarrow$

$$N_{Ar}(1 - x_A) = -c D_{AB} \frac{dx_A}{dr}$$

$$\frac{dx_A}{(1 - x_A)} = \left(\frac{-c_1}{c D_{AB}}\right) \frac{1}{r}\, dr$$

Can we integrate?

D_{AB} = constant (assume)

c_1 = CONSTANT

c = ? if dilute, c = constant (assume dilute since diffusion is slow)

$$(-1)\int \frac{-dx_A}{1-x_A} = \left(-\frac{c_1}{cD_{AB}}\right)\frac{dr}{r}$$

$$\boxed{-\ln(1-x_A) = \left(-\frac{c_1}{cD_{AB}}\right)\ln r + c_2}$$

BC: $r = R$ $x_A = x_A^*$

$r = \delta$ $x_A = x_{A\delta}$ (given)

$$-\ln(1-x_A^*) = \left(-\frac{c_1}{cD_{AB}}\right)\ln R + c_2$$

$$-\ln(1-x_{A\delta}) = \left(-\frac{c_1}{cD_{AB}}\right)\ln \delta + c_2$$

$\overline{\overline{\text{mass stop line}}}$

Solve for c_1 & c_2:

subtract

$$\ln\left(\frac{1-x_{A\delta}}{1-x_A^*}\right) = \left(-\frac{c_1}{cD_{AB}}\right)\underbrace{(\ln R - \ln \delta)}_{\ln\frac{R}{\delta}}$$

$$\frac{\ln\left(\frac{1-x_{A\delta}}{1-x_A^*}\right)}{\ln\left(\frac{R}{\delta}\right)} = \left(-\frac{c_1}{cD_{AB}}\right)$$

$$\boxed{c_1 = -cD_{AB}\left(\frac{\ln\left(\frac{1-x_{A\delta}}{1-x_A^*}\right)}{\ln\left(\frac{R}{\delta}\right)}\right)}$$

note: $\boxed{N_{Az} = \frac{c_1}{r}}$

Substitute back to obtain C_2:

$$-\ln(1-x_A^*) = \left(\frac{\ln\left(\frac{1-x_{A\delta}}{1-x_A^*}\right)}{\ln\left(\frac{R}{\delta}\right)}\right)\ln R + C_2$$

$$-C_2 = \left(\frac{\ln\left(\frac{1-x_{A\delta}}{1-x_A^*}\right)}{\ln\left(\frac{R}{\delta}\right)}\right)\ln R + \ln(1-x_A^*)$$

Substitute back:

$$-\ln(1-x_A) = \left(\frac{\ln\left(\frac{1-x_{A\delta}}{1-x_A^*}\right)}{\ln\left(\ln\frac{R}{\delta}\right)}\right)(\ln r - \ln R)$$

$$-\ln(1-x_A^*)$$

$$\ln\left(\frac{1-x_A^*}{1-x_A}\right) = \left(\frac{\ln\left(\frac{1-x_{A\delta}}{1-x_A^*}\right)}{\ln\left(\frac{R}{\delta}\right)}\right)\ln\left(\frac{r}{R}\right)$$

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$$\boxed{\frac{\ln\left(\dfrac{1-X_A}{1-X_A^*}\right)}{\ln\left(\dfrac{1-X_A^*}{1-X_{A\delta}}\right)} = \frac{\ln\left(\dfrac{r}{R}\right)}{\ln\left(\dfrac{R}{\delta}\right)}}$$

check BC: $r=R \quad X=X_A^* \qquad 0=0$

$r=\delta \quad X=X_{A\delta}$

$-1=-1$ ✓

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