Contents

Short and MCQ's

1. Diffusion of the reactants and products within the pores of a solid catalyst; diffusion of moisture in a wet solid during drying; diffusion through a membrane; diffusion of a solute within a 'rigid' drop in liquid extraction; diffusion of an ionic species in an ion-exchange resin.
2. If the molecular weights of all the species in a mixture are equal.
3. (i) Concentration, (ii) length of the diffusion path, (vi) partial pressure are <u>scalar</u> quantities; others are <u>vectors</u>.
4. (i) ft^2/s ; (ii) $lbmol/ft^2 \cdot s$; (iii) $lbmol/(\cancel{ft}^3)\cdot(\cancel{ft})$
5. (i) If the bulk flow term is small, or (ii) for transport in a dilute solution.
6. Ideal gas mixture.
7. (a) Absorption of a solute from an inert (insoluble) carrier; (b) distillation, if the components have equal molar heats of vaporization.
8. Since $N_B = 0$, $N_A = N_A \cdot p_A/P - \frac{D_{AB}}{RT}\frac{dp_A}{dz} = \text{constant}$ $\begin{pmatrix} A \to \text{ethanol} \\ B \to \text{air} \end{pmatrix}$ p_A is maximum at the liquid surface $\Rightarrow$ contribution of the bulk flow term is the maximum at the liquid surface.
9. From Eq(2.19), $-\frac{dp_A}{dz} = N_A \cdot \frac{P-p_A}{P} \cdot \frac{RT}{D_{AB}}$. At $z=z_2$, $p_A=p_{A2}$ is the minimum and the <u>magnitude</u> of $\frac{dp_A}{dz}$ is <u>maximum</u>.
10. If the other two components are non-diffusing and these are present in the same volume ratio along the diffusion path.
11. Yes, by virtue of the <u>Cauchy's Mean Value Theorem</u>.
12. Compare the fluxes given by Eqs(2.27) and (2.30).

12 contd... $\dfrac{(N_A)_{\text{nondiffusing B}}}{(N_A)_{\text{equimolar counter...}}} = \dfrac{P}{p_{BM}} > 1$. Reason: molecules of B in counterdiffusion offer more 'resistance' to diffusion of A compared to the case when these are non-diffusing.

13. D_{AB} depends inversely with total pressure, P, since at a higher pressure there are more molecular collisions (less mean free path) offering more 'resistance' to diffusion. D_{AB} increases as $T^{3/2}$ to $T^{1.75}$, since a higher temperature means higher velocity or mobility of the molecules.

14. The flux will be very high and pseudosteady state assumption will not be applicable.

15. The diffusivity increases with T and decreases with μ.

16. (a) → (ii) zero; (b) → (i) $u > U$; (c) → (iii) multicomponent...; (d) → (i) -2; (e) → (i) $-78/94 = -0.83$; (f) → Diffusion vel., $v_{A,d}$ $= u_A - U = J_A/C_A = -\dfrac{D_{AB}}{C_A}\cdot\dfrac{dC_A}{dz} = -\dfrac{D_{AB}}{p_A}\cdot\dfrac{dp_A}{dz}$.

Equimolar counterdiffusion for $p_{A_1} = 0.3$ atm, $p_{A_2} = 0.1$ atm midway in the film, $p_A = 0.2$ atm; $\dfrac{dp_A}{dz} = \dfrac{0.1 - 0.3}{1}\,\dfrac{\text{atm}}{\text{cm}} = -0.2\,\dfrac{\text{atm}}{\text{cm}}$;

$$v_{A,d} = -\frac{0.2\ \text{cm}^2/\text{s}}{0.2\ \text{atm}}\cdot\left(-0.2\ \frac{\text{atm}}{\text{cm}}\right) = 0.2\ \text{cm/s} = \underline{2\ \text{mm/s}}\quad (i)$$

(g) $$N_A\left(\frac{P - p_A}{P}\right) = -\frac{D_{AB}}{RT}\cdot\frac{dp_A}{dz} \Longrightarrow \frac{(dp_A/dz)_1}{(dp_A/dz)_2} = \frac{(P - p_A)_1}{(P - p_A)_2}$$
$$= \frac{2 - (2)(0.1)}{2 - (2)(0)} = \frac{1.8}{2} = 0.9,\ \underline{(iii)}.$$

(h) $(dp_B/dz) = -(dp_A/dz) =$ constant everywhere (since $p_A + p_B = P$)
$= -(-7\ \text{atm/m}) = \underline{7\ \text{atm/m}\ (iii)}$

(i) After 10 hr, partial pressures of A and B in bulb1 are: $p_{A_1} = 0.5$ atm; $p_{B_1} = 0.5$ atm (Since half of A diffuses out).

16 (i) contd... Material balance of A: $V_1 \cdot \frac{1\,\text{atm}}{RT} = V_1 \cdot \frac{0.5\,\text{atm}}{RT} + V_2 \frac{p_{A2}}{RT}$.

$\Rightarrow p_{A2} = \frac{(V_1)(0.5)}{V_2} = \left(\frac{5}{10}\right)(0.5) = 0.25$ atm. [I → initial, II → after 10 hour]

$$\frac{(N_A)_I}{(N_A)_{II}} = \frac{(D_{AB}/RTl)(p_{A1}-p_{A2})_I}{(D_{AB}/RTl)\ (p_{A1}-p_{A2})_{II}} = \frac{1-0.0}{0.5-0.25} = \frac{1}{0.25} = \underline{\underline{4}}$$

(j) Equimolar counterdiffusion of A and B occurs. Since the area of diffusion is variable,

$$\pi r_1^2 \cdot (N_A)_I = \pi r_2^2 (-N_B)_{II} \Rightarrow (N_B)_{II} = -(r_1^2/r_2^2)\cdot(N_A)_I = -\left(\tfrac{1}{2}\right)^2 (10^{-6}\ \text{kmol/m}^2\text{s})$$

$= \underline{2.5\times10^{-7}\ \text{kmol/m}^2\text{s}}$ towards vessel 1

(k) → (ii). It is the geometric mean dia $= (1\times4)^{1/2} = \underline{2\text{ cm}}$

(l) → (ii). Since $\pi r^2 N_A$ = constant, N_A is the highest where the radius is the smallest.

(m) For equimolar counterdiffusion through a spherical film,

$4\pi r^2 N_A$ = constant, $N_A = -\frac{D_{AB}}{RT}\cdot\frac{dp_A}{dr} \Rightarrow 4\pi r^2\left(-\frac{D_{AB}}{RT}\frac{dp_A}{dr}\right) = W$

$$\Rightarrow -\int_{p_{A1}}^{p_{A2}} dp_A = \frac{W\cdot RT}{D_{AB}\cdot 4\pi}\int_{r_i}^{r_i+\delta}\frac{dr}{r^2} \Rightarrow p_{A1}-p_{A2} = \Delta p = \frac{WRT}{D_{AB}\,4\pi}\left(\frac{1}{r_i}-\frac{1}{r_i+\delta}\right)$$

$\Rightarrow$ Flux at $r = r_i$ is $(N_A)_I = \frac{W}{4\pi r_i^2} = \frac{D_{AB}}{RT}\cdot\frac{r_i+\delta}{r_i\cdot\delta}\cdot\Delta p_A$

For diffusion through a flat film of this thickness, $(N_A)_{II} = \frac{D_{AB}}{RT\cdot\delta}\cdot\Delta p_A$

$$\frac{(N_A)_I}{(N_A)_{II}} = 1.05\ \text{(given)} \Rightarrow \frac{r_i+\delta}{r_i} = 1.05 \Rightarrow \frac{\delta}{r_i} = 0.05 \Rightarrow \underline{\delta = 0.05\,r_i}$$

(n) → (i), because of spherical symmetry; (o) → (i); (p) → (iii), other values are out of range; (q) → (iii), other values are out of range; (r) → (iii) methanol, since it has the smallest molecular size among the three; (s) → (ii) largest molecular size/weight; (t) → (iii), since $D_{AB}P$ is constant for gas-phase diffusion; (u) → (i); use the relation $\frac{D_1\mu_1}{T_1} = \frac{D_2\mu_2}{T_2}$.

16(v) → (ii), 0·09 cm²/s, use the relation $D_{AB} \propto T^{1.5}/P$;
(w) → (ii), velocity of the interface, $\frac{dz}{dt} \propto \frac{1}{z}$, see Eq (2·51a);
(x) → (i), surface diffusion; (y) → (ii); (z) → (ii).

Problems

(2·1) Water vapor (A) diffuses through a stagnant film of air (B). Use Eq (2·26) to calculate the flux.

Water temp. = 23°C = 296 K, vapor pressure $p_{A0} = 13.8573 - \frac{5160.2}{296}$ $= \underline{0.0280}$ bar

Ambient air temp. = 27°C; $p^v_{A\ell} = 0.0353$ bar

R. Humidity of air = 65% ⇒ partial pressure of moisture in bulk air, $p_{A\ell} = (0.0353)(0.65) = \underline{0.023}$ bar.

Mean value of diffusivity of water vapor in the film $= (0.257 + 0.262)/2$ $= 0.2595$ cm²/s; mean film temperature $= (296 + 300)/2 = \underline{298}$ K.

Film thickness, $l = 3$ mm $= \underline{3 \times 10^{-3}}$ m; P = 1 atm = $\underline{1.013 \text{ bar}}$

Flux of water vapor at steady state, $N_A = \frac{D_{AB} \cdot P}{RTl} \cdot \ln \frac{P - p_{A\ell}}{P - p_{A0}}$

$$\Rightarrow N_A = \frac{(2.595 \times 10^{-5})(1.013)}{(0.08317)(298)(3 \times 10^{-3})} \ln \frac{1.013 - 0.023}{1.013 - 0.028} = 1.79 \times 10^{-6} \frac{\text{kmol}}{\text{m}^2\text{s}}$$

$= \underline{0.116 \text{ kg/m}^2\text{h}}$ = rate of evaporating water per m².
* * * *

(2·2) Use Eq (2·26). The flux of moisture is given, calculate film thickness.

Amount water evaporated per m² of surface in 10 days
= (20 mm)(1 m²) = 0·02 m³ = 20 kg = 20/18, or 1·111 kmol

$$\text{Flux} = \frac{1.111 \text{ kmol}}{(1\text{ m}^2)(10 \times 24 \times 3600\text{ s})} = \underline{1.286 \times 10^{-6}} \text{ kmol/m}^2\text{.s} = N_A$$

Given: $D_{AB} = 1$ ft²/h $= (30.48)^2/3600 \rightarrow 0.258$ cm²/s $= \underline{2.58 \times 10^{-5}}$ m²/s

P = 1·013 bar; R = $\underline{0.08317}$ m³·bar/kmol·K; T = 23°C = $\underline{296}$ K.

Humidity of bulk air = 0·0135 kg moisture/kg dry air.

(2.2) Cond... $y_{Al} = \frac{0.0135/18}{(0.0135/18)+(1/28.9)} = 0.0212$ [mol wt of air = 28.9]

$p_{Al} = P \cdot y_{Al} = (1.013)(0.0212) = 0.0215$ bar.

Vapor pressure of water at 296 K = 0.028 bar = p_{A0} ; $l = ?$
(from Antoine eq)

Substitute in Eq (2.26) → $1.286\times10^{-6} = \frac{(2.58\times10^{-5})(1.013)}{(0.08317)(296)(l)} \cdot \ln\frac{1.013-0.0215}{1.013-0.028}$

$\Rightarrow l = 5.4\times10^{-3}$ m = 5.4 mm = thickness of the air film

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(2.3) Temperature, T = 35°C = 308°C ; vapor press. of water $p_A^v = 0.0552$ bar

Relative humidity of bulk air = 30% $\Rightarrow p_{A0} = (0.0552)(0.3) = 0.01656$ bar

Partial pressure of moisture at the acid surface, $p_{Al} \approx 0$ (Since the acid has a high affinity for water)

Thickness of air film, $l = 1.2\times10^{-3}$ m

P = 1.013 bar

Moisture flux from Eq (2.26),

$D_{AB} = 0.257$ cm²/s at 23°C ; at 308 K, $D_{AB} = (0.257)(308/296)^{1.5} = 0.2728$ cm²/s

$N_A = \frac{(2.728\times10^{-5})(1.013)}{(0.08317)(308)(1.2\times10^{-3})} \cdot \ln\frac{1.013-0.01656}{1.013}$

$= 1.482\times10^{-6}$ kmol/m²·s $= 9.602\times10^{-2}$ kg/m²·h

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(2.4) Temperature, T = 300 K; total pressure = 400 mm Hg (= .533 bar); partial pressure of ammonia in the bulk (40% by volume) = (400)(0.4) = 160 mm Hg

Diffusivity of NH_3 at 1 atm and 333 K = 2.53×10^{-5} m²/s [Table 2.1].

Diffusivity at 400 mm pressure and 300 K $= (2.53\times10^{-5})\left(\frac{760}{400}\right)\left(\frac{300}{333}\right)^{1.5}$
$= 4.11\times10^{-5}$ m²/s ; P = 0.533 bar

$p_{Al} = 0$ at the acid surface; $l = 0.01$ m

$p_{A0} = 160$ mm Hg = 0.2133 bar

Flux of ammonia, $N_A = \frac{(4.11\times10^{-5})(0.533)}{(0.08317)(300)(0.01)} \ln\frac{0.533-0}{0.533-0.2133}$

$= 4.488\times10^{-5}$ kmol/m²s

(i) Rate of absorption of ammonia through an area, $a = 0.1$ m²
$= (4.488\times10^{-5})(0.1) = 4.488\times10^{-6}$ kmol/s

(ii) In order to calculate the partial pressure gradient at

(2.4) contd... a point in the film, calculate the partial pressure of the species at the particular point using Eq.(2.28); and then calculate the gradient, (dp_A/dz), using the Fick's law, Eq.(2.24).

The given point is 4 mm from the acid surface $\Rightarrow \underline{z} = 10 - 4 = 6\text{ mm} = \underline{6\times10^{-3}\text{ m}}$.

Put the values in Eq(2.28) $\rightarrow$ $$4.488\times10^{-5} = \frac{(4.11\times10^{-5})(0.533)}{(0.08317)(300)(0.006)} \ln \frac{0.533 - p_A}{0.533 - 0.2133}$$

$\Rightarrow \underline{p_A = 0.0985\text{ bar}}$

From Eq (2.24),
$$4.488\times10^{-5}\left(1 - \frac{0.0985}{0.533}\right) = -\frac{(4.11\times10^{-5})}{(0.08317)(300)} \cdot \frac{dp_A}{dz}$$

$$\Rightarrow \frac{dp_A}{dz} = \underline{-22.2\text{ bar/m}}$$

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(iii) <u>Acid-side end of the film</u> $\rightarrow z = 0.01\text{ m};\ p_A = 0$

Contribution of 'bulk flow' to the flux [see Eq(2.15)] ; $\boxed{N_B = 0}$

$$= (N_A + N_B)\,C_A/C = N_A \cdot p_A/P = (4.488\times10^{-5})\left(\frac{0}{0.533}\right) = \underline{0}$$

Contribution of the diffusion term $= N_A - N_A \cdot p_A/P = \underline{4.488\times10^{-5}\ \frac{\text{kmol}}{\text{m}^2\text{s}}}$

[i.e. there is no contribution of the bulk flow term at $z = 0.01\text{ m}$]

<u>Gas-side end of the film</u> $\rightarrow \underline{z = 0}$; $\underline{p_A = 0.2133\text{ bar}}$

Contribution of the bulk flow term $= N_A \cdot p_A/P = (4.488\times10^{-5})\left(\frac{0.2133}{0.533}\right)$

$= \underline{1.796\times10^{-5}}\ \text{kmol/m}^2\text{s}$

Contribution of the diffusion term to the flux $= 4.488\times10^{-5} - 1.796\times10^{-5}$

$= \underline{2.692\times10^{-5}\ \text{kmol/m}^2\text{s}}$.

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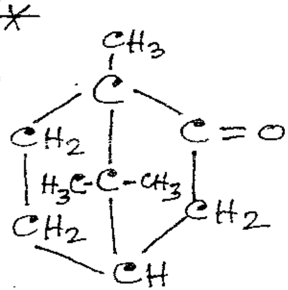
(2.5) <u>Estimation of diffusivity of camphor</u>, $\underline{C_{10}H_{16}O}$ (A)



Camphor

'Diffusion volume', see Table 7.4

10 Carbons $\rightarrow (10)(16.5) = 165$

16 hydrogen atoms $\rightarrow (16)(1.98) = 31.68$

1 oxygen atom $\longrightarrow 5.48$

Total, $(\Sigma v)_A = 165 + 31.68 + 5.48 = \underline{202.16}$

For air, $(\Sigma v)_B = 20.1$; $M_A = \underline{152.13}$; $M_B = \underline{28.9}$; $T = \underline{293\text{K}}$; $\underline{P = 1.013\text{ bar}}$

$$\text{Eq.}(2.57) \rightarrow D_{AB} = \frac{(1.0133\times10^{-7})(293)^{1.75}}{(1.013)\left[(202.16)^{1/3} + (20.1)^{1/3}\right]} \cdot \left[\frac{1}{152.13} + \frac{1}{28.9}\right]^{1/2} = \underline{5.644\times10^{-6}\ \frac{\text{m}^2}{\text{s}}}$$

(2·5) contd... Eq (2·26), $\text{flux} = \dfrac{(5.644\times10^{-6})(1.013)}{(0.08317)(293)(0.12)} \ln\dfrac{1.013-0}{1.013-0.13} = \underline{2.685\times10^{-7}\ \frac{\text{kmol}}{m^2.s}}$

$\boxed{l = 0.12\,m;\ p_{A0} = 97.5\,\text{mm Hg} = 0.13\,\text{bar},\ p_{Al} = 0}$

of camphor in the tube = 0.4 gm $= \dfrac{0.4}{(1000)(152.13)} = \underline{2.63\times10^{-6}}$ kmol $= m_A$

Area of the tube $= \dfrac{\pi}{4}(0.015)^2 = \underline{1.767\times10^{-4}}\ m^2 = a$

$N_A\cdot a\cdot t = m_A = 2.63\times10^{-6} \Rightarrow t = \dfrac{2.63\times10^{-6}}{(2.685\times10^{-7})(1.767\times10^{-4})}\ s = \underline{\underline{15.4\ hr}}$

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(2·6) For diffusion of A through non-diffusing B at steady state in the spherical geometry, we write the following equation [see Eq(2.73)].

$-\dfrac{dp_A}{P-p_A} = \dfrac{WRT}{4\pi D_{AB}P}\cdot\dfrac{dr}{r^2}$; $W = 4\pi r^2\cdot N_A$ = constant rate of transport at steady state.

Integrate from $r = r_i$; $p_A = p_{Ai}$ to $r = r_o = r_i + \delta$, $p_A = p_{A0}$ and simplify.

$W = \dfrac{4\pi D_{AB}P}{RT\,\delta}\cdot r_i(r_i+\delta)\cdot\ln\dfrac{P-p_{A0}}{P-p_{Ai}}$ ...(i)

$= \dfrac{(4)(\pi)(1.744\times10^{-5})(1.013)(0.0035)(0.0035+0.0035)}{(0.0821)(313)(0.0035)}\times$

$\times \ln\dfrac{1-0.3}{1-0} = \underline{-2.13\times10^{-8}}\ \dfrac{\text{kmol}}{s}$

$T = 40^\circ C = 313\,K$; $p_{A0} = \underline{0.3\ \text{atm}}$

D_{AB} at 313K, 1atm

$= (1.62\times10^{-5})\left(\dfrac{313}{298}\right)^{1.5} = \underline{1.744\times10^{-5}}\ \dfrac{m^2}{s}$

$p_{Ai} = \underline{0}$; $\delta = \underline{0.0035\,m}$;

$r_i = 7/2\ \text{mm} = \underline{0.0035\,m}$

Flux of CO_2 midway in the film :

Midway in the film, $r_m = r_i + \delta/2 = 0.0035 + 0.0035/2 = \underline{0.00525\,m}$

$4\pi r^2 N_A = W = 2.13\times10^{-8}$ kmol/s (constant). Put $r = 0.00525$ m to get

N_A (midway in the film) $= \dfrac{-2.13\times10^{-8}}{4\pi\,(0.00525)^2} = \underline{-6.15\times10^{-5}\ \text{kmol}/m^2.s}$

This means that diffusion occurs towards decreasing r, i.e. towards the pellet.

'Diffusion velocity' at $r_m = 0.00525\,m$:

Eq.(2.18) is to be used. (i) Calculate p_A from Eq (i) above written for $r = r_m$, (ii) calculate dp_A/dz from the expression for Fick's law, Eq(2.19).

Eq (i) above written for $r = r_m$ and $p = p_A$ is

$W = \dfrac{4\pi D_{AB}P}{RT\,(\delta/2)}\cdot(r_i)(r_m)\cdot\ln\dfrac{P-p_A}{P-p_{Ai}}$ — (ii). Equate (i) and (ii) to get

$2r_m \ln\dfrac{P-p_A}{P-p_{Ai}} = (r_i+\delta)\ln\dfrac{P-p_{A0}}{P-p_{Ai}}$.

$\Rightarrow (2)(0.00525)\ln\dfrac{1-p_A}{1-0} = (0.007)\ln\dfrac{1-0.3}{1-0} \Rightarrow p_A = \underline{0.2116\ \text{atm}}$, midway in the film.

(2.6) contd... Eq (2.19) $\rightarrow$ $N_A = (N_A + \cancel{N_B}^{0}) \cdot \frac{p_A}{P} - \frac{D_{AB}}{RT}\frac{dp_A}{dr}$

$$\Rightarrow (-6.15 \times 10^{-5})\left(1 - \frac{0.2}{1.0}\right) = -\frac{D_{AB}}{RT} \cdot \frac{dp_A}{dr} = \underline{-4.848 \times 10^{-5} \text{ kmol/m}^2\text{s}}$$

Diffusion velocity [Eq (2.18)] $\rightarrow$ $v_{A,d} = -\frac{D_{AB}}{C_A} \cdot \frac{dC_A}{dr}$

$$\Rightarrow v_{A,d} = -\frac{D_{AB}}{p_A} \cdot \frac{dp_A}{dr} = (-4.848 \times 10^{-5})\left(\frac{(0.0821)(313)}{0.2116}\right) = \underline{-5.9 \times 10^{-3}} \text{ m/s}$$

$\Rightarrow$ The diffusion velocity (5.9 mm/s) is directed towards the pellet, i.e. in the direction of decreasing r.

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(2.7) $N_2 \rightarrow A$; $CO_2 \rightarrow B$; $P = 1.013$ bar

$p_{A1} = 10^4$ Pa $= 0.1$ bar ; $p_{A2} = 0.8$ bar ;

$p_{B1} = 0.913$ bar ; $p_{B2} = 0.213$ bar ; $\underline{l = 0.06 \text{ m}}$

Equimolar counterdiffusion occurs at steady state.

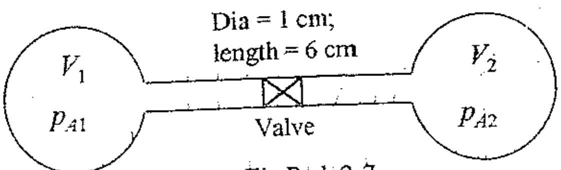


Fig Prob 2.7

(i) Use Eq (2.30) to calculate the flux. Since the vessels are 'large', the partial pressures remain virtually unchanged.

Flux of N_2 (A) $= \frac{D_{AB}}{RTl}(p_{A1} - p_{A2})$; $D_{AB} = 1.69 \times 10^{-5}$ m²/s, calculated from the value at 298 K, Table 2.1.

$$\Rightarrow N_A = \frac{(1.69 \times 10^{-5})}{(0.08317)(303)(0.06)} \cdot (0.1 - 0.8) = \underline{-7.824 \times 10^{-6}} \text{ kmol/m}^2\text{s}$$

(The flux is negative, diffusion occurs from $\underline{\text{vessel 2 to 1}}$)

Velocity of the molecules of species A w.r.t. a stationary observer is $u_A = N_A / C_A$. At vessel 1 end of the tube, $C_{A1} = p_{A1}/RT = \frac{0.1}{(0.08317)(303)}$

$$u_{A1} = \frac{-7.824 \times 10^{-6}}{(0.1)/(0.08317)(303)} = \underline{-0.00197} \text{ m/s}.$$

Similarly, $u_{A2} = \frac{-7.824 \times 10^{-6}}{(0.8)/(0.08317)(303)} = \underline{-2.46 \times 10^{-4}} \text{ m/s}$

Average velocity of the nitrogen molecules $= -\frac{1.97 \times 10^{-3} + 2.46 \times 10^{-4}}{2} = \underline{1.108 \times 10^{-3} \frac{\text{m}}{\text{s}}}$

$\Rightarrow$ velocity of the observer, $u_0 = -1.108 \times 10^{-3}$ m/s

Molar flux of N_2 w.r.t. the observer moving with the above velocity,

$$= (u_A - u_0) C_A = u_A C_A - u_0 C_A = N_A - (-1.108 \times 10^{-3})(p_A / RT)$$

Since the partial pressure is linear in distance for equimolar counterdiffusion, (2.7) contd... $p_A = (p_{A1} + p_{A2})/2 = (0.1 + 0.8)/2 = 0.45$ bar, midway in the tube.

Required flux $= -7.824\times10^{-6} + (1.108\times10^{-3})\left[\dfrac{0.45}{(0.08317)(303)}\right] = \underline{1.19\times10^{-5}\ \dfrac{\text{kmol}}{\text{m}^2\cdot\text{s}}}$

This flux occurs in the direction of vessel 1 → vessel 2.

(ii) To calculate the rate of transport through a tapered tube, (compare, Fig 2.9) use Eq (2.79), $(\pi r^2 N_A) = W = \dfrac{\pi D_{AB}}{RT}\cdot\dfrac{r_1 r_2}{l}(p_{A1} - p_{A2})$

Given; $r_1 = 0.005\,m$, $r_2 = 0.01\,m$. $W = \dfrac{(\pi)(1.69\times10^{-5})}{(0.08317)(303)}\cdot\dfrac{(0.005)(0.01)}{0.06}\cdot(0.1-0.8)$

$= \underline{-1.229\times10^{-9}\ \text{kmol/s}}$

(from vessel 2 to 1, in reality)

(iii) From the above equation it appears that the rate of transport does not change if the tube is reversely fitted.

(iv) The theoretical approach of Section 2.5.1 applies. Start with Eq. (2.49) and integrate from $t=0$, $p_{A10} - p_{A20}$ to $t = t$, $p'_{A1} - p'_{A2}$ $\Rightarrow \ln\dfrac{p_{A10} - p_{A20}}{p'_{A1} - p'_{A2}} = \dfrac{a\cdot D_{AB}}{l}\left(\dfrac{1}{V_1} + \dfrac{1}{V_2}\right)\cdot t \cdots$ (i)

$p_{A10} = \underline{0.1\ \text{bar}}$; $p_{A20} = \underline{0.8\ \text{bar}}$; $a = \frac{\pi}{4}(0.01)^2 = \underline{7.853\times10^{-5}}\,m^2$;

$p'_{A1} = 2p_{A0}$ (given) $\Rightarrow p'_{A1} = \underline{0.2\ \text{bar}}$; $V_1 = \underline{0.005\,m^3}$; $V_2 = \underline{0.003\,m^3}$.

Obtain p'_{A2} by material balance.

$V_1 C_{A10} + V_2 C_{A20} = V_1 C'_{A1} + V_2 C'_{A2} \Rightarrow V_1 p_{A10} + V_2 p_{A20} = V_1 p'_{A1} + V_2 p'_{A2}$

$\Rightarrow (0.005)(0.1) + (0.003)(0.8) = (0.005)(0.2) + (0.003)(p'_{A2}) \Rightarrow p'_{A2} = \underline{0.633\ \text{bar}}$

$$\Rightarrow \ln\frac{0.1-0.8}{0.2-0.633} = \frac{(7.853\times10^{-5})(1.6\_\times10^{-5})}{0.06}\cdot\left(\frac{1}{0.005} + \frac{1}{0.003}\right)\cdot t$$

$\Rightarrow\ t = \underline{11.3}$ hr

<u>Partial pressure of N_2 midway</u> in the connecting tube after $\underline{\underline{20\ hr}}$

Put the values in the above equation (i) to get

$$\ln\frac{0.1-0.8}{p_{A1f} - p_{A2f}} = \frac{(7.853\times10^{-5})(1.69\times10^{-5})}{0.06}\cdot\left(\frac{1}{0.005} + \frac{1}{0.003}\right)\cdot(20\times3600)$$

$\Rightarrow \ln\dfrac{-0.7}{p_{A1f} - p_{A2f}} = 0.85 \Rightarrow (p_{A1f} - p_{A2f}) = \underline{-0.3\ \text{bar}} \cdots$ (ii)

p_{A1f} and p_{A2f} are also related by material balance.

(2.7) Contd... $(0.005)(0.1)+(0.003)(0.8) = (0.005)(p_{A1f})+(0.003)(p_{A2f})$

$\Longrightarrow 5p_{A1f}+3p_{A2f} = 2.9 \quad \cdots \quad \text{(iii)}$

Solve eqs. (ii) and (iii) to get $p_{A1f} = 0.2502$ bar, $p_{A2f} = 0.5496$ bar

Partial pressure of N_2 midway in the tube at $t = 20$ hr,

$$(p_A)_{av} = (0.2502+0.5496)/2 = \underline{0.4 \text{ bar}}$$

* * * *

(2.8) Partial pressures of A and B in the bulk → p_{A0}, p_{B0}; those at the catalyst surface$_{(z=\delta)}$ → $p_{A\delta}$, $p_{B\delta}$; $p_{A\delta}=0$. Also $\underline{P = p_{A0}+p_{B0}}$.

(a) Reaction: $A \rightarrow B$. $N_A = -N_B$ at steady state. Use Eq (2.19).

$$N_A = (N_A+N_B)\frac{p_A}{P} - \frac{D_{AB}}{RT}\frac{dp_A}{dz} \Longrightarrow N_A\int_0^\delta dz = -\frac{D_{AB}}{RT}\int_{p_{A0}}^{p_{A\delta}=0} dp_A$$

$$\Longrightarrow N_A = \frac{D_{AB}}{RT\delta}\cdot p_{A0} \Longrightarrow \text{Reaction rate of A per unit area} = \underline{N_A = \frac{D_{AB}}{RT\delta}\cdot(P-p_{B0})}$$

(b) Reaction: $2A \rightarrow B \Longrightarrow N_A = -2N_B$ at steady state. From Eq (2.19),

$$N_A = (N_A - N_A/2)\frac{p_A}{P} - \frac{D_{AB}}{RT}\frac{dp_A}{dz} \Longrightarrow N_A\cdot\int_0^\delta dz = -\frac{2D_{AB}P}{RT}\int_{p_{A0}}^{0}\frac{dp_A}{2P-p_A}$$

$$\Longrightarrow N_A = \frac{2D_{AB}P}{RT\delta}\ln\frac{2P}{2P-p_{A0}} \Longrightarrow \text{Rate of reaction, } \underline{N_A = \frac{2D_{AB}P}{RT\delta}\ln\frac{2P}{P+p_{B0}}}$$

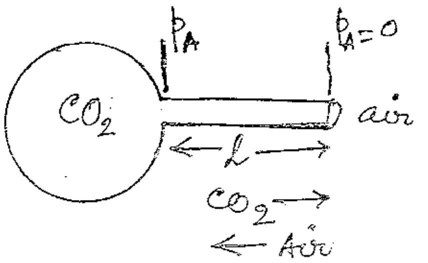
(c) Reaction: $2A \rightarrow 3B \Longrightarrow 3N_A = 2N_B$ (at steady state) $\Rightarrow N_B = -\frac{3}{2}N_A$.

$$N_A = \left(N_A - \frac{3}{2}N_A\right)\frac{p_A}{P} - \frac{D_{AB}}{RT}\frac{dp_A}{dz} \Longrightarrow N_A\int_0^\delta dz = -\frac{2D_{AB}P}{RT}\int_{p_{A0}}^{0}\frac{dp_A}{2P+p_A}$$

$$\Longrightarrow N_A = \frac{2D_{AB}P}{RT\delta}\ln\frac{2P+p_{A0}}{2P} \Longrightarrow \text{Rate of reaction, } \underline{N_A = \frac{2D_BP}{RT\delta}\ln\frac{3P-p_{B0}}{2P}}$$

* * * *

(2.9) Equimolar counterdiffusion of CO_2 and air occurs through the tube. Assume Pseudo-steady state.
Refer to the theoretical analysis in Section 2.5.1.



(2.9) Contd... The time rate of change of the partial pressure of CO_2 in the bulb is given by:

$$-\frac{V}{RT}\frac{dp_A}{dt} = \text{Rate of diffusion of } CO_2 \text{ through the tube} = a \cdot N_A$$

$$\Rightarrow -\frac{V}{RT}\frac{dp_A}{dt} = a \cdot \frac{D_{AB}}{RTl}(p_A - 0)\ ;$$ p_A = CO_2 partial pressure at any time, t. a = area of cross-section of the tube.

The partial pressure of CO_2 at the air-side end of the tube is zero.

Integrate to get $$-\int_{p_{Ai}}^{p_{Af}} \frac{dp_A}{p_A} = \frac{a \cdot D_{AB}}{V \cdot l}\int_0^{t_f} dt \Rightarrow \underline{\ln\frac{p_{Ai}}{p_{Af}} = \frac{aD_{AB}}{V \cdot l} \cdot t_f} \quad \text{...(i)}$$

Given: p_{Ai} = initial partial pressure of CO_2 in the bulb = 1 atm.

p_{Af} = final partial pressure = 0.5 atm ; $V = 2$ litre $= 2\times10^{-3}\ m^3$;

$l = 3$ cm $= 3\times10^{-2}$ m ; $a = \frac{\pi}{4}(0.005)^2 = 1.96\times10^{-5}\ m^2$; $D_{AB} = 1.62\times10^{-5}\ \frac{m^2}{s}$

Substituting in Eq (i) above,

Time of diffusion, $$t_f = \frac{(0.002)(0.03)}{(1.96\times10^{-5})(1.62\times10^{-5})}\ln\frac{1.0}{0.5} = 1.31\times10^5\ s = \underline{\underline{36.38\ hr.}}$$

* * * *

(2.10) Reaction: $2CO + O_2 \longrightarrow 2CO_2$; CO → component 1, O_2 → 2, CO_2 → 3

Flux relation: $N_1 = 2N_2 = -N_3$; y → mole fraction, C = total conc.

Use Eq (2.37) for concentration distribution of component 1 (CO) in the film.

$$-c\frac{dy_1}{dz} = N_1\left(\frac{y_2}{D_{12}} + \frac{y_3}{D_{13}}\right) - y_1\left(\frac{N_2}{D_{12}} + \frac{N_3}{D_{13}}\right)$$

$$\Rightarrow -c\frac{dy_1}{dz} = N_1\left(\frac{y_2}{D_{12}} + \frac{y_3}{D_{13}}\right) - y_1 \cdot N_1\left(\frac{1}{2D_{12}} - \frac{1}{D_{13}}\right) \quad \text{(i)}$$

Similarly, putting the flux relations in Eq (2.38),

$$-c\frac{dy_2}{dz} = \frac{N_1}{2}\left(\frac{y_1}{D_{21}} + \frac{y_3}{D_{23}}\right) - y_2 \cdot N_1\left(\frac{1}{D_{21}} - \frac{1}{D_{23}}\right) \quad \text{(ii)}$$

Put the diffusivity values in Eq (i) and (ii) above, take $D_{ij} = D_{ji}$ for an ideal mixture

For the CO–O_2 pair
$D_{12} = 0.185\ cm^2/s$, at 1 atm and at 273 K
At 250 = 523K,
$D_{12} = (0.185)\left(\frac{523}{273}\right)^{1.5}$
$= \underline{0.363\ cm^2/s}$
Similarly,
$D_{23} = \underline{0.368}$; $D_{12} = \underline{0.49}\ \frac{cm^2}{s}$

and use the relation $y_1 + y_2 + y_3 = 1$ to get

$$-\frac{c}{N_1} \cdot \frac{dy_1}{dz} = 2.755 - 1.02y_1 - 0.714y_2 \quad \text{(iii)}$$

and $$-\frac{c}{N_1}\frac{dy_2}{dz} = 1.359 - 0.338y_1 - 0.682y_2 \quad \text{(iv)}$$

Since the given mixture has three components, two simultaneous ordinary differential equations are to be solved