Question Number II *(25 Marks ~ 30 minutes)*

Part A (/12)

A rigid container of 50 m^3 volume contains CO_2 gas (MW = 44 kg/kmol) at a temperature of 0ºC and pressure of 101 kPa. Assume the CO_2 collision diameter is 3 Å and CO_2 behaves as an ideal gas.

a) What is the density of CO_2 gas? (/4)

$$\rho = ? \qquad Pv = nRT \longrightarrow \frac{n}{v} = \frac{P}{RT} \quad \left(\frac{kmol}{m^3}\right)$$

$$\frac{m}{v} = \frac{PM}{RT} = \frac{(101\ kPa)(44\ kg/kmol)}{(8.314)(273.15)} = \boxed{1.957\ kg/m^3}$$

b) What is the constant pressure specific heat capacity (C_P) of the CO_2 gas at these conditions? (/2)

$$C_p = \frac{5}{2}R = \frac{5}{2}\,8.314 = \boxed{20.785\ \frac{kJ}{kmol\,K}}$$

c) What is the thermal conductivity (k) of the CO_2 at these conditions? (/3)

$$k = \frac{C_v}{N_A \pi \sigma^2}\sqrt{\frac{RT}{\pi M}} \qquad C_v = \frac{3}{2}R = 12.471\ \frac{kJ}{kmol\,K}$$

$$k = \frac{12.471\ kJ/\cancel{kmol}\,K}{(6.023\times10^{26}/\cancel{kmol})(\pi)(3\times10^{-10}\ m)^2}\sqrt{\frac{8314\ \frac{Pa\,m^3}{kmol\,K}\cdot 273.15K}{\pi\ \ 44\ kg/kmol}}$$

$$k = 9.386\times10^{-6}\ \frac{kJ}{m\,s\,K}$$

$$\boxed{k = 9.386\times10^{-6}\ \frac{kW}{m\,K}}$$

d) What is the ratio of the viscosity (μ) of CO_2 at these conditions (0°C and pressure of 101 kPa) to the viscosity at the same pressure but an elevated temperature (20°C)? (/3)

$$\mu = \frac{M}{N_A \pi \sigma^2}\sqrt{\frac{RT}{\pi M}}$$

① 0°C 101 kPa

② 20°C 101 kPa

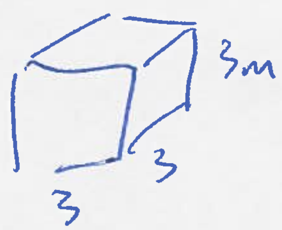
$$\frac{\mu_1}{\mu_2} = \frac{\frac{M}{N_A \pi \sigma^2}\sqrt{\frac{RT_1}{\pi M}}}{\frac{M}{N_A \pi \sigma^2}\sqrt{\frac{RT_2}{\pi M}}} = \frac{\sqrt{T_1}}{\sqrt{T_2}}$$

$$\frac{\mu_1}{\mu_2} = \frac{\sqrt{273.15}}{\sqrt{293.15}} = \boxed{0.965 = \frac{\mu_1}{\mu_2}}$$

Part B (/13)

A closed standard house room (dimension H,W and L: 3m x 3m x 3m) initially holds fresh air at 23°C. You can assume that air is a single ideal gas component. One of the internal walls is coated with a substance that releases phosphine gas, PH_3 (Molar mass M= 34 kg/kmol). The initial concentration of the gas source at the wall surface is measured to be 100 ppm (mg phosphine/L). The wall opposite the phosphine source has a window with a small crack such that the rate of phosphine leaking out of the room does not result in a buildup in the room.

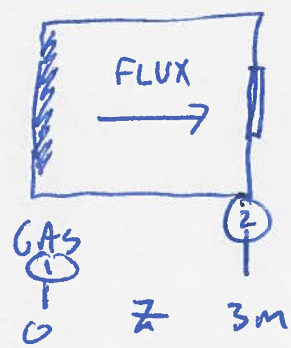
a) The diffusivity of phosphine gas in the air at room conditions is equal to D = 0.381 cm^2/s. Calculate the initial flux of phosphine gas (away from the wall releasing the gas) ($kmol/m^2.s$). (/6)



$T = 23°C$

$D = 0.381 \frac{cm^2}{s}$

$=$



$C_1 = 100 ppm = 100 \frac{mg}{L}$

$C_2 = 0$

$J_A = -D \frac{dC}{dz} = ?$

$$C_1 = \frac{100 \cancel{mg}}{\cancel{L}} \times \frac{1000 \cancel{L}}{m^3} \times \frac{\cancel{g}}{1000 \cancel{mg}} \times \frac{\cancel{kg}}{1000 \cancel{g}} \times \frac{kmol}{34 \cancel{kg}} = 2.94 \times 10^{-3} \frac{kmol}{m^3}$$

$$D = 0.381 \frac{cm^2}{s} \times \left(\frac{m}{100 cm}\right)^2 = 3.81 \times 10^{-5} \frac{m^2}{s}$$

$$j_A = -D \frac{dC}{dz} = -D \frac{\Delta C}{\Delta z} = -D \frac{C_2 - C_1}{\Delta z} =$$

$$j_A = \left(-3.81 \times 10^{-5} \frac{m^2}{s}\right)\left(\frac{0 - 2.94 \times 10^{-5} \, kmol/m^3}{3m}\right)$$

$$\boxed{j_A = 3.735 \times 10^{-8} \frac{kmol}{m^2 s}}$$

b) If the leak in the window is blocked, assuming the initial rate remains constant, find the time in hours at which the concentration of the phosphine gas will become 0.3 ppm in the above mentioned room (3m x3m x 3m). This concentration is the safe limit for domestic use of the room. (/7)

$t = ?$

$C_\circ = 0.3\ ppm$

$C = 0.3 \times \frac{1000}{} \times \frac{1}{1000} \times \frac{1}{1000} \times \frac{1}{34} =$

$C = 8.82 \times 10^{-6}\ \frac{kmol}{m^3}$

$V = 3 \times 3 \times 3 = 27 m^3$

so $n = 8.82 \times 10^{-6}\ \frac{kmol}{m^3} \times 27 m^3 =$ ~~2.38~~

2.382×10^{-4} kmol released

$FLUX = 3.735 \times 10^{-8}\ \frac{kmol}{m^2 s} = \frac{n}{A\,t}$

$A = 3m \times 3m = 9 m^2$

$t = \frac{n}{A \cdot FLUX}$

$t = \frac{2.382 \times 10^{-4}\ kmol}{(9 m^2)(3.735 \times 10^{-8})} = \boxed{708.75 = t}$

(11.8 min)