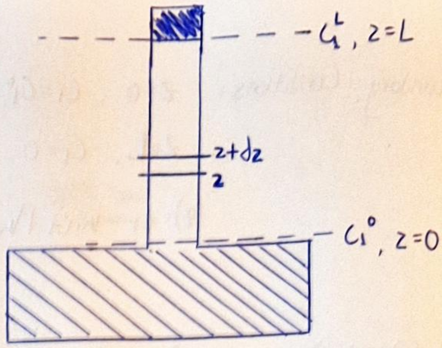
Homework 1 - Solution



1). The system will be the tube between $z=0$ to $z=L$ where we are interested in finding the concentration profile and the flux

- The element will be a small cross-section at height z as shown in the sketch. We have chosen this as an element because the concentration in this small element can be assumed uniform.

Mass Balance

$$\underbrace{\cancel{\text{Accumulation}}}_{\substack{0 \\ \text{(steady state)}}} = \text{Flux}\big|_{in} - \text{Flux}\big|_{out} + \underbrace{\cancel{\text{generation}}}_{0} - \underbrace{\cancel{\text{consumption}}}_{0} \Rightarrow$$

(No reaction)

$$\text{Flux}\big|_{in} - \text{Flux}\big|_{out} = 0 \Rightarrow$$

$$\underbrace{A}_{\text{cross-section area}} \cdot n_1\big|_z - A \cdot n_1\big|_{z+dz} = 0 \Rightarrow \boxed{n_1 = \text{constant}} \quad (1)$$

→ Accumulation is zero as we are in a steady-state

→ Generation, consumption are also zero as we do NOT have any reaction

2) Given that it is steady-state, if we neglect convection, it is a simple steady-state diffusion problem.

The profile will be linear: $D\dfrac{dc_1}{dz} = \text{constant} = k_1 \Rightarrow \boxed{c_1 = k_1 \cdot z + k_2}$ (2) → k_1, k_2 constants that need to be calculated

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Boundary Conditions: $z=0\,,\ c_1=c_1^\circ$
$z=L\,,\ c_1=0$
(2): $c_1 = k_1 z + k_2$
$\Rightarrow$ $k_2 = c_1^\circ$ (3)
$k_1 = -c_1^\circ/L$ (4)

(2), (3), (4) $\Rightarrow c_1 = c_1^\circ - \dfrac{c_1^\circ z}{L} \Rightarrow \boxed{c_1 = c_1^\circ\left(1-\dfrac{z}{L}\right)}$ (5)

So at $\boxed{z=\dfrac{L}{2} \Rightarrow c_1 = \dfrac{c_1^\circ}{2} \simeq 0.25 \text{ bar}} \rightsquigarrow c_1 = 8.47 \text{ mol/m}^3$

3) When convection is present: $\boxed{n_1 = j_1 + c_1 v^a}$ (6)

In this problem, we can assume that air is stagnant $\Rightarrow (v_2 = 0)$

Using velocity of volume: $v^v = c_1\bar{V}_1 v_1 + \cancel{c_2\bar{V}_2 v_2}^{\,0} = c_1 v_1 \bar{V}_1 = n_1\bar{V}_1 \Rightarrow v^v = n_1\bar{V}_1$ (7)

(6), (7): $n_1 = -D\dfrac{dc_1}{dz} + c_1\bar{V}_1 n_1 \Rightarrow$

$$\frac{dc_1}{dz} - \frac{\bar{V}_1 n_1}{D} c_1 + \frac{n_1}{D} = 0 \quad (8)$$

As shown in class the solution to equation (8) is: $\boxed{\dfrac{\bar{c}-c_1}{\bar{c}-c_1^\circ} = \left(\dfrac{\bar{c}-c_1^L}{\bar{c}-c_1^\circ}\right)^{z/L}}$ (9)

Given that $c_1^L = 0$ and $z = L/2$: $\dfrac{\bar{c}-c_1}{\bar{c}-c_1^\circ} = \left(\dfrac{\bar{c}}{\bar{c}-c_1^\circ}\right)^{1/2} \Rightarrow$

$$\bar{c}-c_1 = (\bar{c}-c_1^\circ)\left(\frac{\bar{c}}{\bar{c}-c_1^\circ}\right)^{1/2} \Rightarrow$$

$\boxed{c_1 = \bar{c} - \sqrt{\bar{c}(\bar{c}-c_1^\circ)}}$, in terms of pressure

Partial pressure at $z = L/2 = 1 - \sqrt{1(1-1/2)} =$

$$1 - \frac{1}{\sqrt{2}} = \frac{\sqrt{2}-1}{\sqrt{2}} = \frac{0.414}{1.414} = 0.29 \text{ bar}$$

Error: $\frac{0.29 - 0.25}{0.29} \cdot 100\% = 13.8\%$ → this is a substantial error, mainly because we are at 82°C which is a high temperature

4) Flux of water at $z=0$ and $z=L$ will be the same as flux is constant.

$$n_1 = \frac{D\bar{c}}{L} \ln\left(\frac{\bar{c} - c_1^L}{\bar{c} - c_1^0}\right) =$$

$$\frac{D\bar{c}}{L} \ln\left(\frac{\bar{c} - 0}{\bar{c} - c_1^0}\right) = \frac{D\bar{c}}{L} \ln\left(\frac{\bar{c}}{\bar{c} - c_1^0}\right)$$

We need to find the diffusion coefficient of water at 82°C and at 1 bar

$$D_{12} = \frac{1.86 \cdot 10^{-3} \cdot T^{1.5} (1/M_1 + 1/M_2)^{0.5}}{P \sigma_{12}^2 \cdot \Omega}, \quad \sigma_{12} = \frac{\sigma_1 + \sigma_2}{2}, \quad \varepsilon_{12} = \sqrt{\varepsilon_1 \varepsilon_2}$$

$\sigma_1 = 2.641$ Å, $\sigma_2 = 3.711$ Å $\Rightarrow \sigma_{12} = \frac{\sigma_1 + \sigma_2}{2} = 3.176$ Å

$\frac{\varepsilon_1}{k_B} = 809.1$ K, $\frac{\varepsilon_2}{k_B} = 78.6$ K

$$\frac{\varepsilon_{12}}{k_B} = \sqrt{\frac{\varepsilon_1}{k_B} \cdot \frac{\varepsilon_2}{k_B}} = 252.2 \text{ K}$$

Data:

$T = 82 + 273$ K

$M_1 = 18$ g/mol

$M_2 = 28.97$ g/mol

$P = 1$ bar $= 0.986$ atm

$L = 10$ cm $= 10^{-1}$ m

$$\frac{k_B T}{\varepsilon_{12}} = \frac{(82+273)}{252.2} = 1.41$$

Extrapolating from the table we get: $\boxed{\underline{\Omega} = 1.2318}$

$$D = \frac{1.86 \cdot 10^{-3} \cdot T^{1.5} \left(1/M_1 + 1/M_2\right)^{0.5}}{P \cdot \sigma_{12}^2 \cdot \underline{\Omega}} = \frac{1.86 \cdot 10^{-3} \cdot (82+273)^{1.5} \cdot \left(1/18 + 1/28.97\right)^{0.5}}{0.986 \cdot (3.176)^2 \cdot 1.2318} = \underline{0.305 \text{ cm}^2/\text{s}}$$

$$n_1 = \frac{D\bar{c}}{L} \ln\left(\frac{\bar{c}}{\bar{c}-c_1^\circ}\right) = \frac{D\bar{c}}{L} \ln(2) = \frac{0.305 \cdot 10^{-4} \cdot 33.88}{10^{-1}} \cdot 0.69 = 7.125 \cdot 10^{-3} \frac{\text{mol}}{\text{m}^2 \cdot \text{s}}$$

$$\left.\begin{aligned} \bar{c} &= \frac{P}{RT} = \frac{1 \cdot 10^5 \text{ Pa}}{8.314 \,(\text{J/mol/K})\,(273+82)\,\text{K}} = 33.88 \text{ mol/m}^3 \\ c_1^\circ &= \frac{P_{sat}}{RT} = \frac{0.5 \cdot 10^5 \text{ Pa}}{8.314\,(\text{J/mol/K}) \cdot (273+82)\,\text{K}} = 16.94 \text{ mol/m}^3 \end{aligned}\right\} \Rightarrow \bar{c} = \frac{\underline{2c_1^\circ}}{10}$$