Irrev, Øving 4

1a) $\vec{J} = L\vec{X}$, $\vec{J} = \begin{pmatrix} J_1 \\ J_2 \\ J_q' \end{pmatrix}$, $L = \begin{bmatrix} L_{11} & L_{12} & L_{1q'} \\ L_{21} & L_{22} & L_{2q'} \\ L_{q'1} & L_{q'2} & L_{q'q'} \end{bmatrix}$, $\vec{X} = \begin{pmatrix} -\frac{1}{T}\frac{\partial \mu_1}{\partial x} \\ -\frac{1}{T}\frac{\partial \mu_2}{\partial x} \\ \frac{\partial}{\partial x}\left(\frac{1}{T}\right) \end{pmatrix}$

1b) Mass transport due to a temperature gradient

$\frac{\partial T}{\partial x} \neq 0 \xrightarrow{\text{Soret}} J_i \neq 0$

1c) For a one-component system: $D_T = \frac{L_{\mu q}}{c_1 T^2}$

$S_T := \frac{D_T}{D_{1,2}}$, $D_{1,2} = \frac{L_{\mu\mu} R}{c_1}\left(1 + \frac{\partial \ln \gamma_1}{\partial \ln c_1}\right)$,

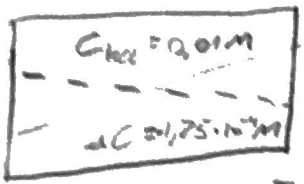
$\alpha_T := S_T T$

1d) Heat transport due to a chemical potential gradient

1e) $q^* := \left(\frac{J_q'}{J_1}\right)_{dT=0} = \frac{L_{q\mu}}{L_{\mu\mu}} = \frac{c_1 D_T T^2}{D_{1,2} T} \frac{\partial \mu_{1,T}}{\partial c_1}$

1f) $D_{1,2}$ can be estimated by $D_{1,1} = D_S$, the self-diffusion coefficient, which can be measured by NMR or calculated for gases using kinetic gas theory.

Oppg 2)



$D_{1,2} = 1{,}9 \cdot 10^{-9} \frac{m^2}{s}$

$T_1 = 293K$ $\quad T_2 = 303K$

2a)

$$S_T = \frac{D_T}{D_{1,2}} = \frac{-\frac{\partial C_1}{\partial x}}{C_1 \frac{\partial T}{\partial x}} \xrightarrow{\text{steady state}} S_T = \frac{-\Delta C_1}{C_1 \Delta T} = -1{,}25 \cdot 10^{-3}\ K^{-1}$$

$d\ln C = \frac{1}{C} dC$

$$q^* = S_T R T^2 \left(1 + \frac{\partial \ln \gamma_1}{\partial \ln C_1}\right),$$

$$= S_T R T^2 \left(1 + C_1 \frac{\partial \ln \gamma_1}{\partial C_1}\right), \quad \gamma_1 \approx \exp\left(z_+ z_- \sqrt{\frac{\mu}{\mu_{DH}}}\right) = 0{,}89$$

$\mu = \frac{1}{2}\sum z_i^2 c_i = C_1 = 0{,}01 M$ can probably assume ideal

$$= S_T R T^2 \left[1 + C_1 \frac{d}{dC_1}\left(-\sqrt{\frac{C_1}{\mu_{DH}}}\right)\right]$$

$$= S_T R T^2 \left[1 - \frac{C_1}{\sqrt{\mu_{DH}}} \frac{C_1^{-\frac{1}{2}}}{2}\right]$$

$$= S_T R T^2 \underbrace{\left(1 - \frac{1}{2}\sqrt{\frac{C_1}{\mu_{DH}}}\right)}_{= 0{,}94} \rightarrow \text{definetely ideal}$$

$$\hookrightarrow \frac{d\ln\gamma}{d\ln C} = \frac{z_+ z_-}{2} \sqrt{\frac{C \sum z_i^2 \nu_i}{2 \mu_{DH}}}$$

For $A_{\nu_A} B_{\nu_B} \ldots Y_{\nu_Y}$ (aq)

$$q^* = -867{,}5 \frac{J}{mol}$$

(Also: Is q^* defined "per component"?)

2b)

$$J_{HCl} = L_{\mu q} \frac{\partial}{\partial x}\left(\frac{1}{T}\right), \quad L_{\mu q} = D_T C_1 T^2, \quad D_T = S_T D_{1,2}$$

$$L_{\mu q} = S_T D_{1,2} C_1 T^2$$

$$J_{HCl} = \frac{-L_{\mu q}}{T^2} \frac{\partial T}{\partial x}$$

$$J_{HCl} = -S_T D_{1,2} C_1 \frac{\Delta T}{\Delta x} = -2{,}25 \cdot 10^{-8} \frac{mol}{m^2 s}$$

Oppg. 3)

$D_{1,2} = 6{,}2 \cdot 10^{-9} \frac{m^2}{s}$

$\alpha_T = 8{,}9$

$$S_T = \frac{\alpha_T}{T}, \quad D_T = S_T D_{1,2}' = \frac{\alpha_T D_{1,2}}{T}$$

$$J_q' = -\frac{L_{q\mu}}{T} \frac{\partial \mu_{1,T}}{\partial x}, \quad L_{q\mu} = L_{\mu q} = D_T C_1 T^2 = \alpha_T D_{1,2} C_1 T$$

$$\mu_1 = \mu_1^0 + RT \ln \gamma_1 \frac{P_1}{P^0} \quad \frac{P_1}{P^0} = \frac{C_1 RT}{C^0 RT} = \frac{C_1}{C^0}$$

$$\frac{\partial \mu_{1,T}}{\partial x} = RT \frac{\partial \ln C_1}{\partial x}, \quad \text{assuming } \gamma = 1$$

$$= \frac{RT}{C_1} \frac{\partial C_1}{\partial x}$$

$$J_q' = -\alpha_T D_{1,2} RT \frac{\Delta C}{\Delta x}$$

$$J_q' = -4{,}76 \cdot 10^{-8} \frac{J}{m^2 s}$$