Matlik, Øving 6, Vegard G. Jervell

1a) $\rho_{H_2O,l} = 0{,}997\ g/ml$

$\rho_{H_2O,s} = 0{,}917\ g/ml$

$\Delta_{trs}H_m = 5{,}128\ kJ/mol$

1b) $H_2O(l) \rightarrow H_2O(s)$

$$\frac{dp}{dT} = \frac{\Delta_{trs}H_m}{T\Delta_{trs}V_m}$$

$$\Delta V_m = M_{m_{H_2O}}\left(\frac{1}{\rho_s} - \frac{1}{\rho_l}\right)$$

$$\Delta V_m = 1{,}575\ \frac{ml}{mol} = 1{,}575 \cdot 10^{-6}\ \frac{m^3}{mol}$$

$$\frac{\Delta_{trs}V_m}{\Delta_{trs}H_m}dp \overset{*}{=} \frac{dT}{T}$$

* Antar at ΔH og ΔV er uavhengig av T

$$3{,}1 \cdot 10^{-10}\ Pa^{-1}\left(100 \cdot 10^5 - 10^5\right)Pa = \ln\left(\frac{T}{278K}\right)$$

$$\ln(T) = 5{,}7$$

$$T = 298{,}867K$$

Oppg 2a)

Clausius-Clapeyrons likning er Clapeyrons likning, innsett antakelse om ideell gass og at $\Delta V \approx V_g$, altså at $V_g >> V_l$ eller V_s, avhengig av om vi ser på $l \rightarrow g$ eller $s \rightarrow g$

2b) $\frac{dp}{dT} = \frac{p\,\Delta_{trs}H}{RT^2}$

$$\frac{dp}{p\,\Delta_{trs}H} = \frac{dT}{RT^2}$$

I) $$\frac{R}{\Delta_{trs}H}\ln\left(\frac{p}{p^\circ}\right) = \left[-\frac{1}{T}\right]_{T_0}^{T}$$

$$\frac{1}{T} = \frac{1}{T_0} - \frac{R}{\Delta_{trs}H}\ln\left(\frac{p}{p_0}\right)$$

$$T = 352\,K$$

2c) From (I): $$\ln\left(\frac{p}{p_0}\right) = \frac{\Delta_{trs}H}{R}\left[\frac{1}{T}\right]_{T}^{T_0}$$

$$\ln\left(\frac{p}{p_0}\right) = -3{,}858$$

$$p = 0{,}02\,atm$$

Opg. 3a) regnar ut $\Delta_{mix}H$ for x_{Al} mellom 0. og 1

negativt avvik

3b) Regular solution model: $\Delta_{mix}H = \Omega x_A x_B$

$$\Delta_{mix}H = -\Omega(x_A - x_A^2)$$

For Al-Y:

$$\Delta_{mix}H = x_{Al}x_Y(a - b(x_{Al} - x_Y))$$

$$= (x_{Al} - x_{Al}^2)(a - b(2x_{Al} - 1)),\ |a| > |b|$$

$$= (x_{Al} - x_{Al}^2)(C_1 + C_2 x_{Al}),\ |C_2| \ll |C_1|$$

Fordi $|\Omega_2| << |\Omega_1|$ vil regulær løsning være en god modell selv om den er kvadratisk i x_i, i stedet for kubisk.

3c)

$$\Delta^E_{mix} G = RT(x_A \ln\gamma_A + x_B \ln\gamma_B), \quad \ln\gamma_i = \frac{\Omega x_j}{RT}$$

$$= x_A \Omega x_B + x_B \Omega x_A$$

$$\Delta^E_{mix} G = \Sigma \Delta_{mix} H = -75{,}1 \frac{kJ}{mol}$$

3d) $\Delta_{mix} S = \Delta^{id}_{mix} S = -R(x_A \ln x_A + x_B \ln x_B)$

$$\Delta_{mix} G = \Delta^{id}_{mix} G + \Delta^E_{mix} G$$

$$\Delta^{id}_{mix} G = -T \Delta^{id}_{mix} S = RT(x_A \ln(x_A) + x_B \ln(x_B))$$

$\Delta^{id}_{mix} G = -9 \frac{kJ}{mol}$, $x_A = 0{,}58$, $x_B = 0{,}42$, $T = 1600\,K$

$\Delta_{mix} G = -84{,}1 \frac{kJ}{mol}$

Dette er et veldig stort avvik fra idealitet. Det gir mening fordi avviket er størst rundt $x_{Al} \approx x_y \approx 0{,}5$