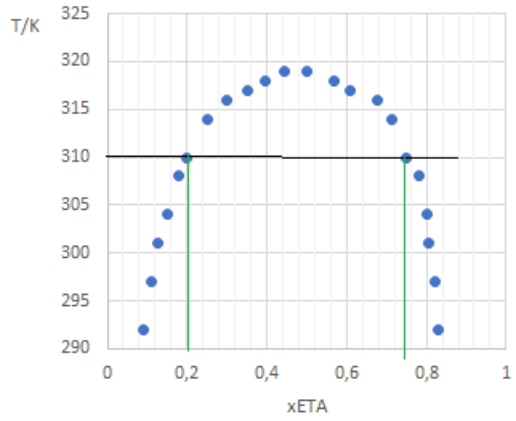
## 4º teste 16 Dezembro 2022

1-a)




Tie-line a 310 K

Fase mais rica em Etanol L1: $x_{ETA} = 0.75$

Fase mais rica em Ciclohexano L2: $x_{ETA} = 0.2$

Regra da alavanca

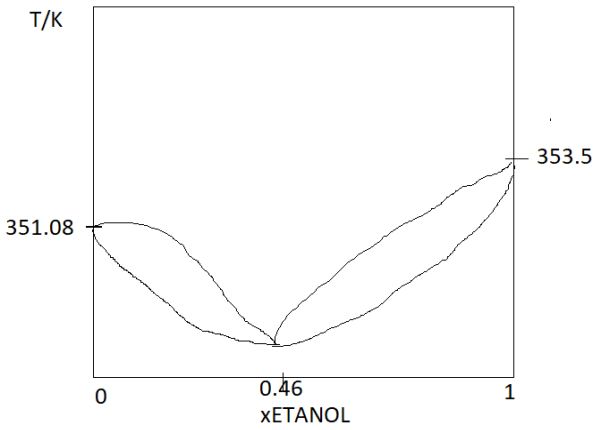
$n^{L1} * \ell^{L1} = n^{L2} * \ell^{L2}$

$n^{L1} *(0.75-x^{T})= nL2 \ *(x^{T}-0.2)$ com $x^{T}$ fracção molar total de etanol na mistura

$n^{L1}/n^{L2}=0.5$; logo $n^{L1}/n^{L2}= (x^{T}-0.2) /(0.75-x^{T}) = 0.5$

obtendo-se $x^{T} =0.383$

1-b)

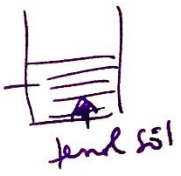


2. $\gamma_I$ mede desvios ao modelo Sol. ideal

a)

$a_{fenol} = x_{fenol}\, \gamma_{I,fenol}$

no eq.;




$\mu^*_{fenol,sól} =$

$= \mu^*_{fenol,liq} + RT \ln a^{a'gua}_{fenol}$

A T e P ctes, $a^{a'gua}_{fenol} = a^{ideal}_{fenol} =$

$= x^{ideal}_{fenol}\, \underbrace{\gamma^{ideal}_{I,fenol}}_{=1} = x^{ideal}_{fenol}$

$$\ln x_{fenol}(sol.\ ideal) = \frac{\Delta_{fus} H_{fenol}}{R}\left(\frac{1}{T_{fus\,fenol}} - \frac{1}{T}\right)$$

$$\ln x^{ideal}_{fenol} = \frac{11510}{8.314}\left(\frac{1}{313.95} - \frac{1}{298.15}\right)$$

$x^{ideal}_{fenol} = 0.792 = a^{ideal}_{fenol} = a^{a'gua}_{fenol}$

$0.792 = x^{a'gua}_{fenol}\, \gamma^{a'gua}_{I,fenol}$

$$\gamma^{a'gua}_{I,fenol} = \frac{0.792}{0.075} = 10.6$$

b) $\ln x_{fenol}(\text{sol. dil. ideal}) = \frac{\Delta_{sol\,fenol}H}{R}\left(\frac{1}{T_{fus\,fenol}} - \frac{1}{T}\right)$

$\ln 0.693 = \frac{\Delta_{sol\,fenol}H}{8.314}\left(\frac{1}{313.95} - \frac{1}{298.15}\right)$

$\Delta_{sol\,fenol}H = 18028\ J\,mol^{-1}$

fenol sól. → fenol líquido

11510 ... ?

18028 → fenol na água

? $= -11510 + 18028$

$= 6510\ J\,mol^{-1}$

3. a) $CO_2(g) + 4\,H_2(g) \rightleftharpoons CH_4(g) + 2\,H_2O(g)$

$$K = \frac{f_{CH_4}\, f_{H_2O}^2}{f_{CO_2}\, f_{H_2}^4} = \frac{P_{CH_4}\, P_{H_2O}^2}{P_{CO_2}\, P_{H_2}^4} \times \frac{\phi_{CH_4}\, \phi_{H_2O}^2}{\phi_{CO_2}\, \phi_{H_2}^4}$$

$$\ln \phi = \int_0^P \frac{Z-1}{P}\, dP = \frac{B}{RT} \times P$$

$B \rightarrow cm^3\,mol^{-1}$

$R \rightarrow J\,K^{-1}\,mol^{-1}$

$T \rightarrow K$

$P \rightarrow MPa$

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$$\ln \phi_{CH_4} = \frac{34.1}{8.314 \times 800} \times 5$$

$$\phi_{CH_4} = 1.03 \qquad \phi_{CO_2} = 1.01 \qquad \phi_{H_2} = 1.01$$

$$\phi_{H_2O} = 0.97$$

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$$K_{800} = 0.126 = \frac{P_{H_2O}^2}{6.8^4} \times \frac{P_{CH_4}}{P_{CO_2}} \times \underbrace{0.914}_{\text{razão } \phi_i}$$

$$P_{H_2O}^2 = \frac{0.126 \times 6.8^4}{0.914} = 301.79$$

$$P_{H_2O} = \sqrt{301.79} = 17.37 \text{ bar}$$

no eq°:

$$P_{CO_2} + P_{CH_4} = 50 - P_{H_2O} - P_{H_2} =$$

$$= 50 - 17.37 - 6.8 = 25.83 \text{ bar}$$

$$P_{CO_2} = P_{CH_4} = \frac{25.83}{2} = 12.91 \text{ bar}$$

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$$Y_{CO_2} = Y_{CH_4} = \frac{12.91}{50} = 0.258$$

$$Y_{H_2} = \frac{6.8}{50} = 0.136 \qquad Y_{H_2O} = \frac{17.37}{50} = 0.347$$

$$\sum_i y_i = 1.000$$

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b) $\Delta G^\circ_{800} = -RT \ln K_{800} = -8.314 \times 800 \times$

$\times \ln 0.126 = \Delta H^\circ - T\Delta S^\circ =$

$= -188.4 \times 10^3 - 800 \times \Delta S^\circ_{800}$

$\Delta G^\circ_{800} = -13778 \text{ J}$

$\Delta S^\circ_{800} = -252.72 \text{ JK}^{-1}$

$$\Delta S^\circ_{800} = \Delta S^\circ_{298} + \int_{298}^{800} \frac{\Delta C_{p_i}}{T} \, dT$$

$$\Delta C_{p_i} = \sum_i m_i C_{p_i}(\text{Prod}) - \sum_i m_i C_{p_i}(\text{Reg})$$

$$= 1 \times 36.8 + 2 \times 34.1 - (1 \times 35 + 4 \times 29.2)$$

$$= -46.8 \ \text{JK}^{-1}$$

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$$-252.72 = \Delta S^\circ_{298} - 46.8 \ln \frac{800}{298}$$

$$\Delta S^\circ_{298} = -206.5 \ \text{JK}^{-1}$$

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4. $(NH_4)_3PO_4 \rightleftarrows 3NH_4^+ + PO_4^{3-}$

$\nu_+ = 3 \quad \nu_- = 1 \quad z_+ = 1 \quad z_- = -3$

$\nu = \nu_+ + \nu_- = 4$

$m_+ = \nu_+ m_i = 3m_i \qquad m_i = 0.005 \text{ mol kg}^{-1}$

$m_- = \nu_- m_i = m_i$

$m_\pm^\nu = m_+^{\nu_+} m_-^{\nu_-} = (3m_i)^3 \times m_i = 27 m_i^4 =$

$= 27 \times 0.005^4 = 1.69 \times 10^{-8}$

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$CaI_2 \rightleftarrows Ca^{2+} + 2I^-$

$\nu_+ = 1 \quad \nu_- = 2 \quad z_+ = 2 \quad z_- = 1$

$m_+ = \nu_+ m = m$

$m_- = \nu_- m = 2m \qquad m = 0.006 \text{ mol kg}^{-1}$

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$I = 0.5 \times \left(3 \times 0.005 \times 1^2 + 1 \times 0.005 \times (-3)^2 + \right.$

$\left. + 1 \times 0.006 \times 2^2 + 2 \times 0.006 \times (-1)^2\right) =$

$= 0.048 \text{ mol kg}^{-1}$

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$\log_{10} \gamma_\pm = -0.509 \times 1 \times |-3| \times \sqrt{0.048} =$

$= -0.3345$

$$\gamma_{\pm} = 10^{-0.3345} = 0.463$$

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$$a_i = a_{(NH_4)_3PO_4} = m_{\pm}^{\nu} \gamma_{\pm}^{\nu} =$$

$$= 1.69 \times 10^{-8} \times 0.463^4 = 7.76 \times 10^{-10}$$