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國立台灣科技大學化工系博士班資格考試　化工熱力學

Part I: 50%

1. The Gibbs-Duhem Equation for a 2-component mixture can be expressed as

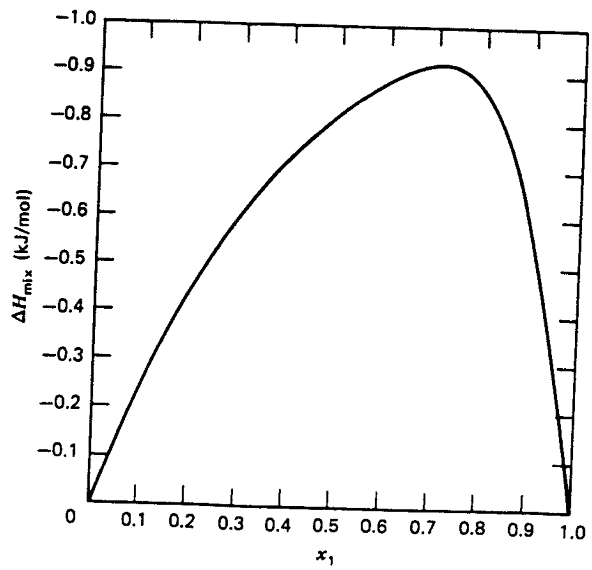
$$x_1\left(\frac{\partial \bar{G}_1}{\partial x_1}\right)_{T,P} + x_2\left(\frac{\partial \bar{G}_2}{\partial x_1}\right)_{T,P} = 0$$

Write down the corresponding equation for a 3 component mixture. (10%)

2. Figure A is the heat of mixing data for water (1)-methanol (2) system at T=19.69℃. Explain (you don't have to do the actual calculation) how to construct a table for $\bar{H}_1$-H_1 vs. x_1 for this system. (10%)

3. The following data are available for water
Ln P^{sub}(ice) = 28.893 – 6140.1/T　　P in Pa
Ln P^{vap}(water) = 26.303 – 5432.8/T　T in K
a. Compute the triple point temperature and pressure of water
b. Compute the heat of vaporization, heat of sublimation and heat of fusion at its triple point. (15%)

4. Find the fugacity of steam at 400℃ and 2 MPa. Given the enthalpy and entropy of steam at 400℃ and 0.01 MPa as 3279.6 kJ/kg and 9.6077 kJ/kg.K. Assume that steam at 400℃ and 0.01 MPa can be treated as an ideal gas. (15%)



Part II. (50%)

1. The second virial coefficient (B) of ethane is given by

$$B = -2.0 \times 10^6 / T^2$$

where B in cm^3/mol and T in K. Calculate the change of internal energy (ΔU) for one mole of ethane in going from very low pressure (P --> 0) to 20 bar at 400 K by using the two-term virial equation

$$Z = 1 + \frac{BP}{RT}$$

where Z is the compressibility factor (= PV/RT), P is pressure, R is the gas constant, and V is the molar volume. (20%)

Hint: $dU = T\,dS - P\,dV$ and $(\partial P / \partial S)_T = -(\partial T / \partial V)_P$

2. For a binary system, the activity coefficient of component 2 (γ_2) can be expressed as

$$\ln \gamma_2 = (a + 1.5b)x_1^2 - bx_1^3$$

where x_1 is the mole fraction of component 1. "a" and "b" are constants. Please derive ln in terms of x_2. (15%)

3. You are asked to calculate the activity coefficient of propanol at infinite dilution (γ_2^∞) in the mixture of ethyl acetate (1) + propanol (2) at 80°C by using the NRTL model:

$$\underline{G}^E / RT = x_1 x_2 [\frac{\tau_{21} G_{21}}{x_1 + x_2 G_{12}} + \frac{\tau_{12} G_{12}}{x_2 + x_1 G_{12}}]$$

where

$$\tau_{12} = (g_{12} - g_{22}) / RT \qquad \tau_{21} = (g_{21} - g_{11}) / RT$$

$$G_{12} = \exp(-\alpha \tau_{12}) \qquad G_{21} = \exp(-\alpha \tau_{21})$$

and $\underline{G}^E$ is the molar excess Gibbs free energy. The optimal values of the parameters for this mixture are given by $g_{12} - g_{22} = -124.48$ bar cm^3/mol, $g_{21} - g_{11} = 436.47$ bar cm^3/mol, and $\alpha = 0.31$.

Note: R = 83.1439 bar $cm^3/(mol\ K)$. (15%)