Additional (Random) Exercises

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December 13, 2024

Exercise 1

Inside a tank in a chemical plant, there is a mixture composed of hydrogen, ammonia, nitrogen, and water. Inside the tank, the pressure is 0.15 [bar] and 25 [°C]. The components are distributed in two different phases: liquid and vapor. Initially, there are 3 moles of hydrogen, 1 of nitrogen, and 5 of water. Calculate the molar fractions of the components in both phases making the following assumptions:

- The gas phase is treated as a perfect gas
- The liquid mixture is ideal

The following table shows the Gibbs free energy of formation values in the pure perfect gas state at 298.15 [K] and 0.15 [bar]. Additionally, the Henry's constant values and Vapor Pressure at 298.15 [K] are reported.

Compound	$\Delta g^{\circ}_{f,j}$ [kJ·mol^{-1}]	**Henry's Constant [Pa]** H_j	**Vapor Pressure [Pa]** (P°_j)
H_2	0	$7.158 \cdot 10^{10}$	
N_2	0	$9.244 \cdot 10^{10}$	
NH_3	-16.33	$9.758 \cdot 10^{4}$	
H_2O			$3.167 \cdot 10^{3}$

In general, using the extent of reaction method, we can write the following system, which relates the extent of reaction (λ) with the moles of species in each phase. (Note: superscript V indicates species j in Vapor phase while superscript L indicates species j in liquid phase)

$$\begin{cases} n_{N_2^V} = 1 - 0.5\lambda_1 - \lambda_2 \\ n_{H_2^V} = 3 - 1.5\lambda_1 - \lambda_3 \\ n_{NH_3^V} = \lambda_1 - \lambda_4 \\ n_{H_2O^V} = 5 - \lambda_5 \\ n_{N_2^L} = \lambda_2 \\ n_{H_2^L} = \lambda_3 \\ n_{NH_3^L} = \lambda_4 \\ n_{H_2O^L} = \lambda_5 \end{cases} \tag{1}$$

Additionally, the following relations hold, where n_T^L is the total moles present in the liquid phase, n_T^V is the total moles present in vapor phase, x_i and y_i are the molar fractions of species i in liquid and vapor phase respectively:

$$n_T^L = \lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 \tag{2}$$

$$n_T^V = 9 - \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4 - \lambda_5 \tag{3}$$

$$x_i = \frac{n_i^L}{n_T^L} \tag{4}$$

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$$y_i = \frac{n_i^V}{n_T^V} \tag{5}$$

Finally, using pure perfect gas at 298.15 [K] and 0.15 [bar] as reference, assuming perfect gas and ideal liquid mixture, the system that solves our problem takes the following form:

$$\begin{cases} \frac{y_{NH_3^V}}{y_{N_2}^{0.5} \cdot y_{H_2}^{1.5}} = \exp\left(-\frac{\Delta g^\circ_{f,NH_3^*}(298.15\text{ K};0.15\text{ bar})}{RT}\right) \\ P y_{H_2} = H_{H_2} \cdot x_{H_2} \\ P y_{N_2} = H_{N_2} \cdot x_{N_2} \\ P y_{NH_3} = H_{NH_3} \cdot x_{NH_3} \\ P y_{H_2O} = P^\circ_{H_2O} \cdot x_{H_2O} \end{cases} \tag{6}$$

TIPS

- The unknowns of our system are the lambda values
- To solve the problem, consider that the system of equations to be solved is (6); it contains the molar fractions of species in both gas and liquid phase, these can be easily written as functions of our problem's unknowns, namely the λ values, as shown in system (1), and the relations reported in equations 2-3-4-5
- Reasonable initial guess values: $\lambda_0 = [1, 0, 0, 0.5, 4.5]$