Department of Chemical Engineering Thapar Institute of Engineering & Technology, Patiala

Course: Material and Energy Balances UCH301

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Calculation of Bubble Point & Dew Pont Temperatures for Ideal Liquid Mixtures

Calculation of bubble point temperature for Ideal Liquid Mixtures

Let the components present in the liquid mixture be A, B and C (there can be any number of components) and the liquid is in equilibrium with the vapor. The composition of the liquid phase is known (i.e., x_A, x_B, & x_C are known)

The partial pressure of gas phase components is given by the Roult's law:

$$p_i = x_i \, p_i^{*}{}_{(Tbp)} , \quad for \; i = A, B, C$$

Then the total pressure must be equal to the sum of partial pressures

$$P = x_A P_A^*{}_{(Tbp)} + x_B P_B^*{}_{(Tbp)} + x_C P_C^*{}_{(Tbp)}$$

Using the above equation, the bubble point temperature of the liquid mixture can be calculated by trial and error.

Step1: Assume T_{bp}

Step2: Calculate the vapor pressure of each component at assumed T_{bp} i.e. $p_i^*(T_{bp})$, using Antoine/any other equation.

Step 3: Calculate total pressure (P) using

$$P = x_A P_{A\,(Tbp)} + x_B P_{B\,(Tbp)} + x_C P_{C\,(Tbp)}$$

Step4: Compare P with total pressure of the system if within tolerance, we have calculated the T_{bp} of the mixture.

Once the T_{bp} is calculated, the composition of vapor phase can be easily calculated using the Roult's law

$$p_i = x_i\, p_{i\,(Tbp)} \;; \quad y_i = p_i/P$$

So bubble point temperature can be used for calculating gas phase composition if the liquid phase composition is known.

Problem

Calculate the bubble point temperature and composition of a vapor in equilibrium with a liquid that is 40 mol% benzene and 60 mol% toluene at 1 atmosphere pressure.

Data:

Benzene: A=6.89272; B=1203.531;C=219.888

Toluene: A=6.95805; B=1346.773; C=219.693

In Antonie equation use T in ^{0}C, and P in mmHg:

$$\log_{10} p^* = A - \frac{B}{T + C}$$

($NBP_{Benzene}$=80 ^{0}C, $NBP_{Toluene}$=110 ^{0}C)

SOLUTION

- Assume a value for TBP of this mixture

(first guess value may be taken as the average of NBPs of Benzene and Toluene)

$$P = x_B P_B{}^*{}_{(Tbp)} + x_T P_T{}^*{}_{(Tbp)}$$

$$P_B^*(T_{BP}) = 10^{6.89272 - \frac{1203.531}{T+219.888}} \qquad P_T^*(T_{BP}) = 10^{6.95805 - \frac{1346.773}{T+219.693}}$$

$$p = 0.4 \times 10^{6.89272 - \frac{1203.531}{T+219.888}} + 0.6 \times 10^{6.95805 - \frac{1346.773}{T+219.693}}$$

In the above equation substitute P =760 mmHg and obtain the value of T (which is TBP of mixture):

$$760 = 0.4 \times 10^{6.89272 - \frac{1203.531}{T+219.888}} + 0.6 \times 10^{6.95805 - \frac{1346.773}{T+219.693}}$$

$$T = 95.1\ ^0C$$

- Composition of vapor phase:

$$y_B = \frac{0.4 \times 10^{6.89272 - \frac{1203.531}{95.1+219.888}}}{760} = 0.62$$

$$y_T = \frac{0.6 \times 10^{6.95805 - \frac{1346.773}{95.1+219.693}}}{760} = 0.38$$

Calculation of dew point temperature for ideal vapor (gas) mixtures

- **Let the components present in the vapor mixture be A, B and C (there can be any number of components) and the composition of liquid in equilibrium with the vapor is to be calculated.**

- **The composition of the vapor phase is known (values of y_A, y_B, y_C are known)**

- **The liquid phase mol fractions may be calculated from the Roult's law:**

$$x_i = \frac{y_i P}{P_i^*(T_{dp})}$$

i = A, B, C

At dew point temperature, $x_A + x_B + x_C = 1.0$

Using the above two equations, the due point temp. of the mixture can be calculated by trial and error.

- **Step1:** Assume T_{dp}
- **Step 2: Calculate pure component vapor pr. at T_{dp}**
- **Step3: Calculate mol fractions of the components A, B,C in the liquid phase**
- **Step4: Check whether the sum $x_i = 1.0$**

So dew point temperature can be used for calculating liquid phase composition if the vapor phase composition is known

PROBLEM

Calculate the dew point temperature and composition of a liquid in equilibrium with a gas mixture containing 10 mol% benzene, 10 mol% Toluene and balance nitrogen at 1 atm.

- Data

Benzene: A=6.89272; B=1203.531;C=219.888

Toluene: A=6.95805; B=1346.773; C=219.639

In Antonie equation use $T\ in\ {}^0C$ and $P\ in\ mm\ Hg$

- In the liquid phase at equilibrium with this vapor:

$$x_i = \frac{y_i P}{P_i^*(T_{dp})}$$

- There will be two components in the liquid phase, N_2 will not condense, therefore:

$$1.0 = \frac{y_B P}{P_B^*(T_{dp})} + \frac{y_T P}{P_T^*(T_{dp})}$$

- The equation for calculation of dew point temperature is to be solved by trail and error

$$1.0 = \frac{0.1 \times P}{P_B^*(T_{dp})} + \frac{0.1 \times P}{P_T^*(T_{dp})}$$

- Where,

$$P_B^*(T_{dp}) = 10^{6.89272 - \frac{1203.531}{T + 219.888}}$$

$$P_T^*(T_{dp}) = 10^{6.95805 - \frac{1346.773}{T + 219.693}}$$

Solving we get, $T_{dp} = 52.4\ ^0C$

- The composition in the liquid phase will be:

$$x_B = \frac{0.1 \times P}{P_B^*(T_{dp})} = \frac{0.1 \times 760}{10^{6.89272 - \frac{1203.531}{52.4+219.888}}} = 0.256$$

$$x_T = \frac{0.1 \times P}{P_T^*(T_{dp})} = \frac{0.1 \times 760}{10^{6.95805 - \frac{1346.773}{52.4+219.693}}} = 0.744$$

Bubble Point Pressure

When a liquid is decompressed at constant temperature the pressure at which first drop of bubble forms is known as bubble point pressure.

Bubble point pressure for an ideal liquid mixture (known composition), and the composition of vapor in equilibrium with this liquid can be calculated using Dalton’s law and Roult’s law

Calculation of bubble point pressure

Step 1. **Calculate the vapor pressure of each component at system temperature using Antoine/Clausius-Clapeyron/other equation.**

Step 2. **Calculate total pressure (P_{bp}) using**

$$P_{bp} = x_A P_A^*(T) + x_B P_B^*(T) + x_C P_C^*(T)$$

Step 3. **Use this calculated pressure to compute composition of vapor phase**

$$y_i = \frac{p_i}{P_{bp}} = \frac{x_i p_i^*(T)}{P_{bp}}$$

Dew Point Pressure

- The dew point pressure is defined as the pressure at which the first drop of liquid is formed when a vapor is compressed at constant temp.
- Dew point pressure (for a mixture of A, B and C) can be calculated using the equations

$$x_A = \frac{y_A P_{dp}}{p_A^*(T)}$$

$$\sum x_i = \sum \frac{y_i P_{dp}}{p_i^*(T)}$$

$$1.0 = \frac{y_A P_{dp}}{p_A^*(T)} + \frac{y_B P_{dp}}{p_B^*(T)} + \frac{y_C P_{dp}}{p_C^*(T)}$$

$$P_{dp} = \frac{1}{\dfrac{y_A}{p_A^*(T)} + \dfrac{y_B}{p_B^*(T)} + \dfrac{y_C}{p_C^*(T)}}$$

Now the liquid phase mol fractions can be calculated using the equation:

$$x_i = \frac{y_i P_{dp}}{P_i^*(T)}$$

The calculation of bubble point pressure and dew point pressure are easier because iterations are not involved in these calculations

PROBLEM

- Calculate the dew point pressure of a gas mixture containing 15 mol% B, 10 mol% T and 75 mol% Nitrogen at 80 ^{0}C. Also calculate the equilibrium composition in the liquid phase.
- Data

Benzene: A=6.89272; B=1203.531;C=219.888

Toluene: A=6.95805; B=1346.773; C=219.693

In Antonie equation use T in ^{0}C , N_2 non condensable

SOLUTION

- Vapor pressure of Benzene at 80 ^{0}C:

$$\log_{10} p^* = A - \frac{B}{T+C}$$

$$\log_{10} p_B^* = 6.89272 - \frac{1203.531}{80+219.888}$$

P_B*= 757.7 mm Hg

- Vapor pressure of Toluene at 80 ^{0}C:

$$\log_{10} p_T^* = 6.95805 - \frac{1346.773}{80+219.693}$$

P_T*= 291.2 mm Hg

Dew point pressure and mol fraction of T & B in liquid phase:

$$P_{dp} = \frac{1}{\dfrac{y_B}{p_B^*(T)} + \dfrac{y_T}{p_T^*(T)}}$$

$$P_{dp} = \frac{1}{\dfrac{0.15}{757.7} + \dfrac{0.1}{291.2}} = 1847 mm\,Hg$$

$$x_B = \frac{y_B P}{p_B^*(T)} = \frac{0.15 \times 1847}{757.7} = 0.366$$

$$x_T = \frac{y_T P}{p_T^*(T)} = \frac{0.1 \times 1847}{291.2} = 0.634$$