ASSIGNMENT CH-301

(SEPARATION PROCESS)

BINARY MIXTURE : Ethanol + 1-Heptane

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INTRODUCTION

In this work, we will:

1. Plot the **total pressure (P)** vs **mole fractions (x, y)** at a constant temperature (345 K) using Raoult's law.
2. Plot the **temperature (T)** vs **mole fractions (x, y)** at a constant pressure (e.g., 1 bar), applying the Antoine equation to find saturation pressures at different temperatures.
3. Plot **vapor phase composition (y)** vs **liquid phase composition (x)** at constant pressure (1 bar) to illustrate the relationship between the phases during equilibrium.

This study will involve numerical calculations performed in Excel to derive pressure, temperature, and composition values for the ethanol-heptane system. The results will be presented in graphical form to visualize the phase behaviour of this non-ideal binary mixture. Additionally, if experimental data for ethanol-heptane VLE behaviour is available, it will be used for comparison with the calculated results to evaluate the validity of the ideal solution assumption.

This approach is crucial for understanding the separation characteristics of ethanol and heptane, which differ significantly in their polarity and intermolecular forces, often leading to deviations from ideal behaviour in real-world applications.

METHODOLOGY

The vapor-liquid equilibrium (VLE) behaviour of the **ethanol + heptane** binary mixture is modeled under the assumption of an ideal gas in the vapor phase and an ideal solution in the liquid phase. To predict the phase behaviour, Raoult's law is applied to the liquid phase, and the ideal gas law is assumed for the vapor phase. The following steps outline the methodology used to calculate and plot the required phase diagrams.

1. Raoult's Law for Ideal Solutions

Raoult's law is applied to model the liquid phase behaviour of the binary mixture. For an ideal solution, the total pressure Ptotal is given by the sum of the partial pressures of each component:

$$P_{\text{total}} = x_1 P_1^{\text{sat}} + x_2 P_2^{\text{sat}}$$

Where:

- x1 and x2 are the mole fractions of ethanol and heptane in the liquid phase, respectively.
- P1sat and P2sat are the saturation vapor pressures of ethanol and heptane at the given temperature, calculated using the Antoine equation.

2. Antoine Equation for Saturation Vapor Pressure

The saturation vapor pressure for each component is calculated using the Antoine equation:

$$\log_{10} P_i^{\text{sat}} = A_i - \frac{B_i}{T + C_i}$$

Where:

- Pisat is the saturation pressure of component i (ethanol or heptane) in bar.
- T is the temperature in °C.
- Ai, Bi, and Ci are Antoine coefficients specific to ethanol and heptane.

3. Vapor Phase Composition

The composition of the vapor phase is calculated using Raoult's law, which gives the partial pressure of each component:

$$y_i = \frac{P_i}{P_{\text{total}}}$$

Where:

- Yi is the mole fraction of component i (ethanol or heptane) in the vapor phase.
- Pi is the partial pressure of component i, determined by $P_i = x_i P_i^{\text{sat}}$.

4. Numerical Calculation in Excel

To calculate the values of pressure, temperature, and composition at various points, an Excel spreadsheet is used.

5. Phase Diagrams

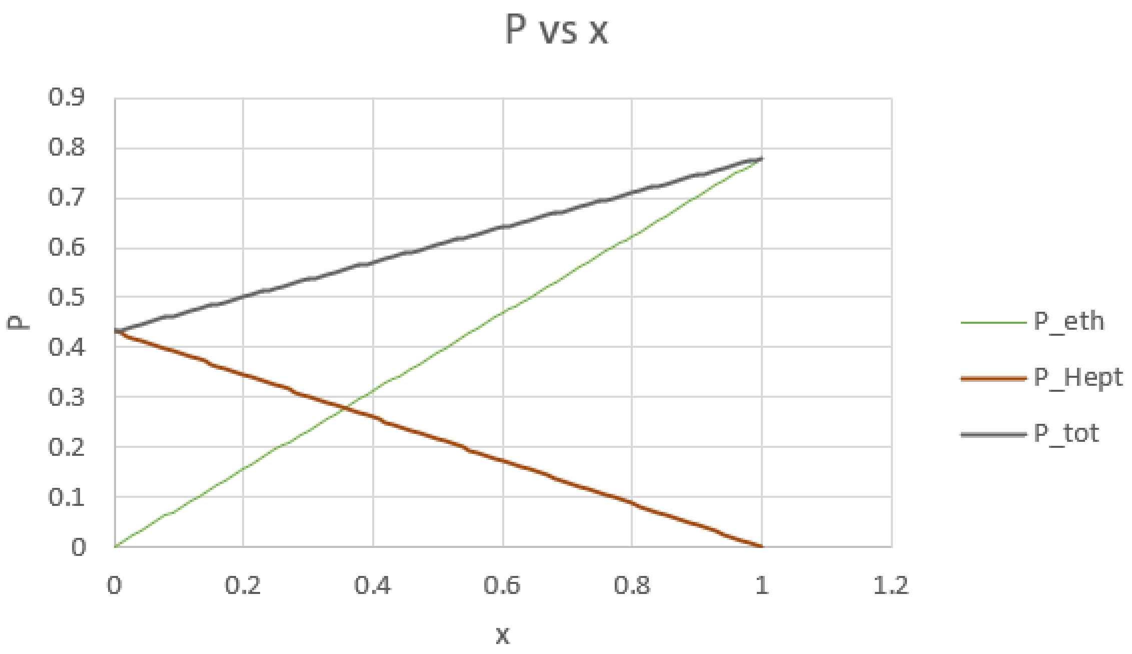
Three different phase diagrams are plotted based on the Excel calculations:

- **P vs x, y (at constant temperature)**: This plot shows the variation of total pressure with mole fractions of ethanol and heptane at a fixed temperature (345 K).
- **T vs x, y (at constant pressure)**: This plot illustrates the temperature variation with mole fractions at a constant pressure (1 bar), helping to identify the boiling points of different compositions.
- **y vs x (at constant pressure)**: This plot shows the relationship between the liquid-phase composition (x) and vapor-phase composition (y) at constant pressure (1 bar).

6. Comparison with Experimental Data

Experimental data was available for only Txy diagram, the theoretical predictions from Raoult's law will be compared against the experimental results.

FIGURES:


P vs x
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0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
P
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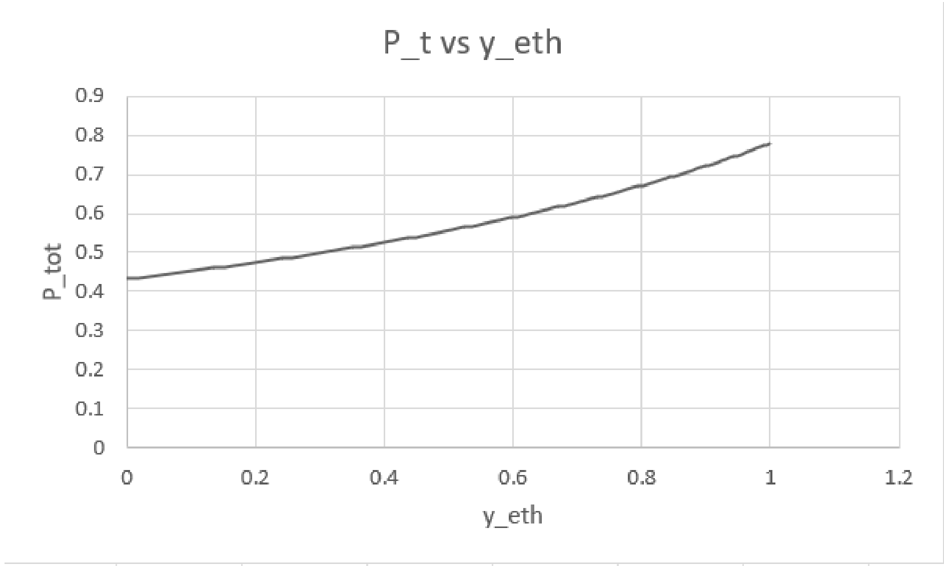
0.2
0.4
0.6
0.8
1
1.2
x
P_eth
P_Hept
P_tot


P_t vs y_eth
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0.6
0.5
0.4
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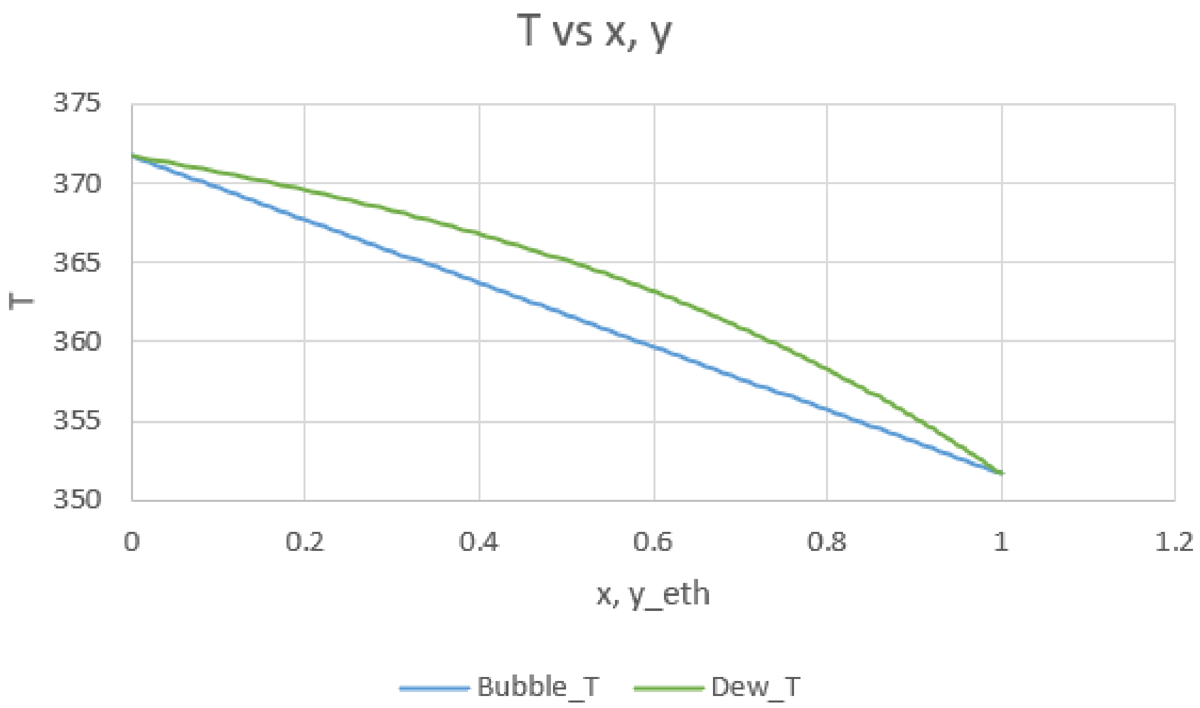
P_tot
0
0.2
0.4
0.6
0.8
1
1.2
y_eth


T vs x, y
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370
365
360
355
350
T
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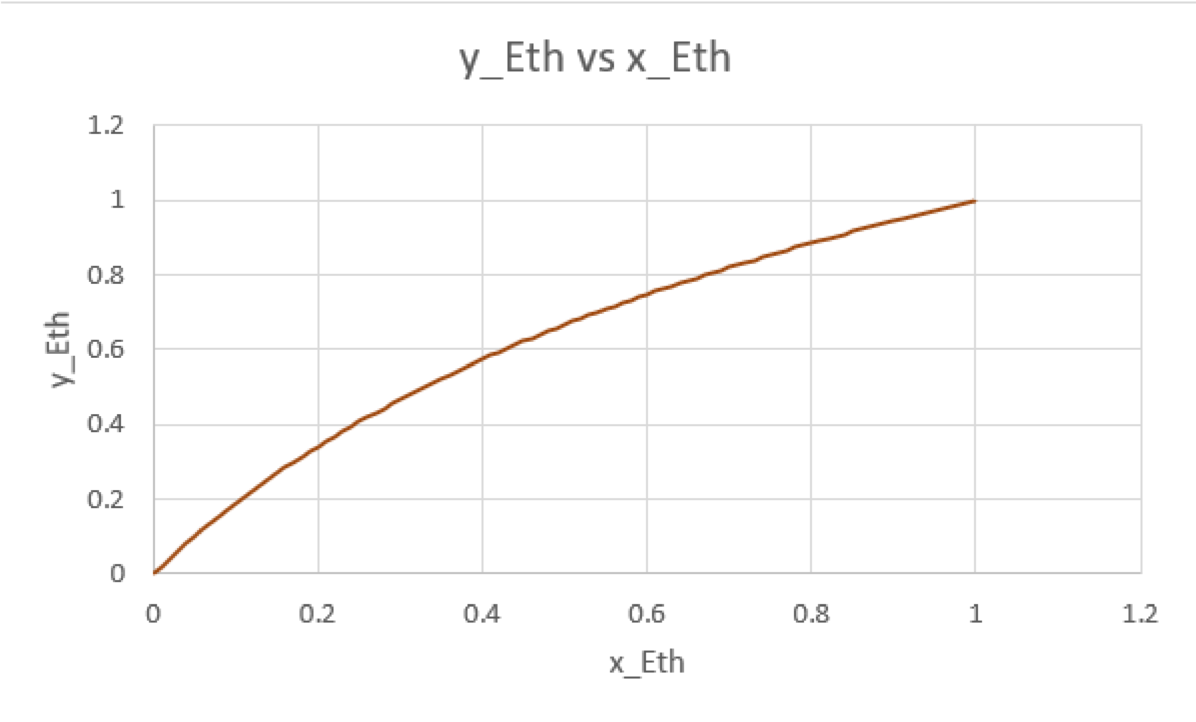
0.2
0.4
0.6
0.8
1
1.2
x, y_eth
Bubble_T
Dew_T


y_Eth vs x_Eth
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1
0.8
0.6
0.4
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0
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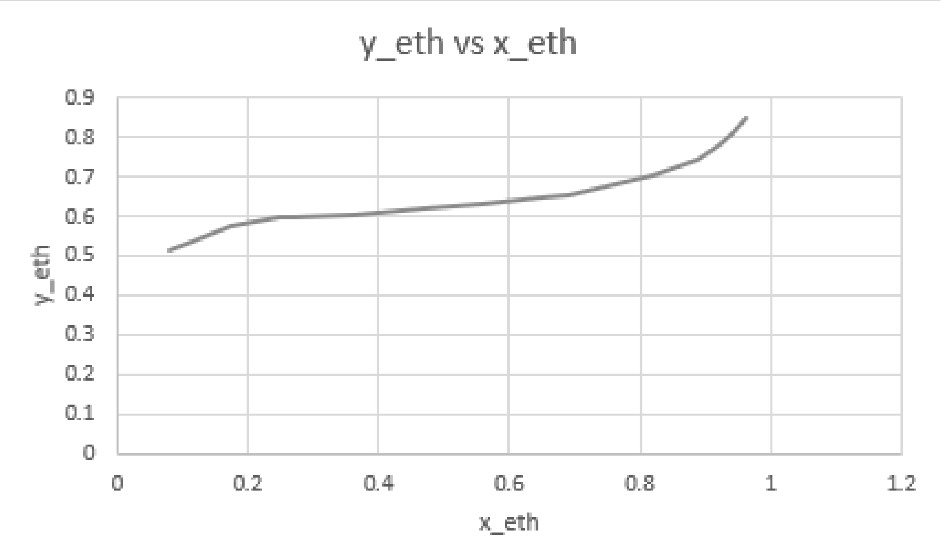
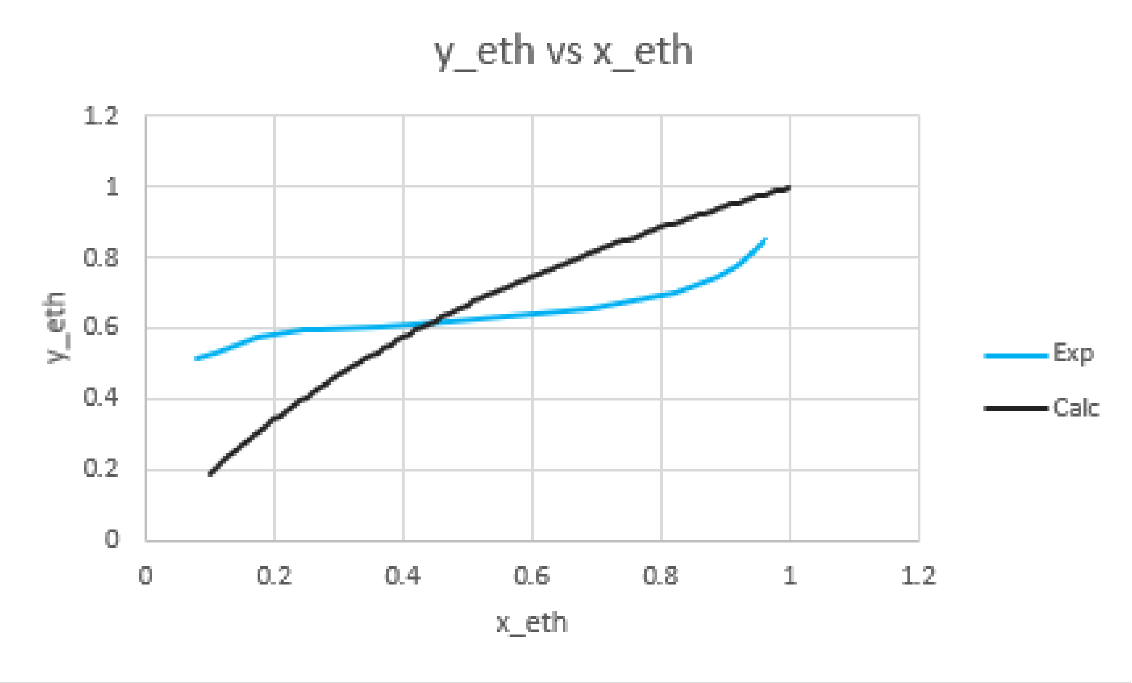
x_Eth



Experimental Txy Diagram



Comparision of Calculated and Experimental Data

CONCLUSION:

With this study we calculated and plotted graphs using the Raoult's Law.

Comparing the calculated data with Experimental data we can see above plot and can say, there is deviation from the ideal condition.