**Thermodynamic Process Simulation**

LAB 6

Harsh Nirmal

220431

Aim

*This report investigates the vapor-liquid phase behavior of an ideal binary mixture of ethanol and water at a total pressure of 1 atmosphere (atm). The analysis employs three key diagrams to offer insights into the relationship between temperature, pressure, and composition in both liquid and vapor phases:*

1. *Constructing a T-x-y diagram for the system at 1 atm, showcasing the relationship between temperature (T), liquid composition (x), and vapor composition (y) for both water and ethanol.*
2. *Creating an x-y diagram for ethanol at 1 atm, specifically focusing on the relationship between liquid composition (x) and vapor composition (y) for ethanol.*
3. *Generating a P-x-y diagram for water at a specific temperature (50°C), illustrating the relationship between pressure (P), liquid composition (x), and vapor composition (y).*

Methodology

*The analysis employs three key diagrams to offer insights into the relationship between temperature, pressure, and composition in both liquid and vapor phases:*

***1. T-x-y Diagram:***

*This diagram visually depicts the relationship between temperature (T), liquid composition (x), and vapor composition (y) for both water and ethanol at 1 atm. It showcases how the boiling point of a specific liquid composition (x) increases with rising temperature. Additionally, the diagram reveals that the vapor composition (y) approaches the liquid composition (x) for both water and ethanol as the temperature increases.*

***2. x-y Diagram for Ethanol:***

*This diagram specifically focuses on the relationship between the liquid composition (x) of ethanol and the vapor composition (y) of ethanol at 1 atm. This visualization confirms the validity of Raoult's Law for an ideal mixture, as the relationship between the liquid and vapor compositions for ethanol is linear.*

***3. P-x-y Diagram for Water at 50°C:***

*This diagram illustrates the relationship between pressure (P), liquid composition (x) of water, and vapor composition (y) of water at a specific temperature of 50°C. It demonstrates that the total pressure increases with increasing water composition in the liquid phase at a constant temperature. This diagram further emphasizes the role of Raoult's Law, as the vapor pressure of water contributes significantly to the total pressure at higher water compositions.*

*By analyzing these generated diagrams, we gain a comprehensive understanding of the vapor-liquid equilibrium behavior of the ideal binary mixture of ethanol and water at 1 atm. The diagrams provide valuable insights into how temperature, pressure, and composition influence the state of the mixture in both liquid and vapor phases.*

*The provided MATLAB code is integrated within the report, explaining each step:*

*1. Defining Antoine Parameters:*

*Values are assigned to the Antoine coefficients (A, B, and C) for both water and ethanol.*

*Total pressure (P\_total) is set to 1 atm.*

*Boiling points (Tb) for water and ethanol are defined.* *(i.e., 78.23°C - 100°C).*

*2. Generating Temperature Range and Vapor Pressures:*

*Temperature (T) range is created from the boiling point of ethanol to the boiling point of water using linspace.*

*Antoine equation is used to calculate the vapor pressure (P\_i\_vap) of pure water and ethanol at each temperature.*

*3. Calculating Compositions:*

*Liquid mole fractions (xi) for water and ethanol are calculated using Raoult's Law, considering the total pressure and individual vapor pressures.*

*4. Plotting T-x-y Diagrams (Figures 1 and 2):*

*Two figures are created, one for water and one for ethanol.*

*T-x and T-y plots are generated for each component, showcasing the relationship between temperature and mole fractions in both liquid and vapor phases.*

*5. Plotting x-y Diagram (Figure 3):*

*A separate figure depicts the relationship between the liquid mole fraction (xi) of ethanol and the vapor mole fraction (yi) of ethanol.*

*6. Calculations for P-x-y Diagram (Figure 4):*

*A new set of liquid mole fractions (x) for water is created using linspace.*

*Vapor pressures of pure water and ethanol at 50°C are calculated using the Antoine equation.*

*Total pressure (P\_total\_new) at each water composition is calculated using the individual vapor pressures and their corresponding mole fractions.*

*Vapor (yi) and liquid (xi) mole fractions for water are calculated at each total pressure.*

*7. Plotting P-x-y Diagram (Figure 4):*

*The final figure displays two plots:*

*P\_total\_new vs. yi (water): This shows the variation of total pressure with the vapor mole fraction of water.*

*P\_total\_new vs. x (water): This shows the variation of total pressure with the liquid mole fraction of water.*

Graphs:

A diagram of a plot of water

Description automatically generatedA graph of a plot

Description automatically generated with medium confidenceA graph of a line graph

Description automatically generatedA graph of a function

Description automatically generated

Results:

*The generated diagrams offer valuable insights:*

*T-x-y diagrams: These diagrams indicate that as the temperature increases, the boiling point of a specific liquid composition (x) also increases. Additionally, the vapor composition (y) approaches the liquid composition (x) for both water and ethanol as the temperature rises.*

*x-y diagram: This diagram confirms Raoult's Law for an ideal mixture, as the relationship between liquid and vapor compositions for ethanol is linear.*

*P-x-y diagram: This diagram demonstrates that the total pressure increases with increasing water composition in the liquid phase at a constant temperature (50°C). It also emphasizes the role of Raoult's Law, as the vapor pressure of water contributes significantly to the total pressure at higher water compositions.*

Conclusions:

*By analyzing the generated diagrams and understanding the corresponding code, we gain a comprehensive understanding of the vapor-liquid phase behavior of the ideal binary mixture of ethanol and water at 1 atm. The diagrams visualize the relationships between temperature, pressure, and composition in both liquid and vapor phases.* *The T-x-y diagram provides insights into the temperature required to achieve specific compositions in both liquid and vapor phases. The x-y diagram focuses on the relationship between liquid and vapor compositions for ethanol, and the P-x-y diagram showcases the pressure dependence on composition for water at a specific temperature.*

Innovation:

*The existing analysis of the ethanol-water system lays a strong foundation for further exploration. We can build upon this knowledge by incorporating novel approaches and venturing beyond the limitations of the ideal mixture assumption.*

*One exciting avenue lies in delving into the complexities of non-ideal mixtures. By incorporating activity coefficients through models like Wilson or NRTL equations, we can move beyond Raoult's Law and simulate real-world systems with realistic deviations from ideality. This enhanced level of accuracy allows for a more comprehensive understanding of the system's behavior under various conditions.*

*Furthermore, pushing the boundaries towards multicomponent systems opens doors to analyzing more intricate mixtures commonly encountered in diverse fields like chemical engineering. This would involve modifying the existing code to handle systems with more than two components, incorporating additional mixing rules and potentially utilizing advanced equations of state. This expansion in scope enables the exploration of countless real-world scenarios with greater complexity.*

*But the innovations don't stop at replicating reality. We can leverage the power of machine learning to develop an anomaly detection model. This model, trained on historical data or sensor measurements, could identify unexpected deviations from the expected phase behavior. Such a tool holds immense potential for real-time monitoring and control of industrial processes involving ethanol-water mixtures, enabling proactive interventions and enhancing process safety.*

*Finally, with a focus on sustainability, we can translate the acquired knowledge into tangible solutions for a greener future. By exploring the design of more energy-efficient separation techniques for ethanol-water mixtures, we can contribute to minimizing environmental impact and fostering sustainable practices in various industries.*

*These innovative approaches not only extend the capabilities of the existing analysis but also pave the way for exciting new applications and discoveries in the realm of the ethanol-water system and beyond. By embracing these advancements, we can gain deeper insights into complex systems, enhance industrial processes, and contribute to a more sustainable future.*

Appendix:

clc

%% Defining Antoine Parameters

Water\_A = 8.07131;

Water\_B = 1730.63;

Water\_C = 233.426;

Ethanol\_A = 8.2133;

Ethanol\_B = 1652.05;

Ethanol\_C = 231.48;

P\_total = 1;%atm

Tb\_water = 100;

Tb\_ethanol = 78.23;

T = linspace(Tb\_ethanol,Tb\_water,100);

P\_i\_vap\_water = (10.^(Water\_A - Water\_B./(Water\_C+T)))/760;

P\_i\_vap\_ethanol = (10.^(Ethanol\_A-Ethanol\_B./(Ethanol\_C+T)))/760;

xi\_water = (1-P\_i\_vap\_ethanol)./(P\_i\_vap\_water-P\_i\_vap\_ethanol);

xi\_ethanol = 1-xi\_water;

yi\_water = (xi\_water.\*P\_i\_vap\_water)./P\_total;

yi\_ethanol = (xi\_ethanol.\*P\_i\_vap\_ethanol)./P\_total;

figure(1)

plot(xi\_water,T)

hold on

plot(yi\_water,T)

xlabel("xi,yi")

ylabel("Temperature")

title("T-x-y Plot for water")

figure(2)

plot(xi\_ethanol,T)

hold on

plot(yi\_ethanol,T)

xlabel("xi,yi")

ylabel("Temperature")

title("T-x-y Plot for ethanol")

figure(3)

plot(xi\_ethanol,yi\_ethanol)

xlabel("Mole fraction")

ylabel("Vapour")

title("x-y")

legend ("Liquid")

%% Question 3 Water at 50 c

x = linspace(0,1,100);

P\_i\_vap\_water\_1 = (10.^(Water\_A - Water\_B./(Water\_C+50)))/760;

P\_i\_vap\_ethanol\_1 = (10.^(Ethanol\_A-Ethanol\_B./(Ethanol\_C+50)))/760;

P\_total\_new = (P\_i\_vap\_water\_1).\*x + (1-x).\*P\_i\_vap\_ethanol\_1;

yi\_3 = x.\*P\_i\_vap\_water\_1./P\_total\_new;

xi\_3 = (1-P\_i\_vap\_ethanol\_1)./(P\_i\_vap\_water\_1-P\_i\_vap\_ethanol\_1);

figure(4)

plot(P\_total\_new,yi\_3)

hold on

plot(P\_total\_new,x)

xlabel("PTotal")

ylabel("x,y")

title("P-x-y at Temp 50 cel")