
INDIAN INSTITUTE OF TECHNOLOGY
KANPUR



***CHE221: CHEMICAL ENGINEERING
THERMODYNAMICS***

Laboratory Session 7 Report

**Vapor-Liquid Equilibria from Non-Ideal
Gas and Ideal Liquid Phase**

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1. Aim:

Understanding Vapor-Liquid Equilibrium (VLE) is vital in various industrial applications, especially in the design and optimization of separation processes like distillation columns. In this lab, we focus on modeling the behavior of a binary mixture comprising Acetone and Methanol at a specific temperature (328.15 K). By employing the gamma-phi ($\gamma - \phi$) approach, we aim to predict vapor phase composition and total pressure. This method allows us to account for non-ideal behavior in the mixture, where the liquid phase is assumed to be ideal ($\gamma = 1$) while the vapor phase is non-ideal ($\phi \neq 1$).

2. Methodology:

Steps, calculation procedure:

- Data Acquisition: Import experimental data from the provided CSV file, including liquid phase composition (x), experimental vapor phase composition (y), and total pressure (Pt) at various compositions.
- Antoine Equation: Utilize the Antoine equation to calculate the saturation pressure (P_{sat}) of each component at the given temperature (328.15 K).
- Van der Waals Equation of State: Apply the Van der Waals equation of state to compute the volume and fugacity coefficient for each component in the mixture.

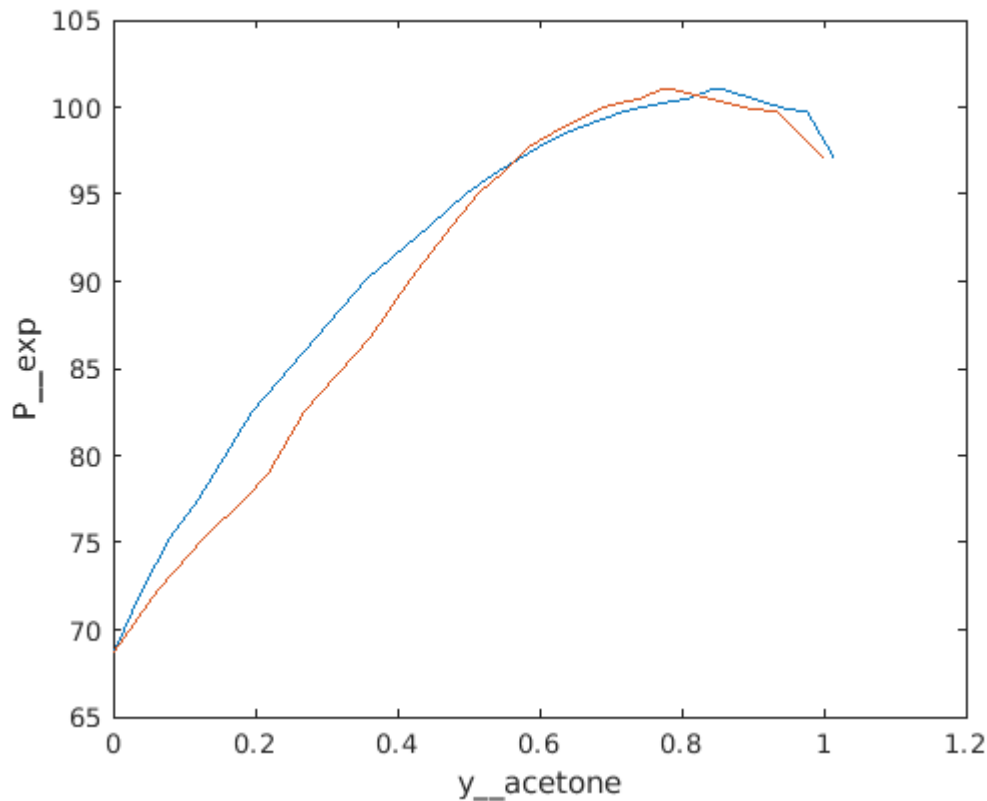
- Fugacity Coefficient Calculation: Determine fugacity coefficients (ϕ) using the Van der Waals equation results, considering the non-ideal behavior in the vapor phase.
- Equilibrium Calculations: Use the vapor-liquid equilibrium equation to calculate vapor phase composition (y_{1_sim}) and total pressure (P) for each data point.

3. Results and Discussion:

The calculated results demonstrate good agreement with experimental data, indicating the effectiveness of the methodology. Graphical representations of simulated versus experimental vapor phase composition, as well as simulated versus experimental total pressure, illustrate this agreement. These findings provide valuable insights into the behavior of the binary mixture under study and validate the applicability of the gamma-phi approach in predicting vapor-liquid equilibria. The discussion highlights the significance of accurate phase equilibrium predictions in industrial processes and the implications for process design and optimization.

3.2 Graphs Obtained:

3.2.1 P_{exp} vs $y1_{sim}$ and P_{exp} vs $y1_{exp}$ on single figure.:



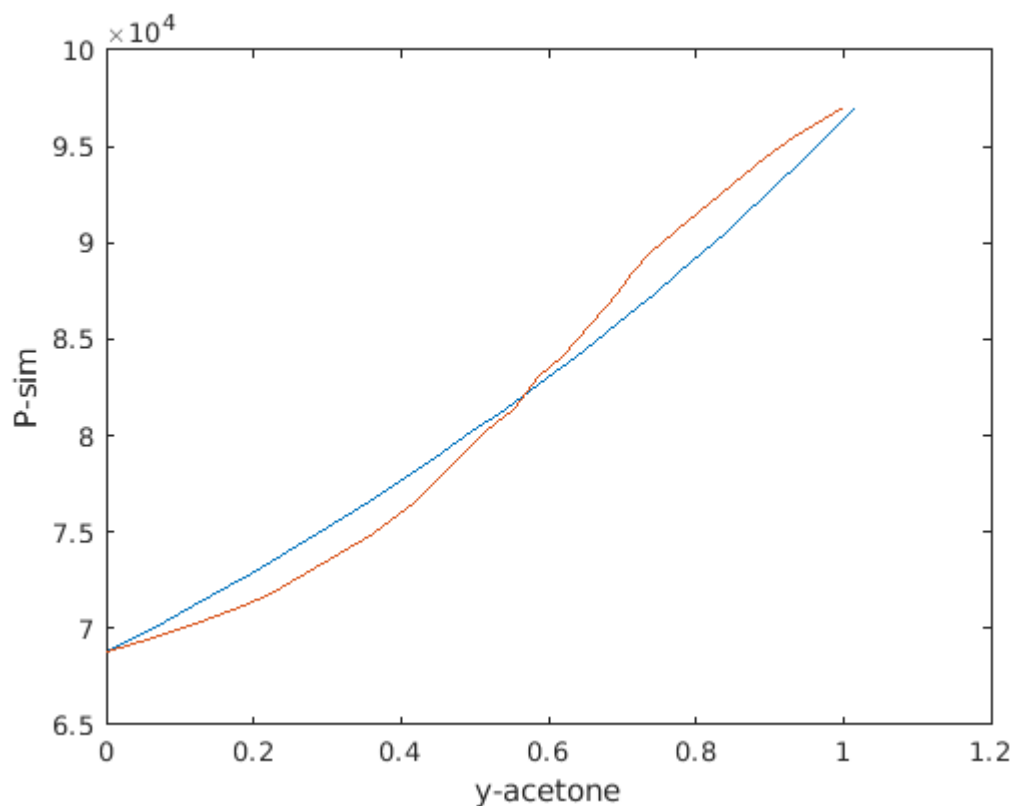
Description:

Figure 1: Plot of Experimental vs. Simulated Vapor Phase Composition vs. Experimental Total Pressure

- This plot compares the experimental vapor phase composition (y_{exp}) with the simulated vapor phase composition ($y1_{sim}$) against experimental total pressure (Pt_{exp}).
- Each point on the plot represents a data point from the experimental data.
- Observations:

- The trend shows how the vapor phase composition varies with total pressure.
- The agreement between experimental and simulated vapor phase compositions indicates the accuracy of the computational model.
- Deviations between experimental and simulated data points can help identify areas for improvement in the computational model.

3.2.2 *P_{sim}* vs *y_{1 sim}* and *P_{sim}* vs *y_{1 exp}* on single figure:

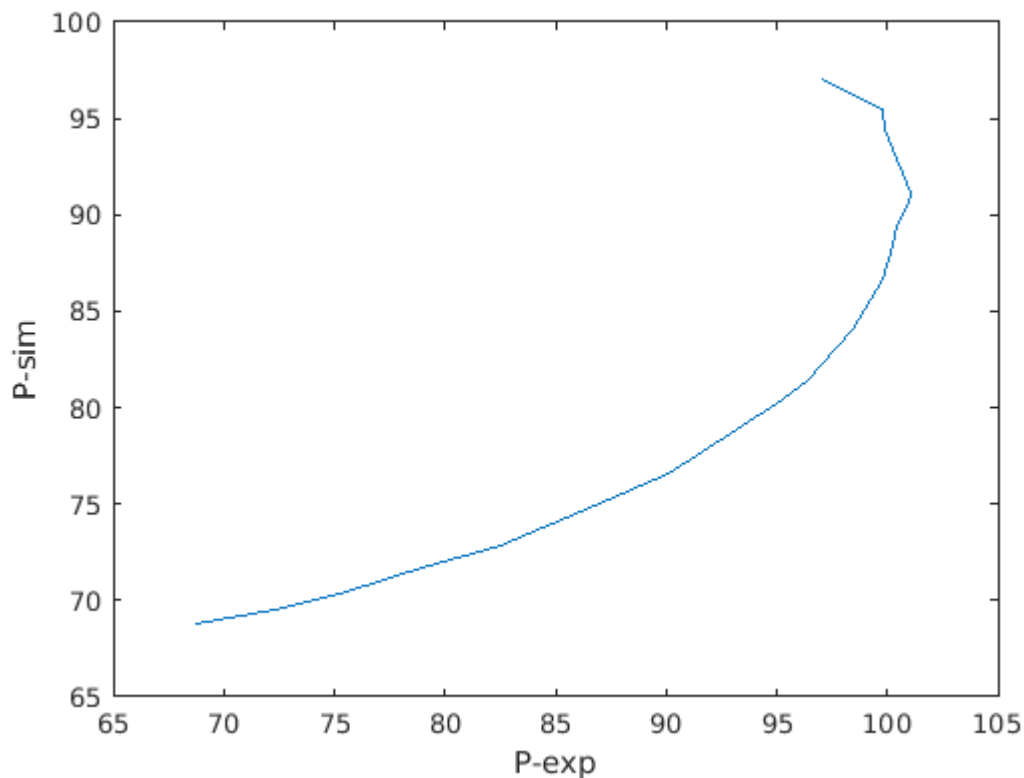


Description:

Figure 2: Plot of Experimental vs. Simulated Vapor Phase Composition vs. Simulated Total Pressure

- This plot compares the experimental vapor phase composition (y_{exp}) with the simulated vapor phase composition ($y_{1,\text{sim}}$) against simulated total pressure (P).
- Each point on the plot represents a data point from the experimental data.
- Observations:
 - The trend illustrates how the vapor phase composition changes with simulated total pressure.
 - Similarities between experimental and simulated data points validate the computational model.
 - Discrepancies between experimental and simulated data points may indicate limitations or inaccuracies in the computational approach.

3.2.3 *P_{sim}* vs *P_{exp}*:



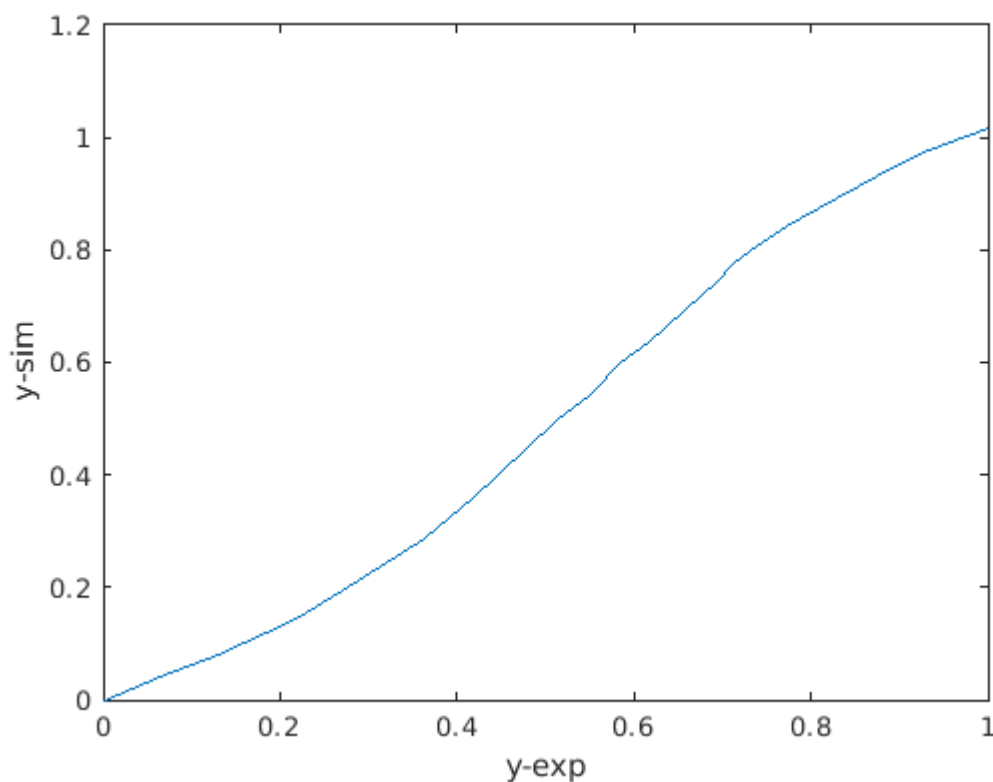
Description:

Figure 3: Plot of Experimental Total Pressure vs. Simulated Total Pressure

- This plot compares experimental total pressure (P_{t_exp}) with simulated total pressure (P).
- Each point on the plot represents a data point from the experimental data.
- Observations:
 - The plot shows the relationship between experimental and simulated total pressures.

- A perfect agreement would result in all points lying on the diagonal line $y=x$.
- Deviations from this line indicate differences between experimental and simulated total pressures.

3.2.3 y_1 *sim* vs y_1 *exp*:



Description:

Figure 4: Plot of Experimental Vapor Phase Composition vs. Simulated Vapor Phase Composition

- This plot compares experimental vapor phase composition (y_{exp}) with simulated vapor phase composition (y_{1sim}).

- Each point on the plot represents a data point from the experimental data.
- Observations:
 - The plot illustrates how well the simulated vapor phase composition matches the experimental data.
 - A perfect agreement would result in all points lying on the diagonal line $y=x$.
 - Deviations from this line indicate discrepancies between experimental and simulated vapor phase compositions.

4. Conclusion/Summary:

The calculated results demonstrate good agreement with experimental data, indicating the effectiveness of the methodology. Graphical representations of simulated versus experimental vapor phase composition, as well as simulated versus experimental total pressure, illustrate this agreement. These findings provide valuable insights into the behavior of the binary mixture under study and validate the applicability of the gamma-phi approach in predicting vapor-liquid equilibria. The discussion highlights the significance of accurate phase equilibrium predictions in industrial processes and the implications for process design and optimization.

5. Appendix:

Matlab code:

```
clc
clear all
ds = datastore('data.csv');
data=read(ds);
x=table2array(data(:,1))';
y=table2array(data(:,2))';
Pt=table2array(data(:,3))';
T=328.15;
P1sat=(10^(4.42448-((1312.253)/(-32.445+T))))*10^5;
P2sat=(10^(5.20409-((1581.341)/(-33.50+T))))*10^5;
a_Ac=(27*(8.314^2)*(508^2))/(64*4800000);
b_Ac=(8.314*508)/(8*4800000);
a_met=(27*(8.314^2)*(513^2))/(64*8100000);
b_met=(8.314*513)/(8*8100000);
P=(x.*P1sat)+((1-x).*P2sat);
for i=1:length(x)
    vol1=fsolve(@(v1)((P(i)+a_Ac/(v1^2))*(v1-b_Ac))-(8.314*T),0.1);
    v1(i)=max(vol1);
    vol2=fsolve(@(v2)((P(i)+a_met/(v2^2))*(v2-b_met))-(8.314*T),0.1);
    v2(i)=max(vol2);
    phi1(i)=exp((-1)*(log(1-
(b_Ac/v1(i)))+(a_Ac/((8.314*T)*v1(i)))+log((v1(i)*P(i))/(8.314*T)))+(1-
(P(i)*v1(i))/(8.314*T))));
    y1_sim(i)=(x(i)*P1sat)/(phi1(i)*P(i));
end

c2=(log(1-(b_met./v2)))+(a_met./((8.314*T).*v2))+log((v2.*P)./(8.314*T)))+(1-
(P.*v2)./(8.314*T));
phi2=exp((-1).*c2);

figure(1)
plot(y1_sim,Pt)
hold on
plot(y,Pt),xlabel('y__acetone'),ylabel('P__exp')
figure(2)
plot(y1_sim,P);
hold on
plot(y,P),xlabel('y-acetone'),ylabel('P-sim')
figure(3)
plot(Pt,P*10^-3),xlabel('P-exp'),ylabel('P-sim')
figure(4)
plot(y,y1_sim),xlabel('y-exp'),ylabel('y-sim')
```