**Thermodynamic Process Simulation**

LAB 5

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Aim

*The objective of this lab experiment is to analyze the fugacity coefficients and evaluate changes in Gibbs energy for ammonia at 100°C using various equations of state (EOS).* *Understanding the behavior of ammonia at different conditions .*

Methodology

*Understanding the behavior of ammonia at different conditions is crucial in various industrial and chemical processes. Fugacity, a measure derived from chemical potential, provides insights into the tendency of a substance to escape into another phase. Gibbs energy is a fundamental property used to characterize phase equilibria. In this experiment, we aim to calculate fugacity coefficients and evaluate changes in Gibbs energy using EOS models for ammonia at 100°C.*

*Fugacity Coefficient Calculation:*

*Fugacity coefficients are calculated using experimental data of compressibility factor (Z) and pressure (P). The Trapezoidal method of numerical integration is applied to obtain the fugacity coefficients.*

*The calculated fugacity coefficients are then compared with experimentally obtained values.*

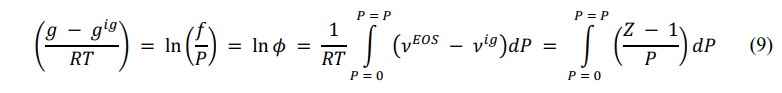
*Evaluation of Δg using Van der Waals EOS:*

*The Van der Waals EOS is employed to calculate changes in Gibbs energy (∆g) at 100°C. The EOS parameters such as critical temperature (Tc) and critical pressure (Pc) are utilized in the calculation.*

*Evaluation of Δg using Peng Robinson EOS:*

*Similarly, the Peng Robinson EOS is used to compute ∆g at 100°C. The EOS parameters including temperature correction (Tc), pressure correction (Pc), and acentric factor (ω) are considered.*

*Equations Used—*

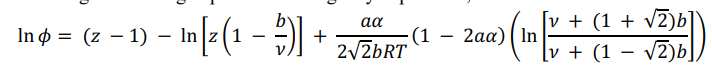
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Description automatically generated with medium confidence **Van der Waals**

A math equations with numbers and symbols

Description automatically generated **Peng Robinson**



Graph:

A graph showing the pressure and pressure

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*a. Fugacity Coefficient Analysis:*

*The experimentally obtained and calculated fugacity coefficients are plotted against pressure. Discrepancies and agreements between the two sets of data are discussed.*

*b. Evaluation of Δg using Van der Waals EOS:*

*The Δg values obtained using the Van der Waals EOS are presented and discussed in comparison with other EOS models.*

*c. Evaluation of Δg using Peng Robinson EOS:*

*The Δg values obtained using the Peng Robinson EOS are presented and compared with the Van der Waals EOS results.*

Conclusions:

*The experiment demonstrates the application of EOS models in calculating fugacity coefficients and evaluating changes in Gibbs energy for ammonia at 100°C. The results contribute to a better understanding of ammonia's phase behavior under specific conditions.* *The obtained results can be used to assess the accuracy of each EOS .* *This report investigates various methods for calculating the fugacity coefficient (ϕ) of ammonia (NH3) at 100°C using different equations of state (EOS). The results obtained from the Van der Waals (VdW), Peng-Robinson (PR) EOS are compared with experimentally obtained fugacity coefficient data. Additionally, the change in Gibbs energy (ΔG) is evaluated using each EOS.*

Appendix:

clc

clear

%% Reading data

data1 = readmatrix("LabThermo5/P-V.csv");

data2 = readmatrix("LabThermo5/Z-P.csv");

%%Q1a

% Calculating Fugacity coeff

Z = data2(:,2);

P = data2(:,1);

phi\_exp = data2(:,3);

for i = 2:size(P)

X = P(1:i);%

Y = (Z(1:i)-1)./X;

ln\_phi\_cal(i) = trapz(X,Y);

end

phi\_cal = exp(ln\_phi\_cal);

figure

plot(P,phi\_exp)

hold on

plot(P,phi\_cal)

xlabel("Pressure")

ylabel("Fugacity Coefficient")

legend('Experimental','Calculated')

%% Q1b

% vander Waals equation of state

P1 = data1(:,1);

V1 = data1(:,2);

R = 0.083;

Tc = 405.6; %K

Pc = 111.5; %atm

a = 27\*(R\*Tc)^2/(64\*Pc);

b = R\*Tc/(8\*Pc);

N = 1;

T = 373;

for i = 1:size(P1)

V\_ideal = R\*T./P1(i);

fun = @(V)(P1(i)+a./V^2).\*(V-b)-R\*T;

v\_sol = fsolve(fun,V\_ideal);

v\_van(i) = max(v\_sol);

z(i) = V1(i)./v\_van(i);

end

ln\_phi\_van = log(v\_van./v\_van-b)+(b./v\_van-b)-2\*a./v\_van\*R\*T-log(z);

del\_g = R\*T\*ln\_phi\_van;

%% Q3

a1 = 0.45724\*R^2\*T^2/Pc;

b1 = 0.0778\*R\*Tc/Pc;

w = 0.253;

Tr = T / Tc;

k = (1 + (0.37464 + 1.54226 \* w - 0.26992 \* w.^2) \* ((1 - Tr).^0.5)).^2;

alpha = (1+k.\*(1+(T/Tc)).^0.5)^2;

for i = 1:size(P1)

V\_ideal = R\*T./P1(i);

fun1 = @(Vpr)(R\*T ./ Vpr - b1) - a1\*alpha ./ 2 .\* sqrt(2) .\* b1\*R\*T\*(1 - 2\*alpha) .\* log((Vpr + (1 + sqrt(2)) .\* b1) ./ (Vpr + (1 - sqrt(2)) .\* b1));

v\_sol1 = fsolve(fun1, V\_ideal);

v\_pr(i) = max(v\_sol1);

z1(i) = V1(i)./v\_pr(i);

end

ln\_phi\_pr = (z1 - 1) - log(z1 .\* (1 - b1 ./ v\_pr)) + (a \* alpha) / (2 \* sqrt(2) \* b1 \* R \* T)\*(1 - 2 \* a1 \* alpha) \* log((v\_pr + (1 + sqrt(2)) .\* b1) ./ (v\_pr + (1 - sqrt(2)) .\* b1));

delg\_pr = R\*T\*ln\_phi\_pr;

% V\_vander(size(P1)) = R\*T./(P1(size(P1))+a./V1(size(P1)).^2)+b;

% V\_vander\_trans = transpose(V\_vander);

%

% z = a-1./V1\*R\*T;

%

%

% for j = 1:size(P1)

% ln\_phi1(j) = log(V1(j)./V1(j)-b)+b./V1(i)-b-2\*a./V1(j)\*R\*T-log(z);

% end

Request---

Sir, please consider this code for evaluation as the submitted code has the issue of dot operation in the peng robbinson equation therefore showing the error. The code is exactly the same with no changement only the dot operations are added in the equations which showed the error.