

CHE221A

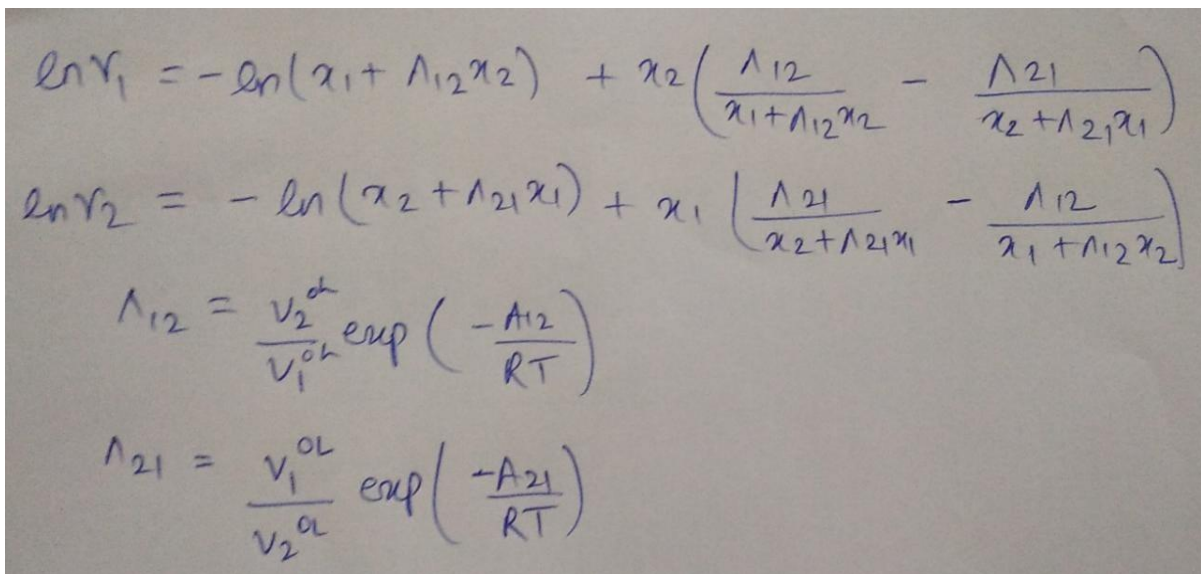
Computational Assignment

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System: Water and Morpholine

Activity Coefficient Model: Wilson

Equations involved in Wilson Model:


$$\ln \gamma_1 = -\ln(x_1 + \Lambda_{12}x_2) + x_2 \left(\frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2} - \frac{\Lambda_{21}}{x_2 + \Lambda_{21}x_1} \right)$$
$$\ln \gamma_2 = -\ln(x_2 + \Lambda_{21}x_1) + x_1 \left(\frac{\Lambda_{21}}{x_2 + \Lambda_{21}x_1} - \frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2} \right)$$
$$\Lambda_{12} = \frac{V_2^{\text{ol}}}{V_1^{\text{ol}}} \exp\left(-\frac{A_{12}}{RT}\right)$$
$$\Lambda_{21} = \frac{V_1^{\text{ol}}}{V_2^{\text{ol}}} \exp\left(-\frac{A_{21}}{RT}\right)$$

The values of A_{12} , A_{21} , V_1^{ol} , and V_2^{ol} are given.

Antoine's Equation:

The values of the parameters of Antoine's Equation for Water and Morpholine are provided.

A dataset consisting of experimental values of T , x_1 , y_1 was also provided. The data in the tabular form is shown below:

EXPERIMENTAL DATA			
T	DEG C	X1	Y1
113.67		.0811	.1758
109.10		.1834	.3427
107.35		.2242	.4458
105.23		.2883	.5115
102.78		.3736	.5928
101.61		.4287	.6370
100.19		.5135	.6949
97.41		.6899	.8211
96.67		.7173	.8398
95.27		.8084	.9042
93.86		.8792	.9457
93.75		.8983	.9554
92.92		.9385	.9747
92.69		.9521	.9803
92.42		.9816	.9923

Analysis of the system:

The system has 2 degrees of freedom, i.e. we need two parameters to solve further. The value of Total Pressure is provided with the data. Now, we need to assume one parameter to make the degree of freedom of the system 0.

I assumed x_1 s (mole fraction in liquid phase) and moved forward with further calculations.

Algorithm Used:

- Made an array of dimensions 50 x 1 consisting of different values of x_i .
- Since the total pressure of the system is known. I calculated T_{1sat} and T_{2sat} for the two components. Thereafter calculated the Temperature of the system using:

$$T = T_1^{sat} * x_1 + T_2^{sat} * (1-x_1)$$

- For each value of x_1 , I calculated corresponding values of γ_1 & γ_2 . Thereafter calculated P_{sat} using Antoine's Equation.
- After calculating the total pressure, I calculated the corresponding y_i s of the system.

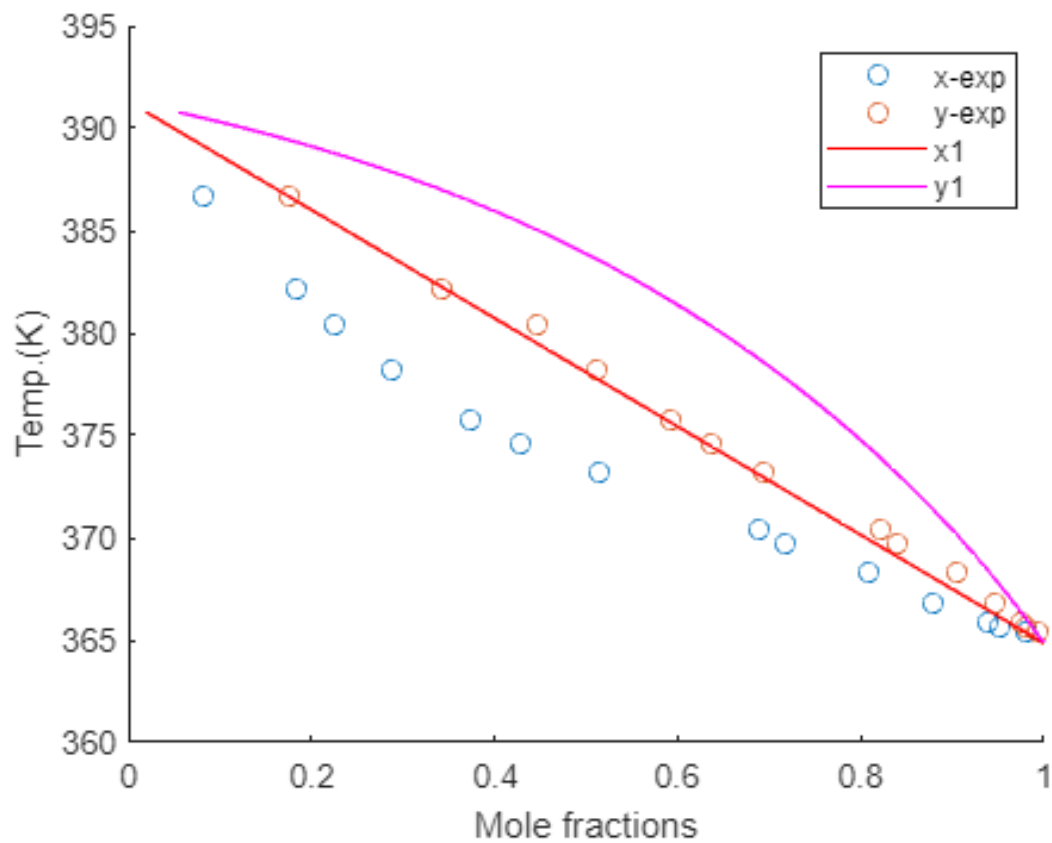
$$P = P_1^{sat} * x_1 + P_2^{sat} * (1-x_1)$$

- Repeat the above step until y_1+y_2 converges to 1. I selected a threshold value of 0.0001 to check for convergence.
- If for a particular iteration,

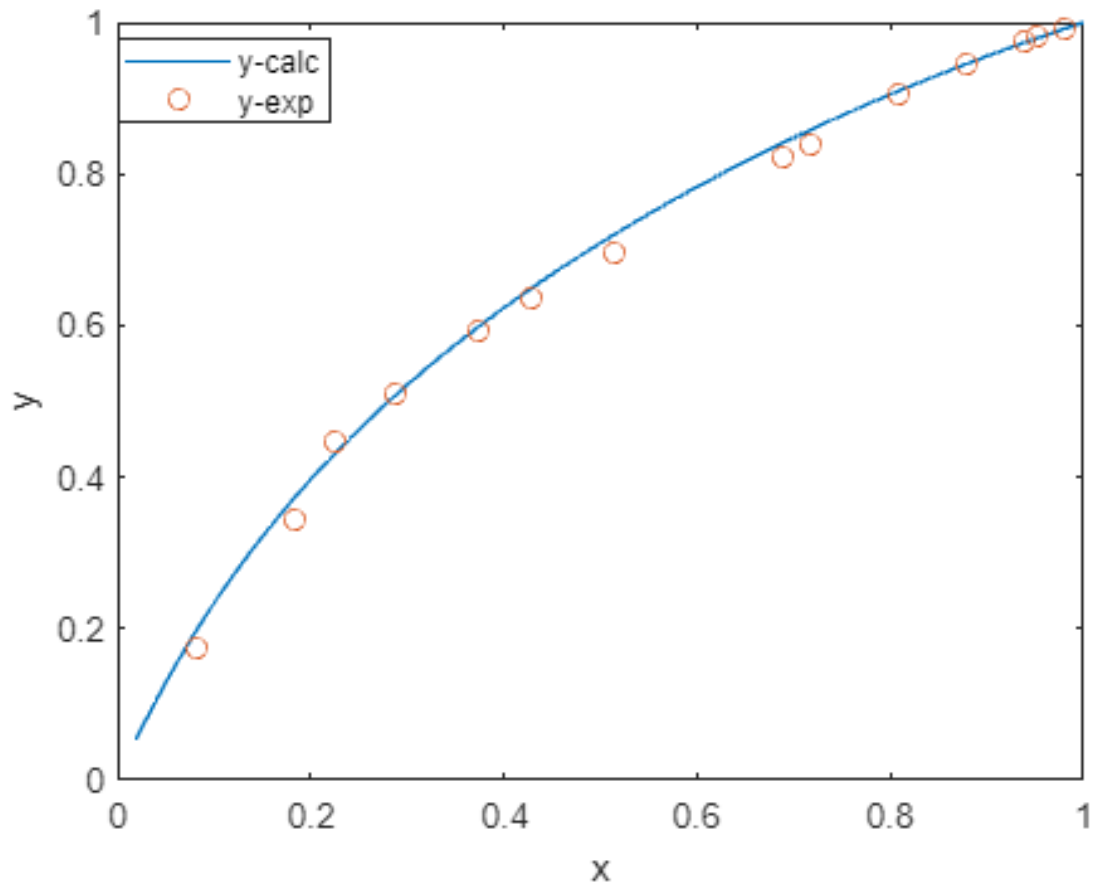
- $y_1 + y_2 > 1$, This implies that there is more vapour in the system. Hence, the temperature is lowered by a small amount (0.001).
- $y_1 + y_2 < 1$, This implies that there is less vapour in the system. Hence, the temperature is increased by a small amount (0.001).
- When $y_1 + y_2$ converges to 1, we store the corresponding value of y_1 in an array.

Required Graphs:

- T vs x,y plot



- x vs y plot



Code:

```
% Writing known Parameters
p=0.751;    % Total Pressure
% Antoine's Equation Parameters

A1=8.07131;

B1=1730.630;

C1=233.426;

A2=7.16030;

B2=1447.700;

C2=210.000;

% Threshold values

eps=1e-4;
```

```

dT=1e-3;

% Wilson Parameters

A12=1675.0732;

A21=-1508.1875;

% Volume of pure liquid components

v1=18.07; %water

v2=87.51; %morpholine

% Initialising x1, y1 & Temp

x1=ones(50,1);

y1=ones(50,1);

Temp=ones(50,1);

x1(1)=0.02;

for i=2:50

    x1(i)=x1(i-1)+0.02;

end

T_sat1=(B1/(A1-log10(p*750.062)))-C1+273;

T_sat2=(B2/(A2-log10(p*750.062)))-C2+273;

% Calculating for each x1

for i=1:50

    x11=x1(i); % x1

    x12=1-x1(i); % x2=1-x1

    Temp(i)=T_sat1*x11+T_sat2*x12;

    % Wilson parameters calculation

    lamda12=(v2/v1)*exp(-A12/(1.9872*Temp(i)));

    lamda21=(v1/v2)*exp(-A21/(1.9872*Temp(i)));

    gamma1=exp(-log(x11+(lamda12*x12))+x12*((lamda12/(x11+(lamda12*x12)))-(lamda
    21/(x12+(lamda21*x11)))));

```

```
gamma2=exp(-log(x12+(lamda21*x11))+x11*((lamda21/(x12+(lamda21*x11)))-(lamda
12/(x11+(lamda12*x12)))));
```

```
P_sat2=0.00133322*(10^(A2-(B2/(C2+(Temp(i)-273)))));
```

```
P_sat1=0.00133322*(10^(A1-(B1/(C1+(Temp(i)-273)))));
```

```
P_t=P_sat1*gamma1*x11+P_sat2*gamma2*x12;
```

```
y11=(gamma1*x11*P_sat1)/P_t;
```

```
y12=(gamma2*x12*P_sat2)/P_t;
```

```
while(abs((y11+y12)-1)>eps)
```

```
    if(y11+y12<1)      %Less vapour, hence increase Temperature
```

```
        Temp(i)=Temp(i)+dT;
```

```
    else                %More vapour, hence decrease Temperature
```

```
        Temp(i)=Temp(i)-dT;
```

```
end
```

```
lamda12=(v2/v1)*exp(-A12/(1.9872*Temp(i)));
```

```
lamda21=(v1/v2)*exp(-A21/(1.9872*Temp(i)));
```

```
gamma1=exp(-log(x1+(lamda12*x12))+x12*((lamda12/(x11+(lamda12*x12)))-(lamda2
1/(x12+(lamda21*x11)))));
```

```
gamma2=exp(-log(x2+(lamda21*x11))+x11*((lamda21/(x12+(lamda21*x11)))-(lamda1
2/(x11+(lamda12*x12)))));
```

```
P_t=P_sat1*gamma1*x11+P_sat2*gamma2*x12;
```

```
y11=(gamma1*x11*P_sat1)/P_t;
```

```
y12=(gamma2*x12*P_sat2)/P_t;
```

```
end
```

```
y1(i)=y11;
```

```
end
```

```
% Reading experimental data
```

```

f="experimental.txt";

M=readmatrix(f);

Texp=M(:,1);

x_exp=M(:,2);

y_exp=M(:,3);

Texp=Texp+273;

% Plotting T vs x,y

figure

scatter(x_exp,Texp);

hold on;

scatter(y_exp,Texp);

hold on;

plot(x1,Temp, '-r');

xlim([0,1]);

hold on;

plot(y1,Temp, '-m')

xlabel('Mole fractions');

ylabel('Temp. (K) ');

legend('x-exp', 'y-exp', 'x1', 'y1');

hold off;

% Plotting x vs y

figure

plot(x1,y1);

xlim([0,1]);

hold on;

scatter(x_exp,y_exp);

xlabel('x');

```

```
ylabel('y');  
  
legend('y-calc','y-exp');  
  
hold off;
```

-----**THANK YOU**-----