# CHE221A
# Computational Assignment

- Sneh Omer
(211041)

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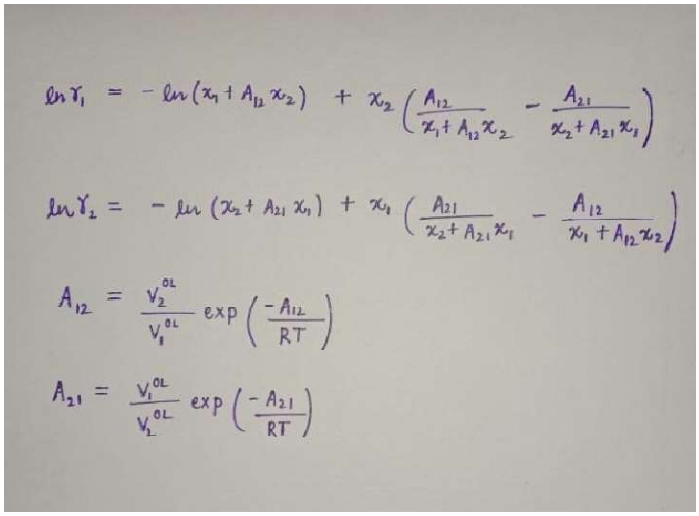
## System – Water and Morphine
## Activity Coefficient Model – Wilson

## Equations involved in Wilson Model




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, x1, y1 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 $x_i$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 xi.
- Since the total pressure of the system is known. I calculated T1sat and T2sat for the two components. Thereafter calculated the Temperature of the system using:

$$T = T_1^{sat} * x1 + T_2^{sat} * (1-x1)$$

- For each value of x1, I calculated corresponding values of gamma1 & gamma2. Thereafter calculated P_sat using Antoine's Equation.
- After calculating the total pressure, I calculated the corresponding $y_i$s of the system.

$$P = P_1^{sat} * x1 + P_2^{sat} * (1-x1)$$

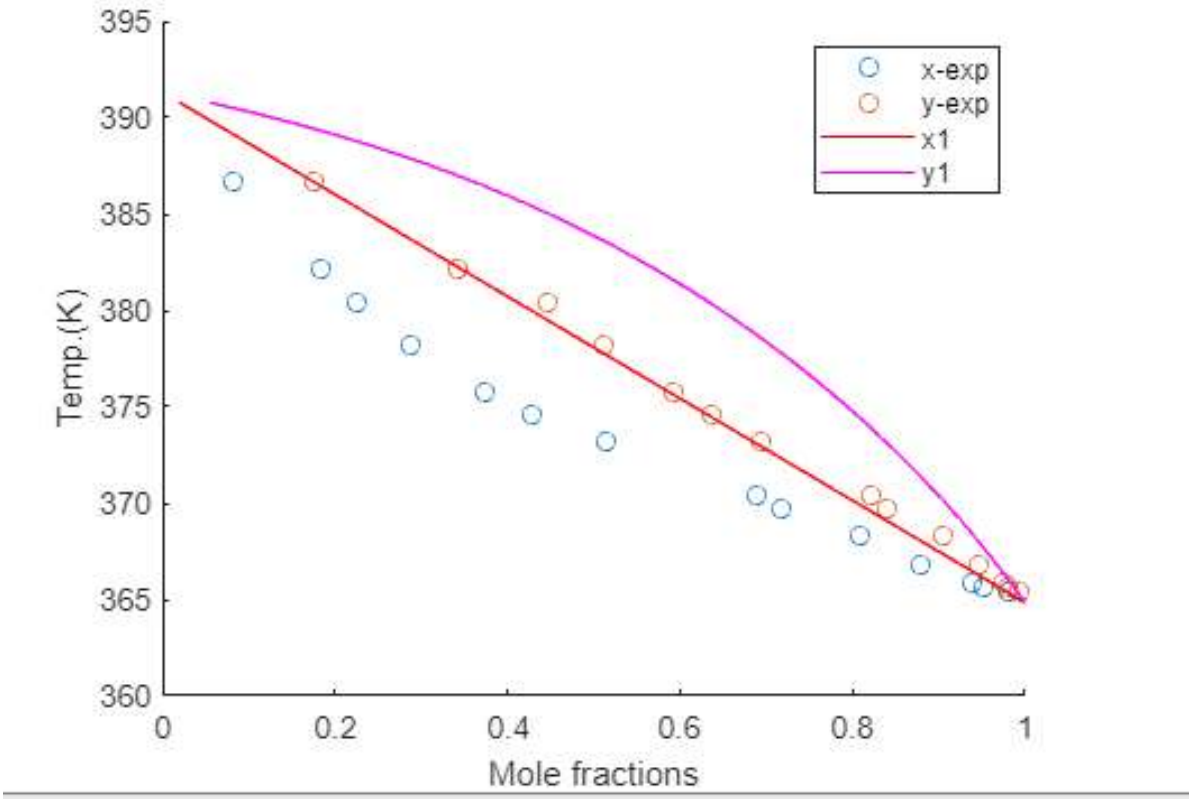
- Repeat the above step until y1+y2 converges to 1. I selected a threshold value of 0.0001 to check for convergence.
- If for a particular iteration,

- y1+y2>1, This implies that there is more vapour in the system. Hence, the temperature is lowered by a small amount (0.001).
- y1+y2<1, This implies that there is less vapour in the system. Hence, the temperature is increased by a small amount (0.001).

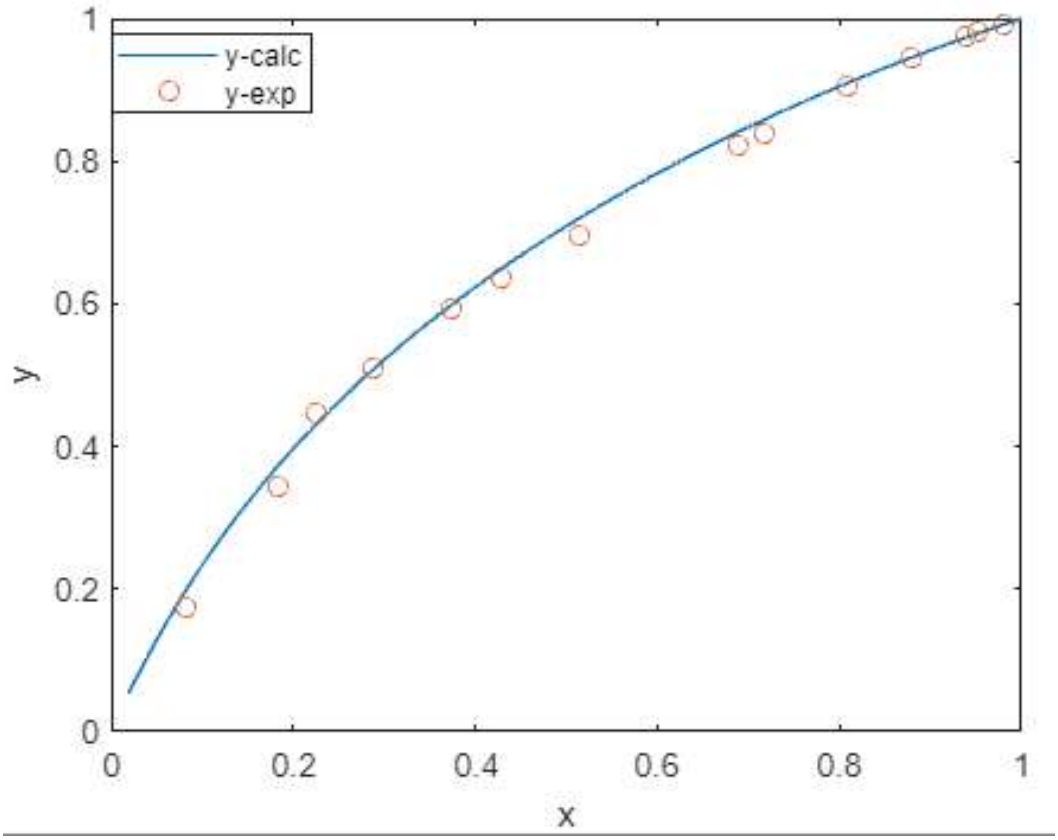
- When y1+y2 converges to 1, we store the corresponding value of y1 in an array.

## 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**----------