Computational Assignment

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AIM- To verify modified Raoult's law with the help of activity coefficients and Antoine's equation.
SYSTEM- Water and 4-Methyl 2-Pentanol
ACTIVITY COEFFICIENT MODEL- Van Laar Model

$$\ln\Upsilon_1=A_{12}\{(A_{21}*x_2)/(A_{12}*x_1+A_{21}*x_2)\}^2$$
$$\ln\Upsilon_2=A_{21}\{(A_{12}*x_1)/(A_{12}*x_1+A_{21}*x_2)\}^2$$

where, $A_{12}=1.2935$ and $A_{21}=5.8737$

ANTOINE's EQUATION (for calculating Saturation Pressure**)**

$$\log[p_i^o]=A-B/(T+C)$$

where for our system
FOR WATER: (for the temperature Range of 1-100^o Celsius)

A=8.07131
B=1730.630
C=233.426

FOR 4-Methyl 2-Pentanol: (for the temp. Range of 25-133^o Celsius)

A=8.46706
B=2174.869
C=257.780

MODIFIED RAOULT's LAW- $Py_i=x_i*\Upsilon_i*P_i^{sat}$
Total Pressure- 760mm Hg (Given)

PROCEDURE -
Degree of Freedom Analysis-
For the system of Water and 4-Methyl 2-Pentanol we have total 5 variables to calculate i.e., x_1, x_2, y_1, y_2 and T(Υ is the function of x and P_{sat} is the function of Temperature). To find the value of these we need 5 equations to solve. But we only have 4 of the equations.

$$Py_1=x_1*\Upsilon_1*P_1^{sat} \quad \text{----------(1)}$$
$$Py_2=x_2*\Upsilon_2*P_2^{sat} \quad \text{----------(2)}$$
$$x_1+x_2=1$$
$$y_1+y_2=1$$

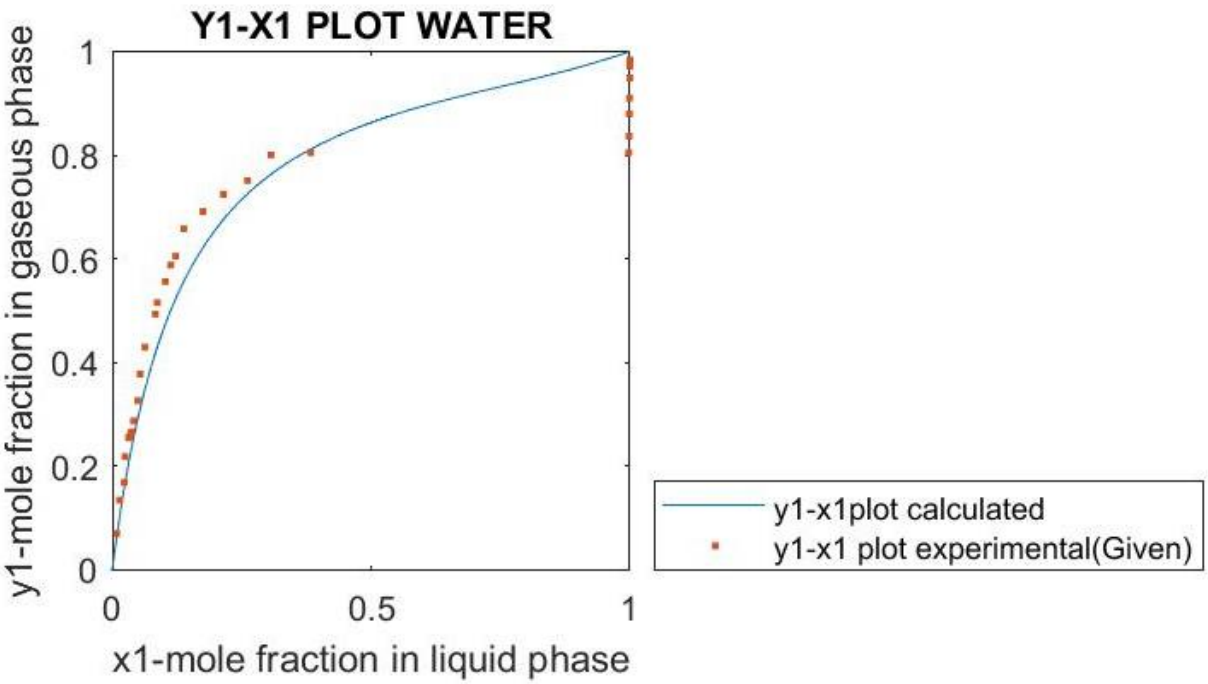
So, in order to find different set of Values for all the variables we have to vary one variable in some range and then calculate other variables with respect to that variable.
I have varied x_1 from 0 to 1 with a gap of 0.01 for this purpose and then calculated Υ_i (as it is the function of x_1). By adding equation (1) and equation (2) we will get

$$P= x_1*\Upsilon_1*P_1^{sat}+ x_2*\Upsilon_2*P_2^{sat}$$

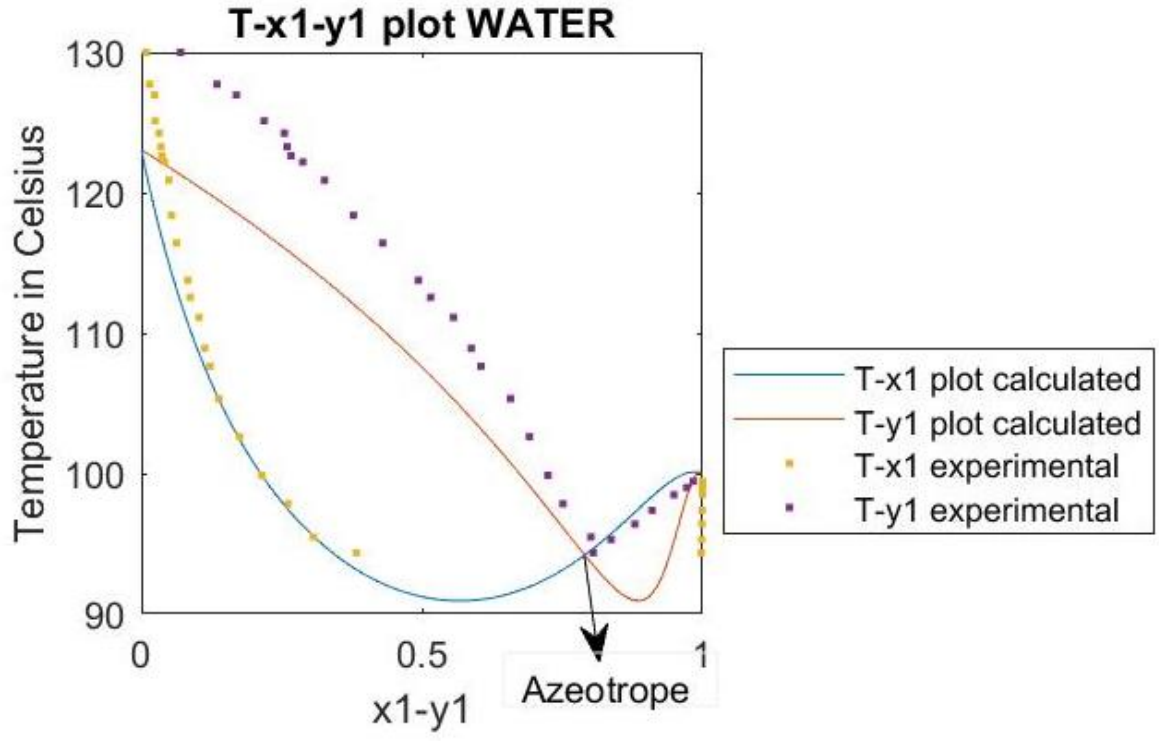
Here we know the total Pressure as it is given in the question (=760mm of Hg) and Υ is the function of x and P^{sat} is the function of Temperature only. Simplifying this equation we will get that only Temperature is the variable here as we are varying x_1.
Therefore, we will calculate respective Temperatures for respective x_1.
Till Now, we have solved for x_1(therefore x_2) and Temperature(T).
For the calculation of y_1 we will use our equation (1) and hence find y_2.
Then we will plot the curves for (y-x) and (T-x-y) by using these values.
And then we will compare our calculated data with the experimental data.

PLOTS-

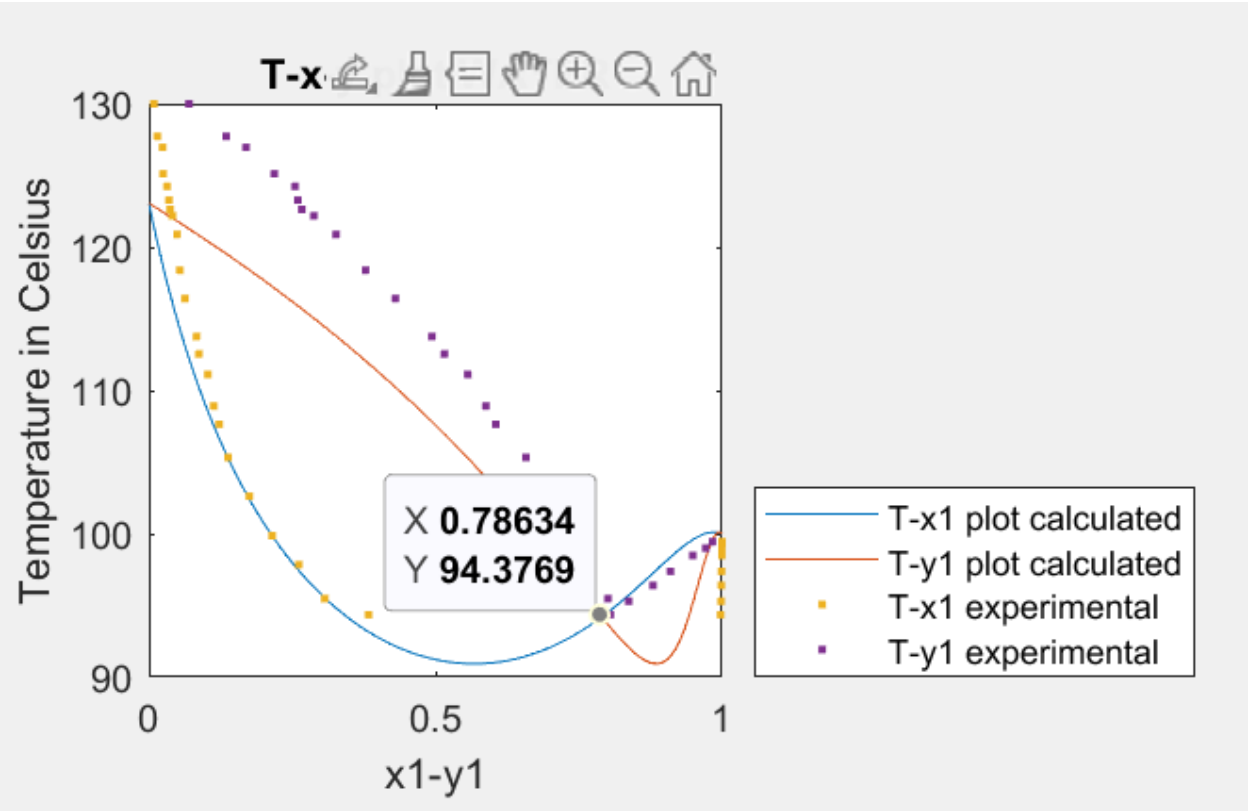
y vs x diagram



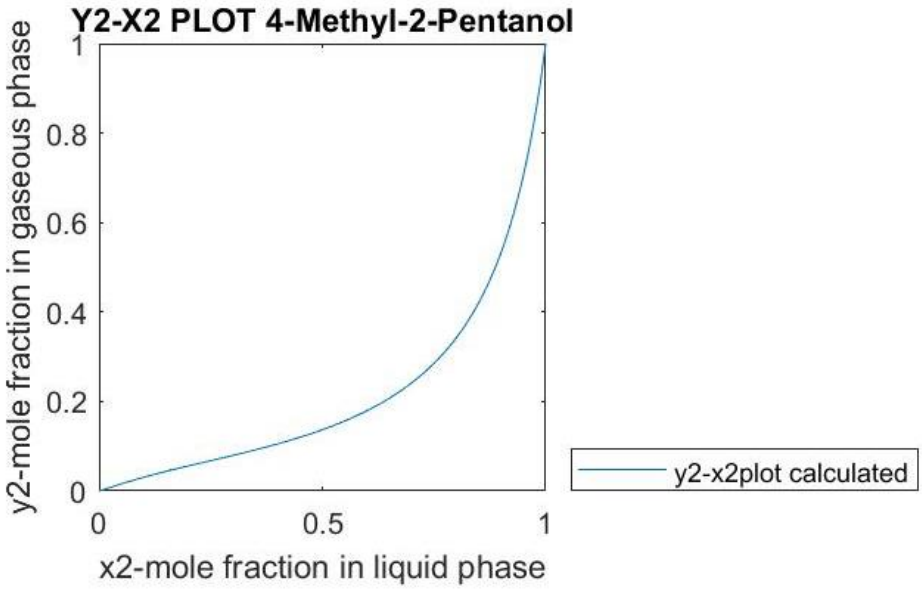
ISOBARIC T vs x,y Diagram

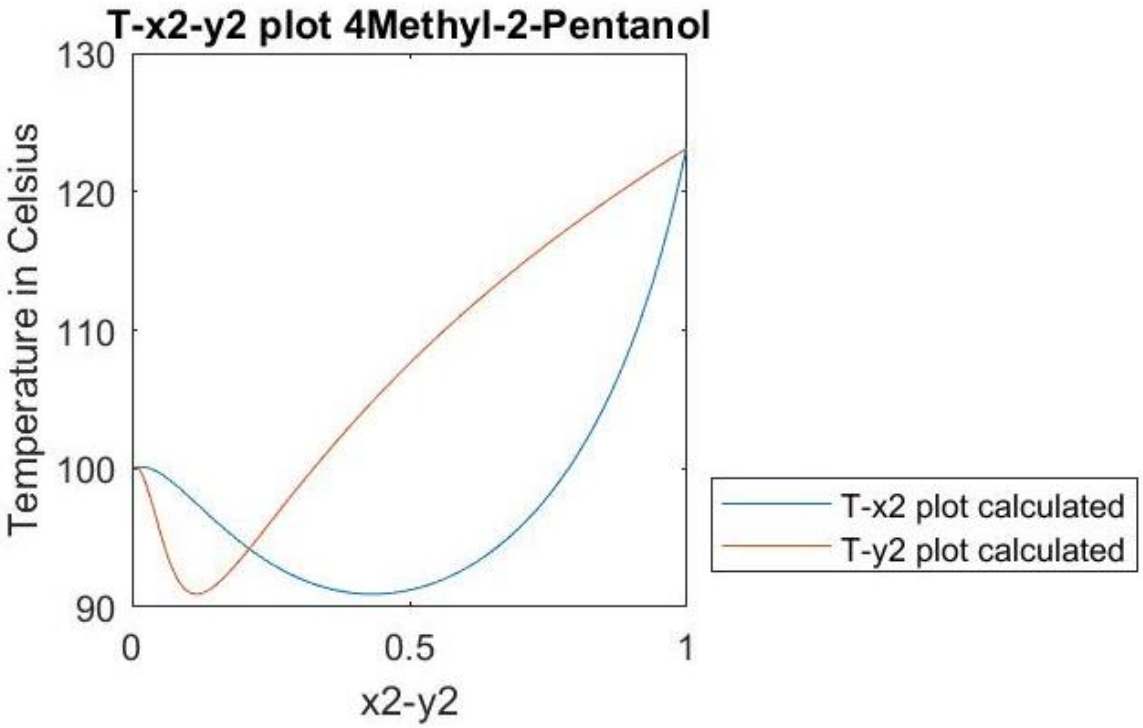


<u>CONCLUSION</u>- We will get a very beautiful curve between T and x-y and y vs x. We can see some deviations in between our results and experimental data, it is because of the saturated pressure that we have calculated. Those values are only limited to a range of temperatures.
Also, in addition to that we can also see the formation of an **azeotropic mixture (minimum boiling)** at the temperature of 94.3769^{o}C.



SOME MORE GRAPHS




T-x2-y2 plot 4Methyl-2-Pentanol
Temperature in Celsius
130
120
110
100
90
0
0.5
1
x2-y2
T-x2 plot calculated
T-y2 plot calculated

THANKS!