Simutech Assignment 1

Project: Distillation Column Design

Group Members:

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2. Sanidhya Singh

System Used:

1-Butanol and Methacrylic acid

Dataset Used: (As a csv file in the .zip folder)

(1-> 1-Butanol and 2-> Methacrylic acid)

	T(deg C)	x1	y1
0	72.50	0.00	0.00
1	67.02	0.05	0.17
2	64.40	0.10	0.32
3	60.23	0.20	0.53
4	56.65	0.30	0.68
5	53.34	0.40	0.80
6	50.40	0.50	0.86
7	48.12	0.60	0.92
8	46.05	0.70	0.95
9	44.15	0.80	0.98
10	42.50	0.90	0.99
11	41.90	0.95	1.00
12	41.20	1.00	1.00

Note:

This dataset is the experimental dataset. We will do our calculations as given in the question and then compare them with this dataset.

Work allotment:

Sanidhya-> Plotting of y v/s x in Q1 and Q2(i)

Harsh-> Plotting in DWsim software Q2(ii)

Q1) For your selected binary system, assuming it is an ideal system (i.e. Raoult's law is directly valid, and there is no deviation from ideal behaviour), Plot y v/s x (Vapour-Liquid equilibrium) curve.

Equation used:

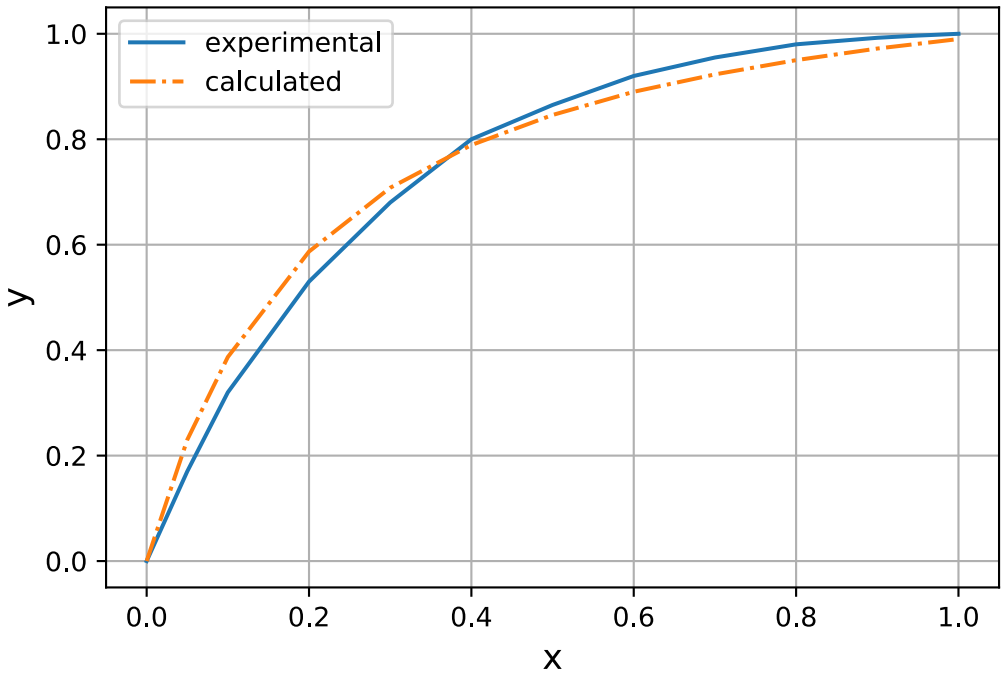
$$y_i P = x_i P_i^{sat}$$

Methodology:

We have 4 parameters here T, P, x, and y.
We have done all the calculations assuming total pressure as constant 20mmHg.
Using the Gibbs phase rule, we have to fix two parameters to fix the system state.
Fixing x, We have calculated T and y.
For calculation purpose, We have fixed x1 and calculated y1 and y2, and in each iteration used three conditions:

1. If y1 + y2> 1 + (some tolerance) -> there are more vapour -> decrease temperature
2. If y1 + y2< 1 - (some tolerance) -> there are less vapour -> increase temperature
3. If y1 + y2= 1, the T obtained is exact.

Graph obtained:



Error obtained from RMSE:

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0.03529
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Q2) For your selected binary system, assume it as a real system (meaning that deviation from ideal behaviour is present in both liquid and vapour phase):

(i) Plot y v/s x (vapour liquid equilibrium) curve for the same, taking into consideration the activity and fugacity coefficient in Roult's law (State all the assumptions)

Equation used:

$$y_i \, \emptyset_i P = x_i \, \gamma_i P_i^{sat} \emptyset_i^{sat}$$

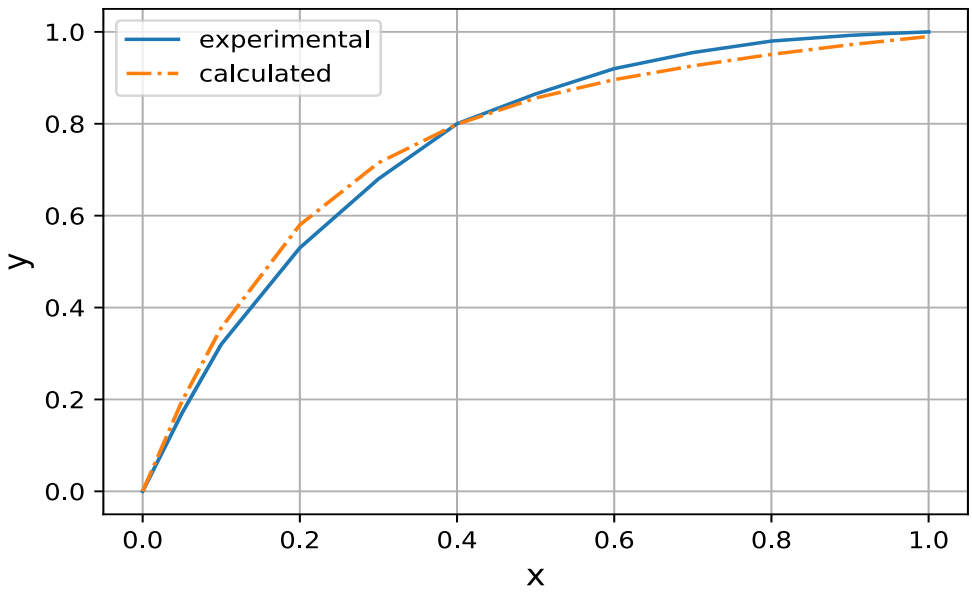
How each part was calculated:

1. $y_i = \ given$
2. $\emptyset_i = \frac{B_i P}{RT}$, $B_i = 2nd\ Virial\ coeff. = \ b_i - \frac{a_i}{RT}$, $where\ b_i \ and\ a_i\ are\ van\ der\ waals\ coeff$
3. $P = given$
4. $x_i = \ given$
5. $\gamma_i = \ from\ NRTL\ model$
6. $P_i^{sat} = \ from\ antoine's\ equation$
7. $\emptyset_i^{sat} = \ same\ as\ \emptyset_i\ but\ P_i = \ P_i^{sat}$

Assumptions:

1. Liquids are miscible in all proportions over a wide range of temperature
2. The system is at low to moderate temperature, thus neglecting the Poynting correction factor (almost equals to 1)
3. Equation of state is well estimated by virial equation up to 2nd coefficient.

Plot:



Error obtained from RMSE:

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0.02600
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(ii) Learn how to plot the vapor equilibrium using DWsim software

Assumptions:

1) Feed stream : 1-Butanol and Methacrylic acid.
2) X_{C4H9OH}=0.5 X_{C4H6O2}=0.5
3) Temp = 32℃
4) Pressure 3.5 bar
5) Mass flow rate = 120kmole/h
6) Property package – Raoult's law

Process:

1) Create a new process modeling file. Select 1-Butanol and Methacrylic acid from the given list of compounds in software. Select Raoult's law in property packages. Select unit C5 that uses metric system units.
2) Now create a material stream (feed). In properties panel of material stream change stream name to feed. Change flash algorithms to nested loops. Change other properties – male fractions, temperature, pressure, mass flow rate, property package according to above assumptions.
3) To plot graph, go to utilities menu, add utility. Select object type -> material streams, utility type –> binary phase envelope, flowsheet object -> feed. And finally click add utility.
4) Now a new window will appear, change its name to T_{xy} plot as first we will plot T_{xy}. Select Envelope type – T_{xy}, T_{xy} diagram options – VLE. Click calculate – x-axis will show mole fractions of 1-Butanol and Methacrylic acid and y-axis will show temperature and the liquid-vapor phase diagram will appear. At this stage you can save the graph.
5) Now in the same window change name to xy plot, Envelope type –T_{xy}. Now click calculate. X-axis and y-axis will show the mole fractions of 1-Butanol and Methacrylic acid depending on what we choose as compound 1 and 2.

6) Now to plot pressure v/s mole fraction plot, change name to P_{xy} in the same window, Envelope type - P_{xy}, temperature – 32°C. Click calculate, the new graph shows mole fractions of 1-Butanol and Methacrylic acid on x-axis and pressure on y-axis.

Hence we have learned how to plot T_{xy}, xy, P_{xy} plot in DWsim software.