Laboratory and Homework Assignment 1

Reading Assignment

1. "Appendix B: Hints when using Matlab" from Finlayson, Bruce A. Introduction to chemical engineering computing. John Wiley & Sons, 2012.
2. "Appendix C: Hints when using ASPEN PLUS" from Finlayson, Bruce A. Introduction to chemical engineering computing. John Wiley & Sons, 2012.

Laboratory Assignment (Due after laboratory session)

1. [100 points] Using Raoult's law, for a benzene/p-xylene binary system, calculate **a)** isobaric T vs x, y diagram; and **b)** isothermal P vs x, y diagram. For both the cases also plot y vs x diagram. Compare with experimental results given in Tables 1 and 2. Also plot $|T_{exp} - Tcal|$ vs x, y for the first case and $|P_{exp} - P_{cal}|$ vs x, y for the second case. Does the system follow Raoult's law? If yes, then why?

   You need to do this exercise first using Matlab and then using ASPEN PLUS. The Antoine equation parameters are (Benzene: A = 6.87987, B = 1196.76, and C = 219.161 for $8 < T < 80$°C; p-xylene: A = 6.99053, B = 1453.430, C = 215.310 for $27 < T < 166$°C). The values are taken from DECHEMA chemical data series. The form of equation used is $\log_{10} P^{sat} = A - B/(T + C)$ with pressure in mmHg and temperature in °C.

Table 1: **Experimental VLE data at T = 308.0 K. Taken from DECHEMA chemical data series.**

P (kPa)	x_1	y_1
3.2744	0.06640	0.41730
4.618	0.13970	0.61830
5.809	0.20550	0.71900
7.050	0.27480	0.78790
8.289	0.34420	0.83620
9.539	0.41440	0.87240
10.812	0.48680	0.90080
12.022	0.55590	0.92240
13.248	0.62650	0.94040
14.512	0.69890	0.95580
14.684	0.70870	0.95770
15.692	0.76710	0.96810
16.849	0.83360	0.97850
16.989	0.84130	0.97970
17.744	0.88520	0.98580

Table 2: **Experimental VLE data at P = 101.33 kPa. Taken from DECHEMA chemical data series.**

T (K)	x_1	y_1
412.09	0.00000	0.00000
405.63	0.05390	0.20390
403.16	0.07920	0.27740
399.51	0.11530	0.36440
394.91	0.16590	0.48480
392.01	0.19100	0.54500
385.91	0.27100	0.66200
381.13	0.34800	0.72900
376.69	0.40500	0.78600
372.02	0.49300	0.84000
369.88	0.53700	0.86700
367.92	0.57900	0.89000
366.62	0.60700	0.91100
363.48	0.68400	0.92800
360.74	0.74800	0.95200
359.12	0.80900	0.96500
358.44	0.82300	0.96900
357.60	0.85300	0.98100
356.91	0.87300	0.98600
353.25	1.00000	1.00000

Practice Homework Assignment

1. Consider a perfectly mixed liquid in a tank. A liquid stream of volumetric flow rate, F_0 (m^3/s), and density, ρ_0 (kg/m^3), flows into the tank. The volumetric hold up at any instant of time in the tank is V(t), and its density is $\rho(t)$. The volumetric flow rate out of the tank is $F(t)$. The liquid stream has three components: C_{A0}, C_{B0}, and C_{C0} ($moles/m^3$). A series chemical reaction takes place inside the tank

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \tag{1}$$

   where k_1 and k_2 are the first order reaction rate constants. Assuming first order reactions, write the component continuity equations for components A, B and C. Clearly state your assumptions.

2. Using Raoult's law, for a Chloroform/ethanol binary system, calculate **a)** isobaric T vs x, y diagram; and **b)** isothermal P vs x, y diagram. For both the cases also plot y vs x diagram. Compare with experimental results given in Tables 3 and 4. Also plot $|T_{exp} - Tcal|$ vs x, y for the first case and $|P_{exp} - P_{cal}|$ vs x, y for the second case. Does the system follow Raoult's law? Provide physical explanation for your answer.

   You need to do this exercise first using Matlab and then using ASPEN PLUS. The Antoine equation parameters are (Chloroform: A = 6.9546, B = 1170.966, and C = 226.232 $-10 < T < 60$°C; Ethanol: A = 8.11220, B = 1592.864, C = 226.184 $20 < T < 93$°C). The values are taken from DECHEMA chemical data series. The form of equation used is $\log_{10} P^{sat} = A - B/(T + C)$ with pressure in mmHg and temperature in °C.

Table 3: **Experimental VLE data at T = 308.15 K. Taken from DECHEMA chemical data series.**

P (kPa)	x_1	y_1
13.703	0.00000	0.00000
13.982	0.00620	0.02540
14.840	0.02410	0.09910
15.147	0.02970	0.12100
16.471	0.05420	0.21540
16.775	0.05940	0.23430
19.766	0.11090	0.38850
23.678	0.17300	0.53040
27.422	0.23610	0.62070
30.006	0.28730	0.67470
30.563	0.30140	0.68700
31.531	0.32270	0.70090
33.783	0.38450	0.73700
34.035	0.39220	0.74120
35.684	0.43840	0.76460
36.536	0.48270	0.77970
38.923	0.61850	0.81810
39.587	0.67830	0.83270
40.403	0.77460	0.85540
40.715	0.82650	0.86980
40.679	0.84230	0.87520
40.830	0.84830	0.87830
40.803	0.93150	0.91610
40.646	0.95600	0.93630
40.553	0.95860	0.93850
40.489	0.96000	0.94030
40.518	0.96160	0.94140
39.345	1.00000	1.00000

Table 4: **Experimental VLE data at P = 94 kPa. Taken from DECHEMA chemical data series.**

T (K)	x_1	y_1
349.7	0.000	0.000
349.0	0.022	0.047
348.2	0.038	0.091
345.9	0.080	0.206
343.7	0.122	0.305
341.7	0.163	0.403
340.4	0.203	0.449
338.9	0.237	0.504
337.5	0.277	0.552
336.6	0.293	0.587
334.3	0.399	0.670
332.1	0.559	0.748
331.1	0.681	0.792
330.6	0.819	0.841
330.7	0.898	0.881
332.3	1.000	1.000