ChE 3063 **Project 2** Due: November 6, 2020

Experimental VLE data for Chloroform (1)/Ethanol (2) system at 35ºC are as follows:

P [kPa]	x_1	y_1
13.703	0.0000	0.0000
13.982	0.0062	0.0254
14.840	0.0241	0.0991
15.147	0.0297	0.1210
16.471	0.0542	0.2154
16.775	0.0594	0.2343
19.766	0.1109	0.3885
23.678	0.1730	0.5304
27.422	0.2361	0.6207
30.006	0.2873	0.6747
30.563	0.3014	0.6870
31.531	0.3227	0.7009
33.783	0.3845	0.7370
34.035	0.3922	0.7412
35.684	0.4384	0.7646
36.536	0.4827	0.7797
38.923	0.6185	0.8181
39.587	0.6783	0.8327
40.403	0.7746	0.8554
40.715	0.8265	0.8698
40.679	0.8423	0.8752
40.830	0.8483	0.8783
40.803	0.9315	0.9161
40.646	0.9560	0.9363
40.553	0.9586	0.9385
40.489	0.9600	0.9403
40.518	0.9616	0.9414
39.345	1.0000	1.0000

Using this data:

1. Calculate values for $\ln \gamma_1$ and $\ln \gamma_2$ and G^E/x_1x_2RT and plot these vs x_1
2. Compute values of A and B for the Margules 3-suffix equation from $\ln \gamma_1^\infty$ and $\ln \gamma_2^\infty$ (extrapolate $\ln \gamma_1$ and $\ln \gamma_2$ to $x_1 = 0$ and $x_2 = 0$ to get these), and plot $\ln \gamma_1$ and $\ln \gamma_2$ and G^E/x_1x_2RT from the Margules 3-suffix equation using these values of A and B all on the same graph as in 1) above for comparison purposes.
3. Simulate the system with HYSYS, extract P and y data from bubble pressure calculations

using the same x's as given in the tabular experimental data. Provide a table with the direct comparison of P, x, and y values that you got from HYSYS to the experimental data (fill in the attached table). Use Margules 3-suffix with ideal gas vapor phase as the fluid package in HYSYS.

4. Plot x_1 vs y_1 from the experimental data, and on the same graph, plot x_1 vs y_1 using the HYSYS simulation. Add the diagonal (a line for $x_1 = y_1$) and compare the azeotrope composition resulting from the experimental data and HYSYS simulation.

Example Table for step 4):

Experimental			HYSYS Simulation		
P [kPa]	x_1	y_1	P [kPa]	x_1	y_1
13.703	0.0000	0.0000		0.0000	
13.982	0.0062	0.0254		0.0062	
14.840	0.0241	0.0991		0.0241	
15.147	0.0297	0.1210		0.0297	
16.471	0.0542	0.2154		0.0542	
16.775	0.0594	0.2343		0.0594	
19.766	0.1109	0.3885		0.1109	
23.678	0.1730	0.5304		0.1730	
27.422	0.2361	0.6207		0.2361	
30.006	0.2873	0.6747		0.2873	
30.563	0.3014	0.6870		0.3014	
31.531	0.3227	0.7009		0.3227	
33.783	0.3845	0.7370		0.3845	
34.035	0.3922	0.7412		0.3922	
35.684	0.4384	0.7646		0.4384	
36.536	0.4827	0.7797		0.4827	
38.923	0.6185	0.8181		0.6185	
39.587	0.6783	0.8327		0.6783	
40.403	0.7746	0.8554		0.7746	
40.715	0.8265	0.8698		0.8265	
40.679	0.8423	0.8752		0.8423	
40.830	0.8483	0.8783		0.8483	
40.803	0.9315	0.9161		0.9315	
40.646	0.9560	0.9363		0.9560	
40.553	0.9586	0.9385		0.9586	
40.489	0.9600	0.9403		0.9600	
40.518	0.9616	0.9414		0.9616	
39.345	1.0000	1.0000		1.0000	

5. Perform an integral test on the experimental data. Plot $\ln(\gamma_{1/}\gamma_2)$ vs. x_1 using the experimental data and make some quantitative assessment of whether or not the data is consistent.

<u>Submitting your Project:</u>

Use Excel to solve the problem except for part 3 where you use HYSYS. *Each student should start with a blank worksheet in preparing their solution.* Turn in a solution in PDF format similar to an exam format. Show intermediate work and results as the problem parts are solved, and organize your solution logically. Your Excel sheet should parallel your hardcopy solution. Be sure to include comments on the sheet and include references to the parts of the problem you are working. Extract data for part 4 from HYSYS and include it in your Excel sheet. Save the Excel sheet as "Project2-FirstName-LastName.xlsx" and HYSYS case as "Project2-FirstName-LastName.hsc" and email them to me *before* class the date it is due with the subject line: "ChE3063 Project 2 Solution". Submit your paper solution at the beginning of class the date it is due.