Capstone Project - 300 points **Due: 12 December at 2359.**

Objectives:

1. Prepare a Txy plot in CHEMCAD and apply regression of binary interaction parameters.
2. Model ideal and nonideal solution behavior with activity coefficient models.
3. Apply machine-learning techniques to build data-based thermodynamic models.
4. Communicate your results in tables and graphs.

Assignments:

1. 40 Points. Use CHEMCAD to prepare a Txy plot using the NRTL equation for K values. The NRTL equation assumes *non-ideal solution* behavior. Follow the guidance for this assignment on page 2. This assignment must be completed for the IPR.
2. 40 Points. Prepare a Txy plot in Mathematica assuming *ideal solution* behavior. This is similar to work you may recall from CH362. The difference is completing the plot in Mathematica. Assignment 2 must be completed for the IPR.
3. 40 Points. Prepare a Txy plot in Mathematica assuming *non-ideal solution* behavior, with activity coefficients calculated from the NRTL equations (textbook equations 13.49 and 13.50). Use the constants obtained from your CHEMCAD results in assignment 1.
4. 40 Points. Your instructor has provided "approved solutions" to confirm your results for assignment 3. The solutions are functions created in Mathematica and deployed to the cloud. Use the instructor-provided functions to confirm your results. Follow the guidance for this assignment on page 3, and complete and submit the skeleton table on page 4.
5. 40 Points. Construct a plot of experimental data and theoretical Txy data from the NRTL equation. For experimental data, include the instructor-provided literature data in your plot. Literature data from Perry's Handbook are provided in Canvas.
6. 40 Points. Construct a plot of excess Gibbs energy versus mole fraction using the NRTL equations. Equation 13.48 is recommended.
7. 60 Points. Machine Learning. Use the "Predict" function in Mathematica to generate a Txy plot. Use your experimental data from Canvas as the training data. Make a plot that compares the results to the experimental data.

IPR Deliverables (pass/fail, due 17 November at 2359):

1. Assignments 1 and 2 complete. Some progress in at least one other assignment.
2. The grade is pass-fail. Failing cadets will have an F entered as a grade until corrections are made.

Final Deliverables (300 points total, due lesson 40):

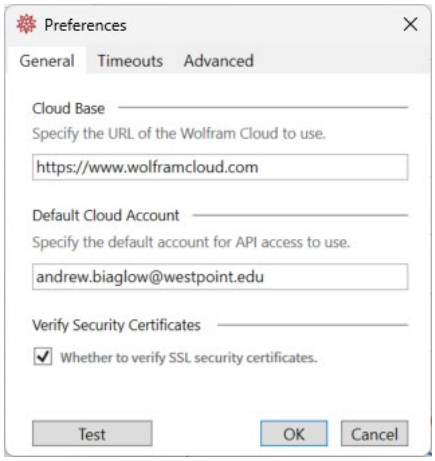
- A pdf of the Mathematica file with cover sheet.
- A Mathematica file with solutions to assignments 2, 3, 6, and 7. Copy and paste screenshots for problem 1, 4, and 5 to this file.
- CHEMCAD file for problem 1 with required charts saved internally in the file.
- Excel solutions for assignments 4 and 5.

Additional Guidance for Assignment 1:

1. Start CHEMCAD and set the engineering units to "Common SI."
2. Select your molecules (either 2-propanol and water or 1-propanol and water).
3. After you select your molecules, CHEMCAD will make suggestions for the thermodynamic settings. Accept the default settings in the thermodynamics suggestions window. CHEMCAD automatically selects NRTL as the K-value method and will import NRTL constants from its internal database.
4. You will refine the NRTL constants using regression to achieve much higher accuracy in subsequent calculations. You will do this using actual data with "BIP Regression." The acronym "BIP" stands for "binary interaction parameter," and the tool is found in the "Thermophysical" tab at "BIP Regression."
5. Once in the tool, select the "Txy" option (3rd option in the list of options, where it says specifically "Regress TPxy/Pxy/Txy VLE data.").
6. The component selection window opens next. When the window opens, select your two molecules. They should be the only molecules available. Click the molecule, then click the "Add" button to add it to the "Selected Components." Either molecule can be chosen first, but I recommend choosing the alcohol first. This identifies subscript "1" as the alcohol in the binary interaction parameters B_{12} and B_{21}. You will see these in the "Regress NRTL Parameters" window that opens next.
7. In the NRTL parameters window, increase the upper bound on the alpha value to .6 and click OK to select all other default values in this window.
8. The regression parameters window opens next. Increase the number of restarts from 1 to 1000 and click OK to accept all other default values.
9. The last window to open is "TPxy Data." The experimental data from Perry's Handbook is posted on Canvas. Add the data for your molecules to the grid in the window. You can enter the numbers one at a time or use "copy and paste" to enter all data all at once. Set all weight factors to 1. Clock "OK" after all data has been entered.
10. The calculation takes some time (14 seconds on my computer). When the calculations are complete, CHEMCAD will generate a report of the results. The refined values are at the very end of the report.
11. When the calculation is finished, proceed to make your Txy plot using "Charts" in the "Home" tab. **Important:** Make sure you use the correct "BIP Set" from your regression.
12. Use the "User Series" tool to add your experimental Tx and Ty data. When the chart is complete, click "Save" in the upper left corner of the chart screen.

Additional Guidance for Assignment 4:

1. Install Wolfram Cloud Connector. The installation file is in the course resources in Canvas: "CloudConnectorForExcel_1.1.0_WIN.msi."
2. The msi will add a Wolfram tab to excel. Once installed, open the Wolfram tab, go to "Preferences," and add your instructor's email address to "Default Cloud Account" as shown here:



3. Click the "Test" button to make sure the connections are good.
4. For **1-propanal plus water**, the instructor's excel functions to calculate the bubble and dew points are listing below and can be copied and pasted from here directly into Excel:

```
=WolframAPI("TbSys11",Parameter("a12",$C$10),Parameter("A",$D$10),Parameter("B",$E$10),Parameter("x",D13))
=WolframAPI("TdSys11",Parameter("a12",$C$10),Parameter("A",$D$10),Parameter("B",$E$10),Parameter("x",E13))
```

   For **2-propanal plus water**, the instructor's excel functions to calculate the bubble and dew points are listing below and can be pasted directly into Excel:

```
=WolframAPI("TbSys12",Parameter("a12",$C$10),Parameter("A",$D$10),Parameter("B",$E$10),Parameter("x",D13))
=WolframAPI("TdSys12",Parameter("a12",$C$10),Parameter("A",$D$10),Parameter("B",$E$10),Parameter("x",E13))
```

5. In these functions, the NRTL parameters are "a12", "A", and "B." These cannot be changed and must be entered exactly as shown. Each of these is followed by an address in your spreadsheet. For example, C10 is the location of "a12," D10 is the location of "A," and E10 is the location of "B." These can be any location you prefer.
6. Mole fractions are represented by a generic "x." That is, in functions TbSys11 and TbSys12, x is the liquid mole fraction, and in functions TdSys11 and TdSys12, x is the vapor mole fraction. The locations shown here are D13 and E13. These correspond to your x and y values (for example C2 and D2 in the provided data sheet). The dollar signs fix the locations of the parameters and mole fractions have floating locations so a table can be calculated.

Complete this table for three different x-values and three different y-values:

Mole fraction		Cadet Mathematica		Instructor Mathematica	
x	y	T_b	T_d	T_b	T_d
Enter your NRTL parameters below:					
a12		A		B	