Capstone Project - 300 points **Due: 13 December**

Objectives:

1. Prepare a Txy plot in CHEMCAD and apply regression of binary interaction parameters.
2. Modeling ideal and nonideal solution behavior in Mathematica.
3. Apply machine-learning techniques to model thermodynamic properties.
4. Communicate your results in tables and graphs.

Questions:

1. 40 Points. Use CHEMCAD to prepare a Txy plot using the NRTL equation for K values, which assumes *non-ideal solution* behavior. Follow the specific guidance for this problem on page 2. This problem should be completed before your IPR.
2. 40 Points. Prepare a Txy plot in Mathematica assuming *ideal solution* behavior. This is similar to work you already did in CH362, but the new requirement is to complete the plot in Mathematica. This problem should be completed before your 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 from Problem 1.
4. 40 Points. Use the instructor-provided Excel Mathematica functions on page 3 to confirm your calculations in Problem 5. There is specific guidance for this problem on page 3 and a skeleton table on page 4 as a guide for the comparison.
5. 40 Points. Construct a plot of experimental data and theoretical Txy data from the NRTL equation. For experimental data, include instructor-provided literature data and cadet data in your plot. Literature data for 1-propanol and 2-propanol plus water are provided in the collaborative spreadsheet in Canvas.
6. 40 Points. Construct a plot of excess Gibbs energy versus mole fraction using the NRTL equations.
7. 60 Points. Machine Learning. Use the Predict function in Mathematica to generate a Txy plot. Use the experimental data references in problem 1 and page 2 as the training data. Make a plot that compares the results to the experimental data.

IPR (pass/fail, due 15 November):

1. Submit a PowerPoint with slides showing progress to date.
2. Identify difficulties encountered in the project, if any.
3. Minimum requirement is complete answers to questions 1 and 2.
4. Your grade is pass-fail. Failing cadets will have an F entered into the project until corrections are made.

Note:

This is a new project. Some changes to this document may occur over the next 1-2 months.

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

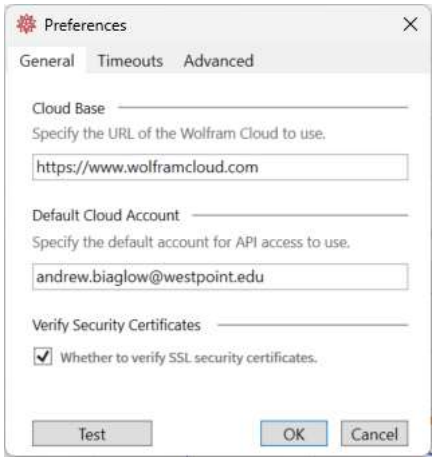
- Lab results entered into collaborative spreadsheet.
- Separate Mathematica files for problems 4 and 5.
- Excel file for problems 6 and 7.
- CHEMCAD file for problem 3 with required charts saved internally in the file.
- PDF file of written report, uploaded to Canvas.

Specific guidance for Problem 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. The NRTL constants can be refined 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.
5. Once in the tool, select the "Txy" option in the regression tool (3rd option in the list of options, 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. 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 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. Add the data found in Canvas for your molecules (originally taken from Perry's Handbook). You do not need to type in the numbers one at a time. You can use "copy and paste" to simplify data entry, entering all data all at once, and minimizing the chance of a transcription error.
10. The calculation takes some time. When the calculations are complete, CHEMCAD will generate a report of the results. The refined values are at the end of the report.

Specific guidance for Problem 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 and add the instructor's email address to the preferences in the Wolfram tab:



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 pasted 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 parameters for the NRTL equations are "a12", "A", and "B", C10 is the location of "a12" in the spreadsheet, D10 is the location of "A" in the spreadsheet, E10 is the location of "B" in the spreadsheet, "x" is the liquid or vapor mole fraction, and D13 and E13 are the locations of the liquid and vapor mole fractions. 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	