Objectives: (1) Measure the boiling point of a liquid mixture, (2) prepare a Txy plot for an ideal solution in Mathematica, (3) prepare a Txy plot for a non-ideal solution in Mathematica, and (4) perform a curve fit of experimental data in CHEMCAD.

Assignment (300 points, due 11 December): Go to the "cadet assignments" link on the course web page to find your assigned solutions, then proceed to the following assignments:

1. 10 points. Schedule and confirm group appointments with Mr. Mathew (Abhilash) by COB Friday 18 August. Include Dr. Biaglow in the calendar invite. A complete experiment takes about an hour. Ensure that you have booked enough time to complete the experiment. Both cadets are encouraged to attend but only one cadet is required. Appointments can be any date up to 15 November, but you are encouraged to complete this requirement as early as possible. Dates for appointments might change depending on availability of chemicals.
2. 40 Points. Experiments must be completed by 15 November. When complete, enter your boiling point results into the collaborative spreadsheet in Canvas and upload your log sheets to Canvas. Remember to obtain Mr. Matthew's electronic initials on your data log sheet before submission. Sheets without initials will not be accepted.
3. 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.
4. 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.
5. 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 study.
6. 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.
7. 40 Points. Construct a plot of experimental data and theoretical Txy data from the NRTL equation. For experimental data, include 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.
8. 50 Points. Writing assignment. Produce a two-page report of your results. The report must include two properly formatted Txy plots. The first includes vapor and liquid calculated results for the ideal solution. The second plot includes (1) literature data, (2) calculated results from Mathematica, (3) calculated data from CHEMCAD, and (4) cadet experimental data. Your write-up must include (1) a comparison of ideal and nonideal solutions using intermolecular forces to explain the differences, and (2) a comparison of cadet measurements and theoretical calculations.

IPR (90 points, due 17 November): Guidance: Submit a PowerPoint with slides showing progress to date and any difficulties encountered. Your grade will be assessed based on your group's progress on problems 1-4 and the quality of your PowerPoint submission.

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

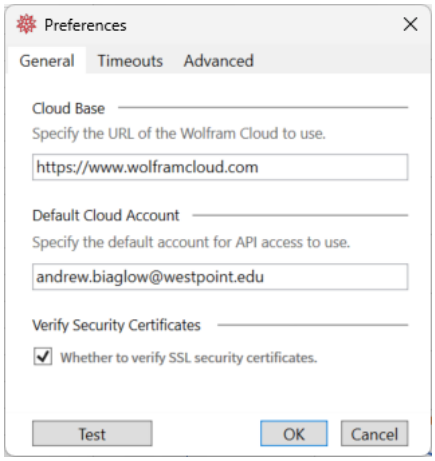
- Lab results entered into collaborative spreadsheet.
- Separate Mathematica files for problems 4 and 5.
- Excel file for problems 6 and 7.
- CHEMCAD file for problem 3 with required charts saved internally in the file.
- PDF file of written report, uploaded to Canvas.

Specific guidance for Problem 3:

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 6:

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	