Capstone Project - 390 points **Due: Lesson 40**

Tasks: (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 with activity coefficients in Mathematica, (4) perform a curve fit of the experimental data, and (5) verify your plots in CHEMCAD.

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. The instructor must be included in the calendar invite. Since a complete experiment takes about an hour, your appointment will need to be at least1.0 hours. One cadet in your group is required to attend. Cadets can stagger attendance to cover the time. Ensure that you have enough time to complete the experiment.
2. 40 Points. Experiments must be completed, and results reported by 15 November. Get started early! Enter your boiling point results into the collaborative spreadsheet in Canvas. Submit experiment data log sheet to Canvas, to include ebulliometer pressure, temperature readings vs time, and initials from Mr. Matthew.
3. 50 Points. Prepare a Txy plot in Mathematica assuming *ideal solution* behavior. This part of the project is similar to work you already did in CH362. That work can be used as a basis for this work, but the new requirement is to complete the plot in Mathematica. This problem can be done before your experiments are complete.
4. 50 Points. Prepare a Txy plot in Mathematica assuming *non-ideal solution* behavior with activity coefficients calculated from the Margules two-parameter equation. Groups assigned 1-propanol and water should useA_{12}=2.357 and A_{21}=0.858. Groups assigned 2-propanol and water should useA_{12}=2.332 and A_{21}=0.898. This problem can also be finished before your experiments are complete.
5. 50 Points. Use the instructor-provided Excel Mathematica function to construct a plot of experimental data with the Margules two-parameter equation. Include literature data in your plot. Data are provided in the collaborative spreadsheet in Canvas.
6. 50 Points. Produce a Txy plot in CHEMCAD to confirm your calculations with the Margules parameters from problem 5.
7. 50 Points. Writing assignment. Produce a two-page report of your results. The report must include three properly formatted plots for the three Txy plots. To save space, individual plots can be consolidated into a single figure. Discuss your experimental procedure, theoretical calculations, and difference between ideal and nonideal solutions using intermolecular forces to explain the differences.

IPR (90 points, due 15 November): Guidance: 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.

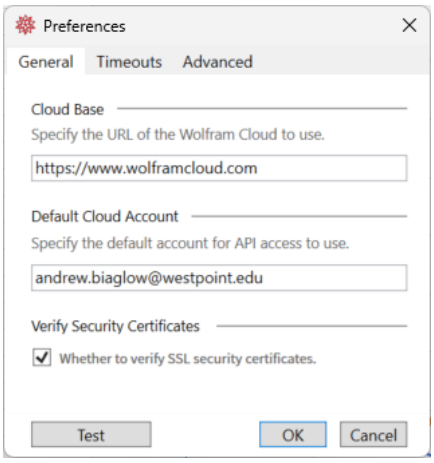
Final Deliverables (300 points total, 290 points for problems 2-7, due lesson 40):

- Lab results entered into collaborative spreadsheet.
- Separate Mathematica files for problems 3 and 4.
- Excel file for problem 5.
- CHEMCAD file for problem 6.
- PDF file of written report, uploaded to Canvas.

Instructions for obtaining the function for problem 5:

Install Wolfram Cloud Connector using the file "CloudConnectorForExcel_1.1.0_WIN.msi" available from the course resources in Canvas.

The msi will add a Wolfram tab to excel. Once installed, add the instructor's email address to the preferences in the Wolfram tab:



You can click the "Test" button to make sure the connections are good.

The excel functions that calculate the boiling point from the mole fraction and Margules parameters are shown here:

1-Propanol+Water:
=WolframAPI("TbSys5",Parameter("A",C10),Parameter("B",D10),Parameter("x",E13))
=WolframAPI("TdSys5",Parameter("A",C10),Parameter("B",D10),Parameter("x",E13))

2-Propanol+Water:
=WolframAPI("TbSys6",Parameter("A",C10),Parameter("B",D10),Parameter("x",E13))
=WolframAPI("TdSys6",Parameter("A",C10),Parameter("B",D10),Parameter("x",E13))

In these functions, "A" and "B" are the Margules activity coefficient parameters, C10 is the location of "A" in the spreadsheet, D10 is the location of "B" in the spreadsheet, "x" is the liquid or vapor mole fraction, and D13 is the location of the mole fraction in the spreadsheet. "A" and "B" have fixed locations and x floats so a table can be calculated.

1-Propanol+Water: $A=A_{12}=2.357$ and $B=A_{21}=0.858$.
2-Propanol+Water: $A=A_{12}=2.332$ and $B=A_{21}=0.898$.

Values for comparison can be found in Perry's Handbook, page 13-20.