General information:

1. Name all function files and scripts using the notation *Q1_function_name* or *Q1_script_name* and so on.
2. **Do not define your functions within the script file**.
3. You do not need to add a separate report. For each question, provide your answers in the form of comments in the code itself. **Marks will be deducted if the comments do not contain answers and explanations, even if you have coded correctly**. Add proper axis labels to help identify what you are plotting.
4. There is **1 bonus question** in this assignment. Full marks will be awarded even if you do not attempt this question and get the others right. Extra points will be awarded if you get the bonus question correct, and these points will be counted in the final grade calculations.
5. Internet access will not be available during the session. However, you are free to access MATLAB documentation. Most, if not all, issues with your code can be fixed if you go through the documentation.
6. TAs will not help clear your conceptual questions. Do not ask them if you are getting the correct answers or not.
7. **Keep all your codes in a single zip file with file name *Name_Roll_number_CHE213_2.*** You will have to upload this zip file to USB drive carried by the TA.
8. **Submissions will start from 4:35 pm. All submissions must be done to the TAs by 4:45 pm**. No submissions will be entertained after that. Submissions will be done using USB drives.

Recovery of ethyl alcohol from sugarcane molasses – Part 1

As the world continues to transition towards sustainable fuel alternatives, the production of biofuels or fuels from biological sources has gained tremendous attention in recent years. One prominent example of biofuel family is ethanol-gasoline blend in which ethanol is combined with gasoline at different compositions.

A common source of the ethanol used in biofuels is sugarcane molasses. The liquid byproduct remaining in the sugarcane juice after extraction of sugar is known as sugarcane molasses. Molasses is rich in fermentable sugars and is a suitable feedstock for fermentation. During the fermentation process, yeast (e.g., *Saccharomyces cerevisiae*) is added to the molasses which converts the sugar into ethanol along with the production of CO_2.

Assume a fermentation process in which the production of gaseous ethanol-CO_2 feedstock, containing 15% mol fraction of ethanol, is 2000 kg/hr. **The ethanol is to be recovered from the ethanol-CO_2 mixture by absorption with pure water** in **(i)** a packed bed column and **(ii)** a stage-wise column. **In Part I of this task, we will focus on determining the operating conditions for the column.** Part II of the task (to be done in the next simulation session) will determine the number of stages, number and height of ideal transfer units, which would aid the design of the two columns.

Assume that the column is operated under isothermal, isobaric conditions and that the water absorbs only ethanol. Use the relevant information provided below.

(i) The ethanol-water equilibrium solubility data is given below. Here x and y are in mole fractions of ethanol. Since, we will be working on a solute-free basis, convert this data to obtain equilibrium data between X and Y, where X and Y are mole ratios. Use your favourite fitting function in MATLAB to fit the X - Y data to the functional form:

$$Y = \frac{aX}{1 + bX}$$

Use this fitted curve for all subsequent calculations. Show both the tabulated and the fitted curve in the same plot (**Name this Figure 1**). **(10 points)**

$\boldsymbol{x}$	0	0.0186	0.0476	0.0673	0.0881	0.1102	0.1424	0.1894	0.2069
$\boldsymbol{y}$	0	0.0105	0.0272	0.0375	0.0492	0.0624	0.0809	0.1078	0.1182

(ii) Use the available information to calculate the necessary flowrates, mole fractions and mole ratios in the system. Clearly define and obtain the following quantities in your MATLAB code with appropriate variable names:

a. Total gas feed rate $G_1 (\frac{kmol}{hr})$

b. Feed rate solute-free basis $G_S (\frac{kmol}{hr})$

c. Mole fraction of ethanol in the feed gas y_1

d. Mole ratio of ethanol in the feed gas Y_1

e. Feed rate of ethanol $G_{1,EtOH}(\frac{kmol}{hr})$

Note: Use the molar average molecular weight to calculate molar flow rate of the feed. **(10 points)**

(iii) To design the column, we need to know how much ethanol needs to be removed. Here, we will look at different extents of ethanol removal and understand how the solvent rates vary with this parameter. Assume that the required recovery of ethanol is between 92% to 98%. For this, you can define an array containing the required recovery values with 2% increments (92%, 94%, 96%, 98%).

(iv) Once we have the recovery required, the next step would be to obtain the remaining flow quantities. Clearly define and obtain the following quantities in your MATLAB code with appropriate variable names:

a. Output rate of ethanol $G_{2,EtOH}\left(\frac{kmol}{hr}\right) = G_{1,EtOH} \times (1 - \%recovery)$

b. Mole ratio of ethanol in the output gas Y_2

c. Mole fraction of ethanol in the output gas y_2

d. Mole ratio of ethanol in the feed water X_2

e. Mole fraction of ethanol in the feed water x_2 **(10 points)**

(v) Next, we need to determine the minimum solvent rate for a required ethanol recovery. **Check the nature of the *X* - *Y* curve (convex downwards or upwards).** Accordingly, for each value of ethanol recovery, use MATLAB to first obtain the **pinch point** and then use this point to calculate the **minimum solvent rate**, $L_{s,min}$. Plot the **minimum solvent rate against the ethanol recovery** (name this Figure 2). How does the minimum solvent rate vary and why?

Hint: You will need to find the point of tangency from (X_2, Y_2) to the equilibrium curve. Remember the training exercise with **fsolve** that you did on determining the point of tangency and the equation of a tangent line to a curve. Here is a snippet of that problem. **(30 points)**

Q5: Determining the point of tangency and the equation of a tangent line to a curve

Write a MATLAB script to determine the equation of a tangent from the point $A(0,1)$ to the curve $y = \frac{2x}{1+x}$. Remember, at the point of tangency, the slope of the tangent is equal to the derivative of the curve. This means, if the point of tangency is $B(x_t, y_t)$ then,

$$\frac{y_t - 1}{x_t} = \left.\frac{dy}{dx}\right|_{x=x_t} = \frac{2}{(1+x_t)^2} \quad (1)$$

Additionally, since the tangent point lies on the curve, we also have

$$y_t = \frac{2x_t}{1+x_t} \quad (2)$$

Solving the system of equations (1) and (2) will provide the point of tangency. Your task is to find out the slope of the tangent and plot the tangent along with y.

Make a separate function file for fsolve. Remember the file name, under which you are saving the function, should be the same as the function name. Call this in your MATLAB script.

(vi) For 94% ethanol recovery, plot the operating line corresponding to the minimum solvent rate along with the equilibrium curve. This is your **Figure 3**. Indicate the **coordinates of the pinch point** and obtain the **maximum mole ratio in the exiting liquid phase ($\boldsymbol{X_1^{max}}$)** also. **(20 points)**

(vii) Assume that in each case, the **actual solvent rate is 1.25 times** the calculated minimum solvent rate. Determine the operating lines for all the recovery values. In **Figure 3**, plot the corresponding operating line for 94% ethanol recovery. **(20 points)**

(viii) **Bonus question:** Repeat steps (iv-vii) for ethanol recovery of 86% and 88%. Make new figures 1* and 2* for these recoveries. **(40 points)**