INDIAN INSTITUTE OF TECHNOLOGY MADRAS
Department of Chemical Engineering

CH 2082
Assignment 6

Deadline: 21/04/2014, 6 pm

1. Attempt all problems on your own.
2. All variables should be declared or initialized within your program
3. **Comment all your files**
4. Name each program using the following convention using a combination of your roll number, assignment number and question number. i.e., if your roll number is CH12B001, name the program in the first question of the first assignment as follows:
CH12B001_A1_Q1.m
5. Submit a single zipped folder containing .m files for each of the questions and a single pdf file that is published. The zip file should be named as follows: if your roll number is CH12B001, then the zip file name would be CH12B001_A1.zip

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1. We will consider a thermodynamic system and dew point, bubble point and flash calculations. Please refer to "Introduction to Chemical Engg. Thermodynamics by Smith and Van Vess, Chapter 10, Section on Raoult's law." We will consider mixtures of acetonitrile (1), nitromethane (2), acetone (3). The Antoine equations are as follows.

$$\ln(Psat_1) = 14.2724 - \frac{2945.47}{(T + 224.00)} \tag{1}$$

$$\ln(Psat_2) = 14.2043 - \frac{2972.64}{(T + 209.00)} \tag{2}$$

$$\ln(Psat_3) = 14.5463 - \frac{2940.46}{(T + 237.22)} \tag{3}$$

where, $Psat_i$ is the vapour pressure in kPa and T is the temperature in ^oC.

a. Write a MATLAB program that outputs a graph showing P vs x_1 and P vs y_1 for temperature of 75^oC for a mixture of acetonitrile (1) and nitromethane (2).

b. Write a MATLAB program that outputs a graph showing T vs x_1 and T vs y_1 for a pressure of 70 kPa for a mixture of acetone (3) and acetonitrile (1).

NOTE: In both the questions x_1 and y_1 corresponds to the liquid and vapour composition respectively of more volatile component.

2. Find the nearest distance of the point (2; 3) from the line x + y + 1.

3. Solve the ODE:

$$\frac{d^2m}{dx^2} + m = 0$$

$$where, \qquad m(0) = 2 \ and \ \frac{dm}{dx}(0) = 3$$

Plot m(x) vs x. Span for x = 0 to 3.142.

4. Water distribution networks, as the name suggests transport water from a source (or multiple sources) and deliver them to demand points. Generally speaking, pressure drives flow, i.e., the upstream pressure is greater than the downstream pressure. Water can also flow aided by gravity, i.e., water flows from a higher level to a lower level. Thus, a difference in elevation and/or pressure provides the driving force for flow. The two are often combined into a single quantity called the head (expressed in meters). If water flows from point A to point B, the head at point A, H_A is greater than the head at point B, H_B. If the flow rate of water Q is known, the head loss $\Delta H = H_A - H_B$ is related to the flow rate, diameter and length of the pipe through the following correlation:

$$H_A - H_B = \Delta H = 4.457 \text{ x } 10^8 \frac{LQ^{1.85}}{D^{4.87}}$$

Where Q is the flow rate in m^3/min, H_A ; H_B ; ΔH are the heads in meters, L is the length of pipe in meter, D is the inner diameter of the pipe in mm.

A network consists of a source node (or multiple sources) and demand points or nodes. The topography of the network (i.e., where the source is situated, where the demand points are located etc.) and the interconnections between the nodes is usually decided beforehand. The water demand at the individual demand points is also known. The task at hand is to decide the diameters of the pipes used to transport the water. There are two competing factors that have to be traded off when deciding the optimum pipe diameters: the capital cost of the pipe and pump operating costs. In the following problems we consider flow by gravity and hence, pump operating costs are zero. A large diameter pipe would result in a high capital cost, but low head loss. Likewise, a smaller diameter pipe would result in small capital cost, high head loss. As expected, one aims to minimize the total cost. Constraints to be enforced are the demand flow rates at the demand points. In addition, it is common to specify a minimum head at the demand nodes. The task at hand is to decide the individual pipe diameters that minimize the total cost while satisfying the constraints.

Consider the network shown in Figure 1. The water distribution network consists of a source node 0 and three demand nodes 1, 2 and 3. Node 0 and node 1 are connected by link I. Likewise, link II connects nodes 1 and 2. Link III connects nodes 1 and 3. The diameters of the pipes are D_1; D_2; D_3 respectively (in mm). Flow is by gravity and it is possible to achieve a head of 100 m at source node 0. Minimum head values at nodes 1, 2 and 3 are 80, 85 and 80 m respectively. The demands at nodes 1, 2 and 3 are 4, 3 and 2 m^3/min respectively. Lengths of links I, II and III are 300, 500 and 400 m respectively. The cost of the pipe per unit length (in Rs./m) can be estimated by the correlation:

$$C = 1.2654\, D^{1.327}$$

Where, D is the diameter of the pipe in mm. Since flow is by gravity, there are no operating costs associated with this network, i.e., total cost is simply the sum of capital costs of the pipes. The task at hand is to decide the diameters of the pipes, D_1; D_2; D_3 respectively using **fmincon** in MATLAB.

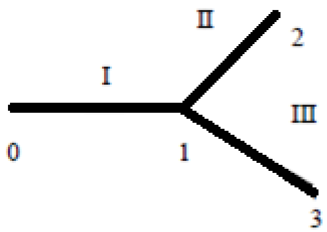


Figure 1. Water distributing pipe network.

Hint: Work backwards from the terminal nodes. Head loss across pipes connected in series is equal to sum of individual head losses.

5. Your team has a cannon that shoots water balloons with a velocity of 100 m/sec. You can adjust its angle of inclination 'α' to change the range. The bull's eye is at a point 10 m high, 300 m away from you. If you hit it with the water balloon, you win. Your plan is to use MATLAB to solve to choose the correct value of α.

6. Consider the following reactions

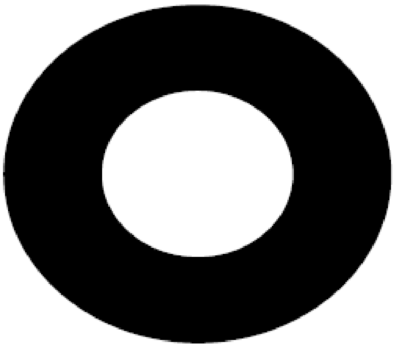
$$A + B \xrightarrow{k_1} R$$
$$R + B \xrightarrow{k_2} S$$

Both reactions are of second order .For C_{A0}= 1 M, C_{B0}=1 M, C_{R0}=0, C_{S0}=0, plot the conc profiles of all components till 2 mins, k_1=0.1 and k_2=0.05. Find the time when the conc of R is maximum.

$$\frac{dC_A}{dt} = -k_1 C_A C_B$$
$$\frac{dC_B}{dt} = -k_1 C_A C_B - k_2 C_R C_B$$
$$\frac{dC_R}{dt} = k_1 C_A C_B - k_2 C_R C_B$$
$$\frac{dC_S}{dt} = -k_2 C_R C_S$$

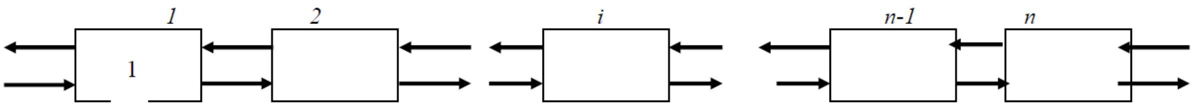
7. Find the nearest point on the shaded area for each of given points.

X	2	2	6	-3	0	11	-4	1	1
Y	2	1	1	-2	0	10	-4	1	4



Shaded region is area between 2 concurrent circles centered (1, 1), with inner radius 3 units and outer radius 5 units.

8. An N stage extraction process is depicted in Fig. 1. In such systems, a stream containing a weight fraction Y_{in} of a chemical enters from the left at a mass flow rate of F_1. Simultaneously a solvent carrying a weight fraction X_{in} of the same chemical enters from the right at a flow rate of F_2. At each stage, equilibrium between X_i and Y_i is assumed that implies that $K = Y_i = X_i$. N is the number of stages. Flow sheet of an extraction process is given below.



For stage i, the mass balance yields the following equation:

$$Y_{i-1} - \left(1 + \frac{F_2}{F_1}K\right) Y_i + \left(\frac{F_2}{F_1}K\right) Y_{i+1} = 0$$

Write down similar equations for other stages. Convert them into matrix form. Use the above developed algorithm to solve for X_{out} and Y_{out} with the following data:

- K = 3
- N = 4
- $F_2/F_1 = 0.5$

Repeat the calculation for N = 5, 6 and F_2/F_1 = 0.75 and 1.

9. This instability can be observed whenever there is at least one of the surfaces of the fluid layer that is an interface. The mechanism for Marangoni instability is that the disturbance in the flow brings slightly warmer fluid from the bottom of the fluid layer, which is initially warmer at the bottom and cooler at the free surface, and thus creates a local disturbance of the temperature, leading to surface tension gradient. Because the interface is cooler away from the perturbed region, the surface tension is higher there, and this tendency to sustain the perturbation by driving fluid motion along the surface away from the perturbed spot, thus pulling more heated fluid up from the bottom of the fluid layer. As fluid moves across the interface it is cooled to temperature of the surroundings and must eventually be drawn backward towards the bottom of the fluid layer to satisfy mass conservation requirements. We therefore expect that the critical parameter for the instability will reflect this competition between the viscous and thermal damping and the surface tension induced motion. It is of course not obvious yet that the fluid layer could be stable to buoyancy-driven motions but still unstable to Marangoni instability.

Solve for the Marangoni number using the function

$$F = \frac{G}{H}$$

$$G = -a^3 * Cosh(a) + (a^2)\big(aCosh(a) - Sinh(a)\big) + \big(2 * a * Coth(a)\big) * (aCosh(a) - Sinh(a) - a^2 Sinh(a) + (M * Bi * e^{-a}) * ((-1 + e^{6a}) + e^{2a}(3 - 4a^3) - (e^{4a})(3 + 4a^3))$$

$$H = 8 * (1 + Bi) * (-1 + e^{2a}) * (Bi(-1 + e^{2a}) + a * (1 + e^{2a}))$$

a is the dimensionless wave number

Bi is the Biot number

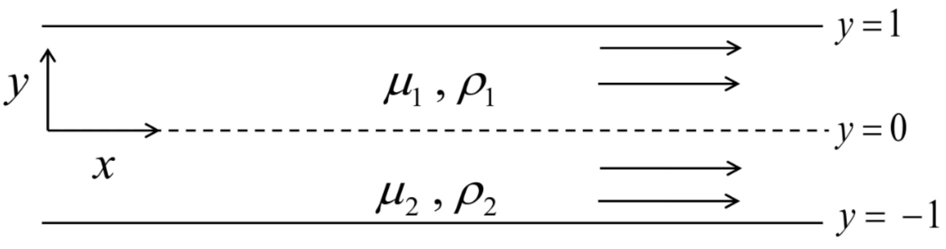
Initial guess value for Marangoni number (M) = 2200

Plot M vs. a for Bi = 2

Plotting range for a is [0, 5]

Plot M vs. a for Bi = 4

10. Plot the velocity profiles for two fluids flowing between two parallel plates.



Boundary conditions

$U_1 = 0$ at y = 1

$U_2 = 0$ at y = - 1

$U_1 = U_2$ at y = 0

$\mu_1 \frac{dU1}{dy} = \mu 2 \frac{dU2}{dy}$ at y = 0; for μ1= μ2 and μ1= 0.5* μ2