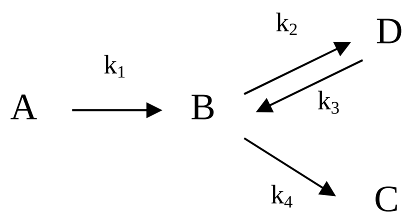
06-623 Mathematical Modeling of Chemical Engineering Processes
Homework Assignment #2
Due by 4:30pm on Monday, Sept 28, 2015

Use Matlab to solve these problems. Generate script which is organized and commented. You can make one m file for the entire assignment or separate m files for each problem. Turn in the m files AND pdf files of the output (using the publish function). Zip files together and turn in one file through blackboard.

Decomposition

1. The reaction scheme below occurs in an isothermal CSTR of volume V. Each reaction is assigned a rate constant and the units of the rate constant will come from the order of the reaction. For this problem, the rates are first order and each takes the form of {rate of production of product in mole/vol time} = $k_iC_{reactant}$ in the reactor. The flow into and out of the reactor is constant at a flow rate of ν and the composition of the exit stream is the same as the composition of the reactor.



Reaction scheme. The k_i terms are the rate constants for the specific reaction steps.

Write a set of balance equations for the moles of the four components in the reactor as a function of time. Your model should take the form $\mathbf{A}\mathbf{c}_{\mathbf{ss}} = \mathbf{c}_{\mathbf{I}}$, where $\mathbf{c}_{\mathbf{ss}}$ is a vector of the steady state concentrations of components in the reactor and $\mathbf{c}_{\mathbf{I}}$ is a vector of the feed concentrations of each component.

Write a script that uses LU decomposition. Input the rate constants and residence time as a single vector. Construct the A matrix and then use the `lu()` function to generate the triangular matrices within the script. For an arbitrary feed vector, have the script perform two steps using the triangular matrices to determine $\mathbf{c}_{\mathbf{ss}}$.

Determine the steady state concentrations in the reactor for the situation that $\mathbf{k}$ = [0.1 0.2 0.1 0.8] sec^{-1} for a 10 L reactor with an inlet/outlet flow rate of 1 L/sec. The feed to the reactor is a mixture of 5M A and 1M D. Your script should output the steady state reactor concentrations and the vector formed as a result of the first multiplication of a triangular matrix by the feed vector.

Eigenvalue Analysis

2. Compute the eigenspace of the following using three different methods as described below.

$$A = \begin{bmatrix} 3 & 2 & 2 & 1 \\ 2 & 3 & 1 & 2 \\ -1 & 1 & 2 & 0 \\ 2 & 4 & 3 & 5 \end{bmatrix}$$

   a. Use the `eig` function in MatLab to determine the eigenspace. Determine the norm of each of the eignevectors calculated; how does Matlab normalize eigenvectors?
   b. Matlab has a symbolic function `sym` that allows symbolic, rather than numerical, calculations to be performed. Use the `sym` function to create symbolic versions of the matrices and find exact solutions for the eigenspace.

3. There are numerical approaches to finding eigenvalues and the power method is one of them. The power method finds the largest eigenvalues for any self-adjoint matrix with distinct eigenvalues. For a matrix **A**, start with the vector $\mathbf{x_0} = [\ 1\ 0\ 0]^T$ and iterate using $\mathbf{x_{i+1}} = \mathbf{A}\ \mathbf{x_i}$. Perform this procedure on a real, symmetric 3x3 matrix **A**. outputting the largest eigenvalue (to within a tolerance that you define) of **A** and corresponding eigenvector.

Solving Nonlinear Algebraic Equations

4. The nonlinear equation $f(x) = x^3 - 5x^2 + 7x - 3$ has three roots, but these are not distinct roots as there is one double root. To solve these problems, the modified Newton-Raphson method is often used. In this problem, we consider the impact of changing the update function, $u(x^{[k]})$, on the speed of convergence of an iterative technique.

$$x^{[k+1]} = x^{[k]} + u(x^{[k]})$$

$$u(x^{[k]}) = -\frac{f(x^{[k]})}{f^{(1)}(x^{[k]})} \quad \text{modified to} \quad u(x^{[k]}) = -\frac{f(x^{[k]})\, f^{(1)}(x^{[k]})}{[f^{(1)}(x^{[k]})]^2 - f(x^{[k]})\, f^{(2)}(x^{[k]})}$$

   a. This is a polynomial, so there are analytical ways to find the roots. Factor the expression for $f(x)$ and determine the three roots.
   b. From the initial guess, $x = 0$, calculate the first 5 values of x (i.e., do 5 iterations) and the error between the actual solution and calculated root using the standard update function.

c. From the initial guess, $x = 0$, calculate the first 5 values of x (i.e., do 5 iterations) and the error between the actual solution and calculated root using the modified update function.

d. Compare the convergence of the two update functions for the initial guess of $x = 4$. Do they approach the same solution?

5. A large tank of water is drained by gravity through a long pipe, L = 5 m, at the bottom of the tank. Assuming that the changes in height of water in the tank do not change the instantaneous velocity, the velocity of fluid leaving the pipe, V(t), is given by:

$$\frac{V(t)}{\sqrt{2gh}} = \tanh\left(\frac{t}{2L}\sqrt{2gh}\right)$$

Determine the height of water, h, needed to have a velocity out of the pipe of 5 m/s after t = 3 sec. Clearly explain the method that you use.

Solving Systems of Nonlinear Algebraic Equations

6. Find at least one real solution to the coupled set of nonlinear algebraic functions below. Solve this as a set of two equations using the Newton-Raphson method. Calculate and use the analytical form of the Jacobian in your method. Clearly state your criteria for convergence. Generate a plot of *x* versus *y* with each of the functions shown as lines and identify your solution (the zero of the system) as a point on the plot.

$$y - (x-1)^2 = 0$$
$$(y+4)^2 - \tan x = 0$$

7. Vapor-liquid equilibrium of mixtures of mixtures requires the calculation of the saturation (or vapor) pressure of the pure components in the mixture. These are tabulated for many components and given as the coefficients (A,B) in Antoine's equation, where A,B are independent of temperature and pressure:

$$P^{sat}(T) = \exp\left(\frac{A}{T(C)+273.15} + B\right) \qquad P_{bubble} = \sum_{i=1}^{N} x_i P_i^{sat}(T \qquad 1/P_{dew} = \sum_{i=1}^{N} y_i \Big/ P_i^{sat}($$

The values of the Antoine coefficients for typical solvents are well known; for example for compound α (A=-3848.09, B=17.5318) and compound β (A=-4328.12, B=17.913). The bubble point pressure is a function of the liquid composition, in terms of mole fractions in the liquid, x_i, for a mixture of N components, and the dew point pressure is a function of the vapor phase composition in terms of mole fractions in the vapor, y_i.

Generate a Txy diagram for α−β mixtures. One line should provide the boiling points (where P_{bubble} is equal to P) while the other should provide the dew points (where P_{dew} is equal to P). Indicate the bubble and dew temperatures for equimolar mixtures on the Txy diagram.

8. A batch gas phase reactor is run at 3000 K at 1 atm with two primary reactions:

$$2CO_2 \rightleftharpoons 2CO + O_2$$
$$O_2 + N_2 \rightleftharpoons 2NO$$

An extent of reaction, ξ_j, is defined for each reaction with units of moles. When run at equilibrium, the mole fractions of each gas in the reactor, y_i, will satisfy:

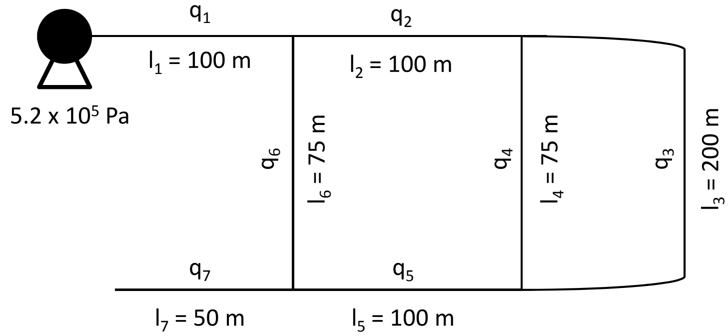
$$\frac{y_{CO}^2 y_{O_2}}{y_{CO_2}^2} = K_1 \text{ and } \frac{y_{NO}^2}{y_{O_2} y_{N_2}} = K_2 .$$

Writing mass balance expressions for the components in the reactor will result in a set of coupled, nonlinear equations in terms of the extents of reaction. This set of equations can be solved to find the solution for the extents of reaction given system parameters and initial feed. Find the solutions for the following sets of conditions using your own iterative approach or a built in function. State the convergence criteria that are used.

a) Solve for the equilibrium extents of reaction for the situation that the feed to the reactor is 1/3 of a mole of CO_2, O_2 and N_2 with values of K_1 = 0.1071 and K_2 = 0.01493.

b) Solve for the equilibrium extents of reaction for the situation that the feed to the reactor is 2 moles of CO_2 and 1/3 of a mole of O_2 and N_2 with values of K_1 = 0.1071 and K_2 = 0.01493.

9. The pipe network below involves seven unknown flow rates, q_i, through loops and junctions. The flow directions and pipe lengths are given on the figure and the flow is driven by a pump delivering a pressure head of 5.2 x 10^5 Pa.



For an incompressible liquid, the flow rates into and out of each junction must balance providing four equations relating the flow rates. The sum of the pressure drops around each loop must also balance providing three more equations:

$$l_3 q_3^2 = l_4 q_4^2$$
$$l_2 q_2^2 + l_4 q_4^2 + l_5 q_5^2 = l_6 q_6^2$$
$$l_1 q_1^2 + l_6 q_6^2 + l_7 q_7^2 = 5.2x10^5 \frac{\pi^2 (0.2)^5}{8(0.02)(998)}$$

Develop the appropriate system of seven nonlinear equations and then solve for q, the vector of flow rates in the flow loop. Assume that the units are consistent. Use an initial guess of q_i = 0.1 for each flow rate.