06-623 Mathematical Modeling of Chemical Engineering Processes
Homework Assignment #3

Due by 4:30pm on Wednesday October 21, 2015

Use Matlab to solve these problems. Generate script which is organized and commented. Please make one m file for the entire assignment. Turn in the m files AND pdf files of the output (using the publish function).

Initial Value Problems

1. Michaelis-Menten kinetics is an established model for enzyme reactions. The reaction mechanism requires two steps, the formation of an enzyme-substrate structure, ES, that reacts to form a product, P. This two step reaction mechanism leads to nonlinear kinetics with a rate of reaction as given below. Assuming that there is initially no product, P, in the reactor, predict the concentration of product as a function of time for the situations below. Assume that the concentration of enzyme is constant and equal to 10% of the initial substrate concentration. For each set of conditions, generate a plot of the concentration of the four species as a function of time. Then plot results for P(t) to compare the impact of different parameters.

$$E + S \rightleftarrows ES \xrightarrow{k_{cat}} E + P$$

$$\text{Reaction rate} = \frac{d[P]}{dt} = \frac{V_{\max}[S]}{K_m + [S]} = k_{cat}[E]_o \frac{[S]}{K_m + [S]}$$

   a) Pepsin catalyzed: k_{cat} = 0.5 s^{-1}; K_m = 0.3 mM; $[S]_o$ = 1 mM
   b) Fumarase catalyzed: k_{cat} = 0.08 s^{-1}; K_m = 5 μM; $[S]_o$ = 1 mM

2. The centerline temperature of a thin copper (ρ=8933 kg/m^3) plate of thickness d = 0.002 m placed in a 1200K furnace (assuming a uniform temperature in the plate and radiative heat transfer, $\sigma = 5.676\ 10^{-8}$ W/m^2 K^4) is given by:

$$\frac{dT}{dt} = \left(\frac{2\sigma}{\rho d}\right)\frac{T_F^4 - T^4}{c_p(T) + T\dfrac{dc_p}{dT}},$$

   where T_F is the furnace temperature and the specific heat of copper, $c_p(T)$, is given by:

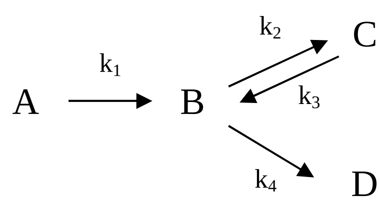
$$c_p(T) = 355.2 + 0.1004T \text{ ; } c_p \text{ [=] J/kg K and T [=] K.}$$

   The initial temperature of the plate is 300K and you have been asked to predict the temperature as a function of time. Assume that the plate dimensions and density are not functions of temperature. Scale the temperature as $\theta = T/T_F$, develop a natural scaling for time using the variables given and define $\tau = t/t^*$ as a dimensionless time. Plot $\theta(\tau)$ for this problem. Be sure to provide the value of t* and a clear description of your method in the comments of your code.

3. The following system describes the trajectory (velocity and position) along a unit circle. This is the DAE system that I discussed in class. Solve this as a DAE using Matlab (see the documentation for `ode15s`) and plot x_2 versus x_1. Choose a value of θ_o and solve the system first using an initial condition of $x_1(t=0) = 0$ and a value of $x_2(0)$ that follows from the algebraic constraint. Then solve it again using $x_1(t=0) = 0$ and $x_2(t=0) = 0.8$; what does this tell you about how the solver computes an initial state that is consistent?

$$\frac{dx_1}{dt} = -[x_1 - \cos(\theta_o)] + [x_2 - \sin(\theta_o)]$$
$$0 = x_1^2 + x_2^2 - 1$$

4. The reaction scheme below occurs in an isothermal, batch reactor. The reactor is initially charged with the reactant A at a concentration of $C_{A,o}$ [=] mol/L and has a volume of 1 L. Each reaction is assigned a rate constant and the rate of formation of the product is proportional to the concentration of the reactant (i.e., first order kinetics).



For the case that the rate constants are $\mathbf{k} = [\ 1 \quad 1 \quad 0.5 \quad 1\ ]^T$ [=] 1/min and the reactor is initially charged with 10 M of reactant A, plot the concentration of each species as a function of time. Use a numerical time marching approach (i.e., do not solve this analytically). Plot each concentration on a separate subplot (four plots) and label the axes. Choose a time range so that the dynamics and the steady state can be seen.

5. Solve the reactor problem above but perform the calculations for a CSTR with a constant flow rate in and out, Q. Choose a flow rate to give a residence time in the reactor of 1 minute. Generate a similar plot of the concentration of each component in the reactor on four subplots. Also provide one plot comparing the batch and CSTR results for the concentration of A as a function of time.

6. A small container and its contents are at 150F. To cool both the container and the liquid to room temperature (70F, the container is immersed in a bath held at 32F. Balancing the rate of change of energy storage between the liquid and the container with the rate of convective heat transfer (liquid – container and container – bath) leads to a coupled system of equations, where L is the temperature of the liquid and C is the temperature of the container. Using the parameters given, plot the temperature of the liquid **and** the container as a function of time. Be careful, the time constants for these two processes are very different!

$$\frac{dL}{dt} = \frac{A_i h}{\rho_1 c_{p,1} V_1}(C - L)$$
$$\frac{dC}{dt} = \frac{A_o h}{\rho_2 c_{p,2} V_2}(32 - C) + \frac{A_i h}{\rho_2 c_{p,2} V_2}(L - C)$$

	Liquid	**Container**
Mass density [lb_m/ft^3]	62	139
Specific heat [Btu/lb_mF]	1.00	0.2
Volume [ft^3]	0.03	0.003

A_i=0.4 ft^2 and A_o=0.5 ft^2
Assume h = 8.8 Btu/hr ft^3 F

Boundary Value Problems

7. The following third order differential equation can be solved as a system of coupled first order differential equations. Write this equation as a system of three coupled first order equations $\underline{u}' = f(\underline{u})$

$$y''' + y'' - 2y = 2x^2 + 2x$$

   (a) Solve with the initial conditions $y(0) = -1; y'(0) = 0; y''(0) = -4$
   (b) Solve using the shooting method and $y(1) = -1; y'(0) = 0; y''(0) = -4$

8. Find the solution to the boundary value problem below using the shooting method. Plot y(x) over the range $1 \le x \le 2$ given the boundary conditions that y(1) = 6.308447 and y(2)=55.430436.

$$y'' - y' + y = 3e^{2x} - 2\sin x$$

9. For linear boundary value problems of the form $y'' = p(x)y' + q(x)y + r(x)$ there is a simple procedure that makes the shooting method very effective. The function $y(x) = y_1(x) + cy_2(x)$ will be an exact solution to the problem where $y_1(x)$ is the solution to to the IVP that corresponds to the nonhomogeneous BVP and $y_2(x)$ is the solution to the corresponding homogeneous IVP (i.e., with $r(x) = 0$). For the following problem:

$$-u'' + \pi^2 u = 2\pi^2 \sin(\pi x)$$
$$u(0) = u(1) = 0$$

   a) Convert this problem into two first order initial value problems to solve for $u_1(x)$ and $u_2(x)$. Show the systems that you plan to solve and the relevant initial value conditions.

b) Use an RK4 method to estimate $u_1(x)$ and $u_2(x)$ at $x_i = 0, 0.25, 0.50, 0.75, 1.00$. Is the prediction for the Dirichlet condition at $x = 1$ correct?

c) Determine the value of c that will give the approximate solution for $y(x)$. Use this to point wise calculate $w(x) = y_1(x) + cy_2(x)$ given the values calculated in part (b).

d) Since the analytical solution is $u(x) = \sin(\pi x)$ calculate the exact error at each point.