CH E 572 - Assignment #1 **Due date: Thursday January 26, 2012**

The objectives for this assignment are:

1. review some material from your math and numerical methods courses,
2. get started on first-principles process modelling,
3. continue to build your MATLAB / Simulink skills.

You may work together in groups to complete the assignment, but you must hand in your own assignment solution. If you work with a group, please identify the people that you worked with on your solution. Computer printout may be included with your solution as an appendix, but please do not provide these as your entire solution.

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1. (5 points) Calculate the Jacobian of the following set of equations, showing all of your work:

$$\mathbf{f}(\mathbf{x}) = \begin{bmatrix} x_1^2 + 6x_1x_2 + x_2^2 + 4x_1 + 3x_2 + 12 \\ 2x_1^2 + 2x_2^2 - 2x_1x_2 \end{bmatrix} = \mathbf{0}$$

   This set of equations could come from a regression analysis. You may use a computer to check your work, but please do the derivations by hand.

2. (5 points) Calculate the gradient of the following function with respect to $\mathbf{x}$ showing all of your work:

$$r(\mathbf{x}) = \frac{\mu_{max} x_1 x_2}{k_m + x_2}$$

   This function is the Monod biochemical reaction rate expression. Both μ_{max} and k_m are constants. You may use a computer to check your work, but please do the derivations by hand.

3. (10 points) Determine the second-order Taylor series expansion for each of the following functions, showing all of your work:

   a) The common function $f(x) = x\ e^{-x}$ about x_0,

   b) The Monod rate expression $r(\mathbf{x}) = \frac{\mu_{max} x_1 x_2}{k_m + x_2}$ about $\mathbf{x}_0$.

   You may use a computer to check your work, but please do the derivations by hand.

4. (10 points) MATLAB has a several ODE solvers. Given the following dynamic process model:

$$\begin{bmatrix} 0 & 1 \\ 2 & 0 \end{bmatrix} \frac{d\mathbf{x}}{dt} = \begin{bmatrix} 10^6 & 0 \\ 0 & 1 \end{bmatrix} \mathbf{x} + \begin{bmatrix} 473 \\ 5 \end{bmatrix} u$$

Please answer each of the following:

a) list all of the ODE solvers available in MATLAB and for each solver, name the algorithm used.

b) Would a solver that uses a Runge-Kutta algorithm be an appropriate choice to numerically solve the given dynamic model? Explain your answer .

c) What would be the best MATLAB solver for the given dynamic model? Explain your answer.

5. (45 points) The ACME Brewing Company uses spherical kettles for brewing their specialty beers. Please note that beer is brewed in batches and that all materials are initially charged into the kettles. Then, the mixture is allowed to ferment for a given amount of time, until the alcohol content reaches the desired level. (Of course this is a very simplistic description of the process). The tank is 2 m in diameter, but is never completely filled. Our beer is brewed in three different batch sizes. For large batches, the kettle is filled to a level or height of 1.5 m from the bottom. For medium and small batches, the kettle is filled to 1.0 m and 0.5 m, respectively. The ingredients for a 20 l batch of our Grandma's Best Pilsner are:

Ingredient	**Amount**
water (room temperature)	17 l
light malt extract	3200 g
ACME Grandma's Secret Hops	100 g

To these ingredients, a small amount of European Lager yeast is added before the mixture is charged to the brewing kettle.

The biochemical reaction kinetics have been found to follow a modified Monod expression and are given by:

$$\mu = \frac{\mu_{max}}{K_m + S}$$

where: $\mu_{max} = 0.54\, days^{-1}$, $K_m = 5\ \frac{g\ substrate}{g\ mixture}$ and S is the *weight fraction* of substrate in the mixture. The substrate is the carbohydrate source for the biochemical reactions (*i.e.*, malt liquor, hops, *etc.*) Then, the rate of substrate consumption is given by $r(S) = \mu S$. For the purposes of this model, you may assume that as substrate is consumed, half of it is used to produce ethanol and half is used for the growth of the yeast culture inside the kettle.

Please answer each of the following questions, showing all of your work:

a) classify the process variables.

b) state your assumptions.

c) develop a dynamic model of the process.

d) is the model linear or nonlinear?

e) plot the transient behaviour of the ethanol concentration for 20 days of brewing time.

f) batches of beer are brewed until the mixture is 5 $wt\%$ ethanol. How long does it take to brew a batch of beer? At the end of a batch what is the composition of the mixture?

g) how does the length of time that it takes to brew a batch of beer depend on the liquid level h in the kettle? Explain.