Practice problems

**Problem 1 (Given ODE, demonstrate ability to computational solve)**

Solve and plot y(x)









**Problem 2 (introduce physical reality to problem)**

The tensile strength of a pasta noodle can be modeled by the following equation. x is the linear deformation distance (mm) and F is force (N).

For this pasta, a force of greater than 3N results in the pasta breaking (undesirable).

Determine the displacement distance (mm) at which the pasta noodle will break.

F"-A\*F'-B\*F-C\*exp(x)=0

F(0)=0 y'(0)=0.1

A, B, C, are constants A=0.01, B=-0.01 C=0.05

F- force

x- displacement

**Problem 3 (problem setup, computational model/solution, and analysis of model)**

You are the process engineer for TAOCO’s batch process that produces a valuable pharmaceutical, B, from an unsaturated lipid, A, via an enzymatic reaction. A also slowly oxidizes chemically into a by-product, C. B is also enzymatically converted into C by normal cellular behavior.

This reaction network is shown below. The rate of reaction equation for each compound is given below, including the initial operating conditions. Reactions 1 and 3 are enzymatic reactions and reaction 2 is a 2nd order chemical reaction. Concentrations, A(t), B(t), and C(t), are in mmol/L. Vi, Ki, and k2 are reaction constants (see data below). The process currently operates using an initial concentration of A of 100 mmol/L. Your task is to obtain A(t), B(t), and C(t).

Rxn 1

V1, K1



A B

Rxn 3

V3, K3

Rxn 2

K2

C

Data values:

V1 = 12 mmol/L-hr K1 = 5 mmol/L

V3 = 1 mmol/L-hr K3 = 0.03 mmol/L

k2 = 0.0008 L/mmol-hr

Part A. (Setup)

Write the set of differential equations to model this situation.

Part B (calculations)

Using your favorite computational platform, solve this set of differential equations to provide numerical models A(t), B(t), and C(t) for 0<t<30 hours. **Provide an appropriate plot of A(t), B(t), and C(t) vs. t over the interval 0<t<30 hr.** Be sure to check your models to make sure they make sense given the physical situation.

Part C (use of model to calculate desired result)

It is desired to set the batch time (time at which the process is stopped) to obtain the highest B:C ratio product. Using your models **provide appropriate plots of the ratio, B(t)/C(t), over the interval 0<t<30 hr** and **determine what the batch time is** to obtain the highest B:C ratio, and the **value of the B/C ratio at this time**. **Also, calculate the % conversion of A at this time).** Be sure to **clearly explain how you obtained the batch time**.

Part D (analysis of model to understand behavior and if system makes sense)

Since B is the desired product and C is a by-product, it is desirable to have as high a B:C ratio as possible. Higher B concentration products would sell for a higher price/better profit (note: it is not possible to separate components in the mixture).

You recently hired a bright young BFPE intern and she suggests that changing the initial process operating conditions might increase the B/C ratio of the product. She reasons that since the 2nd reaction depends more strongly on the concentration of A (2nd order reaction), a higher B/C ratios might be obtained with lower initial concentrations of A. Before you suggest any operating changes to the process to the plant manager (your boss), you want to check her suggestion to see if it makes sense.

**Using your model, examine her suggestion to determine if it is correct**. **Determine how you would change the initial A concentration and batch time to make a product with a maximized B/C ratio. Note that the conversion of A affects the product yield (amount of product made/amount of reactant used) and the batch time affects the process productivity (amount of product made per hour).**

Given this knowledge, **explain whether you would suggest to the plant manager that the initial process operating conditions be changed and to what values,** understanding that your objective is to maximize profitability for TAOCO (and may get a good raise/promotion!).