**Problem 1 (100 points)**

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). Note: A’(t) = dA(t)/dt, etc.

The process currently operates using an initial concentration of A of 100 mmol/L

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

Draw a picture and define the system/flows. Derive the unsteady state differential equation models of the concentrations of A, B and C as a function of time.

Part A. (35 points)

Using Euler’s method on a spreadsheet, solve this set of differential equations to provide numerical models of A(t), B(t), and C(t) for 0<t<30 hours using a **step size of t = 0.5 hr**. Show **calculated values at each step for A(t), B(t), and C(t), as well as A’(t), B’(t), and C’(t).**

**Provide an appropriate plot of A(t), B(t), and C(t) vs. t over the interval 0<t<30 hr.** **Clearly label your submissions for each variable.** Be sure to check your models to make sure they make sense given the physical situation. Note: you may wish to include a column calculating B/C for part C.

Part B (35 points)

Using MathCad, solve this set of differential equations to provide numerical models A(t), B(t), and C(t) for 0<t<30 hours. **Provide the MathCad program** used to solve for the numerical models. **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 (20 points)

It is desired to set the batch time (time at which the process is stopped) to obtain the highest B:C ratio product. Using each of your models **provide appropriate plots of the ratio, B(t)/C(t), over the interval 0<t<30 hr** and **determine at 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**. Compare your solutions from each model (parts A and B) and explain any differences.

Part D (10 points)

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 (who has taken ABE 370) 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 MathCad 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!).