Homework Assignment Number Twelve

Problem 1. (8 points)

Consider the following dimerization reaction

$$2A \rightarrow B$$

The following two mass balances describe the concentrations of A & B in an isothermal reactor as a function of time:

$$\frac{dC_A}{dt} = \frac{F_{in}}{V} C_{A,in} - \frac{F_{out}}{V} C_A - 2r$$

$$\frac{dC_B}{dt} = \frac{F_{in}}{V} C_{B,in} - \frac{F_{out}}{V} C_B + r$$

where the reaction rate, r, is given by

$$r = kC_A^2$$

The following numerical values for the parameters are given in the table below

variable	symbol	value	units
inlet flowrate	F_{in}	0.5	l/s
outlet flowrate	F_{out}	0.5	l/s
inlet concentration of A	$C_{A,in}$	0.8	mol/l
inlet concentration of B	$C_{B,in}$	0.0	mol/l
reactor volume	V	60.0	l
reaction rate	k	14.0	$l/mol/s$

The following initial conditions are given for these two ordinary differential equations

variable	symbol	value	units
Initial reactor concentration of A	$C_{A,o}$	0.0	$mole/l$
Initial reactor concentration of B	$C_{B,o}$	0.0	$mole/l$

(a) Is this system of ordinary differential equations linear or nonlinear?

(b) What is the appropriate technique to solve this system of equations?

(c) Solve the transient behavior of the concentration of A, C_A, and the concentration of B, C_B, up to 1000 seconds, if the initial concentration of A in the reactor is $C_A = C_{A,o}$ and the initial concentration of B in the reactor is $C_B = C_{B,o}$. Plot the concentrations of A & B as a function of time.

(d) Report values of the concentration of A, C_A, and the concentration of B, C_B, at 1000 seconds.

Problem 2. (12 points)

We are testing a polymer membrane designed to catalytically filter microbes. The concentration of microbe *A*, $C_{A,0}$, on one side of the membrane, located at $z = 0$, is $C_{A,0}$. The concentration of microbe *A*, $C_{A,f}$, on the other side of the membrane, located at $z = L$, is $C_{A,f}$. Inside the polymer membrane, a chemical agent kills the microbe. The following equation describes the profile of the microbe concentration within the membrane,

$$0 = D\frac{d^2C_A}{dz^2} - k\sqrt{C_A}$$

Answer the following questions.

(a) Is this ODE problem linear or nonlinear?
(b) Is this ODE problem an initial value problem or a boundary value problem?
(c) Convert this second order ODE into a system of two first order ODEs.
(d) For a membrane of thickness, $L = 5$ cm, and the following numerical values, $D = 1.0 \cdot 10^{-6}\frac{cm^2}{s}$, $k = 2.8 \cdot 10^{-9}\frac{\left(\frac{mol}{\ell}\right)^{1/2}}{s}$, $C_{A,0} = 1.0 \cdot 10^{-2}\frac{mol}{\ell}$ and $C_{A,f} = 2.2 \cdot 10^{-4}\frac{mol}{\ell}$, find the concentration gradient of the microbe at $z = 0$.
(e) Sketch the concentration profile.
(f) Verify that your discretization resolution was sufficient.