Final Exam
Administered: Tuesday, December 10, 2024
10:30 AM – 12:45 PM
24 points

Problem 1. System of Ordinary Differential Equations (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}	1.0	l/s
outlet flowrate	F_{out}	1.0	l/s
inlet concentration of A	$C_{A,in}$	2.0	mol/l
inlet concentration of B	$C_{B,in}$	0.0	mol/l
reactor volume	V	100.0	l
reaction rate	k	20.0	$l/mol/s$

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. System of Algebraic Equations (8 points)
We allow the reactor in problem 1 to reach steady state. In this case, time derivatives in problem 1 become zero. Thus, the ODEs in problem 1 become algebraic equations:

$$0 = \frac{F_{in}}{V} C_{A,in} - \frac{F_{out}}{V} C_A - 2r$$

$$0 = \frac{F_{in}}{V} C_{B,in} - \frac{F_{out}}{V} C_B + r$$

All parameters remain the same as in problem 1.

(a) Is this system of equations linear or nonlinear?
(b) What is the appropriate technique to solve this system of equations?
(c) Determine the steady values of the concentration of A, C_A, and the concentration of B, C_B.
(d) Explain the relationship between the answer for problem 2(c) and problem 1(d).

Problem 3. Numerical Integration (4 points)
Consider the reactor described in problem 1. The total amount of component B, N_B, produced in the first 1000 seconds is given by

$$N_B = \int_{t=0}^{t=1000} F_{out} \left(\frac{dC_B}{dt} \right) dt$$

Substituting in the ODE for C_B and the definition of the reaction rate, r, given in problem 1, yields

$$N_B = \int_{t=0}^{t=1000} F_{out} \left(\frac{F_{in}}{V} C_{B,in} - \frac{F_{out}}{V} C_B + kC_A^2 \right) dt$$

Thus knowing the values of C_A and C_B as a function of time (from the solution of problem 1), we can compute the total moles of B produced through numerical integration. For the purposes of this exam, the entire integrand has been calculated from C_A and C_B and is given as a function of time in the file, https://utkstair.org/clausius/docs/mse301/data/xm4p03_f24.txt, on the course website.

(a) What is the appropriate numerical technique to evaluate this integral?
(b) How many moles of B were produced in the first thousand second of reactor operation?

Problem 4. Project Question. (4 points)
Regarding the course project, answer the following questions.
(a) Which project did you work on?
(b) In your opinion, what was the most significant result of your project?