Exam III
Administered: Monday, November 2, 2020
22 points

For each problem part: 0 points if not attempted or no work shown,
1 point for partial credit, if work is shown,
2 points for correct numerical value of solution

Problem 1. (12 points)

Consider an isothermal flow reactor with a volume, V= 10 liters, in which the following set of elementary reactions take place

reaction 1: $A \rightarrow B$ with rate constant $k_1 = 2$ s^{-1}
reaction 2: $B \rightarrow C$ with rate constant $k_2 = 5$ s^{-1}
reaction 3: $A \rightarrow D$ with rate constant $k_3 = 3$ s^{-1}
reaction 4: $C \rightarrow D$ with rate constant $k_4 = 1$ s^{-1}

The inlet flow rates are given by

$$F_{A,in} = F_{B,in} = 2\frac{mole}{\ell \cdot s} \quad \text{and} \quad F_{C,in} = F_{D,in} = 0\frac{mole}{\ell \cdot s}$$

The outlet flow rates are given by

$$F_{A,out} = \hat{F}_{out}C_A, F_{B,out} = \hat{F}_{out}C_B, F_{C,out} = \hat{F}_{out}C_C \text{ and } F_{D,out} = \hat{F}_{out}C_D \frac{mole}{\ell \cdot s}$$

where $\hat{F}_{out} = 4$ s^{-1} and concentrations are measured in moles/liter.

The steady state mass balances are

accumulation = in – out + generation -consumption

$$0 = F_{A,in} - \hat{F}_{out}C_A - k_1 C_A - k_3 C_A$$
$$0 = F_{B,in} - \hat{F}_{out}C_B + k_1 C_A - k_2 C_B$$
$$0 = F_{C,in} - \hat{F}_{out}C_C + k_2 C_B - k_4 C_C$$
$$0 = F_{D,in} - \hat{F}_{out}C_D + k_3 C_A + k_4 C_C$$

(a) Write this set of equations in matrix notation, $\underline{\underline{A}}\underline{x} = \underline{b}$. Identify all three quantities, $\underline{\underline{A}}$, $\underline{x}$ and $\underline{b}$.
(b) Calculate the determinant of $\underline{\underline{A}}$.
(c) Calculate the rank of $\underline{\underline{A}}$.
(d) Calculate the rank of $\underline{\underline{A}}|\underline{b}$
(e) How many solutions are there to this problem?
(f) Calculate the steady state concentrations of A, B, C and D in this reactor under these conditions.

(over)

Problem 2. (10 points)

If we rework problem 1 with the single change that we replace reaction 4 with

reaction 4: $B + C \rightarrow D$ with rate constant $k_4 = 4 \frac{\text{liter}}{\text{mole} \cdot s}$

Then the steady state mass balances become

accumulation = in – out + generation -consumption

$$0 = F_{A,in} - \hat{F}_{out} C_A - k_1 C_A - k_3 C_A$$
$$0 = F_{B,in} - \hat{F}_{out} C_B + k_1 C_A - k_2 C_B - k_4 C_C C_B$$
$$0 = F_{C,in} - \hat{F}_{out} C_C + k_2 C_B - k_4 C_C C_B$$
$$0 = F_{D,in} - \hat{F}_{out} C_D + k_3 C_A + k_4 C_C C_B$$

(a) Is this system of equation linear or nonlinear?
(b) What numerical technique is appropriate for solving this problem?
(c) Solve for the steady state concentrations. (6 points)