

Exam III

Administered: Friday, November 6, 2015

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 $k_1 = 1 \text{ s}^{-1}$

reaction 2: $B \rightarrow C$ with rate constant $k_2 = 2 \text{ s}^{-1}$

reaction 3: $A \rightarrow C$ with rate constant $k_3 = 3 \text{ s}^{-1}$

reaction 4: $C \rightarrow D$ with rate constant $k_4 = 4 \text{ s}^{-1}$

The inlet flow rates are given by

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

The outlet flow rates are given by

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

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

The steady state mass balances are

accumulation = in – out + generation – consumption

$$0 = F_{A,in} - \hat{F}_{out} C_A - k_1 C_A - k_3 C_A$$

$$0 = F_{B,in} - \hat{F}_{out} C_B + k_1 C_A - k_2 C_B$$

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

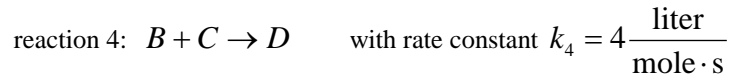
$$0 = F_{D,in} - \hat{F}_{out} C_D + k_4 C_C$$

- Write this set of equations in matrix notation, $\underline{\underline{A}}\underline{\underline{x}} = \underline{\underline{b}}$. Identify all three quantities, $\underline{\underline{A}}$, $\underline{\underline{x}}$ and $\underline{\underline{b}}$.
- Calculate the determinant of $\underline{\underline{A}}$.
- Calculate the rank of $\underline{\underline{A}}$.
- Calculate the rank of $\underline{\underline{A}}|\underline{\underline{b}}$
- How many solutions are there to this problem?
- 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



Then the steady state mass balances become

accumulation = in – out + generation -consumption

$$0 = F_{A,in} - \hat{F}_{out} C_A - k_1 C_A - k_3 C_A$$

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

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

$$0 = F_{D,in} - \hat{F}_{out} C_D + k_4 C_C C_B$$

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