Written Homework #4
ChE 231
Spring 2019

Problem 1. Consider a continuous stirred tank reactor in which the following irreversible reaction occurs: A $\rightarrow$ B, B $\rightarrow$ A. The reaction rates per unit volume of the forward and reverse reactions are $r_f = k_f C_A$ and $r_r = k_r C_B$, respectively. The reactor has two inlet streams, with the first stream having volumetric flow rate q_1 and concentrations C_{A1} and $C_{B1} = 0$ and the second stream having volumetric flow rate q_2 and concentrations C_{A2} and C_{B2}. The reactor has an outlet stream with volumetric flow rate q_3 and concentrations C_{A3} and C_{B3}. The reactor operates isothermally with constant volume V and density ρ. At steady state the reactor is described by the following linear algebraic equations:

$$\begin{aligned} 0 &= \frac{q_1}{V}C_{A1} + \frac{q_2}{V}C_{A2} - \left(k_f + \frac{q_1}{V} + \frac{q_2}{V}\right)C_{A3} + k_r C_{B3} \\ 0 &= \frac{q_2}{V}C_{B2} + k_f C_{A3} - \left(k_r + \frac{q_1}{V} + \frac{q_2}{V}\right)C_{B3} \end{aligned}$$

Given the parameter values $k_f = 2$, $k_r = 1$, $\frac{q_1}{V} = 2$, $\frac{q_2}{V} = 1$, $C_{A1} = 1$, $C_{A2} = 1$ and $C_{B2} = 6$, formulate and solve a matrix problem $\mathbf{Ax} = \mathbf{b}$ by Gaussian elimination to find the steady-state values C_{A3} and C_{B3}.

Problem 2. Consider a continuous stirred tank reactor with the following reaction sequence:

$$2A \rightarrow B, \qquad B \rightarrow C, \qquad 2B \rightarrow D, \qquad 2C + D \rightarrow E$$

The rates of the four reactions per unit volume are denoted r_1, r_2, r_3 and r_4, respectively. Let $r_1 = 2$. Formulate the linear algebraic equation model $\mathbf{Ar} = \mathbf{b}$ where $\mathbf{r} = [r_2\ r_3\ r_4]^T$. Find the solution $\mathbf{r}$ by Gaussian elimination.