Written Homework #5 (Solutions)

ChE 231

Spring 2019

Problem 1. Consider a continuous stirred tank reactor in which the following reactions occur: A $\rightarrow$ B, B $\rightarrow$ C, C $\rightarrow$ B and B $\rightarrow$ D. The reactor has an inlet stream with concentration C_{Af}. The reactor is described by the following steady-state mass balance equations:

$$\begin{aligned} 0 &= -5C_A + 2C_{Af} \\ 0 &= 3C_A - 20C_B + 9C_C \\ 0 &= 6C_B - 11C_C \end{aligned}$$

Use Gauss-Jordan elimination to find the matrix inverse and to find the solution C_A, C_B and C_C.

$$\begin{bmatrix} -5 & 0 & 0 \\ 3 & -20 & 9 \\ 0 & 6 & -11 \end{bmatrix} X = \begin{bmatrix} -2C_{Af} \\ 0 \\ 0 \end{bmatrix} \Rightarrow Ax = b$$

$(x = [C_A, C_B, C_C])$

$$[A \;\; I] = \left[\begin{array}{ccc|ccc} -5 & 0 & 0 & 1 & 0 & 0 \\ 3 & -20 & 9 & 0 & 1 & 0 \\ 0 & 6 & -11 & 0 & 0 & 1 \end{array}\right]$$

$$-\tfrac{1}{5} \times R1 \rightarrow R1 = \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & -\frac{1}{5} & 0 & 0 \\ 3 & -20 & 9 & 0 & 1 & 0 \\ 0 & 6 & -11 & 0 & 0 & 1 \end{array}\right]$$

$$R2 - 3 \times R1 \rightarrow R2 = \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & -\frac{1}{5} & 0 & 0 \\ 0 & -20 & 9 & \frac{3}{5} & 1 & 0 \\ 0 & 6 & -11 & 0 & 0 & 1 \end{array}\right]$$

$$-\tfrac{1}{20} \times R2 \rightarrow R2 = \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & -\frac{1}{5} & 0 & 0 \\ 0 & 1 & -9/20 & -3/100 & -\frac{1}{20} & 0 \\ 0 & 6 & -11 & 0 & 0 & 1 \end{array}\right]$$

$$R3 - 6 \times R2 \rightarrow R3 = \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & -1/5 & 0 & 0 \\ 0 & 1 & -9/20 & -3/100 & -1/20 & 0 \\ 0 & 0 & -83/10 & 9/50 & 3/10 & 1 \end{array}\right]$$

$$-\tfrac{10}{83} \times R3 \rightarrow R3 = \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & -1/5 & 0 & 0 \\ 0 & 1 & -9/20 & -3/100 & -1/20 & 0 \\ 0 & 0 & 1 & -9/415 & -3/83 & -10/83 \end{array}\right]$$

$$R2 - (-\tfrac{9}{20}) \times R3 \rightarrow R2 = \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & -1/5 & 0 & 0 \\ 0 & 1 & 0 & -33/830 & -11/166 & -9/166 \\ 0 & 0 & 1 & -9/415 & -3/83 & -10/83 \end{array}\right]$$

$$A^{-1} = \begin{bmatrix} -1/5 & 0 & 0 \\ -33/830 & -11/166 & -9/166 \\ -9/415 & -3/83 & -10/83 \end{bmatrix} \#$$

$$X = A^{-1} b$$

$$= \begin{bmatrix} -\frac{1}{5} & 0 & 0 \\ -33/830 & -11/166 & -9/166 \\ -9/415 & -3/83 & -10/83 \end{bmatrix} \begin{bmatrix} -2C_{Af} \\ 0 \\ 0 \end{bmatrix}$$

$$X = \left[\tfrac{2}{5} C_{Af}, \; \tfrac{33}{415} C_{Af}, \; \tfrac{18}{415} C_{Af} \right]$$

Thus, $C_A = \frac{2}{5} C_{Af}$

$C_B = \frac{33}{415} C_{Af}$ #

$C_C = \frac{18}{415} C_{Af}$

Problem 2. Consider the following reaction network: $A \to D$, $2A \to 2B$, $4B + 3C \to 2A$. The rates of these three reactions are denoted r_1, r_2 and r_3, respectively. Assume that the reacting species A, B and C are supplied at rates $r_{A0} = 1$, $r_{B0} = 2$ and $r_{C0} = 6$, respectively.

1. Show that mass balances on the species A, B and C yield a linear algebraic equation system that can be written as follows where $\mathbf{x} = [r_1\ r_2\ r_3]^T$,

$$\begin{bmatrix} -1 & -2 & 2 \\ 0 & -2 & 4 \\ 0 & 0 & -3 \end{bmatrix} \mathbf{x} = \begin{bmatrix} -1 \\ 2 \\ -6 \end{bmatrix}$$

$A \xrightarrow{r_1} D$ $\qquad A_0 \xrightarrow{r_{A0}} A$ $\qquad r_{A0} = 1$

$2A \xrightarrow{r_2} 2B$ $\qquad B_0 \xrightarrow{r_{B0}} B$ $\qquad r_{B0} = 2$

$4B + 3C \xrightarrow{r_3} 2A$ $\qquad C_0 \xrightarrow{r_{C0}} C$ $\qquad r_{C0} = 6$

(9)

$A: r_{A0} - r_1 - 2r_2 + 2r_3 = 0$

$B: r_{B0} + 2r_2 - 4r_3 = 0$

$C: r_{C0} - 3r_3 = 0$

$$\begin{bmatrix} -1 & -2 & 2 \\ 0 & 2 & -4 \\ 0 & 0 & -3 \end{bmatrix} \begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix} = \begin{bmatrix} -r_{A0} \\ -r_{B0} \\ -r_{C0} \end{bmatrix} = \begin{bmatrix} -1 \\ -2 \\ -6 \end{bmatrix}$$

$$\begin{bmatrix} -1 & -2 & 2 \\ 0 & -2 & 4 \\ 0 & 0 & -3 \end{bmatrix} x = \begin{bmatrix} -1 \\ 2 \\ -6 \end{bmatrix} \Rightarrow Ax = b$$

2. Perform Gauss-Jordan elimination on the matrix $\mathbf{A}$ to find the inverse matrix $\mathbf{A}^{-1}$.

(b)

$$[A \; I] = \begin{bmatrix} -1 & -2 & 2 & 1 & 0 & 0 \\ 0 & -2 & 4 & 0 & 1 & 0 \\ 0 & 0 & -3 & 0 & 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} -1 & 0 & -2 & 1 & -1 & 0 \\ 0 & -2 & 4 & 0 & 1 & 0 \\ 0 & 0 & -3 & 0 & 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} -1 & 0 & 0 & 1 & -1 & -2/3 \\ 0 & -2 & 4 & 0 & 1 & 0 \\ 0 & 0 & -3 & 0 & 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 & -1 & 1 & 2/3 \\ 0 & 1 & -2 & 0 & -1/2 & 0 \\ 0 & 0 & 1 & 0 & 0 & -1/3 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 & -1 & 1 & 2/3 \\ 0 & 1 & 0 & 0 & -1/2 & -2/3 \\ 0 & 0 & 1 & 0 & 0 & -1/3 \end{bmatrix} \Rightarrow A^{-1} = \begin{bmatrix} -1 & 1 & 2/3 \\ 0 & -1/2 & -2/3 \\ 0 & 0 & -1/3 \end{bmatrix}$$

3. Use $\mathbf{A}^{-1}$ to determine the solution $\mathbf{x}$. Calculate the 2-norm of $\mathbf{x}$.

(c)

$$x = A^{-1}b = \begin{bmatrix} -1 & 1 & 2/3 \\ 0 & -1/2 & -2/3 \\ 0 & 0 & -1/3 \end{bmatrix} \begin{bmatrix} -1 \\ 2 \\ -6 \end{bmatrix} = \begin{bmatrix} -1 \\ 3 \\ 2 \end{bmatrix}$$

$$\|x\|_2 = \sqrt{(-1)^2 + (3)^2 + (2)^2} = \sqrt{14} = 3.74$$