

Exam III
Administered: Friday, November 8, 2018
24 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, if work is shown

Problem 1. (16 points)

Consider a set of three first order reactions occurring in a closed pot (a batch reactor) involving compounds, OX, MX and PX.

number	reaction	rate expression	rate constant
1	$OX \rightarrow MX$	$r_1 = k_1 OX$	$k_1 = 3 \text{ s}^{-1}$
2	$MX \rightarrow PX$	$r_2 = k_2 MX$	$k_2 = 9 \text{ s}^{-1}$
3	$PX \rightarrow OX$	$r_3 = k_3 PX$	$k_3 = 5 \text{ s}^{-1}$

These equations give rise to the following steady state (at infinite time) mass balances.

compound	rate expression
OX	$0 = k_3 PX - k_1 OX$
MX	$0 = k_1 OX - k_2 MX$
PX	$0 = k_2 MX - k_3 PX$

We also recognize that the sum of the mass fractions equal unity.

$$OX + MX + PX = 1$$

Your goal is to find the steady state composition in this reactor. To do so, answer the following questions.

- Are these equations linear or non-linear?
- Since you have three unknowns, which three of the four equations should be used to solve for the composition?
- Construct a matrix, $\underline{A}$, and vector, $\underline{b}$, from which the compositions, $\underline{x}$, can be obtained.
- Provide the determinant of the matrix.
- Provide the rank of the matrix, $\underline{A}$.
- Provide the rank of the augmented matrix, $\underline{A}\underline{b}$.
- How many solutions will $\underline{A}\underline{x}=\underline{b}$ have?
- Provide a solution if it exists.

(over)

Problem 2. (8 points)

Consider a set of three reactions occurring in a closed pot (a batch reactor) involving compounds, OX, MX and PX.

number	reaction	rate expression	rate constant
1	$\text{OX} + \text{OX} \rightarrow \text{MX}$	$r_1 = k_1 \text{OX}^2$	$k_1 = 3 \text{ s}^{-1}$
2	$\text{MX} + \text{OX} \rightarrow \text{PX}$	$r_2 = k_2 \text{OX} \cdot \text{MX}$	$k_2 = 9 \text{ s}^{-1}$
3	$\text{PX} \rightarrow 3\text{OX}$	$r_3 = k_3 \text{PX}$	$k_3 = 5 \text{ s}^{-1}$

These equations give rise to the following steady state (at infinite time) mass balances.

compound	rate expression
OX	$0 = 3k_3 \text{PX} - 2k_1 \text{OX}^2 - k_2 \text{OX} \cdot \text{MX}$
MX	$0 = k_1 \text{OX}^2 - k_2 \text{OX} \cdot \text{MX}$
PX	$0 = k_2 \text{OX} \cdot \text{MX} - k_3 \text{PX}$

We also recognize that the sum of the mass fractions equal unity.

$$\text{OX} + \text{MX} + \text{PX} = 1$$

Your goal is to find the steady state composition in this reactor. To do so, answer the following questions.

- Are these equations linear or non-linear?
- Since you have three unknowns, which three of the four equations should be used to solve for the composition?
- What solution technique should use you to solve this problem?
- Provide a solution.