Exam III
Administered: Wednesday, November 6, 2024
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

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 → MX	$r_1 = k_1 OX$	$k_1 = 7\ s^{-1}$
2	MX → PX	$r_2 = k_2 MX$	$k_2 = 9\ s^{-1}$
3	PX → OX	$r_3 = k_3 PX$	$k_3 = 5\ s^{-1}$

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.

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

Problem 2. (8 points)
The longest relaxation time of a polymer can be measured through an auto-correlation function (acf) of the polymer end-to-end distance.

$$acf = c \cdot exp\left(-\frac{t}{\tau}\right) \tag{1}$$

where t is time (sec), τ is relaxation time (sec) and c is a prefactor. The acf is dimensionless.

For the acf vs t data given in the file, http://utkstair.org/clausius/docs/mse301/data/xm3p02_f24.txt, perform the following tasks. In this data file, the first column is time and the second column contains the values of the acf.

(a) Identify all variables, $y = mx + b$, when equation (1) is linearized.
(b) Report the best value of τ and c.
(c) Report the standard deviations of τ and c.
(d) Report the measure of fit.