Question 2, part 8.1

According to Murray, the Law of Mass Action states that the rate of a reaction is proportional to the product of the reactant concentrations (Murray, 1989).

We already know that:

$$E + S \underset{k_2}{\overset{k_1}{\rightleftharpoons}} ES \overset{k_3}{\rightarrow} E + P \, (0)$$

Set concentrations of the reactants as:

$$\mathrm{s} = [\mathrm{S}], \mathrm{e} = [\mathrm{E}], \mathrm{c} = [\mathrm{ES}], \mathrm{p} = [\mathrm{P}] \qquad (1)$$

Based on the research of Harris and Keshwani, we also know that instantaneous velocity on reactant concentration composed of loss of reactant or gain of product (Harris and Keshwani, 2009).

For rate of change of concentration [S], we first use loss rate proportional to [E][S], which is e and s. Then we use gain rate proportional to [ES], which is c in our case.

$$\frac{ds}{dt} = -k_1 es + k_2 c \qquad (2)$$

For rate of change of concentration [E], we use loss rate proportional to [E][S], which is e and s. Then we use gain rate proportional to [ES], which is c in our case.

$$\frac{de}{dt} = -k_1 es + (k_2 + k_3)c \qquad (3)$$

For rate of change of concentration [ES], we use gain rate proportional to [E][S], which is e and s. Then we use a loss rate proportional to [ES], which is c in our case.

$$\frac{dc}{dt} = k_1 es - (k_2 + k_3)c \qquad (4)$$

For rate of change of concentration [P], we use gain rate proportional to [ES], which is c in our case.

$$\frac{dp}{dt} = k_3 c \qquad (5)$$

From the question we know that enzyme E converts the substrate S into the product P. As a result, we can get the hidden conditions:

$$\mathrm{s}, \mathrm{e}, \mathrm{c}, \mathrm{p} > 0$$

$$k_1, k_2, k_3 > 0$$

Original condition is:

$$\mathrm{s}(0) = \mathrm{s}_0, \mathrm{e}(0) = \mathrm{e}_0, \mathrm{c}(0) = 0, \mathrm{p}(0) = 0$$

Because the enzyme E is only a catalyst that aids the process, its total concentration, free plus combined, remains constant. This conservation law for the enzyme is also obtained by combining the (3) and (4) equations.

$$\frac{de}{dt} + \frac{dc}{dt} = 0 \Rightarrow e(t) + c(t) = e_0 \qquad (6)$$

Use the formula (6) to simplify formula (2), (3), (4), and (5), we get:

$$\frac{ds}{dt} = -k_1 e_0 s + (k_1 s + k_2)c \quad (7)$$

$$\frac{dc}{dt} = k_1 e_0 s - (k_1 s + k_2 + k_3)c \qquad (8)$$

Suppose that the first stage of complex production, c, is very quick, after which it is virtually at equilibrium, that is, dc/dt close to 0, in which case we obtain from (8):

$$c(t) = \frac{e_0 s(t)}{s(t)+K_m}, K_m = \frac{k_2+k_3}{k_1} \quad (9)$$

Combine formula (9) with (7) to simplified rate of change of concentration [S]:

$$\frac{ds}{dt} = -\frac{k_3 e_0 s}{s+K_m} \quad (10)$$

References

Murray, James D. "Reaction Kinetics." *SpringerLink*, Springer Berlin Heidelberg, 1 Jan. 1989, https://link.springer.com/chapter/10.1007/978-3-662-08539-4_5.

Harris, T.K., and M.M. Keshwani. "Methods in Enzymology | Chapter 7 Measurement of Enzyme Activity." *Science Direct*, 463, 57-71., 3 Nov. 2009, https://www.sciencedirect.com/science/article/abs/pii/S007668790963007X.

Please check Question 2 part 8.2 and 8.3 on the html file or ipynb file.