

Answer to Question 2

8.1 According to the mass action law, the speed of the reaction is proportional to the product of the reactants and the rate of changes can be calculated as the stoichiometry of E /S /ES /P multiple the speed of the reaction.

Firstly, I marked the speed of ES generation as V_{ES} , the speed of ES breakdown as V'_{ES} , and the rate of changes of ES as ΔES . Then the rate of changes of ES can be written as :

$$\Delta ES = V'_{ES} - V_{ES}$$

$$\Delta ES = (k_2 + k_3) * ES - k_1 * E * S$$

The other 3 species can also be calculated in the same way, then suppose the speed of **generation** of E, S, P are:

$$V_E, V_S, V_P$$

the speed of **breakdown** of E, S, P are:

$$V'_E, V'_S, V'_P$$

and the **rate of change** of E, S, P are recorded as:

$$\Delta E, \Delta S, \Delta P$$

Then the other 3 rate of change can be written as :

$$\Delta E = V'_E - V_E = k_1 * E * S - (k_2 + k_3) * ES$$

$$\Delta S = V'_S - V_S = k_1 * E * S - k_2 * ES$$

$$\Delta P = V'_P - V_P = k_3 * ES$$

8.2 With the formula I listed above and the numbers given, we can know set the 4 equation of species E, S, ES, and P as below (temporarily ignore unit):

$$\Delta E = 100 * E * S - 750 * ES$$

$$\Delta S = 100 * E * S - 600 * ES$$

$$\Delta ES = 750 * ES - 100 * E * S$$

$$\Delta P = 150 * ES$$

When it comes to the rate of change, we need 3 factors, the value of the termination state of an object, the initial value, and the time experienced from the initial value to the end of the change point. Consequently, the respective rates of change of E, S, ES, and P can be known by calculating the derivative of the time period with their change of concentration. Then the above four formulas can be transformed into equations for finding the value of derivatives:

$$\frac{d(E)}{d(t)} = 100 * E * S - 750 * ES$$

$$\frac{d(S)}{d(t)} = 100 * E * S - 600 * ES$$

$$\frac{d(ES)}{d(t)} = 750 * ES - 100 * E * S$$

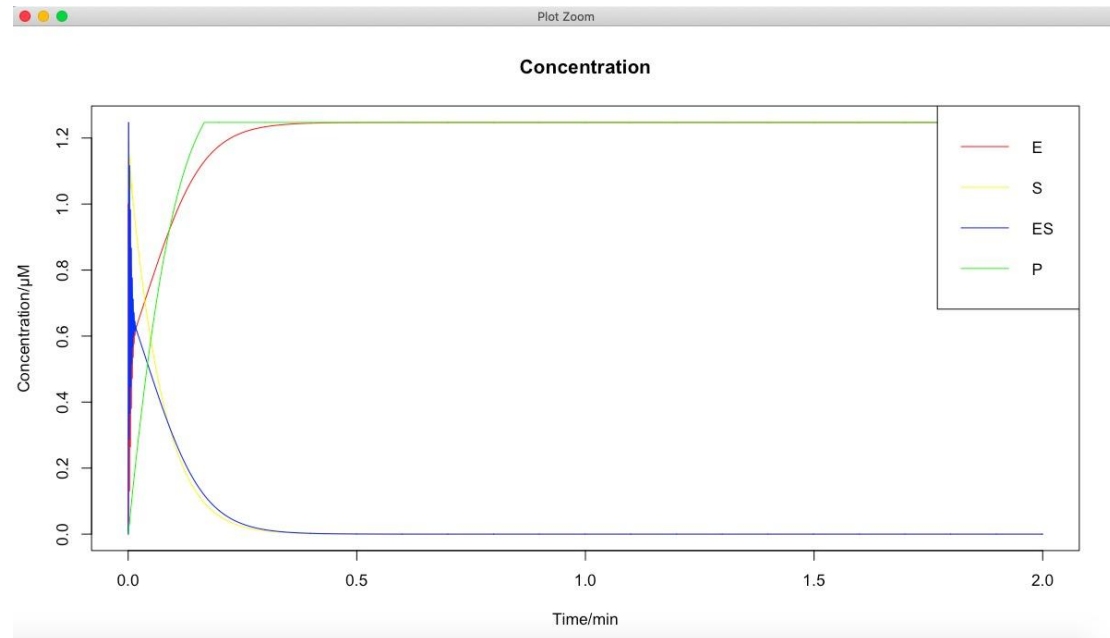
$$\frac{d(P)}{d(t)} = 150 * ES$$

With the given information about the initial concentration of E, S, ES, and P are 1, 10, 0, 0 respectively, I can perform Runge-Kutta method to get the concentration-time curve. Before the function start running, I need to set 2 parameters involved in the formula and they are h and n. The first one, h, stands for the length of step, and the second one, n, stands for the number of iterations.

From my past experience and knowledge, both of them will decide the accuracy of calculation, so I would set h and n smaller (h = 0.001, n = 2000) in

order to get relatively accurate results.

The plots are shown as below:



8.3 In order to get the maximum velocity of the reaction and according to the information given in the title, the velocity of the reaction = $V_p = k_3 \cdot ES$, so we need to plot a curve to find out the relationship between the substrate and the product.

Due to my limited programming ability, this curve is different from the curve I imagined, if you give me more time, I will continue to look for the right plot.

