Q2

Answer 1

According to the information I got from the Internet, the law of mass action is expressed as follows: the rate of the reaction of the substrate is proportional to the product of the powers of the concentrations of the substrate, and the formula is expressed as follows,

$$H_2 + I_2 \rightarrow 2HI$$

The positive reaction rate for this reaction is,

$$v = k_1[H_2][I_2]$$

According to the law of mass action, the four equations for this enzyme reaction are expressed as follows,

$$\frac{d[E]}{dt} = (k_2 + k_3) * [ES] - k_1[E][S] \tag{1}$$

$$\frac{d[S]}{dt} = k_2[ES] - k_1[S][E] \tag{2}$$

$$\frac{d[ES]}{dt} = k_1[E][S] - (k_2 + k_3) * [ES] \tag{3}$$

$$\frac{d[P]}{dt} = k_3[ES] \tag{4}$$

Answer 2

The fourth order Runge-Kutta equation is expressed as follows,

$$y' = f(t, y) \qquad\qquad y(t_0) = y_0 \tag{1}$$

$$k_1 = f(t_n, y_n) \tag{2}$$

$$k_2 = f\left(t_n + \frac{h}{2}, y_n + \frac{h}{2} * k_1\right) \tag{3}$$

$$k_3 = f\left(t_n + \frac{h}{2}, y_n + \frac{h}{2} * k_2\right) \tag{4}$$

$$k_4 = f(t_n + h, y_n + h * k_3) \tag{5}$$

$$y_{n+1} = y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) \tag{6}$$

I implemented the fourth order Runge Kutta method using the C++ programming language, setting the step size to 0.00001, and after 100,000 iterations, the result is as follows,

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E: 0.991771     S: 4.64927e-07  ES: 6.29773e-08 P: 9.99677
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It can be seen that the enzyme is barely consumed, while the substrate S is almost completely consumed, generating a large amount of the product P.

Answer 3

According to the law of mass action, the velocity V given in the question is mainly determined by the concentration of the product ES. The rate of ES production is $v_{produce} = k_1[E][S]$, and the rate of decomposition of the ES is $v_{decomposition} = k_3[ES] + k_2[ES]$. According to the information I found on the Internet, when reaching equilibrium state, the two speeds should be equal, and so we get $k_1[E][S] = k_3[ES] + k_2[ES]$.

According to the information I checked on the Internet because enzymes are not consumed during the reaction, I set the total amount of enzymes as E_t. The above equation can be rewritten as, $k_1(E_t - [ES])[S] = k_3[ES] + k_2[ES]$. The final simplification yields $[ES] = \frac{k_1 E_t[S]}{k_1[S]+k_3+k_2} = \frac{E_t[S]}{[S]+\frac{k_2+k_3}{k_1}}$. According to the law of mass action, the product P is produced at a rate of $V_p = k_3[ES] = \frac{k_3 E_t[S]}{[S]+\frac{k_2+k_3}{k_1}}$. For a chemical reaction, $\frac{k_2+k_3}{k_1}$ is a constant. When the substrate S is very large, this time satisfies, $\frac{k_2+k_3}{k_1[S]} \approx 0$. So, after processing the original formula we get $V_p = \frac{k_3 E_t}{1+\frac{k_2+k_3}{[S]k_1}} \approx \frac{k_3 E_t}{1+0} = k_3 E_t$. So the $V_m = k_3 E_t$