Q2 Answer Report

8.1

*Assume that C[x] represents the concentration of x

We know from the law of mass action,

Change rate of E = (k2 + k3) * C[ES] – k1 * C[E] * C[S]

Change rate of S = k2 * C[ES] – k1 * C[E] * C[S]

Change rate of ES = k1 * C[E] * C[S] – (k2 + k3) * C[ES]

Change rate of P = k3 * C[ES]

8.2

Substitute k1, k2 and k3 into the formula in 8.1 to obtain the following formula,

Change rate of E = 750 * C[ES] – 100 * C[E] * C[S]

Change rate of S = 600 * C[ES] – 100 * C[E] * C[S]

Change rate of ES = 100 * C[E] * C[S] – 750 * C[ES]

Change rate of P = 150 * C[ES]

Write code to follow these formulas and define Runge-Kutta's iterative function. Then define the initial parameter, C[E], C[S], C[ES], C[P] = 1, 10, 0, 0. In order to make the image as accurate as possible, the number of iterations was set as 5000000, and the step length h was set as 0.0000001 min. After the results are obtained, the curves of the concentration of each substance are drawn according to the obtained values. The image was drawn with Matplotlib, as shown in Figure 1.

* All the code involved in this answer is saved in the file ‘Runge-Kutta code for enzyme reaction.ipynb’, in the same folder as this report.

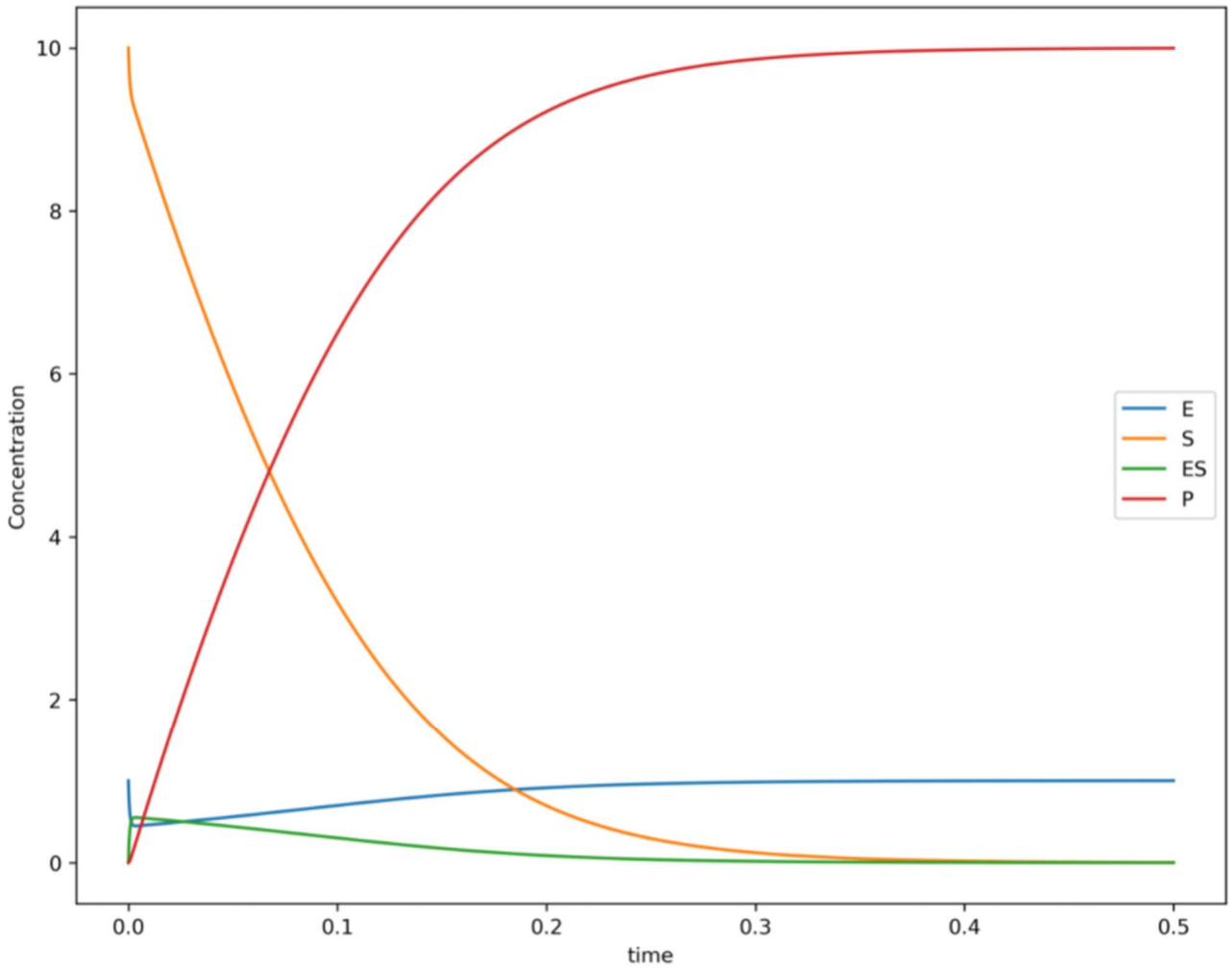

Figure 1. The curves of the concentration of each substance

As can be seen from the figure, the reaction was basically completed after about 0.4 minutes. ES and E were almost exhausted eventually, and the concentration of E recovered to close to 1μM and P to close to 10μM.

8.3

According to the formula obtained in 8.2, V= Change rate of P = 150 * C[ES], so V can be easily calculated from C[ES]. Plot the figure according to the previously obtained C[S] and the converted V, as shown in Figure 2.

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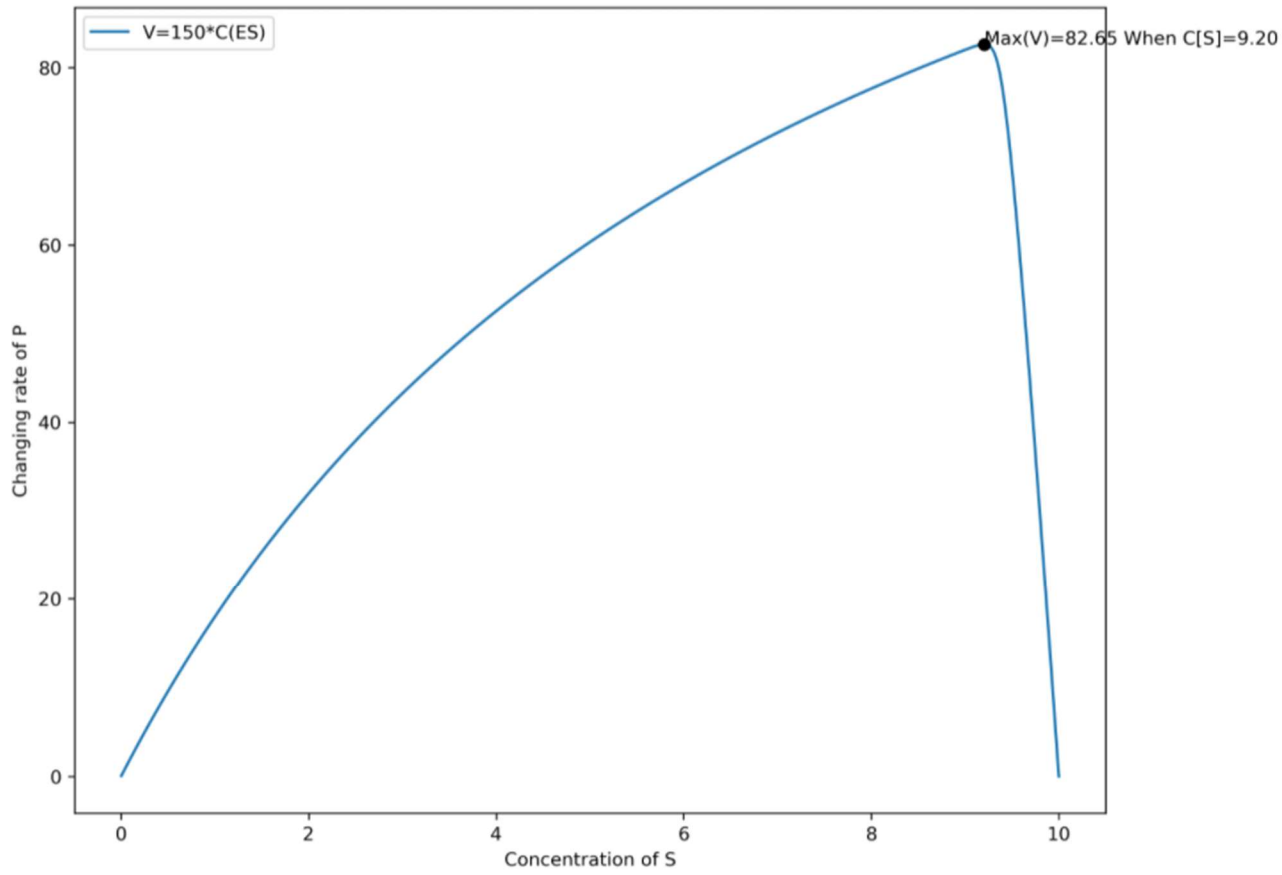

Figure 2. The curve of C[S] – V.

We can easily see from the figure that when C[S] =9.20μM, V reaches the maximum value of 82.65μM/min.