Question 2: Enzyme Kinetics

8.1. Using the law of mass action, write down four equations for the rate of changes of the four species, E, S, ES, and P.

Solution:

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

$$\frac{d[S]}{dt} = -k_1[S][E] + k_2[SE]$$

$$\frac{d[E]}{dt} = -k_1[S][E] + k_2[SE] + k_3[SE]$$

$$\frac{d[SE]}{dt} = k_1[S][E] - k_2[SE] - k_3[SE]$$

$$\frac{d[P]}{dt} = k_3[SE]$$

8.2. Write a code to numerically solve these four equations using the fourth-order Runge-Kutta method. For this exercise, assume that the initial concentration of E is 1 µM, the initial concentration of S is 10 µM, and the initial concentrations of ES and P are both 0. The rate constants are: k1=100/µM/min, k2=600/min, k3=150/min.

Solution:

Using MATLAB function *ode45* to solve the differential equations. *ode45* uses fourth- and fifth-order Runge-Kutta algorithm. It uses the fourth-order method to provide possible solutions and the fifth-order method to control errors. The integration interval is set as [0, 0.5], meaning that the reaction time is 0.5 min. The simulation results are shown in Figure 1.

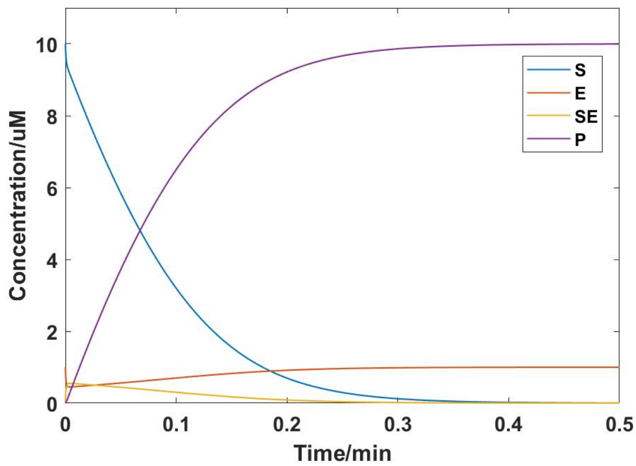

Figure 1: Simulation results for [S]= 10 µM, [E]= 1 µM

8.3. We define the velocity, V, of the enzymatic reaction to be the rate of change of the product P. Plot the velocity V as a function of the concentration of the substrate S. You should find that, when the concentrations of S are small, the velocity V increases approximately linearly. At large concentrations of S, however, the velocity V saturates to a maximum value, Vm. Find this value Vm from your plot.

Solution:

Use the same method to explore the relationship between V and [S] by change the value of [S] from 0 μM to 1000 μM. The velocity of reaction V is defined as the average rate of change of [P] at 0.01min. The simulation result is shown in Figure 2. From Figure 2, the velocity V saturates to a maximum value when [S] is large enough. The maximum of velocity is **150 μM/min.** Then, we changed the range of [S] to [0, 0.5], the result is shown in Figure 3. From Figure 3, it is clear that the V is an approximate linear function of [S].

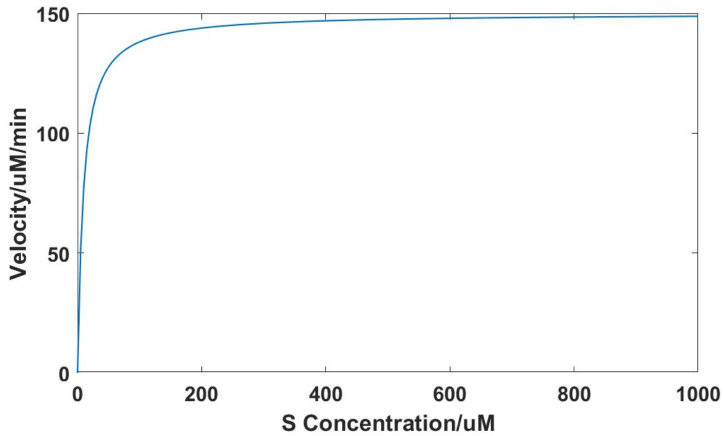

Figure 2: The V-[S] plot

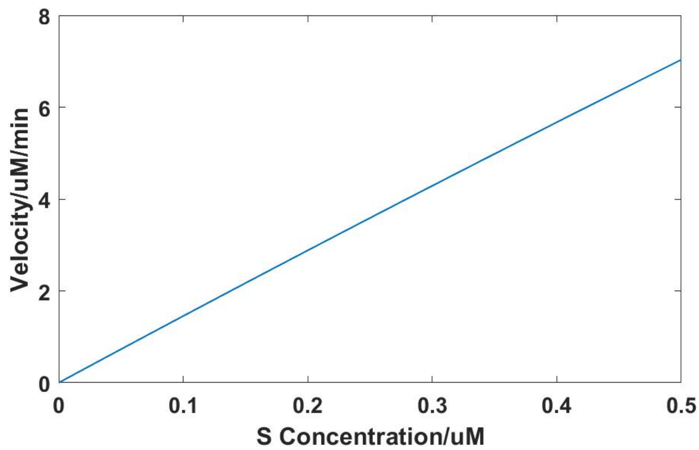

Figure 2: The V-[S] plot at low [S]