Problem 1: Four equations for the rate of changes of *E*, *S*, *ES*, and *P*

Based on the law of mass action, we can get four equations as follows:

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

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

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

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

[*E*], [*S*], [*ES*] and [*P*] represent the concentration of *E*, *S*, *ES* and *P*, respectively.

Problem 2: A code to numerically solve four equations

Using MATLAB R2019a, I finished the code writing to solve the four equations. The code is as follows:

```
clear;
clc;
timespan=[0,1.5];
x0=[1,10,0,0];
[time,X]=ode45(@f1,timespan,x0);

% Concentration of E, S, ES and P
figure;
plot(time, X(:,1),'linewidth',1);
ylim([0,14])
hold on;
title('Concentration of E, S, ES and P');
ylabel('Concentration(uM)'); xlabel('Time(s)');
plot(time,X(:,2),'linewidth',1)
plot(time,X(:,3),'linewidth',1)
plot(time,X(:,4),'linewidth',1)
legend('E','S', 'ES','P')
V=X(:,3);
figure;
plot(X(:,2),V,'linewidth', 1)
xlim([0,15])
ylim([0,0.8])
title('Relationship between S and V')
xlabel('Concentration of S (uM)');
ylabel('Velocity(uM/s)')

% Function definition
function f=f1(t, x)
   f=zeros(4,1);
   f(1)=750*x(3)-100*x(1)*x(2);
   f(2)=600*x(3)-100*x(1)*x(2);
   f(3)=100*x(1)*x(2)-750*x(3);
   f(4)=150*x(3);
end
```

In this problem, I could not write the code to solve these four equations using the fourth-order Runge-Kutta method, but I used the function **ode45** in MATLAB, a general-purpose ODE solver which also uses the Runge-Kutta algorithm. Information from two websites helped my coding:

https://ww2.mathworks.cn/help/matlab/ref/ode45.html?searchHighlight=ode45&s_tid=srchtitle_ode45_1

https://www.zhihu.com/question/395096211/answer/1227935749

In the plot below, we can get the time-concentration change curves of four species:

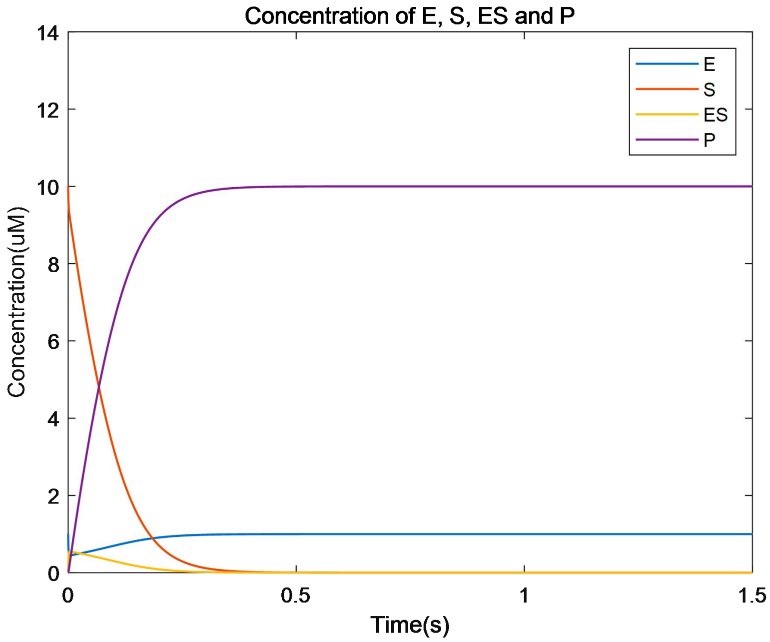

Figure 1 Time-Concentration Plot of E, S, ES and P

Problem 3: The Plot and the Maximum Value *Vm*

Solution 1

Using the code in problem 2, we can also get the relationship between *S* and *V* in figure 2, where we can find the maximum value of velocity is approximately 0.55μM/s at the concentration of *S* = 9μM.

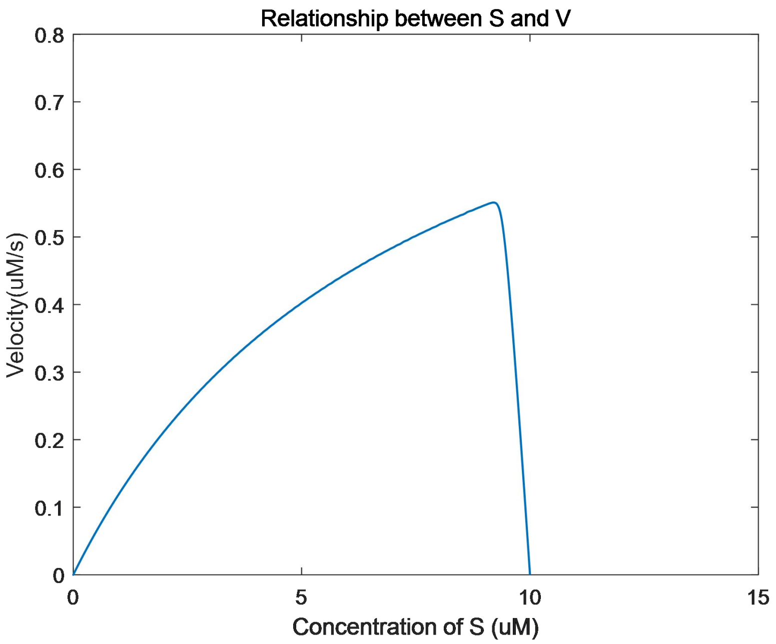

Figure 2 Relationship Between S and V

Solution 2

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

Based on knowledge of enzyme kinetics, when the reaction is at steady state, the rate of *ES* generation is equal to the rate of *ES* decomposition：

$$k_1([E_0] - [ES])[S] = k_2[ES] + k_3[ES]$$

$[E_0]$ represents the total concentration of enzyme;

[*E*], [*S*] and [*ES*] represent the concentration of *E*, *S* and *ES*, respectively.

therefore, we can get

$$[ES] = \frac{[E_0][S]}{[S] + \frac{k_2 + k_3}{k_1}}$$

set

$$k_m = \frac{k_2 + k_3}{k_1}$$

then

$$[ES] = \frac{[E_0][S]}{[S] + k_m}$$

according to the equation in problem 1,

$$V = \frac{d[P]}{dt} = k_3[ES] = k_3\frac{[E_0][S]}{[S] + k_m}$$

at large concentrations of *S*,

$$V_m = k_3[E_0]$$

so,

$$V = \frac{V_m[S]}{[S] + k_m}$$

use double-reciprocal plot

$$\frac{1}{V} = \frac{[S] + k_m}{V_m[S]} = \frac{k_m}{V_m}\frac{1}{[S]} + \frac{1}{V_m}$$

Thus, the vertical axis intercept of the $\frac{1}{[S]} - \frac{1}{V}$ plot equals $\frac{1}{V_m}$, and we can easily get V_m.