$$E + S \stackrel{k_1}{\underset{k_2}{\rightleftharpoons}} ES \stackrel{k_3}{\xrightarrow{}} E + P$$

From the law of mass action, we can indicate that:

$$v_1 = k_1[E] \cdot [S]$$

 $v_2 = k_2[ES]$
 $v_3 = k_3[ES]$

Then, the rate of E, S, ES, P can be inferred that:

$$rate(E) = -k_1[E] \cdot [S] + k_2[ES] + k_3[ES]$$
 (1)

$$rate(S) = -k_1[E] \cdot [S] + k_2[ES]$$
 (2)

$$rate(ES)=k1[E]\cdot[S]-k2[ES]-k3[ES]$$
(3)

$$rate(P) = k3[ES]$$
 (4)

8.2

Use MATLAB solve these four equations using the fourth-order Runge-Kutta method.

Here is the code.

clear

figure(1) %create the plot

plot(T,Y(:,1),T,Y(:,2),T,Y(:,3),T,Y(:,4),'LineWidth',2)

xlabel('time(s)')

ylabel('concentration(uM)')

legend('[E]','[S]','[ES]','[P]')

function dy=fun1218(t,y)

k1=100/60;

k2=600/60;

k3=150/60;

dy=zeros(4,1);% create empty matrix

dy(1)=-k1*y(1)*y(2)+k2*y(3)+k3*y(3);

dy(2)=-k1*y(1)*y(2)+k2*y(3);

dy(3)=k1*y(1)*y(2)-k2*y(3)-k3*y(3);

dy(4)=k3*y(3);

end

The result of equations is shown below in figure 8.2.1, the detail of [E], [ES], [P] at the beginning is shown in figure 8.2.2.

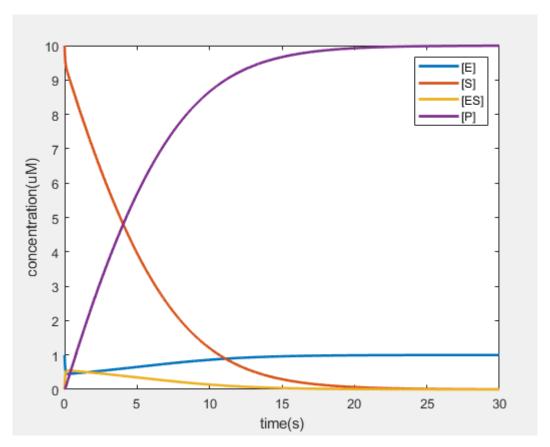


Figure 8.2.1. The result of four equations

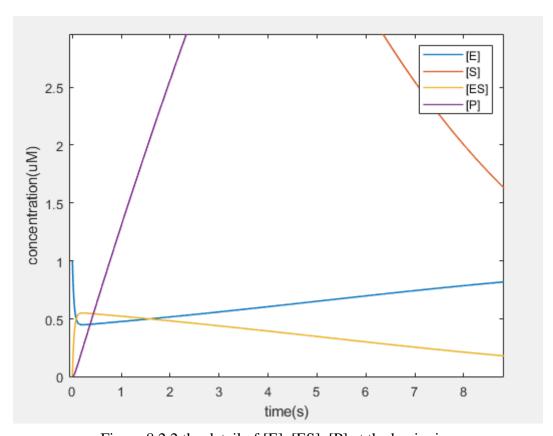


Figure 8.2.2 the detail of [E], [ES], [P] at the beginning

We can inferred from the definition of v that

$$v = rate(P) = k3[ES]$$
 (4)

Here is the code for calculating rates of P in case of different [S], and draw a figure of them.

```
clear
v=[];
k1=100/60;
k2=600/60;
k3=150/60;
km=(k2+k3)/k1;
for s=0:0.1:2000
[T,Y]=ode45(@fun1218,[0:0.001:0.1],[1 s 0 0]);% ode45
v1=(Y(20,4)-Y(1,4))/(T(20)-T(1));
v = [v \ v1];
end
figure(1)
plot([0:0.1:2000],v,'color',[0.18 0.55 0.34],'LineWidth',2)
hold on
plot([0,2000],[2.5,2.5],'--','color',[0.22 0.37 0.06],'LineWidth',2)
ylim([0 \ 2.6]);
xlabel('[S](uM)')
ylabel('v')
function dy=fun1218(t,y)
k1=100/60;
k2=600/60;
k3=150/60;
dy=zeros(4,1);% create empty matrix
dy(1)=-k1*y(1)*y(2)+k2*y(3)+k3*y(3);
dy(2)=-k1*y(1)*y(2)+k2*y(3);
dy(3)=k1*y(1)*y(2)-k2*y(3)-k3*y(3);
dy(4)=k3*y(3);
end
```

The result is showed below in figure 8.3.1.

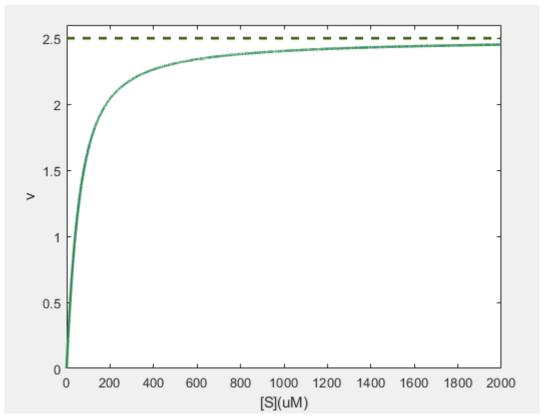


Figure 8.3.1 v-[S]

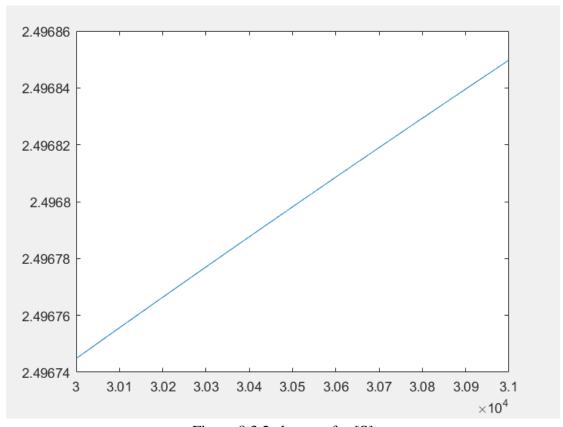


Figure 8.3.2 change of v-[S]

When the concentration of S increases to 31000, v approaches 2.5. The rate of increase in the concentration of 1000 on the basis of the concentration of 30000 has changed smaller than 0.0001. As we can inferred from the figure 8.3.1 and figure 8.3.2, v_m =2.5 μ M/min.