8.1

Suppose the concentration of E, S, ES, P are [E], [S], [ES], [P] respectively.

According to the law of mass action, we can get

the rate of change of E: $r_1 = -k_1[E][S]+k_2[ES]+k_3[ES]$

the rate of change of S: $r_2 = -k_1[E][S]+k_2[ES]$

the rate of change of ES: $r_3 = k_1[E][S]-k_2[ES]-k_3[ES]$

the rate of change of P: $r_4 = k_3[ES]$

8.2

We are given that k_1=100/μM/min, k_2=600/min, k_3=150/min, and the initial concentration of E and S are 1 μM and 10 μM respectively.

Use the fourth-order Runge-Kutta method to solve the four equations numerically:

MATLAB Code

```
clear;
clc;
close all;

%%The rate constants
k1 = 100;
k2 = 300;
k3 = 150;

%Parameter setting
h = 1e-5;                %step size
t = 0:h:1;               %the vector for the argument t

N = length(t);
a = ones(1,N);           %the concentration of E
b = ones(1,N);           %the concentration of S
c = ones(1,N);           %the concentration of ES
b(1,1) = 10;
c(1,1) = 0;

r = zeros(N,4);          %the matrix to store the rate of change

%%The fourth-order Runge-Kutta iteration
for i=2:N
    t_n=t(i-1);
    a_n=a(i-1);
    b_n=b(i-1);
    c_n=c(i-1);

    ka1=-k1*a_n*b_n+k2*c_n+k3*c_n;
    kb1=-k1*a_n*b_n+k2*c_n;
    kc1=k1*a_n*b_n-k2*c_n-k3*c_n;
    kd1=k3*c_n;
```

```
    ka2=(-
k1*(a_n+ka1*h/2)*(b_n+kb1*h/2))+(k2*(c_n+kc1*h/2))+(k3*(c_n+kc1*h/2));
    kb2=(-k1*(a_n+ka1*h/2)*(b_n+kb1*h/2))+(k2*(c_n+kc1*h/2));
    kc2=(k1*(a_n+ka1*h/2)*(b_n+kb1*h/2))+(-k2*(c_n+kc1*h/2))+(-
k3*(c_n+kc1*h/2));
    kd2=k3*(c_n+kc1*h/2);

    ka3=(-
k1*(a_n+ka2*h/2)*(b_n+kb2*h/2))+(k2*(c_n+kc2*h/2))+(k3*(c_n+kc2*h/2));
    kb3=(-k1*(a_n+ka2*h/2)*(b_n+kb2*h/2))+(k2*(c_n+kc2*h/2));
    kc3=(k1*(a_n+ka2*h/2)*(b_n+kb2*h/2))+(-k2*(c_n+kc2*h/2))+(-
k3*(c_n+kc2*h/2));
    kd3=k3*(c_n+kc2*h/2);

    ka4=(-k1*(a_n+ka3*h)*(b_n+kb3*h))+(k2*(c_n+kc3*h))+(k3*(c_n+kc3*h));
    kb4=(-k1*(a_n+ka3*h)*(b_n+kb3*h))+(k2*(c_n+kc3*h));
    kc4=(k1*(a_n+ka3*h)*(b_n+kb3*h))+(-k2*(c_n+kc3*h))+(-k3*(c_n+kc3*h));
    kd4=k3*(c_n+kc3*h);

    a(i)=a_n+h/6*(ka1+2*ka2+2*ka3+ka4);
    b(i)=b_n+h/6*(kb1+2*kb2+2*kb3+kb4);
    c(i)=c_n+h/6*(kc1+2*kc2+2*kc3+kc4);
    r(i-1,:)=[ka1,kb1,kc1,kd1];
end


%%Plot
% figure
% hold on;
% subplot(311);
% plot(t,a,'r');
% xlabel('t');
% ylabel('[E]');
% subplot(312);
% plot(t,b,'g');
% xlabel('t');
% ylabel('[S]');
% subplot(313);
% plot(t,c,'b');
% xlabel('t');
% ylabel('[ES]');
% hold off;

figure
hold on;
subplot(411);
plot(t(1:65000),r(1:65000,1),'r');
xlabel('t');
ylabel('r1');
title('The plot of the rate of change of E');
subplot(412);
plot(t(1:65000),r(1:65000,2),'g');
xlabel('t');
ylabel('r2');
title('The plot of the rate of change of S');
subplot(413);
plot(t(1:65000),r(1:65000,3),'b');
xlabel('t');
ylabel('r3');
```

```
title('The plot of the rate of change of ES');
subplot(414);
plot(t(1:65000),r(1:65000,4),'y');
xlabel('t');
ylabel('r4');
title('The plot of the rate of change of P');
hold off;
```

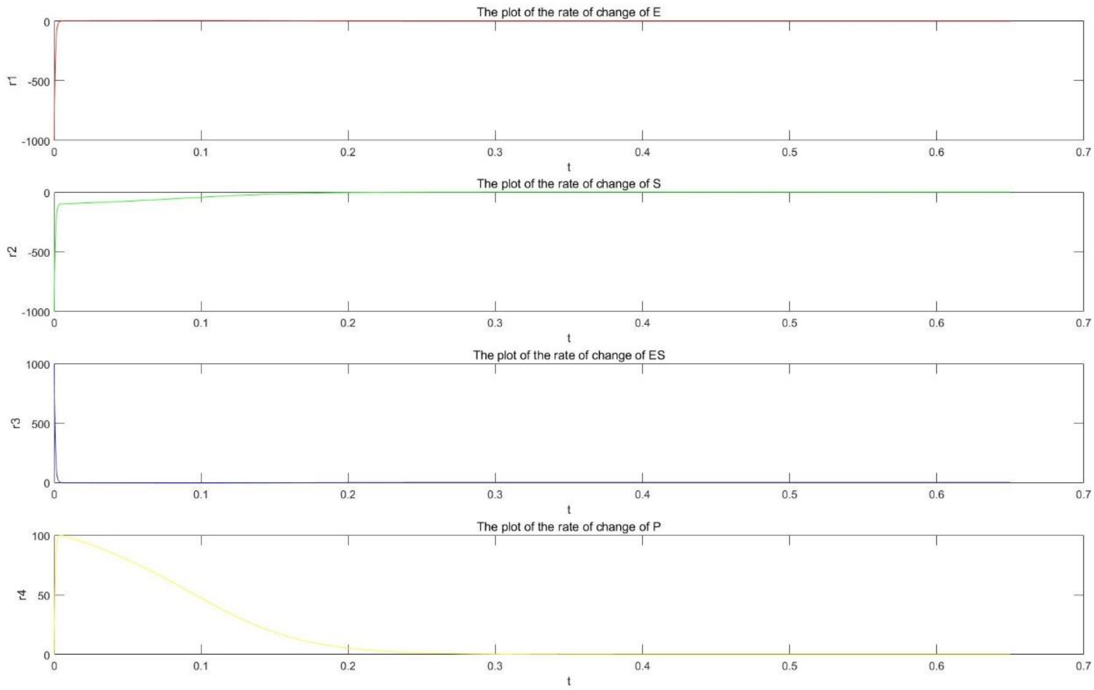
Part of solution

```
ans =

   1.0e+03 *

   -1.0000   -1.0000    1.0000         0
   -0.9846   -0.9861    0.9846    0.0015
   -0.9695   -0.9725    0.9695    0.0030
   -0.9546   -0.9590    0.9546    0.0044
   -0.9400   -0.9458    0.9400    0.0058
   -0.9256   -0.9329    0.9256    0.0072
   -0.9115   -0.9201    0.9115    0.0086
   -0.8976   -0.9075    0.8976    0.0100
   -0.8839   -0.8952    0.8839    0.0113
   -0.8704   -0.8830    0.8704    0.0126
   -0.8572   -0.8711    0.8572    0.0139
   -0.8441   -0.8593    0.8441    0.0152
   -0.8313   -0.8477    0.8313    0.0164
   -0.8187   -0.8364    0.8187    0.0177
   -0.8063   -0.8252    0.8063    0.0189
   -0.7941   -0.8142    0.7941    0.0201
   -0.7821   -0.8033    0.7821    0.0213
   -0.7702   -0.7927    0.7702    0.0224
   -0.7586   -0.7822    0.7586    0.0236
   -0.7472   -0.7719    0.7472    0.0247
   -0.7359   -0.7617    0.7359    0.0258
   -0.7248   -0.7517    0.7248    0.0269
   -0.7139   -0.7419    0.7139    0.0280
   -0.7032   -0.7322    0.7032    0.0291
   -0.6926   -0.7227    0.6926    0.0301
   -0.6822   -0.7134    0.6822    0.0311
   -0.6720   -0.7041    0.6720    0.0322
```

Plot



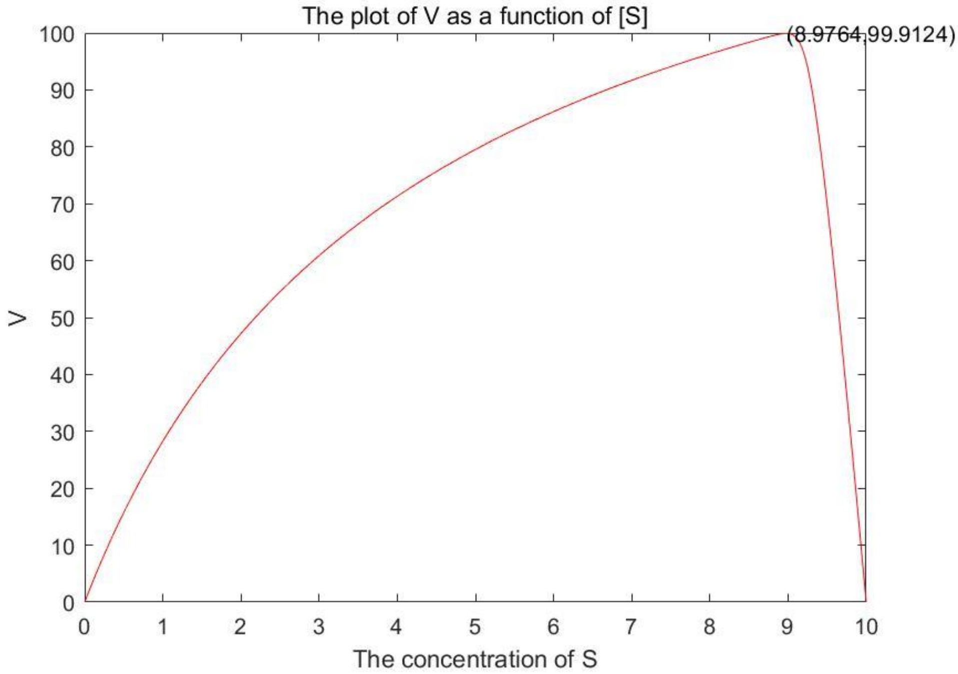
8.3

MATLAB Code

```
Vm = max(r(:,4));             %Find the greatest velocity Vm
index = find(r(:,4)==Vm);
CS = b(index);

% Plot V as a function of the concentration of S
figure
plot(b,r(:,4),'r');
xlabel('The concentration of S');
ylabel('V');
text(CS,Vm,'(8.9764,99.9124)');
title('The plot of V as a function of [S]');
```

Result



We can find that, when the concentrations of S are small, the velocity V increases approximately linearly. The maximum value Vm = 99.9124.