8.1

We can break this reaction down into three elementary reactions.

$E + S \xrightarrow{K1} ES$

$ES \xrightarrow{K2} E + S$

$ES \xrightarrow{K3} E + P$
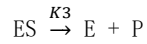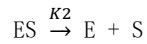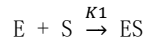
According to the law of mass action, we can obtain four equations about the rate of change of concerntration of E, S, ES, P. In the following answers, E, S, ES, P represent the concentration of E, S, ES, P respectively.

$\frac{dE}{dt} = -K1*(E*S) + (K2+K3)*ES$

$\frac{dS}{dt} = -K1*(E*S) + K2*ES$

$\frac{dES}{dt} = K1*(E*S) - (K2+K3)*ES$

$\frac{dP}{dt} = K3*ES$

8.2

Initially

$E(0) = 1 \mu M$

$S(0) = 10 \mu M$

$ES(0) = 0$

$P(0) = 0$

The rate constants are:

$K1 = 100/\mu M/min$

$K2 = 600/min$

$K3 = 150/min$

It turns out that in every step of the reaction, the reactant has a coefficient of 1, which gives us some relationships and equations, which allows me to reduce the number of differential equations and simplify the calculation.

$\frac{dES}{dt} + \frac{dE}{dt} = 0$

$ES(t) + E(t) = E(0)$

$\frac{dS}{dt} + \frac{dES}{dt} + \frac{dP}{dt} = 0$

$S(t) + ES(t) + P(t) = S(0)$

According to these equations, we can convert the 4 equations obtained in 8.1 into the following 2 differential equations.

$\frac{dES}{dt} = K1*((E(0)-ES)*S) - (K2+K3)*ES$

$\frac{dS}{dt} = -K1((E(0)-ES)*S) + K2*ES$

Therefore, we get:

$\frac{dES}{dt} = f(t,ES,S)$

$\frac{dS}{dt} = g(t,ES,S)$

According to the fourth-order Runge-Kutta method formula, I get:

$ES_{n+1} = ES_n + \frac{1}{6}*h*(K1+2K2+2K3+K4)$

$S_{n+1} = S_n + \frac{1}{6}*h*(L1+2L2+2L3+L4)$

$K1 = f(t_n, ES_n, S_n)$

$K2 = f(t_n + \frac{1}{2}*h, ES_n + \frac{1}{2}*K1, S_n + \frac{1}{2}*K1)$

$K3 = f(t_n + \frac{1}{2}*h, ES_n + \frac{1}{2}*K2, S_n + \frac{1}{2}*K2)$

$K4 = f(t_n + h, ES_n + K3, S_n + K3)$

$$L1 = g(t_n, ES_n, S_n)$$

$$L2 = g(t_n + \frac{1}{2}*h, ES_n + \frac{1}{2}*L1, S_n + \frac{1}{2}*L1)$$

$$L3 = g(t_n + \frac{1}{2}*h, ES_n + \frac{1}{2}*L2, S_n + \frac{1}{2}*L2)$$

$$L4 = g(t_n + h, ES_n + L3, S_n + L3)$$

I use MATLAB to solve the equation obtained through the fourth-order Runge-Kutta method, and the results are expressed in two figures. These two figures respectively reflect the change of concentration and concentration change rate over time.

```matlab
1   clear
2   clc
3
4   %% Initialization
5   h = 0.01;  % Step size
6   t = 0:h:30;
7   x = zeros(length(t),2);
8   x(1,:) = [0,10];  % The original function and the initial derivative
9   % Call function
10  X = FourRK(t,h,x);
11
12  P = 10 - (X(:,1) + X(:,2));
13  E = 1 - X(:,1);
14
15  %% plot
16  figure(1)
17  plot(t,X(:,1),'Linewidth',2)
18  hold on
19  plot(t,X(:,2),'Linewidth',2)
20  hold on
21  plot(t,P,'Linewidth',2)
22  hold on
23  plot(t,E,'Linewidth',2)
24  hold off
25  xlabel('time(s)')
26  ylabel('Concerntration(μM)')
27  legend('ES','S','P','E')
28
29  figure(2)
30  plot(t(1:end-1),diff(X(:,1))/h,'Linewidth',2)
31  hold on
32  plot(t(1:end-1),diff(X(:,2))/h','Linewidth',2)
33  hold on
34  plot(t(1:end-1),diff(P)/h,'Linewidth',2)
35  hold on
36  plot(t(1:end-1),diff(E)/h,'Linewidth',2)
37  hold off
38  xlabel('time(s)')
39  ylabel('Concerntration change rate(μM/s)')
40  legend('dES/dt','dS/dt','dP/dt','dE/dt')
41
42  %% Call function
43
44  % the fourth-order Runge-Kutta method
45  function x = FourRK(t,h,x)
46  for i = 2:length(t)
47      K1 = Fun(t(i-1),x(i-1,:)); % K1
48      K2 = Fun(t(i-1)+1/2*h , x(i-1,:)+1/2*h.*K1); % K2
49      K3 = Fun(t(i-1)+1/2*h , x(i-1,:)+1/2*h.*K2);  % K3
50      K4 = Fun(t(i-1)+h , x(i-1,:)+h.*K3);  % K4
51      x(i,:) = x(i-1,:) + h/6.*(K1 + 2*K2 + 2*K3 + K4);
52  end
53  end
54
55  % Target Function
56  function dx = Fun(t,x)
57  k1 = 100/60; k2 = 600/60; k3 = 150/60;
58  e0 = 1;
59
60  % es = x(1)  s = x(2)
61  dx(1) = k1*(e0 - x(1))*x(2) - (k2 + k3)*x(1);
62  % The first differential function
63  dx(2) = -k1*(e0 - x(1))*x(2) + k2*x(1);
64  % The second differential function
65  end
```
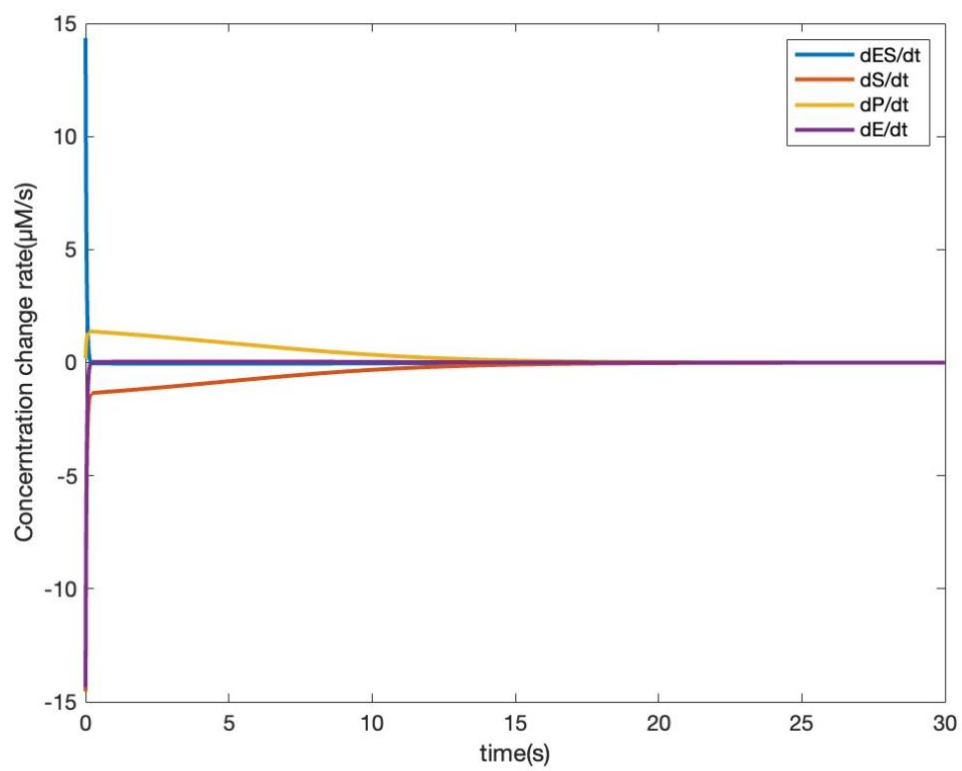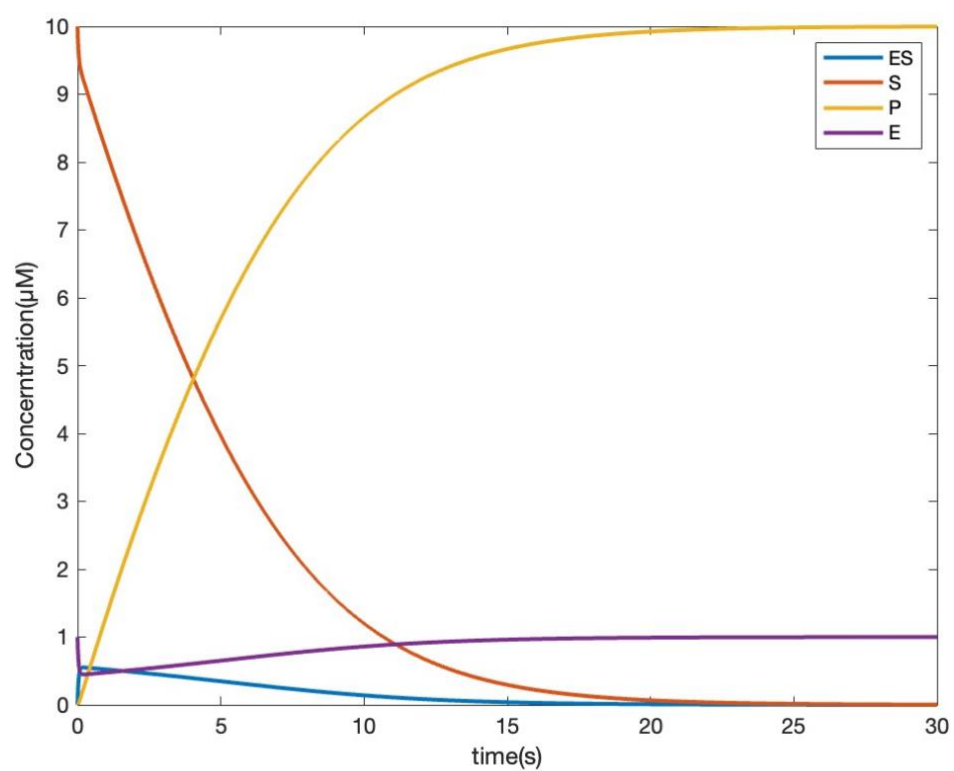
8.3

In a single reaction, V reaches its maximum at equilibrium. At this time:

K2*ES = K1*E*S

$ES = \dfrac{K1*E*S}{K2}$

In 8.2, we get ES+E=E(0), so:

$ES = \dfrac{K1*(S*(E(0))-ES)}{K2}$

$ES = \dfrac{K1*S*E(0)}{K1*S+K2}$

Now let's derive our expression for V

$V = \dfrac{dP}{dt}$

$\quad = K3*ES$

$\quad = \dfrac{K1*K3*E(0)*S}{K1*S+K2}$

$\quad = K3*E(0) - \dfrac{K2*K3*E(0)}{K1*S+K2}$

From this equation, we can conclude: 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.Vm is K3*E(0). Next, I use the data given in 8.2 to draw an image with R for verification.

```
1  K1 <- 100
2  K2 <- 600
3  K3 <- 150
4  E0 <- 1
5  curve(K1*K3*E0*S/(K1*S+K2),from = 0,to = 1000,xname = "S",xlab = "S",ylab = "V")
```