Q2:

$$\underset{[E_0]-[ES]}{E} + \underset{[S]}{S} \underset{k_2}{\overset{k_1}{\rightleftharpoons}} \underset{[ES]}{ES} \xrightarrow{k_3} E + P$$

8.1: Based on mass action, we can describe the rate of change of each following substance:

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

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

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

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

8.2:

Source code using MATLAB： It consists of two parts: the main function RK4 is used for iterative solving, and the subfunction f is used for storing differential equations.

RK4.m:

```
function RK4

clear;clc;
% define initial values
E0=1;
k3=150/60;

% define step width and initial values of ES,S
h=0.001;       % step width is 0.001s
t=0:h:30;      % range is 0-30s
n=length(t);   % quantity of t
Y(1,1)=0;     % initial values of ES put in matrix Y
Y(2,1)=10;     % initial values of S put in matrix Y

% define RK4 to find out the solution of S and ES
for k=1:n-1
    z1=f(t(k),Y(1:2,k));  % Y(1:2,k) means take the 1st and 2nd row of
kth line
    z2=f(t(k)+h/2,Y(1:2,k)+z1*h/2);
    z3=f(t(k)+h/2,Y(1:2,k)+z2*h/2);
    z4=f(t(k)+h,Y(1:2,k)+z3*h);
    Y(1:2,k+1)=Y(1:2,k)+h*(z1+2*z2+2*z3+z4)/6; % iteration of Y
                                                % new ES/S will be added into
matrix Y
                                                % ES to the 1st row, S to the
2nd row
end
```

```
ES=Y(1,:);  % Y's 1st row
S=Y(2,:);  % Y's 2nd row

%solution to E and P
E=E0-ES;

for i=1:1:n  % initial value: step width: final value
   P(i)=k3*sum(ES(1:i))*h;  % P is the integration of ES, ES is
discrete
                        % P(0) = 0
                        % so Pi is the sumption of ES1-ESi * step wid
end

Vp=k3.*ES; % Vp is the change rate of P
        % n2.means conduct every element in matrix

% plot
figure(1);  % 1st picture
plot(t,E,t,S,t,ES,t,P,'LineWidth',3);  % x:t y:E,S,ES,P
legend('E','S','ES','P');
title('Variation of Components Concentration');
xlabel('time/s');
ylabel('concentration/uM');

figure(2);  % 2nd picture
plot(t,Vp,t,S,'LineWidth',3);  % x:t y:Vp,S
legend('Vp','S');
title('Variation of Vp and S');
xlabel('time/s');

figure(3);  % 3rd picture
plot(S,Vp,'LineWidth',3);  % x:s y:Vp
title('Vp changed with the concentration of S');
xlabel('Sconcentration/uM');
ylabel('uM/s');

end
```

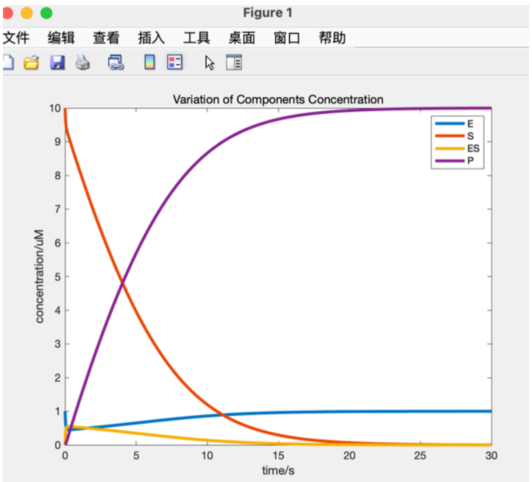
f.m:

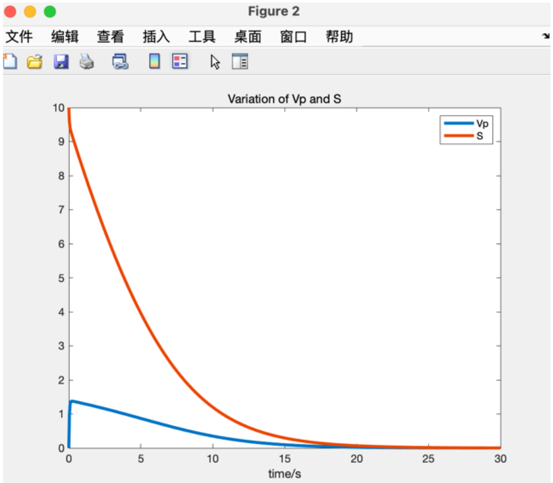
```
function F=f(t,Y)
% input t and matrix Y
% define variables
k1=100/60;
k2=600/60;
```

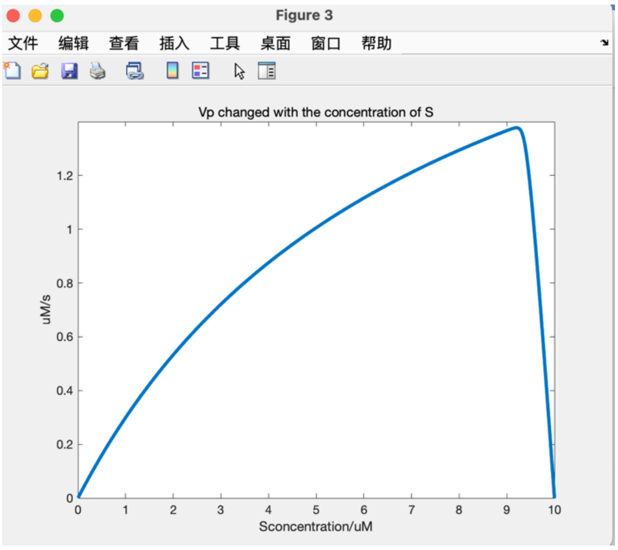
```
k3=150/60;
E0=1;
theta=k2+k3;
lamda=k1*E0;

% define the equation we want to solve
ES=Y(1,1);  % Y is a 1*2 matrix
S=Y(2,1);
f1=lamda*S-(theta+k1*S)*ES;  % equation of dES/dt
f2=-lamda*S+(k1*S+k2)*ES;  % equation of dS/dt
F=[f1;f2];  % output of F is a matrix contain f1(ES) and f2(S)
end
```

The results:







Notes: The above code borrows from:
https://blog.csdn.net/Tonyslp/article/details/122619031

8.3:

[ES] formation rate : $V_1 = k_1([E_t]-[ES])[S]$

[ES] decomposition rate : $V_2 = k_2[ES]+k_3[ES]$

When the enzyme reaction system is in a constant rate: $V_1 = V_2$

Hence: $k_1([E_t]-[ES])[S] = k_2[ES]+k_3[ES]$

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

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

then: $k_m[ES]+[ES][S] = [E_t][S]$

we got: $[ES] = \frac{[E_t][S]}{k_m+[S]}$ (1)

since $v = k_3[ES]$, so: $[ES] = \frac{v}{k_3}$ (2)

Let's put (2) into (1): $\frac{v}{k_3} = \frac{[E_t][S]}{k_m+[S]}$

$$v = \frac{k_3[E_t][S]}{k_m+[S]} \quad (3)$$

when $[E_t]=[ES]$, $v=V_m$,

so: $V_m = k_2[E_t]$ (4)

Put (4) into (3), we got: $v = \frac{V_m[S]}{k_m+[S]}$

a. When the substrate concentration is very low, $[S] \ll k_m$,

then $V \cong \frac{V_m[S]}{k_m}$, the velocity V increases approximately linearly.

b. When the substrate concentration is very high, $[S] \gg k_m$,

then $V \cong V_m$, the velocity V reaches a maximum value.