Question2

8.1

Set the concentration of the four species [E].[S].[ES].[P]

Set the reaction rates of the four species V_E V_S V_{ES} V_P

The four equations:

V_E=V_E(in)-V_E(out)=k_2[ES] + k_3[ES] - k_1[E][S]

V_S=V_S(in)-V_S(out)=k_2[ES] - k_1[E][S]

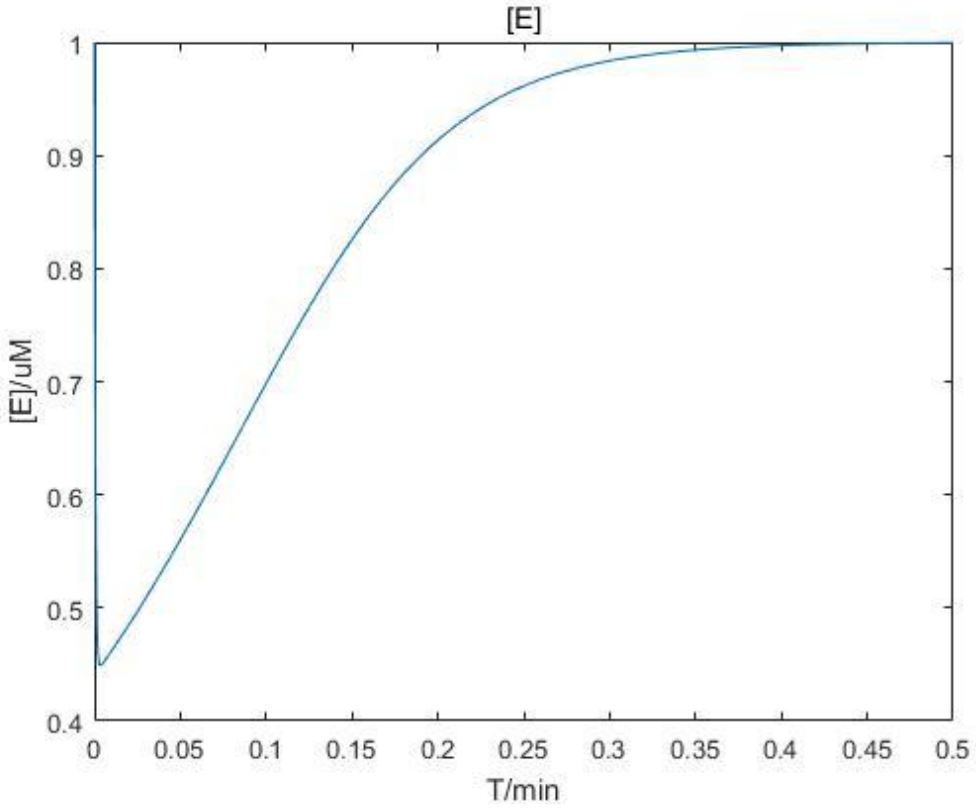
V_{ES}=V_{ES}(in)-V_{ES}(out)=k_1[E][S] - (k_2[ES] + k_3[ES])

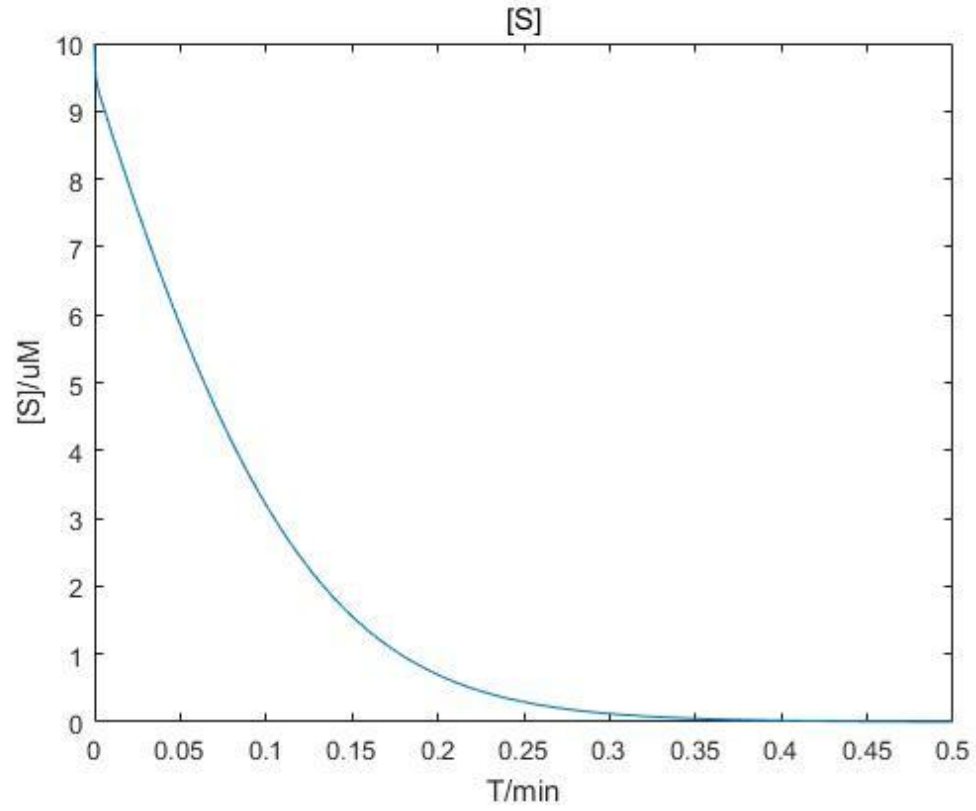
V_P=k_2[ES]

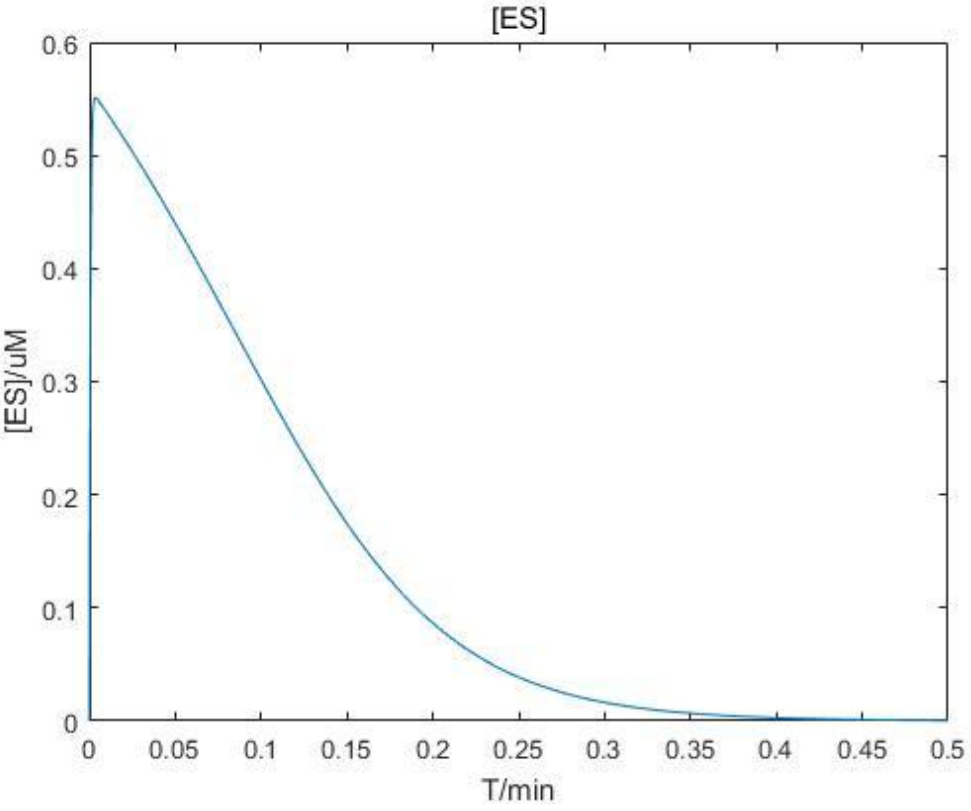
8.2

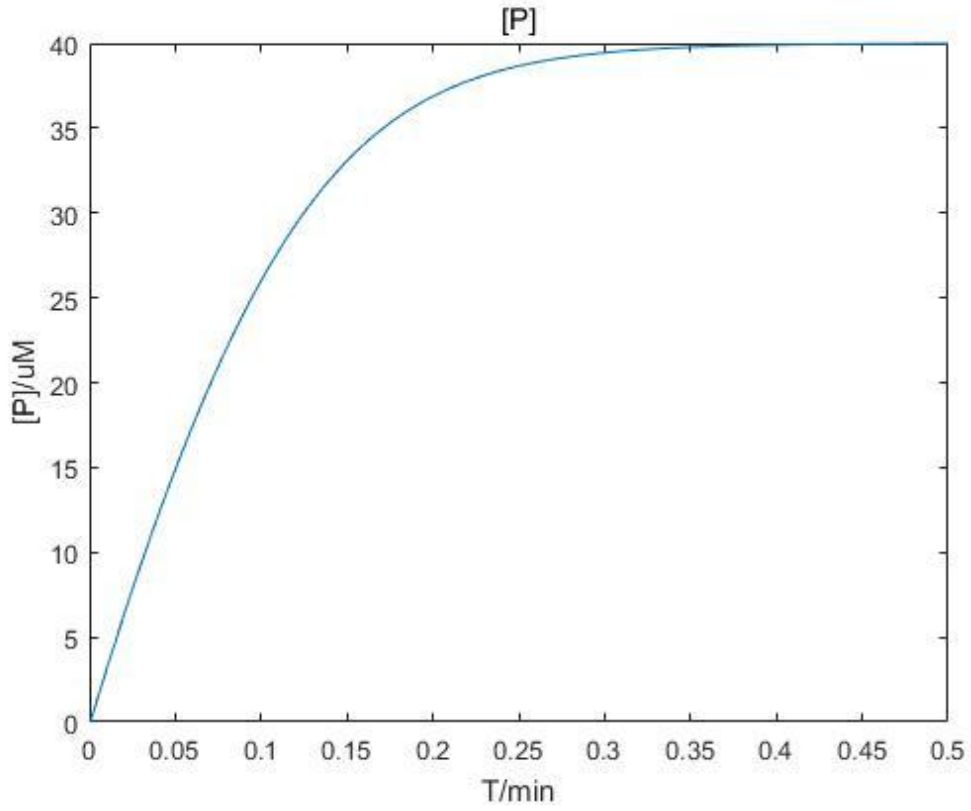
Code in matlab

```
clc
clear
h = 0.000001;
t = 0:h:0.05;
numb = length(t);%set h t , numb
k1 = 100;
k2 = 600;
k3 = 150;
Y(:,1) = [1;10;0;0];% input the given number
fun = @(t,Y)[(k2+k3)*Y(3)-k1*Y(1)*Y(2) ; k2*Y(3)-k1*Y(1)*Y(2) ;
k1*Y(1)*Y(2) - (k2+k3)*Y(3) ;k2*Y(3) ];%Y(1) is [E],Y(2) is [S], Y(3) is
[ES]

%start  RK4
for i=1:numb-1
    z1  = fun( t(i),Y(:,i));
    z2 =  fun( t(i)+h/2 , Y(:,i)+h*z1/2 );
    z3 =  fun( t(i)+h/2 , Y(:,i)+h*z2/2 );
    z4 =  fun( t(i)+h   , Y(:,i)+h*z3 );
    Y(:,i+1) = Y(:,i) + h*(z1+2*z2+2*z3+z4)/6;
end

% figure(1)
% plot(t,Y(1,:))
% hold on
% figure(2)
% plot(t,Y(2,:))
% hold on
% figure(3)
% plot(t,Y(3,:))
% hold on
% figure(4)
% plot(t,Y(4,:))
plot(t,Y(1,:)+Y(3,:)) % [E]add [ES]  ,this figure demonstrates that
[E]+[ES] =1 （+ or -）0.00000000000005
```


[E]
[E]/uM
T/min
1
0.9
0.8
0.7
0.6
0.5
0.4
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5


[S]
[S]/uM
T/min
10
9
8
7
6
5
4
3
2
1
0
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5


[ES]
[ES]/uM
T/min
0
0.1
0.2
0.3
0.4
0.5
0.6
0.05
0.15
0.25
0.35
0.45


[P]
[P]/uM
T/min
0
5
10
15
20
25
30
35
40
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5

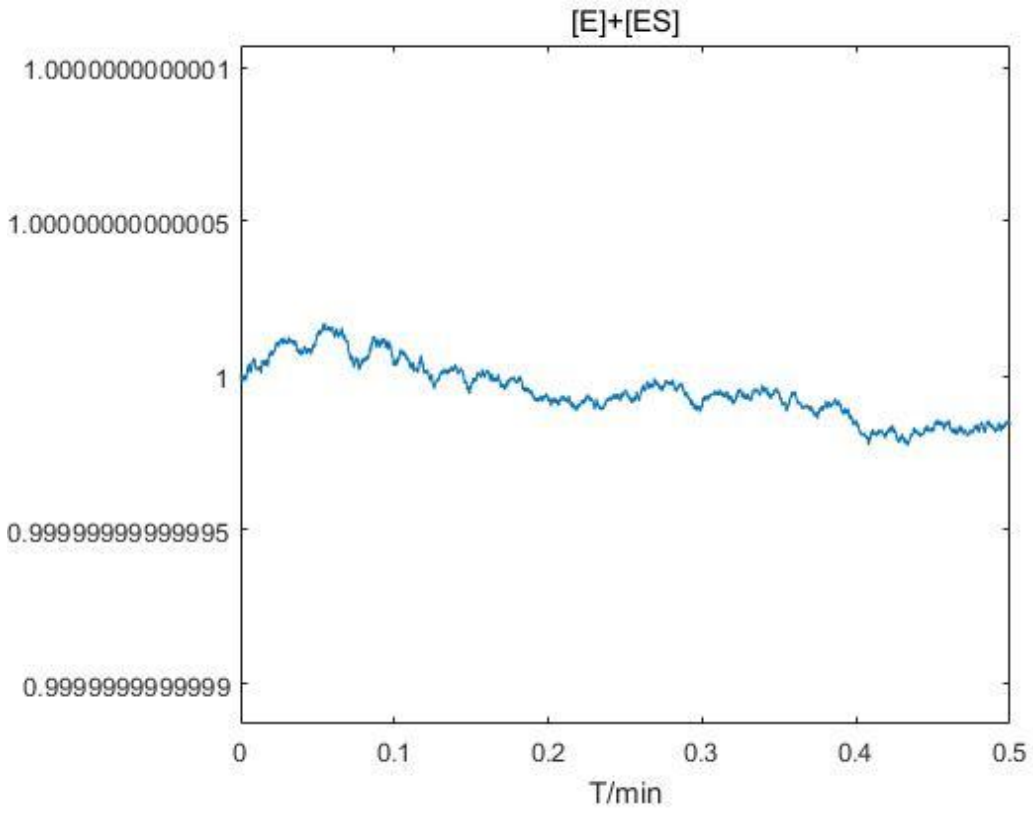

[E]+[ES]
1.0000000000001
1.00000000000005
1
0.99999999999995
0.9999999999999
0
0.1
0.2
0.3
0.4
0.5
T/min

Figure 1

8.3

First, we need the following conditions

1.The concentration value of picture [ES]+[S] obtained from 8.2（figure 1）, we can assume that [ES]+[S] is approximately equal to the constant value , let it be C.

2. V_E and V_{ES} tend to 0 after the reaction has gone on for some time.

3. Provided externally to ensure that [S] maintains its initial concentration during the reaction.

Then we can acquire:

$$[ES] + [S] = C$$

$$V_{ES}=k_1[E][S] - (k_2[ES] + k_3[ES]) = 0$$

By simplification, we get

$$[ES] = \frac{Ck_1[S]}{k_2 + k_3 + k_1[S]}$$

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

Bring in

$$V_P=k_2[ES]$$

$$V_P = \frac{Ck_2[S]}{\frac{k_2 + k_3}{k_1} + [S]}$$

The C, k_1, k_2, k_3 are constant, this function is about [S] and V_P. Set C=1, k_1=100,k_2=600,k_3=150. Use matlab to plot.

```
clc
clear
syms x ;

k1=100;
k2=600;
k3=150;
C=1;
x =0:0.01:300;
num = length(x);
for i=1:num-1

    y(1,i+1)=C*k2*x(1,i)/(((k2+k3)/k1)+x(1,i));

end
% y = C*k2*x/(((k2+k3)/k1)+x);
figure
 plot(x,y)
```