Question2:Enzyme Kinetics

8.1

Solution:

The four equations are below:

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

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

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

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

8.2

Solution:

For simplicity,let $[S]$ equal s,let $[ES]$ equal c, let $[E]$ equal e, let $[P]$ equal p. And the four equations above in code like below:

$$fs(t,s,c,e,p) = k_2c - k_1es$$

$$fe(t,s,c,e,p) = (k_3 + k_2)c - k_1es$$

$$fc(t,s,c,e,p) = k_1es - (k_3 + k_2)c$$

$$fp(t,s,c,e,p) = k_3c$$

We define the function in the code like below:

```
def fs(t, s, c, e, p):
    """ds/dt"""
    return k2*c - k1*s*e

def fe(t, s, c, e, p):
    """de/dt"""
```

```
    return (k3 + k2)*c - k1*s*e

def fc(t, s, c, e, p):
    """dc/dt"""
    return k1*s*e - (k2+k3)*c

def fp(t, s, c, e, p):
    """dp/dt"""
    return k3*c
```

For s,use S_1, S_2, S_3, S_4 represent the four parameters K_1, K_2, K_3, K_4 in the fourth-order Runge-Kutta method. Similiarly, for e, the parameters are E_1, E_2,E_3, E_4, for c, they are C_1, C_2, C_3, C_4, and P_1, P_2, P_3, P_4. After many attempts, set the step size h to 0.00002 and set the range of t as $(0, 0.01)$. In my solution, I use the classic fourth-order Runge-Kutta method, and calculate the parameters like below:

```
S_1 = fs(t, s, c, e, p)
E_1 = fe(t, s, c, e, p)
C_1 = fc(t, s, c, e, p)
P_1 = fp(t, s, c, e, p)

S_2 = fs(t + h/2, s + h*S_1/2, c + h*C_1/2, e + h*E_1/2, p + h*P_1/2)
E_2 = fe(t + h/2, s + h*S_1/2, c + h*C_1/2, e + h*E_1/2, p + h*P_1/2)
C_2 = fc(t + h/2, s + h*S_1/2, c + h*C_1/2, e + h*E_1/2, p + h*P_1/2)
P_2 = fp(t + h/2, s + h*S_1/2, c + h*C_1/2, e + h*E_1/2, p + h*P_1/2)

S_3 = fs(t + h/2, s + h*S_2/2, c + h*C_2/2, e + h*E_2/2, p + h*P_2/2)
E_3 = fe(t + h/2, s + h*S_2/2, c + h*C_2/2, e + h*E_2/2, p + h*P_2/2)
C_3 = fc(t + h/2, s + h*S_2/2, c + h*C_2/2, e + h*E_2/2, p + h*P_2/2)
P_3 = fp(t + h/2, s + h*S_2/2, c + h*C_2/2, e + h*E_2/2, p + h*P_2/2)

S_4 = fs(t + h, s + h*S_3, c + h*C_3, e + h*E_3, p + h*P_3)
E_4 = fe(t + h, s + h*S_3, c + h*C_3, e + h*E_3, p + h*P_3)
C_4 = fc(t + h, s + h*S_3, c + h*C_3, e + h*E_3, p + h*P_3)
P_4 = fp(t + h, s + h*S_3, c + h*C_3, e + h*E_3, p + h*P_3)
```

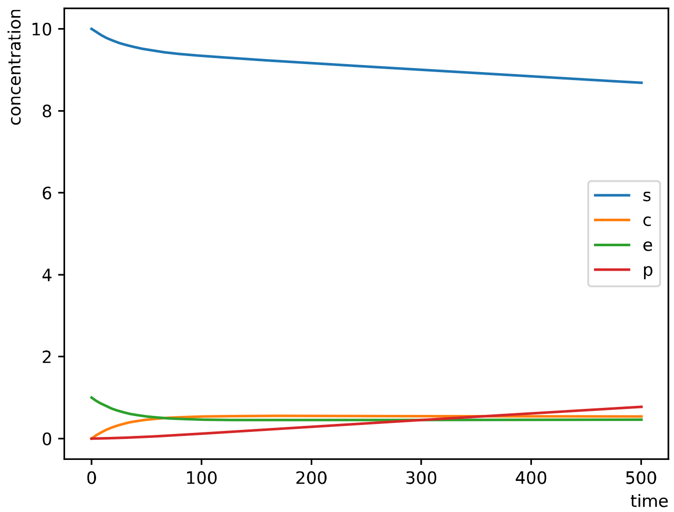
Then get the iteration value like below:

```
s = s + h*(S_1 + 2*S_2 + 2*S_3 + S_4)/6
c = c + h*(C_1 + 2*C_2 + 2*C_3 + C_4)/6
e = e + h*(E_1 + 2*E_2 + 2*E_3 + E_4)/6
p = p + h*(P_1 + 2*P_2 + 2*P_3 + P_4)/6
```

Part of the code running results like below

```
Results of fourth-order Runge-Kutta
----------------------------------------
t               s               c               e               p
0.00000000      10.00000000     0.00000000      1.00000000      0.00000000
0.00002000      9.98033561      0.01963476      0.98036524      0.00002963
0.00004000      9.96132523      0.03855767      0.96144233      0.00011710
0.00006000      9.94294388      0.05679582      0.94320418      0.00026029
0.00008000      9.92516761      0.07437517      0.92562483      0.00045721
0.00010000      9.90797347      0.09132062      0.90867938      0.00070591
0.00012000      9.89133944      0.10765603      0.89234397      0.00100453
0.00014000      9.87524441      0.12340432      0.87659568      0.00135126
0.00016000      9.85966815      0.13858747      0.86141253      0.00174439
0.00018000      9.84459120      0.15322655      0.84677345      0.00218224
......
```

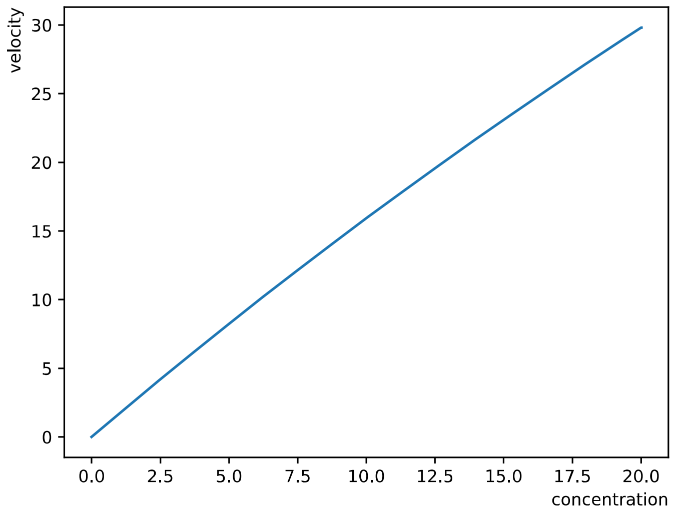
Collect all the data every time, and use the matplotlib python library to plot the concentration of s, c, e and p as funtions of the time t, and we get the image below:



8.3

Solution:

To get the rate of change of the profuct P, I use part of the process of the RK method. As we all konw, to a certain extent, the four parameters are the slope of the curve which is the function between the concertain and the time. And the slope is just the velocity, so I calculate the average of leading ten times parameter of the RK method as what we should get. The code is just similar to the second question. Then use the matplotlib to plot the curve of the concentration and the velocity. When the concentration is small, we can see that the velocity V increases approximately linearly, the image like below:



When the concentration is large, we can see that the velocity V saturates to a maximum value about 160, the image like below: