Q2.1.

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

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

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

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

Where *[E]*, *[S]*, *[ES]* and *[P]* represent the concentration of *E*, *S*, *ES* and *P*

Q2.2.

According to fourth-order Runge Kutta method, the calculation formula for each iteration step is:

$$K_1 = f(y_n, t_n)$$

$$K_2 = f(y_n + dt\frac{K_1}{2}, t_n + \frac{dt}{2})$$

$$K_3 = f(y_n + dt\frac{K_2}{2}, t_n + \frac{dt}{2})$$

$$K_4 = f(y_n + dtK_3, t_n + dt)$$

$$y_{n+1} = y_n + \frac{h}{6}(K_1 + 2K_2 + 2K_3 + K_4)$$

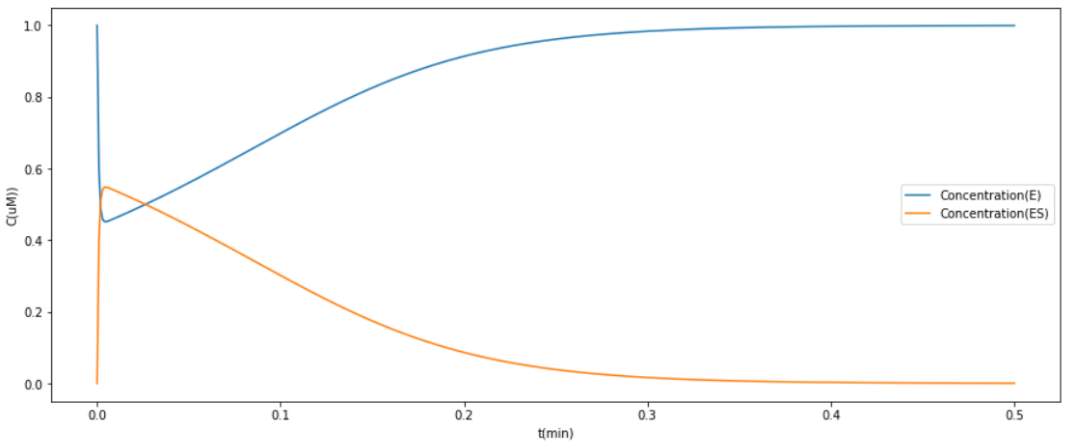
The system of partial differential equations can be implemented as:

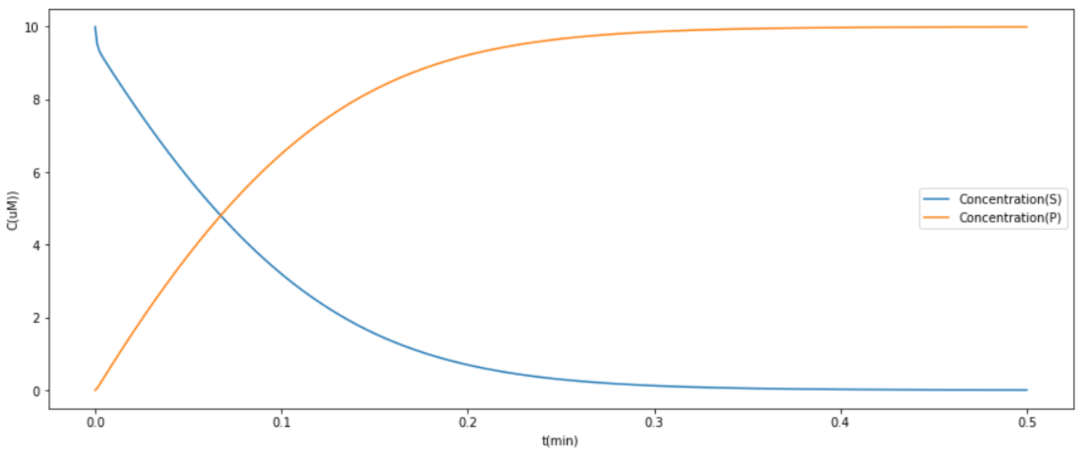
```
# System of partial differential equations
def f(Y, t, K):
    E = Y[0]
    S = Y[1]
    ES = Y[2]
    P = Y[3]
    k1 = K[0]
    k2 = K[1]
    k3 = K[2]

    dE = -k1*E*S + k2*ES + k3*ES
    dS = -k1*E*S + k2*ES
    dES = k1*E*S - k2*ES - k3*ES
    dP = k3*ES

    return np.array([dE, dS, dES, dP])
```

The fourth-order Runge Kutta expression can be implemented as:

```
#fourth-order Runge Kutta expression
def RK4(f, Y0, dt, N):
    Yn = np.zeros((N + 1, len(Y0)))
    Yn[0, :] = Y0
    t = np.linspace(1, dt*N, N)
    for i in range(0, N):
        K1 = f(Yn[i, :], t[i], K0)
        K2 = f(Yn[i, :]+dt*K1/2, t[i]+dt/2, K0)
        K3 = f(Yn[i, :]+dt*K2/2, t[i]+dt/2, K0)
        K4 = f(Yn[i, :]+dt*K3, t[i]+dt, K0)
        #print(K1, K2, K3, K4)
        Yn[i+1, :] = Yn[i, :] + dt/6 * (K1 + 2*K2 + 2*K3 + K4)

    return Yn
```

Let dt = 0.001 and N = 500 (totally 0.5min), the result plots are shown below:





Through which we can find that the reaction stops at about 0.5min, at which the concentration of E is close to the initial value.

The detailed code *Question2 Code.ipynb* is saved in the same folder

Q2.3.

Theoretically, the velocity of enzymatic reaction can be expressed by Michaelis-Menten equation: $V = \frac{k_3[Et][S]}{K_m+[S]}, where\ [Et] = [E] + [ES], K_m = \frac{k2}{k1}$

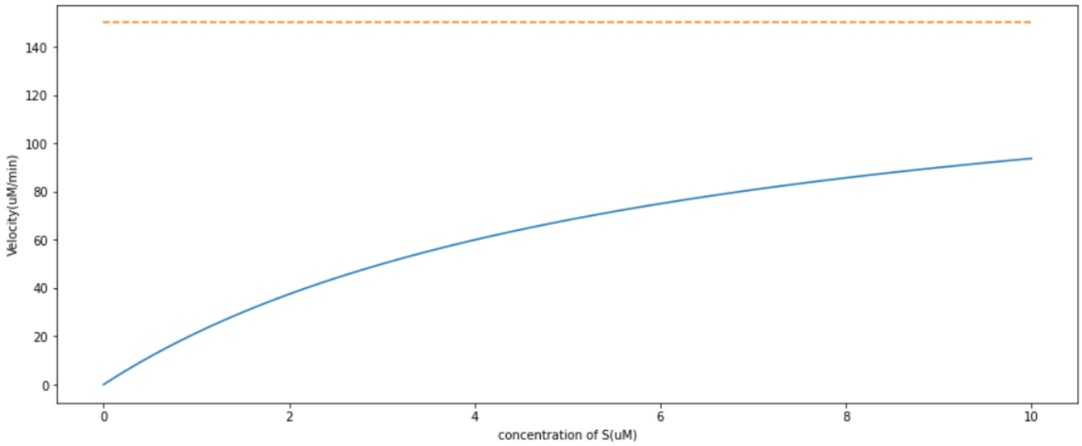
Substitute in known conditions in Q2.2: $[Et] = 1uM, K_m = 6uM, k3 = 150/min$

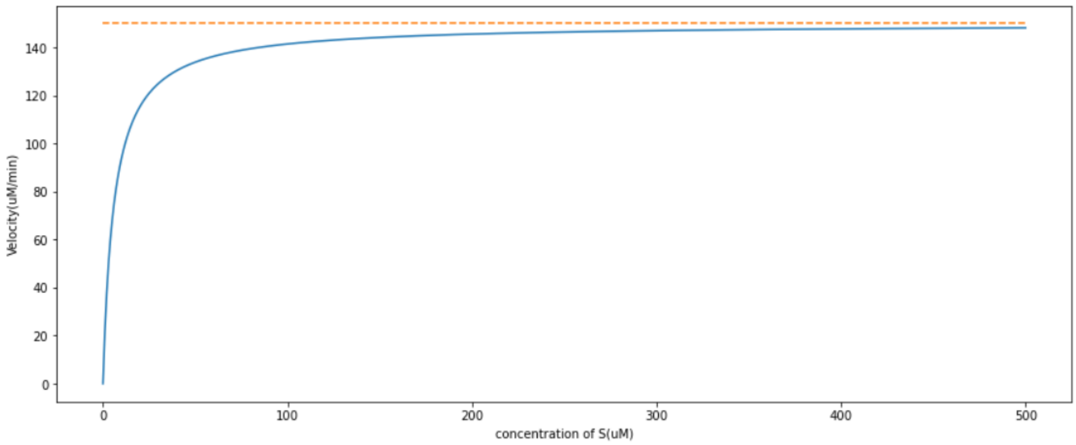
We have $V = \frac{150[S]}{6+[S]} uM/min.$

Besides, the maximal velocity V_{max} can be expressed as

$V_{max} = k3[Et] = 150uM/min$

Plot V in python:





We can see when the concentrations of S are small (upper figure, S < 10uM), the velocity V are approximately linearly, and the velocity *V* saturates to Vmax for large S (lower figure, S < 500uM).