

## 8.1

The law of mass action means that the rate of a chemical or biological reaction is proportional to the effective mass of the reactants. The "effective mass" here is actually the concentration of each reactant.

In this scheme, we have two steps and three reactions



For reaction 1, we have

$$\frac{dc_{E(1)}}{dt} = -k1 c_E c_S \quad (\text{equation 1})$$

$$\frac{dc_{S(1)}}{dt} = -k1 c_E c_S \quad (\text{equation 2})$$

$$\frac{dc_{ES(1)}}{dt} = k1 c_E c_S \quad (\text{equation 3})$$

where  $c_E$  means the concentration of E;  $k1$  means the reaction rate, which depends on many factors in one reaction, such as reaction type, reaction temperature and reaction catalyst

For reaction 2, we have

$$\frac{dc_{ES(2)}}{dt} = -k2 c_{ES} \quad (\text{equation 4})$$

$$\frac{dc_{E(2)}}{dt} = k2 c_{ES} \quad (\text{equation 5})$$

$$\frac{dc_{S(2)}}{dt} = k2 c_{ES} \quad (\text{equation 6})$$

For reaction 3, we have

$$\frac{dc_{ES(3)}}{dt} = -k3 c_{ES} \quad (\text{equation 7})$$

$$\frac{dc_{E(3)}}{dt} = k3 c_{ES} \quad (\text{equation 8})$$

$$\frac{dc_{P(3)}}{dt} = k3 c_{ES} \quad (\text{equation 9})$$

Combing all the equations, we have:

$$\left\{ \begin{array}{l} \frac{dc_E}{dt} = -k_1 c_E c_S + k_2 c_{ES} + k_3 c_{ES} \\ \frac{dc_S}{dt} = -k_1 c_E c_S + k_2 c_{ES} \\ \frac{dc_{ES}}{dt} = k_1 c_E c_S - k_2 c_{ES} - k_3 c_{ES} \\ \frac{dc_P}{dt} = k_3 c_{ES} \end{array} \right.$$

## 8.2

When we solve ordinary differential equations, some ordinary differential equations have analytical methods, but most ordinary differential equations can only be solved numerically. The fourth-order Runge-Kutta method is one of the numerical solutions. The essence of this method is the following equations

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

$$K_1 = f(x_n, y_n) \quad (2)$$

$$K_2 = f(x_n + \frac{h}{2}, y_n + \frac{h}{2} K_1) \quad (3)$$

$$K_3 = f(x_n + \frac{h}{2}, y_n + \frac{h}{2} K_2) \quad (4)$$

$$K_4 = f(x_n + h, y_n + h K_3) \quad (5)$$

According to the equations above, we can have the code using python (see 8.ipynb)

$$\frac{dc_E}{dt} = -100 c_E c_S + 600 c_{ES} + 150 c_{ES}$$

$$\frac{dc_S}{dt} = -100 c_E c_S + 600 c_{ES}$$

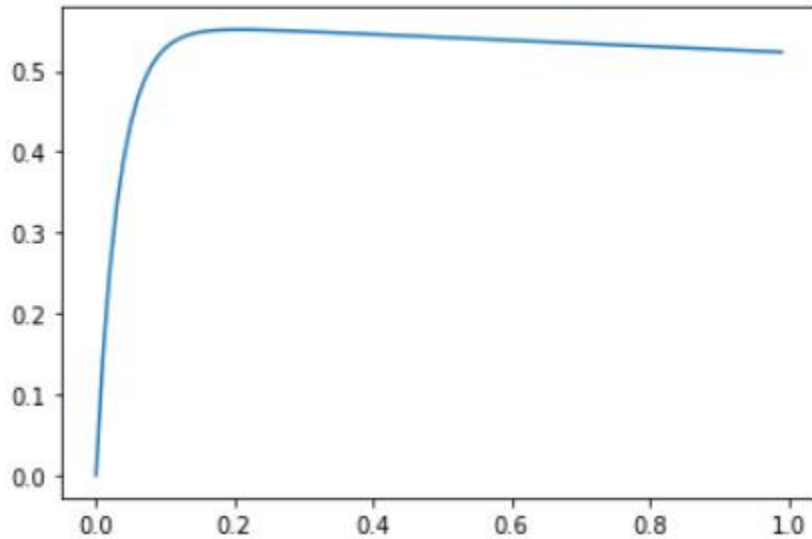
$$\frac{dc_{ES}}{dt} = 100 c_E c_S - 600 c_{ES} - 150 c_{ES}$$

$$\frac{dc_P}{dt} = 150 c_{ES}$$

$$C_{E0} = 1, C_{S0} = 10, C_{ES0} = 0, C_{P0} = 0$$

8.3

Here we have the figure



We can find that, 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,  $V_m$ .

After calculating,  $V_m$  equals about 0.54