## Equations for the rate of changes of the four species

[E] is the concentration of E.

$$E: \frac{d[E]}{dt} = -k_1[E][S] + k_2[ES] + k_3[ES]$$
 (1)

S: 
$$\frac{d[S]}{dt} = -k_1[E][S] + k_2[ES]$$
 (2)

$$ES: \frac{d[ES]}{dt} = k_1[E][S] - k_2[ES] - k_3[ES]$$
 (3)

$$P: \frac{\mathrm{d}[P]}{\mathrm{d}t} = k_3[ES] \tag{4}$$

Solve these four equations using the fourth-order Runge-Kutta method

Using the steady-state approximation, the following equation can get:

$$\frac{d[ES]}{dt} = k_1[E][S] - k_2[ES] - k_3[ES] = 0$$

SO

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

Call  $k_M = \frac{k_2 + k_3}{k_1}$  as Michaelis constant.

If the original concentration of the enzyme is [E], after the reaction reaches E steady state, part of it becomes an intermediate compound [ES], the other part is still free, so

$$[E] = [E_0] - [ES] \tag{5}$$

Substitute this into (4),

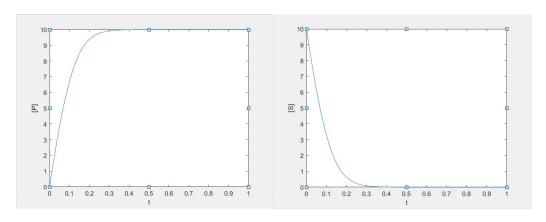
$$[ES] = \frac{[E_0][S]}{k_M[S]} \tag{6}$$

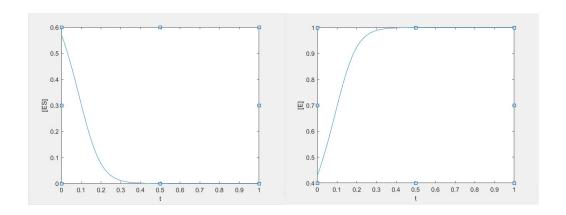
Substitute (5) into (4),

$$P: \frac{d[P]}{dt} = k_3 \frac{[E_0][S]}{k_M[S]}$$
 (7)

The total reaction we could call that  $S \rightarrow P$ , so when you consume a certain amount of S, you get the same amount of P. According to this relationship and the initial concentration of S, we can further simplify the expression for P, as shown in the code. When we get the value of P, also according to this relationship, we can further get the value of S. And based on (6), we can know the value of ES. Finally, based on (6), we can get the value of E.

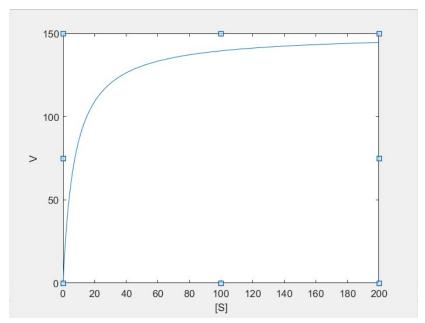
Plug in the values of the coefficients and the initial values, four figures are as follows:





## Find this value Vm from your plot

Based on (7), we know  $\frac{d[P]}{dt} = V$ . Then a plot can be draw



We can find that the value of Vm is 150, which equals the value of  $k_2$ .