2.1 math solution:

2.1 $E + S \underset{k_2}{\overset{k_1}{\rightleftharpoons}} ES \xrightarrow{k_3} E + P$

use C to represent ES, therefore

$$E + S \underset{k_2}{\overset{k_1}{\rightleftharpoons}} C \xrightarrow{k_3} E + P$$

1) E: consumption $= k_1 ES$

production $= k_2 C + k_3 C$

2) S: consumption $= k_1 ES$

production $= k_2 C$

3) C: consumption $= k_2 C + k_3 C$

production $= k_1 ES$

4) P: consumption $= 0$

production $= k_3 C$

therefore

$$\begin{cases} \frac{dE}{dt} = (k_2 + k_3) C - k_1 ES & ① \\ \frac{dS}{dt} = k_2 C - k_1 ES & ② \\ \frac{dC}{dt} = k_1 ES - (k_2 + k_3) C & ③ \\ \frac{dP}{dt} = k_3 C & ④ \end{cases}$$

2.2 math solution :

2.2

use the equations in 2.1, we can know that:

① + ③ $\Rightarrow \frac{dE}{dt} + \frac{dC}{dt} = \frac{d(E+C)}{dt} = 0$

therefore $E+C$ equals to a constant

we also know the initial concentration of E and C,

so $E + C = E_0 + C_0 = E_0 \Rightarrow E = E_0 - C$

bring $E = E_0 - C$ into equation ② and ③, we can have:

$$\begin{cases} \frac{dS}{dt} = -k_1(E_0 - C)S + k_2 C \\ \frac{dC}{dt} = k_1(E_0 - C)S - (k_2 + k_3)C \end{cases}$$

$\Downarrow \quad \theta = k_2 + k_3 \qquad \lambda = k_1 E_0$

$$\begin{cases} \frac{dS}{dt} = -\lambda S + (k_1 S + k_2)C \\ \frac{dC}{dt} = \lambda S - (\theta + k_1 S)C \end{cases}$$

initial conditions
$$\begin{cases} E(0) = 1\ uM \\ S(0) = 10\ uM \\ C(0) = 0\ uM \\ P(0) = 0\ uM \\ k_1 = 100\ uM/min \\ k_2 = 600\ uM/min \\ k_3 = 150\ uM/min \end{cases}$$

so the oringinal equations can be:

$$\begin{cases} \frac{dC}{dt} = \lambda S - (\theta + k_1 S)C \\ \frac{dS}{dt} = -\lambda S + (k_1 S + k_2)C \\ C(0) = 0 \qquad S(0) = 10 \end{cases} \qquad \begin{cases} E = E_0 - C \\ P = k_3 \int C\, dt \end{cases}$$

2.2 python results:

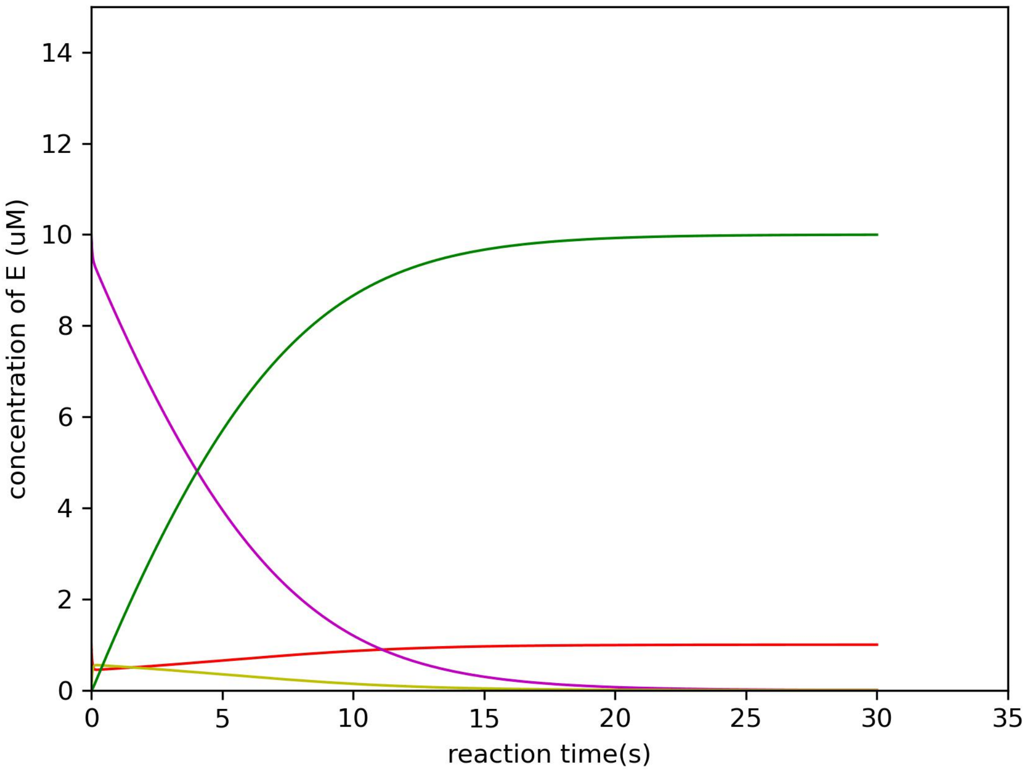

Figure 1: variation of components' concentration in 30s.

We can see from this picture that the enzymatic reaction is really fast at the beginning. There is a huge change both in the concentration of enzyme and intermediate compound during the first second. After that, the concentration of intermediate compound gradually decreases to 0μM while that of enzyme increases and stays about 1μM.

Production is generated quickly during the first 10 second and slows down during 10-20 second. And after that, its concentration comes to a maximum and keep stable.

There is an obvious inverse relationship between the decrease of substrate concentration and the increase of product concentration.

The numeric result of concentration in each second(0-30 second, 30001 steps in total) is demonstrated in the csv file named ' concentration per step(0.001s)'.

	enzyme	substract	compound	product
0	1	10	0	0
1	0.983588	9.983567	0.016412	4.10E-05
2	0.967673	9.967591	0.032327	0.000122
3	0.952239	9.952057	0.047761	0.000241
4	0.937272	9.936952	0.062728	0.000398
5	0.922757	9.922262	0.077243	0.000591
6	0.908679	9.907973	0.091321	0.000819
7	0.895025	9.894074	0.104975	0.001082
8	0.881781	9.880551	0.118219	0.001377
9	0.868935	9.867393	0.131065	0.001705

Figure 2: part of the numeric results of components' concentration in 30s.

2.3 math solution :

2.3

$V = \frac{dP}{dt}$ we want to plot $\frac{dV}{dS}$

$$\frac{dV}{dS} = \frac{d(\frac{dP}{dt})}{dS}$$

from 2.1 equation ④ we know $\frac{dP}{dt} = k_3 C$

therefore $$\frac{dV}{dS} = \frac{d(k_3 C)}{dS} = \frac{k_2\, dC}{dt} \cdot \frac{dt}{dS} = \frac{\frac{k_2 dC}{dt}}{\frac{dS}{dt}}$$

from 2.1 equation ② ③ , we can have :

$$\frac{dV}{dS} = \frac{k_3 [k_1 ES - (k_2 + k_3) C]}{k_2 C - k_1 ES}$$

2.3 python results:

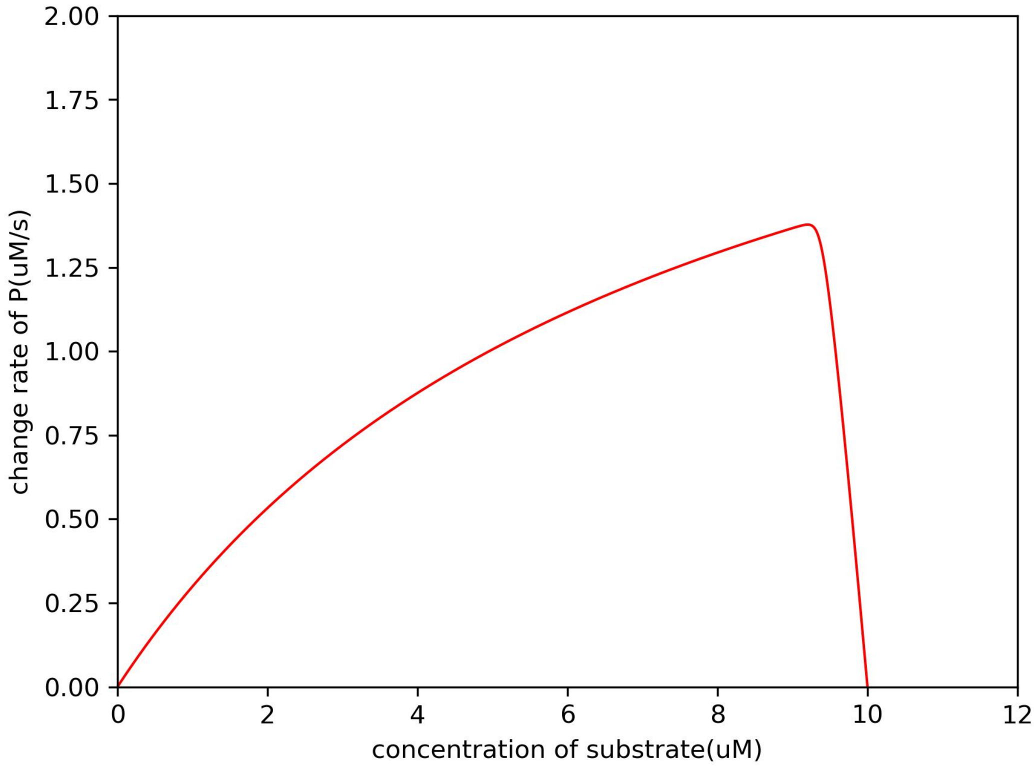

Figure 3: relationship between change rate of product and concentration of substrate

We can see from this picture that the change rate of product increases almost linearly during 0-9s. And it jumped into 0 during 9-10. This is reasonable because at the beginning, 10μM substrate is much large than the concentration of enzyme, therefore, the reaction will go forward, which leads P to increase sharply. And the consumption of substrate lets the concentration of P become stable. That's the reason for the almost linear change of P's rate.

The maximum value of the change rate of product P is 1.392μM/s when the concentration of substrate is 9μM.

Reference

[1] Barazandeh Y , Ghazanfari B . Numerical Solution for Fuzzy Enzyme Kinetic Equations by the Runge–Kutta Method[J]. 2018.