Enzyme Kinetics Modeling

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Answers

8.1 Solution:

The process of an enzyme *E* converts the substrate *S* into the product *P* is Schematically written as follow:

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

The equations for the rate of changes of the four species, *E*, *S*, *ES*, and *P* are:

1) For enzyme *E*: $d[E]/dt = -k_1[E][S] + k_2[ES] + k_3[ES]$
2) For substrate *S*: $d[S]/dt = -k_1[E][S] + k_2[ES]$
3) For intermediate species *ES*: $d[ES]/dt = k_1[E][S] - k_2[ES] - k_3[ES]$
4) For Product *P*: $d[P]/dt = k_3[ES]$

[E], [S], [ES], [P] represent the concentration of E, S, ES, P respectively.

8.2 Solution:

The Given data:

1) The initial concentration of E is 1 µM
2) The initial concentration of S is 10 µM
3) The initial concentrations of ES and P are both 0.
4) k1 = 100/µM/min = $1.67 \mu M^{-1} s^{-1}$
5) k2 = 600/µM/min = $10\ \mu M^{-1} s^{-1}$
6) k3 = 150/µM/min = $2.5\ \mu M^{-1} s^{-1}$

The fourth-order Runge Kutta method

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

$$\begin{cases} K_1 = f(t_n, y_n) \\ K_2 = f(t_n + \frac{h}{2}, y_n + \frac{h}{2}K_1) \\ K_3 = f(t_n + \frac{h}{2}, y_n + \frac{h}{2}K_2) \\ K_4 = f(t_n, y_n + hK_3) \end{cases}$$

Figure 1. Equations for fourth-order Runge-Kutta method[1]

Matlab Code and outputs for this question:

```
% initial conditions, time
yzero=[10, 1, 0, 0];
k1=1.67; k2=10; k3=2.5;
tsp=[0 80];

% using ode45 for RK4
[t,y]=ode45('RK4',tsp,yzero,[],k1,k2,k3);

% Plot the figure
plot(t,y(:,1),'-',t,y(:,4),'-.')
hold on
plot(t,y(:,2),'-',t,y(:,3),'-.')

title('Time-Concentration Plot for 4 species')
xlabel('Time (s)');
ylabel('Concentration(μM)');
legend('S(substrate)','P(product)','E(enzyme)','ES(intermediate)','location', 'east');
```

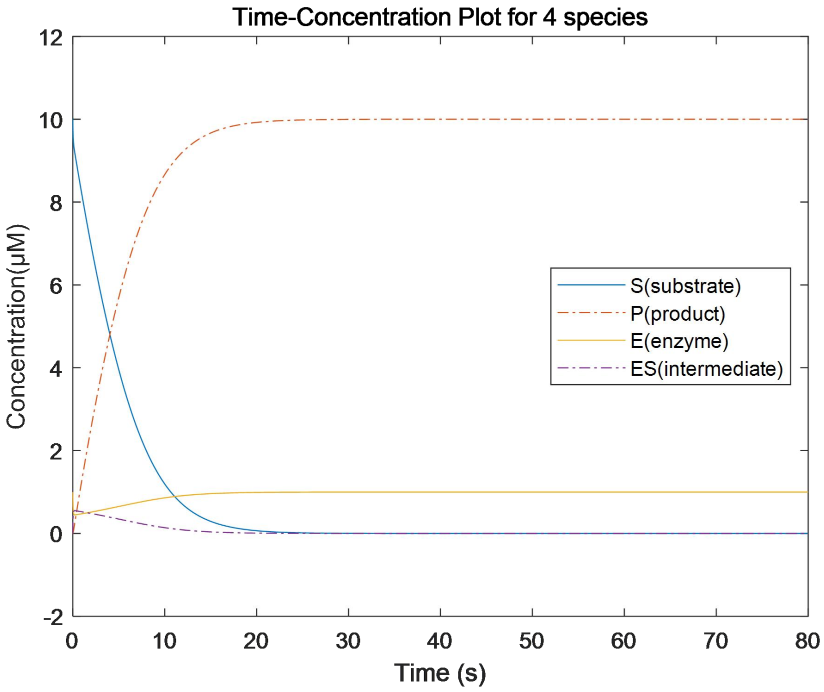

Figure 2. Time-Concentration Plot for 4 species

```
% initial conditions, time
yzero=[10, 1, 0, 0];
k1=1.67; k2=10; k3=2.5;
tsp=[0 1];

% using ode45 for RK4
[t,y]=ode45('RK4',tsp,yzero,[],k1,k2,k3);

% Plot the figure
plot(t,y(:,2),'-',t,y(:,3),'-.')

title('Time-Concentration Plot for enzyme and intermediate')
xlabel('Time (s)');
ylabel('Concentration(μM)');
legend('E(enzyme)','ES(intermediate)');
```

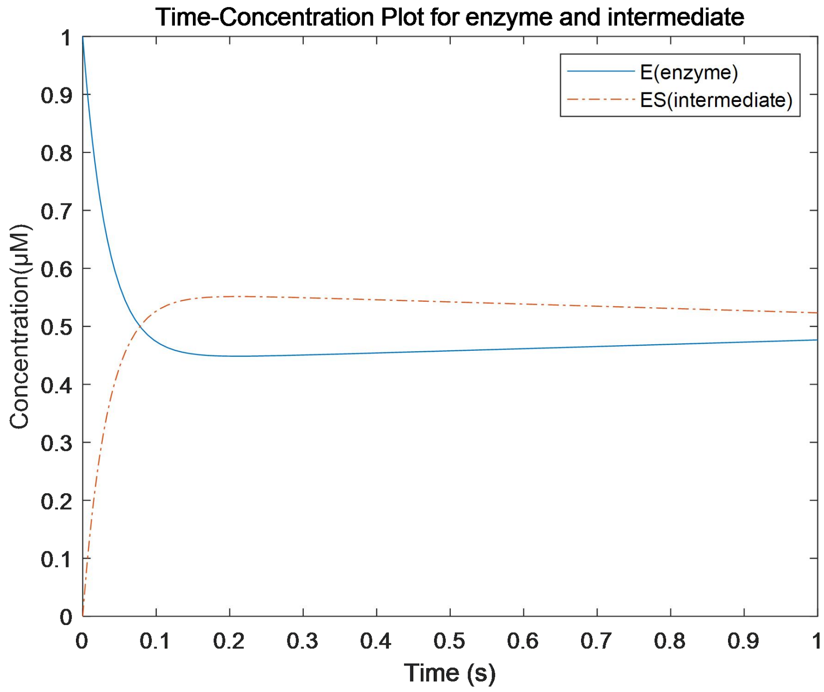

Figure 3. Time-Concentration Plot for enzyme and intermediate

8.3 Solution:

Reference

[1] Song Yezhi. Numerical Analysis and Application of MATLAB [M]. Beijing: China Machine Press,2021