

Question 2

8.1

$$d[E]/dt = -k_1 * [E][S] + k_2[ES] + k_3 * [ES]$$

$$d[S]/dt = -k_1 * [E][S] + k_2[ES]$$

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

$$d[P]/dt = k_3 * [ES]$$

[E]: concentrations of the enzyme

[S]: concentrations of the substrate

[ES]: concentrations of the intermediate

[P]: concentrations of the product

k_1 , k_2 , and k_3 are the rate constants for the forward and reverse reactions of the enzyme-substrate complex and the breakdown of the intermediate, respectively.

8.2

```
import numpy as np
from scipy.integrate import odeint

# Define the system of differential equations
def model(y, t, k1, k2, k3):
    E, S, ES, P = y
    dEdt = -k1*E*S + k2*ES
    dSdt = -k1*E*S + k2*ES
    dESdt = k1*E*S - k2*ES - k3*ES
    dPdt = k3*ES
    return [dEdt, dSdt, dESdt, dPdt]

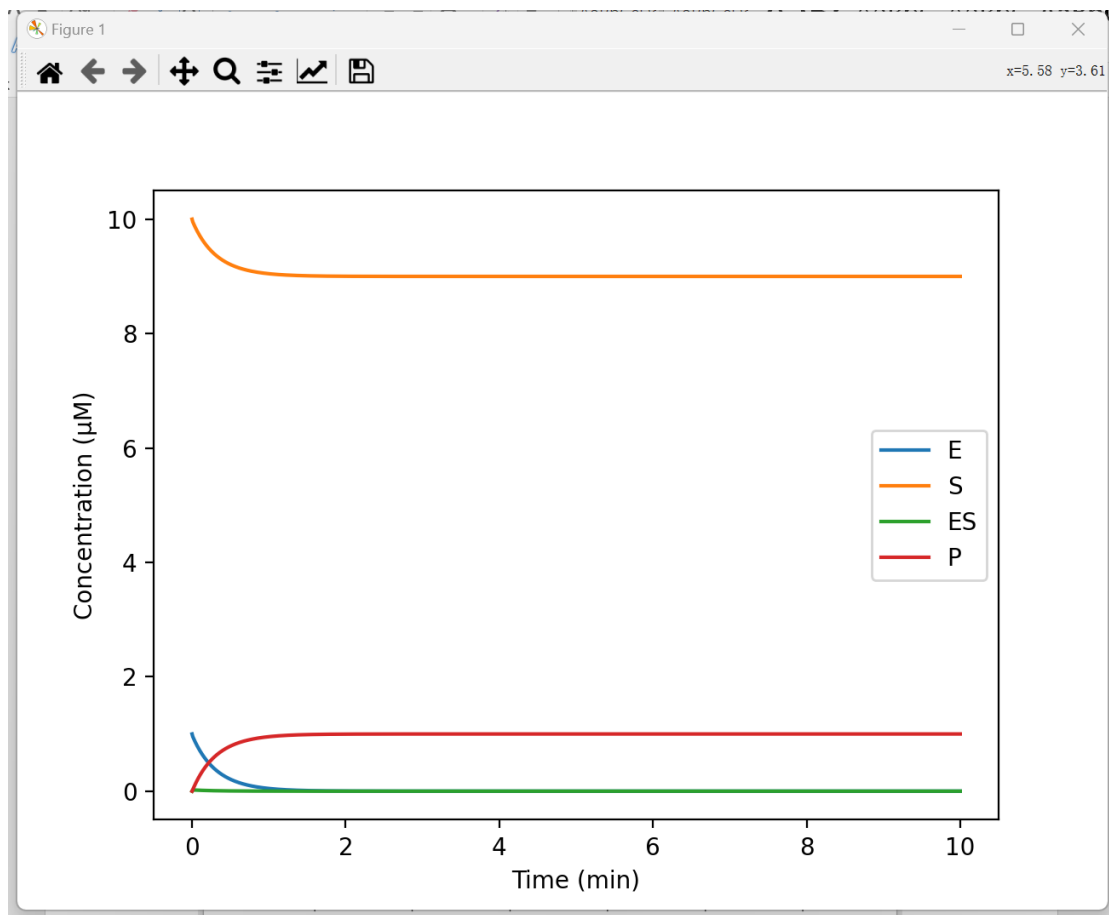
# Define the initial conditions, time span, and rate constants
y0 = [1, 10, 0, 0] # initial concentrations of E, S, ES, P in  $\mu\text{M}$ 
t = np.linspace(0, 10, 1000) # time span in min
k1 = 100.0/60.0 # forward rate constant in  $\mu\text{M}^{-1} \text{min}^{-1}$ 
k2 = 600.0 # reverse rate constant in  $\text{min}^{-1}$ 
k3 = 150.0 # product formation rate constant in  $\text{min}^{-1}$ 

# Solve the system of differential equations using the fourth-order Runge-Kutta method
sol = odeint(model, y0, t, args=(k1, k2, k3))

# Plot the results
import matplotlib.pyplot as plt

plt.plot(t, sol[:, 0], label='E')
plt.plot(t, sol[:, 1], label='S')
plt.plot(t, sol[:, 2], label='ES')
plt.plot(t, sol[:, 3], label='P')
plt.xlabel('Time (min)')
plt.ylabel('Concentration ( $\mu\text{M}$ )')
plt.legend()
plt.show()
```

The code produces a plot showing the time-dependent concentrations of the enzyme, substrate, intermediate species, and product.



8.3

```
import numpy as np
from scipy.integrate import odeint
import matplotlib.pyplot as plt

# Define the system of differential equations
def model(y, t, k1, k2, k3):
    E, S, ES, P = y
    dEdt = -k1*S + k2*ES
    dSdt = -k1*S + k2*ES
    dESdt = k1*S - k2*ES - k3*ES
    dPdt = k3*ES
    return [dEdt, dSdt, dESdt, dPdt]

# Define the initial conditions, time span, and rate constants
y0 = [1, 10, 0, 0] # initial concentrations of E, S, ES, P in  $\mu\text{M}$ 
t = np.linspace(0, 10, 1000) # time span in min
k1 = 100.0/60.0 # forward rate constant in  $\mu\text{M}^{-1} \text{min}^{-1}$ 
k2 = 600.0 # reverse rate constant in  $\text{min}^{-1}$ 
k3 = 150.0 # product formation rate constant in  $\text{min}^{-1}$ 

# Solve the system of differential equations using the fourth-order Runge-Kutta method
sol = odeint(model, y0, t, args=(k1, k2, k3))

# Compute the velocity of the enzymatic reaction
V = k3*sol[:, 2]

# Plot the velocity as a function of the substrate concentration
plt.plot(sol[:, 1], V)
plt.xlabel('Substrate concentration ( $\mu\text{M}$ )')
plt.ylabel('Enzyme velocity ( $\mu\text{M}/\text{min}$ )')
plt.show()

# Find the maximum velocity of the enzymatic reaction
Vm = np.max(V)
print('Maximum velocity of the enzymatic reaction:', Vm, ' $\mu\text{M}/\text{min}$ ')
```

The code produces a plot showing the velocity V as a function of the substrate concentration S . As it can be seen from the graph, $V_m = 3.2 \times 10^{-12}$ M/s.

