Enzyme Kinetics

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1. Problem 1 Answer

The law of mass action states that the rate of a chemical reaction is proportional to the concentration of the reactants. We can use this law to write down the following four equations for the rate of changes of the four species:

d[E]/dt = -k1*[E][S] + k2[ES] + k3*[ES]

d[S]/dt = -k1*[E][S] + k2[ES]

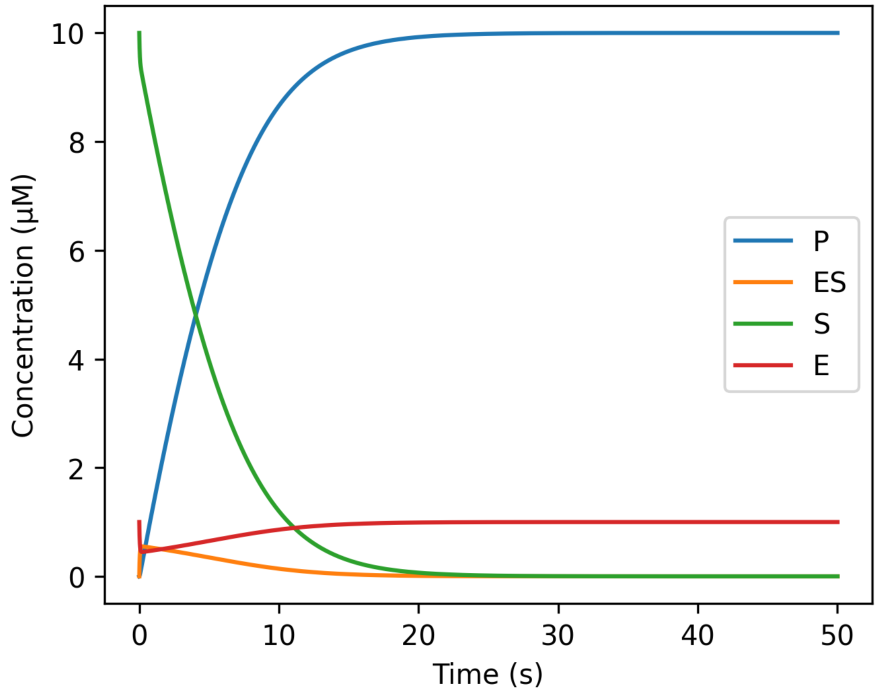
d[ES]/dt = k1*[E][S] - k2[ES] - k3*[ES]

d[P]/dt = k3*[ES]

where [E], [S], [ES], and [P] are the concentrations of enzyme, substrate, enzyme-substrate complex, and product, respectively.

2. Problem 2 Answer

The concentration of each substance changes with time as shown in the figure below:



The final concentration results of each substance are:
1. P = 9.999990632711981 μM
2. ES = 1.1259147027478198e-06 μM
3. S = 8.24137334653992e-06 μM
4. E = 0.9999988740853092 μM

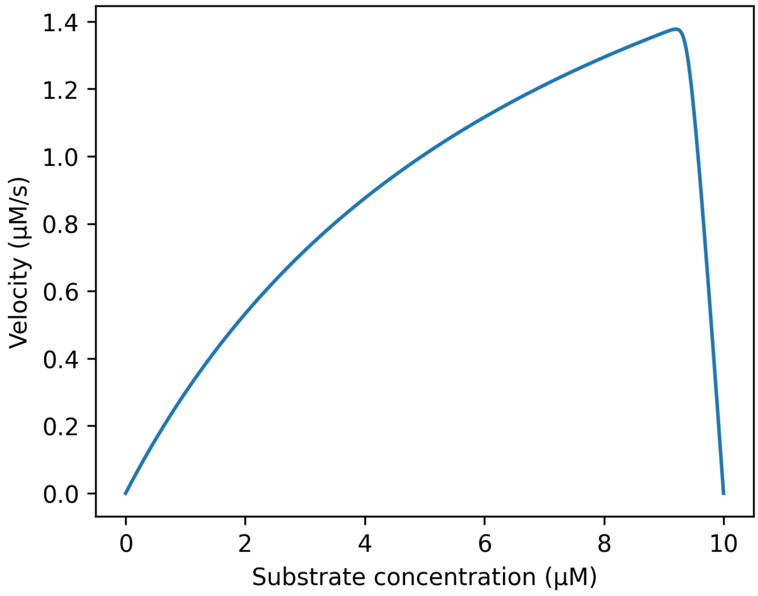
My code to solve problem 8.2 is as follows:

```
import matplotlib.pyplot as plt
import numpy as np

# Set initial conditions
E_0 = 1  # μM
S_0 = 10  # μM
ES_0 = 0  # μM
P_0 = 0  # μM

k1 = 100 / 60  # /s
k2 = 600 / 60  # /s
k3 = 150 / 60  # /s

# Set up the time array
N = 50000
t0 = 0
t_end = 50
t = np.linspace(t0, t_end, N)
dt = t[1] - t[0]


# Initialize the solution array
y = np.zeros((N, 4))
y[0] = [E_0, S_0, ES_0, P_0]

dp_list = [0]

# Define the derivative function
def f(t, y):
    E, S, ES, P = y
    dE = -k1 * E * S + k2 * ES + k3 * ES
    dS = -k1 * E * S + k2 * ES
    dES = k1 * E * S - k2 * ES - k3 * ES
    dP = k3 * ES
    return np.array([dE, dS, dES, dP])

# Use the fourth-order Runge-Kutta method to solve the differential
equations
```

```python
for i in range(N - 1):
    k1_ = f(t[i], y[i])
    k2_ = f(dt/2 + t[i], y[i] + dt/2 * k1_)
    k3_ = f(dt/2 + t[i], y[i] + dt/2 * k2_)
    k4_ = f(dt + t[i], y[i] + dt * k3_)
    y[i + 1] = y[i] + dt/6 *(k1_ + 2*k2_ + 2*k3_ + k4_)
    dp_list.append(k3 * y[i + 1][2])

# Plot the results for 8.2

# Set dpi and image size
fig = plt.figure(figsize=(5, 4), dpi=300)

plt.plot(t, y[:, 3], label='P') # 'Product'
plt.plot(t, y[:, 2], label='ES') # 'Intermediate'
plt.plot(t, y[:, 1], label='S') # 'Substrate'
plt.plot(t, y[:, 0], label='E') # 'Enzyme'

plt.legend()
plt.xlabel('Time (s)')
plt.ylabel('Concentration (μM)')
plt.show()

# Save the image in PNG format
fig.savefig('result1.png', dpi=300, bbox_inches='tight')


print("The Final Concentration (μM) of P is: " + str(y[:, 3][-1]) + ' 
μM')
print("The Final Concentration (μM) of ES is: " + str(y[:, 2][-1]) + ' 
μM')
print("The Final Concentration (μM) of S is: " + str(y[:, 1][-1]) + ' 
μM')
print("The Final Concentration (μM) of E is: " + str(y[:, 0][-1]) + ' 
μM')
```

3. Problem 3 Answer

The following figure is the relationship between Velocity and Substrate concentration:



Maximum Velocity: 1.3774644263606182 μM/s
When Velocity reaches the maximum value, the value of S is: 9.203310016020918 μM

My code to plot the results for 8.3 is as follows:

```
# Plot the results for 8.3

# Set dpi and image size
fig = plt.figure(figsize=(5, 4), dpi=300)

# Plot the velocity as a function of the substrate concentration
plt.plot(list(y[:, 1]), dp_list)
plt.xlabel('Substrate concentration (μM)')
plt.ylabel('Velocity (μM/s)')
plt.show()

# Save the image in PNG format
fig.savefig('result2.png', dpi=300, bbox_inches='tight')


print("Maximum Velocity: " + str(max(dp_list)) + " μM/s")
max_index = dp_list.index(max(dp_list))
s_for_max_v = list(y[:, 1])[max_index]
print("When Velocity reaches the maximum value, the value of S is: " +
str(s_for_max_v) + ' μM')
```

Appendix

The overall Python code for solving Question 2 is as follows:

```
import matplotlib.pyplot as plt
import numpy as np

# Set initial conditions
E_0 = 1  # µM
S_0 = 10  # µM
ES_0 = 0  # µM
P_0 = 0  # µM

k1 = 100 / 60  # /s
k2 = 600 / 60  # /s
k3 = 150 / 60  # /s

# Set up the time array
N = 50000
t0 = 0
t_end = 50
t = np.linspace(t0, t_end, N)
dt = t[1] - t[0]


# Initialize the solution array
y = np.zeros((N, 4))
y[0] = [E_0, S_0, ES_0, P_0]

dp_list = [0]

# Define the derivative function
def f(t, y):
    E, S, ES, P = y
    dE = -k1 * E * S + k2 * ES + k3 * ES
    dS = -k1 * E * S + k2 * ES
    dES = k1 * E * S - k2 * ES - k3 * ES
    dP = k3 * ES
    return np.array([dE, dS, dES, dP])

# Use the fourth-order Runge-Kutta method to solve the differential
equations
for i in range(N - 1):
    k1_ = f(t[i], y[i])
    k2_ = f(dt/2 + t[i], y[i] + dt/2 * k1_)
```

```
    k3_ = f(dt/2 + t[i], y[i] + dt/2 * k2_)
    k4_ = f(dt + t[i], y[i] + dt * k3_)
    y[i + 1] = y[i] + dt/6 *(k1_ + 2*k2_ + 2*k3_ + k4_)
    dp_list.append(k3 * y[i + 1][2])

# Plot the results for 8.2

# Set dpi and image size
fig = plt.figure(figsize=(5, 4), dpi=300)

plt.plot(t, y[:, 3], label='P') # 'Product'
plt.plot(t, y[:, 2], label='ES') # 'Intermediate'
plt.plot(t, y[:, 1], label='S') # 'Substrate'
plt.plot(t, y[:, 0], label='E') # 'Enzyme'

plt.legend()
plt.xlabel('Time (s)')
plt.ylabel('Concentration (μM)')
plt.show()

# Save the image in PNG format
fig.savefig('result1.png', dpi=300, bbox_inches='tight')

print("The Final Concentration (μM) of P is: " + str(y[:, 3][-1]) + '
μM')
print("The Final Concentration (μM) of ES is: " + str(y[:, 2][-1]) + '
μM')
print("The Final Concentration (μM) of S is: " + str(y[:, 1][-1]) + '
μM')
print("The Final Concentration (μM) of E is: " + str(y[:, 0][-1]) + '
μM')

# Plot the results for 8.3

# Set dpi and image size
fig = plt.figure(figsize=(5, 4), dpi=300)

# Plot the velocity as a function of the substrate concentration
plt.plot(list(y[:, 1]), dp_list)
plt.xlabel('Substrate concentration (μM)')
plt.ylabel('Velocity (μM/s)')
plt.show()

# Save the image in PNG format
fig.savefig('result2.png', dpi=300, bbox_inches='tight')
```

```
print("Maximum Velocity: " + str(max(dp_list)) + " µM/s")
max_index = dp_list.index(max(dp_list))
s_for_max_v = list(y[:, 1])[max_index]
print("When Velocity reaches the maximum value, the value of S is: " +
str(s_for_max_v) + ' µM')
```