Loh Hui Wen (C2303110)

Question 2.1

From

$$\mathrm{E} + \mathrm{S} \underset{k_2}{\overset{k_1}{\rightleftharpoons}} \mathrm{ES}$$

Forward reaction gives:

$$\frac{d[\mathrm{E}]}{dt} = -k_1[\mathrm{E}][\mathrm{S}]$$

$$\frac{d[\mathrm{S}]}{dt} = -k_1[\mathrm{E}][\mathrm{S}]$$

$$\frac{d[\mathrm{ES}]}{dt} = k_1[\mathrm{E}][\mathrm{S}]$$

Reverse reaction gives:

$$\frac{d[\mathrm{E}]}{dt} = k_2[\mathrm{ES}]$$

$$\frac{d[\mathrm{S}]}{dt} = k_2[\mathrm{ES}]$$

$$\frac{d[\mathrm{ES}]}{dt} = -k_2[\mathrm{ES}]$$

From

$$\mathrm{ES} \xrightarrow{k_3} \mathrm{E} + \mathrm{P}$$

$$\frac{d[\mathrm{ES}]}{dt} = -k_3[\mathrm{ES}]$$

$$\frac{d[\mathrm{E}]}{dt} = k_3[\mathrm{ES}]$$

$$\frac{d[\mathrm{P}]}{dt} = k_3[\mathrm{ES}]$$

Final rate of change of E :

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

Final rate of change of S :

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

Final rate of change of ES :

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

Final rate of change of P :

$$\frac{d[\mathrm{P}]}{dt} = k_3[\mathrm{ES}]$$

Question 2.2

Let [E] = x1, [S] = x2, and [ES] = x3

$$[\mathrm{E}][\mathrm{S}] = x_1$$

$$[\mathrm{S}] = x_2$$

$$[\mathrm{ES}] = x_3$$

Then,

$$\frac{d[\mathrm{E}]}{dt} = -k_1 x_1 x_2 + (k_2 + k_3)\mathrm{x}_3$$

$$\frac{d[\mathrm{S}]}{dt} = -k_1 x_1 x_2 + k_2\mathrm{x}_3$$

$$\frac{d[\mathrm{ES}]}{dt} = k_1 x_1 x_2 - (k_2 + k_3)\mathrm{x}_3$$

$$\frac{d[\mathrm{P}]}{dt} = k_3 x_3$$

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
```

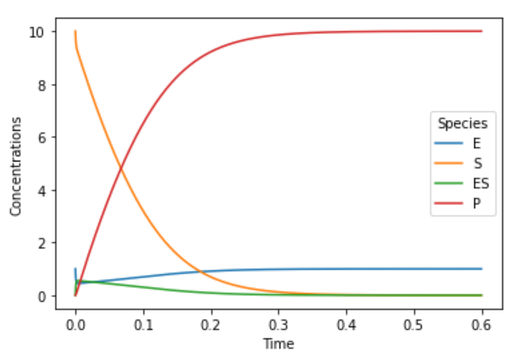
In [2]:
```
# Enzyme kinetic model

def kmodel(x, params):
    K1 = params['K1']
    K2 = params['K2']
    K3 = params['K3']

    xdot = np.array([-K1*x[0]*x[1]+K2*x[2]+K3*x[2],
                     -K1*x[0]*x[1]+K2*x[2],
                     K1*x[0]*x[1]-K2*x[2]-K3*x[2],
                     K3*x[2]])
    return xdot
```

In [3]:
```
# RK4 function

def rk4(f,x0,t0,tf,dt):
    t = np.arange(t0,tf,dt)
    nt = t.size
    nx = x0.size
    x = np.zeros((nx,nt))
    x[:,0] = x0

    for k in range(nt-1):
        k1 = dt * f(t[k], x[:,k])
        k2 = dt * f((t[k]+dt/2), (x[:,k]+k1/2))
        k3 = dt * f((t[k]+dt/2), (x[:,k]+k2/2))
        k4 = dt * f((t[k]+dt), (x[:,k]+k3))
        dx = (k1+2*k2+2*k3+k4)/6
        x[:,k+1] = x[:,k] + dx

    return x, t
```

In [4]:
```
# Define problem

params = {'K1':100, 'K2':600, 'K3':150}

f = lambda t, x : kmodel(x, params)

x0 = np.array([1, 10, 0 , 0])

t0 = 0
tf = 0.6  # (1/100*60s) cause E is limiting reactant
dt = 1.66667e-5 # minutes to milliseconds

x, t = rk4(f,x0,t0,tf,dt)
```

In [5]:
```
plt.plot(t, x[0,:], label = "E")
plt.plot(t, x[1,:], label = "S")
plt.plot(t, x[2,:], label = "ES")
plt.plot(t, x[3,:], label = "P")
plt.legend(title = "Species")
plt.xlabel('Time')
plt.ylabel('Concentrations')
```

Out[5]:
```
Text(0, 0.5, 'Concentrations')
```



Question 2.3

$$v = \frac{d[\mathrm{P}]}{dt}$$

$$k_m = \frac{k_2 + k_3}{k_1}$$

v also equal to

$$v = \frac{V_{max}[\mathrm{S}]}{k_m + [\mathrm{S}]}$$

therefore

$$\frac{d[\mathrm{P}]}{dt} = \frac{V_{max}[\mathrm{S}]}{k_m + [\mathrm{S}]}$$

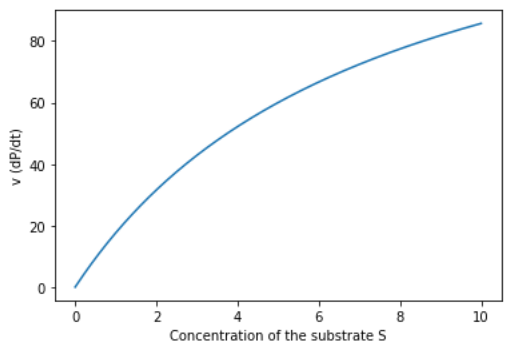
And

$$V_{max} = k_3[\mathrm{E_{total}}]$$

In [6]:

```
K1 = 100
K2 = 600
K3 = 150
km = (K2+K3)/K1
vmax = K3*1
v = vmax*x[1,:]/(x[1,:]+km)
plt.plot(x[1,:], v)
plt.xlabel('Concentration of the substrate S')
plt.ylabel('v (dP/dt)')

print('Vm = {:.3f} uM/min'.format(max(v)))
```

```
Vm = 85.714 uM/min
```



$$V_m = 85.714\mu M/min$$

References

https://www.anotherscienceblog.com/post/the-michaelis-menten-enzyme-kinetics-model (https://www.anotherscienceblog.com/post/the-michaelis-menten-enzyme-kinetics-model)

https://slideplayer.com/slide/17157260/ (https://slideplayer.com/slide/17157260/)

https://www.youtube.com/watch?v=1FYrnwqWQNY (https://www.youtube.com/watch?v=1FYrnwqWQNY)

https://www.mathworks.com/help/simbio/ug/defining-reaction-rates-with-enzyme-kinetics.html (https://www.mathworks.com/help/simbio/ug/defining-reaction-rates-with-enzyme-kinetics.html)