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A
LAB REPORT
ON

Simulation of Chemical Reaction (Continuous System)

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SUBMITTED TO:

SIMULATION AND MODELLING

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OBJECTIVE:

1. To develop the mathematical modeling of the continuous system.
2. To determine the state of the system i.e. the value of reactants and product at different points of time.

THEORY

Chemical reactions exhibit dynamic equilibrium, which means that a combination reaction is also accomplished by the reverse process of a decomposition reaction. At the steady-state, the rates of the forward and the backward reaction are the same. Let's take an example where the two chemicals react together to produce a third chemical.

$$Ch1 + Ch2 = Ch3$$

The rate of reaction depends on a large number of factors such as:

1. The amount of *Ch1* and *Ch2* are mixed.
2. The temperature
3. The pressure
4. The humidity
5. Catalyst used

Let us consider,

Amount of *Ch1 = C1*
Amount of *Ch2 = C2*
Amount of Ch3 = C3

Then,
The rate of increase of *C1, C2, and C3* can be expressed as,

$$-\frac{dC1}{dt} \propto C1.C2 \qquad \text{(Composition)}$$

$$\frac{dC3}{dt} \propto C3 \qquad \text{(Decomposition)}$$

$$\frac{dC1}{dt} = K2.C3 - K1.C1.C2$$
$$\frac{dC2}{dt} = K2.C3 - K1.C1.C2$$
$$\frac{dC3}{dt} = K1.C1.C2 - K2.C3$$

Where $K1,\ K2$ are constants of the chemical reaction.

To keep the problem simple, we assume temperature, pressure, humidity etc maintained constant and have no effect on the rate of formation and decomposition of chemicals.

When the chemicals $Ch1$ and $Ch2$ are mixed, the reaction starts and the amount of $Ch1,\ Ch2,\ and\ Ch3$ in the mixture goes on changing as time development. The simulation of reaction will determine the state of the system. i.e. value of $C1,\ C2,\ and\ C3$ at different points of time. If $C1(t),\ C2(t),\ and\ C3(t)$ are the quantities to there chemicals at time t, then at time $t + \Delta t$, the quantities are given as:

$$C1(t+\Delta t) = C1(t) + \frac{dC1}{dt}$$
$$C2(t+\Delta t) = C2(t) + \frac{dC2}{dt}$$
$$C3(t+\Delta t) = C3(t) + \frac{dC3}{dt}$$

Taking $C1(0),\ C2(0),\ and\ C3(0)$ as quantities of at time zero.

$$C1(\Delta t) = C1(0) + \frac{dC1}{dt}$$
$$= C1(0) + [K2.C3(0) - K1.C1(0).C2(0)]\,\Delta t$$
$$C2(\Delta t) = C2(0) + \frac{dC2}{dt}$$
$$= C3(0) + [K2.C3(0) - K1.C1(0).C2(0)]\,\Delta t$$
$$C3(\Delta t) = C3(0) + \frac{dC3}{dt}$$
$$= C3(0) + [K1.C1(0).C2(0) - K2.C3(0)]\,\Delta t$$

SOURCE CODE FOR SIMULATION

Now I’ve used python programming language with framework numpy, scipy, and matplotlib libraries to simulate the above chemical reaction to determine the concentration of both reactants and products at different points of time.

```
# import of libraries
import numpy as np
from scipy.integrate import odeint
import matplotlib.pyplot as plt
% matplotlib inline
```

```
# function that returns the rate of change of conc (dC/dt)
def model(c0, t, k):
   k1, k2 = k[0], k[1]
   c1, c2, c3 = c0[0], c0[1], c0[2]

   dc1dt = k2 * c3 - k1 * c1 * c2
   dc2dt = k2 * c3 - k1 * c1 * c2
   dc3dt = k1 *  c1 * c2 - k2 *  c3
   return [dc1dt, dc2dt, dc3dt]
```

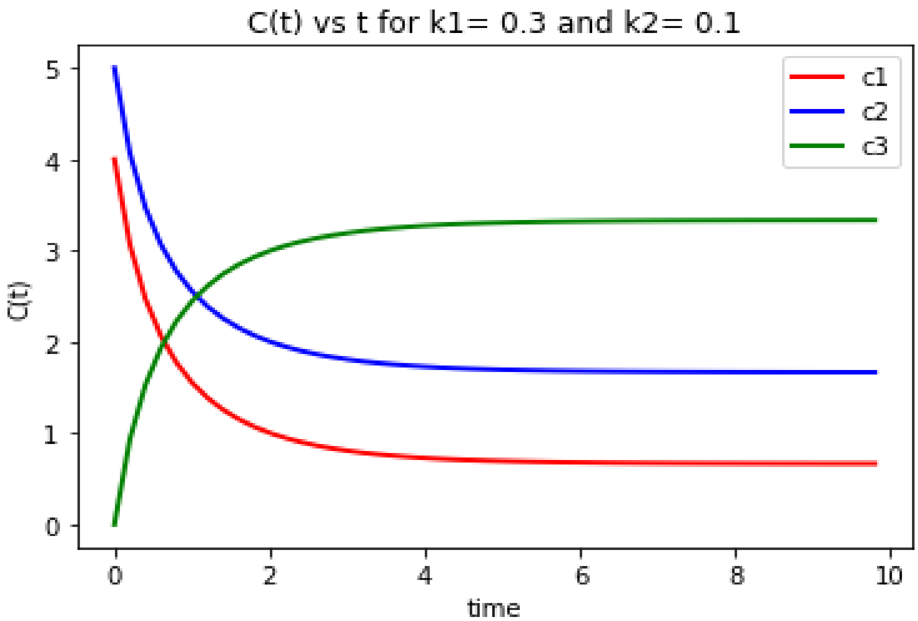
```python
# Initial Conditions
c10 = 4
c20 = 5
c30 = 0
c0 = [c10, c20, c30]

# Reaction Constants
k1 = 0.3
k2 = 0.1
k = [k1, k2]

# Time Points
t = np.arange(0, 10, 0.2)
# solve ODEs
c = odeint(model, c0, t, args=(k, ))
c1, c2, c3 = np.hsplit(c, 3)
```

```python
# plot results
plt.plot(t, c1, 'r-',linewidth=2,label='c1')
plt.plot(t,c2,'b-',linewidth=2,label='c2')
plt.plot(t,c3,'g-',linewidth=2,label='c3')
plt.title(f'C(t) vs t for k1= {k1} and k2= {k2}')
plt.xlabel('time')
plt.ylabel('C(t)')
plt.legend()
plt.show()
```

```
plt.savefig('sim.png')
```

RESULT AND VISUALIZATION

After running the script, the following curve was obtained which shows the time along the x-axis and the concentration of $C1,\ C2,\ and\ C3$ along the y-axis.



DISCUSSION AND CONCLUSION

From this lab session, we became familiar with the concept of a continuous system. We explored the topic with an example of a chemical reaction. We also learned to develop the mathematical model of the chemical reaction and expressed the rate of change of concentration of reactants and products using differential equations. We wrote a script in python programming language to simulate the model of the chemical reaction. We used python's numpy library as a data structure to store an array of values, scipy to solve the ordinary differential equation using *odeint* function, and matplotlib to visualize the graph showing the variation of concentration of reactants and products over a period of time.