Lab - 1

Simulation of the chemical reaction (continuous system)

Objectives:

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

Theory:

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

$Ch_1+Ch_2 = Ch_3$

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

In addition to the forward reaction where Ch_1 and Ch_2 react ton produce Ch_3, there may also be backward reaction, where by, Ch_3 decomposes back into Ch_1 and Ch_2. Let the rate of formation of Ch_3 be proportional to the product of the amounts Ch_1 and Ch_2 present in the mixture and let the rate of decomposition of Ch_3 be proportional to its amount in the mixture.

Let us consider C1, C2 and C_3 Amount of Ch_1, Ch_2 and Ch_3 at any instant of time t, the rate of increase of C_1, C_2 & C_3 are given by the following differential equations:

$$dC_1/dt = K_2C_3 – K_1C_1C_2$$

$$dC_2/dt = K_2C_3 – K_1C_1C_2$$

$$dC_3/dt = 2K_1C_1C_2 - 2k_2C_3$$

Where K_1 and K_2 are constants.

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

As soon as the chemicals Ch_1 and Ch_2 are mixed, the reaction starts and the amount of C_1, C_2, C_3 in the mixture goes on changing as time progresses. The simulation of reaction will determine the state of the system. i.e. value of quantities C_1, C_2 and C_3 at different points in time. Starting at zero time, a very small increment of time is taken in each step. It is assumed to be so small, that all changes in the mixture can be taken to occur at the end of each increment. If C_1 (t), C_2 (t) and C_3 (t) are the quantities to there chemicals at time t, then at time $t + \Delta t$, the quantities are ;

$C_1(t + \Delta t) = C_1(t) + dC_1(t)/dt$

$C_2(t + \Delta t) = C_2(t) + dC_2(t)/dt$

$C_3(t + \Delta t) = C_3(t) + dC_3(t)/dt$

Taking $C_1(0)$, $C_2(0)$ and $C_3(0)$ as quantities of Ch_1, Ch_2 and Ch_3 at time zero, that is when the reaction starts the state of the system at time Δt will be.

$C_1(\Delta t) = C_1(0) + dC_1(t)/dt$

$= C_1(0) + [K_2C_3(0) - K_1C_1(0).C_2(0)]\,\Delta t$ ---------(1)

$C_2(\Delta t) = C_2(0) + [K_2C_3(0) - K_1C_1(0).C_2(0)]\,\Delta t$ ---------(2)

$C_3(\Delta t) = C_3(0) + [2K_1C_1(0).C_2(0) - 2K_2C_3(0)]\,\Delta t$ ---------(3)

Using the state of the system at time $2\Delta t$, the state of the system at time $3\Delta t$ and so on will be computed. This will continue till the specified time of reaction T is reached. At each increment of time , we can either count the number of steps taken or checked the attained time with the prescribed simulation run time.