Lab Sheet - 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

Let us consider,

Amount of $Ch_1 = C_1$

Amount of $Ch_2 = C_2$

Amount of $Ch_3 = C_3$

The rate of increase of C_1, C_2 & C_3 can be expressed as

$-dC_1/dt \propto C_1C_2$ Composition

$dC_3/dt \propto C_3$ Decomposition

$dC_1/dt = K_2C_3 - K_1C_1C_2$

$dC_2/dt = K2C_3 - K_1C_1C_2$

Where K_1, K_2 are constant.

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 Ch_1 and Ch_2 are mixed, the reaction starts and the amount of Ch_1, Ch_2, Ch_3 in the mixture goes on changing as time development. The simulation of reaction will determine the state of the system. i.e. value of C_1, C_2 and C_3 at different point of time. 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 given as

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

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

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

Taking $C_1(0)$, $C_2(0)$ and $C_3(0)$ as quantities of Ch_1, Ch_2 and Ch_3 at time zero.

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

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

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

$C_3(\Delta t) = C_3(0) + [2K_1C_1(0) – 2K_2\ C_3(0)]\ \Delta t$ ---------(3)

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