Chapter-2 Mole Balances and Kinetic Study in Different Reactors

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Kinetic Study and Analysis of Rate Models

1. The rate equation for a reaction with detail knowledge of all kinetic parameters is required for reactor design.

2. To analyze the rate equations, the kinetic data are to be generated in a suitable laboratory reactors. It depends on the type of reactions.

3. Various types of ideal reactor are required which will be discussed in this section.

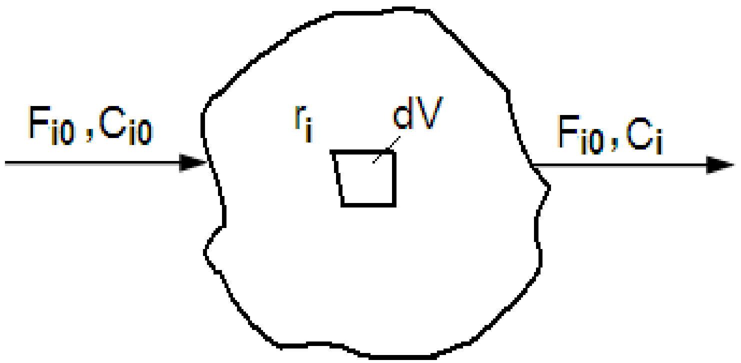
General Mole Balance

Mole balance by considering an infinitesimal volume, *dV*

[Rate of inflow] – [Rate of output] + [Rate of generation by reaction] = [Rate of accumulation within the volume]

- $F_{i0} - F_i + \int_0^V r_i \, dV = \frac{dN_i}{dt}$

- Where F_{i0} and F_i are the inflow and outflow rates in mol/L
- At steady state the rate of accumulation of i is $\frac{dN_i}{dt} = 0$



Kinetic Study in Different Reactors

Three ideal reactors are used to get the kinetic information

1. Batch reactor
2. Continuous stirred tank reactor (CSTR)
3. Plug-flow reactor (PFR).

These are used as laboratory reactors to study the reaction for developing kinetic equation.

This experimentation is called the kinetic study.

Kinetic Analysis

- For example, if the rate equation for a reaction $A \rightarrow B$ is represented by the equation.

$$-r_A = \frac{k_1 C_A}{1 + k_2 C_A}$$

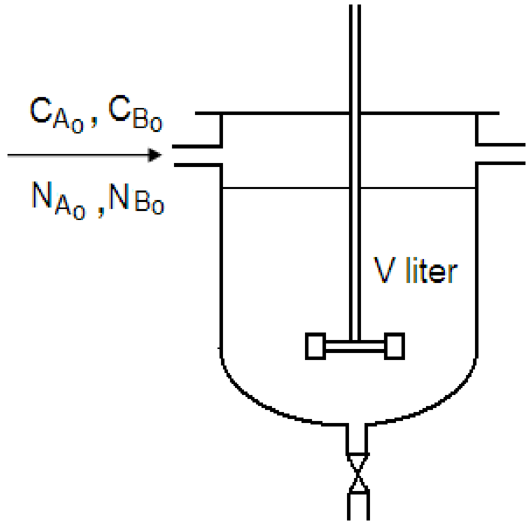
- The estimation of the parameters k_1 and k_2 of the above equation is known as kinetic analysis.
- The rate data of $-r_A$ versus C_A is required.
- An empirical rate equation is also used $-r_A = -\frac{dC_A}{dt} = kC_A^p$
- In this case, k and p are the rate parameters.

Mole Balance in Batch Reactor

Consider the equation aA + bB → mM

$$A + \frac{b}{a}B \rightarrow \frac{m}{a}M$$

- The initial number of moles of A and B are N_{Ao} and N_{Bo} respectively. The number of moles of A after reaction at time t is N_A . The conversion of A is then given by



- $X_A = \frac{N_{Ao} - N_A}{N_{Ao}} = \frac{\text{moles of A reacted}}{\text{moles of A supplied}}$

Schematic view of batch reactor

Batch Reactor

As there is no inflow and outflow in a batch reactor, the mole balance for A is

$$\int_0^V r_i \, dV = \frac{dN_i}{dt}$$

Rate of generation of A = Rate of accumulation of A

$$\int_0^V r_A dV = \frac{dN_A}{dt} = -N_{Ao} \frac{dX_A}{dt}$$

We have, $N_A = N_{Ao}(1 - X_A)$

Batch Reactor

$$-r_A V = N_{Ao} \frac{dX_A}{dt} \qquad (5)$$

or,

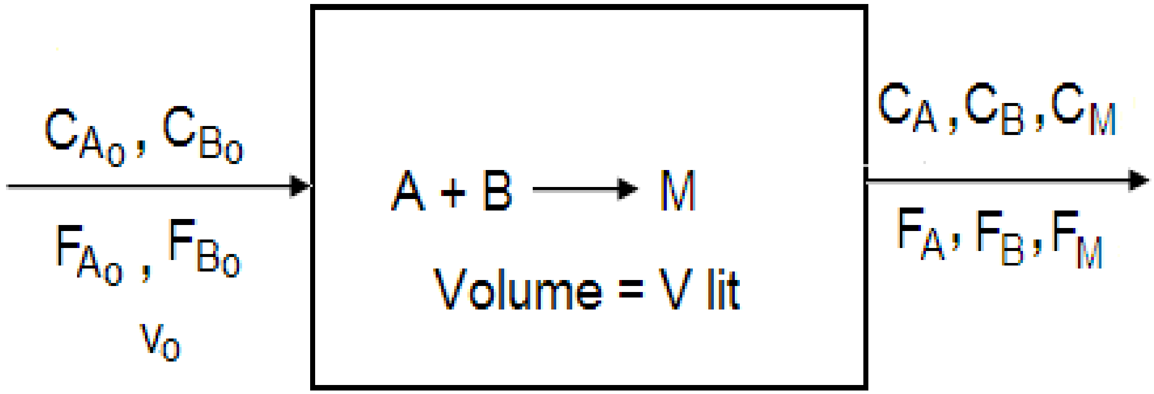
$$\frac{N_{Ao}}{V} \frac{dX_A}{dt} = -r_A \qquad (6)$$

For constant reactor volume (V= constant) we may write,

$$C_{Ao} \frac{dX_A}{dt} = -r_A \qquad (7)$$

Mole balance in Continuous Stirred Tank Reactor(CSTR)

- The mole balance in a CSTR by considering flow reactor is shown in the following figure



Mole balance in a CSTR

Continuous Stirred Tank Reactor(CSTR)

Mole Balance of A in a CSTR of volume V

Rate of input of A – Rate of output of A+ Rate of generation of A by reaction = Rate of accumulation of A in the volume

$$v_o C_{Ao} - v_o C_A + r_A V = \frac{d}{dt}(C_A V) \qquad (8)$$

The accumulation term is zero.

$$v_o(C_{Ao} - C_A) = -r_A V \qquad (9)$$

$$\tau_m = \frac{V}{v_0} = \frac{C_{Ao} - C_A}{-r_A} \qquad (10)$$

Continuous Stirred Tank Reactor(CSTR)

- $F_{Ao} = v_0 C_{Ao}$ $F_A = vC_A$ and $v_0 = v$ if there is no volume change by the reaction.

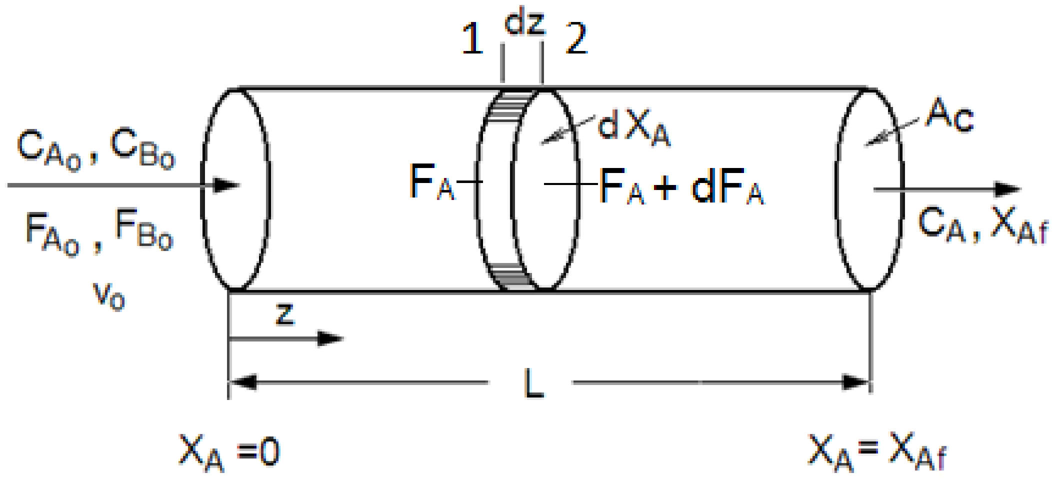
- $-r_A = \frac{F_{Ao} - F_A}{V} = \frac{F_{Ao} X_A}{\mathrm{V}}$ $\quad (11)$

- Equations (10) and (11) are called design equations for CSTR those are used for finding size of the reactor (V) for known reaction rate ($-r_A$).

Mole balance in plug flow reactor

The mole balance is performed over a differential section dz in a tubular reactor.

F_A and $F_A + dF_A$ are the molar flow rate of A at the location 1 and 2 of the section Δz respectively. Inlet feed rate of A is F_{Ao} mol/min.



Mole balance in a PFR

Plug flow reactor

Mole balance in PFR :

- Rate of input – Rate of output + Rate of reaction of A = Rate of accumulation.

$$F_A - (F_A + dF_A) + \int_0^L A_C r_A dz = 0 \qquad (12)$$

- By considering accumulation $= 0$ and $A_C dz = dV$

$$-dF_A + \int_0^{V_t} r_A dV = 0$$

$$-\frac{dF_A}{dV} = -r_A \qquad (13)$$

Substituting $F_A = F_{Ao}(1 - \mathrm{X_A})$ in Eqn.(13),

$$F_{Ao}\left(\frac{dX_A}{dV}\right) = -r_A \qquad (14)$$

Equation (14) is the design equation in differential form. In integral form it may be written as

$$\frac{V}{F_{Ao}} = \int_0^{X_f} \frac{dX_A}{-r_A} \qquad (15)$$

$$\tau_P = \frac{V}{v_0} = C_{Ao} \int_0^{X_f} \frac{dX_A}{-r_A} \qquad (16)$$