# 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.

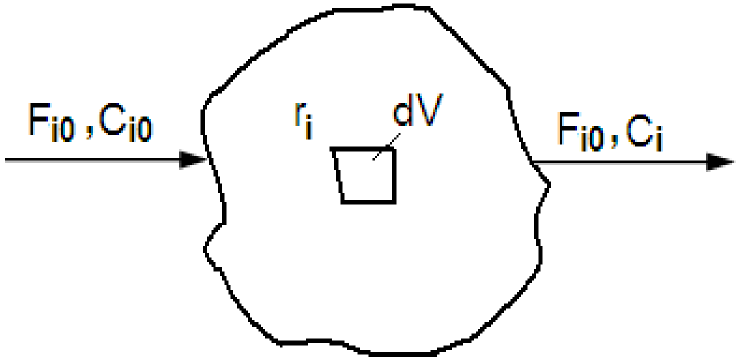
# General Mole Balance

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.

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

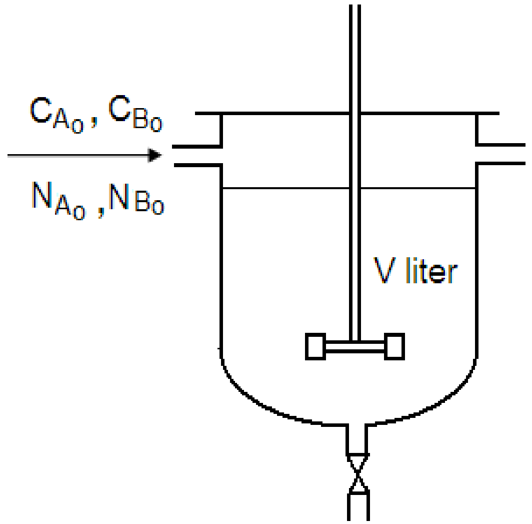
- The estimation of the parameters $k_1$ and $k_2$ of the above equation is known as kinetic analysis.
- The rate data of $-r_A$ versus $C_A$ is required.
- An empirical rate equation is also used $-r_A = -\frac{dC_A}{dt} = kC_A^p$
- In this case, k and p are the rate parameters.

# 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,

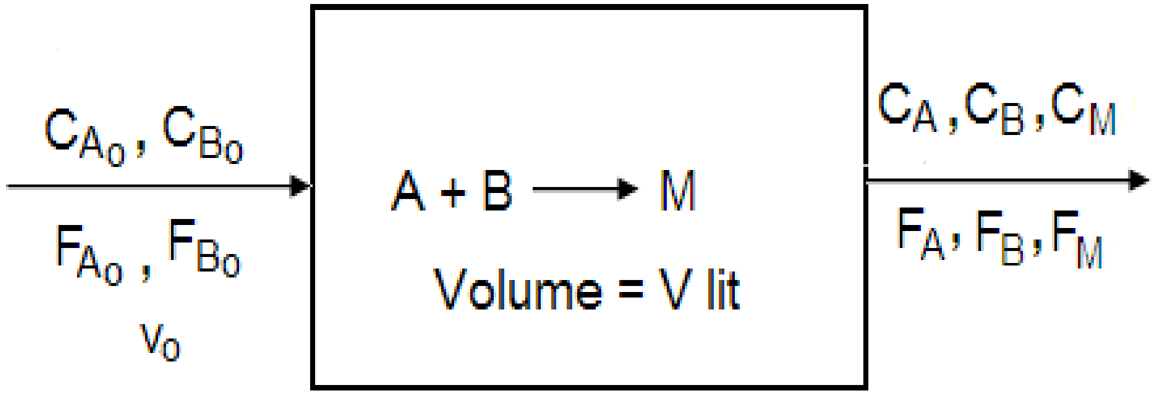
$$\frac{N_{Ao}}{V}\frac{dX_A}{dt} = -r_A \qquad (6)$$

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

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

The accumulation term is zero.

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

$$\tau_m = \frac{V}{v_0} = \frac{C_{Ao} - C_A}{-r_A} \tag{10}$$

# 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.

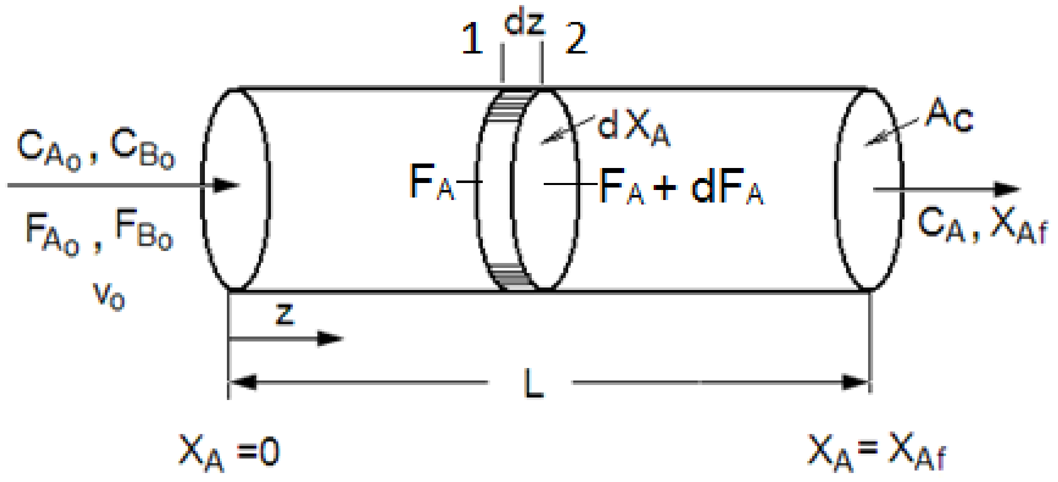
- $-r_A = \frac{F_{Ao} - F_A}{V} = \frac{F_{Ao} X_A}{\mathrm{V}}$ $\qquad (11)$

- 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 $\Delta z$ 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

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

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