

الجامعة التكنولوجية

قسم الهندسة الكيماوية

المرحلة الثالثة

تصميم مفاعل

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# REACTOR DESIGN

3h. Lect. +  
1h. Tut.

## 1 - Mole Balances: Introduction to Chem. Eng. Kinetics

- \* Definition of the Rate of Reaction
- \* Rate Laws and Stoichiometry (Basic Definitions: The Reaction Rate Constant, The Reaction Order, Elementary Reactions, Non-elementary Reactions, Reversible Reactions)
- \* The General Mole Balance Equation.
- \* Reactors:
  - Batch Reactor
  - Continuous-Flow Reactors (CSTR, PFR)
  - Semi-batch Reactor.
  - Industrial Reactor.

## 2 - Conversion and Reactor Sizing

- \* Definition of Conversion
- \* Design Equations (Batch Systems, Flow Systems)
- \* Applications of the Design Equations.
- \* Reactors in Series & in Parallel

## 3 - Stoichiometric Table

- \* Batch Systems.
- \* Constant Volume Reaction Systems.
- \* Flow System.
- \* Volume Change with Reaction.
- \* Reactions with Phase Change.

#### 4 - Reactor Design

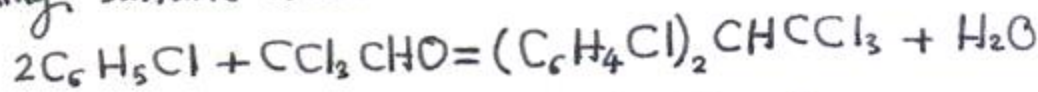
- \* Batch Reactor: Design Equation, Reaction Time, Volume of Reactor for Isothermal and Non-isothermal Operation.
- \* Plug Flow Reactor (PFR): Design Equation, Volume of Reactor, Number of Tubes, Pressure drop (All for Isothermal Operation)
- \* Continuous Stirred Tank Reactor (CSTR): Design Equation, Volume of Reactor, Reactors in series and in parallel
- \* Semi-batch Reactor: Design Equation, Conversion as function of Time

#### References:

1. Fogler, H.S., Elements of Chemical Reaction Engineering, Prentice Hall (2000).
2. Levenspiel, O., Chemical Reaction Engineering, Wiley & Sons (1999).
3. Smith, J.M., Chemical Engineering Kinetics, 3rd ed., McGraw Hill (1981).
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## \* Definition of the rate law, $(-r_A)$

The rate at which a given chemical reaction proceeds can be expressed in several ways. It can be expressed as the rate of disappearance of reactants or rate of formation of products. For example, the insecticide DDT (dichloro diphenyl trichloroethane) is produced from chlorobenzene and chloral in the presence of fuming sulfuric acid.



Letting A represents the chemical chloral, the numerical value of the rate of reaction  $(-r_A)$  is defined as the number of moles of chloral reacting (disappearing) per unit time per unit volume  $\text{mol/dm}^3 \cdot \text{s}$

In heterogeneous reaction systems, the rate of reaction  $(-r_A')$  is usually expressed in reaction surface area or catalyst weight. Thus for a gas-solid catalytic reaction,  $-r_A'$  is the number of moles of A reacted per unit time per unit mass of catalyst ( $\text{mol/s} \cdot \text{g catalyst}$ ).  $[-r_A = \rho_b (-r_A')]$  where  $\rho_b$ : bulk density of catalyst bed.

The mathematical definition of a chemical reaction rate. The reactants were mixed together at time  $t=0$  and the concentration of one of the reactants  $C_A$  was measured at various times  $t$ . The rate of reaction was determined from the slope of a plot of  $C_A$  as a function of time. Letting  $r_A$  be the rate of



formation of A per unit volume (e.g.,  $\text{gmol/s}\cdot\text{dm}^3$ )

$$r_A = \frac{dC_A}{dt} \quad (1-1)$$

This definition is for constant-volume batch reactor.

The chemical rate depends on temperature and concentration.

The reaction rate equation (i.e., the rate law) is essentially an algebraic equation involving concentration, not a differential equation. For example, the algebraic form of the rate law  $-r_A$  for the reaction



may be a linear function of concentration

$-r_A = KC_A$  or it may be some other algebraic

function of concentration, such as

$$-r_A = KC_A^2 \quad \text{or} \quad -r_A = K_1 C_A / (1 + K_2 C_A)$$

The concentration dependence of the rate law must be determined from experimental observations.

By convention,

$r_A$  = is the rate of formation of A  
 $-r_A$  = is the rate of disappearance of A

## - Rate law and Stoichiometry

### Basic Definitions

Homogeneous reaction: is one that involves only one phase.

Heterogeneous reaction: involves more than one phase and the reaction usually occurs at or very near the interface between phases.

Irreversible reaction: is that proceeds in only one direction and continues until the reactants are exhausted.

Reversible reaction can proceed in either directions, depending on the concentrations of reactants and products relative to the corresponding equilibrium concentrations.

Strictly speaking, no chemical reaction is completely irreversible, but in very many reactions the equilibrium point lies so far to the right that they are treated as irreversible reactions.

### The reaction rate constant

We take as the basis of calculation a species A, which is one of the reactants that is disappearing as a result of the reaction. The limiting reactant is usually chosen as our basis for calculation.

The rate law (rate of disappearance of A) gives the relationship between reaction rate and concentration

$$(-r_A) = [K(T)] [f(C_A, C_B, \dots)]$$

$K$  = reaction rate constant, it is merely independent of concentration, but it is strongly dependent on temperature. The unit of  $K$  depends on the order of reaction.

### Arrhenius equation

$$K(T) = A e^{-E/RT}$$

where  $A$  = frequency factor, it has the same units of  $K$ .

$E$  = activation energy, J/mol or cal/mol.

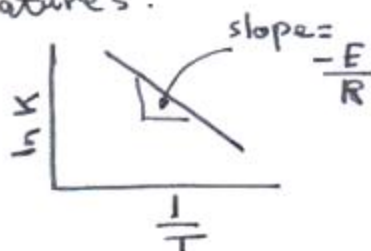
$R$  = gas constant =  $0.082 \frac{\text{atm. lit}}{\text{mol. K}} = 1.987 \frac{\text{cal}}{\text{mol. K}}$

$T$  = absolute temperature.

(E) is determined experimentally by carrying out the reaction at several different temperatures.

$$\ln K = \ln A - \frac{E}{R} \left( \frac{1}{T} \right)$$

$$\ln \frac{K_2}{K_1} = \frac{E}{R} \left( \frac{1}{T_1} - \frac{1}{T_2} \right)$$



The reaction order



(-r<sub>A</sub>) may be  $-r_A = K C_A^\alpha C_B^\beta$

$\alpha = a$  or  $\alpha \neq a$   
 $\beta = b$  or  $\beta \neq b$

The exponents of the concentrations lead to the concept of reaction order. The reaction is  $\alpha$  order with respect to reactant A, and  $\beta$  order with respect to reactant B.

The overall order of the reaction, (n), is

$$n = \alpha + \beta$$

For example, in the gas-phase reaction



the Kinetic rate law is  $-r_{NO} = K C_{NO}^2 C_{O_2}$

This reaction is 2nd order with respect to nitric oxide, 1st order with respect to ( $O_2$ ), and overall is a 3rd order reaction. In general 1st- and 2nd-order reactions are more commonly observed than zero- and 3rd order reactions.

The gas-phase synthesis of Phosgene:  $CO + Cl_2 \longrightarrow COCl_2$   
 in which the Kinetic rate law is  $-r_{CO} = K C_{CO} C_{Cl_2}^{3/2}$ . This reaction is 1st order with respect to ( $CO$ ), three-halves order with respect to ( $Cl_2$ ), and five-halves order as overall.

Sometimes reactions have complex rate expressions that cannot be separated into solely temperature-



dependent and concentration-dependent portions. In the decomposition of nitrous oxide over platinum.



the kinetic rate law is

$$-r_{\text{N}_2\text{O}} = \frac{K C_{\text{N}_2\text{O}}}{1 + K' C_{\text{O}_2}}$$

$K$  and  $K'$  are strongly temperature-dependent. We can only speak of reaction order under certain limiting conditions. For example, at very low concentrations of oxygen, the 2nd term in the denominator would be negligible and the reaction would be "apparent" 1st order with respect to nitrous oxide and 1st order overall. However, if the concentration of  $\text{O}_2$  were large enough so that the number 1 in the denominator were insignificant in comparison with the 2nd term,  $K' C_{\text{O}_2}$ , the apparent reaction order would be -1 with respect to  $\text{O}_2$  and (1) with respect to nitrous oxide.

The units of  $K$  vary with the order of the reaction.

Consider a reaction involving only one reactant as  $\text{A} \longrightarrow \text{products}$ . For this type of reaction, the units of the rate constant are:

Zero order	$-r_A = K$	$\{K\} = \text{mol}/\text{dm}^3 \cdot \text{s}$
1st order	$-r_A = K C_A$	$\{K\} = \text{s}^{-1}$
2nd order	$-r_A = K C_A^2$	$\{K\} = \text{dm}^3/\text{mol} \cdot \text{s}$
3rd order	$-r_A = K C_A^3$	$\{K\} = (\text{dm}^3/\text{mol})^2 \cdot \text{s}^{-1}$



## Elementary Reactions

An elementary reaction is one which the reaction order of each species is identical with the stoichiometric coefficient of the species, for the reaction



## Non-elementary Reactions

The reaction order is not identical with the stoichiometric coefficients.



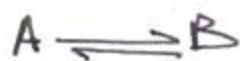
$$+r_{\text{HBr}} = \frac{k_1 C_{\text{H}_2} C_{\text{Br}_2}}{k_2 + C_{\text{HBr}}/C_{\text{Br}_2}}$$

## Reversible Reactions



$$r_{\text{B}} = -r_{\text{B forward}} + r_{\text{B reverse}} = k_1 \left( C_{\text{B}}^2 - \frac{C_{\text{D}} C_{\text{H}_2}}{K_{\text{c}}} \right) \quad , K_{\text{c}} = \frac{k_1}{k_2}$$

where  $K_{\text{c}}$  = concentration equilibrium constant.



$$-r_{\text{A}} = k_{\text{A}} \left( C_{\text{A}} - \frac{C_{\text{B}}}{K_{\text{c}}} \right)$$

$$K_{\text{e}} = f(T)$$

$$K_{\text{e}}(T) = K_{\text{e}}(T_1) \exp \left[ \frac{\Delta H_{\text{R}}^{\circ}}{R} \left( \frac{1}{T_1} - \frac{1}{T} \right) \right] \quad , \text{ for } \Delta C_{\text{p}} = 0$$

$a\text{A} + b\text{B} \longrightarrow c\text{C} + d\text{D}$ , the relationship between the rate of any components with each other.

$$\frac{(-r_{\text{A}})}{a} = \frac{(-r_{\text{B}})}{b} = \frac{(+r_{\text{C}})}{c} = \frac{(+r_{\text{D}})}{d}$$

Conversion (X): fraction of reactant transformed or converted.

For a reactant A: 
$$X_A = \frac{\text{no. of moles of A reacted}}{\text{initial no. of moles of A}}$$
$$= \frac{N_{A0} - N_A}{N_{A0}} = 1 - \frac{N_A}{N_{A0}}$$

Selectivity: In a complex reaction, stable products are produced by more than one reaction.



The overall selectivity of B is the ratio of the yields of B and C

$$S_B = \frac{X_B}{X_C}$$

Yield: For a reactor, the yield is defined as:

$$\text{Yield} = \frac{\text{moles of product produced} \times \text{stoichiometric factor}}{\text{moles of reactant converted}}$$

Excess reactant: The percentage excess reactant is defined by the following equation:

$$\% \text{ excess} = \frac{\text{quantity supplied} - \text{stoichiometric}}{\text{Stoichiometric quantity}} \times 100$$

# Introduction to Reactor Design

## The General Mole Balance Equation

A mole balance on species  $j$  at any instant in time,  $t$ , yield the following equation:

$$\left[ \begin{array}{l} \text{rate of flow} \\ \text{of } j \text{ into the} \\ \text{system} \\ \text{(moles/time)} \end{array} \right] + \left[ \begin{array}{l} \text{rate of generation} \\ \text{of } j \text{ by chemical} \\ \text{reaction within} \\ \text{the system} \\ \text{(moles/time)} \end{array} \right] - \left[ \begin{array}{l} \text{rate of flow} \\ \text{of } j \text{ out of} \\ \text{the system} \\ \text{(moles/time)} \end{array} \right] = \left[ \begin{array}{l} \text{rate of} \\ \text{accumulation} \\ \text{of } j \text{ within} \\ \text{the system} \\ \text{(moles/time)} \end{array} \right]$$
$$F_{j0} + G_j - F_j = \frac{dN_j}{dt} \dots (1-2)$$

where  $N_j$  = the number of moles of species  $j$  in the system at time  $t$ .

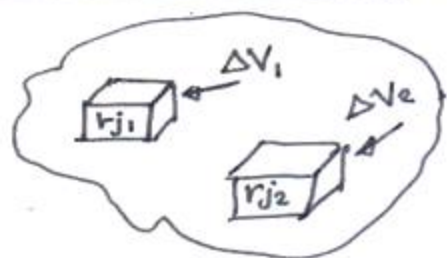
If all the system variables (e.g., temperature, catalytic activity, \* concentration of the chemical species) are uniform [only for Batch & CSTR] throughout the system volume, the rate of generation of species  $j$ ,  $G_j$ , is just the product of the reaction volume,  $V$ , and the rate of formation of species  $j$ ,  $r_j$ .



Fig. 1-1

$$G_j = \sum_i r_{ji} \Delta V_i = r_j \cdot V$$

$$\frac{\text{moles}}{\text{time}} = \frac{\text{moles}}{\text{time} \cdot \text{Volume}} \cdot \text{Volume}$$



\* [only for PFR] Suppose now that the rate of formation of species  $j$  for the reaction varies with the position in the system volume.

That is it has a value  $r_{j1}$  at location 1, which is surrounded by a small volume,  $\Delta V_1$ , within which the rate is uniform. Similarly the rate of generation,  $\Delta G_1 = r_{j1} \Delta V_1$ , similar for  $\Delta G_2$ .



The total rate of generation within the system volume is the sum of the rates of generation in each of the subvolumes.

If the total system is divided into  $M$  subvolumes, the total rate of generation is  $G_j = \sum_{i=1}^M \Delta G_{ji} = \sum_{i=1}^M r_{ji} \Delta V_i$

By taking the appropriate limits (i.e., let  $M \rightarrow \infty$  and  $\Delta V \rightarrow 0$ ) and making use of the definition of integral, we can rewrite the foregoing equation in the form:

$$G_j = \int_V r_j dV$$

From this equation we see that  $r_j$  will be an indirect function of position (volume), since the properties of the reacting materials (e.g., concentration, temperature) can have different values at different locations in the reactor.

We now replace  $G_j$  in Equation (1-2)

$$F_{j0} - F_j + G_j = \frac{dN_j}{dt} \quad (1-2)$$

by its integral form to yield the general mole balance equation for any chemical species  $j$  that is entering, leaving, reacting and/or accumulating within any system volume  $V$ .

$$F_{j0} - F_j + \int_V r_j dV = \frac{dN_j}{dt} \quad (1-3)$$

Equation (1-3) is a basic equation for chem. reaction eng. From this equation we can develop the design for the various types of industrial reactor (Batch, semibatch and continuous flow). We can determine the time (batch) or reactor volume (continuous-flow)

## Batch Reactors

A batch reactor has neither inflow nor outflow of reactants or products while the reaction is being carried out;  $F_{j0} - F_j = 0$



The general mole balance reduces to:

$$\frac{dN_j}{dt} = \int_0^V r_j dV \quad \dots (1.4)$$

If the reaction mixture is perfect mixed so that there is no variation in the rate of reaction throughout the reactor volume, we can take  $r_j$  out of the integral and write the material balance as:

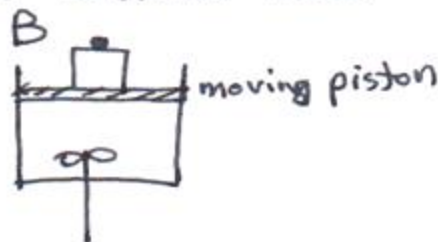
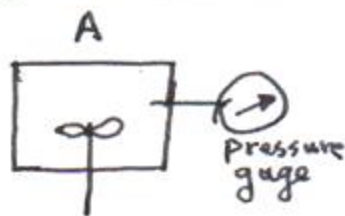
$$\frac{dN_j}{dt} = r_j V \quad \dots (1.5)$$

A is a reactant  
j is a species

Fig. 1-3 shows two different types of batch reactors used for gas-phase reaction. Reactor A is a constant volume (variable-pressure) reactor and reactor B is a constant-pressure (variable-volume) reactor.

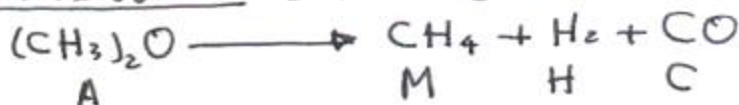
Before the design can be carried out, it is necessary to perform and analyze a batch reactor experiments to determine the reaction rate constant.

Fig(1-3)



### Example 1-2

Write the mole balance for the gas-phase decomposition of dimethylether (A) to methane (M), hydrogen (H) and carbon monoxide (C) in terms of the reactor volume, concentration and rate of formation of dimethylether for both a constant-pressure and a constant-volume batch reactor.



Solution :

For both batch reactors, the mole balance on A is

$$\frac{1}{V} \frac{dN_A}{dt} = r_A$$

For a batch reactor, the only assumption made is no spatial variation in  $r_A$ .

Constant-volume batch reactor: The reactor is perfectly mixed so the concentration of the reacting species is spatially uniform.

Because  $(V)$  is constant, we take it inside the differential and write MB in terms of the concentration of A :

$$\frac{1}{V} \frac{dN_A}{dt} = \frac{d(N_A/V)}{dt} = \frac{dC_A}{dt} = r_A \quad (\text{E1-2-1})$$

Constant-pressure batch reactor: To write the MB in terms of concentration;

$$\begin{aligned} N_A &= C_A V ; \quad \frac{1}{V} \frac{dN_A}{dt} = \left( \frac{1}{V} \right) d \left( \frac{C_A V}{dt} \right) \\ &= \frac{dC_A}{dt} + \frac{C_A}{V} \frac{dV}{dt} = r_A \quad (\text{E1-2-2}) \end{aligned}$$



$$r_A = \frac{dC_A}{dt} + C_A \frac{d(\ln V)}{dt} \quad (E1-2.3)$$

The difference between equations (E1-2.1) and (E1-2.2) is apparent.

## Continuous-Flow Reactors

### Continuous-stirred Tank Reactor (CSTR)

CSTR is normally run at steady state and operated so as to be quite well mixed. As a result of the latter quality, the CSTR is generally modeled as having no spatial variations in concentration, temperature or reaction rate throughout the vessel. Since the temperature and concentration are identical everywhere in tank, they are the same at the exit point as they are elsewhere in the tank. Thus the temperature and concentration in the exit stream are the same as those inside the reactor.

When the general MB eqn. ( ) is applied to a CSTR operated at steady state (i.e., conditions do not change with time)

$$\frac{dN_j}{dt} = 0$$

in which there are no spatial variations in the rate of reaction, i.e.,

$$\int_V r_j dV = V r_j$$

The design equation for a CSTR

$$\boxed{V = \frac{F_{A0} - F_A}{-r_A}} \quad ; \quad \boxed{V = \frac{F_{j0} - F_j}{-r_j}} \quad \text{---(1-6)}$$

The molar flow rate  $F_j = C_j V$

$C_j$ : concentration of species  $j$

$V$ : volumetric flow rate.

$$\boxed{V = \frac{V_0 (C_{A0} - C_A)}{-r_A}}$$

### Tubular Reactor

Another type of reactor commonly used in industry is the tubular reactor. It consists of a cylindrical pipe and is normally operated at (steady state) as is the CSTR.

The flow is highly turbulent and the flow field may be modeled by that of plug flow. That is, there is no radial variation in concentration and the reactor is referred to as Plug-flow reactor (PFR).

In the tubular reactor, the reactants are continually consumed as they flow down the length of the reactor.

The concentration and the reaction rate vary axially (flow direction).

Start with the general MB equation (1-3) ;

$$F_{j0} - F_j + \int r_j dV = \frac{dN_j}{dt}$$

We shall divide (conceptually) the reactor into a number of subvolumes so that within each subvolume  $\Delta V$ , the

reaction rate may be spatially uniform

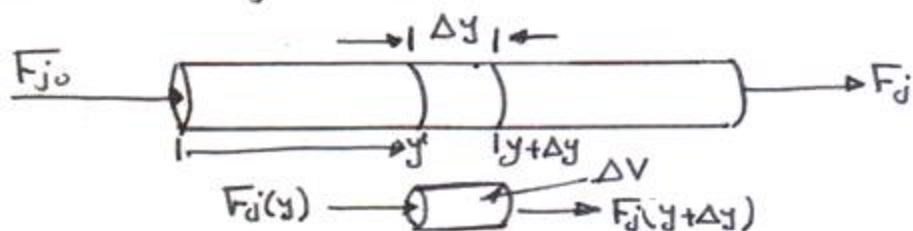


Fig. (1-4) Tubular reactor

The subvolume is located at distance  $y$  from the entrance,  $F_{j1}(y)$  represents the molar flow rate of species  $j$  into volume  $\Delta V$  at  $y$ , and  $F_{j1}(y+\Delta y)$  = the molar flow rate of species  $j$  out of the volume at the location  $(y+\Delta y)$ . In spatially uniform subvolume  $\Delta V$

$$\int_{\Delta V} r_j \Delta V = r_j \Delta V \quad \text{--- (1-7)}$$

For a tubular reactor operated at steady state  $\frac{dN_j}{dt} = 0$ ; Equation (1-3) becomes:

$$F_{j1}(y) - F_{j1}(y+\Delta y) + r_j \Delta V = 0 \quad \text{--- (1-8)}$$

In this expression  $r_j$  is an indirect function of  $y$ . That is,  $r_j$  is a function of reactant concentration, which is a function of the position  $y$  down the reactor.

$$\Delta V = A \Delta y$$

$A$  = cross sectional area

Substitute in Eqn. (1-8) for  $\Delta V$  and then divided by  $\Delta y$ :

$$-\left[ \frac{F_{j1}(y+\Delta y) - F_{j1}(y)}{\Delta y} \right] = -A r_j$$

The term in bracket resembles the definition of the derivation;



$$\lim_{\Delta x \rightarrow 0} \left[ \frac{f(x+\Delta x) - f(x)}{\Delta x} \right] = \frac{df}{dx}$$

Taking the limit as  $\Delta y$  approaches zero,

$$-\frac{dF_j}{dy} = -Ar_j$$

Or dividing by  $(-1)$ , we have  $\frac{dF_j}{dy} = Ar_j \dots (1-9)$

It is most convenient to have  $V$  (reactor volume) rather than  $(y)$  reactor length.

$dV = A dy$ . The design equation for a tubular reactor,

$$\frac{dF_j}{dV} = r_j \dots (1-10)$$

For a reactor in which  $(A)$  varies along the length of the reactor, the design equation remains unchanged

$$\boxed{\frac{dF_A}{dV} = r_A}, \quad \boxed{\frac{dF_j}{dV} = r_j} \dots (1-10)$$

The extent of reaction achieved in a PFR does depend on its shape, only on its total volume.

### Example 1-3

The first-order reaction  $A \rightarrow B$  is carried out in a tubular reactor in which the volumetric flow rate is constant. Derive an equation relating the reactor volume to the entering and exiting concentration of  $A$ , the rate constant  $K$ , and the volumetric flow rate  $V$ . Determine the reactor volume necessary to reduce the exiting concentration to 10% of the entering concentration when the volumetric flow rate is  $10 \text{ dm}^3/\text{min}$

(i.e., liters/min) and the specific reaction rate constant,  $K$ , is  $0.23 \text{ min}^{-1}$ .

### Solution

For a tubular reactor, the MB on species A ( $j=A$ ) was shown to be

$$\frac{dF_A}{dV} = r_A \quad \dots (1-10)$$

The rate law for a 1st order reaction:

$$-r_A = K C_A \quad \dots (E1-3.1)$$

Since  $v_0$  is constant,

$$\frac{dF_A}{dV} = \frac{d(C_A v_0)}{dV} = v_0 \frac{dC_A}{dV} = r_A \quad \dots (E1-3.2)$$

Substituting for  $r_A$  in Eqn. (E1-3.1) yields:

$$-v_0 \frac{dC_A}{dV} = -r_A = K C_A$$

Rearranging gives:

$$\frac{-v_0}{K} \left( \frac{dC_A}{C_A} \right) = dV$$

Using the conditions at entrance of the reactor,

$$V=0 \quad \text{then} \quad C_A = C_{A0}$$

$$-\frac{v_0}{K} \int_{C_{A0}}^{C_A} \frac{dC_A}{C_A} = \int_0^V dV \quad \dots (E1-3.4)$$

This equation gives,

$$V = \frac{v_0}{K} \ln \frac{C_{A0}}{C_A} \quad \dots (E1-3.5)$$

Substituting  $C_{A0}$ ,  $C_A$ ,  $v_0$  and  $K$  in Eqn. (E1-3.5), we have:

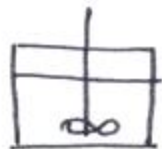
$$V = \frac{10 \text{ dm}^3/\text{min}}{0.23 \text{ min}^{-1}} \ln \frac{C_{A0}}{0.1 C_{A0}} = \frac{10 \text{ dm}^3}{0.23} \ln 10 = 100 \text{ dm}^3$$

We see that a reactor volume of  $0.1 \text{ m}^3$  is necessary to convert 90% of species A entering.

# Industrial Reactors

\* Advantages and disadvantages :

## ① Batch Reactor



- (a) Used for small scale production.
- (b) Used for the manufacture of expensive products.
- (c) Used for process that are difficult to convert to continuous operation.
- (d) Used for obtaining high conversions by increasing residence time of reaction.
- (e) It has high labor cost per unit product.

## ② Continuous-Stirred Tank Reactor (CSTR)

- (a) Used for large scale production.
- (b) Lower conversion per reactor volume than that of batch reactor.
- (c) To increase conversion, the number of reactor in series are increased.
- (d) Mostly used for liquid-phase reaction.

## ③ Tubular Reactor (PFR)



- (a) Easy to maintain (i.e., no moving parts).
- (b) Higher conversion than that of CSTR which has the same volume and operating conditions.
- (c) Mostly used for gas-phase reaction.
- (d) Difficult to control the temperature within the reactor.

Examples Packed-bed (fixed-bed), Trickle-bed, slurry reactor, fluidized bed reactor.



## 2. Reactor Sizing

### 2.1 Design Equations

#### 2.1.1 Batch Systems

In most batch reactors, the longer a reactant is in the reactor, the more reactant is converted to product until either equilibrium is reached or the reactant is exhausted.

Consequently, in batch systems the conversion  $X$  is a function of time the reactants spend in the reactor. If  $N_{A0}$  = the number of moles of A initially,  $X$  = the total number of moles of A that have reacted after time  $t$ .

$$\left[ \begin{array}{c} \text{moles of A} \\ \text{consumed} \end{array} \right] = \left[ \begin{array}{c} \text{moles of A} \\ \text{fed} \end{array} \right] \cdot \left[ \frac{\text{moles of A reacted}}{\text{moles of A fed}} \right]$$

$$\left[ \begin{array}{c} \text{moles of A} \\ \text{reacted} \end{array} \right] = [N_{A0}] \cdot X \quad \text{--- (2.1)}$$

Now,  $N_A$  = the number of moles of A that remain in the reactor after a time  $t$ .

$$\left[ \begin{array}{c} \text{moles of A} \\ \text{in reactor} \\ \text{at time } t \end{array} \right] = \left[ \begin{array}{c} \text{moles of A} \\ \text{in initially fed} \\ \text{to reactor at} \\ t=0 \end{array} \right] - \left[ \begin{array}{c} \text{moles of A that} \\ \text{have been cons-} \\ \text{umed by chemical} \\ \text{reaction} \end{array} \right]$$

$$[N_A] = [N_{A0}] - [N_{A0} X] \quad \text{--- (2.2)}$$

$$\text{--- (2.3)}$$

$$N_A = N_{A0} - N_{A0} X = N_{A0} (1 - X)$$

Mole balance equation for reactant A for a batch system,

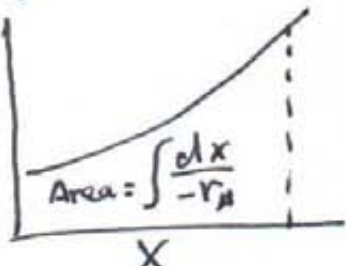
$$\frac{dN_A}{dt} = r_A V \quad \dots \dots (2.4)$$

reactant A is disappearing, we multiply both sides of Equation (2.4) by (-1) to obtain MB for the batch reactor,  $-\frac{dN_A}{dt} = (-r_A)V \dots (2.5)$  from eqn. (2.3)

$$\begin{aligned} \frac{dN_A}{dt} &= 0 - N_{A0} \frac{dx}{dt} \\ \therefore -N_{A0} \frac{dx}{dt} &= r_A V \end{aligned}$$

For a batch reactor the design equation in differential form is :

$$\begin{aligned} N_{A0} \frac{dx}{dt} &= -r_A V \\ t &= N_{A0} \int_0^x \frac{dx}{-r_A V} \quad \dots (2.6) \quad , V = \text{constant} \end{aligned}$$

$$t = \frac{N_{A0}}{V} \int_0^x \frac{dx}{-r_A} = C_{A0} \int_0^x \frac{dx}{-r_A} \quad \dots (2.7) \quad \frac{1}{-r_A}$$


Shut down time ( $t_s$ )

: Time excluding reaction time,

$t_s = \text{Charging time} + \text{Cleaning time} + \text{Discharging time}$

Ex- Typical Cycle Times for a batch Polymerization Process

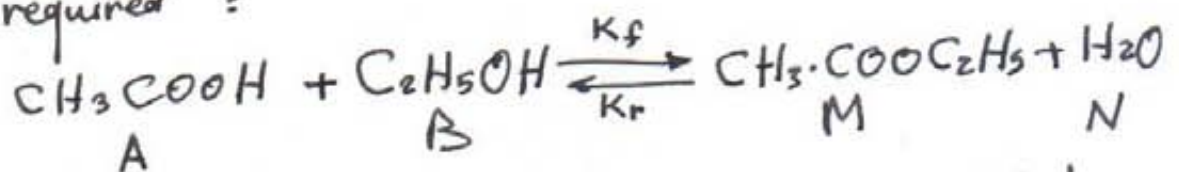
Activity	Time(h)
1. Charge feed to reactor and agitate	1.5 - 3.0
2. Heat to reaction temp.	1.0 - 2.0
3. Carry out reaction	varies
4. Empty and clean reactor	0.5 - 1.0
Total time excluding reaction time	3.0 - 6.0

$$t_{\text{total}} = t_s + t_r \text{ (calculated from Design Eqn.)}$$

Example : Production of Ethyl Acetate in a Batch Reactor

Ethyl acetate is to be manufactured by esterification of acetic acid with ethanol in an isothermal batch reactor.

A production rate of 10 tonne/day of ethyl acetate is required :



The reactor will be charged with a mixture containing 500 kg/m<sup>3</sup> ethanol and 250 kg/m<sup>3</sup> acetic acid, the remainder being water, and a small quantity of hydrochloric acid to act as a catalyst. The density of this mixture is 1045 kg/m<sup>3</sup>, which will be assumed constant