CHEMICAL REACTION ENGINEERING (SKF3223)

Chapter 1: Mole Balances

WAN NORHARYATI WAN SALLEH
hayati@petroleum.utm.my
RAFIZIANA MD. KASMANI
rafiziana@petroleum.utm.my

Rate of Reaction

- The reaction rate is the rate at which a species looses its chemical identity per unit volume.

- **RATE = SPEED**

- The **RATE** of a reaction is the **SPEED** at which a reaction happens.

- If a reaction has a low rate that means the molecules combine at a slower speed than a reaction with a high rate.

Rate of Reaction

- The rate of a reaction can be expressed as the rate of disappearance of a reactant or as the rate of appearance of a product.

- Consider species A:

$$A \longrightarrow B$$

  - r_A = the rate of formation of species A per unit volume
  - $-r_A$ = the rate of a disappearance of species A per unit volume
  - r_B = the rate of formation of species B per unit volume

- r_A tells us how fast a number of moles of one chemical species are being consumed to form another chemical species.

Example:

$$A \longrightarrow B$$

If B is being created at 0.6 moles per decimeter cubed per second, therefore:

The rate of formation of B is : r_B = 0.6 mole/dm^3/s

The rate of a disappearance of species A is :

$-r_A$ = 0.6 mole/dm^3/s

The rate of formation of A is : r_A = -0.6 mole/dm^3/s

Remember.... r_B

- r_B is the rate of formation of species B per unit volume [e.g. mol/dm^{3}s]
- r_B is a function of concentration, temperature, pressure, and the type of catalyst (if any)
- r_B is independent of the type of reaction system (batch, plug flow, etc.)
- r_B is an algebraic equation, not a differential equation

$$A \longrightarrow B$$

Reaction rate

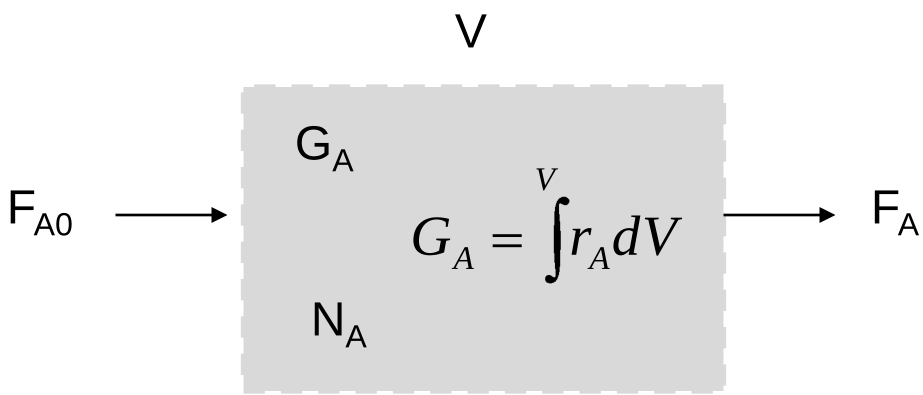
- Reaction rate, *r* is a function of concentration, for example:

$$-r_A = kC_A \text{ (First order reaction)}$$

$$-r_A = kC_A^2 \text{ (Second order reaction)}$$

$$k = \text{specific reaction rate (time}^{-}\text{)}$$

General Mole Balance Equation (GMBE)



F_{A0}= Entering molar flow rate of A (mol/time)
F_A= Exiting molar flow rate of A (mol/time)
G_A= Rate of generation(formation) of A (mol/time)
V = Volume (m^3)
r_A= rate of generation(formation) of A (mole/time.vol)
N_A= number of moles of A inside the system Volume V (mols)

General Mole Balance Equation

[In] + [Generation] - [Out] = [Accumulation]

$$F_{in} + G - F_{out} = \frac{dN}{dt}$$

moles/time moles/time moles/time moles/time

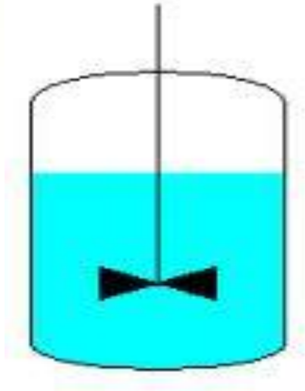
$$F_{in} + \int r.dV - F_{out} = \frac{dN}{dt}$$

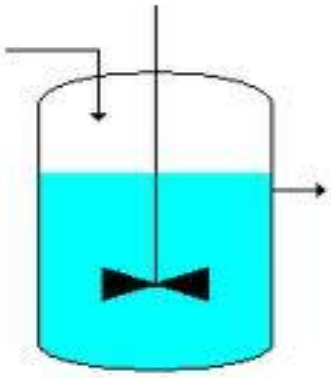
$$\text{moles/time} \quad \frac{\text{moles}}{\text{time.volume}}.\text{volume} \quad \text{moles/time} \quad \text{moles/time}$$

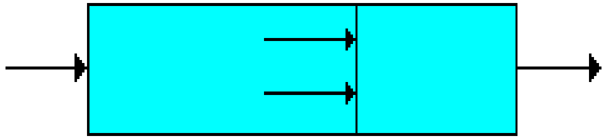
- Develop the design equation for the various types of industrial reactors (batch, semibatch, and continuous-flow)

Types of Reactors

Continuos Flow



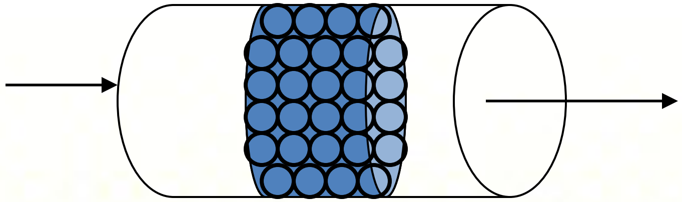




Batch

CSTR

Tubular/Plug Flow



Packed Bed

BATCH REACTOR

No inflow or outflow

$$r = \frac{dN}{dt} \cdot \frac{1}{V}$$

Assumption

- F in =F out = 0
- V is constant (well-mixed)

- Small scale operation
- For testing new processes
- To manufacture expensive product
- ADV: high conversion
- DISADV: high labor cost
- Not reproducible

Batch reactor derivation

Well-mixed
$$\int r_A dV = r_A V$$

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

Differential form

Rearranging and integrating with limits

$t = 0$ $N_A = N_{A0}$

$t = t_1$ $N_A = N_{A1}$

$$t_1 = \int_{N_{A0}}^{N_{A1}} \frac{dN_A}{r_A V}$$

The time necessary to reduce the number of moles from N_{A0} to N_{A1} and also to from N_{B1} mole of B

-- graph of reaction (N_A , t)

Multiplying by -1 and changing the limits of integration

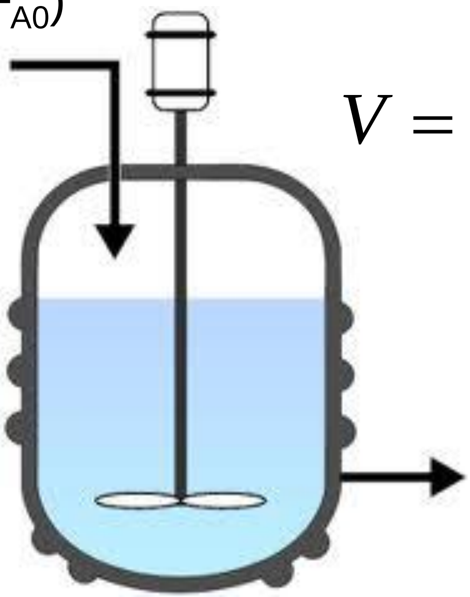
$$t_1 = \int_{N_{A1}}^{N_{A0}} \frac{dN_A}{-r_A V}$$

Integral form

CONTINUOUS- STIRRED TANK REACTOR (CSTR)

Assumption

- ❑ Well mixed – constant concentration, temperature , reaction rate
- ❑ No accumulation



$$V = \frac{F_{out} - F_{in}}{r}$$

- ❑ Commonly used in industry
- ❑ Liquid-phase reaction
- ❑ Advantage: when intense agitation is required
- ❑ Disadvantage: larger reactor are necessary to obtain high conversion

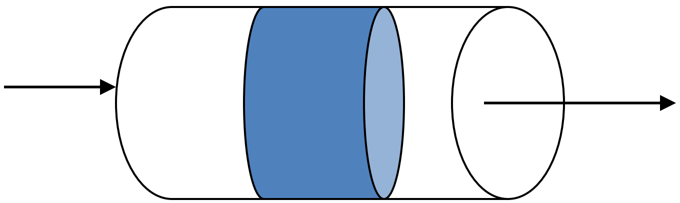
The volume of the reactor

$$V = \frac{F_{A0} - F_A}{-rA}$$

Algebraic form

TUBULAR REACTOR OR PLUG-FLOW REACTOR (PFR)

Assumption: Operated at steady state



- Consists of a cylindrical pipe
- Gas-phase reaction
- Advantages: easy to maintain, provides the highest conversion
- Disadvantage: difficult to maintain the temperature within the reactor

The volume necessary to reduce the entering molar flow rate of A from F_{A0} to F_{A1} or the volume necessary to produce a molar flow rate of B of F_{B1} – graph of reaction (F_{A0} , V)

$$r = \frac{F_{out} - F_{in}}{dV}$$

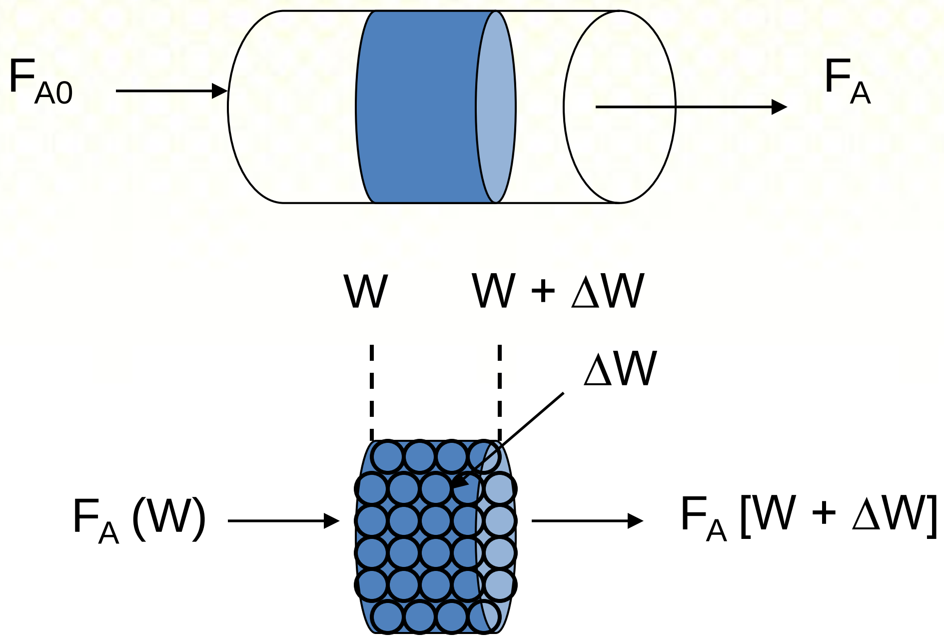
$$\boxed{r_A = \frac{dF_A}{dV}}$$

Differential form

$$\boxed{V_1 = \int_{F_{A1}}^{F_{A0}} \frac{dF_A}{-r_A}}$$

Integral form

PACKED-BED REACTOR (PBR)



- The reaction rate is based on mass of solid catalyst, W
- Fluid-solid heterogeneous reaction
- Essentially tubular reactor that is packed with solid catalyst particles

Differential form

$$\frac{dF_A}{dW} = r'_A$$

Integral form

$$W_1 = \int_{F_{A1}}^{F_{A0}} \frac{dF_A}{-r'_A}$$

Catalyst weight necessary to reduce the entering molar flow rate of A, F_{A0} to F_{A1}
– graph of reaction (F_A , W)

	Differential form	Algebraic form	Integral form
BATCH	$\frac{dN_A}{dt} = r_A V$		$t_1 = \int_{N_{A1}}^{N_{A0}} \frac{dN_A}{-r_A V}$
CSTR		$V = \frac{F_{A0} - F_A}{-rA}$	
PFR	$r_A = \frac{dF_A}{dV}$		$V_1 = \int_{F_{A1}}^{F_{A0}} \frac{dF_A}{-r_A}$
PBR	$\frac{dF_A}{dW} = r'_A$		$W_1 = \int_{F_{A1}}^{F_{A0}} \frac{dF_A}{-r'_A}$

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