B.Tech. Chemical Engineering

Fifth Semester

Sub: Chemical Reaction Engineering

Course No. ChBC-52 **Credit 5**

By

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Books Suggested:

- Levenspiel, O., “Chemical Reaction Engineering”. John Wiley & Sons, New York (1995).
- Fogler, H.S., “Elements of Chemical Reaction Engineering”. Prentice-Hall of India Pvt. Ltd. (1995).
- Smith, J.M. “Chemical Engineering Kinetics”. McGraw-Hill Book Company, New York (1981).

Syllabus

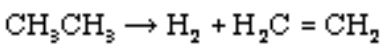
- **Objective:** To provide the comprehensive knowledge of safe reactor design.

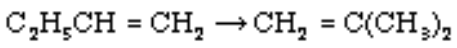
Ideal Reactors: Design equations for ideal reactors, namely batch, CSTR, plug Flow

Design for Single Reaction: Design equation for single reaction systems using batch- and semi batch- reactors, CSTR, PFR and recycle reactor, auto catalytic reactions, reactor choice for single reaction. **Design for Multiple Reactions:** Parallel and series reactions, quantitative treatment of product distribution and of reactor size for different types of ideal reactors, selectivity and yield factors, reactor choice for multiple reactions. **Non-isothermal Operation and Stability of Reactors:** Non-isothermal design of ideal reactors, hot spot in tubular reactor, auto-thermal process, steady state multiplicity optimal temperature progression for first order reversible reaction. **Non-ideal Flow:** Residence time distribution **(**RTD) theory, role of RTD in determining reactor behavior, age distribution (E) of fluid, experimental methods for finding E, relationship between E and F curve, models for non ideal flow – single parameter and multi parameter models (axial dispersion, tanks in series), performance estimation of reactor using reactor models. **Solid and Catalytic Reactions:** Solid reactions-shrinking core model, catalytic reactionshomogeneous and heterogeneous**,** steps in solid catalysed reaction, rate limiting steps, effect of external resistance, effect of diffusion on reaction, Thiele modulus and effectiveness factor, performance equations for catalytic reactors (packed bed, fluidized bed), product distribution in multiple reactions, basic equations for trickle bed and moving bed reactors.

Chemical Identity

- A chemical species is said to have reacted when it has lost its chemical identity.
- The identity of a chemical species is determined by the *kind*, *number*, and *configuration* of that species' atoms.

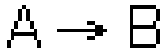
1. Decomposition 

2. Isomerization 

Reaction Rate

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

- 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.

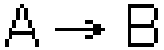
Consider species A: 

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

Reaction Rate

- EXAMPLE: 

  If B is being formed at 0.2 moles per decimeter cubed per second, ie,

  $r_B = 0.2$ mole/dm^3/s

  Then A is disappearing at the same rate:

  $-r_A = 0.2$ mole/dm^3/s

  The rate of formation (generation of A) is

  $r_A = -0.2$ mole/dm^3/s

Reaction Rate

- For a catalytic reaction, we refer to $-r_A'$, which is the rate of disappearance of species A on a per mass of catalyst basis.

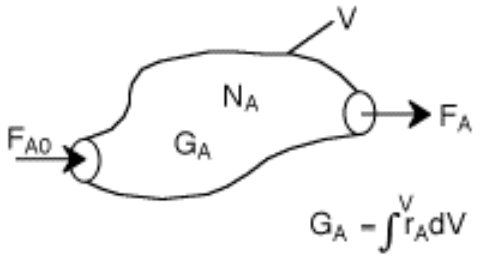
NOTE: dC_A/dt is not the rate of reaction

Reaction Rate

Consider species j:

- r_j is the rate of formation of species j per unit volume [e.g. mol/dm^3*s]
- r_j is a function of concentration, temperature, pressure, and the type of catalyst (if any)
- r_j is independent of the type of reaction system (batch, plug flow, etc.)
- r_j is an algebraic equation, not a differential equation
- We use an algebraic equation to relate the rate of reaction, $-r_A$, to the concentration of reacting species and to the temperature at which the reaction occurs [e.g. $-r_A = k(T)C_A^2$].

General Mole Balance

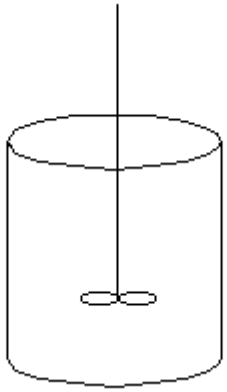


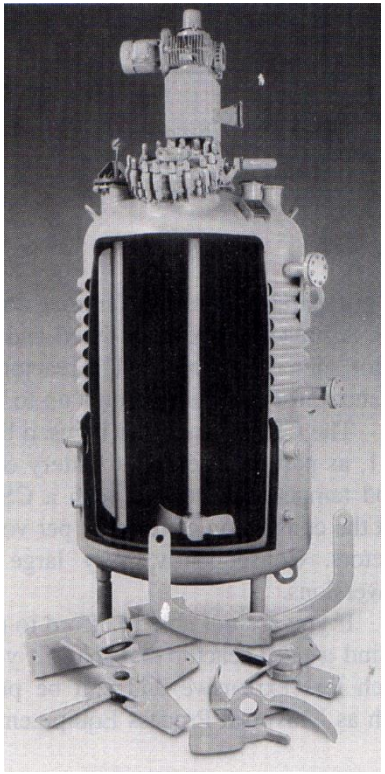
General Mole Balance on System Volume V

In − Out + Generation = Accumulation

$$F_{A0} - F_A + \int r_A dV = \frac{dN_A}{dt}$$

Batch Reactor Mole Balance





Batch

$$F_{A0} - F_A + \int r_A \, dV = \frac{dN_A}{dt}$$

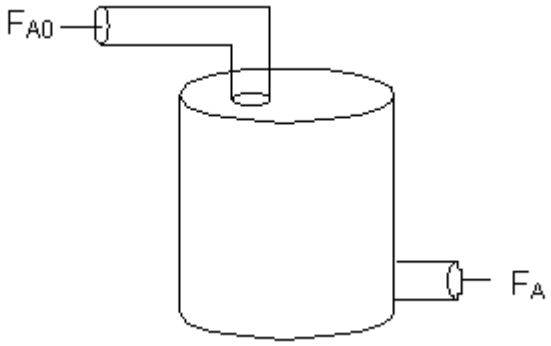
$$F_{A0} = F_A = 0$$

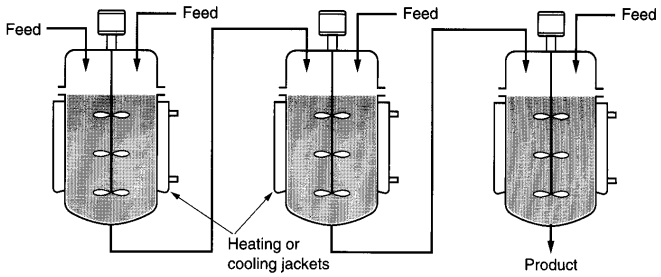
Well mixed

$$\int r_A \, dV = r_A V$$

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

Constantly Stirred Tank Reactor
Mole Balance





CSTR $$F_{A0} - F_A + \int r_A \, dV = \frac{dN_A}{dt}$$

Steady State $$\frac{dN_A}{dt} = 0$$

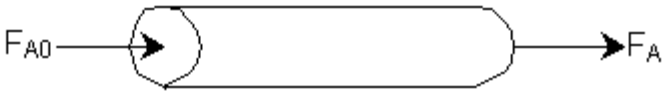
Well mixed $$\int r_A dV = r_A V$$

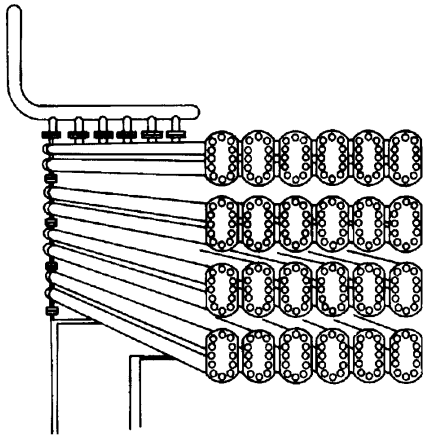
$$F_{A0} - F_A + r_A V = 0$$

$$\boxed{V = \frac{F_{A0} - F_A}{-r_A}}$$

Plug Flow Reactor Mole Balance

PFR:





$$F_{A0} - F_A + \int r_A \, dV = \frac{dN_A}{dt}$$

Steady State $\quad \frac{dN_A}{dt} = 0$

$$F_{A0} - F_A + \int r_A \, dV = 0$$

Differentiate with respect to V

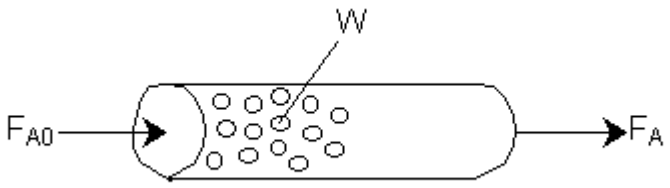
$$0 - \frac{dF_A}{dV} = -r_A$$

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

This is the volume necessary to reduce the entering molar flow rate (mol/s) from F_{A0} to the exit molar flow rate of F_A.

Packed Bed Reactor Mole Balance

PBR



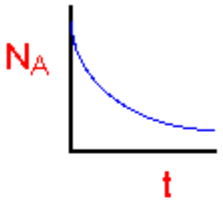
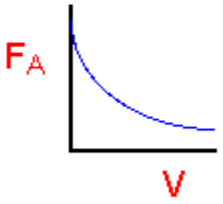
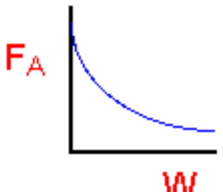
Steady State $$\frac{dN_A}{dt} = 0$$

$$F_{A0} - F_A + \int r'_A \, dW = 0$$

Differentiate with respect to W and rearrange

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

Reactor Mole Balance Summary

Reactor	Differential	Algebraic	Integral	
Batch	$\frac{dN_A}{dt} = r_A V$		$t = \int_{N_{A0}}^{N_A} \frac{dN_A}{r_A V}$	
CSTR		$V = \frac{F_{A0} - F_A}{-r_A}$		
PFR	$\frac{dF_A}{dV} = r_A$		$V = \int_{F_{A0}}^{F_A} \frac{dF_A}{r_A}$	
PBR	$\frac{dF_A}{dW} = r'_A$		$W = \int_{F_{A0}}^{F_A} \frac{dF_A}{r'_A}$	

Thank You