



Lecture (12)

Isothermal Operation

Continuous – Stirred Tank Reactor CSTR

"Back-Mix or Mixed Flow Reactor"

- Operate under steady state
- Flow in is equal flow out
- Reactor composition equal exit stream composition.
- Constant rate of reaction throughout the reactor volume
- Composition $\neq f(\text{Position})$
- Composition $= f(\text{time})$
- Temperature $\neq f(\text{Position})$
- Temperature $\neq f(\text{time})$

ideal restrictions

General Mole Balance

Molar flow rate of A fed to the system - Molar flow rate of A leave the system + Disappearance = Accumulation

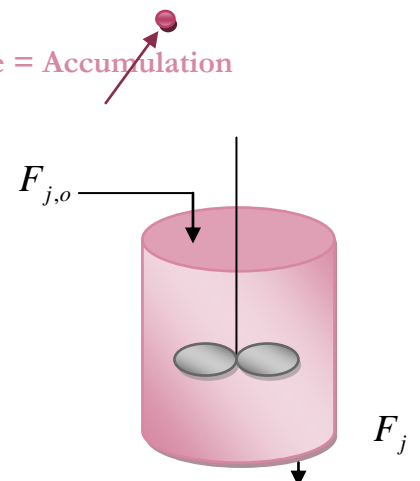
$$F_{j,o} - F_j + \int^V r_j dV = \frac{dN_j}{dt}$$

$$F_{j,o} = \text{Input Feed}$$

$$F_j = \text{Output Stream}$$

$$\frac{dN_j}{dt} = 0 \text{ No accumulation (St.St. Operation)}$$

$$F_{j,o} - F_j + \int^V r_j dV = 0$$



The CSTR is modeled as being well mixed such there are no spatial variations in the rate of reaction :-

$$\int^V r_j dV = V r_j$$

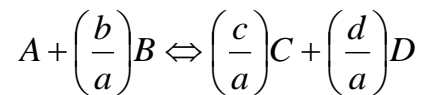


...Design Reactor Equation

for CSTR

- Consider the general reaction;

Stoichiometry set up of equations with A as basis



$$\left[\begin{array}{c} \text{Molar flow rate of species A} \\ \text{reacted or consumed} \\ (F_{Ao}X) \end{array} \right] = \left[\frac{\text{moles of A fed}}{\text{time}} \right] \bullet \left[\frac{\text{moles of A reacted}}{\text{moles of A fed}} \right]$$

$$\left[\begin{array}{c} \text{Molar flow rate of species A} \\ \text{leaves the system} \\ (F_A) \end{array} \right] = \left[\begin{array}{c} \text{Molar flow rate of species A} \\ \text{fed to the system} \\ (F_{Ao}) \end{array} \right] - \left[\begin{array}{c} \text{Molar flow rate of species A} \\ \text{consumed within the system} \\ (F_{Ao}X) \end{array} \right]$$

$$F_A = F_{Ao}[1 - X]$$

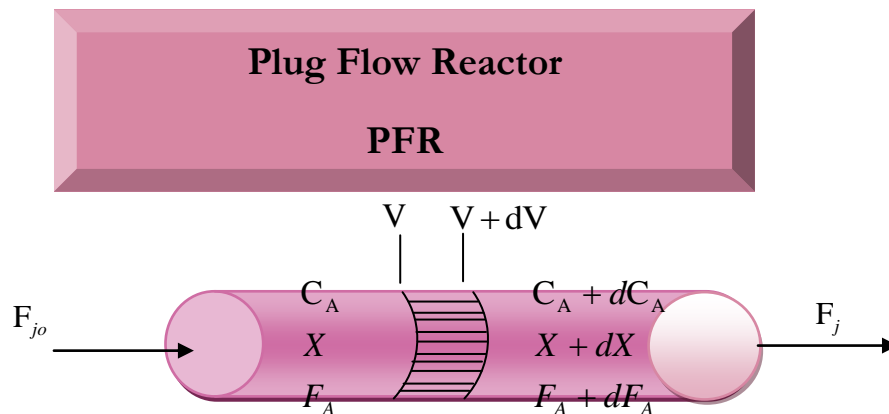
Where v_o entering volumetric flow rate

$$\frac{F_{Ao} - F_A}{-r_A} = V$$

$$V = \frac{F_{Ao}X}{(-r_A)_{exit}}$$

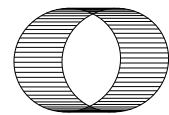
The composition from the reactor is identical to the composition inside the reactor, then the rate of reaction is evaluated at the exit conditions

$$V = \frac{C_{Ao} v_o - C_A v}{(-r_A)}$$



- Operate under steady state
- Flow in is equal flow out (constant mass)
- Conversion increases along the length of reactor
- Composition = $f(\text{Position, or direction of flow})$
- Composition $\neq f(\text{time})$ at a given position
- Composition $\neq f(\text{radial position})$
- Temperature = $f(\text{Position, or direction of flow})$
- Temperature $\neq f(\text{time})$ at a given position
- Temperature $\neq f(\text{radial position})$
- Degree of completion of a reaction depend on reactor volume

ideal restrictions



General Mole Balance

Molar flow rate of A - Molar flow rate of A + Disappearance = Accumulation
fed to the system leave the system

$$F_{jo} - (F_{jo} + dF_j) + \int_V r_j dV = \frac{dN_j}{dt} = 0$$

The balance is made over a finite reactor volume, dV , then

$$F_{jo} - (F_{jo} + dF_j) + r_j dV = 0$$

$$dF_j = r_j dV$$

$$dV = \frac{dF_j}{r_j}$$



Integrating with the limits at $V=0, F_A=F_{Ao}$at $V=V_1, F_A=F_{A1}$

$$V = \int_{F_{Ao}}^{F_{A1}} \frac{dF_j}{r_j}$$

$$V = \int_{F_{A1}}^{F_{Ao}} \frac{dF_j}{-r_j}$$

$$F_A = F_{Ao}[1 - X]$$

Reactor Design Equation

Of PFR

$$V = \int_{F_{Ao}}^{F_{A1}} \frac{dF_j}{r_j}$$

$$V = F_{Ao} \int_0^X \frac{dX}{-r_j}$$

$$V = \int_{F_{A1}}^{F_{Ao}} \frac{dF_j}{-r_j}$$

✚ **Constant Volume (Constant Density) $v = v_0$ ($\epsilon=0$)**

liquid-phase and some of gas phase reaction system fall into this category.

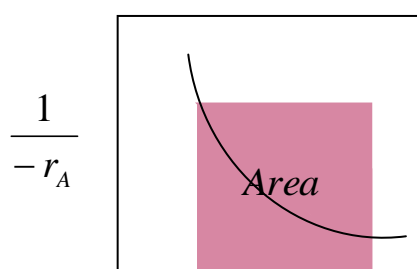
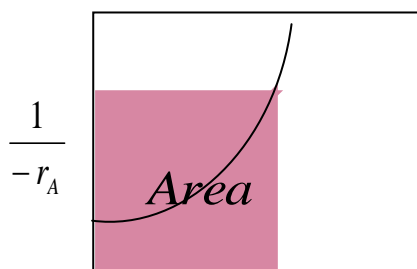
CSTR

$$V = \frac{F_{Ao} X}{(-r_A)}$$

$$V = \frac{C_{Ao} v_o X}{(-r_A)}$$

$$\tau = \frac{C_{Ao} X}{(-r_A)}$$

space time $\tau = \frac{V}{v_o}$





X

C_A

C_{Ao}

$$\text{Area} = \frac{V}{F_{Ao}} = \frac{\tau}{C_{Ao}}$$

$$\text{Area} = \tau = \frac{VC_{Ao}}{F_{Ao}}$$

✚ **Constant Volume (Constant Density)** $v = v_0$ ($\epsilon = 0$)

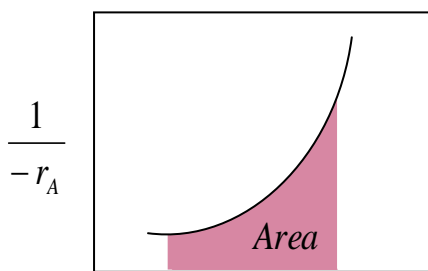
liquid-phase and some of gas phase reaction system fall into this category.

PFR

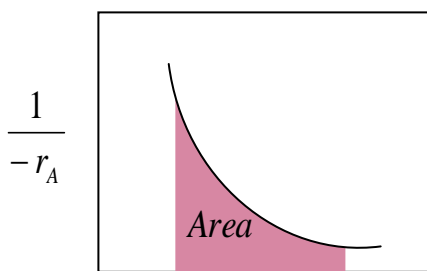
$$V = F_{Ao} \int_0^X \frac{dX}{-r_j}$$

$$\frac{V}{F_{Ao}} = \frac{V}{C_{Ao} v_0} = \frac{\tau}{C_{Ao}} = \int_0^X \frac{dX}{-r_j}$$

$$\tau = C_{Ao} \int_0^X \frac{dX}{-r_j}$$



X



C_A

$$\text{Area} = \frac{V}{F_{Ao}} = \frac{\tau}{C_{Ao}}$$

$$\text{Area} = \tau = \frac{VC_{Ao}}{F_{Ao}}$$



First order and Irreversible :-



CSTR

$$V = \frac{F_{Ao} X}{(-r_A)}$$

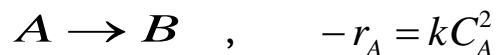
$$C_A = \frac{C_{Ao}}{1 + k\tau}$$

PFR

$$V = F_{Ao} \int_0^X \frac{dX}{-r_A}$$

$$C_A = C_{Ao} e^{-k\tau}$$

Second order and Irreversible :-



CSTR

$$V = \frac{F_{Ao} X}{(-r_A)}$$

$$k\tau = \frac{C_{Ao} - C_A}{C_A^2}$$

PFR

$$V = F_{Ao} \int_0^X \frac{dX}{-r_j}$$

$$\tau = -\frac{1}{k} \left(\frac{1}{C_A} - \frac{1}{C_{Ao}} \right), \quad C_A = \frac{C_{Ao}}{1 + C_{Ao} k\tau}$$

Bimolecular Reactions

Stoichiometric Table Flow System

Specie	Initial	Change	Remaining	Concentration
A	F_{Ao}	$-F_{Ao} X$	$F_A = F_{Ao}(1 - X)$	$C_A = C_{Ao}(1 - X)$
B	$F_{Bo} = F_{Ao} \Theta_B$	$-(b/a)F_{Ao} X$	$F_B = F_{Ao}[\Theta_B - (b/a)X]$	$C_B = C_{Ao} \left(\Theta_B - \frac{b}{a} X \right)$
C	$F_{Co} = F_{Ao} \Theta_C$	$+(c/a)F_{Ao} X$	$F_C = F_{Ao}[\Theta_C + (c/a)X]$	$C_C = C_{Ao} \left(\Theta_C + \frac{c}{a} X \right)$
D	$F_{Do} = F_{Ao} \Theta_D$	$+(d/a)F_{Ao} X$	$F_D = F_{Ao}[\Theta_D + (d/a)X]$	$C_D = C_{Ao} \left(\Theta_D + \frac{d}{a} X \right)$
I	$F_I = F_{Ao} \Theta_I$		$F_I = F_{Ao} \Theta_I$	C_{Io}
	$F_{To} = \sum F_{Ao} \Theta_i$		$F_T = F_{To} + \delta F_{Ao} X$	

$$\Theta_i = F_{io}/F_{Ao} = C_{io}/C_{Ao} = y_{io}/y_{Ao}$$

$$\delta = (d/a) + (c/a) - (b/a) - 1$$



Variable Volume (Variable Density, but with Constant T and P)

$$v = v_0(1 + \varepsilon X)$$

– **Concentration (CSTR, PFR):** $C_j = \frac{F_j}{v} = \frac{P_j}{Z_j RT_j}$

– **Total Concentration** $C_T = \frac{F_T}{v} = \frac{P}{ZRT}$

– **At entrance to the reactor concentration** $C_o = \frac{F_o}{v} = \frac{P_o}{Z_o RT_o}$

$$v = v_0 \left(\frac{F_T}{F_{T0}} \right) \left(\frac{T}{T_0} \right) \left(\frac{P_0}{P} \right) \left(\frac{Z}{Z_0} \right)$$

with constant temperature and pressure, and the compressibility factor will not change significantly during the course of the reaction ,

$$v = v_0 \left(\frac{F_T}{F_{T0}} \right)$$

$$C_j = \left(\frac{F_{T0}}{v_0} \right) \left(\frac{F_j}{F_T} \right)$$

$$C_j = C_{T0} \left(\frac{F_j}{F_T} \right)$$

Total molar flow rates $F_T = F_A + F_B + F_C + F_D + \dots = \sum_{j=1}^n F_j$

$F_T = F_{T0} + \delta F_{A0} X$ sub in $v = v_0 \left(\frac{F_T}{F_{T0}} \right)$

$$v = v_0 \left(\frac{F_{T0} + \delta F_{A0} X}{F_{T0}} \right)$$

$$v = v_0 (1 + \delta y_{A0} X)$$

$$v = v_0 (1 + \varepsilon X)$$

Molar flow rate of species j is $F_j = F_{A0} (\Theta_j + v_j X)$



Stoichiometric Table Flow System

Concentration at variable volume or density

Specie			
$C_A = \left(\frac{N_A}{V} \right)$	$= \frac{F_{A0}(1-X)}{\nu}$	$= \frac{F_{A0}(1-X)}{\nu_o(1+\varepsilon X)}$	$= \frac{C_{A0}(1-X)}{(1+\varepsilon X)}$
$C_B = \left(\frac{N_B}{V} \right)$	$= \frac{F_{A0}(\Theta_B - (b/a)X)}{\nu}$	$= \frac{F_{A0}(\Theta_B - (b/a)X)}{\nu_o(1+\varepsilon X)}$	$= \frac{C_{A0}(\Theta_B - (b/a)X)}{(1+\varepsilon X)}$
$C_C = \left(\frac{N_C}{V} \right)$	$= \frac{F_{A0}(\Theta_C + (c/a)X)}{\nu}$	$= \frac{F_{A0}(\Theta_C + (c/a)X)}{\nu_o(1+\varepsilon X)}$	$= \frac{C_{A0}(\Theta_C + (c/a)X)}{(1+\varepsilon X)}$
$C_D = \left(\frac{N_D}{V} \right)$	$= \frac{F_{A0}(\Theta_D - (d/a)X)}{\nu}$	$= \frac{F_{A0}(\Theta_D - (d/a)X)}{\nu_o(1+\varepsilon X)}$	$= \frac{C_{A0}(\Theta_D - (d/a)X)}{(1+\varepsilon X)}$
$C_I = \left(\frac{N_I}{V} \right)$	$= \frac{F_{A0}\Theta_I}{\nu}$	$= \frac{F_{A0}\Theta_I}{\nu_o(1+\varepsilon X)}$	$= \frac{C_{A0}\Theta_I}{(1+\varepsilon X)}$

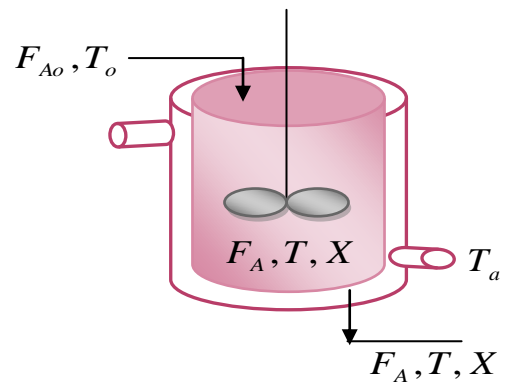


Non-Isothermal Operation Reactor

CSTR

Although the CSTR is well mixed and the temperature is uniform throughout the reaction vessel, these conditions do not mean that the reaction is carried out isothermally. Isothermal operation occurs when the feed temperature is identical to the temperature of the fluid inside the CSTR.

Energy Balance in CSTR



No accumulation in CSTR (steady state operation) then:-

$$F_{Ao} \sum \Theta_i C_{pi} T_{io} - F_{Ao} \sum \Theta_i C_{pi} T + [-\Delta H_r(T) \cdot (-r_A V)] - UA(T - T_a) = 0$$

$$F_{Ao} \sum \Theta_i C_{pi} (T_{io} - T) + [-\Delta H_r(T) \cdot (-r_A V)] - UA(T - T_a) = 0$$

$$T - T_{io} = \frac{[-\Delta H_r(T) \cdot (-r_A V)] - UA(T - T_a)}{F_{Ao} \sum \Theta_i C_{pi}} \dots\dots\dots 1$$



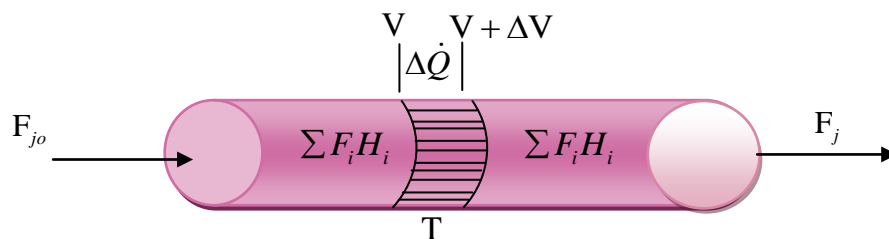
For CSTR design equation

$$V = \frac{F_{A0} X}{(-r_A)}$$

sub for $F_{A0} X = -r_A V$ in energy balance equations then :-

$$X = \frac{F_{A0} \sum \Theta_i C_{pi} (T - T_{io}) + UA (T - T_a)}{[-\Delta H_r(T)]} \dots\dots\dots 2$$

PFR



Tubular reactor with heat gain or loss

Consider a tubular reactor in which heat is either is add or removed through the cylindrical walls of the reactor ,we assume that there are no radial gradients in the reactor and that the heat flux through the wall per unit volume or reactor is shown in figure above.

$$\sum F_i H_i \Big|_V - \sum F_i H_i \Big|_{V+\Delta V} + \Delta \dot{Q} = 0$$

$$\Delta \dot{Q} = UA(T_a - T)$$



T_a = ambient temperature K , T = reactor temperature K

Taking the limit $\Delta V \rightarrow 0$, we get:-

$$UA(T_a - T) - \frac{d \sum (F_i H)_i}{dV} = 0$$

$$UA(T_a - T) - \frac{\sum dF_i}{dV} H_i - \sum F_i \frac{dH_i}{dV} = 0 \dots\dots\dots 3$$

From mole balance of species i , $\frac{dF_i}{dV} = r_i = \nu_i (-r_i) \dots\dots\dots 4$

Enthalpy of each species i , $H_i = H_i^o(T_R) + \int_{T_R}^T C_{p_i} dT = H_i^o(T_R) + C_{p_i}(T - T_R)$

Differentiating enthalpy equation with respect to V : $\frac{dH_i}{dV} = C_{p_i} \frac{dT}{dV} \dots\dots 5$

Sub equation 4 and 5 in 3

$$UA(T_a - T) - \sum \nu_i H_i (-r_i) - \sum F_i C_{p_i} \frac{dT}{dV} = 0$$

$$UA(T_a - T) - \Delta H_R (-r_i) - \sum F_i C_{p_i} \frac{dT}{dV} = 0$$

$$\frac{dT}{dV} = \frac{UA(T_a - T) + (-\Delta H_R)(-r_i)}{\sum F_i C_{p_i}}$$

Heat
generated

Heat
removed

$$\frac{dT}{dV} = \frac{(-\Delta H_R)(-r_i) - UA(T - T_a)}{\sum F_i C_{p_i}}$$