2. Conversion and Reactor Sizing

- **Definition of Conversion, X**
- **Batch Reactor Design Equations**
- **Design Equations for Flow Reactors**
  - CSTR. PFR, PBR
- **Applications of the Design Equations for Continuous-Flow Reactors**
- **Reactors in Series**

1. Definition of Conversion (p.38)

- **Define conversion and space time.**
- **Write the mole balances in terms of conversion for a batch reactor, CSTR, PFR, and PBR.**
- **Size reactors either alone or in series once given the molar flow rate of A, and the rate of reaction, - r_A, as a function of conversion, X**
- **General stoichiometric relationships**

  - Basis of calculation

  $$aA + bB \rightarrow cC + dD$$

  - **limiting reactant**

  $$A + \frac{b}{a}B \rightarrow \frac{c}{a}C + \frac{d}{a}D$$

- **Conversion of species A**

$$X_A = \frac{\text{Moles of A reacted}}{\text{Moles of A feed}}$$

1. Definition of Conversion II

- **The conversion X of species A in a reaction**

  - the number of moles of A reacted per mole of A fed, ie.

$$\mathrm{X} = (\text{moles reacted/moles A fed})$$

$$X_A = \frac{(N_{A0} - N_A)}{N_{A0}} \text{ for Batch}$$

$$= \frac{(F_{A0} - F_A)}{F_{A0}} \text{ for Flow}$$

- **What is the maximum value of conversion?**

  - Irreversible reactions, the complete conversion, i.e. X = 1.0.

  - Reversible reactions, the equilibrium conversion, i.e. X = X_e

2. Batch Reactor Design Equations I

- **General Mole Balance on System Volume V**

$$\begin{bmatrix}\text{Moles of A}\\ \text{reacted}\\ \text{(Consumed)}\end{bmatrix} = [\text{Moles of A fed}]\cdot\left[\frac{\text{Moles of A reacted}}{\text{Moles of A fed}}\right]$$

$$\begin{bmatrix}\text{Moles of A}\\ \text{reacted}\\ \text{(Consumed)}\end{bmatrix} = [N_{A0}] \cdot [X]$$

$$\begin{bmatrix}\text{Moles of A}\\ \text{in reactor}\\ \text{at time } t\end{bmatrix} = \begin{bmatrix}\text{Moles of A}\\ \text{initially fed to}\\ \text{reactor at } t=0\end{bmatrix} - \begin{bmatrix}\text{Moles of A that}\\ \text{have been consumed}\\ \text{by chemical reaction}\end{bmatrix}$$

$$[N_A] = [N_{A0}] - [N_{A0}X]$$

2. Batch Reactor Design Equations II

- **The number of moles of A in the reactor after a conversion X**

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

- No spatial variation

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

- Reactant A is disappearing

$$-\frac{dN_A}{dt} = (-r_A)V$$

- Or

$$-\frac{dN_A}{dt} = 0 - N_{A0}\frac{dX}{dt}$$

$$N_{A0}\frac{dX}{dt} = (-r_A)V$$

2. Batch Reactor Design Equations III

- **For a constant volume batch reactor *V* = *V*$_0$**

$$\frac{1}{V_0}\frac{dN_A}{dt} = \frac{d(N_A/V_0)}{dt} = \frac{dC_A}{dt}$$

- Constant volume batch reactor, $$\frac{dC_A}{dt} = r_A$$

- Rearrangement

$$dt = N_{A0}\frac{dX}{-r_A V}$$

- Time *t* necessary to obtain a conversion *X*

$$t = N_{A0}\int_0^X \frac{dX}{-r_A V}$$

3. Design Equations for Flow Reactor I

○ **At steady state**

$$[F_{A0}]\cdot[X]=\frac{\text{Moles of A fed}}{\text{time}}\cdot\frac{\text{Moles of A reacted}}{\text{Moles of A fed}}$$

$$[F_{A0}\cdot X]=\frac{\text{Moles of A reacted}}{\text{time}}$$

$$\begin{bmatrix}\text{Molar flow rate}\\ \text{at which A is}\\ \text{fed to the system}\end{bmatrix}=\begin{bmatrix}\text{Molar rate at which}\\ \text{A is consumed}\\ \text{within the system}\end{bmatrix}-\begin{bmatrix}\text{Molar flow rate}\\ \text{at which A leaves}\\ \text{the system}\end{bmatrix}$$

$$[F_{A0}] \quad = \quad [F_{A0}X] \quad - \quad [F_A]$$

- Rearrangement $$F_A=F_{A0}(1-X)$$

3. Design Equations for Flow Reactor II

- **For liquid phase system**

$$F_{A0} = C_{A0} v_0$$

- **For gas phase system**

$$C_{A0} = \frac{P_{A0}}{RT_0} = \frac{y_{A0} P_0}{RT_0}$$

- Or

$$F_{A0} = v_0 C_{A0} = v_0 \frac{y_{A0} P_0}{RT_0}$$

where C_{A0}= entering concentration, mol/dm^3

y_{A0}= entering mole fraction of A

P_0= entering total pressure, e.g., kPa

P_{A0}= $y_{A0}P_0$ = entering partial pressure of A, kPa

T_0= entering temperature, K

v_0= volumetric flow rate

R= ideal gas constant

3. Design Equations for Flow Reactor III

- **CSTR**

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

$$F_{A0} - F_A = F_{A0} X$$

$$V = \frac{F_{A0} X}{\left(-r_A\right)_{exit}}$$

- **PFR**

$$F_A = F_{A0} - F_{A0} X$$

$$F_{A0} \frac{dX}{dV} = -r_A$$

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

$$V = F_{A0} \int_0^X \frac{dX}{-r_A}$$

3. Design Equations for Flow Reactor IV

- **PBR**

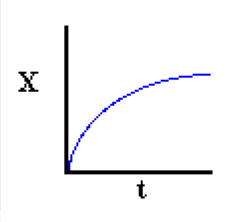
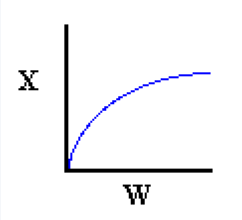
$$F_A = F_{A0} - F_{A0} X$$

$$F_{A0} \frac{dX}{dW} = -r'_A$$

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

$$W = F_{A0} \int_0^X \frac{dX}{-r'_A}$$

Summary of Design Equations

Reactor	Design Equations	Graph
Batch	$N_{A0}\frac{dX}{dt} = -r_A V \quad t = N_{A0}\int_0^X \frac{dX}{-r_A V}$	
CSTR	$V = \frac{F_{A0}X}{-r_A}$	
PFR	$F_{A0}\frac{dX}{dV} = -r_A \quad V = F_{A0}\int_0^X \frac{dX}{-r_A}$	
PBR	$F_{A0}\frac{dX}{dW} = -r'_A \quad W = F_{A0}\int_0^X \frac{dX}{-r'_A}$	

4. Applications of the Design Equations for Continuous-Flow Reactor I

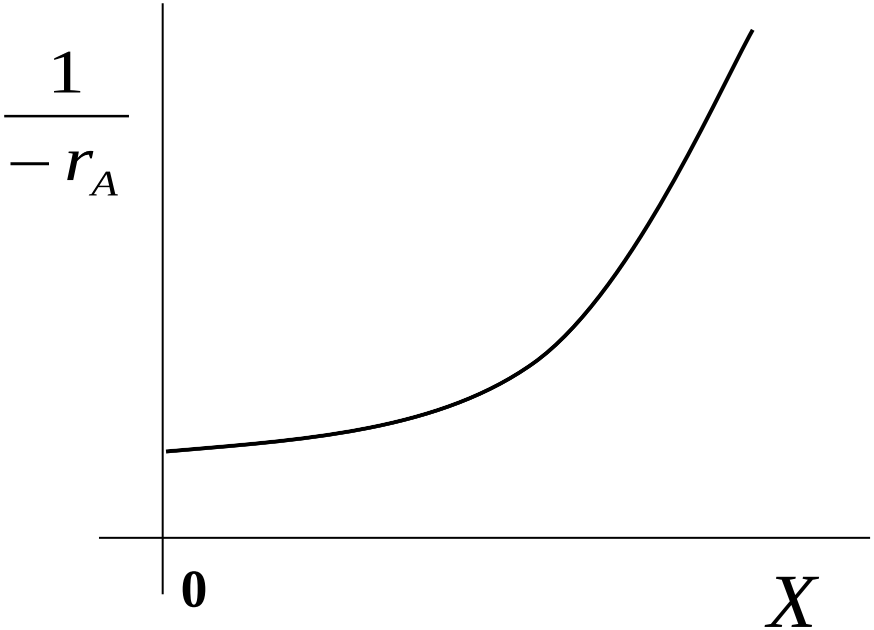
- **1st order dependence**

$$-r_A = kC_A = kC_{A0}(1-X)$$

  - ***k*** **is specific constant, ftn of only Temp.** C_{A0}**, entering concentration**

- Rearrange

$$\frac{1}{-r_A} = \frac{1}{kC_{A0}}\left(\frac{1}{1-X}\right)$$



4. Applications of the Design Equations for Continuous-Flow Reactor II

- Reactor size of CSTR and PFR

- Raw data

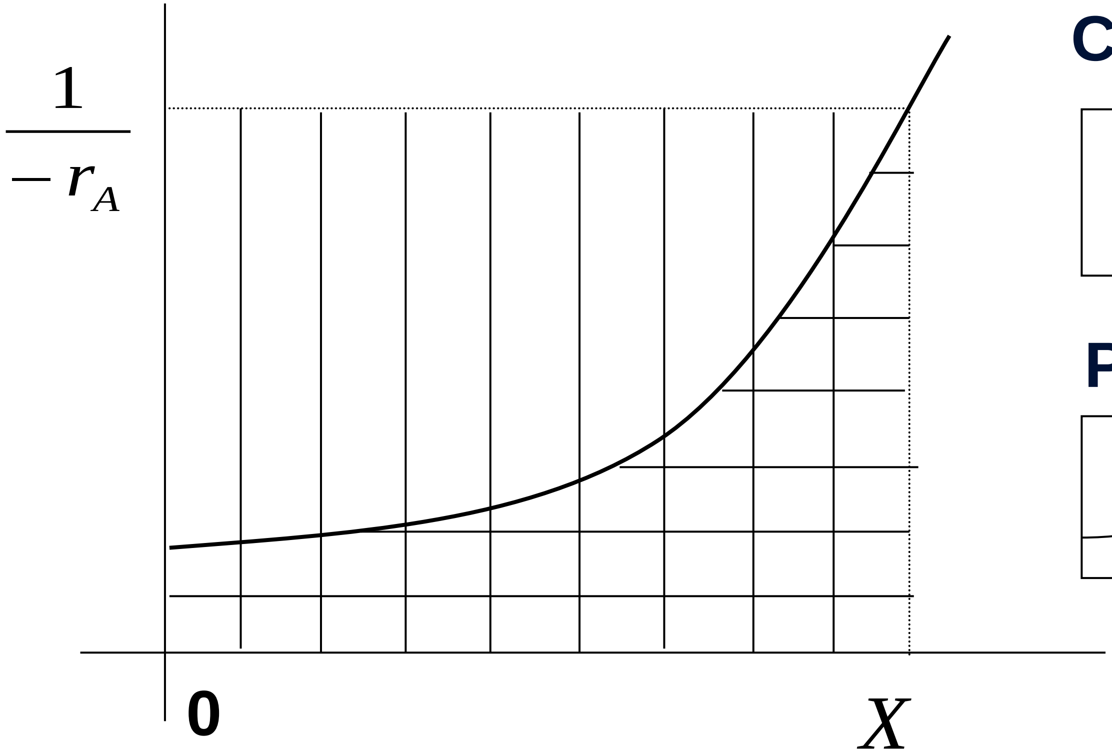
X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$-r_A$(mol/m^{3}s)	0.45	0.37	0.30	0.195	0.113	0.079	0.05
$(1/-r_A)$(m^{3}s/mol)	2.22	2.70	3.33	5.13	8.85	12.7	20

- Manipulated

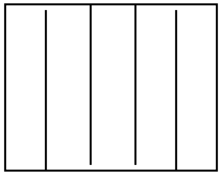
X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$-r_A$(mol/m^{3}s)	0.45	0.37	0.30	0.195	0.113	0.079	0.05
$(1/-r_A)$(m^{3}s/mol)	2.22	2.70	3.33	5.13	8.85	12.7	20
$[F_{A0}/-r_A]$(m^3)	0.89	1.08	1.33	2.05	3.54	5.06	8.0

4. Applications of the Design Equations for Continuous-Flow Reactor II

○ **Reactor sizing**

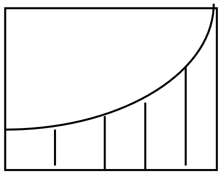


CSTR



$$\frac{1}{-r_A}X$$

PFR



$$\int_0^X \frac{1}{-r_A}dX$$

Plots for sizing CSTR and PFR

5. Reactors in Series

- Given $-r_A$ as a function of conversion, one can also design any sequence of reactors

$$X_i = \frac{\text{moles of A reacted up to a point i}}{\text{moles of A fed to first reactor}}$$

Only valid if there are no side streams

- Consider a PFR between two CSTRs