

Lecture #3.1

- Different reactors for different purposes
- Ideal Reactors and species balance
- Ideal Reactors and more of them

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Ideal reactors and their design equation

Ideal Reactor	Design Equation	Integral form	Conc. given by
BR	$\frac{dN_j}{dt} = r_j.V$	$t = \int \frac{dN_j}{r_j \cdot V}$	$C_j = \frac{N_j}{V}$
CSTR	$V = \frac{F_{j0} - F_j}{-rj}$	algebraic	$C_j = \frac{F_j}{\dot{v}}$
PFR	$\frac{dF_j}{dV} = r_j$	$V = \int \frac{dF_j}{r_j}$	$C_j = \frac{F_j}{\dot{v}}$
PBR	$\frac{dF_j}{dW} = r_j'$	$W = \int \frac{dF_j}{r_j'}$	$C_j = \frac{F_j}{\dot{v}}$



We commonly deal with conversions of a species

- For a reaction following the stoichiometric eqⁿ: aA + bB = cC + dDa, b, c and d are stoichiometric coefficients
- ▶ In terms of limiting reactant A we have $A + \frac{b}{a}B = \frac{c}{a}C + \frac{d}{a}D$
- ► Conversion of species j, X_j , is defined as: $X_j = \frac{moles\ of\ j\ converted}{moles\ j\ fed}$
- ▶ For Batch reactors: $X_j = \frac{N_{j0} N_j}{N_{j0}}$ also $dN_j = -N_{j0}dX_j$
- ► For flow reactors: $X_j = \frac{F_{j_0} F_j}{F_{j_0}}$ also for PFR/PBR $dF_j = -F_{j_0}dX_j$

Design equations can be written in terms of conversions

For BR:
$$\frac{dN_{j}}{dt} = r_{j}.V \rightarrow -\frac{N_{j0}dX_{j}}{dt} = r_{j}.V$$
$$t = N_{j0} \int_{X_{j}}^{X_{j}} at \ t = 0 \frac{dX_{j}}{-r_{j}.V}$$

For CSTR:
$$V = \frac{F_{j0} - F_j}{-r_j} \rightarrow V = \frac{F_{j0} X_j}{-r_j}$$

► For PFR:
$$\frac{dF_j}{dV} = r_j$$
 \rightarrow $-\frac{F_{j0}dX_j}{dV} = r_j$

$$V = F_{j0} \int_{X_j at \ V=0}^{X_j at \ V} \frac{dX_j}{-r_j}$$

► Similarly, for PBR:

$$W = F_{j0} \int_{X_j at W=0}^{X_j at W} \frac{dX_j}{-r'_j}$$

Usually the subscript j is dropped and conversion is based on the limiting reactant $\rightarrow X_j = X$



Design equation in terms of conversion

Reactor	Design Eq ⁿ	Integral form	Conversion	X vs. t or V or W
BR	$\frac{dN_j}{dt} = r_j.V$	$t = \int \frac{dN_j}{r_j}$	$t = N_{j0} \int_{X_j at \ t=0}^{X_j at \ t} \frac{dX_j}{-r_j \cdot V}$	X
CSTR	$V = \frac{F_{j0} - F_{j0}}{-r_{j}}$	^j algebraic	$V = \frac{F_{j0}X_j}{-r_j}$	
PFR	$\frac{dF_j}{dV} = r_j$	$V = \int \frac{dF_j}{r_j}$	$V = F_{j0} \int_{X_j at \ V=0}^{X_j at \ V} \frac{dX_j}{-r_j}$	X V
PBR	$\frac{dF_j}{dW} = r_j'$	$W = \int \frac{dF_j}{r_j'}$	$W = F_{j0} \int_{X_j at W=0}^{X_j at W} \frac{dX_j}{-r_j'}$	X W

Levenspiel plots useful for sizing flow reactors

- ► The function $\frac{F_{j0}}{-r_i}$ or $\frac{F_{A0}}{-r_A}$ is important in sizing \rightarrow **A** is the limiting reactant
- $-r_A = f(X)$ and thus $\frac{F_{A0}}{-r_A}$ is also a function of **X**
- ▶ Thus, a plot of $\frac{F_{A0}}{-r_A}$ or $\frac{1}{-r_A}$ versus X can be used to size the reactor
- ► For a CSTR: $V = \left(\frac{F_{A0}}{-r_A}\right)X$ and for a PFR: $V = \overline{\int_{X \ at \ V=0}^{X \ at \ V} \left(\frac{F_{A0}}{-r_A}\right)dX}$

$$V = \int_{X \text{ at } V}^{X \text{ at } V} \left(\frac{F_{A0}}{-r_A}\right) dX$$



