



# Chemical Reaction Engineering

## Conversion and Reactor Sizing

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## Content

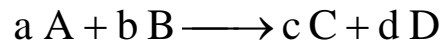


- Definition of Conversion
- Design Equations
  - Batch Reactor
  - CSTR
  - PFR
- Applications for Continuous-Flow Reactors

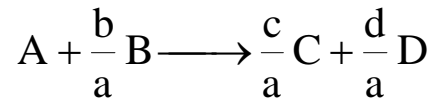


## Definition of Conversion

- In defining conversion, we choose one of the reactants as the basis of calculation and then relate the other species involved in the reaction to this basis



Choose limiting reactant A as basis of calculation



$$X = \frac{\text{moles A reacted}}{\text{moles A fed}}$$

- For irreversible reactions, the maximum conversion is 1.0, i.e., complete conversion.
- For reversible reactions, the maximum conversion is the equilibrium conversion,  $X_e$

(i.e.,  $X_{\max} = X_e$ )

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## Batch Reactor Design Equations

If  $N_{A0}$  is the number of moles of A initially in the reactor,

$$\left[ \text{Moles of A reacted (consumed)} \right] = \left[ \text{Moles of A fed} \right] \cdot \left[ \frac{\text{Moles of A reacted}}{\text{Moles of A fed}} \right]$$

$$\left[ \begin{array}{c} \text{Moles of A} \\ \text{reacted} \\ \text{(consumed)} \end{array} \right] = [N_{A0}] \cdot [X]$$

then the total number of moles of A that have reacted after a time  $t$  is  $[N_{A0}X]$

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## Batch Reactor Design Equations

the number of moles of A that remain in the reactor after a time  $t$ ,  $N_A$ ,

$$\left[ \begin{array}{l} \text{Moles of A} \\ \text{in reactor} \\ \text{at time } t \end{array} \right] = \left[ \begin{array}{l} \text{Moles of A} \\ \text{initially fed} \\ \text{to reactor at} \\ t = 0 \end{array} \right] - \left[ \begin{array}{l} \text{Moles of A that} \\ \text{have been con-} \\ \text{sumed by chemical} \\ \text{reaction} \end{array} \right]$$

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

The number of moles of A in the reactor after a conversion  $X$  has been achieved is

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



## Batch Reactor Design Equations

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

This equation is valid whether or not the reactor volume is constant.

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

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

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

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

The differential form of the design equation for batch reactor



# Batch Reactor Design Equations

For a constant-volume batch reactor,  $V = V_0$ ,

$$\frac{dN_A}{dt} = r_A V \quad \text{and} \quad \frac{1}{V_0} \frac{dN_A}{dt} = \frac{d(N_A/V_0)}{dt} = \frac{dC_A}{dt}$$

$$\rightarrow \frac{dC_A}{dt} = r_A$$

To determine the time to achieve a specified conversion  $X$ ,

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

➤ At time equal zero where there is no conversion initially (i.e.,  $t = 0, X = 0$ )

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

➤ The conversion increases with time spent in the reactor.



# Design Equations for Flow Reactors

➤ For continuous-flow systems, this time usually increases with increasing reactor volume

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

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

The molar feed rate of A to the system *minus* the rate of reaction of A within the system *equals* the molar flow rate of A leaving the system  $F_A$ .

$$\left[ \begin{array}{c} \text{Molar flow rate} \\ \text{at which A is} \\ \text{fed to the system} \end{array} \right] - \left[ \begin{array}{c} \text{Molar rate at} \\ \text{which A is} \\ \text{consumed within} \\ \text{the system} \end{array} \right] = \left[ \begin{array}{c} \text{Molar flow rate} \\ \text{at which A leaves} \\ \text{the system} \end{array} \right]$$

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



## Design Equations for Flow Reactors

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

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

$$(\text{mol/s}) = (\text{mol/dm}^3) (\text{dm}^3/\text{s})$$

For liquid systems,  $C_{A0}$  is commonly given in terms of molarity,  $C_{A0} = 2 \text{ mol/dm}^3$

For gas systems, 
$$C_{A0} = \frac{P_{A0}}{RT_0} = \frac{y_{A0}P_0}{RT_0}$$

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

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## Design Equations for Flow Reactors

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

$y_{A0}$  = entering mole fraction of A

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

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

$T_0$  = entering temperature, K

$R$  = ideal gas constant  $\left( \text{e.g., } R = 8.314 \frac{\text{kPa} \cdot \text{dm}^3}{\text{mol} \cdot \text{K}}; \text{ see Appendix B} \right)$

- The size of the reactor will depend on the flow rate, reaction kinetics, reactor conditions, and desired conversion

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## Design Equations for CSTR

- For species A in the reaction



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

and

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

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



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

- Because the reactor is *perfectly mixed*, the exit composition from the reactor is identical to the composition inside the reactor, and *the* rate of reaction is evaluated at the exit conditions.



## Design Equations for PFR

- No radial gradients in concentration, temperature, or reaction rate.
- As the reactants enter and flow axially down the reactor, they are consumed and *the* conversion increases along the length of the reactor

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

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

differentiating

$$dF_A = -F_{A0}dX$$



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

separate the variables and integrate with the limits  $V = 0$  when  $X = 0$

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

**The volume necessary to achieve a specified conversion X**





# Design Equations for Packed-Bed Reactor

- Packed-bed reactors are tubular reactors filled with catalyst particles

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

In the *absence* of pressure drop, i.e.,  $\Delta P = 0$ ,

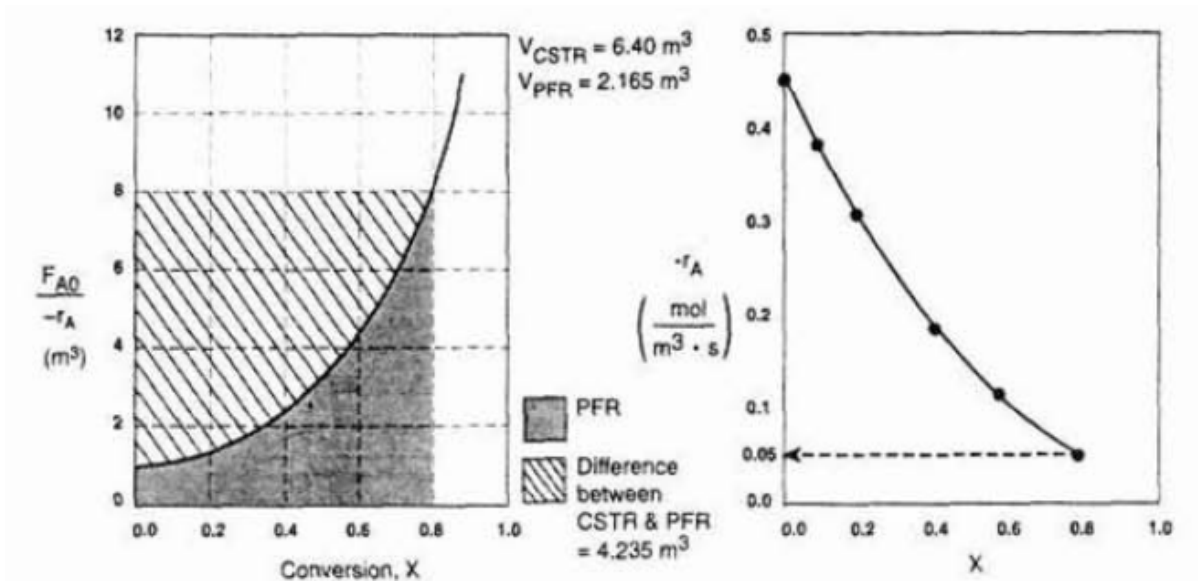
integrate with limits  $X = 0$  at  $W = 0$

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

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## Example Cont.

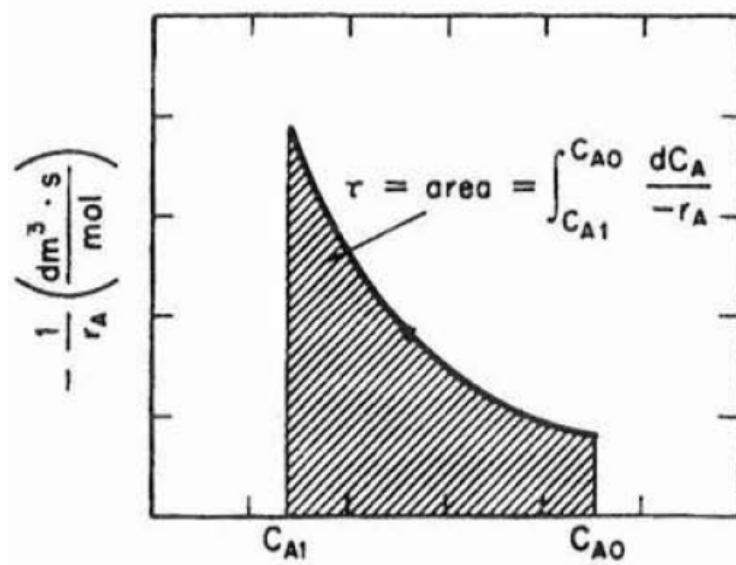


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# Modified Levenspiel Plots

$$\tau = \int_{C_A}^{C_{A0}} \frac{dC_A}{-r_A}$$



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