# Ideal Reactor Design

The *rate equation* for a reacting component i is an intensive measure, and it tells how rapidly component i forms or disappears in a given environment as a function of the conditions there

$$r_i = \frac{1}{V}\left(\frac{dN_i}{dt}\right)_{\text{by reaction}} = f(\text{conditions within the region of volume } V)$$

# Why Design Reactors?

- Want to control reaction conversions
- Cannot arbitrarily control reaction mechanisms or rates
- Issues of reactor size, mass transport, thermal control vs. economics

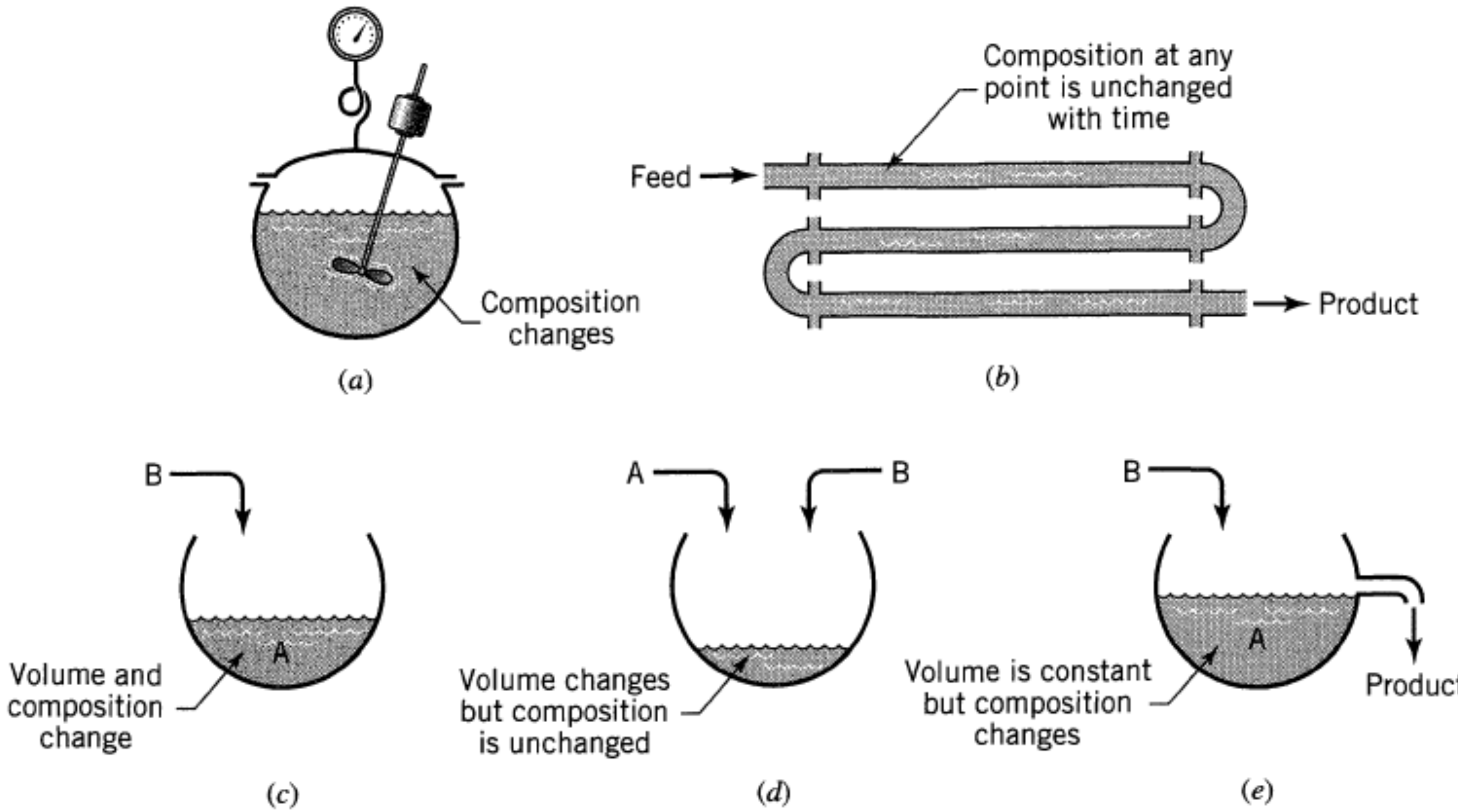
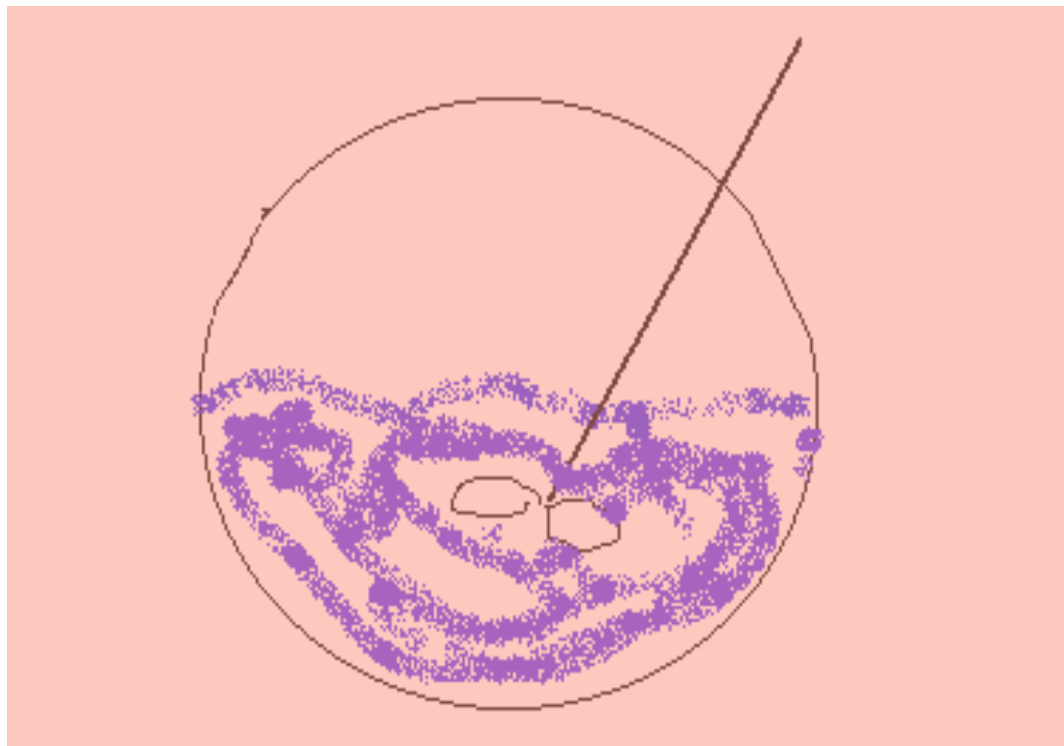



**Figure 4.1** Broad classification of reactor types. (*a*) The batch reactor. (*b*) The steady-state flow reactor. (*c*), (*d*), and (*e*) Various forms of the semibatch reactor.

# Ideal batch reactor

Assumptions:
Composition varies with time
Uniform composition
Constant volume

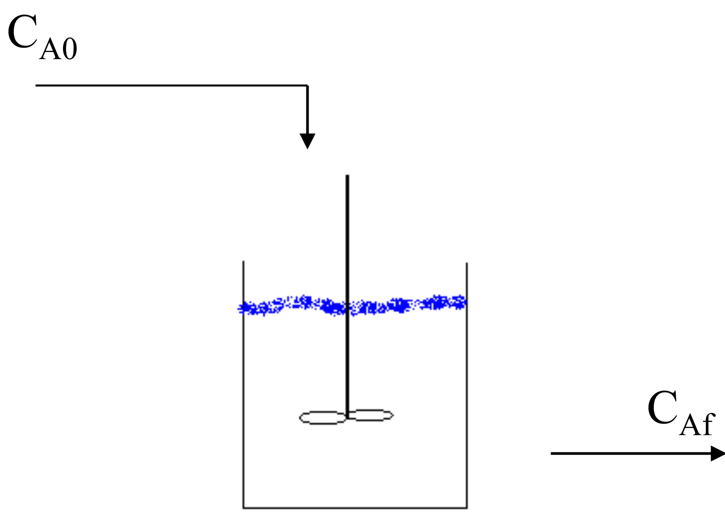


- Very simple
- Need very little supporting equipment
- Ideal for small-scale experimental studies on rxn kinetics

# Steady-State Flow

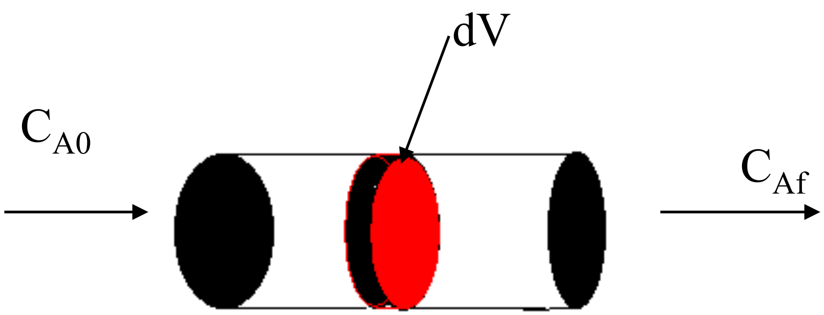
- Ideal for industrial purposes when large quantities of material are to be processed, and rxn rate is high
- Needs a large amount of supporting equipment
- Very good product quality control can be obtained
- Examples are mixed flow and plug flow reactors

# Steady-state flow reactors




MIXED FLOW REACTOR

Assumptions:
Uniform composition in position
Composition does not vary with time
Outlet conc. = reactor conc.
Constant volume

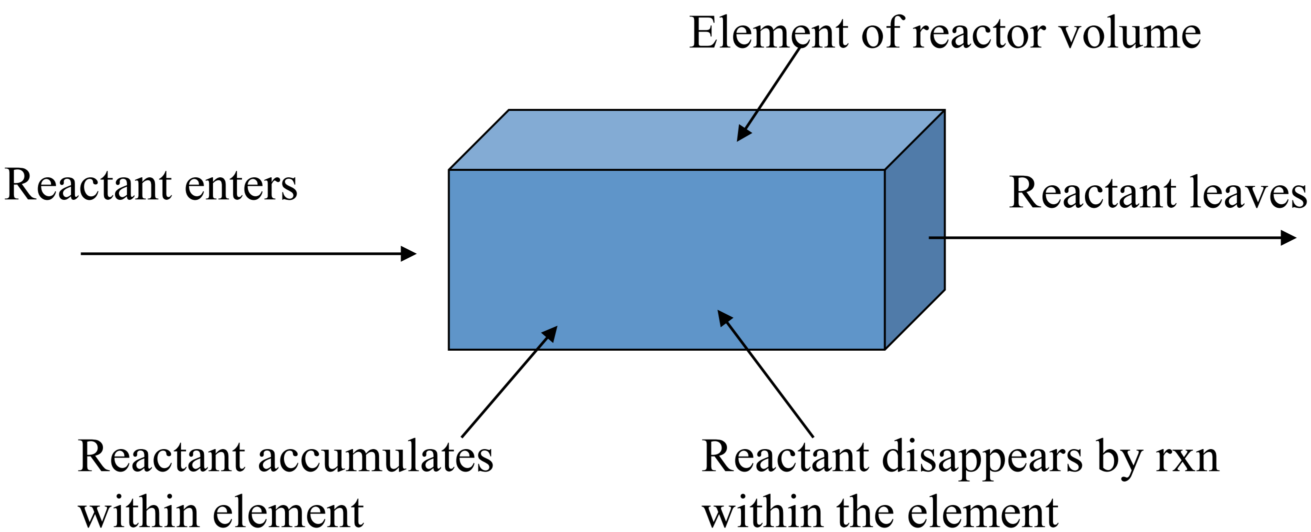



PLUG FLOW REACTOR

Assumptions:
Composition varies with axial position
Composition does not vary with time
Constant volume
No axial mixing
Homogeneous radial composition

The first step in designing a reactor is applying the **material balance** for any reactant (or product).

| | | | | | | |
|---|---|---|---|---|---|---|
| Rate of accumulation of reactant in element of volume | = | Rate of reactant flow into element of volume | + | Rate of reactant flow out of element volume | + | Rate of reactant loss due to chemical rxn within the element of volume |



# Nomenclature

V – reactor volume

t – time

$\nu$ or q – volumetric flow rate

$C_i$ – concentration of species i

$X_i$ – fractional conversion of species i

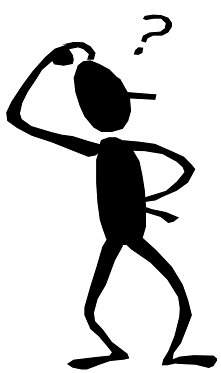
$r_i$ – rate of reaction of species i

$F_i$ – molar/mass flow rate of species i = $\nu * C_i$

Mass Balance:
Consider a general case of a constant density reactor system, with a feed $C_{A0} = 150$, and $C_{B0} = 315$. ($C_{A0}$ = inlet concentration of A and $C_{B0}$ = inlet concentration of B).

The rxn is: $A + 2B = 5R$

The outlet concentration of A ($C_A$) is 30.




What are $C_B$, $X_A$, and $X_B$?

For the various reactor types, the material balance equation is simplified and integrated to get the basic performance equation.

- For Batch Reactor

  Flow terms are zero

  - For steady-state flow (MFR and PFR)

    Accumulation term is zero

# Ideal Batch Reactor

A -> products

$$\text{accumulation} = \underbrace{\cancel{\text{Input}}}_{0} - \underbrace{\cancel{\text{output}}}_{0} + \text{disappearance}$$

$$\left(\begin{array}{l}\text{Rate of loss of reactant A}\\ \text{within reactor due to chemical}\\ \text{reaction}\end{array}\right) = -\left(\begin{array}{l}\text{Rate of accumulation}\\ \text{of reactant A within}\\ \text{the reactor}\end{array}\right)$$

$$\begin{array}{c}\text{disappearance of A}\\ \text{by reaction,}\\ \text{moles/time}\end{array} = (-r_A)V = \left(\frac{\text{moles A reacting}}{(\text{time})(\text{volume of fluid})}\right)(\text{volume of fluid})$$

$$\begin{array}{c}\text{accumulation of A,}\\ \text{moles/time}\end{array} = \frac{dN_A}{dt} = \frac{d[N_{A0}(1 - X_A)]}{dt} = -N_{A0}\frac{dX_A}{dt}$$

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

To get time (t) required to achieve a conversion $X_A$, rearrange and integrate the above formula to get:

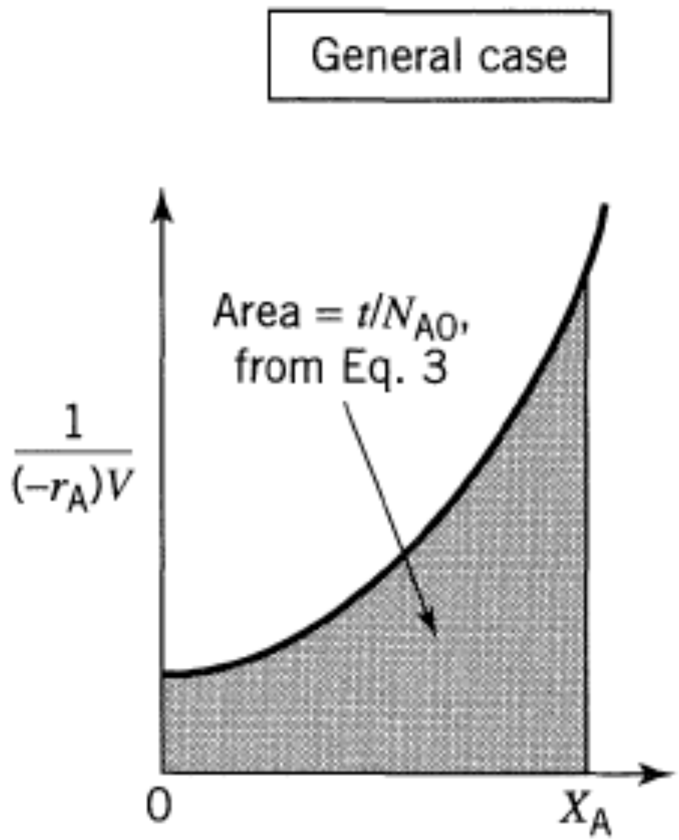
$$t = N_{A0}\int_0^{X_A} \frac{dX_A}{(-r_A)V}$$

For a constant density fluid this becomes:

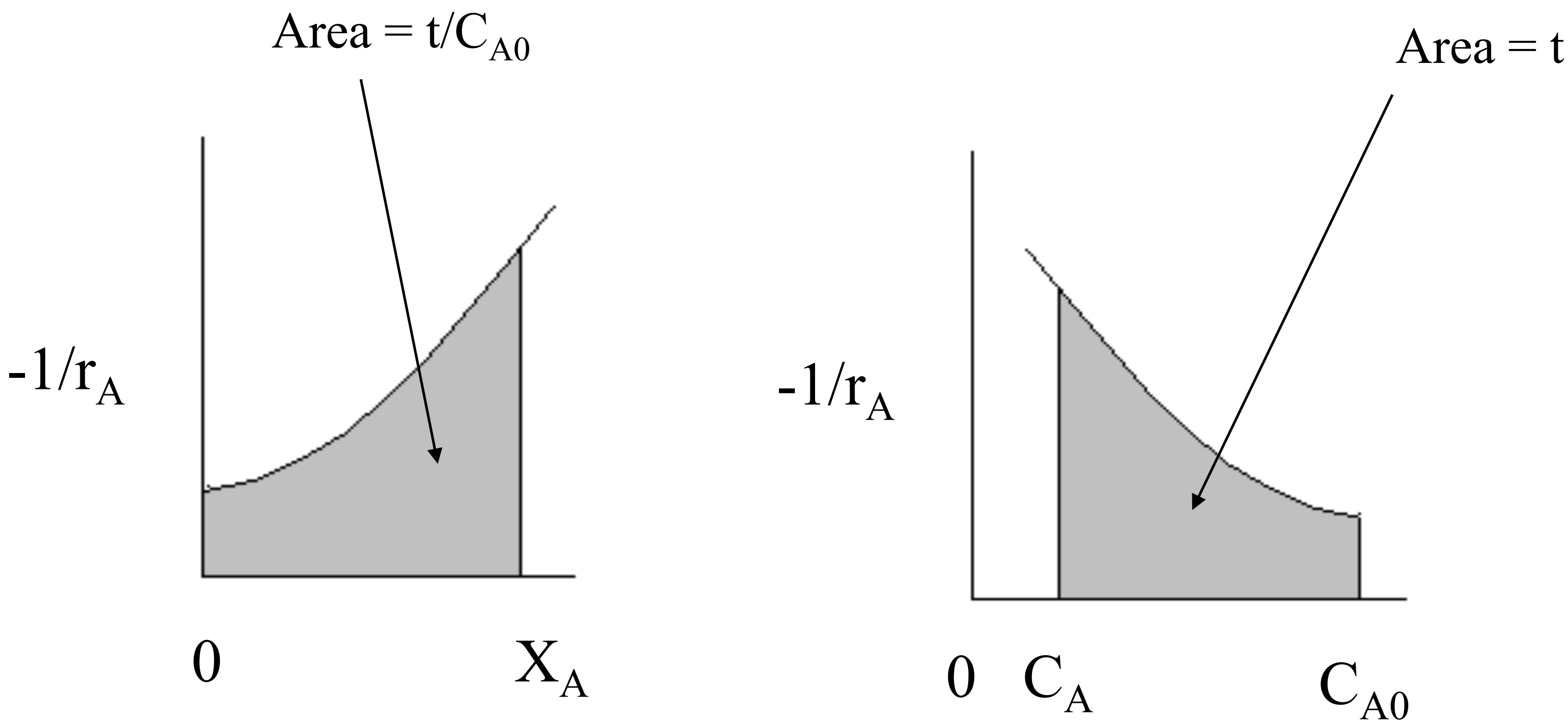
$$t = C_{A0} \int_{0}^{X_A} \frac{1}{-rA} \, dXA = -\int_{C_{A0}}^{C_A} \frac{1}{-rA} \, dCA = \textbf{reaction time}$$

These integrals can be graphically represented as the area underneath the reaction curve.

$$t = N_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A)V} \qquad \textbf{(3)}$$



# Graphical representation for constant-density batch reactor systems.




$$t = C_{A0} \int_0^{X_A} \frac{dX_A}{-r_A} = -\int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A}$$