INTRODUCTION TO REACTOR DESIGN
LEARNING OBJECTIVES

- At the end of this week’s lecture, students should be able to:
  - Understand the essentials of reactor design.
  - Differentiate between a batch, steady-state flow and unsteady state flow reactors
  - Know the symbols and relationships between $C_A$ and $X_A$
ESSENTIALS OF REACTOR DESIGN

- The focus of reactor design are
  - Knowing the size of the reactor, and
  - The type of reactor and
  - The best method of operation.

- Factors of importance in reactor design include:
  - The reacting conditions in the reactor
  - The time taken for the reaction to occur
  - The temperature,
  - The composition of the reacting fluid
  - The thermal character of the reaction, either endothermic or exothermic, the rate of heat addition or removal from the system, and
  - The flow pattern of fluid through the vessel.

- All these factors must be accounted for in predicting the performance of a reactor.
To arrive at a well fitted design:

- we must be able to predict the response of the reacting system to changes in operating conditions (i.e. how rates and equilibrium conversion change with temperature and pressure),

- we must be able to compare yields for alternative designs (adiabatic versus isothermal operations, single versus multiple reactor units, flow versus batch system), and

- we must be able to estimate the economics of the various alternatives.
CLASSIFICATION OF REACTOR TYPES

- The batch reactor is
  - is used for small-scale experimental studies on reaction kinetics
  - used industrially when relatively small amounts of material are to be treated.
  - needs little supporting equipment
  - An ideal reactor

- The steady-state flow reactor is
  - used industrially when large quantities of material are to be processed
  - used when the rate of reaction is fairly high to extremely high
  - extremely good product quality control can be obtained
  - supporting equipment needs are great
  - widely used in the oil industry.
**CLASSIFICATION OF REACTOR TYPES**

- The semi-batch reactor
  - is a flexible system but is more difficult to analyze than the other reactor types
  - It offers good control of reaction speed because the reaction proceeds as reactants are added
  - Such reactors are used in a variety of applications from the calorimetric titrations in the laboratory to the large open hearth furnaces for steel production.
## Comparison of Types of Chemical Reactors

<table>
<thead>
<tr>
<th>Type of Reactor</th>
<th>Characteristics</th>
<th>Usage</th>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td>Batch</td>
<td>• Reactor is charged (filled) via two holes in the top of the tank; while reaction is carried out, nothing else is put in or taken out until reaction is done; tank easily cooled or heated by jacket</td>
<td>• Small-scale production • Intermediate or one-shot productions • Pharmaceuticals • Fermentations</td>
<td>• High conversion per unit volume for one pass • Same reactor can be used to produce one product one time and a different product the next</td>
<td>• High operating cost (labor) • Product quality more variable than with continuous operation</td>
</tr>
<tr>
<td>Sembatch</td>
<td>• Either one reactant is charged and the other is fed continuously (at small concentrations) or else one of the products can be removed continuously (to avoid side reactions)</td>
<td>• Small-scale production • Competing reactions</td>
<td>• Good selectivity; feed can be controlled so as to minimize side runs.</td>
<td>• High operating labor cost • Product quality more variable than with continuous operation</td>
</tr>
<tr>
<td>Continuously stirred tank reactor (CSTR)</td>
<td>• Run at steady state with continuous flow of reactants and products; the feed assumes a uniform composition throughout the reactor, exit stream has the same composition as in the tank</td>
<td>• When agitation is required • Series configuration for different concentration streams</td>
<td>• Continuous operation • Good temperature control • Good control • Simplicity of construction • Low operating (labor) cost</td>
<td>• Lowest conversion per unit volume • Bypassing and channeling possible with poor agitation</td>
</tr>
<tr>
<td>Plug flow reactor (PFR)</td>
<td>• Arranged as one long reactor or many short reactors in a tube bank; no radial variation in reaction rate (concentration); concentration charges with length down the reactor</td>
<td>• Large-scale production • Homogeneous reactions • Heterogeneous reactions • Continuous production • High temperature</td>
<td>• Highest conversion per unit volume • Low operating labor cost • Continuous operation • Good heat transfer</td>
<td>• Undesired thermal gradients may exist • Poor temperature control • Shutdown, cleaning may be expensive</td>
</tr>
<tr>
<td>Tubular packed bed reactor (PBR)</td>
<td>• Tubular reactor that is packed with solid catalyst particles</td>
<td>• Used primarily in heterogeneous gas phase reactions with a catalyst</td>
<td>• Highest conversion per unit mass of catalyst • Low operating cost • Continuous operation</td>
<td>• Undesired thermal gradients may exist • Poor temperature control • Channeling may occur</td>
</tr>
</tbody>
</table>
MATERIAL AND ENERGY BALANCES IN A REACTOR

- In any design process, the first thing to do is to carry out material and energy balances over the equipment to be designed.

- For the material balance, consider an element of volume of the reactor,

- The material balance for any reactant (or product) can be expressed as

\[
\begin{align*}
\text{rate of reactant flow into element of volume} &= \text{rate of reactant flow out of element of volume} + \text{rate of reactant loss due to chemical reaction within the element of volume} + \text{rate of accumulation of reactant in element of volume}
\end{align*}
\]
MATERIAL AND ENERGY BALANCES IN A REACTOR

- For constant composition within the reactor (i.e. independent of position),
  - the accounting is made over the whole reactor (synonymous to integral method).

- For variable composition,
  - the accounting must be made over a differential element of volume and then integrated across the whole reactor for the appropriate flow and concentration conditions (i.e. combining both the differential and integral method of analysis).

- For the various reactor types this material balance equation simplifies to the basic *performance equation* for that type of reactor.
  - in the batch reactor the first two terms are zero;
  - in the steady-state flow reactor the fourth term disappears;
  - in the semi-batch reactor all four terms may have to be considered.
ENERGY BALANCE IN A REACTOR

- In non-isothermal operations energy balances must be used in conjunction with material balances.

- Considering the element of volume of the reactor,

  ![Diagram of energy balance](image)

  - The energy balance for any reactant (or product) is expressed as:

    \[
    \left( \frac{\text{rate of heat flow into element of volume}}{\text{volume}} \right) = \left( \frac{\text{rate of heat flow out of element of volume}}{\text{volume}} \right) + \left( \frac{\text{rate of disappearance of heat by reaction within element of volume}}{\text{volume}} \right) + \left( \frac{\text{rate of accumulation of heat within element of volume}}{\text{volume}} \right)
    \]
For a batch reactor,

While for a steady state flow reactor,

\[ F_{A0} = \text{moles fed/hr} \]
\[ v_0 = \text{m}^3 \text{ fluid entering/hr} \]
\[ C_{A0} = \text{concentration of A in the feed stream} \]
For the reaction: \( aA + bB \rightarrow rR \).

The previous figures show that there are two related measures of the extent of reaction, the concentration \( C_A \) and the conversion \( X_A \).

The relationship between \( C_A \) and \( X_A \) depends on a number of factors.

**Case 1. Constant Density Batch and Flow Systems.** It includes most liquid reactions and gas reactions run at constant temperature and density. Here \( C_A \) and \( X_A \) are related as follows:

\[
X_A = 1 - \frac{C_A}{C_{A0}} \quad \text{and} \quad dX_A = -\frac{dC_A}{C_{A0}} \quad \left\{ \begin{array}{l}
\frac{C_A}{C_{A0}} = 1 - X_A \quad \text{and} \quad dC_A = -C_{A0}dX_A.
\end{array} \right.
\]

where \( \varepsilon_A \) is the fractional volume change on complete conversion of \( A \), and

\[
\frac{C_{A0} - C_A}{a} = \frac{C_{B0} - C_B}{b} = \frac{C_R - C_{R0}}{r} \quad \text{or} \quad \frac{C_{A0}X_A}{a} = \frac{C_{B0}X_B}{b}
\]
Case 2. Batch and Flow Systems of Gases of Changing Density but with \( T \) and \( \pi \) Constant. Here the density changes because of the change in number of moles during reaction. The volume of a fluid element changes linearly with conversion, or \( V = V_0 \left( 1 + \epsilon_A X_A \right) \)

\[
X_A = \frac{C_{A0} - C_A}{C_{A0} + \epsilon_A C_A} \quad \text{and} \quad dX_A = -\frac{C_{A0}(1 + \epsilon_A)}{(C_{A0} + \epsilon_A C_A)^2} dC_A
\]

\[
\frac{C_A}{C_{A0}} = \frac{1 - X_A}{1 + \epsilon_A X_A} \quad \text{and} \quad \frac{dC_A}{C_{A0}} = -\frac{1 + \epsilon_A}{(1 + \epsilon_A X_A)^2} dX_A
\]

For \( \epsilon_A = \frac{V_{X_A=1} - V_{X_A=0}}{V_{X_A=0}} \neq 0 \)

To follow changes in the other components we have

between reactants

\[
\begin{align*}
\epsilon_A X_A &= \epsilon_B X_B \\
\frac{a \epsilon_A}{C_{A0}} &= \frac{b \epsilon_B}{C_{B0}}
\end{align*}
\]

for products and inerts

\[
\begin{align*}
\frac{C_R}{C_{A0}} &= \frac{(r/a)X_A + C_{R0}/C_{A0}}{1 + \epsilon_A X_A} \\
\frac{C_I}{C_{I0}} &= \frac{1}{1 + \epsilon_A X_A}
\end{align*}
\]
Case 3. Batch and Flow Systems for Gases in General (varying \( p, T, \pi \)) which react according to

\[
aA + bB \rightarrow rR, \quad a + b \neq r
\]

Selecting a key reactant, \( A \) as the basis for determining the conversion, then for ideal gas behavior,

\[
X_A = \frac{1}{1 + \varepsilon_A} \left( \frac{C_A}{C_{A0}} \right) \left( \frac{T\pi_0}{T_0\pi} \right)
\]

or

\[
\frac{C_A}{C_{A0}} = \frac{1 - X_A}{1 + \varepsilon_A X_A} \left( \frac{T_0\pi}{T\pi_0} \right)
\]

\[
X_A = \frac{C_{B0} - C_B}{b + \varepsilon_A} \left( \frac{C_A}{C_{A0}} \right) \left( \frac{T\pi_0}{T_0\pi} \right)
\]

or

\[
\frac{C_B}{C_{A0}} = \frac{C_{B0} - b X_A}{a + \varepsilon_A X_A} \left( \frac{T_0\pi}{T\pi_0} \right)
\]

\[
\frac{C_R}{C_{A0}} = \frac{C_{R0} + r X_A}{a} \frac{T_0\pi}{T\pi_0}
\]
For high-pressure non-ideal gas behavior replace

\[
\left( \frac{T_0 \pi}{\tau_0 \pi_0} \right) \text{ by } \left( \frac{z_0 T_0 \pi}{z T \pi} \right)
\]

where \( z \) is the compressibility factor.

To change to another key reactant, say B, note that

\[
\frac{a \varepsilon_A}{C_{A0}} = \frac{b \varepsilon_B}{C_{B0}} \quad \text{and} \quad \frac{C_{A0} X_A}{a} = \frac{C_{B0} X_B}{b}
\]

For liquids or isothermal gases with no change in pressure and density

\[
\varepsilon_A \to 0 \quad \text{and} \quad \left( \frac{T_0 \pi}{T \pi_0} \right) \to 1
\]
Example 1:

Consider a feed $C_{A0} = 100$, $C_{B0} = 200$, $C_{i0} = 100$ to a steady-flow reactor. The isothermal gas-phase reaction is

$$A + 3B \rightarrow 6R$$

If $C_A = 40$ at the reactor exit, what is $C_B$, $X_A$, and $X_B$ there?

SOLUTION:

- First sketch what is known

- Next recognize that this problem concerns Case 2.

- So evaluate $\mathcal{E}_A$ and $\mathcal{E}_B$. 
Remember

\[ \varepsilon_A = \frac{V_{X_A=1} - V_{X_A=0}}{V_{X_A=0}} \text{ and } \varepsilon_B = \frac{\varepsilon_A C_{B0}}{bC_{A0}} \]

Let’s take volumes of entering gas to be 400

at \( X_A = 0 \), \( V = 100A + 200B + 100i = 400 \)

at \( X_A = 1 \), \( V = 0A - 100B + 600R + 100i = 600 \)

So

\[ \varepsilon_A = \frac{600 - 400}{400} = \frac{1}{2} \]

And

\[ \varepsilon_B = \frac{\varepsilon_A C_{B0}}{bC_{A0}} = \frac{(1/2)(200)}{3(100)} = \frac{1}{3} \]

Therefore, calculating for \( X_A \),

\[ X_A = \frac{C_{A0} - C_A}{C_{A0} + \varepsilon_A C_A} = \frac{100 - 40}{100 + (1/2)40} = \frac{60}{120} = 0.5 \]
Calculating for XB,

\[ X_B = \frac{bC_{A0}X_A}{C_{B0}} = \frac{3(100)(0.5)}{200} = 0.75 \]

And calculating for CB,

\[ C_B = C_{B0} \left( \frac{1 - X_B}{1 + \varepsilon_B X_B} \right) = \frac{200(1 - 0.75)}{1 + (1/3)(0.75)} = 40 \]
THANK YOU FOR YOUR ATTENTION! ANY QUESTIONS?
Case 2. Batch and Flow Systems of Gases of Changing Density but with $T$ and $\pi$ Constant. Here the density changes because of the change in number of moles during reaction. The volume of a fluid element changes linearly with conversion, or $V = V_0 (1 + \varepsilon_A X_A)$

$$X_A = \frac{C_{A0} - C_A}{C_{A0} + \varepsilon_A C_A} \quad \text{and} \quad dX_A = -\frac{C_{A0}(1 + \varepsilon_A)}{(C_{A0} + \varepsilon_A C_A)^2} dC_A$$

$$\frac{C_A}{C_{A0}} = \frac{1 - X_A}{1 + \varepsilon_A X_A} \quad \text{and} \quad \frac{dC_A}{C_{A0}} = -\frac{1 + \varepsilon_A}{(1 + \varepsilon_A X_A)^2} dX_A$$

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