Chapter 2: Conversion and Reactor Sizing

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To quantify how far a reaction has progressed
How many moles of C are formed for every mole A consumed

Consider: \[ aA + bB \rightarrow cC + dD \]

The basis of calculation is always the limiting reactant

Irreversible reaction: \( X_{\text{max}} = 1.0 \) (complete conversion)
Reversible reaction: \( X_{\text{max}} = X_{\text{equilibrium}} \) (equilibrium conversion)
CONVERSION

**Batch system (X,t)**

\[ X_A = \frac{N_{A0} - N_A}{N_{A0}} \]

\[ N_A (mol) = N_{A0} - N_{A0}X \]

\[ = N_{A0} (1 - X) \]

\( N_{A0}X = \) moles of A consumed / reacted

**Flow system (X,V/W)**

\[ X_A = \frac{F_{A0} - F_A}{F_{A0}} \]

\[ F_A (mol / s) = F_{A0} - F_{A0}X \]

\[ = F_{A0} (1 - X) \]

\( F_{A0}X = \) molar flow rate at which A is consumed / reacted
For batch reactor, we are interested in determining how long to leave the reactants in the reactor to achieve a certain conversion.

From mole balance: \[ r_A V = \frac{dN_A}{dt} \]

From the conversion: \[ N_A = N_{A0} - N_{A0} X \]

This is how the Design Equation derived from mole balance equation in terms of conversion.

Differentiating with respect of time:

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

\[ N_{A0} = 0 : \text{constant with respect of time} \]

\[ r_A V = -N_{A0} \frac{dX}{dt} \rightarrow -r_A V = N_{A0} \frac{dX}{dt} \rightarrow t = N_{A0} \int_{0}^{X} \frac{dX}{-r_A V} \]
The entering molar flow rate, $F_{A0}$ (mol/s)

\[ F_{A0} = C_{A0} \nu_0 \]

\[ \frac{mol}{s} = \frac{mol}{dm^3} \cdot \frac{dm^3}{s} \]

$C_{A0}$ for gas system

\[ C_{A0} = \frac{P_{A0}}{RT_0} = \frac{y_{A0}P_0}{RT_0} \]

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

$Y_{a0}$ = entering mole fraction of A

$P_0$ = entering total pressure, kPa

$T_0$ = entering temperature, K

$P_{a0}$ = entering partial pressure

$R$ = ideal gas constant = 8.314 kPa dm$^3$/mol.K
From mole balance:

\[ V = \frac{F_{A0} - F_A}{-r_A} \]

Design Equation:

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

\[ V = \frac{F_{A0} - F_{A0} + F_{A0}X}{-r_A} \]

From the conversion:

\[ F_A = F_{A0} - F_{A0}X \]
From mole balance:

\[ \frac{dF_A}{dV} = r_A \]

Design Equation:

Differentiating with respect of volume:

\[ \frac{dF_A}{dV} = 0 - F_{A0} \frac{dX}{dV} \]

\[ r_A = -F_{A0} \frac{dX}{dV} \]

From the conversion:

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

\[ F_{A0} = 0 \text{ : constant with respect of volume} \]

\[ V = F_{A0} \int_{0}^{X} \frac{dX}{-r_A} \]
From mole balance:

\[
\frac{dF_A}{dW} = r'_A
\]

From the conversion:

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

Design Equation:

Differentiating with respect of weight of catalyst:

\[
\frac{dF_A}{dW} = 0 - F_{A0} \frac{dX}{dW}
\]

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

\[
-W = F_{A0} \int_{0}^{X} \frac{dX}{-r'_A}
\]
### Design Equations for Isothermal Reactors

<table>
<thead>
<tr>
<th>REACTOR</th>
<th>DIFFERENTIAL FORM</th>
<th>ALGEBRAIC FORM</th>
<th>INTEGRAL FORM</th>
</tr>
</thead>
<tbody>
<tr>
<td>CSTR</td>
<td>( N_{AO} \frac{dX}{dt} = (-r_A)V )</td>
<td>( V = \frac{F_{AO}(X)}{(-r_A)_{Exit}} )</td>
<td>( t = N_{AO} \int_{0}^{X} \frac{dX}{-r_A V} )</td>
</tr>
<tr>
<td>PFR</td>
<td>( F_{AO} \frac{dX}{dV} = (-r_A) )</td>
<td>( V = F_{AO} \int_{0}^{X} \frac{dX}{-r_A} )</td>
<td></td>
</tr>
<tr>
<td>PBR</td>
<td>( F_{AO} \frac{dX}{dW} = (-r'_A) )</td>
<td>( W = F_{AO} \int_{0}^{X} \frac{dX}{-r'_A} )</td>
<td></td>
</tr>
</tbody>
</table>
By sizing a chemical reactor we mean we're either determine the reactor volume to achieve a given conversion or determine the conversion that can be achieved in a given reactor type and size.

Normally, the process / experimental data will be given \((X, -r_A)\)

PFR

Simpson's One-Third Rule is one of the more common numerical methods.

Other numerical methods (see Appendix A.4, pp 1013-1015):
(i) Trapezoidal Rule (2 data points)
(ii) Simpson's Three-Eighth's Rule (4 data points)
(iii) Five-Point Quadrature Formula (5 data points)
Reactor Sizing

Levenspiel Plot

\[ \frac{F_{A0}}{-r_A} \]

\[ \frac{F_{A0}}{-r_A} \]

CSTR

PFR
REACTORS IN SERIES

Why?

- Sometimes 2 CSTR reactor volumes in series is less than the volume of 1 CSTR to achieve the same conversion.

- Can model a PFR with a large number of CSTR in series.

- In the case of PFR, whether you place 2 PFR in series or have 1 PFR, the total reactor volume required to achieve the same conversion is identical.
REACTORS IN SERIES

\[ X = 0 \]

\[ X_1 = \text{conversion achieved in the PFR} \]

\[ F_{A0} \rightarrow V_1 \rightarrow F_{A1} \rightarrow V_2 \rightarrow V_3 \rightarrow F_{A3} \]

\[ X_2 = \text{conversion achieved in the PFR & CSTR} \]

Valid only for NO side streams:

\[
\begin{align*}
F_{A1} &= F_{A0} - F_{A0} X_1 \\
F_{A2} &= F_{A0} - F_{A0} X_2 \\
F_{A3} &= F_{A0} - F_{A0} X_3
\end{align*}
\]

\[ X_3 = \text{total conversion achieved by all 3 reactors} \]
(i) CSTR in series:

\[ V_1 = \frac{F_{A0} X_1}{-r_{A1}} \]

\[ V_2 = \frac{F_{A0} (X_2 - X_1)}{-r_{A2}} \]

(ii) PFR in series:

\[ V_1 = F_{A0} \int_{0}^{X_1} \frac{dX}{-r_A} \]

\[ V_2 = F_{A0} \int_{X_1}^{X_2} \frac{dX}{-r_A} \]
(iii) CSTR + PFR in series:

\[ V_1 = \frac{F_{A0} X_1}{-r_{A1}} \]

\[ V_2 = F_{A0} \int_{X_1}^{X_2} \frac{dX}{-r_{A2}} \]

\[ V_3 = \frac{F_{A0} (X_3 - X_2)}{-r_{A3}} \]
SPACE TIME, $\tau$

☐ The time necessary to process one reactor volume by the volumetric rate entering the reactor

☐ Also called the *holding time* or *mean residence time*

\[
\tau = \frac{V}{\nu_0}
\]

\[
time = \frac{volume}{volumetric \ rate}
\]

☐ *where* $\nu_0$ *is entrance volumetric rate*
**SPACE VELOCITY (SV)**

\[
SV \equiv \frac{\nu_0}{V} = \frac{1}{\tau}
\]

- Reciprocal of the space time, \( \tau \)
- Two SV commonly used in industry:

  - **GHSV**  
    Gas Hourly Space Velocity, h\(^{-1}\)  
    \( \nu_0 \) at STP (standard temp. and pressure)

  - **LHSV**  
    Liquid Hourly Space Velocity, h\(^{-1}\)  
    \( \nu_0 \) at some reference temperature
REFERENCES

Main Reference:


Other References: