“Why, a four year old child could understand this. Someone get me a four year old child.” -- Groucho Marx

Chapter 4: Isothermal Reactor Design

Combine reactors and reactions

**Goal:** Develop a *logical* structure for designing reactors. Very hazardous to apply ‘formula plugging’ when designing reactors.

PART 1: Mole Balances in Terms of Conversion

PART 2: Mole Balances in Terms of Concentration, and Molar Flowrates
THE ALGORITHM

1. Mole Balance
2. Rate Law
3. Stoichiometry
4. Combine
5. Evaluate
   • Analytically
   • Graphically
   • Numerically
   • Software Package (polymath, mathcad, mathematica, etc)
Sec. 4.1  Design Structure for Isothermal Reactors

Figure 4-1  Isothermal reaction design algorithm for conversion.
PFR volume for a first order gas-phase reaction

1. MOLE BALANCES

PFR: \[ \frac{dX}{dV} = -\frac{\tau_A}{F_{A0}} \]

CSTR: \[ V = \frac{F_{A0}X}{-\tau} \]

BATCH: \[ \frac{dX}{dt} = \frac{-\tau_A V}{N_{A0}} \]

2. RATE LAWS

\[ -\tau_A = kC_A \]

3. STOICHIOMETRY

FLOW: \[ C_A = \frac{F_A}{V} \]

3. STOICHIOMETRY

FLOW: \[ C_A = \frac{F_A}{V} \]

4. COMBINE (First Order Gas-Phase Reaction in a PFR)

From mole balance \( \frac{dX}{dV} = -\frac{\tau_A}{F_{A0}} \)

From rate law \[ \frac{dX}{dV} = \frac{kC_A}{F_{A0}} \]

From stoichiometry \[ \frac{k}{F_{A0}} \left( \frac{C_A}{C_{A0}} \right)^{(1-X)T_0} \frac{P}{P_0} T \]

\[ \frac{dX}{dV} = \frac{k}{V_0 (1+eX)} \frac{1}{T} \]

where \( y = \frac{P}{P_0} \)

Integrating for the case of constant temperature and pressure gives

\[ V = \frac{V_0}{k} \left( 1 + \frac{1}{1-X} \right) -eX \]

Figure 4-2 Algorithm for isothermal reactors.
Scale up of liquid phase batch reactor to the design of a CSTR

**Batch Operation**

**Assumptions**

- No inflow or outflow
- Well mixed
- For liquid phase density change small, \( V = V_0 \)
- For gas phase reactions the batch reactor volume stays constant, \( V = V_0 \)

**CLOSED METAL VESSELS**

\[
\frac{1}{V} \left( \frac{dN_A}{dt} \right) = r_A
\]

Mole Balance - Batch

\[
\frac{1}{V} \left( \frac{dN_A}{dt} \right) = \frac{1}{V_0} \left( \frac{dN_A}{dt} \right) = \left( \frac{d(N_A / V_0)}{dt} \right) = \frac{dC_A}{dt} = r_A
\]

In terms of concentration

\[
- \frac{dC_A}{dt} = -r_A
\]

Form data is usual taken in
Let's take a look at a very simple example – Constant volume batch reactor

**EXAMPLE:** Calculate time necessary to achieve a given conversion, $X$ for the irreversible second order reaction.

$A \xrightarrow{} B$

**Step 1: Mole Balance**

\[ N_{A0} \frac{dX}{dt} = -r_A V_0 \]

**Step 2: Rate Law**

\[-r_A = kC_A^2 \]

**Step 3: Stoichiometry**

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

**Step 4: Combine**

\[ \frac{dX}{dt} = kC_{A0} (1 - X)^2 \]

**Step 5: Evaluate**

\[ \int_0^X \frac{dX}{kC_{A0} (1 - X)^2} = \int_0^t dt \]

\[ t = \frac{1}{kC_{A0}} \frac{(X)}{(1 - X)} \]
The following reaction takes place in a CSTR: \[ A \rightarrow B \]

Pure A is fed to the reactor under the following conditions:

- \( F_{Ao} = 10 \text{ mol/min} \)
- \( C_{Ao} = 2 \text{ mol/dm}^3 \)
- \( V = 500 \text{ dm}^3 \)
- \( k = 0.1/\text{min} \)
- Rate Law: \( -r_A = kC_A \)

What is the conversion in the CSTR?
The elementary liquid phase reaction $2A \rightarrow B$

is carried out isothermally in a CSTR. Pure A enters at a volumetric flow rate of 25 dm$^3$/s and at a concentration of 0.2 mol/dm$^3$. What CSTR volume is necessary to achieve a 90% conversion when $k = 10$ dm$^3$/(mol*s)?

1. Mole Balance
OTHER – VERY IMPORTANT STUFF

Remember HW is due on Wednesday

You have the rest of the week to redo test and submit to me

(DUE February 16th by 4 pm).

You are to work alone on this and may have the assistance of myself or Dr. Jan
Puszynski. You must sign that only YOU worked on it. A resubmitted 100 %
correct test is worth 20 pts added to your original score.

Office Hours: MF 3-4 JAP, W 10-11

T, TH LJG 1-2