CHEE 321: Chemical Reaction Engineering

Module 3: Isothermal Reactor Design

3a: Solving Reactor Design Problems
(Single Reaction in batch, CSTR, PFR)
Chapter 4.1-4.4, Fogler
Module 3a: Isothermal Reactor Design

Topics to be covered in this module

• 4-Step Algorithm for solving reactor design problem

• CSTR in-series
  – Damkohler Number \((\text{Application to design of CSTR-in-series})\)

• Still working with ideal reactors and single reactions

  “In perhaps no area of engineering is mere formula plugging more hazardous; the number of physical conditions that can arise appear infinite, and the chances of a simple formula being sufficient for the adequate design of a real reactor are vanishingly small.”

  \(\text{From Fogler, Ch 4 intro}\)
General Algorithm for Solving Isothermal Reactor Problems

1. **General Mole Balance Equation (GMBE)**
2. **Rate Laws**
   - Write down rate law in terms of limiting reactant
3. **Stoichiometry**
   - Relate concentration to volume and number of moles (for batch reactors) or to volumetric flow rate and molar flow rate (for flow reactor)
   - Relate volume or volumetric flow rate to conversion, pressure and temperature
4. **Combine and Solve**
   - Substitute rate law and stoichiometry in to the GMBE

See Fogler Figure 4.1
General Algorithm (Fogler, Figure 4-2)
Reactor Design (Single Reaction)

- **Constant volume (or volumetric flow) systems**
  - Generally easier to set up and solve
  - Liquid-phase or gas phase systems with no change in moles

  Example 1: Batch Reactor
  Example 2: Gas-Phase PFR with reversible reaction

- **Systems with changing volume (or volumetric flow)**
  - Gas phase systems with change in moles due to reaction

  Example 3: Gas-Phase reaction in a PFR
  Example 4: Gas-Phase reaction in a CSTR
Example 1

Constant volume batch reactor with reaction $A \rightarrow B$ and 2nd order reaction

**GMBE:**

$$\frac{dN_A}{dt} = r_A V ; \quad N_A = N_{A0} \text{ at } t = 0$$

**Rate Law:**

$$-r_A = kC_A^2$$

**Stoichiometry:**

$$C_A = C_{A0}(1 - X_A)$$

**Combine:**

$$N_A = C_A V ; \quad \frac{dN_A}{dt} = V \frac{dC_A}{dt} = VC_{A0} \left( -\frac{dX_A}{dt} \right)$$

$$-r_A = kC_A^2 = kC_{A0}^2 (1 - X_A)^2$$

$$\frac{dX_A}{dt} = kC_{A0}(1 - X_A)^2$$

**Integrate and Solve:**

$$t = \frac{1}{kC_{A0}} \left( \frac{X_A}{1 - X_A} \right)$$
Example 1 (cont’d):
constant volume batch reactor

For 2\textsuperscript{nd} order reaction
\[ t = \frac{1}{kC_{A0}} \left( \frac{X_A}{1 - X_A} \right) \]

For a 1\textsuperscript{st} order reaction
\[ t = \frac{1}{k} \ln \left( \frac{1}{1 - X_A} \right) \] (see Fogler Ex. 4.1)

Time to reach 90\% conversion can vary from hours to less than a second, depending on the magnitude of \( k \) (or \( kC_{A0} \)) [See Table 4.2 in Fogler]

1\textsuperscript{st} order: if \( k=10^{-4} \text{ s}^{-1} \), 6.4 h to reach 90\% conversion
2\textsuperscript{nd} order: if \( kC_{A0}=10^{-4} \text{ L/(mol-s)} \), 25 h to reach 90\% conversion

Practical issues with batch reactors:
- Table 4.3 in Fogler
- Can you think of others?
Example 2
(CSTR, constant volumetric flow)

The elementary liquid-phase reaction

\[ A + B \xrightleftharpoons[k_1]{k_2} R + S \]

is to take place in a 120 L steady-state mixed reactor. Two feed streams, one containing 2.8 mol-A/L and the other containing 1.6 mol-B/L, are to be introduced in equal volumes into the reactor, and 75% conversion of the limiting component is desired. What should be the flow rate of each stream? Assume a constant density throughout, with \( k_1 = 7 \text{ Lmol}^{-1}\text{min}^{-1} \) and \( k_2 = 3 \text{ Lmol}^{-1}\text{min}^{-1} \).
**CSTR in series**

Liquid-phase ($v = v_0$), first-order reaction

**Mole Balance on CSTR-1**

\[ V_1 = \frac{F_{A0} - F_A}{-(r_A)_{at \ X=X_1}} = v_0 \left[ C_{A0} - C_{A1} \right] \frac{1}{k_1 C_{A1}} \]

\[ \tau_1 k_1 = \frac{[C_{A0} - C_{A1}]}{C_{A1}} = \frac{C_{A0}}{C_{A1}} - 1 \]

\[ C_{A1} = \frac{C_{A0}}{1 + \tau_1 k_1} \]

**Mole Balance on CSTR-2**

\[ V_2 = \frac{F_{A1} - F_{A2}}{-(r_A)_{at \ X=X_2}} = v_0 \left[ C_{A1} - C_{A2} \right] \frac{1}{k_2 C_{A2}} \]

\[ \tau_2 k_2 = \frac{[C_{A1} - C_{A2}]}{C_{A2}} = \frac{C_{A1}}{C_{A2}} - 1 \]

\[ C_{A2} = \frac{C_{A1}}{1 + \tau_2 k_2} \]

\[ C_{A2} = \frac{C_{A0}}{[1 + \tau_1 k_1][1 + \tau_2 k_2]} \]
\( n \)-Equal Sized CSTR in series

\[ \tau = \frac{V}{v_0} \]

All CSTR’s are operated at same temperature

\[ \therefore k \text{ is same in all reactors} \]

\[
\begin{align*}
C_{A1} &= \frac{C_{A0}}{1 + \tau k} \\
C_{A2} &= \frac{C_{A1}}{1 + \tau k} \\
C_{A3} &= \frac{C_{A2}}{1 + \tau k} \\
C_{An} &= \frac{C_{An-1}}{1 + \tau k}
\end{align*}
\]

\[
C_{An} = \frac{C_{A0}}{(1 + \tau k)^n} = \frac{C_{A0}}{(1 + Da)^n}
\]
Da is a *dimensionless* number that can provide a *quick* estimate of the degree of conversion in continuous flow reactors.

\[
Da = \frac{(-r_{A0})}{F_{A0}} V
\]

*Note: rate is calculated at inlet conditions*

**First-order reaction**

\[
Da = \frac{-r_{A0}}{F_{A0}} \frac{V}{v_0 C_{A0}} = \tau k
\]

**Second-order reaction**

\[
Da = \frac{-r_{A0}}{F_{A0}} \frac{V}{v_0 C_{A0}^2} = \tau k C_{A0}
\]

*Da \leq 0.1* usually results in conversion less than 10%

*Da \geq 10* usually results in conversion greater than 90%
Figure 4-4  Conversion as a function of the number of tanks in series for different Damköhler numbers for a first-order reaction.
If you had n-equal sized reactors available and had the option of setting them in series or parallel, which configuration would you choose to achieve maximum conversion for a first-order reaction occurring in liquid phase?

\[ X = X_{\text{mix}} \]

- See Fogler 4.3, Ex. 4-2
- Remember your Levenspiel plots

Why run reactors in parallel?
Example 3 (PFR, variable flow)

Estimate the volume of a plug-flow reactor (in m3) required for production of ethylene from ethane \((\text{C}_2\text{H}_6 \rightarrow \text{C}_2\text{H}_4 + \text{H}_2)\) based on the following data and assumptions:

a. The feed is pure ethane at 1 kg s\(^{-1}\), 1000K and 2 bar (abs).

b. The reaction is first-order and irreversible at low conversion, with \(k = 0.254 \text{ s}^{-1}\) at 1000 K.

c. The reactor is operated isothermally and isobarically.

d. Conversion of ethane is 20% at the outlet.

(Similar to Fogler Ex. 4.3)

Effect of changing \(N_T\): Examine Fogler Fig 4.7 and 4.8)
Example 3.4 (CSTR, variable flow)

It is being considered that the following gas-phase reaction be carried out in a CSTR: \( \text{A} + 2\text{B} \rightarrow 4\text{C} \)

The reactor will be operated isobarically and isothermally. The rate law for the reaction is given as: \( (-r_A) = k \cdot C_A \cdot C_B \)
where, \( k = 8 \text{ L/mol-min} \) at the operating temperature.

The total feed volumetric flow rate to the reactor at operating temperature and pressure is 10 L/min. The feed consists of A, B and an inert (I). The feed molar flow rates are \( F_{A0} = F_{B0} = 1 \text{ mol/s} \) and \( F_{I0} = 2 \text{ mol/s} \).

a) Calculate the volume of reactor required to achieve 80% conversion of the limiting reactant.

b) If all other conditions are kept constant (including total volumetric flow rate) but no inert is present in the feed, calculate the reactor volume required to achieve 80% conversion of limiting reactant.
Week 5: Design Week

• Special lectures by design team (see topics at http://www.chemeng.queensu.ca/courses/integratedDesign/)

• Intro to UNISIM software in tutorial(s)

• Work on CHEE 321 Design Assignment 1
  – Design TAs Raul Moraes and Devon Lehrer

• Dr. Hutchinson will be back on Wed 15Oct
  – I’m giving Polymer Reaction Engineering talks in Germany (×2) and in Chicago

• Happy Thanksgiving!