Chemical Reaction Engineering (CRE) is the field that studies the rates and mechanisms of chemical reactions and the design of the reactors in which they take place.
Lecture 7 – Tuesday 1/29/2013

- Block 1: Mole Balances
- Block 2: Rate Laws
- Block 3: Stoichiometry
- Block 4: Combine

California Professional Engineers Exam

In the past, the exam has not been curved, 75% or better to pass

Problem 4-12
1. MOLE BALANCES

- **PFR**
  \[ \frac{dX}{dV} = \frac{-r_A}{F_{Ao}} \]

- **CSTR**
  \[ \frac{dX}{dt} = \frac{-r_A}{N_{AD}} \]

- **BATCH**
  \[ \frac{dX}{dt} = \frac{-r_A V}{N_{AD}} \]

2. RATE LAWS

- \[ -r_A = kC_A \]
- \[ -r_A = \frac{kC_A}{1 + K_A C_A} \]
- \[ -r_A = k \left[ \frac{C_A - \frac{C_B C_C}{K_0}}{K_0} \right] \]

3. STOICHIOMETRY

- **FLOW**
  \[ F_A = F_{Ao} (1 - x) \]

- **LIQUID**
  \[ N_A = N_{Ao} (1 - x) \]

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

   From mole balance
   \[ \frac{dX}{dV} = \frac{-r_A}{F_{Ao}} = \frac{kC_A}{F_{Ao}} = \frac{k}{F_{Ao}} \left( \frac{C_{Ao} (1 - x)}{(1 + \varepsilon X)} \right) \frac{T_0}{P_0} \]

   From rate law
   \[ \frac{dX}{dV} = \frac{k (1 - x) y T_0}{P_0 (1 + \varepsilon X) T} \]

   Integrating for the case of constant temperature and pressure gives
   \[ V = \frac{c_0}{k} \left[ (1 + \varepsilon) \ln \left( \frac{1}{1 - x} \right) - \varepsilon x \right] \]
General Guidelines for the California Professional Engineering Exam

Some hints:

1. Group unknown parameters/values on the same side of the equation
   
   example: \[ \text{[unknowns]} = \text{[knowns]} \]

2. Look for a Case 1 and a Case 2 (usually two data points) to make intermediate calculations

3. Take ratios of Case 1 and Case 2 to cancel as many unknowns as possible

4. Carry all symbols to the end of the manipulation before evaluating, UNLESS THEY ARE ZERO
**P. E. Example**

**P5-17B California Professional Exam Problem**

\[
A \rightleftharpoons B \quad K_C = 5.8
\]

\[
X_1 = 0.55
\]

\[
W_1 = W_2
\]

\[
X_2 = \frac{\text{Total moles reacted at Point 2}}{\text{Mole fed to first reactor}}
\]

**Knowns:** Intermediate Conversion, \( X_1 \), \( K_C \), and \( W_1 = W_2 \)

**Unknowns:** \( F_{A0} \), \( W_1 \), \( C_{A0} \)
P. E. Example

1) Mole Balances

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

2) Rate Laws

\[-r_A = k \left[ C_A - \frac{C_B}{K_C} \right] \]

3) Stoichiometry

**Liquid**, \( \nu = \nu_0 \)

\[ C_A = \frac{F_A}{\nu_0} = \frac{F_{A0}(1 - X)}{\nu_0} = C_{A0}(1 - X) \]

\[ C_B = \frac{F_B}{\nu_0} = \frac{F_{A0}X}{\nu_0} = C_{A0}X \]
P. E. Example

4) Combine

\[-r_A = kC_{A0} \left[ 1 - X - \frac{X}{K_C} \right] \]

\[
\frac{dX}{dW} = \frac{-r'_A}{F_{A0}} = \frac{kC_{A0}}{F_{A0}} \left[ 1 - \left( 1 + \frac{1}{K_C} \right) X \right]
\]

5) Evaluate

\[W_1 = W_2\]

\[W_1 = \frac{F_{A0}}{kC_{A0}} \int_0^X \frac{dX}{1 - \left( 1 + \frac{1}{K_C} \right) X} = W_2 = \frac{F_{A0}}{kC_{A0}} \int_{X_1}^{X_2} \frac{dX}{1 - \left( 1 + \frac{1}{K_C} \right) X}\]
P. E. Example

\[
W_1 = \frac{F_{A0}}{kC_{A0}} \ln \left( 1 + \frac{1}{K_C} \right) \frac{1}{1 - \left( 1 + \frac{1}{K_C} \right) X_1} = \frac{F_{A0}}{kC_{A0}} \ln \left( \frac{1 - \left( 1 + \frac{1}{K_C} \right) X_1}{1 - \left( 1 + \frac{1}{K_C} \right) X_2} \right)
\]

Cancel unknowns \( F_{A0}, k \) and \( C_{A0} \)

\[
X_2 = \left[ 1 - \left( 1 - \left( 1 + \frac{1}{K_C} \right) X_1 \right) \right] ^2
\]

Substitute \( X_1 = 0.55 \) and \( K_C = 5.8 \)

\[
X_2 = 0.745
\]
P. E. Example

Part 2

\[
X_{\text{overall}} = \frac{F_{A0} - F_{A2}}{F_{A0}}
\]

\[
F_{A2} = F_{A1} (1 - X'_2)
\]

Conversion \(X_2\) based on \(F_{A1}\)
P. E. Example

\[ W_1 = \frac{F_{A0}}{kC_{A0}} \left( \frac{1}{1 + \frac{1}{K_C}} \right) \ln \left( \frac{1}{1 - \left(1 + \frac{1}{K_C}\right)X_1} \right) \]

\[ W_2 = \frac{F_{A1}}{kC_{A0}} \int_0^{X_2'} \frac{dX}{1 - \left(1 + \frac{1}{K_C}\right)X} = \frac{F_{A1}}{kC_{A0}} \left( \frac{1}{1 + \frac{1}{K_C}} \right) \ln \left( \frac{1}{1 - \left(1 + \frac{1}{K_C}\right)X'} \right) \]

\[ W_1 = W_2 \]

\[ F_{A1} = F_{A0} \left(1 - X_1 \right) \]

Substitute for \( F_{A1} \) and cancel \( F_{A0}, C_{A0}, k \)

\[ \ln \left( \frac{1}{1 - \left(1 + \frac{1}{K_C}\right)X_1} \right) = (1 - X_1) \ln \left( \frac{1}{1 - \left(1 + \frac{1}{K_C}\right)X'} \right) \]

\[ X_1 = 0.55 \quad K_C = 5.8 \]
P. E. Example

One equation and one unknown

Solving for $X_2'$

$$X_2' = 0.768$$

$$X_{overall} = \frac{F_{A0} - F_{A2}}{F_{A0}} = \frac{F_{A0} - F_{A1}(1 - X_2')}{F_{A0}} = \frac{F_{A0} - F_{A0}(1 - X_1)(1 - X_2')}{F_{A0}}$$

$$= 1 - (1 - X_1)(1 - X_2') = 0.895$$

$$X_{overall} = 0.895$$
End of Lecture 7