Lecture 7

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 e*xam has not been curved,*

  75% or better to pass

  Problem 4-12

Choices

1. MOLE BALANCES

PFR	CSTR	BATCH
$\frac{dX}{dV} = \frac{-r_A}{F_{A0}}$	$V = \frac{F_{A0}X}{-r_A}$	$\frac{dX}{dt} = \frac{-r_A V}{N_{A0}}$

2. RATE LAWS

$-r_A = kC_A$

$-r_A = \frac{kC_A}{1 + K_A C_A}$

$-r_A = k\left[C_A - \frac{C_B C_C}{K_e}\right]$

3. STOICHIOMETRY

FLOW: $C_A = \frac{F_A}{v}$, $F_A = F_{A0}(1 - X)$

BATCH: $C_A = \frac{N_A}{V}$, $N_A = N_{A0}(1 - X)$

LIQUID Constant flow rate	IDEAL GAS Variable flow rate	IDEAL GAS Variable volume	LIQUID OR GAS Constant volume
$v = v_0$	$v = v_0(1 + \varepsilon X)\frac{P_0}{P}\frac{T}{T_0}$	$V = V_0(1 + \varepsilon X)\frac{P_0}{P}\frac{T}{T_0}$	$V = V_0$
$C_A = C_{A0}(1 - X)$	$C_A = \frac{C_{A0}(1 - X)}{(1 + \varepsilon X)}\frac{P}{P_0}\frac{T_0}{T}$	$C_A = \frac{C_{A0}(1 - X)}{(1 + \varepsilon X)}\frac{P}{P_0}\frac{T_0}{T}$	$C_A = C_{A0}(1 - X)$

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

From mole balance — From rate law — From stoichiometry

$$\frac{dX}{dV} = \frac{-r_A}{F_{A0}} = \frac{kC_A}{F_{A0}} = \frac{k}{F_{A0}}\left(C_{A0}\frac{(1 - X)}{(1 + \varepsilon X)}\right)\frac{P}{P_0}\frac{T_0}{T}$$

$$\frac{dX}{dV} = \frac{k}{v_0}\frac{(1 - X)}{(1 + \varepsilon X)}\, y\, \frac{T_0}{T}, \text{ where } y = \frac{P}{P_0} \qquad \text{(A)}$$

Integrating for the case of constant temperature and pressure gives

$$V = \frac{v_0}{k}\left[(1 + \varepsilon)\ln\left(\frac{1}{1 - X}\right) - \varepsilon X\right] \qquad \text{(B)}$$

General Guidelines for the California Professional Engineering Exam

Some hints:

1. Group unknown parameters/values on the same side of the equation

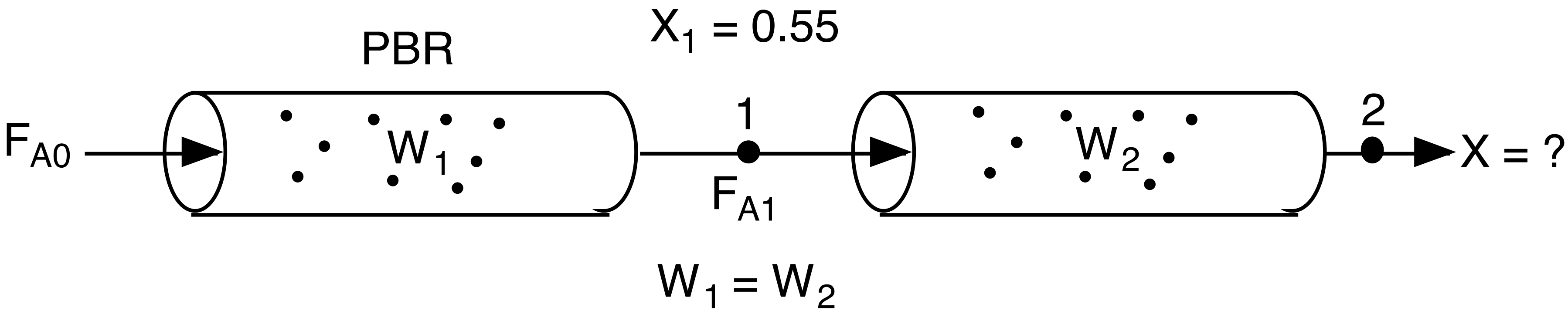
   <u>example:</u> [unknowns] = [knowns]

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

P5-17$_B$ California Professional Exam Problem

$$A \rightleftarrows B \quad K_C = 5.8$$



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

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, $\upsilon = \upsilon_0$

$$C_A = \frac{F_A}{\upsilon_0} = \frac{F_{A0}(1-X)}{\upsilon_0} = C_{A0}(1-X)$$

$$C_B = \frac{F_B}{\upsilon_0} = \frac{F_{A0}X}{\upsilon_0} = C_{A0}X$$

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

$$W_1 = W_2$$

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

P. E. Example

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

Cancel unknowns F_{A0}, k and C_{A0}

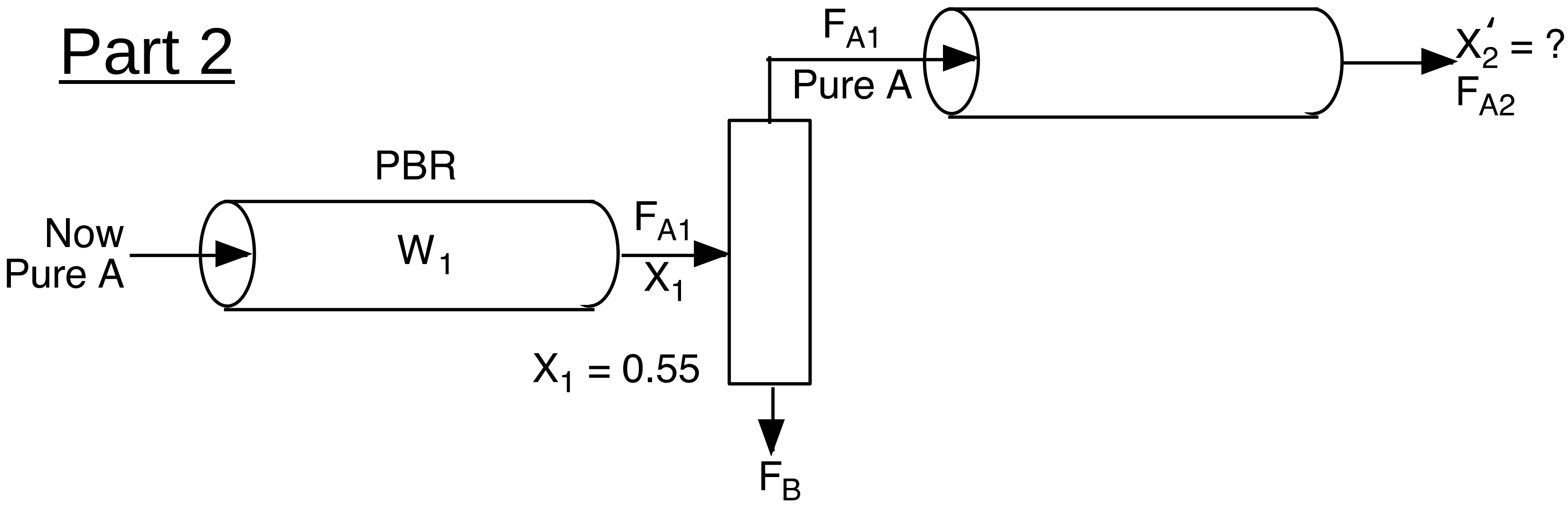
$$X_2 = \frac{\left[1-\left(1-\left(1+\frac{1}{K_C}\right)X_1\right)^2\right]}{1+\frac{1}{K_C}}$$

Substitute $X_1 = 0.55$ and $K_C = 5.8$

$$\boxed{X_2 = 0.745}$$

P. E. Example

Part 2



$$X_{overall} = \frac{F_{A0} - F_{A2}}{F_{A0}}$$

$$F_{A2} = F_{A1}(1 - X'_2)$$

Conversion X'_2 based on F_{A1}

P. E. Example

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

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

$$W_1 = W_2$$

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

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

$$\ln \frac{1}{\left(1-\left(1+\frac{1}{K_C}\right)X_1\right)} = \left(1-X_1\right) \ln \frac{1}{1-\left(1+\frac{1}{K_C}\right)X_2'}$$

$$X_1 = 0.55 \qquad K_C = 5.8$$

P. E. Example

One equation and one unknown

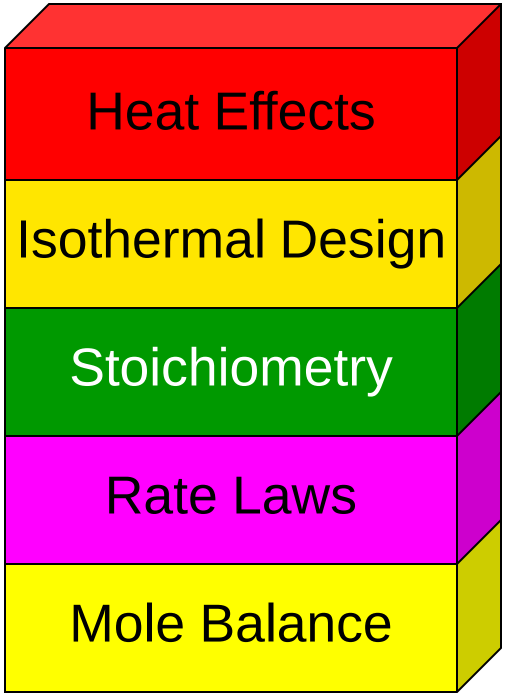
Solving for X_2'

$$X_2' = 0.768$$

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

$$= 1 - \left(1 - X_1\right)\left(1 - X_2'\right) = \underline{0.895}$$

$$\boxed{X_{overall} = 0.895}$$


Heat Effects
Isothermal Design
Stoichiometry
Rate Laws
Mole Balance

End of Lecture 7