ChE 349 – Review of Reactor Design with Heat Effects

IMPORTANT ISSUES YOU NEED TO CONSIDER

• Species Balance equation (batch, CSTR, PFR)
• Constant or variable density
• Kinetics /concentrations /conversion
• Energy balance equation (batch, CSTR, PFR)
• Heat effect (adiabatic or isothermal)
• Heat capacities (variable or constant)
• Heat of reaction (variable or constant)
• Solve simultaneous balance equations
• Math solution (analytical or numerical)

BATCH SPECIES BALANCE

\[ r_A V = \frac{dN_A}{dt} \]

→ Usually write \( N_A, r_A \) in terms of \( C_A \) or \( X_A \)
→ \( r_A = f(X_A, T) \)

BATCH ENERGY BALANCE

\[ \dot{Q} - \dot{W}_s + (-r_A)(-\Delta H_{rA})V = V \sum_i C_i C_{pi} \left( \frac{dT}{dt} \right) \]

→ How to write \( Q, C_{pi}, \) and \( \Delta H_{rA} \)
→ Common form: \( \dot{Q} = UA(T_a - T) \)
→ Usually write \( \sum_i C_i C_{pi} = C_A \left( \sum_i \theta_{C_{pi}} + X_A \Delta c_p \right) \)
**CSTR SPECIES BALANCE** *(steady state)*

\[ F_{A0} - F_A + r_A V = 0 \]

→ Usually, write \( F_A \) and \( r_A \) in terms of \( X_A \)
→ \( r_A = f(X_A, T) \)

**CSTR ENERGY BALANCE** *(steady state)*

\[
\dot{Q} - \dot{W}_S - \sum_{i=1}^{n} \left[ F_{io} \int_{T_o}^{T} C_{pi} dT + (-r_A)(-\Delta H_{rA}) \right] V = 0
\]

→ How to write \( Q \), \( C_{pi} \), and \( \Delta H_{rA} \)
→ Common form: \( \dot{Q} = UA(T_a - T) \)
→ Can write: \( F_{io} = F_{Ao} \theta_i \)
→ Can write: \( -r_A V = F_{Ao} X_A \)

**PFR SPECIES BALANCE** *(steady state)*

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

→ Usually, write \( F_A \) and \( r_A \) in terms of \( X_A \)
→ \( r_A = f(X_A, T) \)

**PFR ENERGY BALANCE** *(steady state)*

\[
\frac{dT}{dV} = \frac{-r_A(-\Delta H_R) + d\dot{Q}/dV}{F_{Ao}(\sum_{i=1}^{n} \theta_i C_{pi} + X_A \Delta C_p)}
\]
→ How to write $dQ/dV$, $C_{pi}$, $\Delta C_p$, and $\Delta H_R$

Typical form: $dQ/dV = U_a(T_a - T)$

**HEAT CAPACITIES AND HEAT OF REACTION**

- $C_{pi}$ typically constant for liquids
- For gases, $C_{pi}$ varies with $T$
  (e.g. $C_{pi} = \alpha_i + \beta_i T + \gamma_i T^2$)
- $\Delta H_R = \Delta H_R \Big|_T + \int_{T_i}^{T_f} \Delta C_p dT$
- For reaction $A + \frac{b}{a} B \rightarrow \frac{c}{a} C + \frac{d}{a} D$, overall change in heat capacity due to reaction:
  
  $$\Delta C_p = \frac{c}{a} C_{pC} + \frac{d}{a} C_{pD} - \frac{b}{a} C_{pB} - C_{pA}$$

**CONSTANT OR VARIABLE DENSITY**

Flow Reactor (CSTR or PFR)
- * Liquids $\rightarrow$ constant density $\rightarrow$ constant volumetric flow rate $v$
- * Gases $\rightarrow$ possible variable density $\rightarrow$ volumetric flow rate $v$

$$v = v_o \left( \frac{P_o}{P} \right) \left( \frac{T}{T_o} \right) (1 + \xi_A X_A)$$

**KINETICS /CONCENTRATIONS /CONVERSION**

Stoichiometry: $A + \frac{b}{a} B \rightarrow \frac{c}{a} C + \frac{d}{a} D$

$\nu_A = -1$, $\nu_B = -\frac{b}{a}$, $\nu_C = \frac{c}{a}$, $\nu_D = \frac{d}{a}$,
For gas phase systems only: \( \varepsilon_A = \delta_A y_{Ao} \)
\[
\delta_A = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1
\]

Rate Expression
- \(-r_A = \text{function}\ (T, C_i)\)
- Elementary vs. global, kinetic orders
- Rate constant \( k = A_t \exp(-E_{\text{act}}/RT) \)

Conversion (flow reactor)
\[
X_A = \frac{F_{Ao} - F_A}{F_{Ao}}
\]

Species Concentrations (flow reactor)
\[
C_i = \frac{F_i}{V} = \frac{F_{Ao}(\Theta_i + \eta_i X_A)}{V}
\]
\[
\theta_i = \frac{F_{io}}{F_{Ao}} \quad \eta_i \text{ from stoichiometry}
\]

Conversion (batch reactor)
\[
X_A = \frac{N_{Ao} - N_A}{N_{Ao}}
\]

Species Concentrations (batch reactor)
\[
C_i = \frac{N_i}{V} = \frac{N_{Ao}(\Theta_i + \eta_i X_A)}{V}
\]
\[
\theta_i = \frac{N_{io}}{N_{Ao}} \quad \eta_i \text{ from stoichiometry}
\]