CSTR Algorithm

1.) Given X
Find T and V
Solution: linear progression of calc T \( \rightarrow \) cal k \( \rightarrow \) calc \( K_C \) \( \rightarrow \) calc \( -r_A \) \( \rightarrow \) calc V

2.) Given T
Find X and V
Solution: linear progression of calc k \( \rightarrow \) cal \( K_C \) \( \rightarrow \) calc X \( \rightarrow \) calc \( -r_A \) \( \rightarrow \) calc V

3.) Given V
Find X at T
Solution: plot \( X_{EB} \ vs. \ T \) and \( X_{MB} \ vs. \ T \) on the same graph:

Can exclude if irreversible
Second Order Reaction Carried Out Adiabatically in a CSTR

The acid-catalyzed irreversible liquid-phase reaction

\[ A \rightarrow B \]

\[ \Delta H_{\text{RX}}(300 \text{ K}) = -3300 \text{ cal/mol} \cdot ^\circ \text{C} \]

\[ C_{P_A} = 15 \text{ cal/mol} \cdot ^\circ \text{C} \]

\[ C_{P_B} = 15 \text{ cal/mol} \cdot ^\circ \text{C} \]

\[ C_{P_S} = 18 \text{ cal/mol} \cdot ^\circ \text{C} \]

\[ k(300 \text{ K}) = 0.0005 \text{ dm}^3/\text{mol} \cdot \text{min} \]

\[ E = 15,000 \text{ cal/mol} \]

is carried out adiabatically in a CSTR.

The reaction is second order in A. The feed, which is equimolar in a solvent (which contains the catalyst) and A, enters the reactor at a total volumetric flow rate of 10 dm$^3$/min with the concentration of A being 4M. The entering temperature is 300 K.

(a) What CSTR reactor volume is necessary to achieve 80% conversion?
Energy Balance CSTR with heat effects

\[ \dot{Q} - \dot{W}_s - F_{A0} \sum_{i=1}^{n} \Theta_i C_{Pi} [T - T_{i0}] - [\Delta H^\circ_{Rx}(T_R) + \Delta C_P(T - T_R)]F_{A0} X = 0 \]

Substitute expression for Q in and divide by Fa0, neglecting Ws

\[ \frac{UA}{F_{A0}} (T_{a1} - T) - \sum_{i=1}^{n} \Theta_i C_{Pi} [T - T_{i0}] - [\Delta H^\circ_{Rx}(T_R) + \Delta C_P(T - T_R)] X = 0 \]

\[ X = \frac{\frac{UA}{F_{A0}} (T - T_a) + \sum_{i=1}^{n} \Theta_i C_{Pi} [T - T_{i0}]}{\frac{UA}{F_{A0}} - [\Delta H^\circ_{Rx}(T_R) + \Delta C_P(T - T_R)]} \]

\[ T = \frac{F_{A0} X[-\Delta H^\circ_{Rx}(T_R)] + UAT_a + F_{A0} \sum \Theta_i C_{Pi} T_{i0}}{UA + F_{A0} \sum \Theta_i C_{Pi}} \]
Energy Balance CSTR – for multiple reactions, $W_s = 0$

$$UA(T_{a1} - T) - F_{A0} \sum_{i=1}^{n} \theta_i C_{pi} [T - T_{i0}] - [\Delta H^\circ_{Rx}(T_R) + \Delta C_p(T - T_R)]F_{A0}X = 0$$

From the mole balance

$$V = \frac{F_{A0}X}{-r_A(X, T)}$$

$$UA(T_{a1} - T) - F_{A0} \sum_{i=1}^{n} \theta_i C_{pi} [T - T_{i0}] - [\Delta H^\circ_{Rx}(T_R) + \Delta C_p(T - T_R)](-r_AV) = 0$$

So for multiple reactions what do we do?

For $q$ reactions, and $n$ species we sum up

$$UA(T_{a1} - T) - F_{A0} \sum_{i=1}^{n} \theta_i C_{pi} [T - T_{i0}] - V \sum_{i=1}^{q} r_{ij} \Delta H^\circ_{Rxij}(T_R) + \Delta C_p(T - T_R) = 0$$
Preparation for the test:

2 questions –

**Chapter 6**  Series or Parallel reactions in various reactors

  Rate law expressions, selectivity, combined with mole balances

  Review quiz

**Chapter 8**

  Energy Balances with and without heat effects

  CSTR –

  go thru example 8-8 and 8-9 to prepare

Homework due date extended to Wednesday!