Lecture # 22 CHE331A

Energy Balance for reactors

Adiabatic Flow Reactors

Determined relationship between T and X

Species and Energy balance for an adiabatic PFR

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Adiabatic PFR as an example for Design/Analysis

- Example 8.3: $A \rightleftharpoons B$, e.g., $nC_4H_{10} \rightleftharpoons i - C_4H_{10}$ (gasoline additive)
- Reaction in a high-pressure adiabatic PFR species in liquid-phase
- $F_{A0} = 163\ kmol/h$; $C_{A0} = 9.3\ kmol/m^3$; $X = 0.70$

  Inlet is 90 mol% n-butane and 10 mol% i-pentane (inert); $T_0 = 330\ K$

  $\Delta h^0_{Rxn} = -6900 \frac{\mathrm{J}}{\mathrm{mol\ butane}}$ (exothermic reaction)

  $E = 65.7 \frac{kJ}{mol}$; $k = 31.1 h^{-1}$ at 360 K; $K_C = 3.03\ at\ 60℃\ (= 333\ K)$

  $C_{P,n-B} = 141 \frac{J}{mol}$; $C_{P,i-B} = 141 \frac{J}{mol}$; $C_{P,i-P} = 161 \frac{J}{mol}$

Design/Analysis of a PFR operating under adiabatic conditions

- Mol Balance equation for PFR: $F_{A0}\frac{dX}{dV} = -r_A$
- Rate law: $nC_4H_{10} \rightleftharpoons i - C_4H_{10}$ $-r_A = k\left(C_A - \frac{C_B}{K_C}\right)$
- Temperature effect of k and K_C given by:
  - $k = k_1.exp\left[\frac{E}{R}\left(\frac{1}{T_1} - \frac{1}{T}\right)\right]$
  - $K = K_{C,2}.exp\left[\frac{\Delta H_{Rxn}}{R}\left(\frac{1}{T_2} - \frac{1}{T}\right)\right]$
- Liquid-phase reaction: $C_A = C_{A0}.(1 - X)$ and $C_B = C_{A0}.X$

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

The relationship between temperature and conversion

- $F_{A0}\frac{dX}{dV} = -r_A$ with $-r_A = kC_{A0}\left[1-(1+\frac{1}{K_C})\right]$ need $T = T(X)$
- Energy balance: $T = \frac{X[-\Delta h^0_{Rxn}(T_R)]+\sum[\theta_i C_{P,i} T_0]+X\Delta C_p T_R}{\sum \theta_i C_{P,i}+X\Delta C_P}$
- With $\Delta C_p = 0$ since $C_{P,n-B} = 141\frac{J}{mol} = C_{P,i-B}$
- And $\sum \theta_i C_{P,i} = C_{P,n-B} + \frac{1}{9}C_{P,i-P} = 141 + \frac{1}{9} * 161 = 159\frac{J}{mol.K}$
  - since 90% $C_{P,n-B}$ and 10% $C_{P,i-P}$
- $T = T_0 + \frac{X[-\Delta h^0_{Rxn}]}{\sum \theta_i C_{P,i}} = 330 + \frac{-(-6900)*X}{159}$; $\boxed{T = 330 + 43.4X}$ in Kelvin

Reversible reactions posses additional constraints

- For $T = 330 + 43.4X$ the temperature at X = 0.7 is T = 360.3
- Important to check the temperature when the equilibrium conversions (X_e) will reach 0.7
- For $nC_4H_{10} \rightleftharpoons i - C_4H_{10};$ $K_C = \frac{Xe}{1-Xe}$ and for $X_e = 0.7; K_C = 2.33$
- $K_C = K_{C,2}.exp\left[\frac{\Delta H_{Rxn}}{R}\left(\frac{1}{T_2} - \frac{1}{T}\right)\right]$; and $K_{C,2} = 3.03\ at\ T_2 = 333\ K$
- And, $ln\left(\frac{K_C}{3.03}\right) = -830.3\left(\frac{T-333}{333*T}\right)$ T = 372 K
- Thus, 372 K is the maximum possible temperature permissible, which is less than the temperature as per the energy balance equation

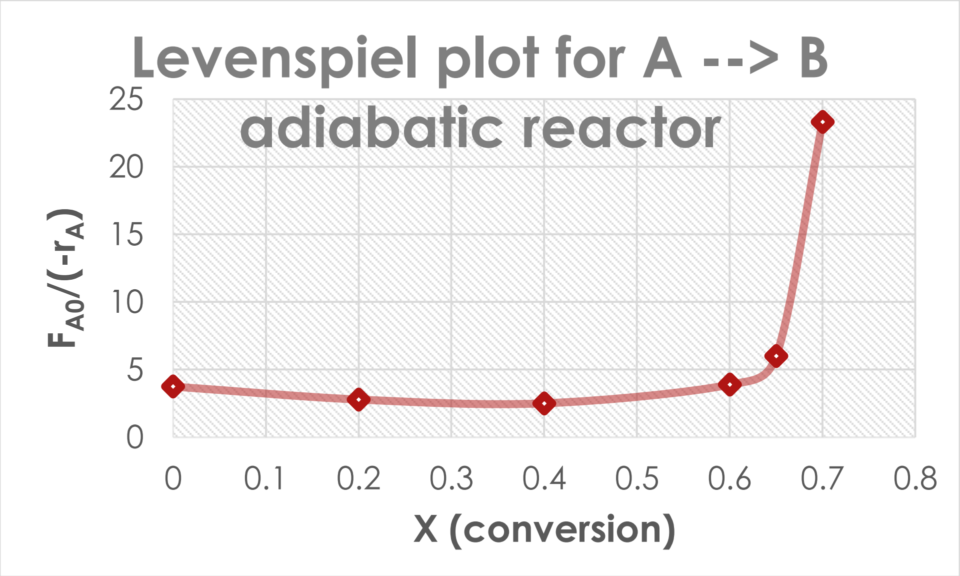
The Levenspiel plot for determining the reactor volume

- To make the Levenspiel plot we need the value of $\frac{F_{A0}}{-r_A}$ as a function of X
- To determine $\frac{F_{A0}}{-r_A}$, $-r_A = kC_{A0}\left[1-\left(1+\frac{1}{K_C}\right)X\right]$ is required for different X (or T)
- To generate such a plot the rate and equilibrium constant as a function of temperature needs to be determined
  - $k = k_1.exp\left[\frac{E}{R}\left(\frac{1}{T_1}-\frac{1}{T}\right)\right]$; $k = 31.1exp\left[7906\left(\frac{T-360}{360T}\right)\right]h^{-1}$
  - $K_C = K_{C,2}.exp\left[\frac{\Delta H_{Rxn}}{R}\left(\frac{1}{T_2}-\frac{1}{T}\right)\right]$; $K_C = 3.03exp\left[-830.3\left(\frac{T-333}{333T}\right)\right]$

The table for making the Levenspiel plot

X	T (K)	k (h^{-1})	K_C	$-r_A$	$F_{A0}/(-r_A)$ m^3
0.00	330.0	4.22	3.1	39.2	3.74
0.20	338.7	7.66	2.9	52.8	2.78
0.40	347.3	14.02	2.73	58.6	2.50
0.60	356.0	24.27	2.57	37.7	3.88
0.65	358.1	27.74	2.54	24.5	5.99
0.70	360.3	31.67	2.50	6.2	23.29

Volume for conversion of 0.7 is 2.60 m^3



Analysis of an adiabatic CSTR

- For a CSTR, the volume to achieve 70% conversion is:
- $V = \frac{F_{A0}}{-r_A} X = 23.29 * 0.7 = 16.3\ m^3$
- For a CSTR, the volume to achieve 40% conversion is:
- $V = \frac{F_{A0}}{-r_A} X = 2.5 * 0.4 = 1\ m^3$
- For PFR, the volume is given by integration (about 1.15 m^3)