Lecture # 7.1 CHE331A

Mole balance equations for reactors

Rate law and its dependence on concentration and temperature

Rate law in terms of conversion (stoichiometric table) for constant and variable volume

Analysis of n-CSTRs in series and parallel and the manufacture of EG

Analysis of PFRs for gas-phase reactions with variable volume

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Gas phase reactions are primarily carried out in PFRs

▶ In PFRs (Tubular Reactors) flow is turbulent, and there are NO radial gradients of T, P, velocity or conc $\rightarrow$ flow in reactor is like a plug

▶ Mole balance equation for PFR: $\qquad F_{A0}\dfrac{dX}{dV} = -r_A$

▶ Rate law for A $\rightarrow$ products: $\qquad -r_A = kC_A^2$, then

$$\frac{dX}{dV} = \frac{k.C_A^2}{F_{A0}}$$

▶ For $\dot{v} = \dot{v}_0$ then $C_A = C_{A0}(1-X)$, and after substituting

$$V = \frac{F_{A0}}{k.C_{A0}^2}\int_0^X \frac{dX}{(1-X)^2}$$

Design equation for PFR in Damkohler number

$$V = \frac{F_{A0}}{k.C_{A0}^2} \int_0^X \frac{dX}{(1-X)^2} = \frac{\dot{v}_0}{k.C_{A0}} \cdot \frac{X}{(1-X)}$$

▶ Thus, $V = \frac{\dot{v}_0}{k.C_{A0}} \frac{X}{(1-X)}$ $\rightarrow$ $\tau = \frac{V}{\dot{v}_0} = \frac{1}{k.C_{A0}} \frac{X}{(1-X)}$

▶ Then, $k.\tau.C_{A0} = D_{a2} = \frac{X}{(1-X)}$

$$\boxed{X = \frac{D_{a2}}{(1+D_{a2})}}$$

▶ $D_{a2} \rightarrow$ Damkohler number for 2nd order reaction

Considering change in $\dot{v}$ with conversion has an effect on the concentration

▶ For gas-phase reactions under $T = T_0$, $P = P_0$, and $Z = Z_0$

  ○ Then, $\dot{v} = f(X)$ (change in volumetric flow due to $\delta \neq 0$)

▶ $\dot{v} = \dot{v}_0(1 + \varepsilon.X)$ and $F_A = F_{A0}(1 - X)$

where, $\varepsilon = y_{A0}\delta$ and $\delta = \dfrac{d}{a} + \dfrac{c}{a} - \dfrac{b}{a} - 1$

▶ Then, $C_A = \dfrac{F_A}{\dot{v}} = \dfrac{F_{A0}(1-X)}{\dot{v}_0(1+\varepsilon.X)}$ and

$$C_A = C_{A0}\frac{(1 - X)}{(1 + \varepsilon.X)}$$

Considering change in $\dot{v}$ with conversion has an effect on the volume of the PFR

▶ With $C_A = C_{A0}\dfrac{(1-X)}{(1+\varepsilon.X)}$ then $V = F_{A0}\displaystyle\int_0^X \dfrac{dX}{-r_A} = \dfrac{F_{A0}}{k.C_{A0}^2}\int_0^X \dfrac{(1+\varepsilon X)^2\,dX}{(1-X)^2}$

▶ $F_T = F_{T0} + \delta.F_{A0}.X \quad \rightarrow \quad F_T - F_{T0} = \delta.F_{A0}.X$

▶ Dividing by F_{T0} and $y_{A0} = \dfrac{F_{A0}}{F_{T0}}$ we have for X = 1 (complete conversion)

$$\varepsilon = \frac{F_T - F_{T0}}{F_{T0}} = \frac{change\ in\ molar\ flowrate\ for\ complete\ conversion}{total\ number\ of\ moles\ fed\ to\ the\ reactor}$$

▶ And

$$V = \frac{\dot{v}_0}{k.C_{A0}}\left[2\varepsilon(1+\varepsilon)\ln(1-X) + \varepsilon^2 X + \frac{(1+\varepsilon)^2.X}{(1-X)}\right]$$

Change in V or v must be considered for proper design of reactor

▶ For $\varepsilon = 0;\ \delta = 0$ then $\dot{v} = \dot{v}_0(1 + \varepsilon.X) = \dot{v}_0$

   ○ no change in vol. flowrate

$$V = \frac{\dot{v}_0}{k.C_{A0}}\left[2\varepsilon(1 + \varepsilon)\ln(1 - X) + \varepsilon^2 X + \frac{(1 + \varepsilon)^2.X}{(1 - X)}\right]$$

▶ For $\varepsilon < 0,\ \ \delta < 0$ then $\dot{v} = \dot{v}_0(1 + \varepsilon.X)$ will decrease with X

   ○ Lower flowrate, higher residence time and higher conversion, relative to $\varepsilon = 0$ are achieved

▶ For $\varepsilon > 0,\ \ \delta > 0$ then $\dot{v} = \dot{v}_0(1 + \varepsilon.X)$ will increase with X

   ○ Higher flowrate, lower residence time and lower conversions achieved