Lecture # 6.1 CHE331A

▶ Rate law is a function of concentration and temperature

▶ Concentration is a function of conversion (stoichiometric table)

▶ Rate law in terms of constant and variable volume
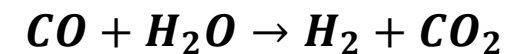
▶ Isothermal Reactor Design for a CSTR
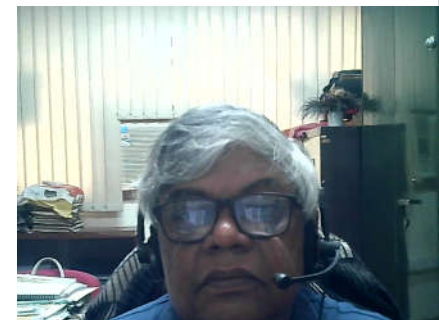
GOUTAM DEO

CHEMICAL ENGINEERING DEPARTMENT

IIT KANPUR

High temperature Shift Reactor

$$CO + H_2O \rightarrow H_2 + CO_2$$

Packed bed Reactor

Catalyst: Iron oxide + Chromium oxide

Calculation methodology for designing a CSTR

▶ Mole balance: design equation for CSTR in terms of X

$$V = \frac{F_{A0} \cdot X}{(-r_A)_{exit}}$$

▶ Rate law, e.g., $\qquad -r_A = k \cdot C_A$

▶ Stoichiometry → Stoichiometric table (Please make one yourself!)

   ○ This will give the relation between concentration and conversion

$$C_j = f(X)$$

   ○ $A + B \rightarrow C$ Liquid phase reaction, no volume change

$$C_A = C_{A0}(1 - X); \quad C_B = C_{A0}(\theta_B - X); \quad C_C = C_{A0}(\theta_C + X)$$

Design equation in terms of space time for convenience

▶ $V = \frac{F_{A0}.X}{(-r_A)_{exit}}$, which can be put in terms of $\tau = \left(\frac{V}{\dot{v}_0}\right)$ the space time

▶ Since $\dot{v} = \dot{v}_0$ (constant volume liquid system) $\rightarrow V = \frac{\dot{v}_0 C_{A0}.X}{(-r_A)_{exit}}$

▶ Thus, $\tau = \frac{C_{A0}.X}{(-r_A)_{exit}}$, which with the given rate law of $-r_A = k.C_A$

$$\tau = \frac{C_{A0}.X}{(-r_A)_{exit}} = \frac{C_{A0}.X}{k.C_A} = \frac{C_{A0}.X}{k.C_{A0}(1-X)} = \frac{X}{k.(1-X)}$$

▶ Or in terms of conversion and outlet concentration

$$X = \frac{k.\tau}{(1+k,\tau)}$$
and
$$C_A = \frac{C_{A0}}{k.(1-X)}$$

Damkohler number, a reaction related dimensionless number

▶ For a 1st order reaction the product $k\tau$ is dimensionless and called the Damkohler number, $D_a \rightarrow k \; in \; (time)^{-1}$ and $\tau \; in \; time$

$$D_a = \frac{\text{reaction rate based on entrance}}{\text{Flow of A at entrance}} = \frac{-r_{A0}V}{F_{A0}} = \frac{kC_{A0}V}{\dot{v}_0 C_{A0}} = k\tau$$

▶ For 2nd order reaction: $\quad D_a = \frac{kC_{A0}^2 V}{\dot{v}_0 C_{A0}} = k\tau C_{A0}$

▶ Conversions are related to D_a

  ○ Low values of D_a conversions are low, e.g., $D_a < 0.1$ then $X < 0.1$

  ○ High values of D_a conversions are high, e.g., $D_a > 10$ then $X > 0.9$

$$X = \frac{D_a}{1 + D_a} = 1 - \frac{1}{1 + D_a}$$

Revisiting CSTRs in series

▶ $\tau_1 = \dfrac{V}{\dot{v}_0}$ and $C_{A1} = \dfrac{C_{A0}}{1+k_1\tau_1}$
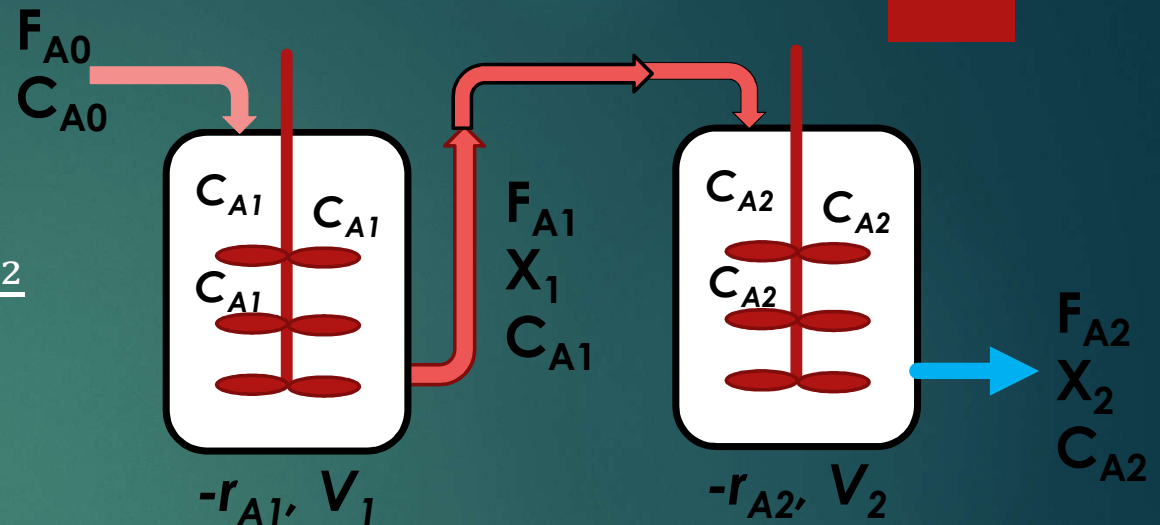
▶ For the 2nd reactor: $V_2 = \dfrac{F_{A1}-F_{A2}}{-r_{A2}}$

▶ In terms of concentration:

$$V_2 = \dfrac{\dot{v}_0(C_{A1}-C_{A2})}{k_2 C_{A2}} \quad \text{and} \quad C_{A2} = \dfrac{C_{A1}}{1+k_2\tau_2} \quad \text{and} \quad C_{A2} = \dfrac{C_{A0}}{(1+k_1\tau_1)(1+k_2\tau_2)}$$

▶ If both reactors are equal size and operate at the same temperature

▶ $k_1 = k_2 = k$ and $\tau_1 = \tau_2 = \tau$ $\rightarrow$ $C_{A2} = \dfrac{C_{A0}}{(1+k\tau)^2}$

The concentration and conversion can be generalized for n-CSTRs in series

▶ For n-CSTRs of equal volume operating in series at the same temperature

$$C_{An} = \frac{C_{A0}}{(1 + k\tau)^n} = \frac{C_{A0}}{(1 + D_a)^n}$$

▶ Or in terms of conversion

$$X = 1 - \frac{1}{(1+k.\tau)^n} = 1 - \frac{1}{(1+D_a)^n}$$

▶ When D_a is small then the conversion increases significantly when the number of reactors increase

▶ For large values of D_a (e.g., =1) then increasing beyond a certain number might not be justified

X

$D_a = 1$
$D_a = 0.5$
$D_a = 0.1$

Number of CSTRs