Lecture # 6.2 CHE331A

- Rate law is a function of conc and temp
- Concentration is a function of conversion (stoichiometric table)
- Rate law in conv terms for constant volume
- Isothermal n-CSTRs in series
- Isothermal n-CSTRs in parallel and the manufacture of Ethylene Glycol

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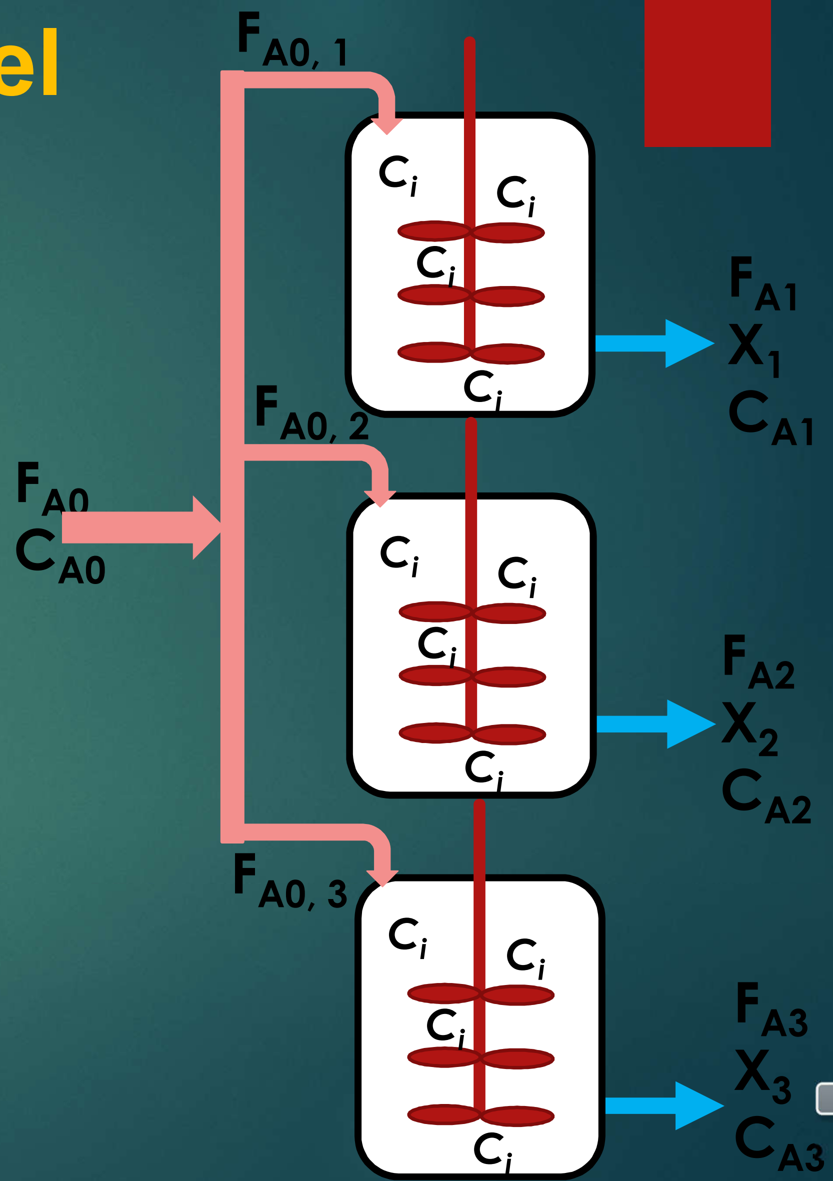
Number of CSTRs in Parallel

$$V_i = \frac{V}{n} \text{ and } F_{A0i} = \frac{F_{A0}}{n}$$

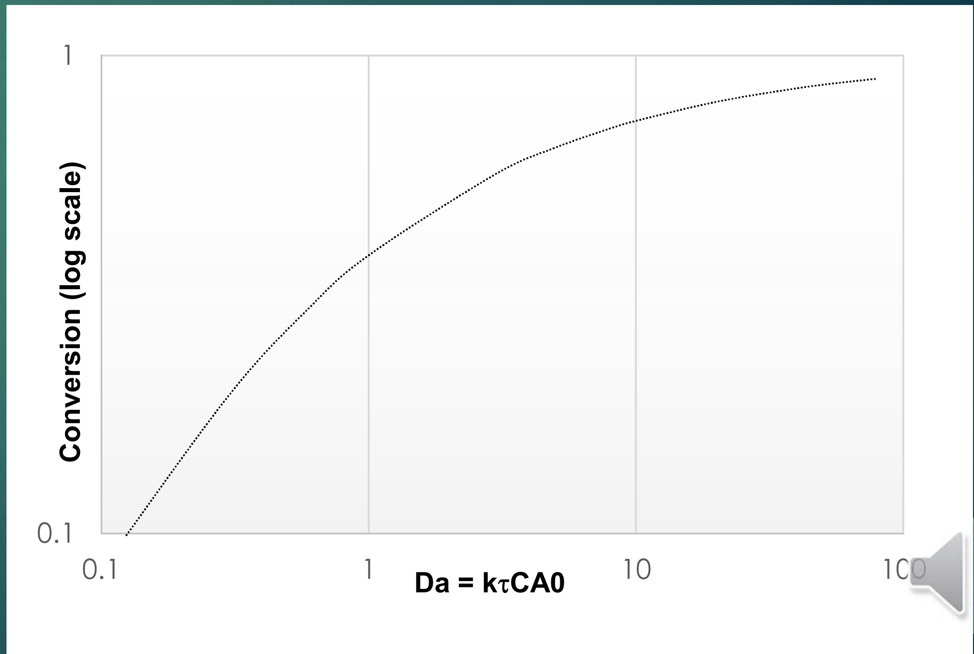
- For each reactor: $V_i = F_{A0i} \frac{X_i}{-r_{Ai}}$
- For each reactors at same temperature: all $-r_{Ai}$ are the same
- And → $X_1 = X_2 = \ldots = X_n = X$
- The total volume of the CSTRs in series $V = \sum V_i = \sum_n F_{A0,i} \frac{X_i}{-r_{Ai}} = \frac{F_{A0}X}{-r_A}$
- This is the same volume as a single reactor to achieve a conversion of X



Single CSTR and second order reaction

- For constant volume: $V = \frac{F_{A0}.X}{-r_A} = \frac{F_{A0}.X}{kC_A^2} = \frac{\dot{v}_0 C_{A0}.X}{kC_{A0}^2(1-X)^2}$
- In terms of space time: $\tau = \frac{V}{\dot{v}_0} = \frac{X}{kC_{A0}(1-X)^2} \rightarrow D_a = k.\tau.C_{A0} = \frac{X}{(1-X)^2}$
- Thus, $X^2 D_a - X(2D_a + 1) + D_a = 0$
  - Valid only for $X < 1$
- A tenfold increase in D_a by

increase reactor vol or temp increases the conversion from 0.67 to 0.88



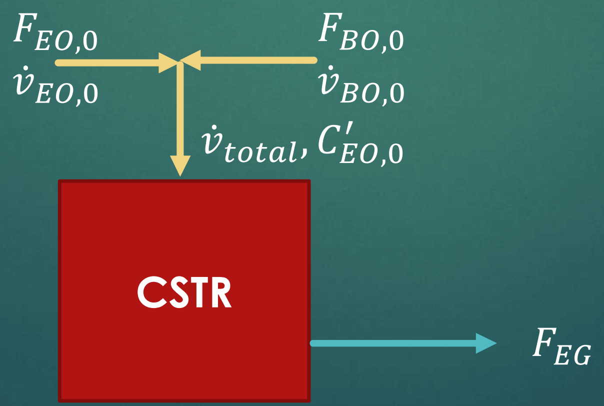
Reactor sizing for a specific chemical reaction - CSTRs

- Ethylene glycol is produced in large quantities for a variety of uses
  - Used for manufacture of polyester and antifreeze
  - For polyesters about 88% is used for making fibers and 12% for manufacture of bottles and films
- We are required to design (size) a CSTR to produce 200 million lbs per year of ethylene glycol (EG) by hydrolyzing ethylene oxide (EO). Inlet concentration of EO = 1 lbmol/ft^3 in water and equal volumetric flow rate of water containing 0.9% H_2SO_4
- The reaction is: $C_2H_4O(EO) + H_2O(B) \xrightarrow{Catalyst} C_2H_4(-OH)_2(EG)$
  - Catalyst is H_2SO_4

CSTR volume for X = 0.80

- 200 million lbs per year of EG $\rightarrow F_{EG} = 6.137 \ \frac{lbmol}{min}$
- For X = 0.8, then $F_{EG} = F_{EO,0}.X \ \rightarrow F_{EO,0} = \frac{6.137}{0.8} = 7.67 \ \frac{lbmol}{min}$
- With $C_{EO,0} = 1 \ \frac{lbmole}{ft^3} \rightarrow \dot{v}_{EO,0} = 7.67 \frac{ft^3}{min}$

$$\dot{v}_{total} = \dot{v}_{EO,0} + \dot{v}_{B,0} = 2.\dot{v}_{EO,0}, \qquad \rightarrow C'_{EO,0} = \frac{1}{2} C_{EO,0}$$



CSTR volume calculation contd.

- **Mole balance:** $V = \frac{F_{A0}.X}{-r_A}$

- **Rate law** was determined experimentally by the R&D section as
  - $-r_A = k.C_A$, water was in used in excess, no subscript on k required
  - $-r_A = 0.311.C_A \frac{lbmol}{ft^3.min}$ at a reaction temperature of 55°C

- Stoichiometry: $C_{E0} = C_{EO,0}(1 - X)$, and

$$V = \frac{F'_{EO,0}.X}{-r_A} = \frac{\dot{v}_{total}.X}{k.(1 - X)} = \frac{2 * 7.67 * 0.8}{0.314 * (1 - 0.8)} = 197.3\ ft^3$$

- For example a tank 5 ft in diameter and approximately 10 ft tall

Volume for 2 CSTRs in series for the same conversion

- Reactors of the same volume and operating at the same temperature

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

- For 2 reactors in series and X = 0.8: $0.8 = 1 - \frac{1}{(1+D_a)^2}$

$$D_a = \sqrt{5} - 1 = 1.23 \rightarrow k\tau = 1.23 \rightarrow \tau = \frac{1.23}{0.311} = 4\,min$$

- Volume of each reactor is $V = \dot{v}_{total}.\tau = 15.34 * 4 = 61.36\ ft^3$
- The total volume = 122.72 ft^3 which is < 197 ft^3 for a single reactor
- Choice between the two may be based on cost