Lecture # 7.2 CHE331A

- Design of ideal reactors - Basics
- Reaction kinetics and Rate law as a function of conversion
- Design/Analysis of a PFR with variable volume
- Cracking of Ethane in a PFR as an example of variable volume flow

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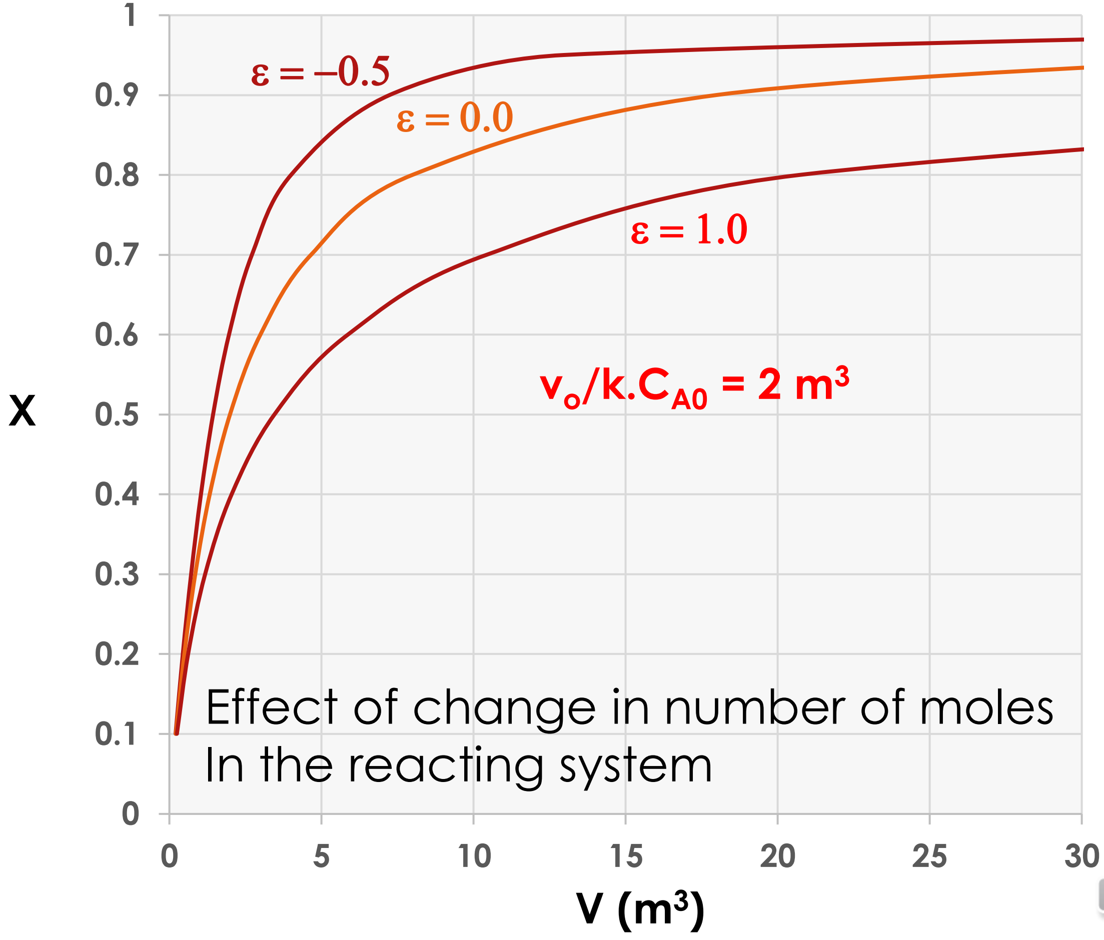
$$V = \frac{\dot{v}_0}{k.C_{A0}}\left[2\varepsilon(1+\varepsilon)\ln(1-X) + \varepsilon^2 X + \frac{(1+\varepsilon)^2.X}{(1-X)}\right]$$



Tubular reactor design for Ethane Cracking to Ethylene

- Required to produce 300 million lbs per year of ethylene in a PFR at 6 atm and 1100 K (isothermal and isobaric) with 0.80 conversion
- Gas phase reaction: $C_2H_6(A) \rightarrow C_2H_4(B) + H_2(C)$
- $F_B = 300\ million \frac{lb}{year} = 0.340 \frac{lbmol}{s}$ and $F_{A0} = \frac{0.340}{0.8} = 0.425 \frac{lbmol}{s}$
- $C_{A0} = y_{A0} C_{T0} = \frac{y_{A0} P_0}{RT_0} = \frac{1 * 6\ atm}{0.73 \frac{ft^3.atm}{lbmol.R} * 1980\ R} = 0.00415 \frac{lbmol}{ft^3}$ and
- For pure ethane feed: $y_{A0} = 1$, and for the reaction: $\delta = 1 + 1 - 1 = 1$
- Thus, $\varepsilon = y_{A0}\delta = 1$

In Ethane Cracking the number of moles change and concentration is affected

- Mole balance for PFR in terms of conversion:

$$F_{A0}\frac{dX}{dV} = -r_A$$

- Rate law: $-r_A = k.C_A$ with $k = 3.07\ s^{-1}$

$$V = F_{A0}\int_0^X \frac{dX}{-r_A} = F_{A0}\int_0^X \frac{dX}{kC_A}$$

- Stoichiometry: $\dot{v} = \dot{v}_0(1 + \varepsilon X)$ $P = P_0,\ T = T_0,\ Z = Z_0$

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

Number of moles change affects the volume of PFR

- With $C_A = \frac{F_A}{\dot{v}} = \frac{F_{A0}(1-X)}{\dot{v}_0(1+\varepsilon.X)} = C_{A0}\frac{(1-X)}{(1+\varepsilon X)}$ then

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

- And,

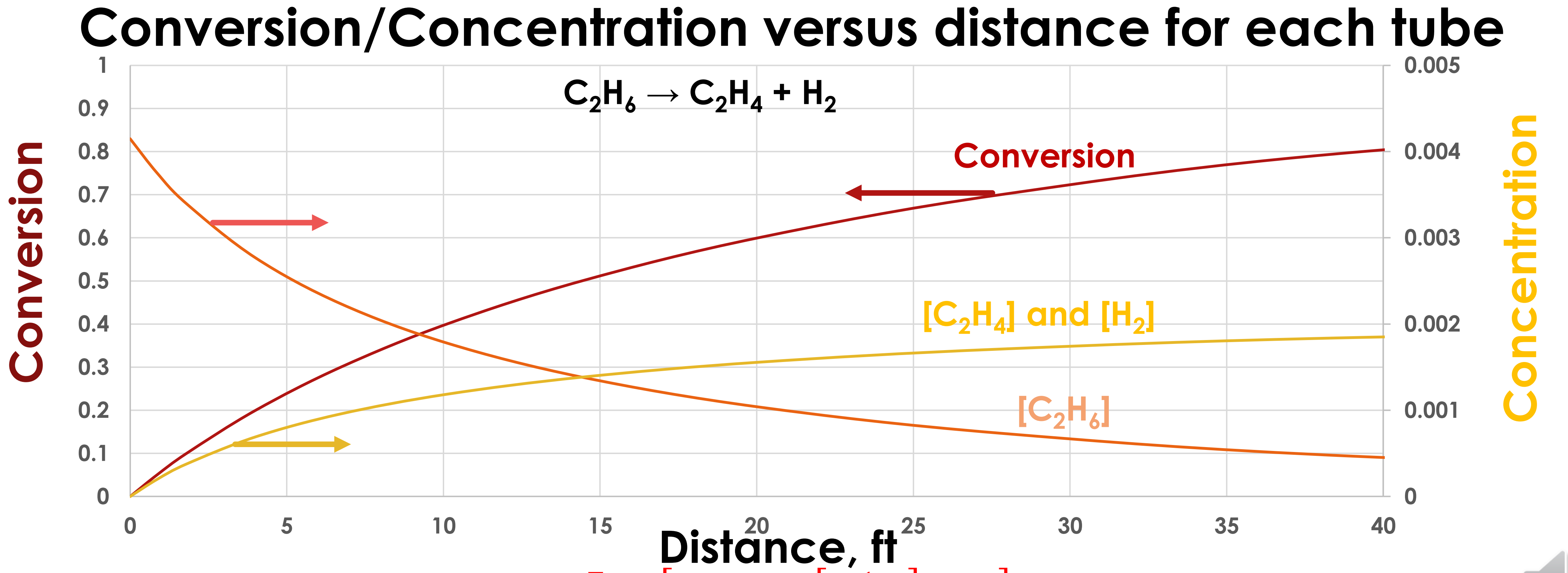
$$V = F_{A0}\int_0^X \frac{dX}{kC_A} = \frac{F_{A0}}{k.C_{A0}}\int_0^X \frac{(1+\varepsilon X)}{(1-X)}dX$$

$$\boxed{V = \frac{F_{A0}}{k.C_{A0}}\left[(1+\varepsilon)\ln\left[\frac{1}{1-X}\right] - \varepsilon X\right]}$$

Calculation for volume continued

- $V = \frac{F_{A0}}{k.C_{A0}}\left[(1+\varepsilon)\ln\left[\frac{1}{1-X}\right] - \varepsilon X\right] = \frac{0.425}{3.07*0.0045}\left[(1+1)\ln\left[\frac{1}{1-0.8}\right] - 1*0.8\right]$
- $V = 80.7\ ft^3$ (about 2.28 m^3)
- PFRs are usually in the form of tubes/pipes.
  - Pipes are available with definite diameter as per pipe schedule
  - Pipe schedule 80 gives a cross-sectional area = 0.0205 ft^2
  - For a length of 40 ft the number of tubes can be found out
  - Number of tubes: $n = \frac{80.7}{0.0205*40} \approx 100$
- Thus, using 100 tubes of schedule 80 one has the reactor volume necessary to produce 300 million lbs of ethylene from ethane

Conversion and concentration profile along the length can be calculated with distance, Z



$$V = \frac{F_{A0}}{k.C_{A0}}\left[(1+\varepsilon)\ln\left[\frac{1}{1-X}\right] - \varepsilon X\right]$$