P 6-4

$$A \longrightarrow B + 2C$$

- isothermal
- elementary
- $\Delta P = 0$
- k @ 50°C $= 1 \times 10^{-4}$ 1/min
- $E = 85$ kJ/mol
- $P_0 = 10$ atm
- $y_A = 1$
- $T_0 = 127$ °C
- $F_{A0} = 2.5$ mol/min

k @ 127 °C

$$k = k_0 \exp\left[\frac{E}{R}\left(\frac{1}{T_0} - \frac{1}{T_1}\right)\right]$$

$$= 1 \times 10^{-4} \exp\left[\frac{85000}{8.31} \times \left(\frac{1}{323} - \frac{1}{400}\right)\right]$$

$$= 0.044 \text{ 1/min}$$

(A) → **PFR**

$$-r_A = kC_A$$

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

$$\varepsilon = y_{A0}\delta = 1 \times (1+2-1) = 2$$

$$C_{A0} = \frac{P_0}{RT_0} = \frac{10}{0.082 \times 400} = 0.3 \ \frac{\text{mol}}{\text{dm}^3}$$

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

$$= \frac{F_{A0}}{kC_{A0}} \int_0^X \frac{\epsilon(1+\epsilon X)}{(1-X)} dX$$

$$V = \frac{F_{A0}}{kC_{A0}} \left[(1+\epsilon) \ln \frac{1}{1-X} - \epsilon X \right]$$

↖ Use this equation to plot X Vs V

F_A, F_B, and F_C can be calculated from x using stoichiometry.

(B) PFR volume for $X = 0.9$

$$V = \frac{F_{A0}}{kC_{A0}} \left[(1+\epsilon) \ln \frac{1}{1-X} - \epsilon X \right]$$

$$V = \frac{2.5}{0.044 \times 0.3} \left[(1+2) \ln \frac{1}{1-0.9} - 2 \times 0.9 \right]$$

$$V = 967 \text{ dm}^3$$

CSTR volume

$$V = \frac{F_{A0}\, X}{-r_A|_{exit}}$$

$$= \frac{F_{A0} \times (1 + \epsilon X)}{k\, C_{A0} (1 - X)}$$

$$= \frac{2.5 \times 0.9 \times (1 + 2 \times 0.9)}{0.044 \times 0.3 \times (1 - 0.9)}$$

$$V = 4772 \text{ dm}^3$$

$$v_0 = \frac{F_{A0}}{C_{A0}} = \frac{2.5}{0.3} = 8.33 \ \frac{\text{dm}^3}{\text{min}}$$

$$v = v_0 (1 + \epsilon X)$$

$$= 8.33 (1 + 2 \times 0.9)$$

$$v = 23.33 \text{ dm}^3/\text{min}$$

$$\tau = \frac{V}{v} = \frac{4722}{23.33} = 202.3 \text{ min}$$