Josh whitehead

HW II 1

19 Jan 2022

1) Find conversions in CSTR and PFR

$\dot{V} = 10 \frac{L}{sec}$

$k = 0.05 \frac{1}{sec}$

$V = 100\ L$

1° order: $-r_A = kC_A$

For CSTR

$$V = \frac{F_{A0} - F_A}{-r_A} \rightarrow F_A = F_{A0} - F_{A0}X_A \therefore V = \frac{F_{A0}X_A}{-r_A}$$

$\downarrow$

$r_A = kC_A$

$\downarrow$

$C_A = C_{A0} - C_{A0}X_A$

$$\rightarrow V = \frac{\dot{V}\cancel{C_{A0}}X_A}{k\cancel{C_{A0}}(1-X_A)} \rightarrow kV - kVX_A = \dot{V}X_A$$

$$kV = X_A(\dot{V} + kV)$$

$\downarrow$

$$X_A = \frac{kV}{\dot{V} + kV} = \frac{0.05 \cdot 100}{10 + 0.05 \cdot 100} = \boxed{0.333}$$

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1) PFR $V = F_{A0}\int_0^{x_A} \frac{dx_A}{-r_A} = F_{A0}\int \frac{dx_A}{kC_A} = \frac{F_{A0}}{k}\int \frac{dx_A}{C_A}$

$$V = \frac{\dot{V}C_{A0}}{k}\int \frac{dx_A}{C_A} = \frac{\dot{V}C_{A0}}{k}\int \frac{dx_A}{C_{A0}(1-x_A)} = \frac{\dot{V}\cancel{C_{A0}}}{k\cancel{C_{A0}}}\int \frac{dx_A}{1-x_A}$$

$$\rightarrow V = \frac{-\dot{V}}{k}\ln(1-x_A) \rightarrow x_A = 1-\exp\left(\frac{-Vk}{\dot{V}}\right) \boxed{= 0.393}$$

Residence Time: $\tau = \frac{V}{\dot{V}} = \frac{100}{10} = 10\text{ sec} \rightarrow \boxed{10.0\text{ sec}}$

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2) a.) Find units of K $\rightarrow$ $-r_A = K_1 \dfrac{C_A C_B^2}{C_C^2}$

$$\left.\begin{aligned} r_A &= \frac{mol}{m^3 \cdot sec} \\ C &= \frac{mol}{m^3} \end{aligned}\right\} \longrightarrow K_1 = \frac{-r_A C_C^2}{C_A C_B^2} \Rightarrow \frac{-\left(\frac{\cancel{mol}}{\cancel{m^3} \cdot sec}\right)\cancel{\left(\frac{mol^2}{m^6}\right)}}{\left(\frac{\cancel{mol}}{\cancel{m^3}}\right)\cancel{\left(\frac{mol^2}{m^6}\right)}}$$

$$= -\frac{1}{sec}$$

$$\boxed{\text{units of } K_1 = \frac{1}{sec}}$$

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2.) b.) find units of K_1, K_2, K_3, K_4

$r_A' = \frac{mol}{g \cdot sec}$

$-r_A' = \frac{K_1\left(P_A - \frac{P_B P_C}{K_3}\right)}{1 + K_2 P_B^2 + K_4 P_C}$

$C = \frac{mol}{m^3}$

$P = Pa$

K_4

$K_4 P_C = \text{unitless} = 1$

$\boxed{\therefore K_4 (=) \frac{1}{Pa}}$

K_1

$K_1 P_A (=) r_A'$

$\boxed{K_1 (=) \frac{mol}{g \cdot sec \cdot Pa}}$

K_2

$K_2 P_B^2 = \text{unitless} = 1$

$\boxed{\therefore K_2 (=) \frac{1}{Pa^2}}$

K_3

$\frac{P_B P_C}{K_3} (=) P_A$

$\rightarrow \frac{Pa^2}{K_3} (=) Pa$

$\boxed{\therefore K_3 (=) Pa}$

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2.) c.) find units of $k_N, k_{-N}, k_S, k_P, k_I$

$$-r_N'' = \left(\frac{k_N k_S K_P}{k_{-N} + k_S}\right) \cdot \frac{C_N C_P}{\left(1 + \frac{k_N}{k_{-N} + k_S}\left(1 + \frac{k_S}{k_I}\right) C_N + K_I C_I^{0.5}\right)^2}$$

$r_N'' (=) \frac{mol}{m^2 \cdot sec}$

$C = \frac{mol}{m^3}$

K_I | $K_I C_I^{0.5} (=) 1$ $\therefore$ $\boxed{K_I (=) \frac{m^{1.5}}{mol^{0.5}}}$

K_S | $\frac{K_S}{K_I} (=) 1$ $\therefore$ $K_S (=) K_I \rightarrow \boxed{K_S (=) \frac{m^{1.5}}{mol^{0.5}}}$

K_{-N} | $K_{-N} (=) K_S$ $\therefore$ $\boxed{K_{-N} (=) \frac{m^{1.5}}{mol^{0.5}}}$

K_N | $\frac{K_N C_N}{K_{-N} + K_S} (=) 1 \rightarrow \frac{K_N \frac{mol}{m^3}}{\frac{m^{1.5}}{mol^{0.5}}} \longrightarrow K_N \frac{mol}{m^3} \cdot \frac{mol^{0.5}}{m^{1.5}}$

$\rightarrow K_N \frac{mol^{1.5}}{m^{4.5}}$

$\therefore \boxed{K_N (=) \frac{m^{4.5}}{mol^{1.5}}}$

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2)(c) $-r_N'' \; (=) \left(\dfrac{k_N k_S K_P}{k_{-N} + k_S} \right) \cdot \dfrac{C_N C_P}{1}$

$\boxed{K_P}$ $\rightarrow \dfrac{mol}{m^2 \cdot sec} \; (=) \left(\dfrac{\dfrac{m^{4.5}}{mol^{0.5}} \cdot \cancel{\dfrac{m^{1.5}}{mol^{0.5}}} \cdot K_P}{\cancel{\dfrac{m^{1.5}}{mol^{0.5}}}} \right) \left(\dfrac{mol^2}{m^9} \right)$

$\rightarrow \dfrac{mol}{m^2 \cdot sec} \; (=) \left(\dfrac{\dfrac{m^6}{mol^2} \cdot K_P}{\dfrac{m^{1.5}}{mol^{0.5}}} \right) \left(\dfrac{mol^2}{m^9} \right)$

$\rightarrow \dfrac{mol}{m^2 \cdot sec} \; (=) \; \dfrac{m^{4.5}}{mol^{1.5}} \; K_P \; \dfrac{mol^2}{m^9}$

$\dfrac{mol}{m^2 \cdot sec} \; (=) \; K_P \; \dfrac{mol^{0.5}}{m^{4.5}} \rightarrow \boxed{K_P \; (=) \; \dfrac{mol^{0.5} \cdot m^{2.5}}{sec}}$

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3) a) find V_{CSTR} when $X_A = 0.40$

$k'' = 10^{-6} \frac{m}{sec}$

$F_{A0} = 200 \frac{mol}{sec}$

$\rho_A = 500 \frac{kg}{m^3}$

$M_A = 500 \frac{g}{mol}$

$S_g = 5 \frac{m^2}{g}$

$\rho_{cat} = 30 \frac{kg}{m^3}$

$$V = \frac{F_{A0} X_A}{-r_A'' S_g \rho_{cat}} = \frac{F_{A0} X_A}{k'' C_A S_g \rho_{cat}} = \frac{F_{A0} X_A}{k C_{A0} (1 - X_A) S_g \rho_{cat}}$$

$$\rightarrow V = \frac{\dot{v} \cancel{C_{A0}} X_A}{k \cancel{C_{A0}} (1 - X_A) S_g \rho_{cat}} = \frac{\dot{v} X_A}{k (1 - X_A) S_g \rho_{cat}}$$

$$\dot{v} = \frac{F_{A0} \cdot M_A}{\rho_A} = \frac{200 \cdot 500}{500000} = \underline{0.2 \frac{m^3}{sec}}$$

$$\therefore V = \frac{0.2 \cdot 0.4}{10^{-6} (1 - 0.4) \cdot 5 \cdot 30000} \boxed{= 0.889 \ m^3}$$

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3) b)

PBR $V = F_{A0}\int_0^{x_A} \frac{dx_A}{k'' C_A S_g \rho_{cat}} \rightarrow V = \frac{-F_{A0}}{k C_{A0} S_g \rho_{cat}} \ln(1-x_A)$

$\rightarrow V = \frac{-\dot{V} \cancel{C_{A0}}}{k \cancel{C_{A0}} S_g \rho_{cat}} \ln(1-x_A) \boxed{= 0.681\ m^3}$

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c) $\tau_{CSTR} = \frac{V}{\dot{V}} = \frac{0.889}{0.2} \boxed{= 4.45\ sec}$

$\tau_{PBR} = \frac{V}{\dot{V}} = \frac{0.681}{0.2} \boxed{= 3.41\ sec}$

$\tau_{w\,CSTR} = \frac{V \rho_{cat}}{\dot{V}} = \frac{0.889 \cdot 30}{0.2} \boxed{= 133.\ \frac{kg \cdot sec}{m^3}}$

$\tau_{w\,PBR} = \frac{V \rho_{cat}}{\dot{V}} = \frac{0.681 \cdot 30}{0.2} \boxed{= 102.\ \frac{sec \cdot kg}{m^3}}$

Residence time is lower for PBR than for CSTR of equal volumes because PBR is more efficient for first order reactions

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3) d) if $\dot{v} = 2\dot{v}$ what happens to X_A

CSTR

$$V = \frac{F_{A0} X_A}{K C_A S_g \rho_{cat}} = \frac{\cancel{F_{A0}} X_A \cancel{C_{A0}} \dot{v}}{K \cancel{C_{A0}} S_g \rho_{cat} (1 - X_A)}$$

$$\rightarrow X_A = \frac{V K S_g \rho_{cat}}{\dot{v} + V K S_g \rho_{cat}} = \frac{0.889 \cdot 10^{-6} \cdot 30000 \cdot 5}{0.4 + 0.889 \cdot 10^{-6} \cdot 30000 \cdot 5} \boxed{= 0.250}$$

PBR

$$V = \frac{-\dot{v}}{K S_g \rho_{cat}} \ln (1 - X_A) \rightarrow X_A = 1 - \exp\left(\frac{-\dot{v}}{V K S_g \rho_{cat}}\right)$$

$$\rightarrow X_A = 1 - \exp\left(\frac{-0.4}{0.681 \cdot 10^{-6} \cdot 30000 \cdot 5}\right) \boxed{= 0.980}$$

For CSTR the conversion decreases

For PBR the conversion increases

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4) a) Calculate time for 95% conversion

assume:
- liquid phase
- irriversible
- isothermal

$k = 0.2 \frac{L}{mol \cdot min}$

$V = 2L$

$n_0 = 10 \, mol$

$n_f = \cancel{??} \, 0.5 \, mol$

$C_0 = \frac{10}{2} = 5 \frac{mol}{L}$

$C_f = \frac{0.5}{2} = 0.25 \frac{mol}{L}$

$$t = \int_{N_A}^{N_{A0}} \frac{dN_A}{-r_A V} = \frac{1}{\cancel{V}k} \int_{C_A}^{C_{A0}} \frac{\cancel{V} \, dC_A}{C_A^2}$$

$$\rightarrow t = \frac{1}{k}\left(\frac{1}{C_A} - \frac{1}{C_{A0}}\right) = \frac{1}{0.2}\left(\frac{1}{0.25} - \frac{1}{5}\right)$$

$$\boxed{= 19.0 \, \cancel{sec} \; min}$$

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4) b)

PFR

find τ_{PFR} @ $x_A = 0.95$

$\dot{V} = 2 \frac{L}{min}$

$F_{A_0} = 10 \frac{mol}{min}$

$C_{A_0} = 5 \frac{mol}{L}$

$$V = \frac{\dot{V} C_{A_0}}{k} \int_0^{x_A} \frac{dx_A}{(C_{A_0}(1-x_A))^2}$$

$$\rightarrow V = \frac{\dot{V} \cancel{C_{A_0}}}{k\, C_{A_0}^{\cancel{2}} (1-x_A)} = \frac{2}{0.2 \cdot 5 (1-0.95)} = 40 L$$

$$\tau = \frac{V}{\dot{V}} = \frac{40 L}{2 \frac{L}{min}} \boxed{= 20.0 min}$$

4) c)

~~Batch ≈ τ_{PFR} because a PFR is like a long batch reactor~~

$\tau_{Batch} \approx \tau_{PFR}$ because a PFR is like a really long batch reactor or many batches stacked end to end

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4)d) $V = \frac{F_{A0} X_A}{k C_A^2} = \frac{F_{A0} X_A}{k (C_{A0}(1-X_A))^2}$

$F_{A0} = 10 \frac{mol}{min}$

$X_A = 0.95$

$C_{A0} = \frac{10}{2} = 5 \frac{mol}{L}$

$\boxed{V = 760.\ L}$

4) e) $\tau_{CSTR} = \frac{V}{\dot{V}} = \frac{760}{2} = \boxed{380\ min}$

$\boxed{\tau_{CSTR} >> \tau_{PFR}}$

I will use PFR because it is much smaller and has lower residence time.

PFR yields higher conversion with same residence time

4) f) For a negative order reaction, I would choose CSTR because for negative order $r_A \propto \frac{1}{C_A}$

4) g) For zero order reactions, it would not depend on concentration so I would choose PFR because it is smaller

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5) find C_A

$$-r_A = \frac{k_1 C_A}{(1+k_2\sqrt{C_A})^2}$$

$$V = \frac{F_{A0} X_A}{-r_A} = \frac{F_{A0} X_A (1+k_2\sqrt{C_A})^2}{k_1 C_A}$$

$k_1 = 2\ \frac{1}{min}$

$k_2 = 2\ \left(\frac{L}{mol}\right)^{0.5}$

$$\rightarrow \frac{V k_1 \cancel{C_A}}{F_A X_A} = 1 + 2 k_2 \sqrt{C_A} + k_2^2 \cancel{C_A}$$

$V = 10 L$

$F_{A0} = 5\ \frac{mol}{min}$

$X_A = 0.90$

$$\underbrace{\frac{V k_1}{F_A X_A} - k_2^2 = \frac{1}{C_A} + \frac{2 k_2}{\sqrt{C_A}}}$$

$$\boxed{C_A = 85.5\ \frac{mol}{L}}$$