PROBLEM #1

CSTR

$$V = \frac{F_{A0} X_A}{-r_A} = \frac{v \cancel{C_{A0}} X_A}{k \cancel{C_{A0}}(1-X_A)} \rightarrow \tau k = \frac{X_A}{1-X_A}$$

$$\tau = \frac{V}{v} = \frac{100\,L}{10\,L/s} = 10\,s$$

$$(10\,s)(0.05) = \frac{X_A}{1-X_A} = 0.5$$

$$\boxed{X_A = \frac{1}{3} \text{ FOR CSTR}}$$

PFR

$$V = F_{A0} \int \frac{dX_A}{-r_A} = v \cancel{C_{A0}} \int \frac{dX_A}{k \cancel{C_{A0}}(1-X_A)}$$

$$\tau k = \int_0^{X_A} \frac{dX_A}{1-X_A} = -\ln(1-X_A) = \tau k$$

$$1 - X_A = \exp(-\tau k)$$

$$X_A = 1 - \exp(-\tau k) = 1 - \exp(-0.5)$$

$$\boxed{X_A = 0.393 \text{ FOR PFR}}$$

TIME IN A BATCH REACTOR FOR $X_A = 0.393$ IS EQUAL TO $\tau_{PFR} = 10\,s$.

Problem #2

2a. $-r_A \; [=] \; \frac{mol}{m^3 s}$

$$\frac{C_A C_B^2}{C_C^2} \; [=] \; \frac{mol}{m^3}$$

$$\boxed{k \; [=] \; \frac{1}{s}}$$

2b. UNITS OF P_A AND $\frac{P_B P_C}{K_3}$ ARE THE SAME.

K_3 HAS UNITS OF Pa^{+1}

$K_2 P_B^2$ AND $K_4 P_C$ ARE UNITLESS, SO K_2 HAS UNITS OF $\frac{1}{Pa^2}$, K_4 HAS UNITS OF $\frac{1}{Pa}$

$$-r_A' \; [=] \; \frac{mol}{g \cdot s}$$

$$\frac{P_A - \frac{P_B P_C}{K_3}}{1 + K_2 P_B^2 + K_4 P_C} \; [=] \; Pa$$

$$\boxed{k_1 \; [=] \; \frac{mol}{Pa \cdot g \cdot s}}$$

2c $k_I, k_{-N}, k_s \;[=]\; \left(\frac{m^3}{mol}\right)^{1/2}$

FIND UNITS ON k_N

$$\frac{k_N}{k_{-N}+k_s} \;[=]\; \left(\frac{m^3}{mol}\right)$$

$$\frac{k_N}{\left(\frac{m^3}{mol}\right)^{1/2}} \;[=]\; \frac{m^3}{mol}$$

$$k_N \;[=]\; \left(\frac{m^3}{mol}\right)^{3/2}$$

$$r_N'' \;[=]\; \frac{mol}{m^2 \cdot s}$$

$$K_p = \frac{(k_{-N}+k_s)(-r_N'')}{\cancel{k}_N \cancel{k}_s C_N C_p} = \frac{\cancel{\left(\frac{mol}{m^3}\right)^{-1/2}}\left(\frac{mol}{m^2 \cdot s}\right)}{\cancel{\left(\frac{mol}{m^3}\right)^{-1/2}}\left(\frac{m^3}{mol}\right)^{3/2}\left(\frac{mol}{m^3}\right)^2}$$

$$K_p \;[=]\; \frac{mol^{1/2}}{s \cdot m^{1/2}}$$

3a.

$$F_{A0} - F_A + r_A V = 0$$

$$F_A = F_{A0}(1-X)$$

$$F_{A0}X + r_A V = 0$$

$$F_{A0}X = -r_A V = -r_A'' S_g \rho V$$

$$F_{A0}X = -k_A'' C_A S_g \rho V$$

$$C_A = C_{A0}(1-X)$$

$$F_{A0}X = k_A'' C_{A0}(1-X) S_g \rho V$$

$$C_{A0} = \frac{1\,mol}{500g}\left(\frac{1000g}{kg}\right)\left(\frac{500kg}{m^3}\right)$$

$$C_{A0} = 1000\,mol/m^3$$

$$V = \frac{F_{A0}X}{k_A'' C_{A0}(1-X) S_g \rho} = \frac{\frac{200\,mol}{s}(0.4)}{\frac{1E\text{-}6\,m}{s}\left(\frac{1000\,mol}{m^3}\right)(0.6)\left(\frac{5m^3}{g}\right)\left(\frac{30kg}{m^3}\right)\left(\frac{1000g}{kg}\right)}$$

$$\boxed{V = 0.889\,m^3}$$

b) $$\lim_{\Delta V \to 0} \frac{F_A|_V - F_A|_{V+\Delta V} + r_A \Delta V}{\Delta V} = \cancel{\frac{dN_A}{dt}}$$

$$\frac{dF_A}{dV_{cat}} = r_A$$

$$F_A = F_{A0}(1-X)$$

$$C_A = C_{A0}(1-X)$$

$$F_{A0}\frac{dX}{dV} = k_A C_{A0}(1-X) S_g \rho$$

$$\int_0^{0.4} \frac{1}{1-X}\, dX = \int_0^{V_f} \frac{k_A'' C_{A0} S_g \rho \, dV}{F_{A0}}$$

$$\underbrace{-\ln(1-X)\Big|_0^{0.4}}_{0.5108} = \frac{k_A'' C_{A0} S_g \rho V_f}{F_{A0}}$$

$$V_f = 0.5108\left(\frac{200\,\text{mol}}{s}\right)\left(\frac{10^6\, s}{m}\right)\left(\frac{m^3}{1000\,\text{mol}}\right)\left(\frac{g}{5m^2}\right)\left(\frac{m^3}{30\,kg}\right)\left(\frac{kg}{1000\,g}\right)$$

$$\boxed{V_f = 0.681\ m^3}$$

3c. $$\frac{V}{V_0} = \tau$$

$$V_0 = \frac{F_{A0}}{C_{A0}} = \frac{200 \text{ mol/s}}{1000 \text{ mol}/m^3} = \frac{0.2\, m^3}{s}$$

$$\boxed{\begin{aligned} \tau_{CSTR} &= \frac{0.889\, m^3}{0.2\, m^3/s} = 4.44\, s \\ \tau_{PBR} &= \frac{0.681\, m^3}{0.2\, m^3/s} = 3.41\, s \end{aligned}}$$

$$W = \rho V_f$$

$$W_{CSTR} = 26.7\, kg \qquad W_{PFR} = 20.4\, kg$$

$$\boxed{\begin{aligned} \tau_{w,CSTR} &= \frac{26.7\, kg}{0.2\, m^3/s} = 133\, \frac{kg \cdot s}{m^3} \\ \tau_{w,PBR} &= \frac{20.4\, kg}{0.2\, m^3/s} = 102\, \frac{kg \cdot s}{m^3} \end{aligned}}$$

THE RESIDENCE TIME FOR THE CSTR IS DIFFERENT FROM THAT OF A PBR BECAUSE THE CSTR DILUTES THE ENTERING FEED, LOWERING THE CONCENTRATION OF C_A + LOWERING THE REACTION RATE.

3d. THE CONVERSION IN THE PBR + CSTR WILL BOTH DECREASE

CSTR: $F_{A0}X = -r_A V = k_A'' C_A S_g \rho V$

$F_{A0} \leftarrow \frac{400\,mol}{s}$

$$C_A = C_{A0}(1-X) = \frac{F_{A0}}{v}(1-X)$$

$$v = \frac{400\ mol/s}{1000\ mol/m^3} = \frac{0.4\,m^3}{s}$$

$$X = \frac{k_A''(1-X) S_g \rho V}{v}$$

$$\frac{X}{1-X} = \left(\frac{1(10^{-6})\,m}{s}\right)\left(\frac{s}{0.4\,m^3}\right)\left(\frac{5\,m^2}{g}\right)\left(\frac{30\,kg}{m^3}\right)(0.889\,m^3)\left(\frac{1000\,g}{kg}\right)$$

$$X = 0.25$$

PBR: $-\ln(1-X)\Big|_0^{X_f} = \frac{k_A'' C_{A0} S_g \rho V_f}{F_{A0}} = \frac{k_A'' S_g \rho V_f}{v}$

$$-\ln(1-X_f) = 0.255375$$

$$\boxed{X_f = 0.225}$$

4a.

ASSUME CONSTANT VOLUME

$$\cancel{IN}_0 - \cancel{OUT}_0 + GEN - CONS = ACCUM$$

BATCH

$$r_A V = \frac{dN_A}{dt}$$

$$-k c_A^2 V = \frac{dN_A}{dt}$$

$$N_A = N_{A0}(1-X) \; ; \; c_A = \frac{N_A}{V}$$

$$-\frac{k N_{A0}^2 (1-X)^2}{V} = \frac{d(N_{A0}(1-X))}{dt}$$

$$+\frac{k N_{A0}^2 (1-X)^2}{V} = +N_{A0}\frac{dX}{dt}$$

$$\int_0^{t_f} \frac{k N_{A0}}{V} dt = \int_0^{.95} (1-X)^{-2} dX$$

$$\frac{k N_{A0} t_f}{V} = (1-X)\Big|_0^{0.95} = \frac{1}{0.05} - 1 = 19$$

$$\boxed{t_f = 19 \text{ min}}$$

4b.

ASSUME STEADY-STATE
WELL-MIXED RADIALLY
CONSTANT DENSITY LIQUID

$$F_{A0}\Big|_V - F_A\Big|_{V+\Delta V} + r_A \Delta V = \cancel{\frac{dN_A}{dt}}^{\,0}$$

$$\lim_{\Delta V \to 0}\left(\frac{F_{A0}|_V - F_A|_{V+\Delta V}}{\Delta V} + r_A\right) = 0$$

$$-\frac{dF_A}{dV} + r_A = 0$$

$$-kC_A^2 = \frac{dF_A}{dV}$$

$$F_A = C_A v_0 = F_{A0}(1-X)$$

$$-k\left(\frac{F_A}{v_0}\right)^2 = \frac{dF_A}{dV}$$

$$+\frac{kF_{A0}^{\cancel{2}}(1-X)^2}{v_0^2} = +\cancel{F_{A0}}\frac{dX}{dV}$$

$$\int_0^{V_f}\frac{kF_{A0}}{v_0^2}\,dV = \int_0^{0.95}(1-X)^{-2}\,dX = 19$$

$$\frac{kF_{A0}V_f}{v_0^2} = 19$$

$$V_f = \frac{19\,(2\,L/min)^2}{\frac{0.2\,L}{mol \cdot min}\,(10\,mol/min)} = 38\,L$$

$$\boxed{\tau = \frac{V_f}{v_0} = \frac{38\,L}{2\,L/min} = 19\,min}$$

4c. RESIDENCE TIME IN A PFR IS EQUAL TO THE AMOUNT OF TIME THAT THE FLUID MUST STAY IN THE REACTOR TO ACHIEVE THE SAME CONVERSION. THE FORMS OF THE EQUATIONS FOR A PFR AND A BATCH REACTOR ARE SIMILAR IF WE DRAW THE ANALOGY BETWEEN THE TRADITIONAL CONCEPT OF TIME IN A BATCH REACTOR + POSITION (OR VOLUME) IN A PFR.

4d. ASSUME STEADY-STATE
CONSTANT ρ LIQUID

$$F_{A0} - F_A + r_A V = 0$$

$$F_A = F_{A0}(1-X)$$

$$F_{A0} X = -r_A V$$

$$F_{A0} X = k C_A^2 V$$

$$C_A = \frac{F_A}{v_0} = \frac{F_{A0}(1-X)}{v_0}$$

$$F_{A0}X = \frac{k F_{A0}^2 (1-X)^2}{v_0^2} V$$

$$V = \frac{v_0^2 X}{k F_{A0}(1-X)^2} = \frac{(2L/min)^2\ 0.95}{\frac{0.2L}{mol\ min}\left(\frac{10\ mol}{min}\right) 0.05^2}$$

$$V = 760L$$

4e. $$\tau = \frac{V}{v_0} = \frac{760L}{2L/min} = 380\ min$$

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

USE PFR WHICH NEEDS A SHORTER RESIDENCE TIME TO ACHIEVE THE SAME CONVERSION AS A CSTR.

SINCE THE RATE EQN. WAS POSITIVE ORDER IN C_A, LOWERING C_A WILL RESULT IN A LOWER RATE, AND A LARGER VOLUME TO ACHIEVE THE SAME CONVERSION

4f. CHOOSE CSTR BECAUSE THE CSTR WILL HAVE A HIGHER CONVERSION FOR THE SAME RESIDENCE TIME. LOWERING C_A WILL RESULT IN A HIGHER RATE.

4g. If the reaction was zero order, the PFR & CSTR WOULD BE THE SAME SINCE THE RATE is NOT DEPENDENT ON CONCENTRATION FOR A 0 ORDER REACTION.

PROBLEM #5

$$F_{A0} - F_A + r_A V = 0$$

$$F_A = F_{A0}(1 - X)$$ ASSUME CONSTANT ρ LIQUID

$$F_{A0} X = -r_A V$$

$$\frac{F_{A0} X}{V} = \frac{k_1 C_A}{\left(1 + k_2 \sqrt{C_A}\right)^2}$$

$$\frac{F_{A0} X}{k_1 V} = \frac{5\,\text{mol/min}\,(0.9)}{\frac{2}{\text{MIN}}(10\,\text{L})} = \frac{0.225\,\text{MOL}}{\text{L}} = \frac{C_A}{\left(1 + k_2 \sqrt{C_A}\right)^2}$$

Solve USING EQUATION SOLVER

$$C_A = 85.4\ \text{MOL/L}$$