Solution, Assignment #1

Problem1

Constant volumetric flow rate; isothermal; continuous flow reactor

$$F_{A0} = 5.0\, mol/hr,\ \upsilon_0 = 10\, dm^3/hr\ ,\ F_{A0} = \upsilon_0 \times C_{A0},\ C_{A0} = \frac{5.0\, mol/hr}{10\, dm^3/hr} = 0.5\, mol/dm^3$$

$$(a)\ -r_A = k,\ with\ \ k = 0.05\ mol/h.dm^3$$

CSTR

For CSTR mole balance equation is:

$$V = \frac{F_{A0} - F_A}{-r_A},\quad \text{Rate Law}: \quad -r_A = k$$

$$V = \frac{F_{A0} - 0.01F_{A0}}{-r_A} = \frac{\left(5.0\frac{mol}{h}\right)\times(0.99)}{\left(0.05\frac{mol}{h.dm^3}\right)} = 99.0\ \ dm^3$$

PFR

$$\frac{dF_A}{dV} = r_A$$

$$\frac{dF_A}{dV} = -k\ \ ,\ \ -\frac{1}{k}\int_{F_{A0}}^{F_A} dF_A = \int_0^V dV\ ,\ V = -\frac{1}{k}\left[0.01F_{A0} - F_{A0}\right] = \frac{\left(5\frac{mol}{h}\right)\times(0.99)}{\left(0.05\frac{mol}{h.dm^3}\right)} = 99\, dm^3$$

(b) $-r_A = kC_A$

CSTR

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

$$V = \frac{v_0(C_{A0} - C_A)}{kC_A} = \frac{\left(10\frac{dm^3}{h}\times\frac{h}{3600s}\right)\times(0.99)\times(C_{A0})}{(0.0001s^{-1})\times(0.01)\times(C_{A0})} = 2750dm^3$$

PFR

$$\frac{dF_A}{dV} = r_A \rightarrow\ \frac{dF_A}{dV} = -kC_A\, , dF_A = d(\upsilon_0 C_A) = \upsilon_0 dC_A \rightarrow \frac{\upsilon_0 dC_A}{dV} = -kC_A$$

$$\frac{dC_A}{C_A} = \frac{-k}{\upsilon_0}dV \rightarrow \int_{C_{A0}}^{C_A}\frac{dC_A}{C_A} = \frac{-k}{\upsilon_0}\int_0^V dV \rightarrow \ln\frac{C_A}{C_{A0}} = \frac{-kV}{\upsilon_0} \rightarrow V = \frac{\upsilon_0}{-k}\ln\frac{C_A}{C_{A0}}$$

$$V = \frac{\left(10\frac{dm^3}{h}\right)}{\left(-0.0001\frac{1}{s}\times\frac{3600s}{h}\right)}\ln\frac{0.01C_{A0}}{C_{A0}} = 127.92\ dm^3$$

(c) $-r_A = kC_A^2$

<u>CSTR</u>

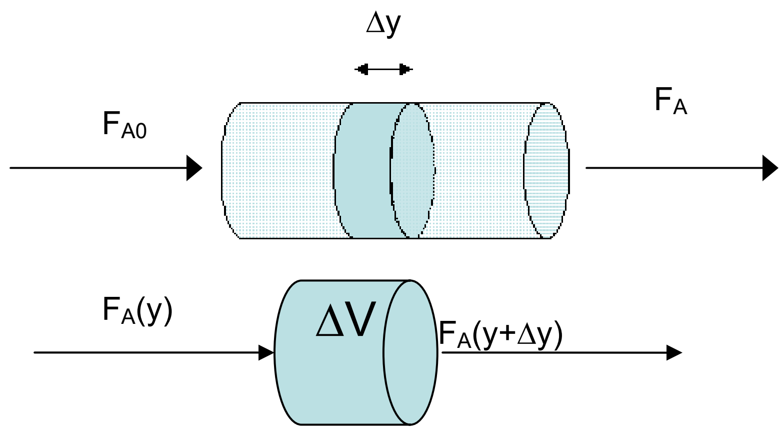
$$V=\frac{F_{A0}-F_A}{-r_A}\rightarrow V=\frac{\upsilon_0\left(C_{A0}-C_A\right)}{kC_A^2}\rightarrow V=\frac{\upsilon_0\times 0.99\times C_{A0}}{kC_{A0}^2(0.01)^2}\rightarrow V=\frac{\left(10\frac{dm^3}{h}\right)\times 0.99}{\left(3\frac{dm^3}{mol.h}\right)\times(0.01)^2\times(0.5\frac{mol}{dm^3})}=66,000\,dm^3$$

<u>PFR</u>

$$\frac{dF_A}{dV}=r_A\rightarrow\frac{\upsilon_0 dC_A}{dV}=-kC_A^2\rightarrow\frac{dC_A}{C_A^2}=-\frac{k}{\upsilon_0}dV\rightarrow\int_{C_{A0}}^{C_A}\frac{dC_A}{C_A^2}=-\frac{k}{\upsilon_0}\int_0^V dV$$

$$-\left[\frac{1}{C_A}-\frac{1}{C_{A0}}\right]=-\frac{k}{\upsilon_0}V\rightarrow V=\frac{\upsilon_0}{kC_{A0}}\left[\frac{1}{0.01}-1\right]\rightarrow V=\frac{\left(10\frac{dm^3}{h}\right)\times 99.0}{\left(3\frac{dm^3}{h.mol}\right)\times\left(0.5\frac{mol}{dm^3}\right)}=660dm^3$$

<u>Problem 2</u>



Consider a differential element ΔV of the reactor :
By material balance

$$F_A|_y - F_A|_{y+\Delta y} + r_A(1-\varepsilon)\Delta V = 0$$

where: $(1-\varepsilon)\Delta V$ = fraction of reactor element which is liquid.

$$-\Delta F_A + r_A(1-\varepsilon)\Delta V = 0\rightarrow\frac{\Delta F_A}{\Delta V}=r_A(1-\varepsilon)\rightarrow\lim_{\Delta V\to 0}\frac{\Delta F_A}{\Delta V}=r_A(1-\varepsilon)$$

$$\frac{dF_A}{dV}=r_A(1-\varepsilon)$$

b) For constant-pressure batch reactor:

$$r_A V = \frac{dN_A}{dt} \rightarrow r_A V = \frac{d(C_A V)}{dt} \rightarrow r_A V = \frac{VdC_A + C_A dV}{dt} \rightarrow r_A = \frac{VdC_A + C_A dV}{Vdt} \rightarrow r_A = \frac{dC_A}{dt} + \frac{C_A dV}{Vdt}$$

$$V = V_0 + V_1 \sin \omega t, \frac{dV}{dt} = V_1 \omega \cos \omega t$$

Combine above equations:

$$r_A = \frac{VdC_A + C_A dV}{Vdt} = \frac{dC_A}{dt} + \frac{C_A}{V_0 + V_1 \sin \omega t} V_1 \omega \cos \omega t$$

<u>Problem 3</u>

(a) $-r_A = kC_A$

$$C_{A0} = \frac{N_{A0}}{V} = \frac{20mol}{20dm^3} = 1\frac{mol}{dm^3}, \ C_A = \frac{N_A}{V} = \frac{0.2mol}{20dm^3} = 0.01\frac{mol}{dm^3}$$

$$r_A V = \frac{dN_A}{dt} \rightarrow r_A V = \frac{d(C_A V)}{dt} \rightarrow r_A = \frac{dC_A}{dt} \rightarrow -kC_A = \frac{dC_A}{dt} \rightarrow dt = -\frac{dC_A}{kC_A}$$

$$\int_0^t dt = -\frac{1}{k}\int_{C_{A0}}^{C_A} \frac{dC_A}{C_A} \rightarrow t = -\frac{1}{k}\ln\frac{C_A}{C_{A0}} \rightarrow t = -\frac{1}{0.865\min^{-1}}\ln\frac{0.01}{1} \rightarrow t = 5.32\min$$

(b) $-r_A = kC_A^2$

$$C_{A0} = \frac{N_{A0}}{V} = \frac{20\,mol}{20\,dm^3} = 1\frac{mol}{dm^3}, \ C_A = \frac{N_A}{V} = \frac{1mol}{20dm^3} = 0.05\frac{mol}{dm^3}$$

$$r_A V = \frac{dN_A}{dt} \rightarrow r_A V = \frac{d(C_A V)}{dt} \rightarrow r_A = \frac{dC_A}{dt} \rightarrow -kC_A^2 = \frac{dC_A}{dt} \rightarrow dt = -\frac{dC_A}{kC_A^2}$$

$$\int_0^t dt = -\frac{1}{k}\int_{C_{A0}}^{C_A} \frac{dC_A}{C_A^2} \rightarrow t = \frac{1}{k}\left[\frac{1}{C_A} - \frac{1}{C_{A0}}\right] \rightarrow t = \frac{1}{2\frac{dm^3}{mol.\min}}\left[\frac{1}{0.05} - 1\right](\frac{dm^3}{mol}) \rightarrow t = 9.5\min$$

(c)

$$Gas\,cons\tan t = R = 0.082\frac{dm^3 atm}{molK}$$

$$nRT = PV \rightarrow P_0 = \frac{n_0 RT}{V} = \frac{(20mol)\times\left(0.082\frac{dm^3 atm}{molK}\right)\times(400.15K)}{(20dm^3)} = 32.8\,atm$$

$$nRT = PV \rightarrow P_{final} = \frac{n_{final} RT}{V} = \frac{(20\times 2mol)\times\left(0.082\frac{dm^3 atm}{molK}\right)\times(400.15K)}{(20dm^3)} = 65.62\,atm$$