CHE 4063 Exam II Nov. 7, 2002

solution

I. a) $-r_A = k_1 C_A + k_2 C_A^2$

$$\tau = \frac{C_{A0}(f_{A,OUT} - f_{A,IN})}{-r_A} = \frac{C_{A0} f_{A1}}{k_1 C_{A0}(1-f_{A1}) + k_2 C_{A0}^2 (1-f_{A1})^2}$$

$$\frac{0.4}{0.6} = 6.6667 = \tau = \frac{f_{A1}}{k_1(1-f_{A1}) + k_2 C_{A0}(1-f_{A1})^2}$$

1:1 stoichiometry, so $C_{A1} = 1.8 - 1.2 - 0.4 = 0.2$

$$f_{A1} = \frac{1.8-0.2}{1.8} = 0.8889$$

$$6.6667 = \frac{0.8889}{k_1(0.1111) + k_2(1.8)(0.0123568)} = \frac{0.8889}{0.1111k_1 + 0.2222k_2}$$

But:

$$\tau = \frac{C_{V,IN} - C_{V,OUT}}{-r_V} = \frac{0-1.2}{-k_1 C_{A1}} = \frac{1.2}{k_1(0.2)}$$

$0.6667 k_1 (0.2) = 1.2$

$$\boxed{k_1 = 0.9000 \text{ min}^{-1}}$$

$$6.6667 = \frac{0.4}{k_2(0.2)^2}$$

$$\boxed{k_2 = 1.500 \text{ lt/mole-min}}$$

check: $$6.6667 \stackrel{?}{=} \frac{0.8889}{(0.9)(0.1111) + 1.5(0.02)}$$ yes ✓

b) $\tau = C_{A0}\int_0^{f_A} \frac{df_A}{-r_A} = -\int_{C_{AIN}}^{C_{AOUT}} \frac{dC_A}{-r_A}$

$$6.67 = -\int_{1.8}^{C_A} \frac{dC_A}{k_1 C_A + k_2 C_A^2} = -\int_{1.8}^{C_A} \frac{dC_A}{C_A(k_1 + k_2 C_A)}$$

$$6.67 = -\left[-\frac{1}{k_1}\ln\left(\frac{k_1 + k_2 C_A}{C_A}\right)\right]_{1.8}^{C_A}$$

$$6.67 = \frac{1}{k_1}\ln\left[\left(\frac{k_1 + k_2 C_A}{C_A}\right)\left(\frac{1.8}{k_1 + k_2(1.8)}\right)\right]$$

$k_1 = 0.9$
$k_2 \quad 1.5$

$$6.67 = \frac{1}{0.9}\ln\left[\left(\frac{0.9 + 1.5 C_A}{C_A}\right)\left(\frac{1.8}{0.9 + 1.5(1.8)}\right)\right]$$

$$6.00 = \ln\left[\frac{0.9 + 1.5 C_A}{C_A}(0.5)\right]$$

$$403.43 = \left(\frac{0.9 + 1.5 C_A}{C_A}\right)\left(\frac{1}{2}\right)$$

$$806.86 = (0.9 + 1.5 C_A)/C_A$$

$$806.86 C_A = 0.9 + 1.5 C_A$$

$$805.35 C_A = 0.9$$

$$C_A = 1.12 \times 10^{-3} = 0.00112$$

$$f_A = \frac{1.8 - 1.12 \times 10^{-3}}{1.8} = 0.9994$$

$$\boxed{C_{A1} = 1.8(1-0.9994) = 0.00108}$$

$$\frac{dC_V}{dC_A} = \frac{-k_1 C_A}{k_1 C_A + k_2 C_A^2} = -\frac{k_1}{k_1 + k_2 C_A}$$

$$-\int_0^{C_{V1}} dC_V = \int_{1.8}^{0.0016} \frac{k_1 \, dC_A}{k_1 + k_2 C_A} = \frac{k_1}{k_2} \ln\left(k_1 + k_2 C_A\right)\Big]_{1.8}^{0.00108}$$

$$= \frac{k_1}{k_2}\Big[-\ln\left(k_1 + k_2(1.8)\right) + \ln\left(k_1 + k_2(0.00108)\right)\Big]_{1.8}^{0.00108}$$

$$-C_{V1} = \frac{0.9}{1.5}\left(-\ln(0.9 + 1.8(1.5)) + \ln\left(0.9 + 1.5(0.00108)\right)\right)$$

$$-C_{V1} = \frac{0.9}{1.5}\Big[-1.2809 - 0.1035\Big].$$

$$\boxed{C_{V1} = 0.830}$$

$$\boxed{C_{W1} = 1.8 - 0.830 - 0.00108 = 0.9683}$$

c) $$\boxed{Y_V = \frac{0.830}{1.8 - 0.00108} = 0.4615 \quad \text{PFR}}$$

$$\boxed{Y_V = \frac{1.2}{1.8 - 0.2} = 0.750 \quad \text{CSTR}}$$

II. a) $A \rightarrow \frac{1}{2} B$

$$T = T_0 + \Delta H^\circ_R F_{A0} f_A / r_A \sum F_i C_{pi}$$

$$T = 350^\circ K + (-100{,}000)(10 \text{ mols/lt}) f_A / (-1)\left[10(1-f_A)15 + (10/2) f_A (19) + 100(17)\right]$$

$$T = 350 + 10^5 f_A / (1850 - 55 f_A)$$

@ $f_A = 0.7$

$$\boxed{T = 350 + 10^5 (0.7) / (1850 - 55(0.7)) = 388.6^\circ K}$$

b) $\tau = C_{A0}(f_{A\,OUT} - f_{A\,IN}) / -r_A$

@ $388.6^\circ K$, $k = 8 \times 10^{16} e^{-22000/1.987(388.6)}$

$k = 3.38 \times 10^4 \text{ min}^{-1}$

$$C_A = \frac{C_{A0}(1-f_A)}{1+\delta_A f_A} \qquad C_{A0} = \frac{10/110}{(0.08205)(350)} = 3.17 \times 10^{-3} \text{ mols/lt}$$

$$\delta_A = \frac{105-110}{110} = -0.0455$$

$$C_A = \left[3.17 \times 10^{-3}(1-f_A)/(1-0.0455 f_A)\right](T_0/T)$$

$$\tau = \frac{\cancel{3.17 \times 10^{-3}} f_A \left(388.6/350\right)}{\dfrac{(3.38 \times 10^4)\cancel{(3.17 \times 10^{-3})}(1-f_A)}{(1 - 0.0455 f_A)}}$$

for $f_A = 0.7$

$$\tau = \frac{0.7\left[1 - 0.0455(0.7)\right]\left(388.6/350\right)}{(3.38 \times 10^4)(1-0.7)} = 7.417 \times 10^{-5} \text{ min}$$

$$V_R / V_0 = 7.417 \times 10^{-5} \text{ min}$$

$1/0.08205(350) = 3.48 \times 10^{-2}$ mols/lt $\equiv 28.712$ lt/mole

28.712 lt/mole $\times 110$ mols/min $= 3.15 \times 10^3$ lt/min

$V_R = 3.15 \times 10^3 = 7.417 \times 10^{-5}$

$$\boxed{V_R = 0.233 \text{ lt}}$$