Chemical Reaction Engineering—Spring 2020
Homework 3 Solutions

Problem #1

$$A(g) + 2B(g) \longrightarrow C(g,l) + D(g)$$

$$-r_A = k\, C_A C_B$$

$$y_c = 0.25$$

$$v_0 = 1.5 \text{ L min}^{-1}, \quad k = 0.035 \frac{\text{L}}{\text{mol}\cdot\text{s}}$$

a) THIS IS NOT AN ELEMENTRY STEP, THE RATE LAW DOES NOT ~~REPRESENT~~ REPRESENT THE STOICHIOMETRY.

b) Stoichiometric Table:

Species	In	Change	Out (Before Condensation)
A	F_{A0}	$-F_{A0}X_A$	$F_{A0}(1-X_A)$
B	$2F_{A0}$	$-2F_{A0}X_A$	$F_{A0}(2-2X_A)$
C	0	$F_{A0}X_A$	$F_{A0}X_A$
D	0	$F_{A0}X_A$	$F_{A0}X_A$

Before Condensation: $F_T = F_{A0}(3-X_A)$

After Condensation: $F_T' = y_c F_T' + (3-2X_A)F_{A0}$

$$F_T' = \frac{F_{A0}(3-2X_A)}{(1-y_c)}$$

$F_A = F_{A0}(1-X_A)$ $\qquad F_C = y_c F_T'$

$F_B = F_{A0}(2-2X_A)$ $\qquad F_D = F_{A0}X_A$

c. $F_T = F_T'$ WHEN CONDENSATION BEGINS

$$\cancel{F_{A0}}(3 - X_A) = \frac{\cancel{F_{A0}}(3 - 2X_A)}{1 - y_c}$$

$y_c = 0.25$ GIVEN

$$0.75(3 - X_A) = 3 - 2X_A$$

$$\boxed{X_A = 0.6}$$

DEFINITION OF PARTIAL PRESSURE

$$y_c = \frac{P_c^*}{P}$$

$$\boxed{P_c^* = 0.25\,(101\text{ kPa}) = 25.25\text{ kPa}}$$

d. IN TERMS OF X_A, k, C_{A0}, WE CAN WRITE $-r_A$ BEFORE CONDENSATION

$$C_j = \frac{F_{A0}(\Theta_j + \nu_j X)}{v_0\left[(1 + \varepsilon X)\left(\frac{P_0}{P}\frac{T}{T_0}\right)\right]}$$

$P = P_0$ ISOBARIC

$T = T_0$ ISOTHERMAL

$$\varepsilon = y_{A0}\,\delta = \frac{1}{3}(1 + 1 - 1 - 2) = \frac{1}{3}(-1) = \frac{-1}{3}$$

$$C_A = \frac{F_{A0}}{v_0}\frac{(1 - X)}{(1 - \frac{1}{3}X)} = \frac{C_{A0}(1 - X)}{\left(1 - \frac{X}{3}\right)}$$

$$C_B = \frac{F_{A0}}{v_0}\frac{(2 - 2X)}{\left(1 - \frac{X}{3}\right)} = \frac{2C_{A0}(1 - X)}{1 - \frac{X}{3}}$$

$$-r_A = k C_A C_B$$

$$\boxed{-r_A = \frac{2k C_{A0}^2 (1-X)^2}{\left(1 - \frac{X}{3}\right)^2}}$$

AFTER CONDENSATION

$$v = v_0 \left(\frac{F_T'}{F_{T0}}\right) = \frac{v_0 F_{A0}(3-2X_A)}{3F_{A0}(1-y_c)}$$

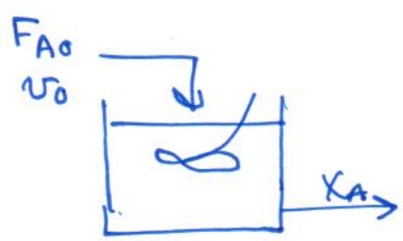
$$\boxed{v = \frac{v_0(3-2X_A)}{3(1-y_c)}}$$

d. $$C_A = \frac{F_A}{v} = \frac{F_{A0}(1-X_A)\cdot 3(1-y_c)}{v_0(3-2X_A)} = \frac{3C_{A0}(1-y_c)(1-X_A)}{3-2X_A}$$

$$C_B = \frac{F_B}{v} = \frac{2F_{A0}(1-X_A)\,3(1-y_c)}{v_0(3-2X_A)} = \frac{6C_{A0}(1-y_c)(1-X_A)}{3-2X_A}$$

$$-r_A = \frac{18k C_{A0}^2 (1-y_c)^2 (1-X_A)^2}{(3-2X_A)^2}$$

e. 90% CONVERSION OF A



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

$$F_{A0} = C_{A0} v_0 = y_{A0} C_{T0} v_0$$

IDEAL GAS $\quad C_{T0} = \dfrac{P_0}{R T_0}$

$$F_{A0} = \frac{y_{A0} P_0}{R T_0} v_0 = \frac{\frac{1}{3}(101\ \text{kPa})(1.5\ \text{L}\cdot\text{min}^{-1})}{\left(8.314 \frac{\text{kPa}\cdot\text{L}}{\text{mol}\cdot\text{K}}\right)(298\ \text{K})}$$

$$F_{A0} = 0.0204\ \frac{\text{mol}}{\text{min}}$$

$$V = \frac{F_{A0} X_A (3-2X_A)^2}{18 k\, c_{A0}^2 (1-y_c)^2 (1-X_A)^2}$$

$$V = \frac{\cancel{F_{A0}} X_A (3-2X_A)^2 v_0^2}{18 k\, F_{A0}^{\cancel{2}} (1-y_c)^2 (1-X_A)^2}$$

$$V = \frac{(0.9)(3-2(0.9))^2 (1.5\ \text{L/min})^2}{18(0.035\ \text{L}\cdot\text{mol}^{-1}\text{s}^{-1})\left(0.0204 \frac{\text{mol}}{\text{min}}\right)\left(60 \frac{\text{s}}{\text{min}}\right)(0.75)^2(0.1)^2}$$

$$\boxed{V = 672\ \text{L}}$$

PROBLEM #2

ARRHENIUS TEMPERATURE DEPENDENCE OF RATE CONSTANT

$$k = A \,\mathrm{EXP}\left[\frac{-E_A}{RT}\right]$$

$$\ln k = \ln A - \frac{E_A}{RT}$$

PLOT $\ln k$ VS. $\frac{1}{T}$

y-INT $= \ln A$ SLOPE $= \frac{-E_A}{R}$

FIT DATA TO LINEAR EQUATION

$\ln A = 28.51 \longrightarrow \boxed{A = 2.4(10^{12}) \frac{\text{mol}}{\text{L} \cdot \text{min ATM}^2}}$

$-\frac{E_A}{R} = -13351 \longrightarrow \boxed{E_A = 111 \text{ kJ/mol}}$

VAN'T HOFF EQN.

$$K(T) = K(T_{REF}) \,\mathrm{EXP}\left[\frac{\Delta H}{R}\left(\frac{1}{T_{ref}} - \frac{1}{T}\right)\right]$$

$$\ln\left(\frac{K(T)}{K(T_{ref})}\right) = \frac{\Delta H}{R}\left(\frac{1}{T_{ref}} - \frac{1}{T}\right)$$

SLOPE IS $\frac{\Delta H}{R}$ WHEN PLOTTING

$$\ln\left(\frac{K(T)}{K(T_{ref})}\right) \text{ VS } \left(\frac{1}{T_{ref}} - \frac{1}{T}\right)$$

CHOOSE $T_{ref} = 303K$

$$\frac{\Delta H}{R} = -7577.6 \qquad \Delta H = \frac{-63\,kJ}{mol}$$

b) $C_6H_6 + C_3H_6 \underset{k_r}{\overset{k_f}{\rightleftharpoons}} C_9H_{12}$

$F_{T0} = F_{A0} + 2F_{A0}$

$F_{A0} = 4.8\ mol/MIN \qquad F_{B0} = 9.6\ MOL/MIN$

DESIGN EQN $\quad F_{A0}\dfrac{dX}{dV} = -r_A$

$-r_A = r_{forward} - r_{rev.}$

$-r_A = k_f P_A P_B - k_r P_C$

CALCULATE k_f at 373K

$$k_f = 2.4E12\ EXP\left[\frac{-111\ kJ/MOL}{0.008314\frac{kJ}{MOL\cdot K}(373K)}\right]$$

$$k_f = 6.83\times10^{-4}\ \frac{MOL}{MIN\ L\ ATM^2}$$

FOR AN ELEMENTARY STEP, k_r CAN BE CALCULATED FROM THE EQUILIBRIUM CONSTANT.

$$K(373K) = 9.09E2 \ EXP\left[\frac{-63 \ kJ/mol}{0.008314 \ \frac{kJ}{mol \cdot K}}\left(\frac{1}{303K} - \frac{1}{373K}\right)\right]$$

$$K(373K) = 8.32 \ ATM^{-1}$$

$$k_r = 8.22E\text{-}5 \ \frac{MOL}{L \cdot MIN \ ATM}$$

$$F_{A0}\frac{dX}{dV} = k_f P_A P_B - k_r P_C$$

IDEAL GAS* LAW

$$P_A = C_A RT \ ; \ P_B = C_B RT \ ; \ P_C = C_C RT$$

STOICHIOMETRIC TABLE

SPECIES	INITIAL	CHANGE	FINAL	CONC.
A	F_{A0}	$-F_{A0}X_A$	$F_{A0}(1-X_A)$	$\frac{F_{A0}(1-X_A)}{v_0(1+\varepsilon X_A)}$
B	F_{B0}	$-F_{A0}X_A$	$F_{A0}\left(\frac{F_{B0}}{F_{A0}}-X_A\right)$	$\frac{F_{A0}\left(\frac{F_{B0}}{F_{A0}}-X_A\right)}{v_0(1+\varepsilon X_A)}$
C	0	$+F_{A0}X_A$	$F_{A0}X_A$	$\frac{F_{A0}X_A}{v_0(1+\varepsilon X_A)}$

$$\underset{A}{C_6H_6} + \underset{B}{C_3H_6} \rightleftharpoons \underset{C}{C_9H_{12}}$$

$$\varepsilon = y_{A0}\delta = \frac{1}{3}(-1) = \frac{-1}{3}$$

SOLVE THE DESIGN EQN. NUMERICALLY

FOR $V = 0L$ TO $150L$

$$\boxed{X_A = 0.089}$$

c. SAME AS PART B EXCEPT k_f, k_r, AND K MUST BE CALCULATED AT 423K

$$k_f = 0.0471 \frac{\text{mol}}{\text{L}\cdot\text{min atm}^2}$$

$$k_r = 0.0625 \frac{\text{mol}}{\text{L}\cdot\text{MIN}\cdot\text{ATM}}$$

$$K = 0.754 \ \text{ATM}^{-1}$$

$$X_A = 0.682$$

d. TO SOLVE FOR X_{EQ}, USE EQUATION FOR K

$$K = \frac{P_C}{P_A P_B} = \frac{C_C RT}{C_A C_B (RT)^2}$$

$$K = \frac{\frac{F_{A0}}{v_0} X_A \left(\frac{1}{1+\varepsilon X_A}\right)}{RT\left[\frac{F_{A0}^2 (1-X_A)\left(\frac{F_{B0}}{F_{A0}} - X_A\right)}{v_0^2 (1+\varepsilon X_A)^2}\right]}$$

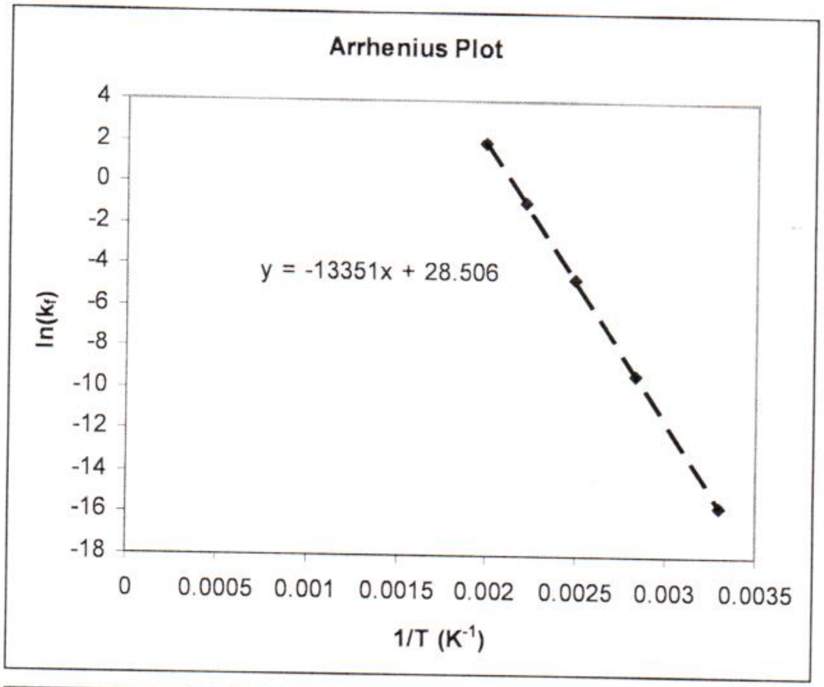
$$K = \frac{v_0 (1 + \varepsilon X_A) X_A}{RT\, F_{A0} (1 - X_A) \left(\frac{F_{B0}}{F_{A0}} - X_A \right)}$$

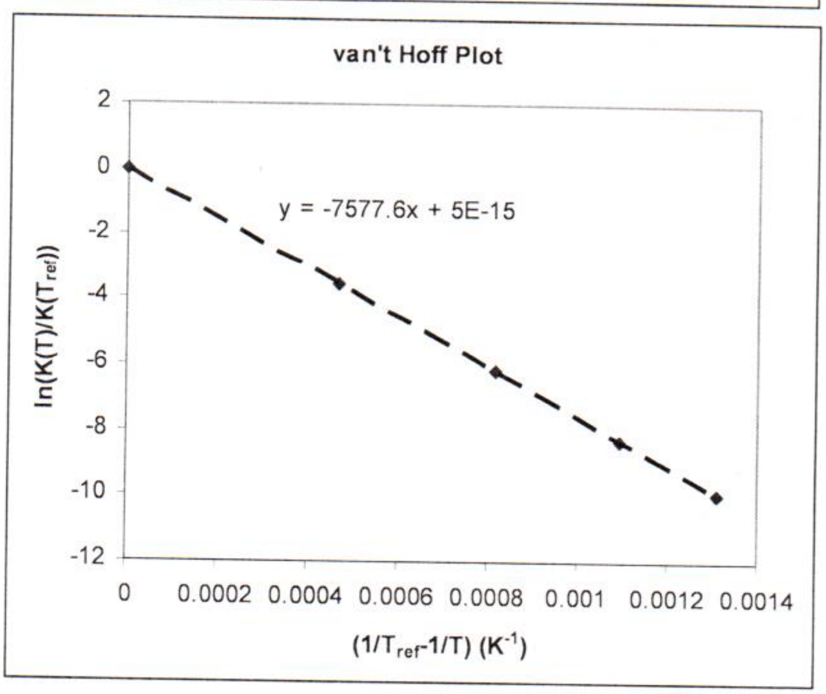
$X_{EQ}(373K) = 0.949$

$X_{EQ}(423K) = 0.682$

Problem 2 Solutions.

Part (a):





PROBLEM #3

$A \rightarrow 3B$ IN A BATCH REACTOR

$k = 0.45\ s^{-1}\ M^{-1}$

$$C_{A0} = \frac{0.5\,(50\ \text{MOL})}{10\ L} = 2.5\ M$$

STOICHIOMETRIC TABLE

SPECIES	INITIAL	FINAL
A	N_{A0}	$N_{A0}(1-X_A)$
B	0	$3N_{A0}X_A$
I	N_{A0}	N_{A0}
TOTAL	$2N_{A0}$	$(2+2X_A)N_{A0}$

a. CONSTANT PRESSURE

$$\varepsilon = y_{A0}\,\delta = \tfrac{1}{2}(3-1) = 1$$

$$V = V_0(1+X_A)$$

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

$$-\frac{k N_A^2}{V_0(1+X_A)} = \frac{dN_A}{dt}$$

$$-\frac{k N_{A0}^2(1-X_A)^2}{V_0(1+X_A)} = -N_{A0}\frac{dX}{dt}$$

$$\frac{k N_{A0} (1-X_A)^2}{V_0 (1+X_A)} = \frac{dX}{dt}$$

$$\frac{k t N_{A0}}{V_0} = \int_0^{X_f} \frac{1+X}{(1-X)^2} \, dX$$

$$\boxed{X_f = 0.973}$$

PROBLEM #4

a. ASSUME ISOTHERMAL, ISOBARIC REACTOR OPERATION

$$C_j = \frac{C_{A0}\left(\Theta_j + \frac{\nu_j}{\nu_A} X_A\right)}{1 + \varepsilon X_A}$$

$$C_A = \frac{C_{A0}\left(1 - X_A\right)}{1 - \frac{1}{2} X_A}$$

$$C_A = \frac{4 \frac{mol}{L}\left(1 - 0.6\right)}{1 - \frac{1}{2}(0.6)} = 2.29 \frac{mol}{L}$$

$$C_B = \frac{C_{A0}\left(0 + \frac{1}{2} X_A\right)}{1 - \frac{1}{2} X_A} = \frac{\frac{1}{2} C_{A0} X_A}{1 - \frac{1}{2} X_A}$$

$$C_B = \frac{4 \frac{mol}{L}\left(\frac{1}{2}\right)\left(0.6\right)}{1 - \frac{1}{2}(0.6)} = 1.71 \frac{mol}{L}$$

$$K_c = \frac{C_B}{C_A^2} = \frac{1.71 \frac{mol}{L}}{\left(2.29 \frac{mol}{L}\right)^2} = \boxed{0.326 M^{-1}}$$

$$K_c = \frac{C_C^{\,3}}{C_A} = 0.25\,M^2 = \frac{\left(C_{A0}(3X)\right)^3}{C_{A0}(1-X)}$$

USE AN NLE SOLVER

$$\boxed{X = 0.393}$$

d) CONSTANT PRESSURE

$$\varepsilon = y_{A0} \cdot \delta = 1(2) = 2$$

$$C_A = \frac{C_{A0}(1-X)}{1+2X}$$

ASSUME ISOTHERMAL, ISOBARIC REACTOR

$$C_C = \frac{C_{A0}(3X)}{1+2X}$$

$$K_c = \frac{C_C^{\,3}}{C_A} = \frac{\dfrac{C_{A0}^{\,3}(3X)^3}{(1+2X)^3}}{\dfrac{C_{A0}(1-X)}{1+2X}} = 0.25\,M^2$$

$$\boxed{X = 0.58}$$

b. FOR LIQUID PHASE, THERE IS NO VOLUME CHANGE

$$C_A = C_{A0}(1-X) \qquad C_B = \frac{C_{A0}X}{2}$$

$$C_A = \frac{4\,\text{MOL}}{L}(1-0.6) = 1.6\ \frac{\text{MOL}}{L}$$

$$C_B = \frac{1}{2}\left(4\ \frac{\text{MOL}}{L}\right)(0.6) = 1.2\ \frac{\text{MOL}}{L}$$

$$K_C = \frac{C_B}{C_A^2} = \frac{1.2\ \frac{\text{MOL}}{L}}{\left(1.6\ \frac{\text{MOL}}{L}\right)^2}$$

$$\boxed{K_C = 0.469}$$

c. $A \rightleftharpoons 3C \qquad K_C = 0.25\ M^2$

$$C_{A0} = \frac{y_{A0}P}{RT} = \frac{1\,(10\ \text{ATM})}{\left(0.082\ \frac{L\cdot\text{ATM}}{\text{MOL}\cdot K}\right)(400K)}$$

$$C_{A0} = 0.305\ \frac{\text{MOL}}{L}$$

FOR CONSTANT VOLUME

$$C_A = C_{A0}(1-X) \qquad C_C = C_{A0}(3X)$$