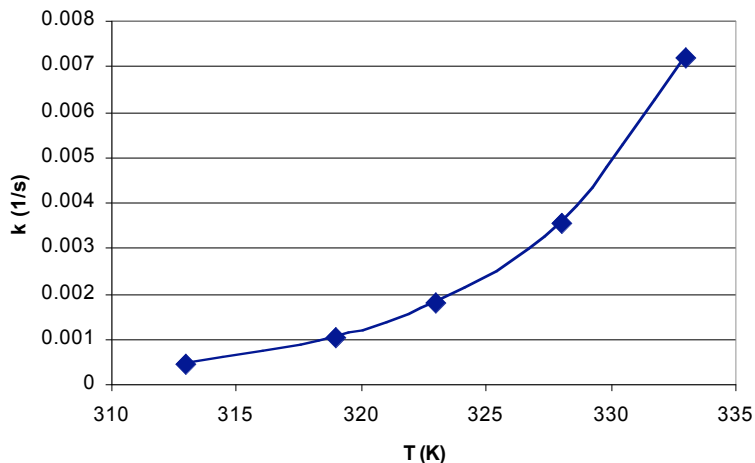


Solutions for Chapter 3 – Rate Law and Stoichiometry

P3-1 Individualized solution.

P3-2 (a) Example 3-1



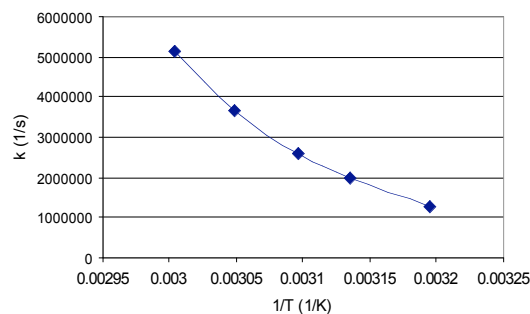
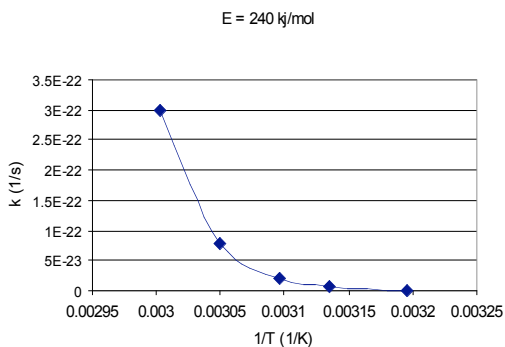
For $E = 60\text{kJ/mol}$

$$k = 1.32 \times 10^{16} \exp\left(\frac{-60000J}{RT}\right)$$

For $E_1 = 240\text{kJ/mol}$

$$k_1 = 1.32 \times 10^{16} \exp\left(\frac{-240000J}{RT}\right)$$

$E = 60\text{ kJ/mol}$



P3-2 (b) Example 3-2 Yes, water is already considered inert.

P3-2 (c) Example 3-3

The solution to the example at a conversion of 20% would remain unchanged. For 90% conversions of the caustic soda, the final concentration of glyceryl sterate is 0 instead of a negative concentration. Therefore 90% of caustic soda is possible.

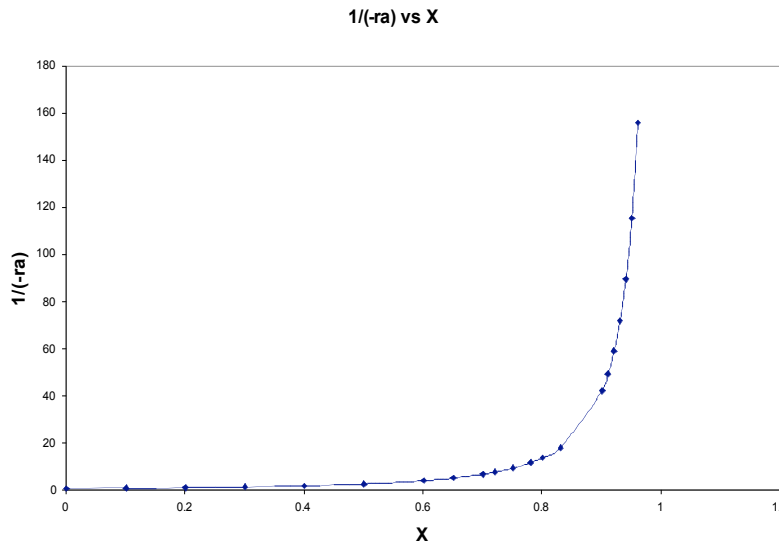
P3-2 (d) Example 3-4 $A + \frac{b}{a}B \rightarrow \frac{c}{a}C + \frac{d}{a}D$

So, the minimum value of $\Theta_B = b/a = \frac{1/3}{1} = 0.33$

P3-2 (e) Example 3-5

For the concentration of N_2 to be constant, the volume of reactor must be constant. $V = V_0$.

Plot: $\frac{1}{-r_A} = \frac{0.5(1 - 0.14X)^2}{(1 - X)(0.54 - 0.5X)}$

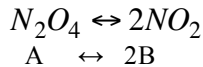


The rate of reaction decreases drastically with increase in conversion at higher conversions.

P3-2 (f) Example 3-6

For a given conversion, concentration of B is lower in flow reactor than a constant volume batch reactor. Therefore the reverse reaction decreases.

C_{T0} = constant and inerts are varied.



Equilibrium rate constant is given by: $K_C = \frac{C_{B,e}^2}{C_{A,e}}$

Stoichiometry: $\epsilon = y_{A0}\delta = y_{A0}(2 - 1) = y_{A0}$

Constant volume Batch:

$$C_A = \frac{N_{A0}(1 - X)}{V_0} = C_{A0}(1 - X) \quad \text{and} \quad C_B = \frac{2N_{A0}X}{V_0} = 2C_{A0}X$$

Plug flow reactor:

$$C_A = \frac{F_{A0}(1 - X)}{v_0(1 + \epsilon X)} = \frac{C_{A0}(1 - X)}{(1 + \epsilon X)} \quad \text{and} \quad C_B = \frac{2F_{A0}X}{v_0(1 + \epsilon X)} = \frac{2C_{A0}X}{(1 + \epsilon X)}$$

$$C_{AO} = \frac{y_{AO}P_O}{RT_O} = y_{AO}(0.07176) \text{ mol/dm}^3$$

Combining: For constant volume batch:

$$K_C = \frac{C_{B,e}^2}{C_{A,e}} = \frac{4C_{AO}^2 X^2}{C_{AO}(1-X)} \quad \Rightarrow X_e = \sqrt{\frac{K_C(1-X_e)}{4C_{AO}}}$$

For flow reactor:

$$K_C = \frac{C_{B,e}^2}{C_{A,e}} = \frac{4C_{AO}^2 X^2}{C_{AO}(1-X)(1+\epsilon X)} \quad \Rightarrow X_e = \sqrt{\frac{K_C(1-X_e)(1+\epsilon X_e)}{4C_{AO}}}$$

See Polymath program [P3-2-f.pol](#).

POLYMATH Results

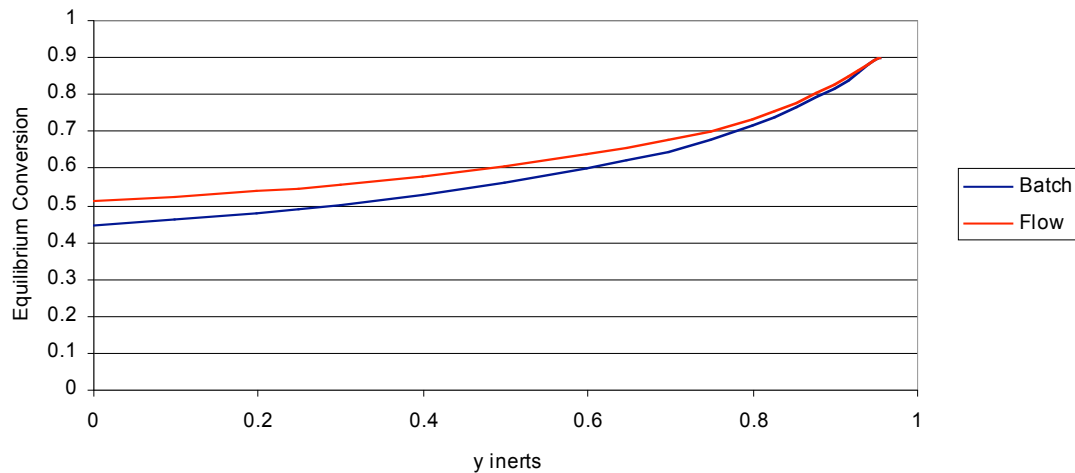
NLES Report (safenewt)

Nonlinear equations

- [1] $f(X_{eb}) = X_{eb} - (kc*(1-X_{eb})/(4*C_{ao}))^{0.5} = 0$
- [2] $f(X_{ef}) = X_{ef} - (kc*(1-X_{ef})*(1+eps*X_{ef})/(4*C_{ao}))^{0.5} = 0$

Explicit equations

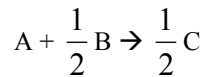
- [1] $y_{ao} = 1$
- [2] $kc = 0.1$
- [3] $C_{ao} = 0.07174*y_{ao}$
- [4] $eps = y_{ao}$



| Y _{inert} | Y _{ao} | X _{eb} | X _{ef} |
|--------------------|-----------------|-----------------|-----------------|
| 0 | 1 | 0.44 | 0.508 |
| 0.1 | 0.9 | 0.458 | 0.5217 |
| 0.2 | 0.8 | 0.4777 | 0.537 |
| 0.3 | 0.7 | 0.5 | 0.5547 |
| 0.4 | 0.6 | 0.525 | 0.576 |
| 0.5 | 0.5 | 0.556 | 0.601 |
| 0.6 | 0.4 | 0.5944 | 0.633 |
| 0.7 | 0.3 | 0.6435 | 0.6743 |
| 0.8 | 0.2 | 0.71 | 0.732 |
| 0.9 | 0.1 | 0.8112 | 0.8212 |
| 0.95 | 0.05 | 0.887 | 0.89 |
| 0.956 | 0.044 | 0.893 | 0.896 |

P3-2 (g) No solution will be given

P3-2 (h)

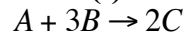


$$\text{Rate law: } -r_A = k_A C_A^2 C_B \text{ and } k_A = 25 \frac{1}{s} \left(\frac{dm^3}{mol} \right)^2$$

$$\frac{r_A}{-1} = \frac{r_B}{-1/2} = \frac{r_C}{1/2} \Rightarrow 25 C_A^2 C_B = \frac{k_B C_A^2 C_B}{1/2} = \frac{k_C C_A^2 C_B}{-1/2}$$

$$k_C = k_B = 12.5 \frac{1}{s} \left(\frac{dm^3}{mol} \right)^2$$

P3-2 (i)



Rate law: $-r_A = k_A C_A C_B$ at low temperatures.

At equilibrium,

$$K_C = \frac{C_{C,e}}{C_{A,e}^{1/2} C_{B,e}^{3/2}} \Rightarrow C_A^{1/2} C_B^{3/2} - \frac{C_C}{K_C} = 0$$

At equilibrium, $-r_A = 0$, so we can suggest that $-r_A = k_A \left(C_A^{1/2} C_B^{1/2} - \frac{C_C}{K_C} \right)$

But at $t = 0$, $C_C = 0$

So the rate law is not valid at $t = 0$.

Next guess:

$$K_C^2 = \frac{C_{C,e}^2}{C_{A,e} C_{B,e}^3}, \text{ or } C_A C_B - \frac{C_C^2}{K_C^2 C_B^2} = 0$$

$$\Rightarrow -r_A = k_A \left(C_A C_B - \frac{C_C^2}{K_C^2 C_B^2} \right)$$

which satisfies both the initial conditions and equilibrium rate law.

Hence $-r_A = k_A \left(C_A C_B - \frac{C_C^2}{K_C^2 C_B^2} \right)$ is the required rate law.

P3-3 Solution is in the decoding algorithm available separately from the author.

P3-4 (a)

Note: This problem can have many solutions as data fitting can be done in many ways.

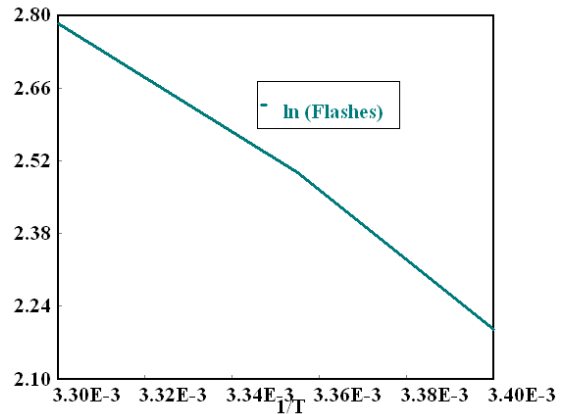
Using Arrhenius Equation

For Fire flies:

| T(in K) | 1/T | Flashes/min | ln(flashes/min) |
|---------|----------|-------------|-----------------|
| 294 | 0.003401 | 9 | 2.197 |
| 298 | 0.003356 | 12.16 | 2.498 |
| 303 | 0.003300 | 16.2 | 2.785 |

Plotting ln(flashes/min) vs 1/T, we get a straight line.

See Polymath program [P3-4-fireflies.pol](#).



For Crickets:

| T(in K) | 1/T x10 ³ | chirps/min | ln(chirps/min) |
|---------|----------------------|------------|----------------|
| 287.2 | 3.482 | 80 | 4.382 |
| 293.3 | 3.409 | 126 | 4.836 |
| 300 | 3.333 | 200 | 5.298 |

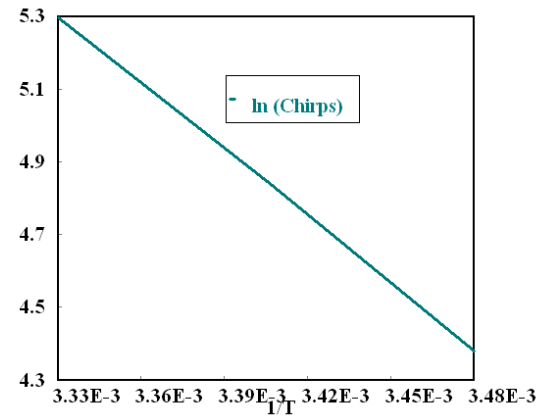
Plotting ln(chirps/min) Vs 1/T, we get a straight line.

→ Both, Fireflies and Crickets data

follow the Arrhenius Model.

ln y = A + B/T, and have the same activation energy.

See Polymath program [P3-4-crickets.pol](#).



P3-4 (b)

For Honeybee:

| T(in K) | 1/T x10 ³ | V(cm/s) | ln(V) |
|---------|----------------------|---------|--------|
| 298 | 3.356 | 0.7 | -0.357 |
| 303 | 3.300 | 1.8 | 0.588 |
| 308 | 3.247 | 3 | 1.098 |

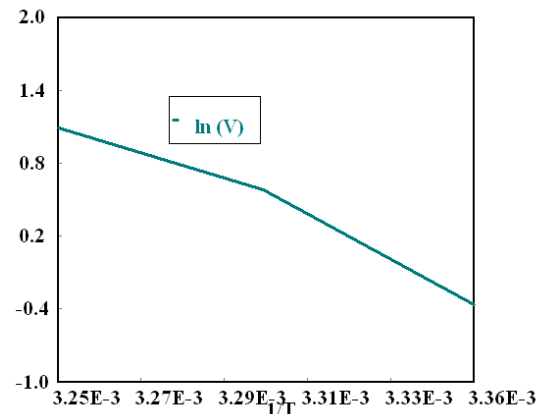
Plotting ln(V) Vs 1/T, almost straight line.

$$\ln(V) = 44.6 - 1.33E4/T$$

At T = 40°C(313K) V = 6.4cm/s

At T = -5°C(268K) V = 0.005cm/s(But bee would not be alive at this temperature)

See Polymath program [P3-4-bees.pol](#).



P3-4 (c)

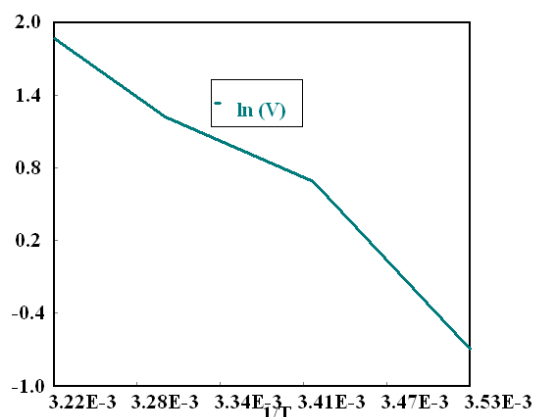
For ants:

| T(in K) | 1/T x10 ³ | V(cm/s) | ln(V) |
|---------|----------------------|---------|-------|
| 283 | 3.53 | 0.5 | -0.69 |
| 293 | 3.41 | 2 | 0.69 |
| 303 | 3.30 | 3.4 | 1.22 |
| 311 | 3.21 | 6.5 | 1.87 |

Plotting ln(V) Vs 1/T,
almost straight line.

See Polymath program [P3-4-ants.pol](#).

So activity of bees, ants, crickets and fireflies follow Arrhenius model. So activity increases with an increase in temperature. Activation energies for fireflies and crickets are almost the same.



| Insect | Activation Energy |
|----------|-------------------|
| Cricket | 52150 |
| Firefly | 54800 |
| Ant | 95570 |
| Honeybee | 141800 |

P3-4 (d)

There is a limit to temperature for which data for any one of the insect can be extrapolate. Data which would be helpful is the maximum and the minimum temperature that these insects can endure before death. Therefore, even if extrapolation gives us a value that looks reasonable, at certain temperature it could be useless.

P3-5

There are two competing effects that bring about the maximum in the corrosion rate: Temperature and HCN-H₂SO₄ concentration. The corrosion rate increases with increasing temperature and increasing concentration of HCN-H₂SO₄ complex. The temperature increases as we go from top to bottom of the column and consequently the rate of corrosion should increase. However, the HCN concentrations (and the HCN-H₂SO₄ complex) decrease as we go from top to bottom of the column. There is virtually no HCN in the bottom of the column. These two opposing factors results in the maximum of the corrosion rate somewhere around the middle of the column.

P3-6 Antidote did not dissolve from glass at low temperatures.

P3-7 (a)

If a reaction rate doubles for an increase in 10°C, at T = T₁ let k = k₁ and at T = T₂ = T₁+10, let k = k₂ = 2k₁. Then with k = Ae^{-E/RT} in general, k₁ = Ae^{-E/RT₁} and k₂ = Ae^{-E/RT₂}, or

$$\frac{k_2}{k_1} = e^{-\frac{E}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)} \quad \text{or} \quad \frac{E}{R} = -\frac{\ln\left(\frac{k_2}{k_1}\right)}{\left(\frac{1}{T_2} - \frac{1}{T_1}\right)} = -\frac{\ln\left(\frac{k_2}{k_1}\right)}{\frac{T_1 - T_2}{T_1 T_2}}$$

Therefore:

$$E = R \frac{\ln\left(\frac{k_2}{k_1}\right)(T_1(T_1 + 10))}{(T_2 - T_1)} = R \frac{(\ln 2)(T_1(T_1 + 10))}{10}$$

$$T_1(T_1 + 10) = \frac{10E}{R \ln 2}$$

which can be approximated by $T = \frac{10E^{0.5}}{R \ln 2}$

P3-7 (b)

Equation 3-18 is $k = Ae^{-\frac{E}{RT}}$

From the data, at $T_1 = 0^\circ\text{C}$, $k_1 = Ae^{-E/RT_1}$, and at $T_2 = 100^\circ\text{C}$, $k_2 = Ae^{-E/RT_2}$

Dividing gives $\frac{k_2}{k_1} = e^{-\frac{E}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)}$, or

$$E = -\frac{R \ln\left(\frac{k_2}{k_1}\right)}{\left(\frac{1}{T_2} - \frac{1}{T_1}\right)} = -\frac{RT_1 T_2}{(T_1 - T_2)} \ln\left(\frac{k_2}{k_1}\right)$$

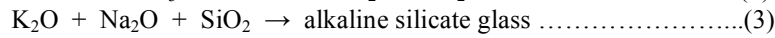
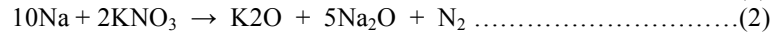
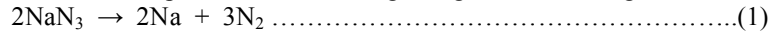
$$E = \frac{\left[1.99 \frac{\text{cal}}{\text{mol K}}\right] [273 \text{ K} \text{ } \text{ } 373 \text{ K}]}{100 \text{ K}} \ln\left(\frac{.050}{.001}\right) = 7960 \frac{\text{cal}}{\text{mol}}$$

$$A = k_1 e^{\frac{E}{RT_1}} = 10^{-3} \text{ min}^{-1} \exp\left[\frac{7960 \frac{\text{cal}}{\text{mol}}}{\left(1.99 \frac{\text{cal}}{\text{mol K}}\right)(273 \text{ K})}\right] = 2100 \text{ min}^{-1}$$

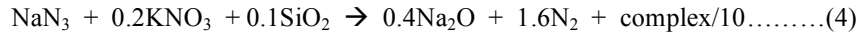
P3-7 (c) Individualized solution

P3-8

When the components inside air bag are ignited, following reactions take place,



$$5 \times rxn(1) + rxn(2) + rxn(3) = rxn(4)$$



Stoichiometric table:

| Species | Symbol | Initial | Change | Final |
|-------------------|--------|-------------------------------|----------------------|----------------------------------------|
| NaN ₃ | A | N _A | -N _A X | N _A (1-X) |
| KNO ₃ | B | N _A θ _B | -0.2X N _A | N _A (θ _B - 0.2X) |
| SiO ₂ | C | N _A θ _C | -0.1XN _A | N _A (θ _C - 0.1X) |
| Na ₂ O | D | 0 | 0.4XN _A | 0.4XN _A |
| N ₂ | E | 0 | 1.6XN _A | 1.6XN _A |

Given weight of NaN₃ = 150g

M_{wt} of NaN₃ = 65

Therefore, no. of moles of NaN₃ = 2.3

1 moles of NaN₃ requires 0.2 mole of KNO₃

=> Moles of B, KNO₃ = 0.2(2.3) = 0.46 moles M_{wt} of KNO₃ = 101.1

Therefore, grams of KNO₃ required = 0.46 x 101.1 = 46.5 g

1 moles of NaN₃ requires 0.1 mole of SiO₂.

Moles of C, SiO₂ = 0.1(2.3) = 0.23 moles M_{wt} of SiO₂ = 60.08

Therefore, grams of SiO₂ required = 0.23 x 60.08 = 13.8 g

Following proposals are given to handle all the un-detonated air bags in cars piling up in the junkyards:

- Store cars in cool, dry, ventilated areas.
- Avoid Physical damage of the bag in car.
- It is stable under ordinary conditions of storage. Decomposes explosively upon heating (over 221 ° F or 105 ° C), shock, concussion, or friction.
- Conditions to avoid: heat, flames, ignition sources and incompatibles.

P3-9 (a)

From the web module we know that $\frac{dX}{dt} = k(1-x)$ and that k is a function of temperature, but not a

linear function. Therefore doubling the temperature will not necessarily double the reaction rate, and therefore halve the cooking time.

P3-9 (b)

When you boil the potato in water, the heat transfer coefficient is much larger, but the temperature can only be 100°C.

When you bake the potato, the heat transfer coefficient is smaller, but the temperature can be more than double that of boiling water.

P3-9 (c) No solution will be given

P3-10 (a)

- 1) $C_2H_6 \rightarrow C_2H_4 + H_2$ Rate law: $-r_A = kC_{C_2H_6}$
- 2) $C_2H_4 + 1/2O_2 \rightarrow C_2H_4O$ Rate law: $-r_A = kC_{C_2H_4} C_{O_2}^{1/2}$
- 3) $(CH_3)_3COOC(CH_3)_3 \rightarrow C_2H_6 + 2CH_3COCH_3$
 A → B + 2C
 Rate law: $-r_A = k[C_A - C_B C_C^2 / K_c]$
- 4) $n-C_4H_{10} \leftrightarrow I-C_4H_{10}$ Rate law: $-r_A = k[C_{nC_4H_{10}} - C_{iC_4H_{10}} / K_c]$
- 5) $CH_3COOC_2H_5 + C_4H_9OH \leftrightarrow CH_3COOC_4H_9 + C_2H_5OH$
 A + B ↔ C + D
 Rate law: $-r_A = k[C_A C_B - C_C C_D / K_c]$

P3-10 (b)



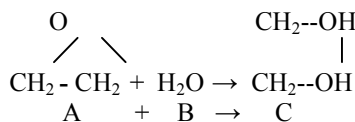
- (1) $-r_A = kC_A C_B^2$
 (2) $-r_A = kC_B$
 (3) $-r_A = k$
 (4) $-r_A = kC_A C_B^{-1}$

P3-10 (c)

- (1) $C_2H_6 \rightarrow C_2H_4 + H_2$ Rate law: $-r_A = kC_{C_2H_6}$
- (2) $H_2 + Br_2 \rightarrow 2HBr$ Rate law: $-r_{HBr} = \frac{k_1 C_{H_2} C_{Br_2}^{1/2}}{k_2 + \frac{C_{HBr}}{C_{Br_2}}}$
- (3) $H_2 + I_2 \rightarrow 2HI$ Rate law: $-r_{H_2} = kC_{H_2} C_{I_2}$

P3-11 (a)

Liquid phase reaction,



$$C_{A0} = 1 \text{ lbmol/ft}^3$$

$$C_{B0} = 3.47 \text{ lbmol/ft}^3$$

Stoichiometric Table:

| Species | Symbol | Initial | Change | Remaining |
|----------------|--------|-----------------------------------------------------------|------------|-----------------------------------------------------------------|
| Ethylene oxide | A | $C_{A0} = 1 \text{ lbmol/ft}^3$ | $-C_{A0}X$ | $C_A = C_{A0}(1-X)$ $= (1-X) \text{ lbmol/ft}^3$ |
| Water | B | $C_{B0} = 3.47 \text{ lbmol/ft}^3$, $\theta_B = 3.47$ | $-C_{A0}X$ | $C_B = C_{A0}(\theta_B - X)$ $= (3.47-X) \text{ lbmol/ft}^3$ |
| Glycol | C | 0 | $C_{A0}X$ | $C_C = C_{A0}X$ $= X \text{ lbmol/ft}^3$ |

$$\text{Rate law: } -r_A = kC_A C_B$$

Therefore, $-r_A = k C_{AO}^2 (1-X)(\theta_B - X) = k(1-X)(3.47-X)$

At 300K $E = 12500 \text{ cal/mol}$, $X = 0.9$,

$$k = 0.1 \text{ dm}^3/\text{mol.s} = 1.6018 \text{ ft}^3 / \text{lbmol.s}$$

$$\tau_{CSTR} = \frac{C_{AO} X}{-r_A} = \frac{(1)(0.9)}{(1.6018)(1)^2 (1-0.9)(3.47-0.9)} = 2.186 \text{ sec}$$

At 350K,

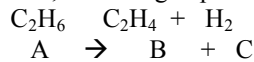
$$k_2 = k \exp((E/R)(1/T-1/T_2)) = 1.6018 \exp((12500/1.987)(1/300-1/350)) = 32.034 \text{ dm}^3/\text{mol.s}$$

Therefore,

$$\tau_{CSTR} = \frac{C_{AO} X}{-r_A} = \frac{(1)(0.9)}{(32.034)(1)^2 (1-0.9)(3.47-0.9)} = 0.109 \text{ sec}$$

P3-11 (b)

Isothermal, isobaric gas-phase pyrolysis,



Stoichiometric table:

| Species | symbol | Entering | Change | Leaving |
|-------------------------------|--------|----------------------------------|--------------------|---------------------------------------|
| C ₂ H ₆ | A | F _{AO} | -F _{AO} X | F _A =F _{AO} (1-X) |
| C ₂ H ₄ | B | 0 | +F _{AO} X | F _B =F _{AO} X |
| H ₂ | C | 0 | +F _{AO} X | F _C =F _{AO} X |
| | | F _{TO} =F _{AO} | | F _T =F _{AO} (1+X) |

$$\varepsilon = y_{AO} \delta = 1(1+1-1) = 1$$

$$v = v_o(1 + \varepsilon X) \Rightarrow v = v_o(1+X)$$

$$C_{AO} = y_{AO} C_{TO} = y_{AO} \frac{P}{RT} = \frac{(1)(6 \text{ atm})}{\left(0.082 \frac{\text{m}^3 \text{ atm}}{\text{K.kmol}}\right)(1100 \text{ K})} = 0.067 \text{ kmol/m}^3 = 0.067 \text{ mol/dm}^3$$

$$C_A = \frac{F_A}{v} = \frac{F_{AO}(1-X)}{v_o(1+X)} = C_{AO} \frac{(1-X)}{(1+X)} \text{ mol/dm}^3$$

$$C_B = \frac{F_B}{v} = \frac{F_{AO}(X)}{v_o(1+X)} = C_{AO} \frac{X}{(1+X)} \text{ mol/dm}^3$$

$$C_C = \frac{F_C}{v} = \frac{F_{AO}(X)}{v_o(1+X)} = C_{AO} \frac{X}{(1+X)} \text{ mol/dm}^3$$

Rate law:

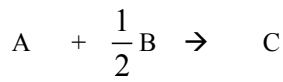
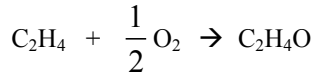
$$-r_A = k C_A = k C_{AO} \frac{(1-X)}{(1+X)} = 0.067 k \frac{(1-X)}{(1+X)}$$

If the reaction is carried out in a constant volume batch reactor, $\Rightarrow (\varepsilon = 0)$

$$C_A = C_{AO}(1-X) \text{ mol/dm}^3 \quad C_B = C_{AO} X \text{ mol/dm}^3 \quad C_C = C_{AO} X \text{ mol/dm}^3$$

P3-11 (c)

Isothermal, isobaric, catalytic gas phase oxidation,



Stoichiometric table:

| Species | Symbol | Entering | Change | Leaving |
|---------------------------------|--------|-----------------|-----------------------------------|-----------------------------------------------------|
| C ₂ H ₄ | A | F _{AO} | -F _{AO} X | F _A =F _{AO} (1-X) |
| O ₂ | B | F _{BO} | -θ _B F _{AO} X | F _B =F _{AO} (θ _B -X) |
| C ₂ H ₄ O | C | 0 | +F _{AO} X | F _C =F _{AO} X |

$$\theta_B = \frac{F_{BO}}{F_{AO}} = \frac{\frac{1}{2} F_{AO}}{F_{AO}} = \frac{1}{2} \quad y_{AO} = \frac{F_{AO}}{F_{TO}} = \frac{F_{AO}}{F_{AO} + F_{BO}} = \frac{2}{3}$$

$$\varepsilon = y_{AO} \delta = \frac{2}{3} \left(1 - \frac{1}{2} - 1 \right) = 0.33$$

$$C_{AO} = y_{AO} C_{TO} = y_{AO} \frac{P}{RT} = \frac{2}{3} \frac{(6 \text{ atm})}{\left(0.082 \frac{\text{atm} \cdot \text{dm}^3}{\text{mol} \cdot \text{K}} \right) (533 \text{ K})} = 0.092 \frac{\text{mol}}{\text{dm}^3}$$

$$C_A = \frac{F_A}{v} = \frac{F_{AO}(1-X)}{v_O(1+\varepsilon X)} = \frac{C_{AO}(1-X)}{(1-0.33X)} = \frac{0.092(1-X)}{(1-0.33X)}$$

$$C_B = \frac{F_B}{v} = \frac{F_{AO} \left(\theta_B - \frac{X}{2} \right)}{v_O(1+\varepsilon X)} = \frac{0.046(1-X)}{(1-0.33X)}$$

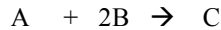
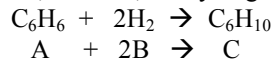
$$C_C = \frac{F_C}{v} = \frac{F_{AO} X}{v_O(1+\varepsilon X)} = \frac{0.092(X)}{(1-0.33X)}$$

If the reaction follow elementary rate law

$$\text{Rate law: } -r_A = k C_A C_B^{0.5} \quad \Rightarrow \quad -r_A = k \left\{ \frac{0.092(1-X)}{(1-0.33X)} \right\} \left\{ \frac{0.046(1-X)}{(1-0.33X)} \right\}^{0.5}$$

P3-11 (d)

Isothermal, isobaric, catalytic gas phase reaction in a PBR



Stoichiometric table:

| Species | Symbol | Entering | Change | Leaving |
|--------------------------------|--------|-----------------------------------|---------------------|------------------------------------------------------|
| Benzene | A | F _{AO} | -F _{AO} X | F _A =F _{AO} (1-X) |
| H ₂ | B | F _{BO} =2F _{AO} | -2F _{AO} X | F _B =F _{AO} (θ _B -2X) |
| C ₆ H ₁₀ | C | 0 | F _{AO} X | F _C =F _{AO} X |

$$\theta_B = \frac{F_{BO}}{F_{AO}} = \frac{2F_{AO}}{F_{AO}} = 2$$

$$y_{AO} = \frac{F_{AO}}{F_{TO}} = \frac{F_{AO}}{F_{AO} + F_{BO}} = \frac{1}{3}$$

$$\varepsilon = y_{AO}\delta = \frac{1}{3}(1 - 2 - 1) = -\frac{2}{3}$$

$$C_{AO} = C_{TO}y_{AO} = \frac{P}{RT} \left(\frac{1}{3} \right) = \frac{6 \text{ atm}}{\left(0.082 \frac{\text{atm} \cdot \text{dm}^3}{\text{mol} \cdot \text{K}} \right) (443.2 \text{ K})} \left(\frac{1}{3} \right) = 0.055 \text{ mol} / \text{dm}^3$$

$$C_A = \frac{F_A}{v} = \frac{F_{AO}(1-X)}{v_o(1+\varepsilon X)} = \frac{C_{AO}(1-X)}{\left(1 - \frac{2}{3}X \right)} = \frac{0.055(1-X)}{\left(1 - \frac{2}{3}X \right)}$$

$$C_B = \frac{F_B}{v} = \frac{F_{AO}(\theta_B - 2X)}{v_o(1+\varepsilon X)} = \frac{0.11(1-X)}{\left(1 - \frac{2}{3}X \right)}$$

$$C_C = \frac{F_C}{v} = \frac{F_{AO}X}{v_o(1+\varepsilon X)} = \frac{C_{AO}X}{\left(1 - \frac{2}{3}X \right)} = \frac{0.055X}{\left(1 - \frac{2}{3}X \right)}$$

If the reaction follow elementary rate law.

Rate law:

$$-r_A' = kC_A C_B^2$$

$$-r_A' = 0.0007k \frac{(1-X)^3}{\left(1 - \frac{2}{3}X \right)^3}$$

For a fluidized CSTR:

$$W = \frac{F_{AO}X}{-r_A'}$$

$$W = \frac{F_{AO}X}{0.0007k \frac{(1-X)^3}{\left(1 - \frac{2}{3}X \right)^3}}$$

$$k = 53 \frac{\text{mol}}{\text{kgcat min atm}^3} \text{ at } 300\text{K}$$

@ T = 170oC

$$k = k_1 \exp\left(\frac{E}{R} \left(\frac{1}{T_1} - \frac{1}{T} \right) \right) = 53 \exp\left(\frac{80000}{8.314} \left(\frac{1}{300} - \frac{1}{443} \right) \right) = 1663000 \frac{\text{mol}}{\text{kgcat min atm}^3}$$

$$F_{A0} = C_{A0}^* v_0$$

$$v_0 = 5 \text{ dm}^3/\text{min}$$

$$W = \frac{C_{A0} v_0 X}{0.0007k \frac{(1-X)^3}{\left(1 - \frac{2}{3}X\right)^3}}$$

at $X = 0.8$

$$W = 2.4 \times 10^{-3} \text{ kg of catalyst}$$

@ $T = 270^\circ\text{C}$

$$k = k_1 \exp\left(\frac{E}{R} \left(\frac{1}{T_1} - \frac{1}{T}\right)\right) = 53 \exp\left(\frac{80000}{8.314} \left(\frac{1}{300} - \frac{1}{543}\right)\right) = 90787719 \frac{\text{mol}}{\text{kgcat} \cdot \text{min} \cdot \text{atm}^3}$$

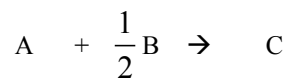
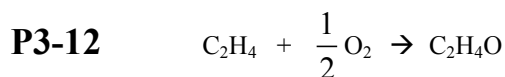
$$F_{A0} = C_{A0}^* v_0$$

$$v_0 = 5 \text{ dm}^3/\text{min}$$

$$W = \frac{C_{A0} v_0 X}{0.0007k \frac{(1-X)^3}{\left(1 - \frac{2}{3}X\right)^3}}$$

at $X = 0.8$

$$W = 4.4 \times 10^{-5} \text{ kg of catalyst}$$



Stoichiometric table for the given problem will be as follows

Assuming gas phase

| Species | Symbol | Entering | Change | Leaving |
|--------------------------------|--------|----------------------------|----------------|--------------------------|
| C_2H_4 | A | F_{A0} | $-F_{A0}X$ | $F_{A0}(1-X)$ |
| O_2 | B | $F_{B0} = \Theta_B F_{A0}$ | $-1/2 F_{A0}X$ | $F_{A0}(\Theta_B - X/2)$ |
| N_2 | I | $F_{I0} = \Theta_I F_{A0}$ | ----- | $F_{A0}\Theta_I$ |
| $\text{C}_2\text{H}_4\text{O}$ | C | 0 | $F_{A0}X$ | $F_{A0}X$ |

$$\theta_B = \frac{\frac{1}{2} F_{A0}}{F_{A0}} = \frac{1}{2}$$

$$\theta_I = \frac{F_{I0}}{F_{A0}}, F_{I0} = \frac{0.79}{0.21} F_{B0} \Rightarrow \theta_I = \theta_B \frac{0.79}{0.21} = 1.88$$

$$y_{A0} = \frac{F_{A0}}{F_{T0}} = 0.30, \quad \varepsilon = y_{A0}\delta = -0.15$$

$$C_{A0} = \frac{y_{A0}P}{RT} = 0.041 \frac{\text{mol}}{\text{dm}^3}$$

$$C_A = \frac{F_{A0}}{v} = C_{A0} \frac{(1-X)}{(1+\varepsilon X)} = \frac{0.041(1-X)}{1-0.15X}$$

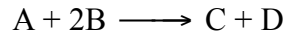
$$C_B = \frac{F_B}{v} = C_{A0} \frac{\left(\frac{1}{2} - \frac{1}{2}X\right)}{1-0.15X} = \frac{0.020(1-X)}{1-0.15X}$$

$$C_C = \frac{F_C}{v} = \frac{C_{A0}X}{1-0.15X} = \frac{0.041X}{1-0.15X}$$

P3-13 (a)

Let A = ONCB
B = NH₃

C = Nibroaniline
D = Ammonium Chloride



$$-r_A = kC_A C_B$$

P3-13 (b)

| Species | Entering | Change | Leaving |
|---------|-------------------------------------------------------------------------------|----------------------|-------------------------------------------|
| A | F _{A0} | - F _{A0} X | F _{A0} (1-X) |
| B | F _{B0} = Θ _B F _{A0} = 6.6/1.8 F _{A0} | -2 F _{A0} X | F _{B0} - F _{A0} (2X) |
| C | 0 | F _{A0} X | F _{C0} = F _{A0} X |
| D | 0 | F _{A0} X | F _{D0} = F _{A0} X |

P3-13 (c)

For batch system,

$$C_A = N_A/V$$

$$-r_A = kN_A N_B / V^2$$

P3-13 (d)

$$-r_A = kC_A C_B$$

$$F_A = \frac{N_A}{V} = \frac{N_A}{V_0} = \frac{N_{A0}}{V_0} (1-X) = C_{A0} (1-X), \quad C_A = \frac{F_A}{v} = \frac{F_A}{v_0} = C_{A0} (1-X)$$

$$F_B = \frac{N_B}{V} = \frac{N_B}{V_0} = \frac{N_{A0}}{V_0} (\theta_B - 2X) = C_{A0} (\theta_B - 2X), \quad C_B = \frac{F_B}{v} = C_{A0} (\theta_B - 2X)$$

$$-r_A = kC_{A0}^2 (1-X)(\theta_B - 2X)$$

$$\theta_B = \frac{C_{B0}}{C_{A0}} = \frac{6.6}{1.8} = 3.67$$

$$C_{A0} = 1.8 \frac{\text{kmol}}{\text{m}^3}$$

$$-r_A = k(1.8)^2(1-X)(3.67-2X)$$

P3-13 (e)

1) At X = 0 and T = 188°C = 461 K

$$-r_{A0} = kC_{A0}^2 \Theta_B = 0.0017 \frac{\text{m}^3}{\text{kmol min}} \left(1.8 \frac{\text{kmol}}{\text{m}^3}\right)^2 3.67 = 0.0202 \frac{\text{kmol}}{\text{m}^3 \text{ min}}$$

$$-r_{A0} = 0.0202 \frac{\text{kmol}}{\text{m}^3 \text{ min}}$$

2) At X = 0 and T = 25°C = 298 K

$$k = k_0 \exp\left(\frac{E}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\right)$$

$$k = 0.0017 \frac{\text{m}^3}{\text{kmol min}} \exp\left(\frac{11273 \frac{\text{cal}}{\text{mol}}}{1.987 \frac{\text{cal}}{\text{mol K}}}\left(\frac{1}{461} - \frac{1}{298}\right)\right)$$

$$= 2.03 \times 10^{-6} \frac{\text{m}^3}{\text{kmol min}}$$

$$-r_{A0} = kC_{A0}C_{B0} = 2.41 \times 10^{-5} \text{ kmol/m}^3\text{min}$$

3)

$$k = k_0 \exp\left[\frac{E}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\right]$$

$$k = 0.0017 \frac{\text{m}^3}{\text{kmol min}} \exp\left[\frac{11273 \frac{\text{cal}}{\text{mol}}}{1.987 \frac{\text{cal}}{\text{mol K}}}\left(\frac{1}{461 \text{ K}} - \frac{1}{561 \text{ K}}\right)\right]$$

$$k = 0.0152 \frac{\text{m}^3}{\text{kmol min}}$$

$$-r_{A0} = kC_{A0}C_{B0}$$

$$-r_A = 0.0152 \frac{\text{m}^3}{\text{kmol min}} \left(1.8 \frac{\text{kmol}}{\text{m}^3}\right) \left(6.6 \frac{\text{kmol}}{\text{m}^3}\right)$$

$$-r_A = 0.1806 \frac{\text{kmol}}{\text{m}^3 \text{ min}}$$

P3-13 (f)

$$r_A = kC_{A0}^2(1-X)(\Theta_B-2X)$$

At X = 0.90 and T = 188C = 461K

1) at T = 188 C = 461 K

$$\begin{aligned} -r_A &= \left(0.0017 \frac{m^3}{kmol \cdot min} \right) \left(1.8 \frac{kmol}{m^3} \right)^2 (1 - 0.9)(3.67 - 2(0.9)) \\ &= 0.00103 \frac{kmol}{m^3 \cdot min} \end{aligned}$$

2)

At X = 0.90 and T = 25C = 298K

$$\begin{aligned} -r_A &= \left(2.03 \times 10^{-6} \frac{m^3}{kmol \cdot min} \right) \left(1.8 \frac{kmol}{m^3} \right)^2 (1 - 0.9)(3.67 - 2(0.9)) \\ &= 1.23 \times 10^{-6} \frac{kmol}{m^3 \cdot min} \end{aligned}$$

3)

At X = 0.90 and T = 288C = 561K

$$\begin{aligned} -r_A &= \left(0.0152 \frac{m^3}{kmol \cdot min} \right) \left(1.8 \frac{kmol}{m^3} \right)^2 (1 - 0.9)(3.67 - 2(0.9)) \\ &= 0.0092 \frac{kmol}{m^3 \cdot min} \end{aligned}$$

P3-13 (g)

$F_{AO} = 2 \text{ mol/min}$

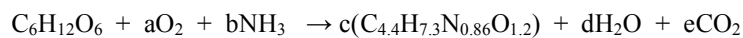
1) For CSTR at 25°C $-r_A = 1.23 \times 10^{-6} \frac{kmol}{m^3 \cdot min}$

$$\begin{aligned} V &= \frac{F_{AO}(1 - X)}{-r_{A:X=0.9}} \\ &= \frac{2 \text{ mol/min} \times 0.1}{1.23 \times 10^{-3} \frac{\text{mol}}{m^3 \cdot min}} = 162.60 m^3 \end{aligned}$$

2) At 288°C, $-r_A = 0.0092 \frac{kmol}{m^3 \cdot min}$

$$\begin{aligned} V &= \frac{F_{AO}(1 - X)}{-r_{A:X=0.9}} \\ &= \frac{2 \text{ mol/min} \times 0.1}{0.0092 \frac{\text{mol}}{m^3 \cdot min}} = 21.739 m^3 \end{aligned}$$

P3-14



To calculate the yields of biomass, you must first balance the reaction equation by finding the coefficients a, b, c, d, and e. This can be done with mass balances on each element involved in the reaction. Once all the coefficients are found, you can then calculate the yield coefficients by simply assuming the reaction

proceeds to completion and calculating the ending mass of the cells.

P3-14 (a)

Apply mass balance

$$\text{For C} \quad 6 = 4.4c + e$$

$$\text{For N} \quad b = 0.86c$$

For O

$$6 + 2a = 1.2c + d + 2e$$

For H

$$12 + 3b = 7.3c + 2d$$

Also for C, $6(2/3) = 4.4c$ which gives $c = \mathbf{0.909}$

Next we solve for e using the other carbon balance

$$6 = 4.4(0.909) + e$$

$$e = \mathbf{2}$$

We can solve for b using the nitrogen balance

$$b = 0.86c = 0.86 * (0.909)$$

$$b = \mathbf{0.78}$$

Next we use the hydrogen balance to solve for d

$$12 + 3b = 7.3c + 2d$$

$$12 + 3(0.78) = 7.3(0.909) + 2d$$

$$d = \mathbf{3.85}$$

Finally we solve for a using the oxygen balance

$$6 + 2a = 1.2c + d + 2e$$

$$6 + 2a = 1.2(0.909) + 3.85 + 2(2)$$

$$a = \mathbf{1.47}$$

P3-14 (b)

Assume 1 mole of glucose (180 g) reacts:

$$Y_{c/s} = \text{mass of cells} / \text{mass of glucose} = \text{mass of cells} / 180 \text{ g}$$

$$\text{mass of cells} = c * (\text{molecular weight}) = 0.909 \text{ mol} * (91.34 \text{ g/mol})$$

$$\text{mass of cells} = 83.12 \text{ g}$$

$$Y_{c/s} = 83.12 \text{ g} / 180 \text{ g}$$

$$Y_{c/s} = \mathbf{0.46}$$

$$Y_{c/o_2} = \text{mass of cells} / \text{mass of O}_2$$

If we assume 1 mole of glucose reacted, then 1.47 moles of O₂ are needed and 83.12 g of cells are produced.

$$\text{mass of O}_2 = 1.47 \text{ mol} * (32 \text{ g/mol})$$

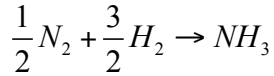
$$\text{mass of O}_2 = 47.04 \text{ g}$$

$$Y_{c/o_2} = 83.12 \text{ g} / 47.04 \text{ g}$$

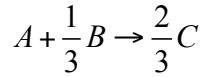
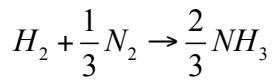
$$Y_{c/o_2} = \mathbf{1.77}$$

P3-15 (a)

Isothermal gas phase reaction.



Making H_2 as the basis of calculation:



Stoichiometric table:

| Species | Symbol | Initial | change | Leaving |
|---------|--------|----------------------------|---------------|--------------------------------|
| H_2 | A | F_{AO} | $-F_{AO}X$ | $F_A = F_{AO}(1-X)$ |
| N_2 | B | $F_{BO} = \theta_B F_{AO}$ | $-F_{AO}X/3$ | $F_B = F_{AO}(\theta_B - X/3)$ |
| NH_3 | C | 0 | $+2F_{AO}X/3$ | $F_C = (2/3)F_{AO}X$ |

P3-15 (b)

$$\delta = \left(\frac{2}{3} - \frac{1}{3} - 1 \right) = -\frac{2}{3}$$

$$\varepsilon = y_{AO}\delta = 0.5 \times \left(-\frac{2}{3} \right) = -\frac{1}{3}$$

$$C_{AO} = 0.5 \frac{(16.4 \text{ atm})}{\left(0.082 \frac{\text{atm} \cdot \text{dm}^3}{\text{mol} \cdot \text{K}} \right) (500 \text{ K})} = 0.2 \text{ mol/dm}^3$$

$$C_{H_2} = C_A = \frac{C_{AO}(1-X)}{(1+\varepsilon X)} = \frac{0.2(1-X)}{\left(1 - \frac{X}{3} \right)} = 0.1 \text{ mol/dm}^3$$

$$C_{NH_3} = C_C = \frac{2}{3} \times \frac{C_{AO}(1-X)}{(1+\varepsilon X)} = \frac{2}{3} \times \frac{0.2(X)}{\left(1 - \frac{X}{3} \right)} = 0.1 \text{ mol/dm}^3$$

P3-15 (c)

$$k_{N_2} = 40 \text{ dm}^3/\text{mol} \cdot \text{s}$$

(1) For Flow system:

$$\begin{aligned} -r_{N_2} &= k_{N_2} [C_{N_2}]^{1/2} [C_{H_2}]^{3/2} \\ &= 40(C_{AO})^2 \left[\frac{\left(1 - \frac{X}{3} \right)}{\left(1 - \frac{X}{3} \right)} \right]^{1/2} \left[\frac{(1-X)}{\left(1 - \frac{X}{3} \right)} \right]^{3/2} \end{aligned}$$

$$-r_{N_2} = 1.6 \left[\frac{(1-X)}{\left(1-\frac{X}{3}\right)} \right]^{3/2}$$

(2) For batch system, constant volume.

$$\begin{aligned} -r_{N_2} &= k_{N_2} [C_{N_2}]^{1/2} [C_{H_2}]^{3/2} \\ &= 40 (C_{A0})^2 \left[\left(1-\frac{X}{3}\right) \right]^{1/2} [(1-X)]^{3/2} \\ -r_{N_2} &= 1.6 \left[1-\frac{X}{3} \right]^{1/2} [1-X]^{3/2} \end{aligned}$$

P3-16 (a)

Liquid phase reaction → assume constant volume

Rate Law (reversible reaction):

$$-r_A = k \left[C_A C_B - \frac{C_C}{K_C} \right]$$

Stoichiometry:

$$C_A = C_{A0} (1-X), \quad C_B = C_{A0} (1-X), \quad C_C = C_{A0} X$$

To find the equilibrium conversion, set $-r_A = 0$, combine stoichiometry and the rate law, and solve for X_e .

$$C_A C_B K_C = C_C$$

$$C_{A0}^2 (1-X_e)^2 K_C = C_{A0} X_e$$

$$X_e^2 - \left(2 + \frac{1}{C_{A0} K_C} \right) X_e + 1 = 0$$

$$X_e = 0.80$$

To find the equilibrium concentrations, substitute the equilibrium conversion into the stoichiometric relations.

$$C_A = C_{A0} (1-X) = 2 \frac{\text{mol}}{\text{dm}^3} (1-0.80) = 0.4 \frac{\text{mol}}{\text{dm}^3}$$

$$C_B = C_{A0} (1-X) = 2 \frac{\text{mol}}{\text{dm}^3} (1-0.80) = 0.4 \frac{\text{mol}}{\text{dm}^3}$$

$$C_C = C_{A0} X = 2 \frac{\text{mol}}{\text{dm}^3} * 0.80 = 1.6 \frac{\text{mol}}{\text{dm}^3}$$

P3-16 (b)

Stoichiometry:

$$\varepsilon = y_{A0}\delta = (1)(3-1) = 2 \text{ and } \theta_c = 0$$

$$C_A = \frac{N_A}{V} = \frac{N_{A0}(1-X)}{V_0(1+\varepsilon X)} = C_{A0} \frac{(1-X)}{(1+2X)}$$

$$C_C = \frac{N_C}{V} = \frac{3N_{A0}X}{V_0(1+\varepsilon X)} = C_{A0} \frac{3X}{(1+2X)}$$

Combine and solve for X_e .

$$K_C C_{A0} \frac{(1-X_e)}{(1+2X_e)} = \left[C_{A0} \frac{3X_e}{(1+2X_e)} \right]^3$$

$$K_C (1-X_e)(1+2X_e)^2 = 27C_{A0}^2 X_e^3$$

$$-\left(4 + \frac{27C_{A0}^2}{K_C}\right) X_e^3 + 3X_e + 1 = 0$$

$$X_e = 0.58$$

Equilibrium concentrations:

$$C_{A0} = \frac{P_0}{RT_0} = \frac{10 \text{ atm}}{(400 \text{ K}) \left(0.082 \frac{\text{dm}^3 \text{ atm}}{\text{mol K}}\right)} = 0.305 \frac{\text{mol}}{\text{dm}^3}$$

$$C_A = 0.305 \frac{(1-0.58)}{(1+2(0.58))} = 0.059 \frac{\text{mol}}{\text{dm}^3}$$

$$C_C = \frac{3(0.58)(0.305)}{(1+2(0.58))} = 0.246 \frac{\text{mol}}{\text{dm}^3}$$

P3-16 (c)

Same reaction, rate law, and initial concentration as part (b) gas phase, batch reaction.

Stoichiometry:

$$C_A = \frac{N_A}{V} = \frac{N_{A0}(1-X)}{V_0} = C_{A0}(1-X)$$

$$C_C = \frac{N_C}{V} = \frac{3N_{A0}X}{V_0} = 3C_{A0}X$$

Combine and solve for X_e

$$K_C C_{A0} (1-X_e) = (3C_{A0} X_e)^3$$

$$X_e = 0.39$$

Equilibrium concentrations

$$C_A = (0.305)(1 - 0.39) = 0.19 \frac{\text{mol}}{\text{dm}^3}$$

$$C_C = (0.305)(0.39) = 0.36 \frac{\text{mol}}{\text{dm}^3}$$

P3-16 (d)

Gas phase reaction in a constant pressure, batch reactor

Rate law (reversible reaction):

$$-r_A = k \left[C_A - \frac{C_C^3}{K_C} \right]$$

Stoichiometry:

$$\varepsilon = y_{A0} \delta = (1)(3 - 1) = 2 \text{ and } \theta_C = 0$$

$$C_A = \frac{N_A}{V} = \frac{N_{A0}(1 - X)}{V_0(1 + \varepsilon X)} = C_{A0} \frac{(1 - X)}{(1 + 2X)}$$

$$C_C = \frac{N_C}{V} = \frac{3N_{A0}X}{V_0(1 + \varepsilon X)} = 3C_{A0} \frac{X}{(1 + 2X)}$$

Combine and solve for X_e :

$$\frac{K_C C_{A0} (1 - X_e)}{1 + 2X_e} = \left[\frac{3C_{A0} X_e}{1 + 2X_e} \right]^3$$

$$X_e = 0.58$$

Equilibrium concentrations:

$$C_A = \frac{0.305(1 - 0.58)}{1 + 2(0.58)} = 0.059 \frac{\text{mol}}{\text{dm}^3}$$

$$C_C = \frac{3(0.305)(0.58)}{1 + 2(0.58)} = 0.246 \frac{\text{mol}}{\text{dm}^3}$$

P3-17

Given: Gas phase reaction $A + B \rightarrow 8C$ in a batch reactor fitted with a piston such that

$$V = 0.1P_0$$

$$k = 1.0 \frac{(\text{ft}^3)^2}{\text{lb mol}^2 \text{ sec}}$$

$$-r_A = k C_A^2 C_B$$

$$N_{A0} = N_{B0} \text{ at } t = 0$$

$$V_0 = 0.15 \text{ ft}^3$$

$$T = 140^\circ\text{C} = 600^\circ\text{R} = \text{Constant}$$

P3-17 (a)

$$y_{A0} = \frac{N_{A0}}{N_{A0} + N_{B0}} = 0.5$$

$$\delta = 8 - 1 - 1 = 6$$

$$\varepsilon = y_{A0}\delta = 3$$

Now $V = \frac{V_0 P_0}{P \left(\frac{T}{T_0} \right)} (1 + \varepsilon X)$ and $\frac{T}{T_0} = 1$, $P_0 = 10V_0$, and $P = 10V$

Therefore $V = \frac{10V_0^2}{10V} (1 + \varepsilon X)$ or $V^2 = V_0^2 (1 + \varepsilon X)$

$$N_A = N_{A0} [1 - X] \quad N_B = N_{A0} [\theta_B - X] \quad \theta_B = \frac{N_{B0}}{N_{A0}} = 1$$

$$-r_A = k C_A^2 C_B = \frac{k N_A^2 N_B}{V^3} = \frac{k N_{A0}^3 [1 - X]^3}{V_0^3 (1 + \varepsilon X)^2} \quad N_{A0} = \left(\frac{y_{A0} P_0}{RT} \right) V_0$$

Therefore

$$-r_A = k \left(\frac{y_{A0} P_0}{RT} \right) \frac{[1 - X]^3}{(1 + \varepsilon X)^2}$$

$$-r_A = 5.03 * 10^{-9} \frac{[1 - X]^3}{(1 + 3X)^2} \frac{lb mol}{ft^3 sec}$$

P3-17 (b)

$$V^2 = V_0^2 (1 + \varepsilon X)$$

$$0.2^2 = 0.15^2 (1 + \varepsilon X)$$

$$X = 0.259$$

$$-r_A = 8.63 * 10^{-10} \frac{lb mol}{ft^3 sec}$$

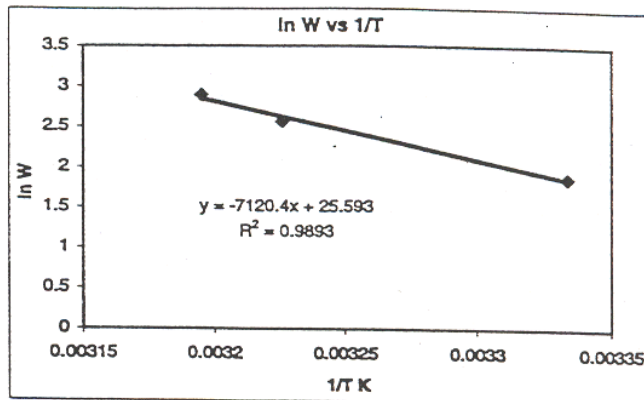
P3-18 No solution will be given.

P3-19 No solution will be given.

P3-20 No solution will be given.

CDP3-A

| W | lnW | T | 1/T |
|-----|----------|-----|----------|
| 6.5 | 1.871802 | 300 | 0.003333 |
| 13 | 2.564949 | 310 | 0.003226 |
| 18 | 2.890372 | 313 | 0.003195 |



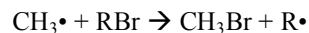
From the graph:
 $E = 7120$

$$\ln W = -7120.4 \cdot \left(\frac{1}{41.5 + 273} \right) + 25.593 = 2.95$$
$$W(41.5^\circ\text{C}) = 19.2 \text{ cm/s}$$

CDP3-B

Polanyi equation: $E = C - \alpha(-\Delta H_R)$

We have to calculate E for the reaction



Given: $\Delta H_R = -6 \text{ kcal/mol}$

From the given data table, we get

$$6.8 = C - \alpha(17.5)$$

and $6.0 = C - \alpha(20)$

$\Rightarrow C = 12.4 \text{ KJ/mol}$ and $\alpha = 0.32$

Using these values, and $\Delta H_R = -6 \text{ kcal/mol}$, we get $E = 10.48 \text{ KJ/mol}$

CDP3-C (a)



Rate law at low temperature: $-r_A = kC_A$

The rate law at higher temperature must:

- 1) Satisfy thermodynamics relationships at equilibrium, and
- 2) Reduce to irreversible rate law when the concentration of one or more of the reaction products is zero.

Also, We know,
$$K_C = \frac{C_{Be}}{C_{Ae}}$$

Rearranging, we get
$$C_{Ae} - \frac{C_{Be}}{K_C} = 0$$

So, let's assume rate law as
$$-r_A = k_A \left(C_A - \frac{C_B}{K_C} \right)$$

Also when $C_B = 0$, it satisfies the given rate law. Hence the proposed rate law is correct.

CDP3-C (b)



Rate law at low temperature:
$$-r_A = k C_A^{1/2} C_B$$

Here,
$$K_C = \frac{C_{De}^2}{C_{Ae} C_{Be}^2}$$

$$C_{Ae} C_{Be}^2 - \frac{C_{De}^2}{K_C} = 0$$

$$-r_A = k_A \left(C_{Ae} C_{Be}^2 - \frac{C_{De}^2}{K_C} \right)$$

But it does not satisfy the irreversible rate law at low temperatures.

Hence it is not correct

So, taking square root of K_C

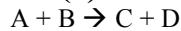
$$\sqrt{K_C} = \frac{C_{De}}{C_{Ae}^{1/2} C_{Be}}, \quad C_{Ae}^{1/2} C_{Be} - \frac{C_{De}}{\sqrt{K_C}} = 0$$

$$-r_A = k_A \left(C_{Ae}^{1/2} C_{Be} - \frac{C_{De}}{\sqrt{K_C}} \right)$$

Which satisfies the irreversible rate law.

Hence it is the required rate law.

CDP3-C (c)



Irreversible rate law:
$$-r_A' = \frac{k P_A P_B}{1 + K_A P_A + K_B P_B}$$

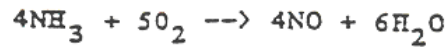
We know, $K_P = \frac{P_C P_D}{P_B P_A}$ or $P_B P_A - \frac{P_C P_D}{K_P} = 0$

Hence assume rate law as:

$$-r_A = \frac{k \left(P_A P_B - \frac{P_C P_D}{K_P} \right)}{1 + K_A P_A + K_B P_B + K_C P_C + K_D P_D}$$

Which satisfies both the above mentioned conditions.

CDP3-D

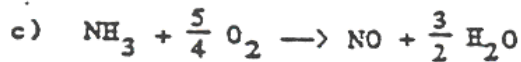


$$Y_{\text{NH}_3,0} = 0.15 \quad P=8.2 \text{ atm} \quad T = 227^\circ\text{C} = 500\text{K}$$

a) Assuming ideal gas law

$$C_{\text{to}} = \frac{n_{\text{to}}}{V_0} = \frac{P_0}{RT_0} = \frac{8.2 \text{ atm}}{0.082 \frac{\text{latm}}{\text{gmol}^\circ\text{K}} (500\text{K})} = 0.2 \text{ gmol/l}$$

b) $C_{\text{NH}_3,0} = Y_{\text{NH}_3,0} C_{\text{to}} = (0.15)(0.2 \text{ gmol/l}) = 0.03 \text{ gmol/l}$



| Compound | Symbol | Initial | Change | Final |
|----------------------|--------|---------|-----------------------|-----------------------------|
| NH_3 | A | 0.15 | -0.15X | 0.15(1-X) |
| O_2 | B | 0.18 | $-\frac{5}{4}(0.15X)$ | $0.18 - \frac{5(0.15X)}{4}$ |
| NO | C | 0 | +0.15X | 0.15X |
| H_2O | D | 0 | $+\frac{3}{2}(0.15X)$ | $+\frac{3}{2}(0.15X)$ |
| N_2 | I | 0.67 | 0 | 0.67 |
| Total | T | 1.00 | $+1/4(0.15X)$ | $1 + 1/4(0.15X)$ |

$$\text{Initial } \text{N}_2 = 0.79(1-0.15) = 0.79(0.85) = 0.67$$

$$\text{Initial } \text{O}_2 = 0.85 - 0.67 = 0.18$$

1) $P_i = y_i P = \frac{n_i}{n_T} P = 8.2 \text{ atm} \left(\frac{n_i}{1 + [0.15/4]X} \right)$

$$C_i = \frac{n_i}{V} = \frac{P_i}{RT} = \frac{n_i}{1 + 0.15/4 X} \frac{8.2 \text{ atm}}{0.082 \frac{\text{latm}}{\text{gmol}^\circ\text{K}} (500\text{K})} = 0.2 \frac{\text{gmol}}{\text{l}} \left(\frac{n_i}{1 + 0.15/4 X} \right)$$

| i | η_i | P_i (atm) | C_i |
|---|------------------------------|------------------------------------------------------------|-------------------------------------------------------|
| A | $0.15(1-X)$ | $1.23 \frac{1-X}{1+[0.15/4]X}$ | $0.03 \frac{1-X}{1+[0.15/4]X}$ |
| B | $0.18 - \frac{5}{4} (0.15X)$ | $8.2 \left(\frac{0.18 - 5/4(0.15X)}{1+[0.15/4]X} \right)$ | $(0.036 - \frac{0.15}{4} X) / (1 + \frac{0.15}{4} X)$ |
| C | $0.15X$ | $1.23 \frac{X}{1 + \left[\frac{0.15}{4} \right] X}$ | $0.03X / (1 + \frac{0.15}{4} X)$ |
| D | $\frac{3}{2} (0.15X)$ | $1.85 \frac{X}{1+[0.15/4]X}$ | $0.045 / (1 + \frac{0.15}{4} X)$ |
| I | 0.67 | $5.49 \frac{1}{1+[0.15/4]X}$ | $0.133 / (1 + \frac{0.15}{4} X)$ |

$$\text{check } P_{\text{TOT}} = \frac{1.23 - 1.23X + 8.2(0.18) - (8.2)(5/4)(0.15X) + 1.23X + 1.85X + 5.49}{1 + (0.15/4)X}$$

$$= \frac{8.2 - 0.313X}{1 + (0.15/4)X} = 8.2$$

$$V = V_0 \left(1 + \frac{0.15}{4} X \right)$$

2) Constant volume

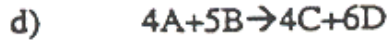
$$C_i = 0.2 \eta_i$$

$$P_i = C_i RT = (0.082)(500)(0.2)\eta_i = 8.2 \eta_i$$

| i | η_i | C_i | P_i |
|---|------------------------------|---------------------------------------------|-----------------------------------|
| A | $0.15(1-X)$ | $0.03 (1-X)$ | $1.23 (1-X)$ |
| B | $0.18 - \frac{5}{4} (0.15X)$ | $0.036 - \frac{0.15}{4} X$ | $8.2(0.18 - \frac{5}{4} (0.15X))$ |
| C | $0.15 X$ | $0.03 X$ | $1.23 X$ |
| D | $\frac{3}{2} (0.15X)$ | $0.045 X$ | $1.85 X$ |
| I | 0.67 | 0.133 | 5.49 |
| | | <hr/> | <hr/> |
| | | $0.199 + 0.008X$ | $8.2 - 0.313 X$ |
| | | $= 0.2 \left(1 + \frac{0.15}{4} X \right)$ | |

$$P_{\text{TOT}} = 8.2 - 0.313 X \text{ atm}$$

3) Same as (1)



Mole balance for a PFR

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

$$\frac{dF_B}{dV} = -r_B$$

$$\frac{dF_C}{dV} = -r_C$$

$$\frac{dF_D}{dV} = -r_D$$

Rate Law (assume elementary):

$$-r_A = k C_A^4 C_B^5$$

Combine with equation 3-40 and 3-48

$$\frac{dF_A}{dV} = k \left(\frac{P_{T0}}{RT_0} \right)^9 \left(\frac{F_A}{F_A + F_B + F_C} \right)^4 \left(\frac{F_B}{F_A + F_B + F_C} \right)^5$$

$$\frac{dF_B}{dV} = \frac{5}{4} k \left(\frac{P_{T0}}{RT_0} \right)^9 \left(\frac{F_A}{F_A + F_B + F_C} \right)^4 \left(\frac{F_B}{F_A + F_B + F_C} \right)^5$$

$$\frac{dF_C}{dV} = -k \left(\frac{P_{T0}}{RT_0} \right)^9 \left(\frac{F_A}{F_A + F_B + F_C} \right)^4 \left(\frac{F_B}{F_A + F_B + F_C} \right)^5$$

$$\frac{dF_D}{dV} = -k \left(\frac{P_{T0}}{RT_0} \right)^9 \left(\frac{F_A}{F_A + F_B + F_C} \right)^4 \left(\frac{F_B}{F_A + F_B + F_C} \right)^5$$

CDP3-E



a)

| Species | Symbol | Initial moles | Change | Final moles | Concentration |
|-------------------|--------|------------------|-------------|-------------------------|---------------------------|
| Benzoyl chloride | A | N_{A0} | $-N_{A0}X$ | $N_{A0}(1-X)$ | $N_{A0}(1-X)/V$ |
| Ammonia | B | $N_{A0}\theta_B$ | $-2N_{A0}X$ | $N_{A0}(\theta_B - 2X)$ | $N_{A0}(\theta_B - 2X)/V$ |
| Benzylamide | C | $N_{A0}\theta_C$ | $N_{A0}X$ | $N_{A0}(\theta_C + X)$ | $N_{A0}(\theta_C + X)/V$ |
| Ammonium Chloride | D | $N_{A0}\theta_D$ | $N_{A0}X$ | $N_{A0}(\theta_D + X)$ | $N_{A0}(\theta_D + X)/V$ |

b) $C_{A0} = N_{A0}/V = 2 \text{ gmol/l}$

$$\theta_B = C_{B0}/C_{A0} = 6/2 = 3$$

$$X = \frac{N_{A0} - N_A}{N_{A0}}$$

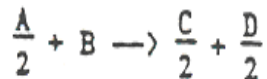
$$\theta_C = \theta_D = 0$$

$$X = 0.25$$

$$\text{Final conc. of ammonia} = \frac{N_{A0}}{V} (\theta_B - 2X) = 2(3 - 2(0.25)) = 5 \text{ gmol/l}$$

$$\text{Final conc. of benzylamide} = \frac{N_{A0}}{V} (\theta_C + X) = 2(0 + 0.25) = 0.5 \text{ gmol/l}$$

c) Stoichiometric table for a flow system using ammonia as the basis



| Species | Symbol | Entering | Change | Exit | Concentration |
|-------------------|--------|-------------------|--------------|--------------------------|------------------------------|
| Ammonia | B | F_{B0} | $-F_{B0}X$ | $F_{B0}(1-X)$ | $F_{B0}(1-X)/v_0$ |
| Benzo chloride | A | $\theta_A F_{B0}$ | $-F_{B0}X/2$ | $F_{B0}(\theta_A - X/2)$ | $F_{B0}(\theta_A - X/2)/v_0$ |
| Benzylamide | C | $\theta_C F_{B0}$ | $F_{B0}X/2$ | $F_{B0}(\theta_C + X/2)$ | $F_{B0}(\theta_C + X/2)/v_0$ |
| Ammonium Chloride | D | $\theta_D F_{B0}$ | $F_{B0}X/2$ | $F_{B0}(\theta_D + X/2)$ | $F_{B0}(\theta_D + X/2)/v_0$ |

Table for the flow system using ammonia as the basis is different from the original in the following ways.

- 1) Molar flow rates considered rather than number of moles.
- 2) $\theta_i = F_{i0}/F_{B0}$, as opposed to N_{i0}/N_{A0}
- 3) Concentration found by dividing the exiting molar flow rate by the volumetric flow rate v_0 .

CDP3-F

Given : $A + B \rightarrow C$ taking place in a square duct.

$$P_0 = 1 \text{ atm.} = \text{constant}$$

$$k = 10^6 \text{ ft}^3/(\text{lb.mole})(\text{sec.})$$

$$T = T_0 = 540^\circ\text{F} = 1000^\circ\text{R}$$

$$P_B^\circ = 0.25 \text{ atm.}$$

$$F_{A0} = 1.5 \text{ lb mole/sec.}$$

(a) If B is at equilibrium in the gas phase throughout the reactor

$C_B = \frac{P_B^\circ}{RT} = \text{constant}$. Since B maintains its equilibrium vapor pressure throughout the reactor, as soon as 1 molecule of B is consumed by the reaction, it is replaced by a molecule of B in the liquid. Hence, $\delta = 1 - 1 = 0$, $z = Y_{A0}^\delta$

$-r_A = k C_A C_B = k C_{B0} C_{A0} [1-X]$; Just inside the reactor,

$$C_{A0} = \frac{y_{A0} P_0}{RT} = \frac{(1-y_{B0}) P_0}{RT}$$

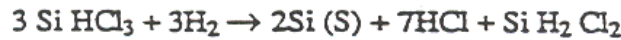
$$\therefore -r_A = k C_A C_B = k y_{B0} [1-y_{B0}] \left[\frac{P_0}{RT} \right]^2 (1-X)$$

(b) At $X = 0.5$

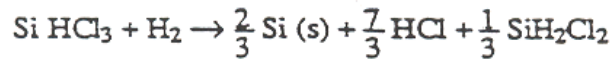
$$-r_A = \frac{10^6 \text{ ft}^3}{(\text{lbmole})(\text{sec})} \left[\frac{(.25 \text{ atm})(.75 \text{ atm})}{\left(\frac{.730 \text{ atm ft}^3}{\text{lb mole } ^\circ\text{R}} \times 1000^\circ\text{R} \right)^2} \right] [0.5] = .174 \frac{\text{lbmole}}{\text{ft}^3 \text{ sec.}}$$

CDP3-G

a)



Take Si HCl_3 as basis



| Species | Symbol | Entering | Change | Leaving |
|--------------------------------|--------|----------------------------|------------------------|------------------------------|
| Si HCl_3 (g) | A | F_{AO} | $-F_{AO}X$ | $F_A = F_{AO}(1-X)$ |
| H_2 (g) | B | $F_{BO} = \theta_B F_{AO}$ | $-F_{AO}X$ | $F_B = F_{AO}(\theta_B - X)$ |
| H_2HCl (g) | C | 0 | $+\frac{7}{3} F_{AO}X$ | $F_C = \frac{7}{3} F_{AO}X$ |
| $\text{Si H}_2\text{Cl}_2$ (g) | D | 0 | $+\frac{1}{3} F_{AO}X$ | $F_D = \frac{1}{3} F_{AO}X$ |
| Si (s) | S | 0 | $\frac{2}{3} F_{AO}X$ | — |

Assume isothermal and constant pressure. Neglect the vapor pressure of $\text{Si}_i(\text{s})$

$$\theta_B = 1 \text{ Stoichiometric feed}$$

δ only involves the changes in gas phase

$$\varepsilon = y_{AO} \delta = \frac{1}{2} \left(\frac{1}{3} + \frac{7}{3} - 1 - 1 \right)$$

$$\varepsilon = \frac{1}{2} \left(\frac{2}{3} \right) = \frac{1}{3}$$

$$C_{AO} = y_{AO} \frac{P_0}{R T_0} = \frac{1}{2} \left(\frac{2.0}{(0.082)(1327)} \right) \quad C_{AO} = 0.0088 \text{ mol/dm}^3$$

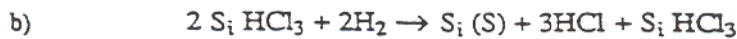
$$C_A = \frac{F_A}{v} = C_{A0} \frac{(1-X)}{(1+\epsilon X)} = \frac{0.0088(1-X)}{1+X/3}$$

$$C_B = \frac{F_B}{v} = C_A \frac{(\theta_B - X)}{(1+\epsilon X)} = \frac{0.0088(1-X)}{1+X/3}$$

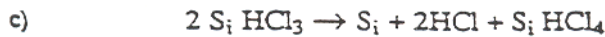
$$C_C = \frac{F_C}{v} = \frac{7}{3} \frac{F_{A0} X}{v_0(1+\epsilon X)} = \frac{7}{3} C_{A0} \frac{X}{(1+\epsilon X)} = 0.021 \frac{X}{(1+X/3)}$$

$$C_D = \frac{F_D}{v} = \frac{1}{3} \frac{F_{A0} X}{v_0(1+\epsilon X)} = 0.0031 \frac{X}{1+X/3}$$

The solution to parts (b) and (c)

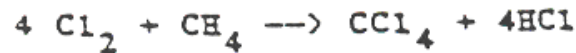


and



are similar to Part (a).

CDP3-H



$$T = 75^\circ\text{C} = 348 \text{ K}$$

$$P = 950 \text{ kPa} = 9.39 \text{ atm}$$

$$\text{Cl}_4 \text{ vapor pressure} = 95 \text{ kPa} = 0.94 \text{ atm} = P_V$$

$$C_i = \frac{F_i}{v} = \frac{F_i}{v_0(1+sX)} = \frac{F_i}{v_0}$$

So we can use the stoichiometric table, substituting C's for F's

| i | $\frac{F_i}{v}$ | $\frac{C_i}{v}$ |
|---|-----------------|-----------------|
| A | $F_{A0}(1-X)$ | $C_{A0}(1-X)$ |
| B | $4F_{A0}(1-X)$ | $4C_{A0}(1-X)$ |
| C | $4F_{A0} X$ | $4C_{A0} X$ |
| D | $F_{A0} X$ | $C_{A0} X$ |
| | $5 F_{A0}$ | $5 C_{A0}$ |

where $C_{A0} = 0.0658 \text{ gmol/l}$ and $F_{A0} = 0.02631 \text{ gmol/s}$

After condensation

$$v = v_0 \frac{F_t}{F_{t0}} = v_0 \frac{F_{A0} (5-X)}{5 F_{A0} (0.90)} = v_0 \frac{5-X}{4.5}$$

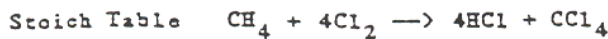
$$C'_i = \frac{F_i}{v} = \frac{F_i (4.5)}{v_0 (5-X)}$$

Note: at $X = 0.5$ (beginning of condensation) $C_i = C'_i$

| i | F_i | C_i |
|-------|-------------------------------|----------------------------------------|
| A | $5F_{A0} - F_{A0}X$ | $C_{A0}(1-X)(4.5)/(5-X)$ |
| B | $F_{A0}(5-X)$ | $4C_{A0}(1-X)(4.5)/(5-X)$ |
| C | $4F_{A0}X$ | $4C_{A0}X(4.5)/(5-X)$ |
| D | $0.1F_{A0}(5-X)/0.9$ | $C_{A0}(5-X)(4.5)/(5-X)/9 = 0.5C_{A0}$ |
| Total | $F_{A0}(5-X) + F_{A0}(5-X)/9$ | $C_{A0}(5-X)^2/40.5$ |

where $F_{A0} = 0.02631 \text{ gmol/S}$ and $C_{A0} = 0.0658 \text{ gmol/l}$

$$y_{DE} = \frac{P_v}{P} = \frac{95}{950} = 0.10$$



Assume stoichiometric feed F_i

| Species | Symbol | In | Change | Before Condensation $P_D < P_v$ remaining | After Condensation $P_D = P_v$ remaining |
|----------------|--------------------|-----------|-------------|----------------------------------------------|---------------------------------------------|
| CH_4 | A | F_{A0} | $-F_{A0}X$ | $F_A = F_{A0}(1-X)$ | $F_{A0}(1-X)$ |
| Cl_2 | B | $4F_{A0}$ | $-4F_{A0}X$ | $F_B = 4F_{A0}(1-X)$ | $4F_{A0}(1-X)$ |
| HCl_4 | C | 0 | $+4F_{A0}X$ | $F_C = 4F_{A0}X$ | $4F_{A0}X$ |
| CCl_4 | D(g) | 0 | $+F_{A0}X$ | $F_D = F_{A0}X$ | $0.10F_T$ |
| | D(l) | 0 | -- | -- | -- |
| | $F_{T0} = 5F_{A0}$ | | | $F_T = 5 F_{A0}$ | $F'_T = 5F_{A0} - F_{A0}X + 0.10F'_T$ |
| | | | | | $F'_T = \frac{F_{A0} (5-X)}{0.90}$ |

When condensation first begins $F_T = F'_T$

$$5 F_{A0} = F_{A0} \frac{(5-X)}{0.90} \rightarrow X_c = 0.50$$

Before Condensation

$$z = y_{A0} \delta \quad \delta = 0 \quad \rightarrow \quad z = 0$$

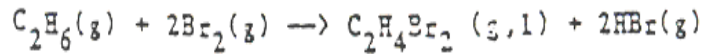
$\Delta T = \Delta P = 0 \rightarrow$ Total concentration is constant

$$C_T = C_{T0} = \frac{P_o}{RT_o} = \frac{9.39 \text{ atm}}{0.08205 \frac{\text{atm lit}}{\text{gmol K}} \times 348 \text{ K}} = 0.329 \frac{\text{gmol}}{\text{lit}}$$

$$C_{A0} = \frac{1}{5} C_{T0} = \frac{0.329}{5} \text{ gmol/l} = 0.0658 \text{ gmol/l}$$

$$F_{A0} = C_{A0} v_o = (0.0658) \text{ gmol/l} (0.4) \text{ l/s} = 0.02631 \text{ gmol/s}$$

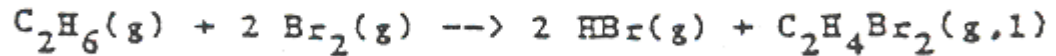
CDP3-I



$$T + 200^\circ C = 473 \text{ K} \quad P = 2500 \text{ kPa} = 24.7 \text{ atm}; \quad P_{v, C_2H_4Br_2} = 506.5 \text{ kPa}$$

$$y_{DE} = \frac{P_v}{P} = \frac{506.5}{2500} = 0.203$$

Stoich table



assume stoichiometric feed

| Species | Symbol | In | Change | F_i before condensation $P_D < P_v$ remaining | F'_i After condensation $P_D = P_v$ remaining |
|--------------|--------|--------------------|-------------|-------------------------------------------------|-------------------------------------------------|
| C_2H_6 | A | F_{A0} | $-F_{A0}X$ | $F_A = F_{A0}(1-X)$ | $F_{A0}(1-X)$ |
| Br_2 | B | $2F_{A0}$ | $-2F_{A0}X$ | $F_B = 2F_{A0}(1-X)$ | $2F_{A0}(1-X)$ |
| HBr | C | 0 | $2F_{A0}X$ | $F_C = 2F_{A0}X$ | $2F_{A0}X$ |
| $C_2H_4Br_2$ | D(g) | 0 | $F_{A0}X$ | $F_D = F_{A0}X$ | $0.203F'_T$ |
| | D(l) | 0 | - | - | - |
| | | $F_{T0} = 3F_{A0}$ | | $F_T = 3F_{A0}$ | $F'_T = 3F_{A0} - F_{A0}X + 0.203F'_T$ |

When condensation first begins $F_T = F_T'$

$$F_T' = \frac{F_{A0}(3-X)}{0.797}$$

$$3F_{A0} = \frac{F_{A0}(3-X)}{0.797} \rightarrow X_C = 0.609$$

Before condensation

$$z = y_{A0} \delta \quad \delta = 0 \quad \rightarrow \quad z = 0$$

$\Delta T = \Delta P = 0$ So total concentration is constant

$$C_T = C_{T0} = \frac{P_0}{RT_0} = \frac{24.7 \text{ atm}}{0.08205 \frac{\text{atm lit}}{\text{gmol K}} \times 473 \text{ K}} = 0.673 \text{ gmol/l}$$

$$C_{A0} = \frac{1}{3} C_{T0} = \frac{0.673}{3} \text{ gmol/l} = 0.212 \text{ gmol/l}$$

| i | F_i | C_i |
|-------|---------------------|----------------------------|
| A | $F_{A0}(1-X)$ | $C_{A0}(1-X)(2.39)/(3-X)$ |
| B | $2F_{A0}(1-X)$ | $2C_{A0}(1-X)(2.39)/(3-X)$ |
| C | $2F_{A0}X$ | $2C_{A0}(X)(2.39)/(3-X)$ |
| D | $F_{A0}(3-X)/3.93$ | $C_{A0}(0.609)$ |
| Total | $F_{A0}(3-X)/0.797$ | |

where $F_{A0} = 0.106 \text{ gmol/s}$ and $C_{A0} = 0.212 \text{ gmol/l}$

| X | F_A gmol/s | F_B gmol/s | F_C gmol/s | F_D gmol/s | F_T gmol/s | C_A gmol/l |
|-------|-----------------|-----------------|-----------------|-----------------------------|------------------------------|------------------------------------|
| 0 | $F_{A0}(1-X)$ | $2F_{A0}(1-X)$ | $2F_{A0}X$ | $F_{A0}X$ | $3F_{A0}$ | $C_{A0}(1-X)$ |
| 0 | 0.106 | 0.212 | 0 | 0 | 0.318 | 0.212 |
| 0.2 | 0.085 | 0.170 | 0.042 | 0.021 | 0.318 | 0.170 |
| 0.4 | 0.064 | 0.127 | 0.085 | 0.042 | 0.318 | 0.127 |
| 0.609 | 0.041 | 0.083 | 0.129 | 0.065 | 0.318 | 0.083 |
| X | $F_{A0}(1-X)$ | $2F_{A0}(1-X)$ | $2F_{A0}X$ | $F_{A0} \frac{(1-X)}{3.93}$ | $F_{A0} \frac{(3-X)}{0.797}$ | $C_{A0} \frac{(1-X)(2.39)}{(3-X)}$ |
| 0.609 | 0.041 | 0.083 | 0.129 | 0.065 | 0.318 | 0.083 |
| 0.8 | 0.021 | 0.042 | 0.170 | 0.059 | 0.293 | 0.039 |
| 1.0 | 0 | 0 | 0.212 | 0.054 | 0.266 | 0 |

| C_B gmol/l | C_C gmol/l | C_D gmol/l |
|-------------------------------------|----------------------------------|------------------|
| $2C_{AO}(1-X)$ | $2C_{AO}X$ | $C_{AO}X$ |
| 0.424 | 0 | 0 |
| 0.339 | 0.085 | 0.042 |
| 0.254 | 0.170 | 0.085 |
| 0.166 | 0.258 | 0.129 |
| $2C_{AO} \frac{(1-X)(2.39)}{(1-X)}$ | $2C_{AO} X \frac{(2.39)}{(1-X)}$ | $C_{AO} (0.609)$ |
| 0.166 | 0.258 | 0.129 |
| 0.073 | 0.312 | 0.109 |
| 0 | 0.312 | 0.090 |

$$F_{AO} = C_{AO} v_o = (0.212) \text{ gmol/l} (0.5) \text{ l/s} = 0.106 \text{ gmol/s}$$

$$C_i = \frac{F_i}{v} = \frac{F_i}{v_o(1+zX)} = \frac{F_i}{v_o}$$

So we can first use the stoichiometric table, substituting C's for F's

| i | F_i | C_i |
|-------|----------------|----------------|
| A | $F_{AO}(1-X)$ | $C_{AO}(1-X)$ |
| B | $2F_{AO}(1-X)$ | $2C_{AO}(1-X)$ |
| C | $2F_{AO} X$ | $2C_{AO} X$ |
| D | $F_{AO} X$ | $C_{AO} X$ |
| Total | $3 F_{AO}$ | $3 C_{AO}$ |

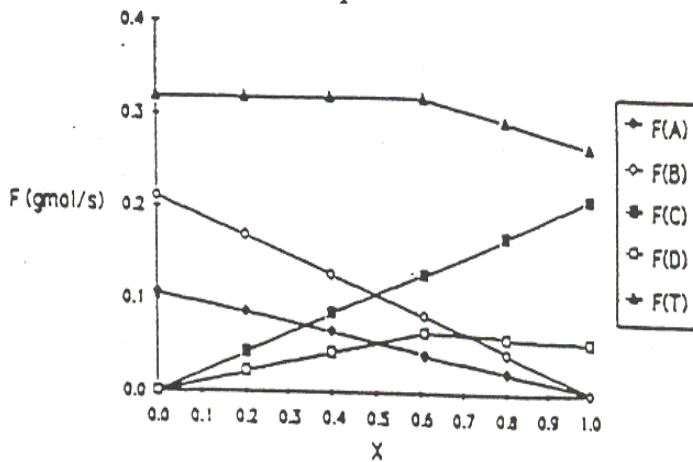
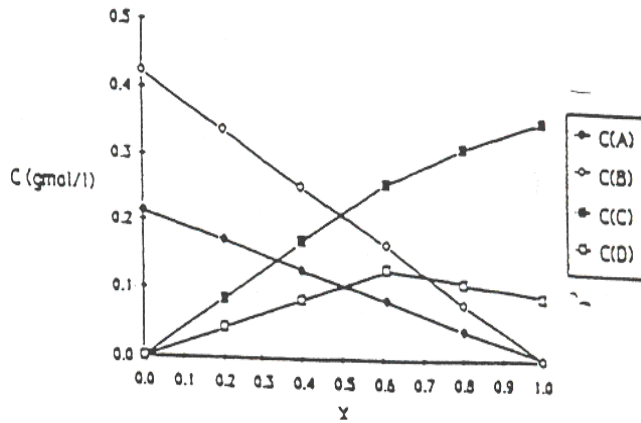
where $F_{AO} = 0.106 \text{ gmol/s}$ and $C_{AO} = 0.212 \text{ gmol/l}$

After condensation

$$v = v_o \frac{F_t'}{F_{t0}} = v_o \frac{F_{A0} (3-X)}{3F_{A0} \cdot 0.797} = v_o \frac{(3-X)}{2.39}$$

$$C'_i = \frac{F_i}{v} = \frac{F_i (2.39)}{v_o (3-X)}$$

Note that at $X = 0.609$ (beginning of condensation) $C_i = C'_i$



CDP3-J

| Species | Symbol | Entering | Change | Leaving |
|--------------------------------|--------|--------------------------------------------------|---------------------|----------------------------|
| SiH ₄ | A | F _{A0} | -3F _{A0} | F _{A0} (1-X) |
| NH ₃ | B | F _{B0} = Θ _B F _{A0} | -4F _{A0} X | F _{A0} (Θ - 4X/3) |
| Si ₃ N ₄ | C | 0 | F _{A0} X | F _{A0} X/3 |
| H ₂ | D | 0 | 12F _{A0} X | 4F _{A0} X |

$$\Theta_B = \frac{F_{B0}}{F_{A0}} = 1$$

$$y_{A0} = 0.5$$

$$\varepsilon = y_{A0}\delta = 0.5(12 - 3 - 4) = 2.5$$

$$C_{A0} = y_{A0}C_{T0} = 0.5 \left(\frac{P_0}{RT_0} \right) = 0.5 \left(\frac{1 \text{ Pa}}{8314 \frac{\text{Pa} \cdot \text{dm}^3}{\text{mol} \cdot \text{K}} * 973 \text{ K}} \right) = 6.18 * 10^{-8}$$

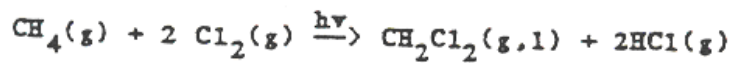
$$C_A = \frac{C_{A0}(1-X)}{1+\varepsilon X} = \frac{6.18 * 10^{-8}(1-X)}{1+2.5X}$$

$$C_B = \frac{1.68 * 10^{-8} \left(1 - \frac{4X}{3} \right)}{1+2.5X}$$

$$C_C = \frac{2.06 * 10^{-8} X}{1+2.5X}$$

$$C_D = \frac{2.47 * 10^{-7} X}{1+2.5X}$$

CDP3-K



| (a) | <u>Component</u> | <u>Symbol</u> | <u>Initial moles</u> | <u>Change</u> | <u>Out</u> |
|-----|---------------------------------|---------------|----------------------|---------------|------------|
| | Cl ₂ | A | 1.0 | -X | 1-X |
| | CH ₄ | B | 0.5 | -0.5X | 0.5(1-X) |
| | CH ₂ Cl ₂ | C | 0 | +0.5X | 0.5X |
| | HCl | D | 0 | +X | X |
| | <u>Total</u> | <u>T</u> | <u>1.5</u> | | <u>1.5</u> |

$$(b) \quad \delta = 1 + 2 - 1 - 2 = 0 ; y_{A0} = 1.0$$

$$\varepsilon = y_{A0} \delta = 0$$

(c) System is gas phase until $P_c = 400$ mmHg

$$\frac{0.5X'}{1.5} (760) = 400$$

$\therefore X' = 1.5789 \rightarrow \text{CH}_2\text{Cl}_2$ does not condense at 1 atm.

$$k = 0.2 \left(\frac{\text{dm}^3}{\text{gmole}} \right)^2 \frac{1}{\text{s}} \rightarrow \text{3rd order}$$

$$-r_A = k C_A^2 C_B$$

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

$$C_B = \frac{1}{2} C_{A0} (1-X_A)$$

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

(d) $C_{A0} = y_{A0} \frac{P}{RT}$

$$C_{A0} = \frac{1}{1.5} = \frac{1}{0.08206} \frac{1}{298.2} = 0.02724 \frac{\text{gmol}}{\text{dm}^3}$$

$$C_A = C_{A0} (1-X_A) = 0.02724 (1-0.6) = 0.01090 \frac{\text{gmol}}{\text{dm}^3}$$

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

$$-r_A = \frac{1}{2} (0.2)^3 (0.02724)^3 (1-0.6)^3$$

$$-r_A = 1.297 \times 10^{-7} \frac{\text{gmol}}{\text{dm}^3 \text{ s}}$$

$$(f) \quad k = A \exp \left\{ - \frac{E}{RT} \right\}$$

$$A = 2 \times 10^{12} \frac{\text{dm}^6}{\text{s gmol}^2}$$

$$0.2 = 2 \times 10^{12} \exp \left\{ \frac{-E}{(8.314)(298.2)} \right\} \quad \text{at } 25^\circ\text{C}$$

$$E = 74212 \frac{\text{J}}{\text{gmol}}$$

$$(g) \quad \text{At } 100^\circ\text{C} = 373.2 \text{ }^\circ\text{K}$$

$$\frac{k_{100}}{k_{25}} = \exp \left\{ - \frac{E}{R} \left(\frac{1}{373.2} - \frac{1}{298.2} \right) \right\} = 409.8$$

$$k_{100^\circ\text{C}} = 81.95 \left(\frac{\text{dm}^3}{\text{gmol}} \right)^2 \frac{1}{\text{S}}$$
