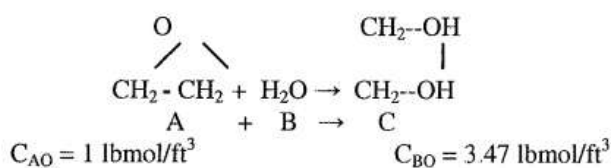


P3-11 (a)

Liquid phase reaction,



Stoichiometric Table:

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

Rate law: $-r_{\text{A}} = k C_{\text{A}} C_{\text{B}}$

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

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

$$k = 0.1 \text{ dm}^3/\text{mol.s} = \frac{0.1}{1000} \times 35.315 \text{ ft}^3/\text{lbmol.s} = 0.0035 \text{ ft}^3/\text{lbmol.s}$$

$$\tau_{\text{CSTR}} = \frac{C_{\text{AO}}X}{-r_{\text{A}}} = \frac{(1)(0.9)}{(0.0035)(1)^2(1-0.9)(3.47-0.9)} = 1000.56 \text{ s}^{-1}$$

At 350K,

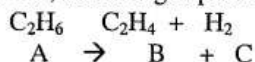
$$k_2 = k \exp((E/R)(1/T - 1/T_2)) = 0.0035 \exp((12500/1.987)(1/T - 1/T_2)) = 0.071 \text{ dm}^3/\text{mol.s}$$

Therefore,

$$\tau_{\text{CSTR}} = \frac{C_{\text{AO}}X}{-r_{\text{A}}} = \frac{(1)(0.9)}{(0.071)(1)^2(1-0.9)(3.47-0.9)} = 49.3 \text{ s}^{-1}$$

P3-11 (b)

Isothermal, isobaric gas-phase pyrolysis,



Stoichiometric table:

Species	symbol	Entering	Change	Leaving
C_2H_6	A	F_{AO}	$-F_{\text{AO}}X$	$F_{\text{A}} = F_{\text{AO}}(1-X)$

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:

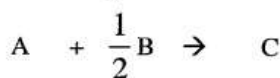
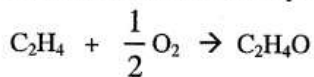
$$-r_A = kC_A = kC_{AO} \frac{(1-X)}{(1+X)} = 0.067 k \frac{(1-X)}{(1+X)}$$

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}	$-\theta_B F_{AO} X$	F _B =F _{AO} (θ_B -X)
C ₂ H ₄ O	C	0	+F _{AO} X	F _C =F _{AO} X

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

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

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

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

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

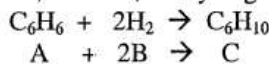
$$C_C = \frac{F_C}{v} = \frac{F_{AO}X}{v_O(1+\varepsilon X)} = \frac{0.092(X)}{(1-0.33X)}$$

If the reaction follow elementary rate law

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

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	$F_{BO} = 2F_{AO}$	$-2F_{AO}X$	$F_B = F_{AO}(\theta_B - 2X)$
C_6H_{10}	C	0	$F_{AO}X$	$F_C = F_{AO}X$

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

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

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

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

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

$$C_B = \frac{F_B}{v} = \frac{F_{A0}(\theta_B - 2X)}{v_0(1 + \varepsilon X)} = \frac{0.11(1 - X)}{\left(1 - \frac{2}{3}X\right)}$$

$$C_C = \frac{F_C}{v} = \frac{F_{A0}X}{v_0(1 + \varepsilon X)} = \frac{C_{A0}X}{\left(1 - \frac{2}{3}X\right)} = \frac{0.055X}{\left(1 - \frac{2}{3}X\right)}$$

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:

$$W = \frac{F_{A0}X}{-r_A'}$$

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

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

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

$$F_{A0} = C_{A0} \cdot v_0$$

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

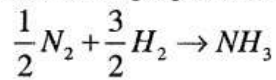
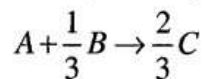
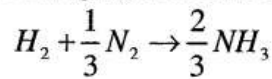
$$W = \frac{C_{A0}v_0X}{0.0007k \frac{(1 - X)^3}{\left(1 - \frac{2}{3}X\right)^3}}$$

at $X = 0.8$

$$W = 0.0024 \text{ kg of catalyst}$$

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:

$$-r_{N_2} = k_{N_2} [C_{N_2}]^{1/2} [C_{H_2}]^{3/2}$$

$$= 40 (C_{AO})^2 \left[\frac{\left(1 - \frac{X}{3}\right)}{\left(1 - \frac{X}{3}\right)} \right]^{1/2} \left[\frac{(1-X)}{\left(1 - \frac{X}{3}\right)} \right]^{3/2}$$

$$-r_{N_2} = 8.3 \left[\frac{(1-X)}{\left(1 - \frac{X}{3}\right)} \right]^{3/2}$$

(2) For batch system, constant volume.

$$-r_{N_2} = k_{N_2} [C_{N_2}]^{1/2} [C_{H_2}]^{3/2}$$

$$= 40 (C_{AO})^2 \left[\left(1 - \frac{X}{3}\right) \right]^{1/2} [(1-X)]^{3/2}$$

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



Edit

Annotate

Fill & Sign

Convert

All

P3-13 (a)

Let A = ONCB
B = NH₃

C = Nitroanaline
D = Ammonium Chloride



$$-r_A = kC_A C_B$$

3-14

3

P3-13 (b)

Species	Entering	Change	Leaving
A	F_{A0}	$-F_{A0}X$	$F_{A0}(1-X)$
B	$F_{B0} = \Theta_B F_{A0}$ $= 6.6/1.8 F_{A0}$	$-2 F_{A0}X$	$F_{B0} - 2F_{A0}X$ $F_{A0}(\Theta_B - 2X)$
C	0	$F_{A0}X$	$F_{A0}X$
D	0	$F_{A0}X$	$F_{A0}X$

P3-13 (c)

For batch system,
 $C_A = N_A/V$

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

P3-13 (d)

$$-r_A = kC_A C_B$$

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

$$F_B = \frac{N_B}{V} = \frac{N_B}{V_0} = \frac{N_{B0}}{V_0} (\theta_B - 2X) = C_{A0} (\theta_B - 2X), \quad C_B = \frac{F_B}{v} = \frac{F_B}{v_0} = C_{A0} (\theta_B - 2X)$$

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

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

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

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

P3-13 (e)

1) At $X = 0$ and $T = 188^\circ\text{C} = 461 \text{ K}$

$$-r_{A0} = kC_{A0}^2 \theta_B = k_A C_{A0} C_{B0} = 0.0017 \frac{\text{m}^3}{\text{kmol min}} \left(1.8 \frac{\text{kmol}}{\text{m}^3} \right) \left(6.6 \frac{\text{kmol}}{\text{m}^3} \right)$$

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

2) At $X = 0$ and $T = 25^\circ\text{C} = 298 \text{ K}$



$$k = k_o \exp\left(\frac{E}{R}\left(\frac{1}{T_o} + \frac{1}{T}\right)\right)$$

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

$$= 2.12 \times 10^{-6} \frac{m^3}{kmol \cdot min}$$

$$-r_{AO} = k C_{AO} C_{BO} = 2.52 \times 10^{-5} kmol/m^3 min$$

3)

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

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

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

$$-r_{AO} = k C_{AO} C_{BO}$$

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

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

P3-13 (f)

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

At $X = 0.90$ and $T = 188^\circ C = 461 K$

1) at $t = 188^\circ C$

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

2)

At $X = 0.90$ and $T = 25^\circ C = 298 K$

3

3

$$\begin{aligned}
 -r_A &= \left(2.12 \times 10^{-6} \frac{m^3}{kmol \cdot min} \right) \left(1.8 \frac{kmol}{m^3} \right)^2 (1 - 0.9)(3.67 - 2(0.9)) \\
 &= 1.28 \times 10^{-6} \frac{kmol}{m^3 \cdot min}
 \end{aligned}$$

3)

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

$$\begin{aligned}
 -r_A &= \left(0.0152 \frac{m^3}{kmol \cdot min} \right) \left(1.8 \frac{kmol}{m^3} \right)^2 (1 - 0.9)(3.67 - 2(0.9)) \\
 &= 0.00333 \frac{kmol}{m^3 \cdot min}
 \end{aligned}$$

P3-13 (g)

$$v_o = 2m^3/min = 0.002m^3/min$$

$$1) \text{ For CSTR at } 25C \quad -r_A = 1.28 \times 10^{-6} \frac{kmol}{m^3 \cdot min}$$

$$\begin{aligned}
 V &= \frac{v_o C_{AO} (1 - X)}{-r_{A: X=0.9}} \\
 &= \frac{0.002m^3/min \times 1.8kmol/m^3 \times 0.1}{1.28 \times 10^{-6} \frac{kmol}{m^3 \cdot min}} = 281.25m^3
 \end{aligned}$$

$$2) \text{ At } 288C, -r_A = 0.00333 \frac{kmol}{m^3 \cdot min}$$

$$\begin{aligned}
 V &= \frac{v_o C_{AO} (1 - X)}{-r_{A: X=0.9}} \\
 &= \frac{0.002m^3/min \times 1.8kmol/m^3 \times 0.1}{0.00333 \frac{kmol}{m^3 \cdot min}} = 0.108m^3
 \end{aligned}$$