

Chapter 4

Introduction to Reactor Design



Introduction

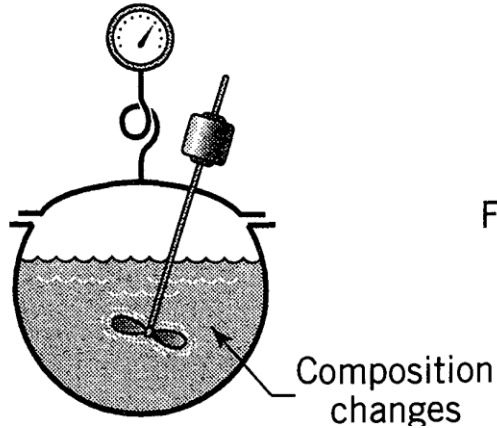
- ▶ The **rate equation** for a reacting component i is an intensive measure

$$r_i = \frac{1}{V} \left(\frac{dN_i}{dt} \right)_{\text{by reaction}}$$

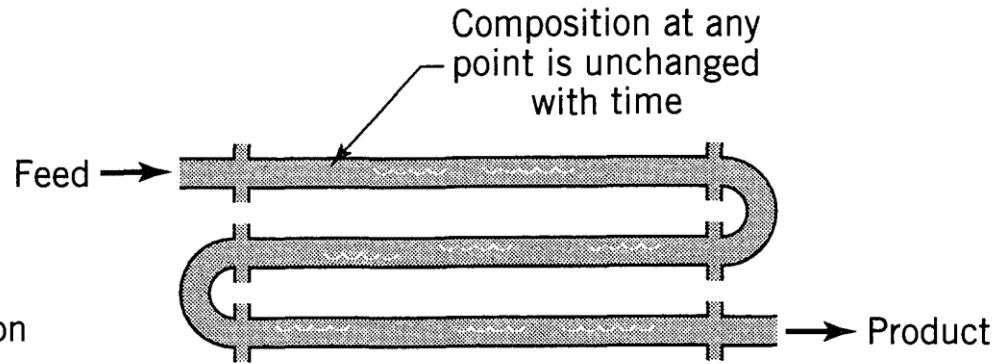
Rate=f (conditions within the **region of volume V**)

- ▶ Equipment in which homogeneous reactions are effected can be one of **three general** types
 - ▶ The batch
 - ▶ The steady-state flow
 - ▶ The semibatch reactor

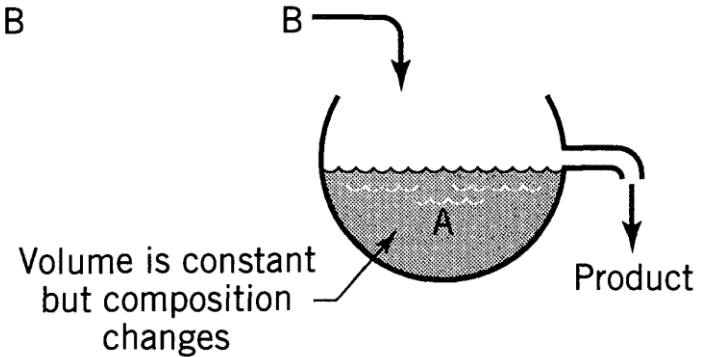
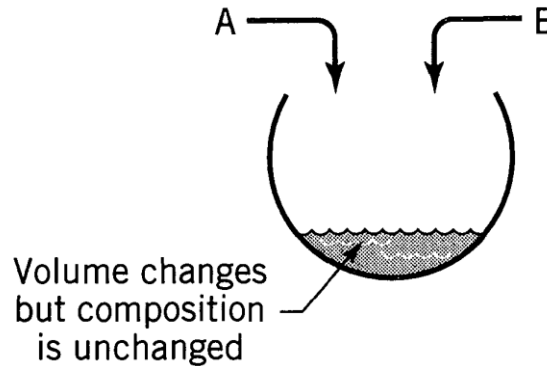
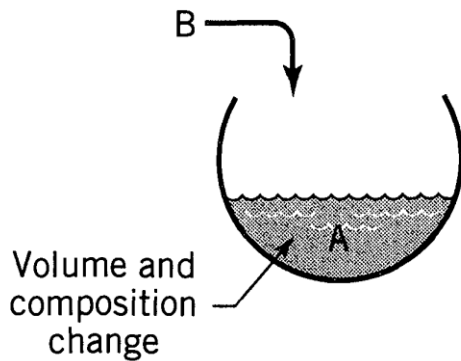
Classification of reactor types



The **batch** reactor



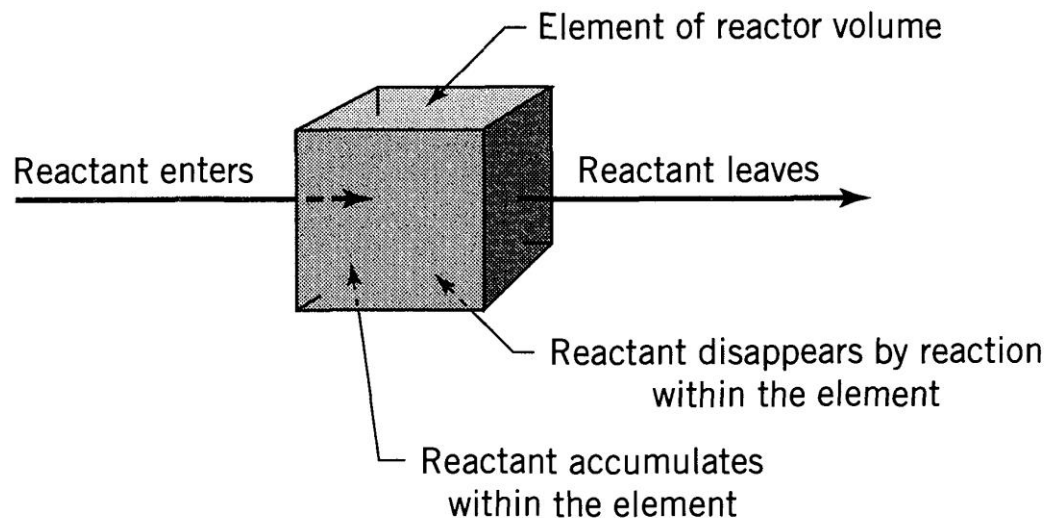
The **steady-state flow** reactor



Various forms of the **semibatch** reactor

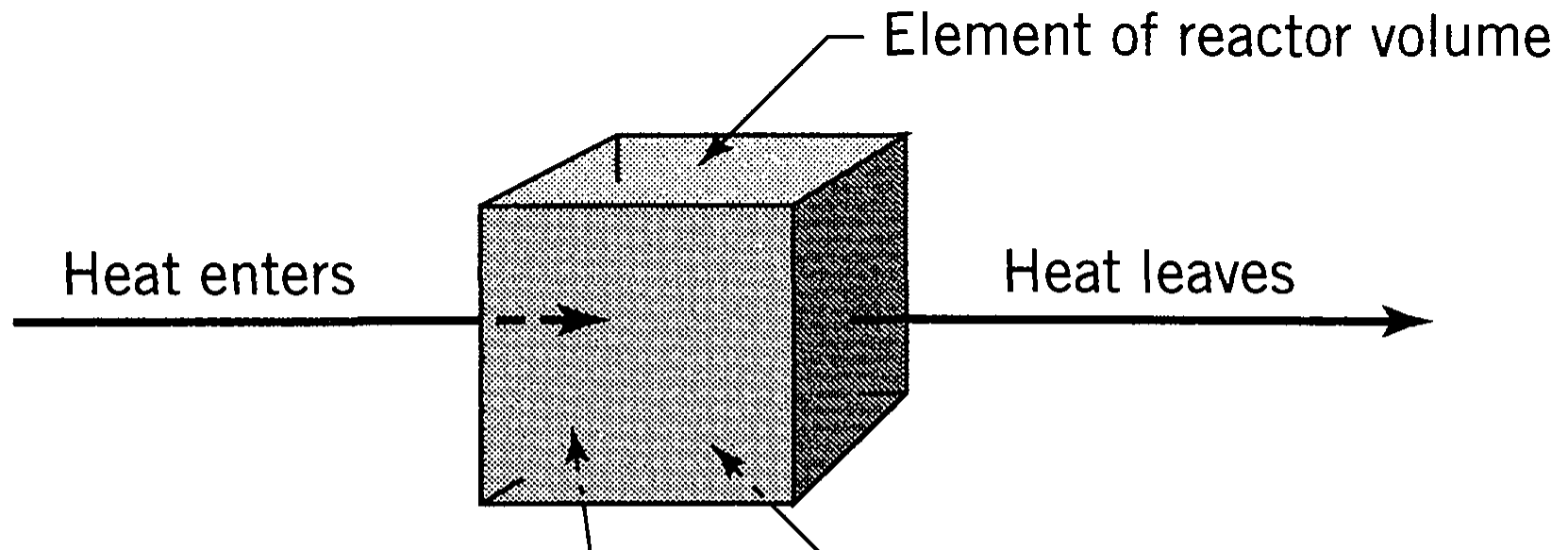
Material balance for an element of volume of the reactor

All design is the *material balance* expressed for any reactant (or product)



$$\left(\begin{array}{c} \text{rate of} \\ \text{reactant} \\ \text{flow into} \\ \text{element} \\ \text{of volume} \end{array} \right) = \left(\begin{array}{c} \text{rate of} \\ \text{reactant} \\ \text{flow out} \\ \text{of element} \\ \text{of volume} \end{array} \right) + \left(\begin{array}{c} \text{rate of reactant} \\ \text{loss due to} \\ \text{chemical reaction} \\ \text{within the element} \\ \text{of volume} \end{array} \right) + \left(\begin{array}{c} \text{rate of} \\ \text{accumulation} \\ \text{of reactant} \\ \text{in element} \\ \text{of volume} \end{array} \right)$$

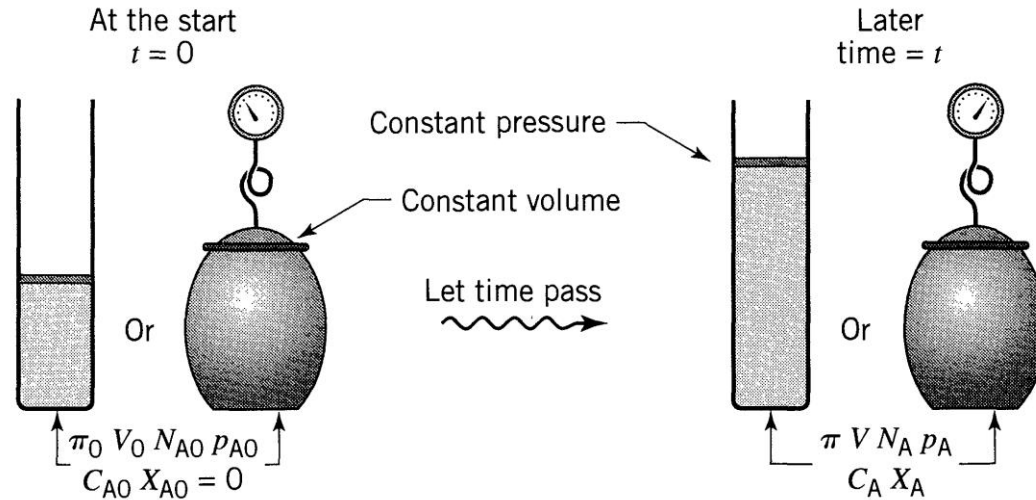
Energy balance for an element of volume of the reactor



$$\left(\begin{array}{c} \text{rate of heat} \\ \text{flow into} \\ \text{element of} \\ \text{volume} \end{array} \right) = \left(\begin{array}{c} \text{rate of heat} \\ \text{flow out of} \\ \text{element of} \\ \text{volume} \end{array} \right) + \left(\begin{array}{c} \text{rate of} \\ \text{disappearance} \\ \text{of heat by} \\ \text{reaction within} \\ \text{element of} \\ \text{volume} \end{array} \right) + \left(\begin{array}{c} \text{rate of} \\ \text{accumulation} \\ \text{of heat within} \\ \text{element of} \\ \text{volume} \end{array} \right)^1$$

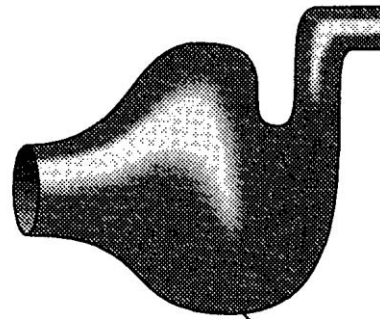
Symbols used for reactors

Batch reactors



Flow reactors

F_{A0} = moles fed/hr
 v_0 = m^3 fluid entering/hr
 C_{A0} = concentration of A
in the feed stream



$$F_A = F_{A0}(1 - X_A)$$

v, C_A, X_A

If there is any ambiguity call these
 $F_{Af}, v_f, C_{Af}, X_{Af}$

$V = \text{volume}$

Relationship between C_A and X_A

Constant Density Batch and Flow Systems

$$X_A = 1 - \frac{C_A}{C_{A0}} \quad \text{and} \quad dX_A = -\frac{dC_A}{C_{A0}}$$

$$\frac{C_A}{C_{A0}} = 1 - X_A \quad \text{and} \quad dC_A = -C_{A0}dX_A$$

For the reaction $aA + bB \rightarrow rR$

$$\frac{C_{A0} - C_A}{a} = \frac{C_{B0} - C_B}{b} = \frac{C_R - C_{R0}}{r}$$
$$\frac{C_{A0}X_A}{a} = \frac{C_{B0}X_B}{b}$$

Changing Density but with T and Pressure Constant
fluid element changes linearly with conversion

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

Changing **Density** system

$$X_A = \frac{C_{A0} - C_A}{C_{A0} + \varepsilon_A C_A}$$

$$\frac{C_A}{C_{A0}} = \frac{1 - X_A}{1 + \varepsilon_A X_A}$$

$$dX_A = -\frac{C_{A0}(1 + \varepsilon_A)}{(C_{A0} + \varepsilon_A C_A)^2} dC_A$$

$$\frac{dC_A}{C_{A0}} = -\frac{1 + \varepsilon_A}{(1 + \varepsilon_A X_A)^2} dX_A$$

$$\varepsilon_A = \frac{V_{X_A=1} - V_{X_A=0}}{V_{X_A=0}} \neq 0$$

Between reactant

Products and inerts

$$\varepsilon_A X_A = \varepsilon_B X_B$$

$$\frac{a\varepsilon_A}{C_{A0}} = \frac{b\varepsilon_B}{C_{B0}}$$

$$\frac{C_R}{C_{A0}} = \frac{(r/a)X_A + C_{R0}/C_{A0}}{1 + \varepsilon_A X_A}$$

$$\frac{C_I}{C_{I0}} = \frac{1}{1 + \varepsilon_A X_A}$$

Gases in General (varying ρ, P, T)

Equation of state

$$PV=ZNRT$$

At time $t=0$

$$P_0 V_0 = Z_0 N_0 R T_0$$

At time $t=t$

$$PV = Z_0 N R T$$

$$\frac{P_0 V_0}{PV} = \frac{Z_0 N_0 T_0}{ZNT}$$
$$V = V_0 \left(\frac{P_0}{P}\right) \left(\frac{Z}{Z_0}\right) \left(\frac{T}{T_0}\right) \left(\frac{N}{N_0}\right)$$



► Batch Systems

At time $t = 0$, moles of species A, B, C, D, and I

N_{A0} , N_{B0} , N_{C0} , N_{D0} and N_{I0} respectively

Number of moles remaining in the reactor after conversion X

Species	Initially (mol)	Change (mol)	Remaining (mol)
A	N_{A0}	$-(N_{A0}X)$	$N_A = N_{A0} - N_{A0}X$
B	N_{B0}	$-\frac{b}{a}(N_{A0}X)$	$N_B = N_{B0} - \frac{b}{a}N_{A0}X$
C	N_{C0}	$\frac{c}{a}(N_{A0}X)$	$N_C = N_{C0} + \frac{c}{a}N_{A0}X$
D	N_{D0}	$\frac{d}{a}(N_{A0}X)$	$N_D = N_{D0} + \frac{d}{a}N_{A0}X$
I (inerts)	N_{I0}	—	$N_I = N_{I0}$
Totals	N_{T0}		$N_T = N_{T0} + \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1\right)N_{A0}X$

Volume Change with Reaction

- ▶ Increase in the total number of moles per mole of A reacted

$$\delta = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1$$

$$N_T = N_{T0} + \delta N_{A0} X$$

$$\frac{N_T}{N_{T0}} = 1 + \frac{N_{A0}}{N_{T0}} \delta X = 1 + \delta y_{A0} X$$

$$\varepsilon = \frac{\text{change in total number of moles for complete conversion}}{\text{total number of moles fed to the reactor}}$$

$$\varepsilon = \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1 \right) \frac{N_{A0}}{N_{T0}} = y_{A0} \delta$$

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

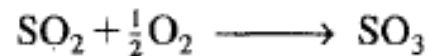
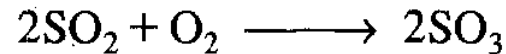
$$V = V_0 \left(\frac{P_0}{P} \right) \frac{T}{T_0} \left(\frac{Z}{Z_0} \right) (1 + \varepsilon X)$$

compressibility factor will not change

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

Volume Change with Reaction

- ▶ A mixture of 28% SO_2 and 72% air is charged to a flow reactor in which SO_2 is oxidized.



$$\varepsilon = y_{A0} \delta = (0.28) \left(1 - 1 - \frac{1}{2}\right) = -0.14$$

We further simplify these equations by defining the parameter Θ_i , allows us to factor N_{A0} in each of the expressions for concentration:

$$\Theta_i = \frac{N_{i0}}{N_{A0}} = \frac{C_{i0}}{C_{A0}} = \frac{y_{i0}}{y_{A0}}$$

$$C_B = \frac{N_{A0} [N_{B0}/N_{A0} - (b/a)X]}{V} = \frac{N_{A0} [\Theta_B - (b/a)X]}{V} \quad \Theta_B = \frac{N_{B0}}{N_{A0}}$$

Variable-volume batch reactor

$$C_{T0} = \frac{F_{T0}}{v_0} = \frac{P_0}{Z_0 R T_0}$$

$$C_T = \frac{F_T}{v} = \frac{P}{ZRT}$$

$$v = v_0 \left(\frac{F_T}{F_{T0}} \right) \frac{P_0}{P} \left(\frac{T}{T_0} \right)$$

$$v = v_0 (1 + \varepsilon X) \frac{P_0}{P} \left(\frac{T}{T_0} \right)$$

$$F_T = F_{T0} + F_{A0} \delta X$$

$$v = v_0 \frac{F_{T0} + F_{A0} \delta X}{F_{T0}} \left(\frac{P_0}{P} \right) \frac{T}{T_0}$$

$$= v_0 \left(1 + \frac{F_{A0}}{F_{T0}} \delta X \right) \frac{P_0}{P} \left(\frac{T}{T_0} \right)$$

$$= v_0 (1 + y_{A0} \delta X) \frac{P_0}{P} \left(\frac{T}{T_0} \right)$$

$$C_j = \frac{F_j}{v} = \frac{F_j}{v_0 \left(\frac{F_T}{F_{T0}} \frac{P_0}{P} \frac{T}{T_0} \right)}$$

$$= \left(\frac{F_{T0}}{v_0} \right) \left(\frac{F_j}{F_T} \right) \left(\frac{P}{P_0} \right) \left(\frac{T_0}{T} \right)$$

$$C_j = C_{T0} \left(\frac{F_j}{F_T} \right) \left(\frac{P}{P_0} \right) \left(\frac{T_0}{T} \right)$$

CONCENTRATIONS IN A VARIABLE-VOLUME GAS FLOW SYSTEM

$$C_A = \frac{F_A}{v} = \frac{F_{A0}(1-X)}{v} = \frac{F_{A0}(1-X)}{v_0(1+\epsilon X)} \left(\frac{T_0}{T} \right) \frac{P}{P_0} = C_{A0} \left(\frac{1-X}{1+\epsilon X} \right) \frac{T_0}{T} \left(\frac{P}{P_0} \right)$$

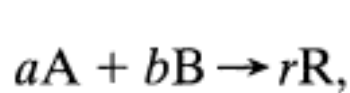
$$C_B = \frac{F_B}{v} = \frac{F_{A0}[\Theta_B - (b/a)X]}{v} = \frac{F_{A0}[\Theta_B - (b/a)X]}{v_0(1+\epsilon X)} \left(\frac{T_0}{T} \right) \frac{P}{P_0} = C_{A0} \left(\frac{\Theta_B - (b/a)X}{1+\epsilon X} \right) \frac{T_0}{T} \left(\frac{P}{P_0} \right)$$

$$C_C = \frac{F_C}{v} = \frac{F_{A0}[\Theta_C + (c/a)X]}{v} = \frac{F_{A0}[\Theta_C + (c/a)X]}{v_0(1+\epsilon X)} \left(\frac{T_0}{T} \right) \frac{P}{P_0} = C_{A0} \left(\frac{\Theta_C + (c/a)X}{1+\epsilon X} \right) \frac{T_0}{T} \left(\frac{P}{P_0} \right)$$

$$C_D = \frac{F_D}{v} = \frac{F_{A0}[\Theta_D + (d/a)X]}{v} = \frac{F_{A0}[\Theta_D + (d/a)X]}{v_0(1+\epsilon X)} \left(\frac{T_0}{T} \right) \frac{P}{P_0} = C_{A0} \left(\frac{\Theta_D + (d/a)X}{1+\epsilon X} \right) \frac{T_0}{T} \left(\frac{P}{P_0} \right)$$

$$C_I = \frac{F_I}{v} = \frac{F_{A0}\Theta_I}{v} = \frac{F_{A0}\Theta_I}{v_0(1+\epsilon X)} \left(\frac{T_0}{T} \right) \frac{P}{P_0} = \frac{C_{A0}\Theta_I}{1+\epsilon X} \left(\frac{T_0}{T} \right) \frac{P}{P_0}$$

Batch and Flow Systems for Gases in General (varying ρ , T , p)



$$a + b \neq r$$

$$X_A = \frac{1 - \frac{C_A}{C_{A0}} \left(\frac{T\pi_0}{T_0\pi} \right)}{1 + \varepsilon_A \frac{C_A}{C_{A0}} \left(\frac{T\pi_0}{T_0\pi} \right)} \quad \text{or} \quad \frac{C_A}{C_{A0}} = \frac{1 - X_A}{1 + \varepsilon_A X_A} \left(\frac{T_0\pi}{T\pi_0} \right)$$

$$X_A = \frac{\frac{C_{B0}}{C_{A0}} - \frac{C_B}{C_{A0}} \left(\frac{T\pi_0}{T_0\pi} \right)}{\frac{b}{a} + \varepsilon_A \frac{C_B}{C_{A0}} \left(\frac{T\pi_0}{T_0\pi} \right)} \quad \text{or} \quad \frac{C_B}{C_{A0}} = \frac{\frac{C_{B0}}{C_{A0}} - \frac{b}{a} X_A}{1 + \varepsilon_A X_A} \left(\frac{T_0\pi}{T\pi_0} \right)$$

$$\frac{C_R}{C_{A0}} = \frac{\frac{C_{R0}}{C_{A0}} + \frac{r}{a} X_A}{1 + \varepsilon_A X_A} \left(\frac{T_0\pi}{T\pi_0} \right)$$

- For high-pressure non-ideal gas behaviour replace

$$\left(\frac{T_0\pi}{T_0\pi_0} \right) \text{ by } \left(\frac{z_0 T_0\pi}{z T\pi} \right)$$

- To change to another key reactant, say B

$$\frac{a\varepsilon_A}{C_{A0}} = \frac{b\varepsilon_B}{C_{B0}} \quad ; \quad \frac{C_{A0}X_A}{a} = \frac{C_{B0}X_B}{b}$$

- For liquids or isothermal gases with no change pressure and density

$$\varepsilon_A \rightarrow 0 \quad \text{and} \quad \left(\frac{T_0\pi}{T\pi_0} \right) \rightarrow 1$$

Example

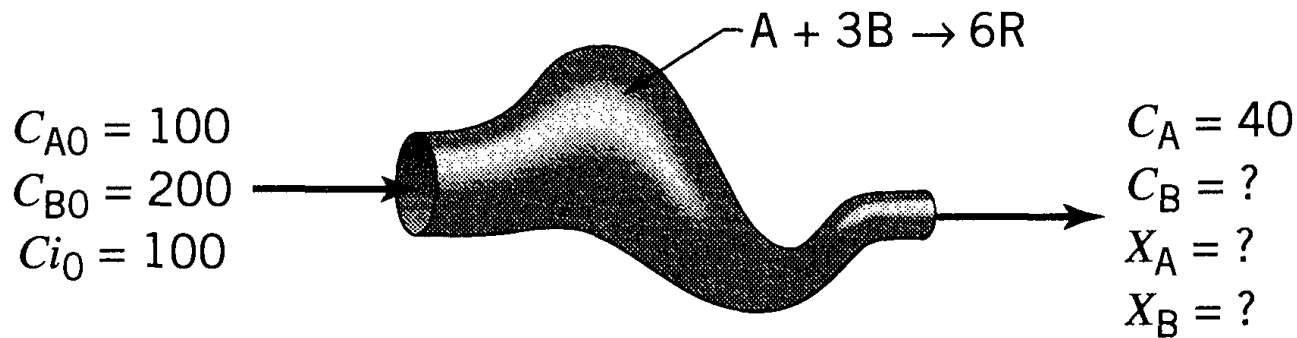
- ▶ Feed to a **steady-flow reactor**. The isothermal gas-phase reaction is

$$C_{A0} = 100, C_{B0} = 200, C_{i0} = 100$$

If $C_A = 40$ at the reactor exit, what is C_A , X_A , and X_B there?



- ▶ **Solution:**





	Inert	A	B	R
x=0	100	100	200	0

$$\delta = (6-3-1)$$

$$\varepsilon = 2 * 1/4 = 0.5$$

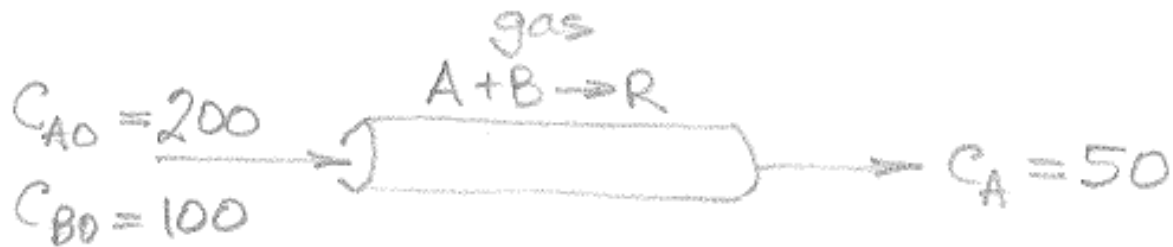
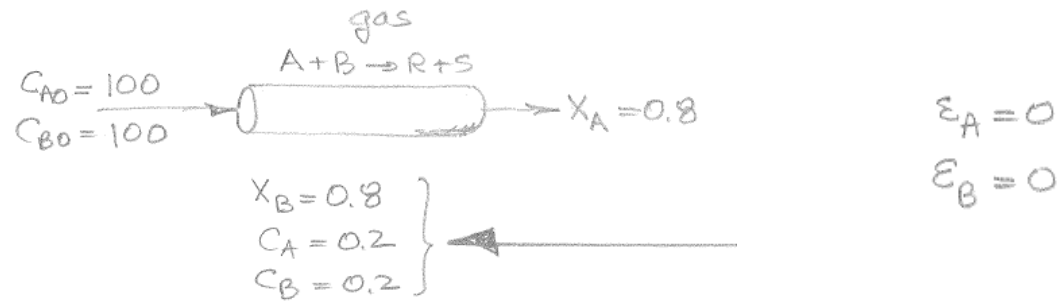
$$\varepsilon_B = \frac{\varepsilon_A C_{B0}}{b C_{A0}} = \frac{(1/2)(200)}{3(100)} = \frac{1}{3}$$

$$X_A = \frac{C_{A0} - C_A}{C_{A0} + \varepsilon_A C_A} = \frac{100 - 40}{100 + (1/2)40} = \frac{60}{120} = \underline{\underline{0.5}}$$

$$X_B = \frac{b C_{A0} X_A}{C_{B0}} = \frac{3(100)(0.5)}{200} = \underline{\underline{0.75}}$$

$$C_B = C_{B0} \left(\frac{1 - X_B}{1 + \varepsilon_B X_B} \right) = \frac{200(1 - 0.75)}{1 + (1/3)(0.75)} = \underline{\underline{40}}$$

Example



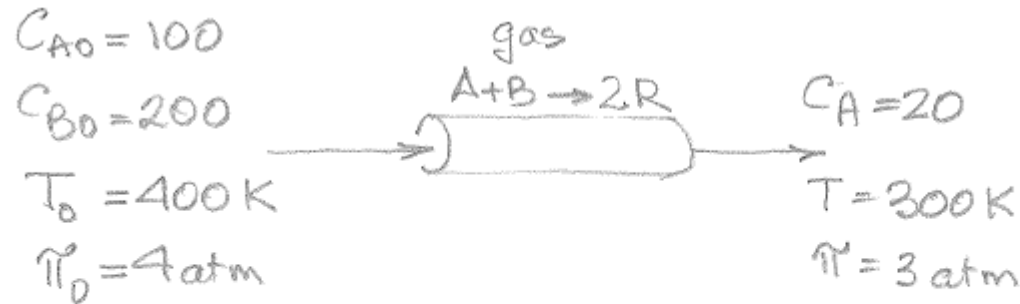
Take 300 moles of feed gas. Consider A

$$\left. \begin{array}{l} \text{at } X_A = 0 \quad V = 200A + 100B + 0R = 300 \\ \text{at } X_A = 1 \quad V = 0A - 100B + 200R = 100 \end{array} \right\} \varepsilon_A = \frac{100 - 300}{300} = -\frac{2}{3}$$

Now consider B

$$\left. \begin{array}{l} \text{at } X_B = 0 \quad V = 300 \\ \text{at } X_B = 1 \quad V = 100A + 0B + 100R = 200 \end{array} \right\} \varepsilon_B = \frac{200 - 300}{300} = -\frac{1}{3}$$

Example



Since the number of moles is unchanged $\epsilon_A = 0$ and $\epsilon_B = 0$